

61st Electronic Materials Conference

SESSION A: EMC Awards Ceremony and Plenary Session
Session Chairs: Kris Bertness and Suzanne Mohney
Wednesday Morning, June 26, 2019
Michigan League, 2nd Floor, Lydia Mendelssohn Theatre

* Plenary Paper

8:20 AM EMC Awards Ceremony

8:30 AM *A01

Programmable Quantum Materials Dmitri N. Basov; Columbia University, New York, New York, United States.

Experimentally realizing quantum phases of matter and controlling their properties is a central goal of the physical sciences. Novel quantum phases with controllable properties are essential for new electronic, photonic, and energy management technologies needed to address the growing societal demands for rapid and energy efficient information processing and transduction[1]. *Quantum materials* offer particularly appealing opportunities for the implementation of on-demand quantum phases. This class of materials host interacting many-body electronic systems featuring an intricate interplay of topology, reduced dimensionality, and strong correlations that leads to the emergence of “quantum matter” exhibiting macroscopically observable quantum effects over a vast range of length and energy scales. In this talk I will overview recent efforts to discover, characterize and deploy new forms of quantum matter controllable by light, gating, and nano-mechanical manipulation, effectively programming their properties. I will focus on enticing opportunities to investigate novel quantum phenomena using nascent nano-optical methods developed in my group[2],[3]. [1] D.N. Basov, R.D. Averitt and D. Hsieh, “Towards properties on demand in quantum materials” *Nature Materials* 16, 1077 (2017). [2] S. S. Sunku, G. X. Ni, B. Y. Jiang, H. Yoo, A. Sternbach, A. S. McLeod, T. Stauber, L. Xiong, T. Taniguchi, K. Watanabe, P. Kim, M. M. Fogler, D. N. Basov “Photonic crystals for nano-light in moiré graphene superlattices” *Science* 362, 1153–1156 (2018). [3] G. X. Ni, A. S. McLeod, Z. Sun, L. Wang, L. Xiong, K. W. Post, S. S. Sunku, B.-Y. Jiang, J. Hone, C. R. Dean, M. M. Fogler & D. N. Basov “Fundamental limits to graphene plasmonics” *Nature* 557, 530 (2018).

9:20 AM REFRESHMENT BREAK

SESSION B: Control of Quantum Systems
Session Chairs: Steven Cundiff and Kris Bertness
Wednesday Morning, June 26, 2019
Michigan League, 2nd Floor, Lydia Mendelssohn Theatre

** Invited Paper

10:00 AM **B01

Coherent Control of Graphene-Based Van der Waals Heterostructures Joel I-Jan Wang¹, Daniel Rodan-Legrain², Charlotte Böttcher³, Landry Bretheau⁴, Daniel L. Campbell¹, Bharath Kannan⁷, David Kim⁵, Morten Kjaergaard¹, Philip Krantz¹, Gabriel O. Samach⁵, Fei Yan¹, Jonilyn L. Yoder⁵, Megan Yamoah^{2,7}, Kenji Watanabe⁶, Takashi Taniguchi⁶, Terry P. Orlando^{1,7}, Simon Gustavsson¹, Pablo Jarillo-Herrero² and William D. Oliver^{1,2,5}. ¹Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; ²Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; ³Department of Physics, Harvard University, Cambridge, Massachusetts, United States; ⁴Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA, Palaiseau, France; ⁵Lincoln Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States; ⁶Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan; ⁷Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

Van der Waals (vdW) materials – a family of layered crystals with various functionalities, can be assembled in specific arrangements to create new electronic devices called vdW heterostructures. The extraordinary and versatile electronic properties of these heterostructures, in combination

with their epitaxial precision, make vdW-based devices a promising alternative for constructing key elements of novel solid-state quantum computing platforms. In particular, these new material systems have the potential to improve coherent characteristics in quantum systems while reducing the footprint of individual qubit — both are keys to realizing extensible quantum computing schemes. We demonstrate quantum coherent control of a superconducting circuit incorporating graphene-based vdW heterostructures. We show that this device can be operated as a voltage-tunable transmon qubit, whose spectrum reflects the electronic properties of massless Dirac fermions traveling ballistically. In addition to the potential for advancing extensible quantum computing technology, our results represent a new approach to studying vdW materials using microwave photons in coherent quantum circuits.

10:40 AM B02

(Student) Nonperturbative Multiphoton Absorption in Gallium Nitrides Haiyi Liu¹, Qile Wu¹, Ping Wang¹, Zetian Mi¹, Steven T. Cundiff^{1,2} and Mackillo Kira¹; ¹Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ²Department of Physics, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

Gallium nitride (GaN) nanostructures can be designed to have a bandgap from near infrared to ultraviolet (UV) regime by using suitable heterostructures. By utilizing the large bandgap differences between heterostructure layers, one can realize extreme confinement, even single-monolayer structures that exhibit very strong excitonic binding energy up to hundreds of meV [Appl. Phys. Lett. **109**, 241102 (2016)] due to enhanced Coulomb interactions. We will present new ways of exciting such GaN nanostructures with strong light fields to drive multiphoton transitions and eventually make the onset of high-harmonic generation [Nat. Phys. **7**, 138 (2011)] as a foundation for optically driven UV sources and lightwave electronics [Nat. Phot. **11**, 227 (2017), *Nature* **557**, 76 (2018)]. Even though multiphoton transitions in solids can be qualitatively understood with perturbative approaches we clearly need to address the massive Coulombic and nonperturbative modifications which strong-field excitations will create in GaN. We will present new quantum-theory insights for multiphoton absorption with respect to excitonic as well as plasma emission properties. The results are compared with our first experiment on GaN monolayers. Our realistic quantum theory is based on dynamic cluster expansion which allows for a completely systematic inclusion of the nonperturbative light-matter and Coulombic interactions. In a solid, a strong non-resonant light excitation creates a large set of optical coherences, polarization, as well as electron and hole densities. As we have shown earlier [Nat. Phot. **8**, 119 (2014)], the polarization and densities mix together to generate a significant and transient carrier production for high-harmonic conditions. Especially, considering only either polarization or densities would essentially eliminate the relevant excitations. At the same time, the simultaneous presence of polarization and densities yields excitation induced dephasing for coherences, initiated by scattering of polarization with densities. These scattering events need some time to build up, typically a few to hundreds of femtoseconds, such that dephasing will acquire quantum memory, i.e. dephasing of polarization at a given time depends on polarization at earlier times. This ultrafast onset of dephasing matches the timescales relevant for high-harmonic generation/multiphoton transitions, therefore must be included for a realistic quantum theory. We will demonstrate that the quantum-memory effects indeed play a crucial role in determining the yield of multiphoton transitions. In particular, we find that the multiphoton carrier production becomes incorrectly dominated by non-resonant single-photon absorption when quantum-memory effects are ignored. This yields not only quantitative inaccuracy but also a qualitatively incorrect prediction that multiphoton resonances cannot be detected, contradicting with experiments. Only a theory that fully includes quantum-memory effects can predict qualitatively and quantitatively correct multiphoton absorption resonances dominated by high-order processes. We will show how including quantum memory at the correct level produces distinct multiphoton resonances and scaling at the perturbative regime, and how they are modified in the nonperturbative regime. Our quantitatively correct approach also allows us to quantify a massive Coulomb enhancement of multiphoton transitions near and below the bandgap as a function of driving field strength. We also show how perturbative results are modified as excitations are made stronger, approaching the regime of lightwave electronics and high-harmonic generation. In summary, our theory advancements will provide a new framework for designing GaN-based lightwave electronics realistically.

11:00 AM B03

Semiconducting Carbon Nanotube Polaritonics Jialiang Wang¹, Abitha Dhavamani¹, Louis Haeberlé², Stéphane Kena-Cohen² and Michael S. Arnold¹; ¹Materials Science and Engineering, University of Wisconsin-Madison, Madison, Wisconsin, United States; ²Engineering Physics, Polytechnique Montréal, Montréal, Quebec, Canada.

Polaritons are quasiparticles that emerge in semiconductor microcavities due to strong light-matter coupling between a cavity photon mode and semiconductor excitons. They possess properties inherited from both of these constituents such as the small effective mass of the photon and the strong nonlinear character of the exciton. While most polariton research has focused on microcavities containing group III-V or II-VI quantum wells at cryogenic temperatures, recent research has turned towards systems that will readily allow for room-temperature operation. For example, transition metal dichalcogenides, organic semiconductors, and hybrid organic-inorganic materials all possess highly stable excitons with binding energies >100 meV and large oscillator strengths – thereby enabling the exploitation of polariton phenomena at room-temperature. A promising route, which is only beginning to be explored, is the use of carbon nanotubes for polaritonics. Carbon nanotubes are highly stable and easily processed, have large exciton binding energy (0.3 eV), large oscillator strength, narrow homogeneous linewidth, and tunable bandgap that can be tailored from 1000 – 2000 nm, which is a spectral range of importance for communications and remote sensing technologies. One challenge to fabricating semiconducting carbon nanotube microcavities is nanotubes' polydispersity. Another challenge is controlling the smoothness and quality of the nanotube-mirror interfaces, due to the roughness inherent to nanotube network thin films. Here, we demonstrate how these challenges can be overcome. Electronics-grade (6,5) semiconducting carbon nanotubes are extracted from polydisperse mixtures of metallic and semiconducting nanotubes of various diameters, using conjugated polymer wrappers as selective agents. Dense thin films of these nanotubes, with optical bandgaps of 1.2 eV, are cast and integrated into microcavities with smooth interfaces. Strong exciton-microcavity photon coupling is realized, with a Rabi splitting energy of 0.4 eV at room-temperature. We show how the microstructure and composition of the semiconducting nanotube layers can be tuned to tailor the polariton dispersion and control light-matter interactions. Nanotube polaritons in the future could lead to the development of transformative optoelectronic devices such as low threshold lasers and ultra-efficient optical switches. Nanotubes' strong exciton-phonon scattering characteristics and sizeable third-order susceptibility are expected to promote rapid polariton relaxation – critical for realizing ultralow thresholds and overcoming the relaxation bottleneck that has limited many material systems. At the same time, nanotubes can be integrated onto almost any substrate via simple solution-phase processing, allowing for device integration with conventional technological platforms (e.g., Si, III-V) without the challenges of heteroepitaxial crystal growth.

11:20 AM B04

(Student) Bright Triplet State Dynamics in Lead-Halide Perovskite Nanocrystals Albert Liu¹, Diogo Almeida², Luiz Bonato², Gabriel Nagamine², Luiz Zagonel², Ana Nogueira², Lazaro Padilha² and Steven T. Cundiff¹; ¹University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Universidade Estadual de Campinas, Campinas, Brazil.

Metal-halide perovskites comprise a class of materials that have garnered tremendous interest due to their potential applications in photovoltaic devices. Recently, cesium lead-halide perovskites were synthesized in colloidal nanocrystal (NC) form [Protesescu et al., *Nano Lett.* **15**, 6 (2015)], which exhibit highly efficient luminescence with near-unity quantum efficiency. The unusual brightness of perovskite NCs has since been attributed to a unique exciton fine-structure comprised of a bright-triplet state that forms the band-edge [Becker et al., *Nature* **553**, (2018)], in contrast to lowest-energy dark states that inhibit emission in other colloidal nanocrystals. Understanding this triplet exciton fine-structure is essential to exploiting the unique properties of perovskite NCs in optoelectronic devices. Just as other colloidal materials, however, perovskite NCs suffer from unavoidable inhomogeneous broadening due to NC size dispersion, precluding study of their ensemble homogeneous properties via linear spectroscopic techniques such as absorption and photoluminescence spectroscopy. Here, we circumvent the inhomogeneous broadening of a CsPbI₃ NC ensemble by use of the 2D coherent spectroscopy technique at cryogenic temperatures, which correlates absorption and emission dynamics between different energy levels. By cross-polarizing the excitation beams, quantum superpositions between triplet states were observed that exhibit polarization selectivity and dephasing times on picosecond timescales. Co-polarizing the excitation beams further suppresses the inter-triplet coherence response and reveals

signatures of exciton-phonon coupling in perovskite nanocrystals. These attractive properties suggest that the triplet states in these NCs have potential for a perovskite analogue of valleytronics [Langer et al., *Nature* **557**, (2018)], in which quantum information protocols involving circularly polarized valley excitons in 2D materials instead use linearly polarized triplet excitons in perovskite NCs. Our work motivates further research of inter-triplet coherences and their properties to advance perovskite nanocrystals as a new material platform for quantum computation.

11:40 AM B05

Optical Nonlinearities in Room-Temperature Exciton-Polariton Platforms Fabio Barachati¹, Antonio Fieramosca², Giovanni Lerario², Dario Ballarini², Vinod Menon³, Daniele Sanvitto² and Stéphane Kena-Cohen¹; ¹Engineering Physics, Polytechnique Montréal, Montreal, Quebec, Canada; ²CNR Nanotec, Lecce, Italy; ³Physics, The City University of New York, New York, New York, United States.

Exciton-polaritons are quasiparticles that form in optical microcavities when the light-matter interaction rate exceeds the dissipation rate. These hybrid light-matter particles combine the small effective mass of the photon with the strong resonant optical nonlinearities of the exciton. This has allowed for a broad range of exotic effects to be demonstrated using semiconductor microcavities such as parametric oscillation, optical bistability, superfluidity and recently signatures of the polariton blockade effect. However, the vast majority of these effects have been demonstrated in epitaxially-grown microcavities containing III-V semiconductors. An important disadvantage of these structures is that the low exciton binding energy prevents the observation of these phenomena at elevated temperatures. Evidence for strong nonlinearities in room-temperature systems such as Group III-N, organic semiconductors and monolayers of transition metal dichalcogenides (TMDs) has been scarce. We will review the source of optical nonlinearities in these room-temperature systems and describe our recent observations of room-temperature superfluidity of polaritons in organic microcavities, enhanced third harmonic generation from polaritons, nonlinearities in 2D TMD polaritons and theoretical predictions of other nonlinear effects which have as yet to be observed in polaritonic systems. To conclude we will benchmark room-temperature polaritonic systems and highlight some of their strengths and disadvantages.

SESSION C: 2D Growth and Characterization

Session Chairs: Susan Fullerton-Shirey and Lincoln Lauhon
Wednesday Morning, June 26, 2019
Michigan League, 2nd Floor, Hussey

10:00 AM C01

(Student) Substrate Engineered and Thermodynamically Controlled Growth of Large Area Hexagonal Boron Nitride (h-BN) via Chemical Vapor Deposition Ankit Rao and Srinivasan Raghavan; Centre for Nano Science and Engineering, Indian Institute of Science, Bangalore, India.

Hexagonal boron nitride (h-BN) has been established as the preferred substrate for nanodevices based on 2-dimensional (2D) materials owing to its atomically flat interface, excellent thermal conductivity and suitable dielectric characteristics. Thus, there is a fundamental requirement to manufacture wafer scale h-BN for large area applications and the most scalable method is chemical vapor deposition (CVD). The current approaches for CVD growth of h-BN are by and large empirical due to which there is lack of control over the deposition. Our research involves thermodynamic control of the B-N-H system by identifying the appropriate windows of process parameters for controlled growth of h-BN. Within the thermodynamic windows, the control over gas phase supersaturation would allow better kinetic control over crystal growth. Physico-chemical modelling of the gas phase chemistry is carried out by correlating the growth parameters with the properties of the deposited film. A simple, relatively non-toxic and non-pyrophoric chemistry, consisting of ammonia borane (BH₃-NH₃) has been chosen for vapor phase synthesis of h-BN over copper (Cu) substrate. Thermodynamic control is exercised over gas phase supersaturation by use of carrier gases such as hydrogen (H₂) and argon (Ar) and by controlling the precursor flux via a simple vaporizer setup. This approach allows us to tune the supersaturation and partial pressures of the gases in the chamber. We employ substrate engineering for obtaining preferential nucleation to control the nucleation density and reduce the surface impurity which arise due to precursor chemistry. We obtain control over grain size and number of layers from multilayer films to monolayer, by exercising supersaturation control by

regulating the gas phase chemistry via variation in the H₂ and Ar partial pressures. Preferential nucleation would allow control over the nucleation density and defect density, and additional control over supersaturation would allow tuning of the electrical characteristics. The growth of h-BN layers is accompanied with undesired nanocrystalline BN (n-BN) particles due to the precursor chemistry which degrades the film quality. So, to obtain preferential nucleation and reduce the n-BN density, we employ a 2 step substrate engineering method of nickel (Ni) deposition on copper substrates by RF sputtering, followed by subsequent annealing in H₂ environment to disperse Ni in Cu matrix. We observe a significant reduction in n-BN particles and also preferential nucleation at location of Ni segregation, this indication of nucleation preference at locations of Ni segregation can be attributed to the energetic potential difference at various sites of the Ni incorporated annealed surface. This site selectivity is of thermodynamic nature as the energy barrier for nucleation at different sites are finite at a supersaturation value or at a BH₃NH₃ partial pressure greater than a certain critical value which is the equilibrium partial pressure. The effect of supersaturation on control over defect density is studied with the help of HR-TEM and also by electrical characterization of vertical graphene/h-BN heterostructures. Thus, the effect of growth parameters on the quality of hBN film deposited via CVD is observed with change in partial pressures and flux of precursor, the quality of film significantly changes with all other parameters being same. This can be attributed to the fact that partial pressure of reactants has an exponential effect on supersaturation, hence precise control over growth parameters yield controlled growth of h-BN layers. Thus, we report controllable and scalable growth of h-BN over large areas by implementing thermodynamic control and substrate engineering.

10:20 AM C02

(Student) 2D to 3D Fractal Growth of WSe₂ Using Chemical Vapor Deposition Sayema Chowdhury, Anupam Roy and Sanjay Banerjee; Department of Electrical and Computer Engineering, Microelectronics Research Center, The University of Texas at Austin, Austin, Texas, United States.

Transition metal dichalcogenides are a class of two-dimensional (2D) layered materials that have recently attracted tremendous attention due to their versatile applications in low power electronic, optoelectronic and flexible devices. Among them, tungsten diselenide (WSe₂) is being thoroughly investigated because of its thickness-dependent electronic band structure and *p*-type transistor behavior with high hole mobilities both in bulk as well as monolayer flakes. However, large scale device applications still require an optimized growth method for large area WSe₂ films. Previous studies have reported growth of WSe₂ by direct reaction of W and Se [1] or selenization of WO₃ powder in presence of hydrogen [2] and various others by molecular beam epitaxy (MBE) and chemical vapor deposition (CVD) processes. A recent work demonstrates MBE growth of WSe₂ and the effect of incident Se flux on the lateral (2D) or vertical (3D) growth of WSe₂ domains [3]. However, the limited grain size in MBE limits its application for device purposes [4]. CVD growth can be used to get larger area yields, but it has its own challenges, the most important one being accurately optimizing various parameters to ensure reproducibility of the grown films. To ensure repeatable large area growth, a detailed study of parameter optimization is of utmost importance. In this work we demonstrate CVD growth of WSe₂ on Si/SiO₂ substrates, and investigate the effect of Se flux on the growth of WSe₂ fractal domains. A deviation from optimized growth parameters resulted in the transition from the compact triangular domains to fractal domains of WSe₂. This is in agreement with a recent theoretical work which uses first principles calculations and Monte Carlo simulations to show that, depending on the temperature and the flux, WSe₂ domains can be either fractal, or dendritic, or compact triangular [5]. Two different types of growths are analyzed here, one in a Se-rich and the other in a Se-deficient environment. Raman and photoluminescence (PL) spectroscopy confirms the formation of monolayer WSe₂ of high crystalline quality in the sample grown under Se-rich environment which helps restrict W-rich nuclei formation during growth, hence promoting lateral 2D growth. Depending on the temperature, the grown sample was largely populated with fractal-type domains. For the sample, grown in Se-deficient environment (all other conditions were kept the same), it also demonstrated fractal type growth mostly but the domains were much thicker (~60 nm thick), showing vertical growth of multilayer WSe₂ which can be attributed to insufficient Se-passivation of W-rich nuclei, hence promoting vertical growth. Atomic force microscopy (AFM) images show the lateral (monolayer) versus vertical growth (> 60 nm thick multilayer WSe₂) under Se-rich and Se-deficient conditions, respectively. This work promises a facile route toward finding an optimized recipe for synthesis of TMD compounds with tunable structural properties and can be useful to understand the complex growth mechanism in TMDs. This work was supported by the Army

Research Office (ARO) Grant # W911NF-17-1-0312 (MURI). **References** [1] W. T. Hicks *et al.*, *J. Electrochem. Soc.*, **1964**, *111*, 1058-1065. [2] J. Huang, *et al.* *ACS nano*, **2013**, *8*, 923-930. [3] R. Yue, *et al.*, *2D Mater.*, **2017**, *4*, 045019. [4] A. Roy *et al.*, *ACS Appl. Mater. Interfaces*, **2016**, *8*, 7396-7402. [5] Y. Nie, *et al.*, *2D Materials*, **2016**, *3*, 025029.

10:40 AM C03

(Student) Optical Performance of Hexagonal Boron Nitride Light Emitting Devices Grown by Molecular Beam Epitaxy David A. Laleyan¹, Eric T. Reid², Kelsey Mengle³, Emmanouil Kioupakis⁴ and Zetian Mi⁵; ¹Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ²Electrical and Computer Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ³Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; ⁴University of Michigan, Ann Arbor, Michigan, United States; ⁵Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

Hexagonal boron nitride (h-BN) has shown tremendous promise when used alongside other two-dimensional (2D) materials such as graphene, and as a wide-bandgap semiconductor for deep-ultraviolet optoelectronics and quantum photonics. Owing to its large bandgap energy comparable or higher than Al(Ga)N, h-BN can be used to form heterostructures to address some of the critical challenges of Al(Ga)N-based systems. To date, however, many fundamental material properties of h-BN remain unknown. For example, its bandgap energy remains under debate, with reports spanning from 5.9 to 6.5 eV. There is also strong controversy as to whether h-BN has a direct or indirect bandgap. In this context, we have studied the epitaxy of h-BN by using plasma-assisted molecular beam epitaxy (MBE) on both Ni(111) and sapphire substrates. Epitaxial domains of exceptional crystalline quality were obtained at a high substrate temperature of ~1300 °C on Ni(111), which was validated by in situ reflection high electron energy diffraction (RHEED) monitoring, micro-Raman analysis and strong excitonic photoluminescence (PL) emission. Furthermore, our atomistic calculations revealed that, even though the gap of h-BN is indirect, it luminesces as strongly as direct-gap materials, because of the unusually strong phonon-assisted optical matrix element, which is nearly 600 times larger than that of Si. And indeed, we experimentally found that the luminescence intensity (~220 nm) of such a h-BN sample with a thickness on the order of 10 nm is 10 to 100 times stronger than that of a high-quality 4 μm thick commercially grown direct-bandgap AlN, demonstrating the extraordinary potential of epitaxial h-BN for deep ultraviolet (UV) optoelectronics and quantum photonics. To better understand and further analyze these unique properties, we have conducted in-depth optical measurements of such h-BN samples, including temperature-dependent PL over a wide range of excitation powers. From there, we correlate the different emission peaks to the calculated bandstructure and calculate the internal quantum efficiency (IQE) extracted based on a revised ABC model. An IQE ~50% is obtained at room temperature, which is significantly higher than that of AlGaIn emitting at similar wavelengths. From polarization-dependent PL, we found that the h-BN emission is predominantly transverse electric (TE) polarized light, which is in direct contrast to the dominant TM polarized emission of AlN and Al-rich AlGaIn. This offers significant advantages in achieving high light extraction efficiency (LEE) for potential deep UV light-emitting diodes (LEDs) and lasers, compared to Al(Ga)N-based LED structures which exhibit extremely low external quantum efficiency (<1%) in the wavelength range of <240 nm. By forming a p-i-n structure using this high-quality h-BN as the active region, the current-voltage (I-V) and electroluminescence characteristics of a first demonstration of a h-BN deep UV LED will be reported.

11:00 AM C04

(Student) Role of Surface Processes in Growth of Monolayer MoS₂ for Device Applications Shashwat Rathkantiwar¹, Kranthi V. Kumar¹, Sukanya Dhar¹, Tanushree H. Choudhury², S. A. Shivashankar¹ and Srinivasan Raghavan¹; ¹Centre for Nano Science and Engineering, Indian Institute of Science, Bangalore, India, Bangalore, India; ²The Pennsylvania State University, State College, Pennsylvania, United States.

While considerable progress has been made in the synthesis of 2D materials, optimization of growth, to obtain the desired microstructure, has been a very empirical one. Though physico-chemical models of graphene growth have now been reported, they are almost non-existent for the more complicated systems such as MoS₂, the most popular 2D semiconductor. In this work, we have analyzed the nucleation and growth of MoS₂ by a CVD method in which all precursors are introduced from outside the growth chamber. While the actual chemistry may vary, such a “true” CVD method—most current vapor phase methods involve physical transport of

precursors placed within the reactor from a hot zone to a cold zone- is essential for technological exploitation of all 2D materials in general, to grow heterostructures and for doping in devices. Regardless of these advantages of “true” CVD, the approach presented in this work should be valid for all vapor phase synthesis of 2D materials. While the vapor phase supersaturation (related to Gibbs free energy change) is determined by experimental parameters -pressure, temperature and flow rates- levers that are available to the grower, actual nucleation and edge growth are determined by surface supersaturation. At steady state, the adsorption-diffusion-growth-desorption kinetics determines the relationship between the two. A quantitative understanding of this relationship is thus essential for the grower to assert control on the processes occurring on the growth surface. Such understanding has allowed us to vary the grain size in MoS₂ monolayers from 10 nm to 100 μm in a predictable fashion. The steady state nucleation rates and the edge growth rates were found to be diffusion controlled by a > 1 eV barrier. The different dependencies of nucleation rates and edge growth rates on surface kinetics and supersaturation have been exploited to reduce nucleation density from 10⁷ to 10³ cm⁻² while simultaneously ensuring very large edge growth rates of up to 3.3 μm/s. We demonstrate in this work, that to attain large grain sizes in reasonable time frames one needs to operate in a physico-chemical window in which the kinetics of nucleation are suppressed but those of crystal edge growth are not. In addition, within this window controlling supersaturation in the very early stages of growth is found to have a significant influence. This has been done by adding a reaction product, CO, to the inlet chemistry, a procedure that can only be done in such “true” CVD synthesis. The microstructural improvement is shown to help increase field effect electronic mobility from 0.1 to 17 cm²/V-sec. This research thus enables a straightforward way to prepare large-area single crystals of MoS₂ and highlights the importance of physico-chemical modeling as a predictive approach for the same. We acknowledge funding support from Ministry of Human Resource Development (MHRD) through NIEIN project, from Ministry of Electronics and Information Technology (MeitY) and DST through NNetRA. This work would not have been possible without support from the Research and Development work undertaken under the Ph.D. scheme of Media Lab Asia, Ministry of Electronics and Information Technology (MeitY). We would also like to thank Micro and Nano Characterization Facility (MNCF) and National Nano Fabrication Centre (NNfC) staff at CeNSE, IISc for their help and support in carrying out this work.

11:20 AM C05

(Student) The Effect of Nickel on MoS₂ Crystallization and Growth Revealed with *In Situ* TEM Neha Kondekar¹, Matthew Boebinger¹, Mengkun Tian² and Matthew McDowell^{1,3}; ¹Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States; ²Institute for Electronics and Nanotechnology, Georgia Institute of Technology, Atlanta, Georgia, United States; ³G.W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States.

MoS₂ has an anisotropic crystal structure, with different chemical and electronic environments at basal planes vs. edge sites. Doping MoS₂ crystals with other species through atomic substitution or surface adsorption has been shown to improve electronic properties. While prior studies have investigated the altered chemical and electronic properties induced by additions of metal atoms into the MoS₂ lattice, there is a significant lack of understanding and control over the growth pathways of MoS₂ in the presence of these additional species. Thus, new methods are necessary to understand the growth processes of transition metal dichalcogenides to enable greater control over synthesis. In this study, we use *in situ* transmission electron microscopy (TEM) to observe the crystallization and growth of MoS₂ crystals during heating of a solid-state precursor in the presence of nickel. Nickel is chosen since it is an important additive to enable high catalytic activity of MoS₂ for various reactions. Low concentrations of Ni are observed to cause significant differences in the MoS₂ crystallization and growth process compared to the Ni-free case, leading to an increase in MoS₂ crystal size. This is observed to be due to increased mobility of MoS₂ grain boundaries at high temperatures, which is likely due to Ni binding at edge sites and affecting atomic diffusion dynamics. Higher concentrations of Ni disrupt the MoS₂ crystallization process, with nickel sulfides being the primary product. These findings demonstrate the important role of additional elements in controlling the evolution of TMDCs during synthesis, which should be considered when designing these materials for a variety of applications.

11:40 AM C06 **WITHDRAWN**

Bottom-Up Synthesis of Mixed-Edge Nitrogen-Doped Graphene Nanoribbons Zhijing Feng; Chemical Engineering, University of California, Irvine, Irvine, California, United States.

Graphene nanoribbons (GNRs), which are narrow strips of graphene featuring a quantum confinement-induced bandgap, constitute a promising class of materials for the next generation of semiconductor devices. The bottom-up strategy is a promising approach to precisely synthesize narrow GNRs with the desired structure. To date, these bottom-up strategies have primarily focused on all-carbon systems, with only a limited number of studies describing the preparation of doped GNR frameworks. Moreover, all of the doped GNRs prepared to date feature a limited number of edge motifs. Given the immense potential of width and edge modification for the tailoring of the electronic properties of GNRs, there is value in developing alternative edge structures for this purpose. Consequently, the development of doped GNRs and with alternative edge motifs is an important synthetic challenge. We present the synthesis and characterization on surface of a new class of nitrogen-doped GNRs with a mixed zigzag and armchair edge structure. First, we synthesize a GNR precursor monomer from simple precursors. Second, we evaporate the monomer onto a hot Au(111) substrate under ultra-high vacuum (UHV) conditions, thus obtaining GNR-precursor polymers on surface upon deposition. Third, we form a nitrogen-doped GNR by cyclodehydrogenating the polymer precursor on Au(111) *via* thermal annealing to higher temperatures. We confirm the identity and morphology of our monomer, polymer precursor, nitrogen-doped GNR and bending GNR *via* scanning tunneling microscopy (STM) and inelastic tunneling probe (itProbe). Moreover, we determine the ensemble properties of our monomer, polymer precursor, and nitrogen-doped GNR *via* X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure spectroscopy (NEXAFS). Overall, we demonstrate the formation of a previously unknown nitrogen-doped GNR that contains a novel and unique edge morphology.

SESSION D: Materials for Memory and Neuromorphic Computing Applications

Session Chair: Angel Yanguas-Gil

Wednesday Morning, June 26, 2019

Michigan League, 2nd Floor, Michigan

10:00 AM D01

(Student) Impact of Alloying Contact Metal on Non-Volatile Performance of Lithium Niobate Memristors for Neuromorphic Computing Aheli Ghosh¹, Bill Zivasatienraj², Alex S. Weidenbach² and W. Alan Doolittle²; ¹ECE, Georgia Tech, Atlanta, Georgia, United States; ²Georgia Institute of Technology, Atlanta, Georgia, United States.

Memristors are a key enabling technology for neuromorphic computing due to their application as synaptic analogues and signal propagation elements. Lithium Niobate (LiNbO₃) based memristors demonstrate tunable electrical properties resulting from changes to its electronic band structure as lithium (Li) is redistributed within the crystal or removed (delithiation) from the crystal. This ionic diffusion based resistance switching mechanism in LiNbO₃ memristors does not induce large structural changes such as filament formation or amorphous-to-crystalline phase transformation, enabling lower power consumption and higher scalability for neuromorphic computing applications. LiNbO₃ memristors are natively volatile, however, employing a lithium-alloying contact induces non-volatile behavior in these devices by delithiation of the Li_{1-x}NbO₃ channel under applied bias. Candidate metals for the Li alloying contact in non-volatile LiNbO₃ memristors based on electrochemical potential, solubility limits, and alloy phases include but are not limited to aluminum (Al), chromium (Cr), silver (Ag), tin (Sn), lead (Pb), gold (Au), platinum (Pt), and zinc (Zn). To evaluate the role of alloying contact metal on the non-volatile behavior of these devices, sputtered LiNbO₃ memristors were fabricated with a Li blocking contact/electrode consisting of titanium (Ti) and Au, and a second alloying/Li absorbing contact with Al, Ag and Cr metals. A control device was also fabricated with both Li blocking Ti/Au electrodes. Non-volatile device characteristics investigated include resistance change, retention time, required bias voltage and device repeatability/cycleability. This study aims to better understand the mechanism of resistance modulation in a LiNbO₃ channel, determine if it is strictly dopant extraction or has an electrochemical component, and optimize the electrode material selection for non-volatile LiNbO₃ memristors with high resistance change between set and reset states, stable

and repeatable resistance states, high retention time and potential for scalability. The change in resistance in a large linear 700x200 μm LiNbO₂ memristor with 300 nm Ag electrode was ~ 100 W and for a 300 nm Al electrode < 10 W. Binary phase diagrams for Ag-Li¹ and Al-Li¹ indicate that in contrast to aluminium which only supports $< 1\%$ dissolved lithium without a phase change, silver can support a significant concentration of lithium without forming an alloy. The solid solubility of Li in Ag is ~ 45.6 atomic percent at room temperature indicating greater capacity for modulating LiNbO₂ channel resistance for same device dimensions and LiNbO₂ thin-film, consistent with these observed measurements. ¹ T.B. Massalski, H. Baker, L.H. Bennet, and J.L. Murray, Binary Alloy Phase Diagrams (ASM International, 1986).

10:20 AM D02

(Student) Evidence of a Second-Order Peierls-Driven Metal-Insulator Transition in Crystalline NbO₂—An Electroforming-Free Switching Mechanism for Analog Memristors Matthew Wahila¹, Galo J. Paez Fajardo¹, Christopher Singh¹, Jatinkumar Rana¹, Shawn Sallis¹, Jerzy T. Sadowski², M. Brooks Tellekamp⁴, W. Alan Doolittle⁴, Wei-Cheng Lee¹ and Louis Piper^{2,3}; ¹Physics, Binghamton University, The State University of New York, Binghamton, New York, United States; ²Binghamton University, Binghamton, New York, United States; ³Materials Science and Engineering, Binghamton University, The State University of New York, Binghamton, New York, United States; ⁴Georgia Institute of Technology, Atlanta, Georgia, United States; ⁵Center for Functional Nanomaterials, Brookhaven National Laboratory, Brookhaven, New York, United States.

The metal-insulator transition of NbO₂ is thought to be important for promising, new niobium oxide-based memristor and neuristor devices, and has often been attributed to Mott physics in these contexts.[1–4] However, confusion arises due to the use of multi-phase, electro-formed NbO_x in these memristor devices, whose switching has been explained in the literature both in terms of a Poole-Frenkel mechanism[5] and a Mott-transition associated with NbO₂ nanostructures.[3, 6, 7] By investigating phase-pure, crystalline NbO₂, we avoid the uncertainty created by investigating electro-formed NbO_x-based devices. Using surface sensitive techniques like low energy electron diffraction (LEED), hard x-ray photoelectron spectroscopy (HAXPES), and low energy electron microscopy (LEEM) on NbO₂(440)/Al₂O₃(006) thin films, we show that the phase transition does not extend to film surface, which prefers to form an inactive Nb⁵⁺ containing reconstruction even after annealing to 1600 Celsius degree under high vacuum. X-ray photoemission spectroscopy (XPS) of the crystalline NbO₂ across the metal-to-insulator transition then reveals a second-order Peierls transition in the bulk, in agreement with density functional theory results, indicating electron correlation effects (Mott physics) do not play a significant role in the transition. In addition, the observed temperature dependence of the Nb-Nb dimer distance which controls the NbO₂ resistivity suggests that the switching of future phase-pure NbO₂ memristors could be controlled by resistive heating in an analog rather than digital fashion. [1] S. Kumar, J. P. Strachan, and R. S. Williams, Nature 548, 318 (2017). [2] L. Gao, P.-Y. Chen, and S. Yu, Applied Physics Letters 111, 103503 (2017), <https://doi.org/10.1063/1.4991917>. [3] M. D. Pickett, G. Medeiros-Ribeiro, and R. S. Williams, Nature Materials 12, 114 (2012). [4] Y. Zhou and S. Ramathan, Proceedings of the IEEE 103, 1289 (2015). [5] Z. Wang, S. Kumar, Y. Nishi, and H.-S. P. Wong, Applied Physics Letters 112, 193503 (2018), <https://doi.org/10.1063/1.5027152>. [6] M. D. Pickett and R. S. Williams, Nanotechnology 23, 215202 (2012). [7] S. Kumar, Z. Wang, N. Davila, N. Kumari, K. J. Norris, X. Huang, J. P. Strachan, D. Vine, A. L. D. Kilcoyne, Y. Nishi, and R. S. Williams, Nature Communications 8, 658 (2017). This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-18-1-0024

10:40 AM D03

Energy Efficient Operation Schemes of Nonlinear Selectorless RRAM for Crossbar Array Applications Ying-Chen Chen¹, Chih-Yang Lin², Hui Chun Huang² and Jack C. Lee¹; ¹Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas, United States; ²National Sun Yat-Sen University, Kaohsiung City, Taiwan.

With increasing demand for high-density memory applications, emerging memory technology has been intensively investigated for replacing charge-based flash memory. Resistive random-access memory (RRAM) device attracts great potential because of its simple design, high-speed operation, excellent scalability, and low power consumption. However, the sneak path current through unselected neighboring cells is a major problem in crossbar RRAM array configuration, which significantly affects the read operation and accuracy. To address the sneak path current issue, a switch device is typically integrated with the memory device. However, integrating an additional selector device i.e. 1T-1R and 1S-1R

configurations considerably increase the manufacturing complexity and cost. In order to reduce the process complexity and cost for future microelectronic scaling, the selectorless 1R-only RRAM are proposed for suppressing the sneak path current without utilizing a selector device (Fig. 1). The intrinsic nonlinear nature in a selectorless RRAM can alleviate the sneak path current because the on-state of the selected cell (SC) is read at a high-voltage region, while the sharp conductance decreases at low-voltage region effectively suppress the sneak current through the unselected cells (USC). In this work, we present a bilayer 1R-only selectorless RRAM i.e. high-k/low-k stacking engineering for realizing the self-selective behaviors with high scalability, intrinsic nonlinear nature, and operation schemes. Titanium nitride (TiN) of 200 nm was deposited as the bottom electrode on heavily-doped N⁺ Si wafers. Then, 5 nm of graphite and 7 nm of HfO_x were deposited as resistive switching dielectric layers for bilayer structures by radio frequency (RF) sputtering. The RRAM devices with various via lengths of 0.4 μm , 0.6 μm , 0.8 μm , 1 μm , have been fabricated. The graphite oxide (GO) was examined as formed after HfO_x deposition. Platinum of 165 nm was then deposited as top electrodes, as followed by lift-off process for RRAM devices (Fig. 2). The abbreviations for various devices are listed (Fig. 3). The nonlinear nature of selectorless RRAM is investigated by voltage sweep (V-sweep), and current sweep (I-sweep) (Fig. 4). The I-sweep operation provides the accessible nonlinearity with reduced high resistance state (HRS) current due to lower operation current with suggested thinner filament. The gap design method by SET compliance current limit (CCL) during the SET process has been reported [1-2]. Besides, the current sweep operation enlarges the operation window with accessible nonlinearity (~ 40) and maintained as CCL up to 5 mA. Multilevel cell (MLC) is demonstrated on H7G5 selectorless RRAM by I-sweep (Fig. 5, red arrows in dark pink curve), and the pulse waveform modulations (Fig. 5, inset). The switching energy of various selectorless RRAMs in this work (right panel) is compared with different emerging memory categories (left panel) (Fig. 6). The read margin increases with the number of word line decreasing, which is owing to lower sneak path current through the unselected cells. The equivalent circuit of an N \times N crossbar array for the one bitline pull-up read scheme [3]. The simulation results suggest that the nonlinearity behavior itself can guarantee the N of 120 for H7G5, N of 80 for H4S9 on the premise of 10% read margin, which is improved in comparison to HfO_x single layer devices (N=2) under the same read margin criterion (Fig. 7). The benchmarks of bilayer selectorless RRAMs are summarized by nonlinearity as a function switching energy (Fig. 8) [4-10], showing that the H7G5 is an excellent candidate for bilayer selectorless RRAM with high nonlinearity (~ 120), good memory window ($\sim 10^2$), and low switching energy (~ 40 pJ/bit). The scalability of bilayer structures with intrinsic nonlinearity for suppressing sneak path current is desirable in the low-power selectorless memory array, high-density storage memory-integrated applications.

11:00 AM D04

(Student) Scalability of Non-Volatile Lithium Niobite Memristors—Potential for Millivolt Operation of Neuromorphic Devices Bill Zivasatienraj, Alex S. Weidenbach, Aheli Ghosh, Timothy M. McCrone and W. Alan Doolittle; Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States.

Neuromorphic computing is a rapidly growing research area that aims to achieve the energy-efficient computational power of the brain. By utilizing a biologically inspired neuron-synapse system, many computational tasks that are difficult for present Von Neumann architectures are implemented significantly faster and with less resource consumption. The memristor has been considered a promising element for the realization of a solid-state neuristor circuit because its ability to retain memory inherently provides a low-power solution and leads to adaptive learning. In addition to memristive and non-volatile characteristics, the scalability of memristors is important for the design of high-density neural networks. Lithium niobite (LiNbO₃), a lithium intercalated sub-oxide of the maturely studied lithium niobate (LiNbO₃), is a memristive material that utilizes lithium intercalation and deintercalation to produce hysteretic characteristics. Mobile lithium ions within LiNbO₃ create vacancies that act as dopants as they intercalate through the material under the influence of an electric field. In volatile memristors, the resulting non-uniform distribution of vacancies causes a change in conductivity, which relaxes to equilibrium upon removal of electrical bias. In nonvolatile memristors, rather than allowing the ions to diffuse, metals known to alloy with lithium, such as silver, can trap the ions outside the LiNbO₃ and thereby allow non-volatile conductivity changes. When a positive bias is applied to a titanium lithium-blocking contact, positively charged lithium ions drift towards and are trapped by the silver contact. The delithiation of LiNbO₃ increases the lithium vacancy concentration resulting in an increase in conductivity. Conversely, a positive bias applied to the silver lithium-alloying contact

releases the trapped lithium ions back into the bulk material, decreasing the conductivity due to lithiation. In this study, we report on the scaling of non-volatile LiNbO₂ memristors from devices with device lengths ranging from 25 to 1000 μm. LiNbO₂ non-volatile two-terminal memristors were fabricated using a titanium lithium-blocking contact for one terminal and a silver lithium-alloying contact for the other terminal, with gold as a final cap layer on both contacts. The rectangular mesa-isolated devices have widths ranging from 5 μm to 50 μm, each with varying active area aspect ratios of 5, 10, and 20. Memristors of varying sizes are electrically conditioned to exhibit non-volatile behavior, with observed stable resistance changes of up to $\Delta R/R \sim 2000\%$. Importantly, all devices require a threshold voltage before resistive programming is observed. It is found that regardless of the length memristor used, the critical electric field for the onset of programming is a mere 535 ± 3 V/cm. This implies that future efforts for nanoscale devices can be operated at millivolts. While nanoscale devices are still under development, and energy consumption is not yet measured, present microscale devices program at ~ 137 μWatts DC for 25 μm lengths. Thus, 25 nm future devices should reach ~ 137 pWatt DC programming with a threshold voltage for programming of only 1.3 millivolts. Nanoscale devices will be presented at the meeting to refute or support these projections obtained from the current microscale data. The mechanism of lithium intercalation into and out of silver, how it scales as the nanometer device regime is approached, and the tunability of the non-volatile LiNbO₂ memristors will be discussed.

11:20 AM D05

Phase-Change Nano-Clusters Embedded Nitride Films Capable of Adaptive Learning and Signal Modulation Qin Wan, Fei Zeng, Jun Yin, Jialu Liu and Yingcong Wang; School of Materials Sciences & Engineering, Tsinghua University, Beijing, China.

A type of functional film is fabricated by doping transition elements (such as niobium) into nitride and naturally oxidizing them. It is found that the Nb atoms absorb the neighbor oxygen atoms in the film during strong stimulations. This results in the formation of filaments composed of phase-change nano-clusters of NbO in the nitride films. The system state is determined by both oxygen vacancies (V_{O_s}) migration and structure evolution of phase-change nano-clusters. The former controls the formation and rupture of conductive filaments depending on the direction of V_{O_s} migration and electrical stimulation strength, while the later acts as an adaptive switch depending on local heat environment. Strong electrical stimulations will modify the resistance permanently to fulfill memory and learning. Interesting finding is that a set of periodical input can be modified to an output with relative longer periodicity, suggesting signal modulation. The behaviors of this functional nitride film are regarded to replicate the critical dynamics in real synapse, such as the Ca²⁺ flux and transmitter release at the pre-synapse and the ionic flux modulated by the post-synaptic potential (current). Diverse learning protocols proposed in neuroscience, including spike-rate dependent plasticity and spike-timing dependent plasticity. Our work proposes an elementary cell closely approximating biological synapse and usable for brain-like computing.

11:40 AM D06

(LATE NEWS) Effect of Atomic Layer Deposition Grown VO₂ Film Morphology and Crystallinity on Opto-Electronic Phase Transition Jason R. Avila¹, Marc Currie², Brian Downey² and Virginia Wheeler²; ¹Postdoctoral Fellow, American Society of Engineering Education, Washington, District of Columbia, United States; ²U.S. Naval Research Laboratory, Washington, District of Columbia, United States.

VO₂ is a promising material for a variety of electronic and opto-electronic applications due to its metal-to-insulator phase transition, which occurs near room temperature and is accompanied by dramatic changes in electrical resistance and optical transmission. Atomic layer deposition (ALD) is an advantageous technique to deposit VO₂ due to its excellent conformality and ability to deposit thin films at low temperatures allowing for growth on a variety of substrates and device architectures. Such conformality is especially useful for complex optical devices with non-planar structures such as waveguides or diffraction gratings. There is, however, no current ALD method for direct growth of crystalline VO₂, thus post deposition annealing is required to achieve crystallinity. In this study, we examine the impact of annealing conditions on the resulting phase, crystallinity, composition, morphology, and metal-to-insulator transition properties of as-grown amorphous ALD VO₂ films on sapphire. Altering annealing parameters such as temperature, time, and O₂ pressure enables control over film morphologies and phase transition properties of the resulting VO₂ film. For example the VO₂ film roughness is decreasing by an order of magnitude by decreasing the anneal temperature 100 °C, which simultaneously improves the hysteresis of the metal-to-insulator film transition. Through these efforts, the structure-property relationship of

VO₂ will be revealed, which can then provide a guide for tailoring of optimal film properties for specific electronic and optical applications.

SESSION E: Energy Conversion and Storage

Session Chair: Zetian Mi

Wednesday Morning, June 26, 2019

Michigan League, 3rd Floor, Henderson

10:00 AM E01

(Student) Single-Crystalline III-N Thin Film-Based Flexible Piezoelectric Generators and Pulse Sensors Jie Chen^{1,2,3}, Noor Nabulsi², Weijie Wang^{2,3}, Heidi Johnson⁴, Seungkyu Oh^{2,3,5}, Haoran Liu⁶, Wenbo Zhao⁷, Shahab Shervin², Sara Pouladi^{1,2,3} and Jae-Hyun Ryou^{1,2,5}; ¹Materials Science and Engineering Program, University of Houston, Houston, Texas, United States; ²Department of Mechanical Engineering, University of Houston, Houston, Texas, United States; ³Advanced Manufacturing Institute (AMI), University of Houston, Houston, Texas, United States; ⁴Department of Mechanical Engineering, Brigham Young University, Provo, Utah, United States; ⁵Texas Center for Superconductivity at UH (TcSUH), University of Houston, Houston, Texas, United States; ⁶Department of Nanomedicine, Houston Methodist Research Institute, Houston, Texas, United States; ⁷Department of Neurology, Xuanwu Hospital, Capital Medical University, Beijing, China.

Single-crystalline group III-nitride (III-N) thin films obtained by epitaxy have been widely used in electronic and optoelectronic devices, such as transistors, light emitting diodes (LEDs) and photodiodes, as great progress has been made to achieve high crystal quality. Besides, III-N thin films are good candidates to make piezoelectric devices, since high piezoelectric coefficient is readily available without electrical poling as the atoms are already well aligned in the as-grown single-crystalline thin film. Compared with conventional piezoelectric materials such as lead zirconate titanate (PZT), zinc oxide (ZnO) and polyvinylidene fluoride (PVDF), III-N thin films have the advantages of good biocompatibility without containing toxic elements, high durability being chemically stable, and simple process without extra electrical poling. Unfortunately, applications in piezoelectric devices such as generators and sensors which usually require flexibility are still underdeveloped, due to the brittleness of III-N thin film and difficulty to be flexible since they are usually grown on rigid substrates. In this research, flexible piezoelectric generator (F-PEG) and flexible piezoelectric pulse sensor (F-PPS) were developed with single-crystalline III-N thin film, which is composed of an AlN buffer layer, Al_xGa_{1-x}N interlayers and a top GaN layer, by transferring the as-grown thin film from the Si (111) substrate to a foreign flexible substrate. Large-area and defect-free flexible single-crystalline III-N thin film was obtained by this layer-transfer method. The III-N thin-film F-PEG can generate an open-circuit voltage of 50 V, a short-circuit current of 15 μA, and a maximum power of 167 μW with a corresponding optimum load resistance of 5 MΩ. The III-N thin-film F-PEG is able to directly power electronics such as light-emitting diodes and electric watches, and charge commercial capacitors and batteries. The III-N thin-film F-PPS is sensitive enough to convert the subtle deflection caused by the arterial pulse into electrical signal and detect the pulse waveform with detailed characteristic peaks from most arterial pulse sites. Both the F-PEG and the F-PPS showed high durability and stable outputs after being subjected to long-term tests. The piezoelectric devices made from single-crystalline III-N thin films have great potential applications in future flexible wearable electronics, such as the energy harvester and active pulse sensor.

10:20 AM E02

(Student) Ultra-Stable and High Efficiency Si Photocathode Protected by Multifunctional GaN Nanostructures Srinivas Vanka^{1,2}, Baowen Zhou², Nick Pant² and Zetian Mi²; ¹McGill University, Montreal, Quebec, Canada; ²Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

Photoelectrochemical (PEC) water splitting is a promising and environmentally benign method for solar hydrogen generation and has attracted significant attention over past few decades. A key component of a PEC system is an efficient and stable semiconductor photocathode. To date, however, there have been no demonstrations of high efficiency and stable photoelectrodes. In this work, we have investigated the use of GaN nanostructures as a multifunctional passivation layer for Si photocathodes, which not only offers robust protection against photo and chemical corrosion for the underlying Si light absorber but also significantly improves the reaction kinetics and solar-to-hydrogen efficiency. We have

demonstrated that such a monolithically integrated n^+ -GaN nanowire/Si photocathode can exhibit a half-cell solar hydrogen conversion efficiency of 10.5% and ultra-high stability of >2,000 hrs, which are the best values ever reported for a Si photocathode. In this study, GaN nanowire arrays were grown on Si wafer under N-rich conditions to promote the formation of N-terminated surfaces, which can protect against photo-corrosion and oxidation. We have performed detailed X-ray photoelectron spectroscopy measurements and revealed that the conduction band edges of GaN and Si are near-perfectly aligned, which enables efficient extraction of photogenerated electrons from the underlying Si wafer to GaN nanowires. Electrochemical impedance measurements further confirm that, due to the extremely large surface area of GaN nanowires, the charge carrier transfer resistance at the semiconductor/liquid junction is reduced by nearly two orders of magnitude compared to that for a planar Si photocathode. The GaN nanowire protected Si photocathodes exhibit excellent performance, including a saturated photocurrent density of ~38 mA/cm² with onset potential ~0.5 V vs reversible hydrogen electrode (RHE) and a large ABPE of 10.5% in 0.5 M H₂SO₄ under AM 1.5G 1 sun illumination. Chronoamperometry analysis for the photocathode shows a stable photocurrent density of ~38 mA/cm² for >2,000 h, which, to our knowledge, is the best reported stability for any semiconductor photoelectrode. This is in direct contrast to the conventional approaches, wherein the incorporation of an extra surface protection layer for the underlying photoelectrodes often compromises the charge carrier extraction and limits the maximum achievable efficiency. Significantly, both Si and GaN have already been widely produced in the electronics and photonics industries, thereby providing a scalable platform for future solar fuel devices and systems. Our studies offer a viable path in the quest for a high-efficiency and highly stable semiconductor photoelectrode for solar water splitting.

10:40 AM E03

An Artificial Photosynthesis System for Direct Conversion of CO₂ to Formic Acid Under Sunlight Illumination Baowen Zhou², Srinivas Vanka^{3,2}, Nick Pant^{1,2}, Sheng Chu³ and Zetian Mi²; ¹Applied Physics, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Electrical Engineering and Computer Science, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ³McGill University, Montreal, Quebec, Canada.

Photoelectrochemical conversion of CO₂ with H₂O into high-energy fuels and value-added chemicals provides an appealing strategy for storing intermittent solar energy and reducing anthropogenic carbon emissions. However, the chemical inertness of CO₂ and the myriad reaction pathways render the transformation low efficiency. In this work, we report a unique GaN: Sn nanoarchitecture integrated on planar silicon for aqueous photoelectrochemical reduction of CO₂ to formic acid. The sample was synthesized by coupling GaN nanowires (NWs) with electrodeposition of Sn nanoparticles (Sn NPs). Firstly, plasma-assisted MBE was used for growing GaN NWs on planar n^+ -p Si junction. Sn NPs were then electrochemically deposited on GaN NWs. In such a design, the planar n^+ -p Si junction can harvest a large part of the solar spectrum to generate holes and electrons. Photo-generated electrons are readily transferred from Si to Sn NPs via the 1-D defect-free GaN NWs, due to their strong charge carrier extraction effect. Then, Sn NPs catalyze the CO₂-into-HCOOH conversion. High Angle Annular Dark-field Scanning Transmission Electron Microscopy (STEM-HAADF) image further discloses that Sn NPs are uniformly distributed on GaN nanowire with diameter of ca. 2.3 nm and high-density sites. Such a multiscale and multifunctional heterostructure offers a superior configuration for outstanding photoelectrochemical CO₂ reduction towards formic acid. Linear sweep voltammetry (LSV) measurements of Sn NPs/GaN NWs/Si in CO₂-saturated 0.1 M aqueous solution of KHCO₃ under standard one-sun illumination were firstly conducted using a typical three-electrode configuration. A large onset potential of +0.22 V vs. RHE, corresponding to a current density of -0.2 mA/cm², is achieved. The current density can reach -28.2 mA/cm² at a potential of -0.8 V vs. RHE. The faradaic efficiency for various products at different potentials was then studied. At the applied potential of -0.33 V, HCOOH is the predominant product with a maximum faradaic efficiency of 84%. To further evaluate the performance of Sn NPs/GaN NWs/Si photoelectrode, the turnover number (TON) and turnover frequency (TOF) for photoelectrochemical formic acid generation from CO₂ were estimated at different applied potentials under standard one-sun illumination. A maximum TON for formic acid as high as 12800 with a corresponding unprecedentedly high TOF of 107 min⁻¹ was achieved at -0.53 V vs. RHE within two hours, which is much higher than that of state-of-the-art homogeneous metal-based molecular catalysts for solar-driven CO₂-into-HCOOH conversion. These results provide unambiguous evidence that the configuration of Sn NPs/GaN NWs/Si is highly efficient for superior production of formic acid from

photoelectrochemical CO₂ reduction. Stability testing was performed at a fixed potential of -0.53 V vs. RHE in CO₂-saturated 0.1 M KHCO₃ aqueous solution under standard one-sun irradiation. It is observed that the photocurrent density does not show observable degradation after 10 hour irradiation. And the isotopic experiments suggest that formic acid indeed originated from carbon dioxide. In summary, we demonstrate that one-dimensional GaN NWs integrated on planar Si can be used as superior scaffolds for highly efficient loading Sn NPs for artificial photosynthesis of formic acid from CO₂ reduction. The achievement of one-step solar-driven CO₂ reduction to chemical fuels with energy conversion efficiency >10% is in progress and will be reported.

11:00 AM E04

Focusing on the Raman Spectroscopy of Lithium-Ion Batteries Sarah C. Shidler¹, Tim Batten², Ian Hayward² and Tim Prusnick¹; ¹Spectroscopy Products Division, Renishaw Inc, West Dundee, Illinois, United States; ²Spectroscopy Products Division, Renishaw plc, Gloucestershire, United Kingdom.

Raman spectroscopy is a powerful technique for studying lithium-ion batteries. It can identify all the key electrode and electrolyte components, differentiating—for example—the forms of carbon in negative electrodes. It can also determine the spatial distribution of these components and detect the structural changes that occur during battery cycling. Furthermore, it can be used for not only *ex situ*, but also for non-destructive *in situ* and *operando* measurements (in appropriate electrochemical cells). It is therefore ideal for not only studies of the basic chemistry involved, but also for aiding the development of commercial batteries. Lithium-ion batteries do however prove challenging to analyse. A high lateral spatial resolution is needed to map fine detail, but this requires a good focus (to micrometre precision). This is typically difficult to achieve on electrodes because their surfaces are relatively rough and uneven. Here we present results that show the benefit of real-time focus-tracking during Raman measurements. The Raman microscope maintains optimum focus during mapping experiments by continuously adjusting the height of the sample. Examples are taken from both research and commercial batteries. They illustrate how measurements that would normally be very difficult or impossible are now easy to achieve. An additional advantage of the dynamic focus-tracking is that sequential spot measurements may be automatically made on electrodes that are expanding and contracting during cycling, removing the need for continual operator intervention to maintain focus.

11:20 AM E05

(Student) InGaN/Si Tandem Photocathode for High Efficiency Unassisted Solar Water Splitting Srinivas Vanka^{1,2}, Baowen Zhou², Nick Pant², Alexa Roberts², Krishnamurthy Kulkarni², Yongjie Wang² and Zetian Mi²; ¹McGill University, Montreal, Quebec, Canada; ²Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

Solar hydrogen fuel is one of the most sustainable and clean alternatives to address the current global energy needs by using the two most abundant natural resources on earth, i.e., water and sunlight. Photoelectrochemical water splitting is a clean and environmentally friendly method for solar hydrogen generation. III-nitride semiconductors are one of the most promising materials to realize high efficiency photoelectrodes: their energy bandgap can be varied across nearly the entire solar spectrum by changing the alloy compositions and the band edge positions straddle water oxidation and reduction potentials under deep visible light irradiation. To date, however, the previously reported InGaN photoelectrodes generally exhibit very low photocurrent densities, due to the presence of extensive defects, dislocations, and indium phase separation. Here, we demonstrate the epitaxy of high-quality InGaN nanowires (NWs) on a Si p-n junction solar cell wafer by plasma-assisted molecular beam epitaxy to realize, for the first time, a Si-based double-junction photocathode. Such a tandem photoelectrode consists of a top InGaN junction and bottom Si junction. An n^{++}/p^{++} InGaN tunnel junction (TJ) is incorporated within the InGaN nanowire segment. Due to the presence of a downward band bending for p^+ -InGaN NWs, photo-generated electrons can readily diffuse to the nanowire/electrolyte interface to drive proton reduction reaction. Photo-generated holes, on the other hand, migrate towards the TJ, which recombine with photo-generated electrons extracted from the underlying Si solar cell through the n^+ -InGaN buffer segment. The SEM image shows the NWs are vertically aligned on n^+ -p Si substrate with a length of ~600 nm and diameter of ~90 nm. The photoluminance (PL) measurement shows the peak position is at 540 nm (bandgap ~ 2.3eV), corresponding to an In composition of ~30%. We have also shown that proton reduction cocatalyst and passivation techniques play an important role to achieve efficient and stable solar water splitting. With the incorporation of Pt co-

catalyst particles on InGaN nanowire surface, we have demonstrated solar water splitting on InGaN/Si double-band photocathode with a maximum current density of 10 mA/cm² in 0.5 M H₂SO₄ and a half cell conversion efficiency of ~10% under AM1.5G one-sun illumination in three-electrode configuration. Significantly, when measured in two-electrode configuration, i.e., practical solar water splitting conditions, the InGaN/Si double junction photocathode exhibit an onset voltage (V_{on}) of ~2 V vs. IrO₃, which include the photo-voltage generated by both the top p⁺-InGaN and bottom Si junction. At zero-bias, a photocurrent density ~6.2 mA/cm² is measured under AM1.5G one-sun illumination, corresponding to a solar-to-hydrogen (STH) efficiency ~7.6%, which, to the best of our knowledge, is the highest value ever reported for a Si-based photoelectrode, or for any III-nitride based photoelectrode. The double-junction photocathode also shows no degradation during initial long-term stability measurements. Work is currently in progress to achieve Si-based photocathode with STH efficiency >15% and stability >1000 hrs by further optimizing the surface passivation of InGaN NWs to protect against surface recombination and photo-corrosion.

11:40 AM E06

(Student) Increased Collection Efficiency by Design Improvements for Planar GaN-Based Betavoltaic Battery Kasey Hogan², Johnny Russo¹, Marc Litz¹, Isra Mahaboo², Emma Rocco², Sean A. Tozier², Vincent E. Meyers², Benjamin McEwen² and Fatemeh (Shadi) Shahedipour-Sandvik²; ¹U.S. Army Research Laboratory, Adelphi, Maryland, United States; ²Colleges of Nanoscale Science and Engineering, State University of New York Polytechnic Institute, Albany, New York, United States.

Betavoltaic (BV) micro-batteries show promise as a replacement for conventional lithium ion batteries in low power applications due to high energy density, relatively low mass and long lifetime. In a BV device, electron hole pairs are created by incident beta radiation and swept away in the depletion region of a p-n junction as usable current. The (Al)GaN material system shows promise for use in BV configuration due to its diverse properties including wide bandgap, radiation hardness, chemical inertness, and physical hardness. Here we report on the improvements made to a conventional planar design which led to ~7% power conversion efficiency as measured by electron beam induced current (EBIC) at 16 keV - the highest reported for p-i-n GaN BV configuration. The device layer thicknesses were optimized by Monte Carlo simulation of electron penetration to best couple with a ⁶³Ni source. The p-i-n device consisted of 80 nm p-GaN, 500 nm u-GaN, on an n-GaN template grown by metal organic chemical vapor deposition (MOCVD). Due to a low minority carrier diffusion length in p-type GaN material, a semitransparent p-contact was utilized to enable efficient current collection across the full device area. The contact consisted of a Ni (5 nm) /Au (5 nm) spreading layer with a thicker Ni/Au ring surrounding for device probing and wire-bonding. The semitransparent characteristic allows for the passage of incident (beta) electrons with limited attenuation. Limiting leakage current is crucial for BV batteries which operate in the low power regime (nW -μW). The main source of leakage and current loss from planar GaN based devices is due to high dislocation defect density inherent to heteroepitaxial growth, along with the damaged mesa sidewall post dry etch. To overcome this, a potassium hydroxide (KOH) wet etch treatment was added to passivate the sidewall after mesa isolation, reducing the leakage current density to 0.93 μA/cm². BV device fabrication on bulk GaN is also being studied to reduce carrier recombination from bulk defect traps and the results will be presented. Noteworthy is the difference in the use of EBIC technique from a real radioisotope source due to the variable beta energy spectrum. As such, coupling of the device with ⁶³NiCl₂ and ¹⁴⁷PmCl₂ source will also be reported. The limitations in using a planar device are also discussed, while sharing progress towards next generation 3D batteries.

SESSION F: Novel Nitride-Based Materials Session Chairs: Charles Lutz and Christine Wang Wednesday Morning, June 26, 2019 Michigan League, 3rd Floor, Koessler

10:00 AM F01

(Student) Tuning the Optical Properties of ScN Deposited on Al₂O₃ with DC Reactive Magnetron Sputtering by Changing Sputter Power. Zachary Biegler^{1,2}, Hadley Smith^{3,2}, Rachel Adams^{2,3,4}, Kurt Eyink², John S. Cetnar⁵, David Look^{5,6} and Amber Reed²; ¹Electro-Optics and Photonics, University of Dayton, Dayton, Ohio, United States; ²Materials Directorate, Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio, United States; ³Physics, University of Dayton, Dayton, Ohio, United States; ⁴Mechanical Engineering, University of Dayton, Dayton, Ohio, United States; ⁵Sensors Directorate, Air Force Research Laboratory, WPAFB, Ohio, United States; ⁶Semiconductor Research Center, Wright State University, Dayton, Ohio, United States.

Transition metal nitrides (TMNs) have gained significant scientific interest in recent years due to their high chemical and thermal stability, diverse and tunable properties, and potential for use in a wide range of applications. Scandium nitride (ScN), one such TMN, is a semiconducting material that exhibits a high degree of degeneracy due to oxygen incorporation and nitrogen vacancies. It possesses the typical characteristics of the TMN family being that it is corrosion resistant, thermally stable, capable of alloying with other TMN materials, and the material properties may be tuned through deposition conditions. Additionally, ScN (111) is closely lattice matched to GaN (0001) (<1% mismatch). As such, some have shown that an interlayer ScN (111) is capable of reducing the dislocation density in the GaN top layer.^[i] This has led some to consider using ScN substrates for GaN based electronics. Research to date has focused mostly on the electrical properties of ScN and what causes its observed degeneracy. Due to the rock salt structure of ScN, most growth has focused on MgO (100) substrates. However, epitaxial growth of ScN (111) on Al₂O₃ (0001) has not been explored extensively. In addition, the degree to which the optical properties of ScN can be tuned is still largely unknown. To better understand the optical properties of ScN, a series of 50nm ScN layers were grown on Al₂O₃ (0001) by controllably-unbalanced, DC reactive magnetron sputtering. The sputtering power was varied from 25 W to 200 W. The crystallinity of the ScN films were characterized by X-ray diffractometry (XRD), which showed successful growth of ScN (111) on Al₂O₃ (0001). The Pendellösung fringes in the XRD images were used to calculate film thickness and to show high quality growth. The optical properties of the films were obtained through spectroscopic ellipsometry (SE), which showed the ability to tune the peak location in the imaginary part of the dielectric constant. This peak has previously been attributed to interband transitions at the direct band gap near 530nm. ^[ii] Additionally, the zero crossover point in the real part of the dielectric constant (where the film begins to behave metallically) shifted significantly. Finally, carrier concentrations and mobilities of the films were obtained through temperature dependent Hall Effect measurements, which corroborated the values obtained from the SE measurements. ^[i] Kappers, M. J. *et al.* Interlayer methods for reducing the dislocation density in gallium nitride. *Physica B: Condensed Matter* **401-402**, 296-301 (2007). ^[ii] Saha, B. *et al.* Compensation of native donor doping in ScN: Carrier concentration control and p-type ScN. *Appl. Phys. Lett.* **110**, 252104 (2017).

10:20 AM F02

(Student) Polarization Modulation Effect of BeO on AlGaIn/GaN High-Electron-Mobility Transistors Weijie Wang¹, Sara Pouladi², Seung Min Lee³, Jung Hwan Yum⁴, Jie Chen⁵, Shahab Shervin⁶, Jungwoo Oh³ and Jae-Hyun Ryou²; ¹Mechanical Engineering, University of Houston, Houston, Texas, United States; ²Mechanical Engineering, University of Houston, Houston, Texas, United States; ³School of Integrated Technology, Yonsei University, Incheon, Korea (the Republic of); ⁴Multidimensional Carbon Materials, Institute for Basic Science, Ulsan, Korea (the Republic of); ⁵Materials Science and Engineering Program, University of Houston, Houston, Texas, United States; ⁶University of Houston, Houston, Texas, United States.

The excellent characteristics of beryllium oxide (BeO) such as very high thermal conductivity, ultra-wide bandgap energy, and high dielectric constant make it well suited for high power applications. We investigated the polarization modulation effect of single-crystalline BeO layer on AlGaIn/GaN high-electron-mobility transistors (HEMTs) and found that a

BeO layer on top of the AlGaIn Schottky barrier layer increases the 2-dimensional electron gas (2DEG) density inside the triangular quantum well comparing to conventional AlGaIn/GaN HEMTs. Higher transconductance g_m and source-drain current from simulation results indicates that BeO layer can modify the total polarization field at the AlGaIn/GaN interface. A single-crystal BeO thin film of around 24-nm is grown on AlGaIn/GaN HEMT that is grown on Si (111) substrate by atomic-layer deposition (ALD). High-resolution X-ray diffraction (XRD) scan confirms the in-plane 6-fold symmetrical wurtzite structure of BeO layer which is aligned with beneath GaN layer. Room temperature Hall-effect measurement are performed and a 20 % increment of sheet carrier concentration are observed comparing to conventional HEMT with same ohmic contacts. Higher transconductance g_m and source-drain current I_d are also observed in I-V characteristics. The capacitance-voltage (C-V) measurements are undergoing to confirm the increment of 2DEG concentration and the negative shift of threshold voltage. A thin layer of BeO on top of AlGaIn/GaN HEMT can improve heat dissipation as well as enhance 2DEG density at the interface which will significantly improve the HEMT performance for high power applications.

10:40 AM F03

Properties of Bulk Scandium Nitride Crystals Grown by Physical Vapor Transport James H. Edgar¹, Hayder Al-Atabi¹, John S. Cetnar², David Look², Zheng Qiye³ and David Cahill³; ¹Tim Taylor Department of Chemical Engineering, Kansas State University, Manhattan, Kansas, United States; ²Sensors Directorate, Air Force Research Laboratory, WPAFB, Ohio, United States; ³Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, United States.

Scandium nitride an indirect band gap semiconductor ($E_g = 1.3$ eV) of interest as a substrate for gallium nitride epitaxy and as a component in Al_{1-x}Sc_xN layers for piezoelectric devices. In this study, scandium nitride (ScN) single crystal layers were grown via physical vapor transport in the temperature range of 1900 °C to 2140 °C under a nitrogen pressure between 15 to 20 torr. Growth times of up to 20 days were employed, resulting in crystals as thick as 2 mm. Single crystal tungsten (100) was used as seed crystals. The lattice constant mismatch between the ScN and W was reduced to 0.3% by adopting an in-plane orientation of ScN [100] || W[001]. The ScN (200) x-ray rocking curve FWHM decreased with growth temperature and crystal thickness. A FWHM of 820 arcsec was achieved for a 90 μm thick layer. Hall effect measurements revealed the layers were *n*-type with a 300 K electron concentration and mobility of 2.0×10^{21} cm⁻³ and 80 cm²/V-s respectively. Consequently, these ScN crystals had an exceptionally low electrical resistivity, 3.9×10^{-5} Ω-cm. The electronic thermal conductivity was 17-18 W/m-K at 300 K based on the Wiedemann Franz law. The experimental density, hardness, and reduced elastic modulus were 4.15 gm/cm³, 14.5 GPa, and 216 GPa respectively.

11:00 AM F04

(Student) Ternary Heterovalent Alternative Wide Band Gap Semiconductors Krystal R. York¹, Robert Makin², Steve Durbin³, James P. Mathis⁴, Nancy Senabulya⁴, Zihao Deng⁵, Logan D. Williams⁶, Roy Clarke⁷, Emmanouil Kioupakis⁸, Patrice Miska⁹ and Roger Reeves¹⁰; ¹Electrical and Computer Engineering Department, Western Michigan University, Kalamazoo, Michigan, United States; ²Electrical and Computer Engineering, Western Michigan University, Kalamazoo, Michigan, United States; ³Western Michigan University, Kalamazoo, Michigan, United States; ⁴Applied Physics, University of Michigan, Ann Arbor, Michigan, United States; ⁵Material Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; ⁶MSE, University of Michigan, Ann Arbor, Michigan, United States; ⁷Physics, University of Michigan, Ann Arbor, Michigan, United States; ⁸University of Michigan, Ann Arbor, Michigan, United States; ⁹Université de Lorraine, Nancy, France; ¹⁰University of Canterbury, Christchurch, New Zealand.

For short wavelength optoelectronic devices requiring a direct band gap, the III-N family dominates in many applications, despite the fact that gallium and indium are harmful to the environment to extract, expensive, and difficult to recycle. However, a number of potential alternatives have been proposed recently, such as MgSnN₂ - a largely unexplored material comprised of earth abundant elements which benefit from a mature recycling infrastructure. Abundant elements are cheaper, as well, which could help stimulate a global advancement of new technologies. MgSnN₂ has a predicted band gap of 3.43 eV, indicating that it could be a viable substitute for GaN (3.4 eV), although its synthesis has not previously been published. In this work, six samples of MgSnN₂ were grown via plasma-assisted molecular beam epitaxy (PAMBE), a high-precision process for depositing thin-film, crystalline materials. The first four samples were grown on YSZ(111) single crystal substrates; all displayed polycrystalline

reflection high-energy electron diffraction (RHEED) patterns. The fifth growth experiment used YSZ(100) and the final was performed using ZnSnN₂ buffer layers, which represented the best lattice match in the growth plane (approximately 1.79% mismatch as opposed to 62.18% for YSZ(111) and 34.11% for YSZ(100)). With minor tuning of the substrate temperature, streaky RHEED patterns were ultimately obtained, indicative of high-quality crystal growth. All films in the series were confirmed to be stoichiometric to within the ~1-2% accuracy of Rutherford backscattering spectrometry. Hard x-ray diffraction (XRD) was performed to verify lattice constants as well as the degree of cation sublattice ordering. In fact, we have expended significant effort in both quantifying the degree of cation ordering (through the long-range order parameter, *S*), and determining the effects of disorder on the structure and band gap of MgSnN₂. In addition to XRD, both Raman spectroscopy and in-situ RHEED have also been performed on all films, with excellent agreement among the three techniques. The long-range order parameter (quoted here as *S*², as we anticipate a linear relationship between optical properties and this value) can range from 0 (completely disordered) to 1 (completely ordered) and is directly related to the fraction of cation atoms on the correct site. Systematic variation of process parameters led to the realization that the lattice structure of heterovalent ternary materials can be controlled, switching between structures that are orthorhombic (fully ordered sublattice) in nature and wurtzitic. The lattice structure has a direct effect on the band gap since the disorder on the cation sublattice increases the symmetry of the structure and narrows the band gap, providing a means of tuning the gap to a considerable degree without the need for alloying. This is proven with the optical band gap of the six films grown ranging from 2.57 eV to 3.325 eV with a theoretical range from about 1.9 eV (completely disordered) to 3.5 eV (completely ordered). Therefore, this work establishes the process parameters that result in the desired crystal structure, necessary crystal quality for devices, and the fundamental optical and electronic properties of this semiconductor, all as they relate to ordering of the Mg, Sn (cation) sublattice. Furthermore, because of the success seen with the growth of MgSnN₂ films, we have begun exploring MgGeN₂, with one successful growth already completed. MgGeN₂ has never before been synthesized via PAMBE and has a predicted band gap of 5.14 eV, which is of interest to UV-optoelectronic applications.

11:20 AM F05

(Student) MOCVD Growth and Material Characterization of Wide Bandgap ZnGeN₂ Films Md Rezaul Karim², Benthara Hewage Dinushi Jayatunga⁶, Zixuan Feng¹, Micah Haseman³, Brenton A. Noesges³, Menglin Zhu⁴, Jinwoo Hwang⁵, Leonard Brillson², Kathleen Kash⁶ and Hongping Zhao¹; ¹Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ²Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ³Physics, The Ohio State University, Columbus, Ohio, United States; ⁴Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States; ⁵Materials Science, The Ohio State University, Columbus, Ohio, United States; ⁶Physics, Case Western Reserve University, Cleveland, Ohio, United States.

Zinc germanium nitride (ZnGeN₂), a group II-IV-N₂ compound, is derived from GaN by replacing every two Ga atoms surrounding N atoms in GaN by one Zn and one Ge atoms. ZnGeN₂ has a similar bandgap as GaN, and the difference is within 100 meV. The lattice mismatch between ZnGeN₂ and GaN is less than 0.1%. First principles calculations predict a large band offset (~ 1.1 eV) between the ZnGeN₂/GaN heterostructure [1]. Using the closely lattice-matching ZnGeN₂/GaN heterostructures with large band offset opens up a new territory of designing novel heterostructures with band structure engineering for optoelectronic device applications. Modeling of the InGaN quantum well structures with the insertion of a thin ZnGeN₂ layer has predicted a 6-7 times enhancement of the radiative recombination rate, which is promising to address the “green gap” issue - one of the key challenges in light-emitting diodes for solid state lighting [2]. To date, there has been only a handful of literature on the synthesis of ZnGeN₂ using various growth techniques including vapor-liquid-solid synthesis [3], radio frequency sputtering [4], and metalorganic chemical vapor deposition (MOCVD) [5]. However, the experimental development and fundamental understanding of ZnGeN₂ is still at the very early stage. In this work, MOCVD growth of ZnGeN₂ on c-, r- and a-plane sapphire substrates was investigated. Diethylzinc (DEZn), germane (GeH₄) and ammonia (NH₃) were used as the precursors for Zn, Ge and N, respectively. N₂ was used as the carrier gas. 2θ-ω X-ray diffraction (XRD) spectra confirmed the growth of single crystalline ZnGeN₂ with orthorhombic crystal structure along the [001] direction on c- and a-plane sapphire and along the [010] direction on r-plane sapphire. Studies revealed that the Zn/Ge atomic ratio is highly dependent on the growth temperature, a result attributed to the high vapor pressure of Zn. Characterization of the as-grown ZnGeN₂ films revealed the presence of

'V-defects' on the films grown on c- and a-sapphire whereas the films grown on r-sapphire had stepped surface morphology. The room temperature (RT) photoluminescence (PL) peak at ~ 2.05 eV indicates the existence of deep level defects in the films. The RT PL excitation (PLE) peak at 3.4 eV is in excellent agreement with the predicted bandgap of ZnGeN₂. RT Hall mobility up to 17 cm²/V-s was measured in the n-type films, with 10¹⁸-10¹⁹ cm⁻³ background concentrations. The valence band offset between ZnGeN₂ and GaN was determined to be ~ 1.45 -1.65 eV using X-ray photoemission spectroscopy (XPS). Scanning transmission electron microscopy (STEM) will be used to characterize the crystalline quality at the atomic scale. The experimental verification of the large band offset between ZnGeN₂ and GaN sets the important foundation for future exploration of device applications. In summary, MOCVD growth of ZnGeN₂ films on sapphire substrates with different crystal orientations was investigated. Fundamental materials properties of the as-grown ZnGeN₂ films were probed comprehensively. The crystal structure, optical and electronic transport properties of ZnGeN₂ grown on sapphire substrates were characterized. Band alignment at the ZnGeN₂/GaN interface was determined experimentally. The results from this work indicate that ZnGeN₂ can play an important role for future device designs based on III-N/II-IV-N₂ heterostructures. **References** 1. A. P. Jaroenjittichai, S. Lyu, and W. R. L. Lambrecht, Phys. Rev. B., 96, 079907(E) (2017). 2. L. Han, K. Kash, and H. Zhao, J. Appl. Phys., 120, 103102 (2016). 3. K. Du, C. Bekele, C. C. Hayman, J. C. Angus, P. Pirouz, and K. Kash, J. Cryst. Growth, 310, 1057 (2008). 4. S. Kikkawa, and H. Morisaka, Solid State Commun., 112, 513 (1999). 5. L. D. Zhu, P. H. Maruska, P. E. Norris, W. Yip, and L. O. Bouthilllette, MRS Internet J. Nitride Semicond. Res., 4S1, G3.8 (1999).

11:40 AM F06

(Student) Effects of Controlled Cation Ordering on Optical Properties of ZnSnN₂, Robert Makin¹, Krystal R. York¹, Steve Durbin², Nancy Senabulya³, James P. Mathis³, Roy Clarke⁴, Patrice Miska⁵, Sébastien Diliberto⁶, Christina Jones⁵, Zihao Deng⁵, Logan D. Williams⁵, Emmanouil Kioupakis⁶ and Roger Reeves⁷; ¹Electrical and Computer Engineering, Western Michigan University, Kalamazoo, Michigan, United States; ²Western Michigan University, Kalamazoo, Michigan, United States; ³Applied Physics, University of Michigan, Ann Arbor, Michigan, United States; ⁴Physics, University of Michigan, Ann Arbor, Michigan, United States; ⁵MSE, University of Michigan, Ann Arbor, Michigan, United States; ⁶University of Michigan, Ann Arbor, Michigan, United States; ⁷School of Physical and Chemical Sciences, University of Canterbury, Christchurch, New Zealand; ⁸Institut Jean Lamour, Université de Lorraine, Nancy, France.

ZnSnN₂, a member of the family of II-IV-N₂ ternary heterovalent semiconductors, has recently received considerable interest as a potential earth-abundant element based compound semiconductor for photovoltaic device applications. A major reason for the interest in ZnSnN₂ stems from the constituent elements; they are relatively inexpensive, readily available in high-purity form, non-toxic, and both zinc and tin benefit from mature recycling infrastructure. Although ZnSnN₂ has been synthesized using a variety of techniques, there remain many open questions regarding its fundamental properties. Using plasma-assisted molecular beam epitaxy (PAMBE), we have synthesized crystalline thin films of this ternary heterovalent compound in order to gain a better understanding of its optical and electronic properties. Density functional theory (DFT) calculations for ZnSnN₂ predict an orthorhombic lattice belonging to the Pna2₁ space group, with a band gap between 1.78 and 2.0 eV. These predictions are for a completely ordered cation sublattice, however, as in binary alloys such as GaInP₃, heterovalent ternary materials like ZnSnN₂ can have varying degrees of ordering on the cation sublattice. For ZnSnN₂ with a completely disordered cation sublattice, DFT calculations, using special quasi-random structures (SQS) to model the random distribution of Zn and Sn on the cation sublattice, predict the lattice structure will be wurtzitic and the band gap to be 0.46 eV. We have previously confirmed that it is possible to obtain both orthorhombic and hexagonal lattice structures via plasma-assisted molecular beam epitaxy (PAMBE), and that the band gaps for each structure are close to the DFT predicted values. Here, we now show that the degree of cation ordering can be quantified, and in conjunction with an Ising model based approach, be used to accurately predict the optical band gap. Cation ordering is quantified through the long-range order parameter, S, which varies between 1.0 (for an ordered cation lattice) and 0.0 (for a fully disordered cation sublattice). By systematically adjusting the PAMBE growth parameters over a series of six stoichiometric films we varied the order parameter from 0.98 to 0.26. For these six films, we determined the long-range order parameter using three different techniques – x-ray diffraction, Raman spectroscopy, and in-situ reflection high-energy electron diffraction – and the results from the different techniques were in excellent agreement up to two

decimal places. We have also measured the optical band gap of these films using absorption edge measurements and found the band gap varied between 1.94 to 1.17 eV. Furthermore, we have found, both theoretically and experimentally, that the optical band gap energy exhibits a linear relationship with S², allowing us to determine the full range of possible band gap energies (1.98 to 1.12 eV) accessible via ordering of the cation sublattice (which span the optimal values for a terrestrial single junction solar cell). We can now tune the cation ordering via PAMBE growth parameters over essentially the entire range of possible long-range order parameter values and have demonstrated reproducibility of a few percent, making it possible to repeatedly synthesize ZnSnN₂ with the desired band gap energy.

SESSION G: III-Nitride Electronics

Session Chair: Andrew Koehler

Wednesday Morning, June 26, 2019

Rackham Building, 4th Floor, Amphitheatre

10:00 AM G01

(Student) Electron Transport in N-Polar GaN-Based Heterostructures

Sandra M. Diez Pinzon¹, Alexa Rakoski², Haoran Li³, Stacia Keller³, Cagliyan Kurdak^{2,1} and Elaheh Ahmadi^{1,5}; ¹Applied Physics, University of Michigan, Ann Arbor, Michigan, United States; ²Department of Physics, University of Michigan, Ann Arbor, Michigan, United States; ³Department of Electrical and Computer Engineering, University of California, Santa Barbara, Santa Barbara, California, United States; ⁴Electrical and Computer Engineering, University of California, Santa Barbara, Santa Barbara, California, United States; ⁵Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

N-polar GaN HEMTs have several advantages over their Ga-polar counterparts which make them promising candidates for highly scaled devices as well as high power applications[1]–[3]. In N-polar HEMTs, the two-dimensional electron gas (2DEG) forms on top of the barrier (larger bandgap material) whereas in Ga-polar HEMTs the 2DEG is positioned below the barrier. Formation of the 2DEG above the barrier results in inducing a natural backbarrier in N-polar HEMTs and, consequently, better confinement of the 2DEG. The enhanced confinement of the 2DEG improves the output resistance and pinch-off characteristics of the device [4]. Moreover, the charge centroid of the 2DEG is closer to the gate in N-polar GaN HEMTs, allowing for better gate control, especially for scaled channels. In addition, since there is no large-bandgap barrier between the ohmic metal and the 2DEG in N-face HEMTs, achieving Ohmic contacts with very low resistance is easier. In this work, electron transport in N-polar GaN-based HEMT structures with a combination of In_{0.18}Al_{0.82}N-AIN as barrier was studied via temperature-dependent van der Pauw Hall and Shubnikov-de Haas (SdH) measurements. In contrast to Ga-polar HEMT structures, no persistent photoconductivity could be detected. Three samples (A, B and C) with different back-barrier structures were fabricated by MBE on vicinal semi-insulating GaN templates with 4° miscut along GaN. The backbarriers of samples A and B consist of 10 and 20 nm-thick In_{0.17}Al_{0.83}N layers respectively, while on sample C the barrier is formed by a 10 nm-thick In_{0.17}Al_{0.83}N layer with a 2nm of heavily Si-doped (2x10¹⁹ cm⁻³) GaN layer at the backside. Sample A showed single frequency SdH oscillations at magnetic field above 5.5 T, confirming the presence of a 2DEG with one sublevel at the InAlN/GaN interface. From the oscillations, we extracted a carrier density of 8.54x10¹² cm⁻² and a mobility of 4970 cm²V⁻¹s⁻¹ at 1.7 K. Sample B also demonstrated SdH oscillations starting at a magnetic field of 8.5 T, and the extracted carrier density and mobility were 8.54x10¹² cm⁻² and 2670 cm²V⁻¹s⁻¹ respectively. The lower mobility in Sample B is in agreement with the onset of the oscillations at higher field compared to Sample A, and it is attributed to inhomogeneity in the composition of the 20 nm-thick InAlN barrier. Temperature dependent magnetotransport measurements indicated that the carrier density of Samples A and B approaches the same value at low temperatures, and for Sample A it remains nearly constant up to about 200 K, indicating that the 2DEG is the dominant transport mechanism. Sample C showed oscillations in ρ_{xx} but also in ρ_{xy} with a carrier density of 6.03x10¹² cm⁻², suggesting the presence of a parallel conduction mechanism in addition to the 2DEG. Unlike in Ga-polar GaN-based HEMTs, all three samples showed reduced mobility when decreasing carrier density. [1] S. Kolluri, et al. in *69th Device Research Conference*, 2011, pp. 215–216. [2] S. Kolluri, et al. *IEEE Electron Device Lett.*, vol. 33, no. 1, pp. 44–46, Jan. 2012. [3] M. H. Wong et al., *Semicond. Sci. Technol.*, vol. 28, no. 7, p. 074009, Jul. 2013. [4] T. Palacios et al., *IEEE Electron Device Lett.*, vol. 27, no. 1, pp. 13–15, Jan. 2006.

10:20 AM G02

(Student) LPCVD Passivation for High Linearity Graded AlGaN Channel Field Effect Transistors with Improved Dispersion Shahadat H. Sohel¹, Mohammad Wahidur Rahman², Andy Xie³, Edward Beam³, Yongjie Cui¹, Hao Xue¹, Towhidur Razzak⁴, Sanyam Bajaj¹, Yu Cao³, Wu Lu¹ and Siddharth Rajan¹; ¹Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ²ECE, The Ohio State University, Columbus, Ohio, United States; ³Qorvo, Inc., Richardson, Texas, United States; ⁴Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States.

With the advancement of the communication technology, there is an increasing demand for linearity performance of amplifiers. Widely used amplifier AlGaN/GaN HEMTs suffer from gain compression as well as significant non-linearity at higher frequencies. To improve transistor level linearity of power amplifiers, Polarization-graded Field Effect Transistors (PolFETs) are explored extensively. Although promising results have already been reported, poor dispersion is still limiting the full potential of PolFETs. The dispersion behavior has been largely correlated with poor surface passivation. To get sufficient carrier density in the channel, it is necessary to grade up to higher Al composition AlGaN in PolFETs. This makes the conventional PECVD SiN_x passivation less effective, resulting in huge current collapse and knee-walkout. In this work, we report for the first time, the use of low-pressure chemical vapor deposition (LPCVD) grown SiN_x passivation for graded AlGaN channel PolFETs. Graded AlGaN can be used to realize 3D electron channels that provide more constant gain performance than 2D electron gases found in AlGaN/GaN HEMTs. Unlike in an AlGaN/GaN HEMT, the g_m of the PolFETs do not suffer from any significant decrease at a high gate bias. Large signal simulations show that linearity of PolFETs are significantly better than AlGaN/GaN HEMT devices. However, experimental results from PolFETs are still limited by dispersion. Here, we discuss the design and demonstration of LPCVD passivation for PolFETs, which can successfully reduce the current collapse and knee-walkout. The sample structure used for this study consists of a 20 nm thick MOCVD grown AlGaN channel on a GaN buffer grown on SiC. The AlGaN channel composition was linearly graded from 0% to 40%. On the unprocessed sample, 150 nm SiN_x was grown in LPCVD chamber at 790°C and 300mT. Before LPCVD growth, RCA cleaning was done to improve the surface condition. The source-drain metal stack of Ti/Al/Ni/Au was deposited after etching SiN_x layer. The contact was alloyed in RTA at 850°C in N₂ for 30s, resulting in a contact resistance of 0.4 Ω-mm. Hall measurement showed a mobility of 910 cm²/V-s and a sheet charge density of 1.1×10¹³ cm⁻². Gate openings with 0.7 μm width was created using CF₄ based dry etching. After gate-opening, the sample was annealed at 400°C for 1 hour in RTA in N₂ to improve SiN_x quality. Ni-Au-Ni Schottky gate metal stack with 0.3 μm field plate extension towards the drain were then deposited. The field plate helps in reducing dispersion and increasing breakdown voltage. DC measurement showed the expected flat g_m behavior from the graded channel, with a $g_{m,max}$ of 280 mS/mm and $I_{D,max}$ of 600 mA/mm. The 3-terminal breakdown voltage was 45V for 1 mA/mm compliance. The breakdown was due to Schottky gate leakage. Small signal measurement showed peak f_T and f_{max} of 24 and 44 GHz respectively. Measured f_T and f_{max} as a function of drain current showed flat f_T and f_{max} behavior, which is suggestive of improved linearity performance. To show improvement of the dispersion, pulsed IV was measured using 5 μs pulse and 0.1% duty cycle with drain quiescent bias ($V_{DS,Q}$) up to 30 V. Pulsed I-V showed almost no knee-walkout and very small current collapse. As a comparison, for the same channel and device structure, optimized PECVD SiN_x passivation showed ~8 V knee-walkout and 25% current collapse with $V_{DS,Q}$ =30 V, whereas the LPCVD SiN_x passivation showed ~1V knee-walkout and 8% current collapse for same measurement conditions. The improved dispersion is suggestive of improved large signal performance from LPCVD SiN_x passivated graded channel transistors. LPCVD passivation for graded AlGaN channel transistor is reported for the first time. Measurements showed excellent dispersion behavior and potential for high frequency high power amplifier for high linearity applications. Authors would like to acknowledge the funding from the ONR Grant No. N00014-15-1-2363 (Dr. Paul Maki).

10:40 AM G03

AlGaN MOSHFETs with High-k ALD Oxides—Towards Enhancement Mode Ultra-Wide Bandgap Devices Shahab Mollah¹, Richard Floyd¹, Kamal Hussain¹, Mikhail E. Gaevski¹, Iftikhar Ahmad¹, MVS Chandrashekar¹, G Simin¹, Virginia Wheeler², Charles Eddy² and Asif Khan¹; ¹Electrical Engineering, University of South Carolina, Columbia, South Carolina, United States; ²U.S. Naval Research Laboratory, Washington, District of Columbia, United States.

This work presents Al_{0.65}Ga_{0.35}N/Al_{0.4}Ga_{0.6}N metal oxide semiconductor HFETs (MOSHFETs) with high-k ALD TiO₂, Al₂O₃, and ZrO₂ oxides as gate dielectrics. The gate leakage current in fabricated devices is four

orders of magnitude lower than in Schottky-gate HFETs made on the same wafer. This led to an increase in ON/OFF ratio from 10³ for HFETs to ~10⁷ for ALD MOSHFET, while maintaining drain current levels. The subthreshold swing in all devices was 105-200mV/decade, corresponding to a total interfacial trap density of ~2×10¹²cm⁻², in close agreement with that extracted from C-V measurements at different frequencies. All tested ALD oxides caused a positive shift in threshold voltage, up to +4V compared to a Schottky-gate HFET, due to the fixed negative charges in the oxide and/or at the oxide/barrier interface. Positive threshold shift in ALD oxide MOSHFETs may enable enhancement mode high-Al AlGaN devices, particularly for high temperature, high voltage applications where AlGaN is predicted to overcome the limitations of even wide bandgap materials. All devices were pseudomorphic, and were grown using metalorganic chemical vapor deposition (MOCVD) on high quality AlN templates on sapphire, and are illustrated in Fig. 1, with a band diagram for ZrO₂ shown. These had a threading dislocation density ~10⁸cm⁻². Following a 0.5μm thick x=0.4 Al_xGa_{1-x}N channel layer, a ~30nm thick Si-doped barrier was grown with x=0.65. C-V measurements indicated the barrier doping to be ~4-5×10¹⁸cm⁻³, enabling the 2D electron gas to be isolated from the barrier surface. This enabled independent electrical characterization of this oxide-containing interface, from the barrier/channel interface. Thermal ALD of ZrO₂ and Al₂O₃ films on as-received devices were conducted at 200°C and 250°C, respectively, with either trimethylaluminum (TMA) or tetrakis(dimethylamido)zirconium(IV) (TDMAZ) and deionized water precursors. For both films, the deposition was initiated with 15 water pulse prior to the typical AB pulsing sequence to deposit the gate dielectric to ensure saturation of hydroxyl groups at the AlGaN surface required for conformal ALD nucleation. The TiO₂ film was deposited by plasma-enhanced ALD (PE-ALD) in a Veeco CNT Fiji G2 system equipped with a turbo pump used to achieve low pressure (10's of mTorr) during the plasma pulse. For all the oxides, the ON/OFF ratio improved (Fig. 2a), with subthreshold swing as low as 105mV/decade observed, in agreement with hi-lo C-V characteristics of the barrier/channel interface (Fig. 2b). Moreover, the positive shift of the threshold voltage was consistent in I-V and C-V. The C-V characteristic showed three independent regimes: i) Depletion through barrier layer -2V<V_G<0V with linear 1/C² showing constant doping, ii) 2D electron gas at barrier/channel interface ~8V<V_G<-2V and iii) pinch-off, with depletion extending into channel epitaxial layer V_G<<-8V. Electrostatic analysis of the oxide/barrier interface, showed negative fixed charges as high as 1-3×10¹³cm⁻² depleting the 2DEG density of 2×10¹³cm⁻², causing a positive shift of the threshold voltage. No obvious trapping was seen in the C-V characteristics of the gate dielectric oxides. Using these extracted values of surface fixed charge, and the known dielectric constants, we will present potential architectures that will provide for enhancement-mode devices. This is enabled by the fact that in certain well-prepared oxide/barrier interfaces, ZrO₂ in this study, negative fixed charge greater than the 2DEG sheet density is induced, enabling positive V_{th} with increasing oxide thickness, and decreasing barrier layer thickness.

11:00 AM G04

(Student) Integrated Body-Diode Back-Gate Control in AlGaN/GaN HEMTs Isra Mahaboob, Michael Yakimov, Sean A. Tozier, Kasey Hogan, Emma Rocco and Fatemeh (Shadi) Shahedipour-Sandvik; Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, Clifton Park, New York, United States.

In this work we present the implementation of p-GaN body-diode based back-gate in AlGaN/GaN HEMTs for the first time. We show that this device design enables control of the 2DEG density and shifting of the threshold voltage of the device. The fourth device terminal also the back-gate, is connected to the underlying p-GaN layer of the body-diode. The role of back-gate bias in controlling the performance of HEMTs in both ON and OFF-states of the device operation has been experimentally investigated in this work. AlGaN/GaN HEMT structure used in this study has been epitaxially grown using metal organic chemical vapor deposition (MOCVD) technique. To incorporate body-diode, conventional HEMT structure was epitaxially grown over GaN:Mg layer. The effect of the state of activation of GaN:Mg on the electrical properties of overgrown HEMT has been extensively studied and will be discussed. The difficulties involved with the growth of device structures involving buried p-GaN layers has been reported previously [1]. A series of experiments have been conducted to determine the optimum activation sequence and spacing between the body-diode and the 2DEG channel to enable effective back-gate control through field effect. With the integration of body-diode, the 2DEG current shows modulation with the change in magnitude and polarity of the back-gate voltage. An increase in 2DEG current is measured with the application of a positive back-gate voltage and a decrease is measured with a negative back-gate bias. Moreover, a positive/negative shift in the threshold voltage is observed with the application of

negative/positive back-gate voltage, demonstrating multi-threshold voltage capability. The modulation of 2DEG density is attributed to the modulation of the body diode depletion width. The 3-dimensional control of the 2DEG channel current allows dynamic control of the device ON/OFF characteristics and enables the design of multi-threshold voltage HEMT. In addition to improving HEMT device performance, implementation of this technique is advantageous in enabling the integration of HEMTs in integrated circuit designs requiring normally-ON, normally-OFF and intermediate modes of operation. Along with extensive results of such modulation, a comprehensive study demonstrating 3-terminal and 4-terminal output/transfer characteristics, capacitance-voltage characteristic and breakdown voltage capability of this novel device structure will be presented. [1] Y. Kuwano *et al.*, "Lateral Hydrogen Diffusion at p-GaN Layers in Nitride-Based Light Emitting Diodes with Tunnel Junctions," *Jpn. J. Appl. Phys.*, vol. 52, no. 8S, p. 08JK12, Aug. 2013.

11:20 AM G05

(Student) Experimental and Analytical Determination of Optimum Carbon Doping Level AlGaIn/GaN HEMT on Silicon *Nayana Remesh*, Nagaboopathy K. Mohan, Rangarajan Muralidharan, Srinivasan Raghavan and Digbijoy N. Nath; Center for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India.

High resistive buffer layer is the most vital part in GaN based High Electron Mobility Transistors (HEMTs) on silicon, to achieve high breakdown voltage. Growth conditions for high quality GaN leads to unintentional n-type doping, which results in high vertical as well as lateral leakage. The most commonly adopted method to reduce the leakage is introducing impurity atoms like Iron (Fe) or Carbon (C) in the growth front. Carbon reduces the background doping by compensation method, but in the process introduces killer traps in the devices which degrades the device performance. However, till date, a quantitative analysis of the traps as a function of carbon doping for MOCVD grown GaN buffer on silicon is still lacking. In the present study, we investigate the lateral leakage in C-doped HEMT-on-silicon, and the dependence of carbon doping on leakage. An effort is made to explain the influence of shallow donor traps on leakage with increasing carbon doping. Carbon doped GaN layers are intended to give high breakdown voltage due to auto compensation of acceptor and donor traps. In the samples under study the leakage current is increasing when the carbon doping is increased beyond a limit ($8 \times 10^{18} \text{ cm}^{-3}$) this could be attributed to presence of higher concentration of shallow donor traps compared to acceptor traps. As carbon concentration is increased to 10^{20} cm^{-3} the density of shallow donors will increase and outnumber acceptor traps present, resulting in a leaky GaN layer as evidenced by the CL data. To realise high breakdown carbon doping GaN buffer layer beyond 10^{19} cm^{-3} is not recommended.

11:40 AM G06

(Student) Normally-Off AlGaIn/GaN HEMT on 200 mm Silicon with ON-Current 500 mA/mm and $V_{th} > 5 \text{ V}$ Sandeep Kumar¹, Sandeep Vura¹, Vanjari Charan¹, Surani Dolmanan², Sudhiranjan Tripathy², Rangarajan Muralidharan¹, Digbijoy N. Nath¹ and Nayana Remesh¹; ¹Centre for Nano Science and Engineering (CeNSE), Indian Institute of Science (IISc), Bengaluru, India; ²Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology, and Research (A*STAR), Innovis, Singapore.

III-N HEMTs offer superior power figure of merits compared to Si power devices [1-4]. Here, we demonstrate a normally-off AlGaIn/GaN HEMT based on gate recess technology with a $V_{th} > 5 \text{ V}$ and ON-current=500 mA/mm. The excellent ON-current with high V_{th} were achieved simultaneously by employing deep sub-micron recess etched region ($L_G \sim 200 \text{ nm}$). This is the maximum ON current and V_{th} combination reported till date to the best of our knowledge [5]. MOCVD grown AlGaIn/GaN HEMT stack (Fig. 1 (A)) on 200 mm P-type Si was used in this work. Device structure is shown in the Fig. 1 (B). Device fabrication started with EBL process and it was used to define source-drain regions, optical and e-beam alignment marks. Ti/Al/Ni/Au was evaporated to form Ohmic contacts and were RTA annealed at 850° C condition. And then mesa etching ($\sim 300 \text{ nm}$) was done. PMMA EBL resist was used to transfer the recess pattern on blanket deposited PECVD SiNx by EBL lithography and this SiNx was used as mask for recess etching. 30 nm of ALD- Al_2O_3 was used as gate dielectric. Ni/Au metal was deposited for Gate and different post dielectric anneal (PDA) and post gate metal anneal (PMA) were tried for optimum device performances. Different recess depths were also tried to increase the V_{th} . Input and output characteristics for (700° C PMA and 500° C PDA HEMT) are shown in Fig. 2. The total recess depth of the device was 25 nm (AlGaIn barrier) + 40 nm (GaN Channel). The device has shown strong depletion type characteristics with V_{th} of -1V even with

40 nm of the channel over etching. To increase the V_{th} , a different PDA condition (500° C for 1 min) was tried while keeping the PMA at 500° C for 5 min (input and output characteristics are shown in the Fig. 3). Finally, to further increase the V_{th} voltage, the recess depth was increased to 124 nm (Barrier+channel). The device characteristics of deep recess etched HEMT is shown in the Fig. 4. The device has shown excellent device characteristics $V_{th} (> 5 \text{ V})$ and ON-current ($\sim 500 \text{ mA/mm}$) with significant short channel effects. To improve the gate metal coverage on the side walls of the deep recess region, slant metal deposition was used in the e-beam evaporation tool. SEM Images (top view and cross-section of gate region) of the device are shown in the Fig. 5. Etched region roughness was $\sim 0.7 \text{ nm}$ (Fig. 6). [1] Kumar *et al.*, "Interface traps at Al₂O₃/InAlN/GaN MOS-HEMT-on-200 mm Si." *Solid-State Electronics* 137 (2017): 117-122. [2] Kumar *et al.*, "Temperature and Bias Dependent Trap Capture Cross Section in AlGaIn/GaN HEMT on 6-in Silicon With Carbon-Doped Buffer." *IEEE Transactions on Electron Devices* 64, no. 12 (2017): 4868-4874. [3] Kumar *et al.*, "UV detector based on InAlN/GaN-on-Si HEMT stack with photo-to-dark current ratio > 107." *Applied Physics Letters* 111, no. 25 (2017): 251103. [4] Kumar *et al.*, "Investigation of Ta₂O₅ as an alternative high- κ dielectric for InAlN/GaN MOS HEMT on Si." *arXiv preprint arXiv:1806.03291* (2018). [5] ZHOU *et al.*, 7.6 V THRESHOLD VOLTAGE HIGH-PERFORMANCE NORMALLY-OFF Al₂O₃/GaN MOSFET. *IEEE ELECTRON DEVICE LETTERS*, VOL. 37, NO. 2, FEBRUARY 2016

SESSION H: Chalcogenide Quantum Materials
Session Chairs: Rachel Goldman and Stephanie Law
Wednesday Afternoon, June 26, 2019

Michigan League, 2nd Floor, Lydia Mendelssohn Theatre

** Invited Paper

1:30 PM **H01

Observation of Valley Coupled Topological Current in 2D TMDs Terry Y.T. Hung, Kerem Y. Camsari, Shengjiao Zhang, Pramey Upadhyaya and [Zhihong Chen](#); School of Electrical and Computer Engineering and Birck Nanotechnology Center, Purdue University, Lafayette, Indiana, United States.

Electronic devices exploring carrier transport with spin and valley degree of freedom have emerged as promising candidates for next-generation information storage and transport, since pure spin and valley currents do not accompany energy dissipation associated with Joule heating. The spin and valley degree of freedom of electrons in two-dimensional (2D) transition metal dichalcogenides (TMDs) have been extensively studied by theory, optical and optoelectronic experiments. The ability to electrically generate and detect such pure spin and valley currents in these materials is of particular importance. In this talk, we first report that valley current can be electrically induced and detected through the valley Hall effect and inverse valley Hall effect, respectively, in monolayer molybdenum disulfide. We compare temperature and channel length dependence of non-local electrical signals in monolayer and multi-layer samples to distinguish the valley Hall effect from classical Ohmic contributions. Significantly, valley transport is observed over four-micron distance in monolayer samples at room temperature. We then study the valley coupled spin generation in monolayer tungsten disulfide and spin diffusion in a 2D stack device. Our device design approach provides a unique way to integrate charge, spin and valley degrees of freedom, which can be useful for emerging valleytronic applications.

2:10 PM H02

Probing Topological Surface States in Bi₂Te₃-Bi₂Se₃ and Bi₂Te₃-Sb₂Te₃ Alloy Films Gregory Cunningham¹, Christian Greenhill², [Rachel S. Goldman](#)³, Theresa P. Ginley⁴ and Stephanie Law⁵; ¹Electrical Engineering, University of Michigan-Ann Arbor, Southfield, Michigan, United States; ²Materials Science & Engineering, University of Michigan, Ann Arbor, Michigan, United States; ³Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; ⁴Material Science and Engineering, University of Delaware, Newark, Delaware, United States; ⁵University of Delaware, Newark, Delaware, United States.

Topological insulators (TIs) are an intriguing class of quantum materials that exhibit insulating behavior in the bulk, combined with conducting states on the surface, making them desirable for spintronics and quantum computing. For (Bi_{1-x}Sb_x)₂Te₃ and Bi₂Te₃-xSex alloys, tunable surface to bulk conduction has been demonstrated, but direct detection of their topological surface states at room temperature has yet to be observed. We use scanning tunneling microscopy and spectroscopy (STM/S) to investigate the band structure of (Bi_{1-x}Sb_x)₂Te₃ and Bi₂Te₃-xSex alloys at room temperature. STS reveals both the Fermi level and Dirac point located inside the bulk band gap, indicating bulk-like insulating behavior with accessible surface states. This identification of topological surface states at room temperature is critical for practical applications. We report on studies of Bi₂Te₃-xSex alloys with x ranging from 0 to 3 and (Bi_{1-x}Sb_x)₂Te₃ alloys with x = 0.6 and thicknesses ranging from 6 to 30nm. We emphasize correlations between surface morphology, vibrational modes, and the electronic states of the alloys.

2:30 PM H03

Effect of Spin-Orbit Coupling and Magnetic Strength on Weyl Semimetallic and Chern Insulating Phase of Magnetic Bi₂MnX₄ (X=Se, Te) [Sugata Chowdhury](#); MML, NIST, Gaithersburg, Maryland, United States.

Three-dimensional materials with strong spin-orbit coupling (SOC) and broken time reversal symmetry (TRS) due to magnetic ordering have been the subject of enormous interest in the last few years. Two dimensional insulators with broken TRS and strong SOC can be characterized by a topological invariant called the Chern number (C), and these materials display quantized Hall conductance, $\sigma_{xy} = C(e^2/h)$, when C is non-zero.

These kinds of magnetic materials can carry the spin-polarized edge states even in the absence of an external magnetic field. Experimentally, Chern insulators have thus far been limited to magnetically doped Z₂ topological insulators at very low temperatures (~1K). By performing density functional theory and Wannier calculations on recently synthesized Bi₂MnSe₄ (1,2) and Bi₂MnTe₄ in this work we have identified a series of topological phases. Our calculations reveal that the ferromagnetic phase of bulk Bi₂MnTe₄ (X=Se, Te) is either a nodal line or Weyl semimetal, depending on the direction of the spins. When the spins are arranged in a layered antiferromagnetic configuration, the combination of time reversal plus a partial translation is a new symmetry, and the material instead becomes an antiferromagnetic Z₂ topological insulator. However, the intrinsic TRS breaking at the surface of Bi₂MnTe₄ removes the typical Dirac cone feature, allowing the observation of the half-integer quantum anomalous Hall effect (QAHE). Furthermore, we show that in thin film form, for some thicknesses, Bi₂MnTe₄ becomes a Chern insulator with a small band gap. Experimental measurements of the magnetoresistance of pure and hetero structure (Bi₂X₂/Bi₂MnX₄) are also discussed. This combination of properties in a stoichiometric magnetic material makes Bi₂MnX₄ an excellent candidate for displaying robust topological behavior. Our results have the potential to provide an avenue to achieve a magnetic Weyl semimetal and a higher temperature QAHE. Reference: 1. Hagmann, J. A. *et al.* Molecular beam epitaxy growth and structure of self-assembled Bi₂Se₃/Bi₂MnSe₄ multilayer heterostructures. **New Journal of Physics** **19**, 085002 (2017). 2. Chowdhury, S., Garrity, K. F. & Tavazza, F. Prediction of Weyl semimetal, AFM topological insulator, nodal line semimetal, and Chern insulator phases in Bi₂MnSe₄. *arXiv preprint arXiv:1811.01863* (2018). Accepted **Nature Computational Materials**, 2019.

2:50 PM H04

Epitaxial Growth and Characterization of Chromium Selenide Thin-Films on c-Al₂O₃ (0001) [Anupam Roy](#), Tanmoy Pramanik, Rik Dey, Amritesh Rai and Sanjay Banerjee; Microelectronics Research Center, The University of Texas at Austin, Austin, Texas, United States.

Transition-metal chalcogenides are demonstrating burgeoning demand due to their large variety of novel physical, electrical, and magnetic properties. On the one hand, these can be metallic, half-metallic, or semiconducting depending on the anion and on the ratio between the transition metal and chalcogen atoms. On the other hand, these chalcogenides may have ferromagnetic (FM), antiferromagnetic (AFM), or noncollinear spin structure for different crystal structures and compositions.¹⁻³ The chromium-selenium system comprises a large family of compounds with large varieties of stable stoichiometries and all of them have NiAs-type crystal structure. Previously, chromium selenide (Cr_{1-x}Se) systems have been studied to investigate their suitability for different applications in thermoelectrics, electrochemical sensors, *etc.*^{4,5} However, the studies were limited only to the bulk samples⁶ and detailed studies of the growth and distinct physical properties of Cr₂Se₃ thin films are still lacking. In this work, we present the epitaxial growth of Cr₂Se₃ thin films directly on Al₂O₃(0001) surfaces using molecular beam epitaxy (MBE), and study the details of growth, structural, spectroscopic, electrical and magnetic properties characterized by several *in situ* and *ex situ* techniques. Following growth at elevated temperature, sharp streaky reflection high-energy electron diffraction (RHEED) patterns suggest well-structured film growth with high crystalline quality and atomically flat surface morphologies. Interestingly, the growth occurs only along the [001] direction (*c*-axis), as expected for the epitaxial growth of a hexagonal thin film on hcp(0001) substrates. X-ray diffraction (XRD) pattern shows characteristic peaks that correspond to diffraction from (00*l*) family of planes only, and concur very well with the NiAs-type crystal of Cr₂Se₃. The absence of peaks other than the (0 0 *l*) family confirms the epitaxial growth along the *c*-axis of the sapphire substrates. The extracted *c*-axis lattice constant is 17.4 Å, matching very closely with the bulk crystal. The elemental compositions of the grown films are confirmed from *in situ* X-ray photoelectron spectroscopy (XPS). Temperature-dependent resistivity measurement of a 5 nm epitaxial Cr₂Se₃ thin film using a standard van der Pauw geometry shows an insulating behavior with decreasing temperature, confirming the material to be a low-bandgap semiconductor. AFM nature of the as-grown film is confirmed from the magnetoresistance (MR) measurements showing the exchange bias phenomenon in AFM-FM systems by depositing a thin layer of iron (Fe) on the surface of Cr₂Se₃. The exchange bias fields (H_{EB}) at different temperatures show a non-zero H_{EB} below 40 K, indicating the Néel temperature of this material. These results could be useful to understand and evaluate compounds from the chromium-selenium material system for potential spintronic applications. This work was supported by the Army Research Office (ARO) Grant # W911NF-17-1-0312 (MURI). **References** [1] A. Roy *et al.*, *ACS Nano* **2015**, *9*, 3772-3779. [2] T. Pramanik *et al.*, *J.*

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3:10 PM REFRESHMENT BREAK

3:30 PM **H05

Rotationally Controlled van der Waals Heterostructures—Electron Physics and Device Applications G. W. Burg, Kyoungwan Kim, Hema C. Movva and Emanuel Tutuc; Department of Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas, United States.

Heterostructures of atomic layers such as graphene, hexagonal boron-nitride, and transition metal dichalcogenides (TMDs) can serve as testbed for novel quantum phenomena in two-dimensions (2D), and potential device applications. A key ingredient that can add a new dimension to the atomic layer heterostructures palette is the rotational control, and alignment of different 2D layers. We review here an experimental technique that enables rotationally controlled heterostructures with accurate alignment of individual layer crystal axes [1]. We illustrate the applicability of this technique to the realization rotationally aligned double layers of graphene [2], or TMDs [3] separated by a tunnel barrier which display resonant, energy- and momentum-conserving tunneling in vertical transport, consistent with theoretical expectations [4]. When two 2D layers are overlaid with a relative twist, the resulting heterostructure shows a clear periodicity when viewed from a distance. This new type of moiré superlattices are only beginning to be systematically investigated as platform for strongly correlated electron physics owing to flat energy bands [5]. We discuss the electron transport in tunable moiré patterns realized in twisted bilayer graphene [6], and double bilayer graphene heterostructures. Work done in collaboration with S. K. Banerjee, L. F. Register, B. J. LeRoy, A. H. MacDonald, T. Taniguchi, and K. Watanabe. [1] K. Kim *et al.*, *Nano Lett.* **16**, 1989 (2016); [2] G. W. Burg *et al.*, *Nano Lett.* **17**, 3919 (2017); G. W. Burg *et al.*, *Phys. Rev. Lett.* **120**, 177702 (2018). [3] K. Kim *et al.*, *Nano Lett.* **18**, 5967 (2018). [4] S. C. de la Barrera, and R. M. Feenstra, *Appl. Phys. Lett.* **106**, 093115 (2015). [5] R. Bistritzer, and A. H. MacDonald, *Proc. Natl. Acad. Sci. USA* **108**, 12233 (2011). [6] K. Kim *et al.*, *Proc. Natl. Acad. Sci. USA* **114**, 3364 (2017).

4:10 PM H06

Moiré Excitons in WS_2/WSe_2 Heterostructures Feng Wang^{1,2}, Chenhao Jin¹, Emma Regan¹ and Danqing Wang¹; ¹Physics, UC Berkeley, Berkeley, California, United States; ²Material Science Division, Lawrence Berkeley National Laboratory, Berkeley, California, United States.

Moiré superlattices in van der Waals systems provide a powerful tool to engineer the properties of two-dimensional materials by introducing a new energy and length scale. For example, correlated insulating states and superconductivity have been reported in graphene systems, where the moiré superlattice qualitatively changes the behavior of electrons. In addition to their dramatic effects on single particle states, moiré superlattices were recently predicted to host novel exciton states in two dimensional semiconductors. First, I will discuss our observation of intralayer moiré excitons in WS_2/WSe_2 heterostructures and show that the properties of intralayer excitons can be strongly modified by a moiré superlattice. Then I will consider interlayer excitons in a moiré superlattice, where electrons and holes reside in different layers and are particularly sensitive to the local atomic configuration. I will discuss our effort to observe distinct interlayer exciton states and to probe the possible effects of the moiré angular momentum on such states.

4:30 PM H07

Linearly Aligned Hexagonal Boron Nitride Quantum Dots Grown by Molecular Beam Epitaxy Ping Wang¹, David A. Laleyan¹, Eric T. Reid¹, Jiseok Gim², Zhe Liu¹, Zhaohui Zhong¹, Mackillo Kira¹, Robert Hovden² and Zetian Mi¹; ¹Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ²College of Engineering, Materials Science and Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

As a member of the III-nitride semiconductor as well as the two-dimensional (2D) material families, hexagonal boron nitride (hBN) has received tremendous attention in recent years. Due to its extraordinary properties, such as high chemical stability, excellent thermal conductivity, and wide bandgap (~5.8 eV), hBN has emerged as a promising candidate for many applications, including deep ultraviolet (UV) and 2D optoelectronics, 2D transistors, and quantum emitters. In the 2D materials group, graphite, graphene, and hBN are lattice-matched to within 2% and

exhibit complementary electronic properties, with hBN having a wide bandgap and graphene being a gap-less semimetal. Multilayer hybrid heterostructures based on graphene and hBN have been intensively studied by stacking layers exfoliated from highly-ordered pyrolytic graphite (HOPG) and hBN crystals. To realize well-stacked vertical 2D heterostructures and to achieve scalable devices, epitaxial growth of such configuration would be highly beneficial. In this context, we have investigated the epitaxy of hBN on HOPG utilizing ultra-high temperature (up to 1850°C) molecular beam epitaxy (MBE) equipped with a plasma-assisted nitrogen source. We have demonstrated the formation of hBN quantum dots. The epitaxy was performed under N-rich conditions and at temperatures in the range of 1200°C to 1600°C. Under these conditions, we observed the formation of hBN quantum dots, which have lateral sizes ~5-10 nm and heights ~2-5 nm. It is also observed that the initial nucleation of hBN quantum dots takes place primarily at the HOPG atomic steps, where the height fluctuation provides nucleation sites on low surface energy planes. Energy-dispersive X-ray spectroscopy (EDS) confirms the presence of nitrogen element from the quantum dot arrays, whereas no nitrogen signal was observed at the bare terraces, indicating these dot-like nanostructures are BN. From detailed micro-Raman measurements, a clear E2g peak of hBN was observed at 1355 cm⁻¹, providing direct evidence of the formation of hBN. Photoluminescence (PL) spectroscopy of hBN quantum dots was measured using a 193 nm excitation laser at room temperature. The sample exhibits strong excitonic emission at ~215 nm. Significantly, no defect-related emission was measured. For comparison, PL emission of previously reported hBN is often dominated by defect-related emissions in the UV and visible spectra. The absence of defect-related emission confirms the excellent quality of the hBN quantum dots. The controlled epitaxy of hBN based superior quality quantum nanostructures provides distinct opportunities to realize robust quantum emitters, deep UV, and other quantum photonic and electronic devices. A detailed study of the structural, electronic, and optical properties of hBN quantum dots is currently in progress and will be reported.

SESSION I: Solar Cell Materials and Devices Session Chairs: Jamie Phillips and Mark Wistey Wednesday Afternoon, June 26, 2019 Michigan League, 2nd Floor, Hussey

1:30 PM I01

(Student) GaAs Dual Junction Photovoltaic Modules for Bioimplantable Devices Eunseong Moon, Michael Barrow, Inhee Lee, David Blaauw and Jamie Phillips; Electrical Engineering and Computer Science, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

Wireless biomedical implantable devices are prospective technologies that can be applied to a variety of applications for monitoring physiological signals. For these implantable applications, low-power systems on the mm-scale or micrometer-scale with efficient energy harvesters from ambient and stable sources are essential to make these technologies practical. High-efficiency photovoltaic (PV) cells can meet this requirement through optimization of the spectral response in the near-infrared (NIR) transparency window (700 – 1100 nm) for biological tissue. Previously, we demonstrated monolithic PV modules to directly power bio-implantable systems or to directly charge a battery without DC-DC voltage up-conversion, where module efficiency was limited by perimeter recombination for individual cells and shunt leakage current for the series-connected module configuration. We utilized AlGaAs junction barrier isolation between interconnected cells to dramatically reduce shunt leakage current. A photovoltaic module with eight series-connected cells and total area of 1.27-mm² demonstrated a power conversion efficiency of greater than 26 % under low-flux NIR illumination (850 nm at 1 uW/mm²). The output voltage of the module was greater than 5 V, providing a voltage up-conversion efficiency of more than 90 %. Nevertheless, these single-junction based PV cell or module presented new challenges to increase the output voltage above 10 V due to deteriorated shunt leakage and to miniaturize the system to the sub-mm-scale due to increased area losses from device isolation and metal interconnects. In this work, we present dual-junction single PV cells and modules as a means of increasing voltage generation per cell. Two monolithic PV cells connected by tunnel junction are designed for a 50 % current match at a NIR wavelength of 850 nm. Single PV cells (150 um x 150 um) based on the dual-junction design demonstrate power conversion efficiency greater than 22 % with more than 1.2 V output voltage under 850 nm NIR LED

illumination at 6.62 uW/mm², which is sufficient to directly power miniaturized CMOS IC chips subcutaneously. The output voltage of dual junction PV modules with 8 series-connected single cells was greater than 10 V while maintaining an efficiency of more than 18 %. However, in comparison to single-junction modules and device simulation, an undesirable loss of approximately 10 % is observed in photo-generated current. Further discussion of photocurrent loss and application of these monolithic photovoltaic modules to bio-implantable systems will be presented.

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(Student) Leakage Current Mechanisms in Pixelated Solar Cells Vijay Saradhi Mangu^{1,2}, Fatih Ince², Emma J. Renteria³, Sadvikas J. Addamane², Ganesh Balakrishnan^{1,2} and Francesca Cavallo^{1,2}; ¹Electrical and Computer Engineering, The University of New Mexico, Albuquerque, New Mexico, United States; ²Center for High Technology Materials, The University of New Mexico, Albuquerque, New Mexico, United States; ³Center for High Technology Materials, University of New Mexico, Albuquerque, New Mexico, United States.

Pixelated solar cells are based on single-crystalline semiconductor absorbers with lateral sizes ranging between ~100 and ~500 μm and a thickness of few micrometers.¹ Photovoltaic absorbers are grown epitaxially on lattice-matched substrates using molecular beam epitaxy (MBE). The layer stack includes a P-N diode structure grown on top of a sacrificial layer on a bulk substrate. The semiconductor layer is patterned in a 2D array of pixels, which are then released from their growth substrate and can be transferred onto any substrate of choice. The reduced lateral size of the absorbers results in shorter release times and higher resistance to cracking during release and transfer to a new host. Thus, pixelated absorbers of dislocation-free and highly mismatched materials can be integrated via a high yield and cost-effective process. The numerous benefits of pixelated solar cells and our recent progress in the fabrication and characterization of these devices¹ demand for a better understanding and predictive capability of their process-structure-property relationship. We present a systematic study to determine the contributing mechanisms to the leakage current in GaAs and GaSb pixelated solar cells. We focus on devices with ~ 500x500 μm² area and thickness in the range of 3–4 μm. Briefly, we perform dark-current vs voltage measurements at various temperatures between 77 K and 300 K. We analyze the trend of the dynamic resistance vs voltage and temperature to determine process and material dependent parameters (e.g., surface recombination velocity and minority carrier lifetimes). The results of the modeling are correlated with a detailed characterization of the physical and chemical structure of the pixelated solar cells with a specific focus on surfaces and interfaces within the device. We perform characterization via transmission electron microscopy (TEM), energy-dispersive x-ray spectroscopy (EDS), Raman and x-ray photoelectron spectroscopy (XPS). **References:** 1 Mangu, V. S.; Renteria, E. J.; Addamane, S. J.; Mansoori, A.; Armendariz, A.; Deneke, C. F.; Ferreira, S. O.; Zamiri, M.; Balakrishnan, G.; Cavallo, F. Pixelated GaSb Solar Cells on Silicon by Membrane Bonding. *Appl. Phys. Lett.* **2018**. <https://doi.org/10.1063/1.5037800>.

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(Student) GaP Schottky Diodes Solar Cells with High Quantum Efficiencies Fabricated by Liquid Phase Epitaxy (LPE) Hui-Ying Siao¹, Ryan Bunk¹ and Jerry M. Woodall²; ¹Electrical and Computer Engineering, University of California, Davis, Davis, California, United States; ²ECE, University of California, Davis, Davis, California, United States.

Gallium phosphide (GaP) has been researched for more than 60 years. Most of the research focused on optoelectronic applications, such as solar cells and light emitting diodes (LEDs). In the 1960s, researchers found that efficient red emitting GaP LEDs could be produced by liquid phase epitaxy (LPE) using zinc plus oxygen dopants. This was an intriguing result, since GaP is an indirect band gap semiconductor. Later, green emitting LEDs with low quantum efficiency were realized by LPE using isoelectronic nitrogen doping. It was believed that these LED achievements were due the fact that LPE is a near equilibrium epitaxy method that enables the fabrication of epilayers at growth rates of multi-microns per minute with low defect densities and low background impurities. However, the efficient red emitting LEDs could not be made to be bright due to the saturation of the luminescence via a low concentration of mid-gap states. GaP is currently commercially used as a passive, optically transparent transport layer on which to bond GaInP red and yellow LEDs after being removed from the GaAs lattice-matched substrates. GaP has recently been explored as a candidate wide band gap material for the top layer cell of tandem solar cell stacks. It has been explored using MBE and LPE. However, to date both epilayer methods have resulted in AM1.5 efficiencies of less than 3%, while theory predicts efficiencies that approach 17%. In this paper, we present the

results of our GaP solar cell investigations. The GaP is grown by liquid phase epitaxy, which allows very thick layers to be grown with high growth rates. In our work, we present a new method to improve the diffusion length of GaP by adding aluminum to the melt in the LPE system. The aluminum scavenges trace oxygen in the melt, which is known as a deep donor state in GaP. The diffusion length shows 9 times longer than previous work.

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Preparation of AgGaTe₂ Layers on Mo with Sputtered Ag₂Te Buffer Layers Aya Uruno¹ and Masakazu Kobayashi^{1,2}; ¹Electrical Engineering and BioScience, Waseda Univ., Shinjuku, Japan; ²Kagami Memorial Research Institute for Materials Science and Technology, Waseda University, Shinjuku, Japan.

The room temperature bandgap of AgGaTe₂ is about 1.3eV, hence the application of this material to the active layer of novel solar cells attracted the attention. Among various film preparation methods, the closed space sublimation (CSS) method is suitable for the fabrication of mass production solar cells since it has various advantages toward the production cost reduction. The growth of crystallized AgGaTe₂ thin films by this method on Si and Al₂O₃ substrates have performed in past, and it was discovered that the introduction of the two-step sequence was the key to produce high quality thin films. The Ag₂Te layer was deposited as the first step to avoid the melt-back etching related problems of Ga against substrate materials. Then, AgGaTe₂ thin films were formed using the mixed powder source of Ag₂Te and Ga₂Te₃. The first Ag₂Te layer was disappeared during the high temperature growth process of the second sequence, and a single phase AgGaTe₂ of the uniform layer has achieved once the growth parameter was optimized. It was clarified from the X-ray diffraction (XRD) measurement that the inclusion of AgGa₂Te₈ compounds occurred when the fraction of Ga₂Te₃ in the deposits was greater than that of Ag₂Te. On the other hand, AgGaTe₂ and Ag₂Te were formed when the fraction of Ga₂Te₃ was less than that of Ag₂Te. These results corresponded to the phase diagram of the Ag₂Te–Ga₂Te₃ system. A pn-heterojunction solar cell structure was prepared using the AgGaTe₂ layer on the n-Si substrate, and the photovoltaic properties were confirmed. The AgGaTe₂ layer was also prepared on the Mo/quartz substrate using the same growth sequence. Then crack lines were observed in the Mo electrode, and the grown layer was often peeled off from the substrate during the Ag₂Te layer growth at around 800 °C. Since those phenomena were not observed from the Mo/quartz after the high temperature annealing, the thermal stress between Mo and quartz as well as Mo and AgGaTe₂ were considered as the origin. Thin layer of Cr was introduced between the Mo layer and the quartz substrate. This process improved the adhesion of the Mo layer, but the cracking was still observed after the formation of Ag₂Te layers. In order to reduce the thermal stress, the growth temperature of the first layer was lowered. Ag₂Te layer was prepared using the RF sputtering at room temperature, then AgGaTe₂ layer was prepared using the CSS method at around 700 °C. The stoichiometric compound source target was used for this study. The film quality was mainly analyzed using the XRD measurement, and Scanning Electron Microscope (SEM). The thickness of the sputtered Ag₂Te layer was about 1 micron. The surface morphology of Ag₂Te layer prepared by the CSS method was very characteristic, and the rough surface similar to the membrane filter structure was observed. This structure was advantageous as it would act as the nucleation sites for the successive layer. When the Ag₂Te layer was prepared, the surface became essentially featureless, and smooth morphology was observed. The second step was performed at around 700 °C using the mixture of powder Ag₂Te and Ga₂Te₃. The XRD theta-2theta data suggested that diffraction peak originated from 112 AgGaTe₂ was the dominant peak. This result was similar to that obtained from samples prepared using CSS grown Ag₂Te layer. Cross sectional SEM observation confirmed that the uniform layer was grown on the Mo layer. The crack lines observed from CSS grown Ag₂Te layers were not confirmed from both room temperature sputtered Ag₂Te layers and successively grown AgGaTe₂ layers. This work was supported in part by Waseda University Grant for Special Research Projects, Grant-in-Aid for Young Scientists (Early Bird) at Waseda Research Institute for Science and Engineering, and the Sasakawa Scientific Research Grant from The Japan Science Society.

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(Student) Atomic Layer Deposited MoO_x for Controlling O:Mo Ratio to Obtain Passivation and Hole Selectivity in Si Heterojunction Solar Cells Suren Patwardhan^{1,2}, Arpan Dhara¹, Akash Kumar¹, Sandeep Maurya¹, Balasubramaniam Kavaipatti¹ and Shaibal Sarkar¹; ¹Department of Energy Science and Engineering, Indian Institute of Technology Bombay, Mumbai, India; ²Physics, K J Somaiya College of Engineering, Mumbai, India.

Sub-stoichiometric molybdenum oxide (MoO_x) is a promising candidate for hole extraction in dopant-free carrier selective contact type Si heterojunction

solar cells. Efficiencies exceeding 20% have been already achieved using MoO_x in place of p-doped a-Si in a configuration, which is otherwise similar to a HIT cell. However, majority of the reported literature involves MoO_x films deposited by thermal evaporation. There is less work reported by other methods, particularly by atomic layer deposition (ALD). In our work, we did not use any separate passivation scheme (such as intrinsic a-Si) and directly deposited MoO_x films on Si to check their functionality in terms of passivation in addition to basic hole selectivity. We tried both the precursors tested so far one, $(\text{NtBu})_2(\text{NMe}_2)_2\text{Mo}$ as Mo precursor and O_2 plasma as oxidant and two, molybdenum hexacarbonyl [$\text{Mo}(\text{CO})_6$] as Mo precursor and Ozone as oxidant. The former pair yielded low V_{oc} (< 300 mV) while the latter pair resulted in a better performance (around 430 mV). Although, cells made by both the routes could not match performance of our reference cell incorporating evaporated MoO_x film on Si for which the V_{oc} exceeded 600 mV, it highlights the role played by precursors and deposition conditions on device parameters. There were two main observations. The V_{oc} was strongly affected by the mechanism of film deposition while J_{sc} is not as significantly affected. The key point in the carrier selectivity and passivation by transition metal oxides in general, referring to Si heterojunction cells is their high work function, which assists in band bending in Si near interface leading to depletion/inversion region. V_{oc} is a direct consequence of this band bending. Further, the band bending and thus V_{oc} is affected significantly with change in the O:Mo ratio in the MoO_x film. There are several causes for change in this O:Mo ratio including temperature, humidity etc. but the prominent mechanism is the hydrogen-induced reduction of MoO_3 towards MoO_{3-x} . This hydrogen may come from water adsorbed on deposited MoO_x film on exposure to air or from intrinsic a-Si:H used for passivation during annealing. For this reason, we have avoided passivation by intrinsic a-Si:H and directly deposited MoO_x on Si for to test the quality of passivation. With ALD, it gives flexibility in controlling work function of MoO_x to achieve effective passivation. With evaporation, there are hardly any control parameters to achieve this. The ALD grown MoO_x films also showed stable lifetime as compared to evaporated MoO_x films on Si. This is promising in terms of maintaining the work function of deposited films. In case of evaporated films, there was a drastic reduction in the carrier lifetime indicating complete loss of passivation over long (1-week) exposure to ambient conditions. Our ALD-grown MoO_x/Si cells showed about 7% efficiency without using intrinsic a-Si:H or any other kind of passivation scheme. Although low, to our knowledge, this is a first report of its kind. The O:Mo ratio of these films was estimated to be 2.89 while that for evaporated films, it was around 2.69. adjusting the ALD parameters to yield a ratio close to that observed for an evaporated film may improve the V_{oc} value and hence efficiency. All the cells were made of area about 1 cm^2 by scribing from 5 inch as-cut n-type FZ Si wafers. These wafers were first treated in a saw-damage removal solution to smooth-out the surface. No surface texturing was done. Next, phosphorous diffusion was performed followed by etch-back on the front surface to get n^+ back contact. For MoO_x deposited from $\text{Mo}(\text{CO})_6$, the substrate was maintained at 170°C and N_2 was used as carrier and purging gas. Base pressure of the reactor was kept at around 1 Torr. Metal precursor was kept at room temperature and a N_2 overhead assembly was used to carry the precursor into the reactor.

3:10 PM REFRESHMENT BREAK

3:30 PM I06

(Student) Influence of PbS Quantum Dot Sensitization on Action Spectrum of Graphene/SiC Schottky Diodes Joshua Letton¹, Mathew Kelley², Fiaz Ahmed², Andrew B. Greytak² and MVS Chandrashekar¹; ¹University of South Carolina, Columbia, South Carolina, United States; ²Chemistry and Biochemistry, University of South Carolina, Columbia, South Carolina, United States.

We demonstrate that by incorporating PbS quantum dot films (QD-films) with epitaxial graphene (EG)/SiC Schottky diodes new features appear in the action-spectra well below the bandgap of 4H-SiC ($\lambda=387$ nm) and above-bandgap response is enhanced by $\sim 10\times$. These changes were attributed to the QD-film from comparison with similar action spectra on control QD-films on Si/SiO₂, showing similar characteristic peaks in the action spectra. These QD-film sensitization layers were removed using an HF-clean to reset the EG/SiC Schottky diode to its pre-sensitized state. This cleaning enabled the repetition of measurements with fresh PbS QDs which are often susceptible to oxidation in air. The EG/SiC Schottky/QD-film structure (Fig. 1a) is reminiscent of a dye sensitized solar cell, having a wide-bandgap native single crystal interface integrated with a more disordered QD-film that absorbs over a broader spectrum. The QD-film has size-tunable absorption and is low-temperature solution processable, facilitating low-cost implementation of opto-electronic devices, while the native EG on SiC serves as a transparent contact, underscoring the importance of these hybrid structures in flexible electronics and QD-based solar cells [1], [2]. EG/SiC Schottky structures were grown and fabricated

using a chemically accelerated SiF_4 growth on the Si-face of SiC [3]. The PbS QDs were synthesized following the method described by Zhang et al.[4], having a diameter of 3.8 nm and lowest-energy electronic transition at 1280 nm. The QDs, initially protected by alkyl carboxylate surface coating (ligand), were purified by gel permeation chromatography [5]. A thin film was formed by spin-coating followed by in-situ ligand-exchange with ethanedithiol [6]. The resulting film had a 10 nm thickness and 9.716 nm RMS roughness. Separate measurements on control films on Si/SiO₂ revealed a charge mobility of $\sim 10^3\text{-}10^2\text{cm}^2/\text{Vs}$. Fig. 1b shows the responsivity of the QD-film/EG/SiC structure compared to the bare EG/SiC, confirming the increase in the above-bandgap response and sub-bandgap spectral features were due to the QD-film. Increase in the <387 nm responsivity was attributed to a larger charge collection area, as shown in the charge-collection maps recorded by scanning photocurrent spectroscopy near the band-edge of SiC [7]. At the EG-mesa edge, without QD-films, the photoresponse drops sharply but with the QD-film it increases significantly over the background (Fig. 2b). From the increased charge collection at the EG-mesa edge, the lateral carrier diffusion lengths in the QD-films were estimated to be $\sim 10 \mu\text{m}$. The transient response of these devices (Fig. 2a) gave a recombination time in the QD-films of $\sim 5\text{-}82$ ms, implying a mobility in the QD-film of $\sim 10^2\text{-}10^3\text{cm}^2/\text{Vs}$. With the QD-film application a sharp spectral feature of unknown origin emerged at 750 nm and the EG/SiC Schottky barrier height remained relatively unchanged. This assertion was tested by stripping the QD-film off EG/SiC using HF and resetting the device to its bare state, eliminating the 750nm feature (Fig. 1b). Multiple cycles of this procedure show that the device is robust, likely due to the native EG/SiC interface. Leaving the EG/SiC/QD-film structures in air degraded the device performance but was recovered with the cleaning procedure and a new QD-film. In summary, we have demonstrated the potential for hybrid QD/EG/SiC heterostructures to replace dye-sensitized solar cells and related optoelectronic devices. [1] R. A. Taylor *et al.*, *SPR Nanosci.*, vol. 4, pp. 142–168, 2017. [2] M. Graetzel *et al.*, *Nature*, vol. 488, no. 7411, pp. 304–312, 2012. [3] A. Balachandran *et al.*, *J. Cryst. Growth*, vol. 448, pp. 137, 2016. [4] J. Zhang *et al.*, *J. Phys. Chem. Lett.*, vol. 6, no. 10, pp. 1830, 2015. [5] Y. Shen *et al.*, *Chem. Mater.*, vol. 25, no. 14, pp. 2838, 2013. [6] E. J. D. Klem *et al.*, *Appl. Phys. Lett.*, vol. 90, no. 18, pp. 10, 2007. [7] B. G. Barker Jr *et al.*, *2D Mater.*, vol. 5, no. 1, p. 11003, 2017.

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(Student) Influence of Purification Methods on Optoelectronic Properties of PbS-QD Films Fiaz Ahmed¹, Adam Roberge¹, Joshua Letton², Mathew Kelley¹, Cole A. Love-Baker¹, MVS Chandrashekar² and Andrew B. Greytak²; ¹Chemistry and Biochemistry, University of South Carolina, Columbia, South Carolina, United States; ²University of South Carolina, Columbia, South Carolina, United States.

Colloidal quantum dots (CQDs) are promising semiconducting materials for electronic and optoelectronic applications due to tunable size-dependent band gap, multi-exciton generation phenomena, and high photoluminescence (PL) efficiencies. These properties can be tuned to engineer photovoltaic devices, displays and flexible electronics. To fabricate devices from as-synthesized CQDs, post synthetic purification of CQDs is required to remove reaction byproducts and residual precursor compounds. Precipitation and redissolution (PR) techniques, which employ an anti-solvent to enable CQD's separation through agglomeration, is widely used. However, this technique is inconsistent and generally must be repeated to provide clean CQDs with appropriate populations of surface-bound molecules (ligands) for subsequent steps. PR techniques may also result in loss of native ligands bound to the surface, inducing more surface traps and/or compromising the chemical stability of these nanocrystals. Gel Permeation Chromatography (GPC) has been proven to be an effective technique to remove the byproducts and impurities from CQDs. In this study, we have demonstrated the effectiveness of gel permeation chromatography (GPC) in removing byproducts and impurities from PbS QDs as shown by NMR spectra of PR and GPC purified samples (Fig.1b). Furthermore, we show that films fabricated using GPC purified PbS QD solutions exhibit high photoconductivity and ohmic contacts. Oleate-capped PbS quantum dots (lowest energy electronic transition $\lambda_g \sim 1290$ nm, ~ 4.7 nm diameter) were synthesized through an air free synthetic route. Near-infrared absorption spectroscopy shows that despite removal of unbound surfactants, PbS QDs remain stable in solution following GPC (Fig.1a). These purified nanocrystals were used to make $\sim 100\text{nm}$ thick films using layer by layer spin casting and ligand exchange process. Optoelectronic properties were investigated using Au contacts patterned on Si/SiO₂ substrates. As-fabricated devices were tested for in-plane conductivity and photoresponse. The charge carrier mobility was extracted from the mobility lifetime product and recombination lifetime determined by the spatial profiles of the photocurrent obtained through scanning photocurrent

microscopy (SPCM), and transient photocurrent measurements, respectively. Our findings show an improved photoconductivity of PbS devices prepared with GPC purified QDs. These films also show improved physical characteristics including reduced surface roughness, suggesting that impurities play an important role in film morphology and device performance.

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Investigation of Boron Dopant Deactivation Through Atomic Hydrogen Diffusion in Si for Enhancement of Solar Cell Efficiency Seyedeh Fahimeh Banihashemian¹, Aboozar Mosleh², Shui-Qing Yu¹ and Hameed A. Naseem¹; ¹ELEG, University of Arkansas, Fayetteville, Arkansas, United States; ²Chemistry & Physics, University of Arkansas Pine Bluff, Pine Bluff, Arkansas, United States.

Increasing the efficiency of solar cells have been pursued using various methods such as improving the contact quality and reducing the surface recombination. High doping concentrations are essential in order to achieve good contact quality. However, high concentration near the surface would reduce the lifetime of generated charge carriers through Auger and Shockley-Read-Hall recombination. Selective emitter doping has been the method that was developed to overcome the surface recombination for devices such as lasers [1] and solar cells [2]. Recently, it has been shown that atomic hydrogen treatment of the surface would result in the reduction of doping concentration and a concomitant enhancement in the efficiency of the solar cells [3]. However, presence of passivation layers that are used to increase the efficiency of the cells, do not allow the hydrogen atoms pass through the surface. In this work, we have proposed using high hydrogen content Silicon nitride passivation layers and using it as a source for hydrogen diffusion source for further surface treatment. The films were grown using plasma enhanced chemical vapor deposition. The samples were characterized using spectroscopic techniques, such as, ellipsometry and Fourier Transform Infrared Spectroscopy to measure the material and optical properties. In addition to the experimental results, we have theoretically investigated atomic Hydrogen diffusion in boron doped Si. A plasma enhanced CVD system was used for the deposition of silicon nitride films. Experiments were carried out while the substrate was maintained at room temperature and 300°C while deposition pressure was maintained constant at 500 mtorr. Silane flow rate was varied from 0.5 to 2 sccm with and nitrogen flow rate from 18 to 20 sccm to make N₂/SiH₄ ratio of roughly 10, 20 and 40. Total flow was kept constant at 20 sccm. Applied RF power provided sustainable plasma power density (PPD) of 50-650 mW/cm². The growth times were varied from 10-30 min. Material properties and the hydrogen content of the films were investigated. The samples were annealed from 400-700°C for 5-20 minutes and the hydrogen content of the films were measured afterwards. Finally, the samples were annealed at 125°C for 15-30 minutes in atomic hydrogen ambient and the hydrogen content was measured. Grown samples were characterized by a variable angle spectroscopic ellipsometer to measure the thickness and refractive index. The measured data were fitted with the database available for silicon, silicon nitride and silicon oxide. The chemical composition of the films was characterized using a Fourier transform infrared (FTIR) spectrometer. The FTIR characterization of the samples show the Si-H, N-H, and Si-N bond density in deposited layer. Based on the Si-H and N-H stretching bonds, the concentrations of bonded hydrogen were calculated. The hydrogen content of the films have been studied under different conditions. As the solar cells are processed at high temperatures which results in the reduction of hydrogen content of the films, the hydrogen content is measured after annealing. The results show that hydrogen concentration decreases after annealing. Hydrogen diffusion could be found by detection of B-H complex formation in the Si. We have developed a theoretical model to show diffusion of atomic hydrogen into uniformly boron-doped silicon. By comparing the model with the experimental data from literature [4] it can be seen that hydrogen diffusion decays after deactivating all the boron within a diffusion length. Applying the developed model on a boron diffused Si (emitter of a solar cell) shows that boron is deactivated close to the surface. Further details of the experimental and theoretical models will be presented in the full paper submission. [1] Sugianto et al IEEE PVSC, 2010. [2] Dastgheib et al., EPSE Conference, 2008 [3] Shumate et al. , IEEE PVSC, 2013. [4] Herrero et al., Phys Rev B, vol. 43, 1555, 1991

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Trans-Reflective Solar Cells for High-Efficiency Decorative Silicon Solar Panels Chengang Ji¹, Xinliang Chen², Qingyu Cui¹, Taizo Masuda³, Yuki Kudo³, Xiaodan Zhang² and Lingjie J. Guo¹; ¹Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ²Institute of Photoelectronic Thin Film Devices and Technology, Nankai University, Tianjin, China; ³X-Frontier Division, Toyota Motor Corporation, Susono-shi, Japan.

In recent years, tremendous efforts have been made to boost the efficiency performance of photovoltaic (PV) cells by either optimizing the device configuration or utilizing new active materials with larger bandgap. However, the black and unaesthetic appearance of traditional solar cells has limited their installment only in solar field or on building and car rooftops. There is a strong need to develop decorative PVs that can simultaneously offer attractive colors and harvest the otherwise totally wasted solar energy for buildings and vehicles integrated PV solutions. In this work, we present a new approach for high-efficiency colored PVs by topping a crystalline silicon (c-Si) solar panel with a trans-reflective amorphous Si (a-Si) solar cell device, forming a four-terminal PV system. The top a-Si solar cell consisting of 5 layers exhibits a narrowband reflection and transmits the remaining broadband solar radiation onto the c-Si solar panel underneath, leading to the distinctive reflection color and high power conversion efficiency (PCE) of the whole PV system. Different colors can be achieved by simply adjusting the thickness of each layer in the a-Si device. Taking the green colored device for example, the PCE of the a-Si cell with only 11 nm active layer and the whole system are ~ 2.80% and ~ 11.72%, respectively, where the latter is only 4.28% lower than the original c-Si solar panel without any covering. Considering that only deposition method and mechanical integration are required in realizing the final PV system, the proposed method overcomes the low efficiency limitation of typical colored solar cells and holds potential for future building-integrated photovoltaics and automotive applications.

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(LATE NEWS, Student) Progress toward >30% Efficient III-V/Si Tandem Photovoltaics Daniel L. Lepkowski¹, Jacob T. Boyer¹, Daniel J. Chmielewski¹, Chuqi Yi², Ned Western², Hamid Mehrvarz², Anita Ho-Baillie², Stephen P. Bremner³, Christopher Kerestes³, Daniel Derkacs³, Steven G. Whipple³, Alex P. Stavrides³, Tyler J. Grassman¹ and Steven A. Ringel¹; ¹The Ohio State University, Columbus, Ohio, United States; ²School of Photovoltaic and Renewable Energy Engineering, University of New South Wales, Sydney, New South Wales, Australia; ³SolAero Technologies, Corp., Albuquerque, New Mexico, United States.

Si-based tandem solar cells provide a path to surpassing the single-junction efficiency limit while leveraging the low cost of Si substrates and their associated highly-scaled manufacturing infrastructure. The III-V/Si tandem solar cell architecture has a theoretical efficiency of ~45%. While mechanically-stacked and wafer-bonded cells have thus far resulted in impressive AM1.5G efficiencies of 35.9% and 33.3%, respectively, questions remain about their ultimate scalability and manufacturability. Monolithic, epitaxial integration of III-V on Si provides a more promising avenue for scalability. However, III-V/Si integration has its own challenges with respect to material quality that have yet to be completely resolved. Currently these epitaxially-integrated structures have achieved verified efficiencies of 20.1% for a GaAsP/Si dual junction and 22.3% for a GaInP/GaAs/Si triple junction. Although these devices are promising proofs of concept, they still fall far short of the aspirational values provided by the mechanically-stacked and wafer-bonded cells. To this end, we are currently working toward the achievement of III-V/Si material quality and associated device designs that will enable >30% efficient III-V/Si tandem solar cells in the near future. This work specifically focuses on three key aspects of the III-V/Si tandem structure that require further optimization to improve GaAsP/Si tandem efficiency: 1. Si bottom cells that are specifically designed for the truncated incident spectrum and elevated interface recombination velocity (IRV) at the GaP/Si interface. Therefore, we are exploring various design and experimental aspects of the Si bottom cell, including rear surface texturing and the impact of the high IRV at the GaP/Si interface on the performance of homojunction and GaP/Si heterojunction bottom cells. 2. A GaP nucleation layer and GaAsP graded buffer that is optimized to reduce threading dislocation density (TDD) to levels that do not significantly impact the performance of the GaAsP top cell. We have recently developed a GaP/Si nucleation process that yields a TDD of $1-3 \times 10^6$ cm⁻², nearly an order of magnitude lower than our previous results and on par with the best demonstrated to date elsewhere. Work is thus in progress to optimize subsequent epitaxial processes to take advantage. 3. A GaAsP top cell structure that is optimized for the aforementioned low TDD levels and improved material quality. For this, we have worked investigated low-TDD oriented GaAsP

top cell designs that have thus far yielded >20% (ARC-projected) efficiency. Additionally, investigation of GaAsP top cell performance at various TDD values, along with analytical modeling, now provide a better understanding of the impact of threading dislocations on the top voltage and current performance. This work will present the next generation of the authors tandem solar cell, a 21.8% AM 1.5G efficient device (industry-verified) based on the unoptimized high-TDD ($2 \times 10^7 \text{ cm}^{-2}$) platform, underperforming Si bottom cell, and current-mismatched subcells. However, using this point as a reference and considering the multiple points of progress made recently, we have identified a practical pathway to >30% AM1.5G efficiency. Modeled improvements to antireflection layers, integration of demonstrated isotype cells, improved current-matching, and application of the recently-developed low-TDD material together reveal a realistic efficiency projection of greater than 30% at TDD values approaching 10^6 cm^{-2} . We will present up-to-date progress on these various subcomponent development thrusts, as well as an in-depth look at the near-future performance of this architecture and its potential for rapid development over the next few years.

SESSION J: Alloys for IR Applications

Session Chairs: Ganesh Balakrishnan and Sanjay Krishna
 Wednesday Afternoon, June 26, 2019
 Michigan League, 3rd Floor, Henderson

1:30 PM J01

Accurate Unfolding of Dilute Highly Mismatched Alloy Band Structures Istvan A. Gulyas¹, Chad A. Stephenson² and Mark Wistey¹; ¹Physics, Texas State University, San Marcos, Texas, United States; ²Now at Sandia National Laboratories, Albuquerque, New Mexico, United States.

Highly mismatched alloys (HMAs) such as GeC, BGeAs, and GaInNAs are highly promising for photonic devices and tunneling transistors because they allow independent control of lattice constant, bandgap and effective masses. But HMAs are often difficult to grow due to the mismatch between size and/or electronegativity of the different atoms in the alloy, so they are often modeled numerically. Unfortunately, accurate simulation is also difficult because the same mismatch presents severe computational requirements: large numbers of bands, high energy plane waves to represent highly localized electrons/holes, and often large numbers of atoms to represent dilute alloys. In this work, we present the first clear unfolded band structures of dilute, 128-atom germanium carbide (Ge:C) supercells without major artifacts other than symmetry averaging. Although these results agree qualitatively with the band anticrossing model at Gamma, they show a surprising new splitting at the indirect L valley. In particular, a clear gap in energies exists across k-space between the new, lowest conduction band (E-) and the original conduction band (E+). Original calculations used a single k-point (k=0), which was folded four times along each axis by the use of supercells. Adding additional k-points to the calculation verified the splitting at both Gamma and L. We conclude that there is significant mixing of the conduction band with states other than s-like orbitals, causing interaction between the spherically-symmetric electron localized on the carbon atom, and the antisymmetric conduction band states near L. In addition, we tested the convergence of multiple material properties with various calculation parameters such as the number of bands, the maximum energy included in the wavefunction basis set, the number of k-points, and the number of iterations in the electronic and/or ionic convergence loops. We used the Vienna Ab-initio Software Package (VASP) with BandUP and vasp_unfold to unfold bands. A k-point grid of 2x2x2 (Gamma centered) was significantly more computationally costly than 1x1x1 but had notable effects on bandgaps and even lattice constants. A 3x3x3 grid was slightly better and at nearly the same computational cost. System energies varied continuously as the wavefunction basis set was expanded, up to roughly 650 eV. These clean, unfolded band structures allow extraction and prediction of bandgaps, optical transition rates, and reveal the true mixed nature of the carbon state in Ge:C. The splitting in the L valley complicates efforts to create a direct bandgap by adding carbon, but this is partly offset by the increase in effective mass at Gamma, which will reduce confinement energies in quantum wells. We also note in passing that identical jobs required a variable and nondeterministic amount of time to complete, which has implications for researchers seeking to optimize their computational models.

1:50 PM J02

(Student) MOCVD Grown Metamorphic InAsSb Materials for Long Wave Infrared Detectors Vinita Dahiya¹, John A. Carlin², Julia I. Deitz², Ari N. Blumer³, Tyler J. Grassman^{1,3} and Sanjay Krishna¹; ¹Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ²Institute for Materials Research, The Ohio State University, Columbus, Ohio, United States; ³Material Science and Engineering, The Ohio State University, Columbus, Ohio, United States.

Recently, InAs_{1-y}Sb_y ternary alloy system with Sb fraction greater than 40 % has emerged as a promising material in the long wave infrared (LWIR, 8- 14 μm) [1-3]. However, the non-availability of substrates lattice-matched to the target InAs_{1-y}Sb_y compositions, and the desire for use case flexibility in either bulk or superlattice based structures, necessitates the use of metamorphic virtual substrates. These are produced through the careful engineering (expansion) of the effective lattice constant using compositionally graded buffers, enabling control over the formation and evolution of resultant misfit and threading dislocation densities (TDD), which can affect optoelectronic device performance. The majority of work to date in LWIR InAs_{1-y}Sb_y has made use of molecular beam epitaxial growth [1,4,5], while metal-organic chemical vapor deposition (MOCVD) based work has been limited due to the various challenges faced in growth of III-Sb materials, including low growth temperatures (and thus an awkward balance between precursor reactivity and overall growth dynamics), low Sb volatility (results in Sb clustering under Sb rich conditions) [6,7]. In this paper, we employed a conventional step-graded buffer approach within the InAs_{1-y}Sb_y alloy system, grown on GaSb substrates via MOCVD, to reach the target InAs_{0.6}Sb_{0.4} composition. A range of buffer design variables were considered, including average grading rate, individual layer thickness, and compositional step sizes, as well as investigation of the impact of different growth conditions, such as V/III ratio, substrate temperature, and substrate offset. To date, we achieved residual TDD in the terminal InAs_{0.6}Sb_{0.4} as low as $2 \times 10^6 \text{ cm}^{-2}$, with even further reduction likely possible with careful buffer and growth condition optimization. [1] W.L. Sarney *et al.*, J. Appl. Phys., 122 (2017) 02B105. [2] W.L. Sarney *et al.*, J. Vac. Sci. Technol., B, 30 (2011) 02B105. [3] G. Belenky *et al.*, Appl. Phys. Lett., 99 (2011) 141116. [4] S. Tomasulo *et al.*, J. Vac. Sci. Technol., B, 36 (2018) 02D108. [5] V. Dahiya *et al.*, J. Vac. Sci. Technol., B, 36 (2018) 02D111. [6] C.A. Wang, J. Cryst. Growth, 272 (2004) 664-681. [7] R.M. Biefeld, T. Materials Science and Engineering: R: Reports, 36 (2002) 105-142.

2:10 PM J03

Ge_{1-x}Sn_x Alloys on Si, Germanium, and Sapphire Substrates for Mid-IR Detector Applications Produced by Remote Plasma Enhanced Chemical Vapor Deposition (RPECVD) Gordon J. Grzybowski¹, Jay Mathews², Stefan Zollner³, Arnold Kiefer⁴ and Bruce Claffin⁴; ¹KBRWyle, Dayton, Ohio, United States; ²Department of Physics, University of Dayton, Dayton, Ohio, United States; ³Department of Physics, New Mexico State University, Las Cruces, New Mexico, United States; ⁴Air Force Research Laboratory, Dayton, Ohio, United States.

Ge_{1-x}Sn_x alloys are promising materials for a variety of Mid-IR detector applications due to the predicted direct energy gap caused by alloying. The incorporation of Sn into Ge is expected to yield a direct band gap at concentrations near (X= 0.08-0.1) by lowering both the direct and indirect gaps in Ge, with the former decreasing at a higher rate. However, the low solubility limit of Sn in Germanium (~X=0.01) restricts thin film growth to non-equilibrium, low temperature methods, and often non-standard chemical sources are used in order to produce films of desired composition and quality. Here we report the use of a prototype Remote Plasma Enhanced Chemical Vapor Deposition (RPECVD) to produce Ge and Ge_{1-x}Sn_x films with compositions ranging from (X= 0-0.1) and thicknesses up to 1100 nm utilizing inexpensive, commercially available GeH₄ and SnCl₄ precursors. RPECVD produces quality material on a variety of substrates including silicon, germanium, and sapphire with total thickness variation (TTV) less than 20%. X-ray diffraction indicates the films on silicon are partially relaxed, films on germanium are pseudomorphic, and films on sapphire are polycrystalline. Cross-sectional transmission electronic microscopy (X-TEM) indicates that for germanium films grown on silicon an initial layer of highly defective material is produced in the first 60nm, while the defect density is considerably reduced in the subsequent material. Atomic force microscopy (AFM) shows RMS roughness less than 0.5 nm for Ge and as low as 1 nm for up to X=0.07. Photoluminescence measurements using 1034 nm or 780 nm excitation and spectroscopic ellipsometry characterization show a monotonic shift with composition and indicate a band gap as low as 0.45 eV has been achieved in materials produced by RPECVD. A prototype GeSn/Si(001) photoconductor device has been fabricated showing a spectral response up to 2.2 μm.

2:30 PM J04

Prospects of InGaAs/GaAsSb Lattice-Matched to InP for Extended Range SWIR Detection Justin Easley¹, Martin H. Ettenberg³ and Jamie Phillips²; ¹University of Michigan, Ypsilanti, Michigan, United States; ²EECS Department, University of Michigan, Ann Arbor, Michigan, United States; ³Princeton Infrared Technologies, Inc, Monmouth Junction, New Jersey, United States.

Type II superlattices (T2SL) have been developed in recent years as an important infrared material system, primarily as a replacement for existing MWIR and LWIR technologies. They provide an opportunity to utilize mature III-V growth and fabrication technologies, and substrates including GaSb and InP. T2SLs have been aggressively pursued due to predictions for reduced sensitivity to material defects in nBn heterostructure devices and higher predicted operating temperatures via Auger suppression associated with the strained layer superlattice bandstructure. We propose exploring III-V T2SL on InP as a competitive SWIR photodetector, due to a direct lattice match to InP. While the T2SL/InP technology is attractive for SWIR, the tradeoffs associated with the low absorption strength of the indirect optical transition in the T2SL bandstructure and carrier transport through the T2SL present major challenges. This study examines the prospects of T2SL/InP for optimized SWIR detection at 2 μm , operating at or near room temperature, while comparing performance to extended-range In_{0.83}Ga_{0.17}As and HgCdTe technologies. The T2SL of interest in this study is In_{0.53}Ga_{0.47}As/GaAs_{0.51}Sb_{0.49} (5nm/5nm) lattice matched to InP substrates. Eight band k.p simulations were utilized to extract information on the electronic band structure and calculate the optical absorption spectrum. The effective band gap is calculated to be 0.494 eV, which corresponds to a cutoff wavelength of $\lambda_c = 2.51 \mu\text{m}$, and significant optical absorption near 2 μm . Quantum efficiency was calculated using Sentaurus TCAD and a standard InGaAs/T2SL/InGaAs p-i-n structure with a varying absorber layer thickness with doping concentration of $N_D = 1 \times 10^{16} \text{ cm}^{-3}$, where QE at 2 μm is found to be approximately 55%. The two primary sources of dark current are Shockley-Read-Hall (SRH) and radiative recombination. A range of SRH trap densities were simulated, where SRH is found to be the limiting mechanism for SRH trap densities greater than $5 \times 10^{14} \text{ cm}^{-3}$, while fewer traps result in a radiative recombination limited operation. Based on these lifetime values, the resulting dark current density was estimated and compared to extended-range In_{0.83}Ga_{0.17}As and the Rule 07 metric for HgCdTe. With trap densities $\sim 10^{13} \text{ cm}^{-3}$, a T2SL is expected to outperform extended range InGaAs in dark current, and be comparable to HgCdTe, making it a competitive SWIR technology.

2:50 PM J05

Raman Scattering Study to Optimize the Damage Recovery Treatment of Ion-Implanted GaSb Thermophotovoltaic Cells Emma J. Renteria¹, Vijay Saradhi Mangi^{1,2}, Francesca Cavallo^{1,2}, Ganesh Balakrishnan^{1,2} and Reginald Parker³; ¹Center for High Technology Materials, University of New Mexico, Albuquerque, New Mexico, United States; ²Electrical and Computer Engineering, The University of New Mexico, Albuquerque, New Mexico, United States; ³510nano Inc., Durham, North Carolina, United States.

Ion-implantation is an attractive technique for the doping of GaSb Thermophotovoltaic (TPV) cells as it guarantees better reproducibility, dopant profile control, and uniformity compared to diffusion techniques. Ion-implantation is also more cost-effective than epitaxial growth techniques. The main disadvantage of ion-implantation is the damage caused to the crystal lattice during ion bombardment. Nonetheless, such crystal damage can be recovered with thermal treatments. Rapid thermal annealing (RTA) has been widely used as an effective treatment to recover the damage to the crystal and also to activate the dopants. However, annealing treatments for GaSb are challenging since Sb out-diffuses at 370 °C and GaSb melts at 710 °C. In previous work, we have shown that a cap of Si₃N₄ minimizes the out-diffusion of Sb and that the optimal annealing conditions to recover the crystal damage in Be-implanted GaSb samples are an annealing temperature of 600 °C and an annealing time of 10s.^{1,2} However, we have found that the performance of Be-implanted GaSb TPV devices at these annealing conditions is not the best. The open circuit voltage (V_{oc}) is only 0.13 V which is far from the 0.25 V V_{oc} of epitaxial GaSb TPVs. Hence, in this work, we revisit the annealing and doping conditions to optimize the performance of Be-implanted GaSb TPV cells. We use Raman spectroscopy to analyze the effect of annealing conditions in the recovery of crystal damage. The Raman spectra of an un-implanted GaSb sample show well defined LO mode peak at $\sim 235 \text{ cm}^{-1}$. This peak is not as well define for implanted samples. The Raman spectra of samples implanted with high dose of Be ions does not show a strong LO mode peak until at an annealing temperature of 680 °C while samples implanted with lower dose of Be ions show a very strong peak at a temperature of 660 °C which is expected as lower dose of ions causes less damage. Based

on the Raman scattering studies, samples are treated with the best annealing conditions and fabricated into TPV devices. As a result of these optimizations, the V_{oc} of Be-implanted GaSb TPVs is as good as the V_{oc} of epitaxial GaSb TPVs. The presentation will include a more in-depth characterization study of the devices and will provide more insight into the damage and recovery mechanism in ion implanted GaSb TPVs.

3:10 PM REFRESHMENT BREAK

3:30 PM J06

(Student) Microstructural and Morphological Variations in GaAsBi Brandon Carter¹, Veronica Caro¹, Li Yue¹, Joanna Millunchick¹ and Christopher Tait²; ¹Materials Science and Engineering, University of Michigan—Ann Arbor, Ann Arbor, Michigan, United States; ²Sandia National Laboratories, Albuquerque, New Mexico, United States.

GaAsBi and other bismuth containing III-V alloys (bismides) are promising for a wide range of electronic devices, as increasing Bi concentration serves not only to significantly reduce band gap energy, but also to increase the spin orbit coupling effects [1-3]. Due to this, bismides are of significant interest in a variety of fields, including spintronics [1], long wavelength infrared detectors, and photovoltaics, among others [1,4,5]. However, the realization of such devices has been hampered by compositional inhomogeneities within the film, including phase separation and atomic ordering [6], either of which can increase carrier localization. To study this, a series of growths were performed at constant temperature (T) and over a range of Bi/As2 and As2/Ga beam flux ratios. We found that inhomogeneities are a function of the surface morphology present during growth and are sensitive to small variations in growth conditions. Four distinct surface morphologies were observed at T = 325 C, corresponding to four growth regimes. These regimes are also expected to occur at different growth temperatures, however it is expected different T may lead to a shift in the flux ratios where the regimes form. Droplet-free surfaces were seen at high As2/Ga (≥ 2.4) and low Bi/As2 (≤ 0.2) beam flux ratios. Ga droplets were seen at low As2/Ga (≤ 2.0) and low Bi/As2 (≤ 0.1) beam flux ratios. Bi droplets were seen at high As2/Ga (≥ 2.4) and high Bi/As2 (≥ 2.5) beam flux ratios, and biphasic Bi/Ga droplets were seen at low As2/Ga (≤ 1.8) and high Bi/As2 (≥ 0.125) beam flux ratios. X-ray diffraction (XRD) omega-2theta scans suggest that different microstructures exist in each growth regime. For droplet-free films, XRD exhibit sharp, well-defined peaks indicating uniform incorporation throughout the film. Despite this, atom probe tomography (APT) and transmission electron microscopy (TEM) of these films exhibited lateral composition modulation and Bi clustering. For films with Ga droplets, XRD exhibits a sharp film peak with a long tail, indicating a range of compositions and regions of high Bi incorporation. TEM suggests that these high-Bi regions form during growth around the edges of the Ga droplets, where there is high availability of Ga to react with Bi. Films with Bi droplets exhibit a broad low intensity XRD peak with a long tail, indicating poor crystallinity and large variations in composition throughout the film. Finally, biphasic droplets yield XRD with two distinct broad low intensity peaks indicating two preferred compositions. Simulations [7] predict that maximum Bi incorporation is found in the Ga droplet region near the transition to the biphasic regime. Analysis of the XRD omega-2theta scans show this to not necessarily be the case across the entire film. The highest average Bi composition for films with Ga droplets was found to be 2.9%, assuming a Vegard's law and an unstrained lattice. However, regions up to approximately 23.0% are also apparent in the film. For droplet-free films, the highest average Bi composition is 16.4%. Thus, experimental results indicate to attain high Bi incorporation while maximizing compositional uniformity, growths must be performed in the regime where droplets do not form. [1] B. Fluegel, S. Francoeur, A. Mascarenhas, S. Tixier, E. Young, T. Tiedje, Phys. Rev. Lett. 97(6) (2006) 67205. [2] S. Francoeur, M.-J. Seong, A. Mascarenhas, S. Tixier, M. Adamcyk, T. Tiedje, Appl. Phys. Lett. 82(22) (2003) 3874. [3] G. Pettinari et al., Phys. Status Solidi, 250(4) (2013) 779–786. [4] F. Dimroth, Phys. Status Solidi, 379(3) (2006) 373–379. [5] K. Bertulis, A. Krotkus, G. Aleksejenko, V. Pa, R. Adomavi, G. Molis, Appl. Phys. Lett. 88 (2007). 201112 [6] C.R. Tait, L. Yan, J.M. Millunchick, J. Cryst. Growth, 493 (2018) 20–24. [7] G.V. Rodriguez and J.M. Millunchick, J. App. Phys. (2017) 125310.

3:50 PM J07

(Student) Band Structure Influence on Noise Properties of III-V Digital Alloys Ann K. Rockwell¹, Min Ren², Maddison Woodson², Andrew Jones², Stephen D. March¹, Yaohua Tan², Yuan Yuan², Scott J. Maddox¹, Avik Ghosh^{3,2}, Joe Campbell² and Seth Bank¹; ¹Electrical and Computer Engineering, University of Texas, Austin, Texas, United States; ²Electrical and Computer Engineering, University of Virginia, Charlottesville, Virginia, United States; ³Physics, University of Virginia, Charlottesville, Virginia, United States.

An important figure of merit related to device sensitivity for avalanche photodiodes (APD) is the excess noise factor, $F(M)$, which is directly proportional to $k = \alpha/\beta$, the ratio of the electron, α , and hole, β , impact ionization coefficients, for the case of pure electron injection. We recently demonstrated the successful growth of low-noise, $k \sim 0.01$ to 0.05 , $\text{In}_x\text{Al}_{1-x}\text{As}_y\text{Sb}_{1-y}$ digital alloy APDs, which is comparable to that of current state-of-the-art silicon detectors. These devices were lattice-matched to GaSb with Al fractions ranging from 0 to 80% [1] and we employed them to realize the first working staircase APD [2]. We also utilized the digital alloy approach to grow a variety of materials lattice matched to InP, InAs, and GaAs. Interestingly, InAlAs digital alloys grown on InP exhibited dramatically reduced noise compared with conventionally grown InAlAs lattice-matched to InP; specifically, reducing k from ~ 0.2 , the accepted literature and experimental value of the random alloy, to ~ 0.03 [3]. Here, we seek to understand the mechanism that allows for low-noise operation of some materials when grown as digital alloys, such as $\text{In}_x\text{Al}_{1-x}\text{As}_y\text{Sb}_{1-y}$ on GaSb and InAlAs on InP, while others such as InGaAs on InP and AlGaAs on GaAs show no decrease in excess noise. All samples in this work were grown on either GaSb, semi-insulating (SI) InP, SI GaAs, or InAs substrates by solid-source molecular beam epitaxy. In each sample, the digital alloy was strain-balanced to the corresponding substrate by varying the relative thicknesses of the individual (often strained) binary layers. There are several possible explanations for the origin of low-noise in these materials, but we focus here on superlattice band effects. Tight-binding band structure and direct gain measurements to extract the electron and hole impact ionization coefficients from random and digital alloys of InGaAs and InAlAs APDs show that β might be disproportionately suppressed. This could be due to the larger effective mass of holes in the valence band, leading to narrower minibands with higher radii of curvature. This would suggest larger valence band offsets and larger hole masses would be beneficial in materials selection. To test this hypothesis, two 70% Al quaternary InAlAsSb digital alloy APDs were grown on GaSb. One was nominally identical to that reported in Ref. [1], while the other was modified by combining the AISb/AlAs/AISb portion of the digital alloy into a single ternary layer of $\text{AlAs}_{0.10}\text{Sb}_{0.90}$ with identical average composition. This modification eliminates the largest portion of the valence band offset which should greatly reduce miniband formation and modification to the hole transport. However, both samples show nearly identical noise characteristics. We note that modulation of the effective mass between binary layers can also induce miniband formation, even without a band discontinuity between the layers. In order to truly isolate the noise characteristics, experiments on aperiodic digital alloy APDs are ongoing and will be reported at the conference. This work was supported by the Army Research Office (W911NF-17-1-0065) and DARPA (GG11972.153060), as well as a University of Texas Temple Foundation Fellowship. [1] S.J. Maddox, et al., *57th Electronic Materials Conf. (EMC)*, Columbus, OH (2015). [2] M. Ren, et al., *73rd Device Research Conf. (DRC)*, Columbus, OH (2015). [3] A.K. Rockwell, et al., *Appl. Phys. Lett.* 113, 102106 (2018).

4:10 PM J08

Mapping the Composition-Dependence of the Energy Bandgap of GaAsNBi Alloys Jordan Occena¹, Andra Chen¹, T. Jen¹, W. Linhart², Emil-Mihai Pavelescu³, Robert Kudrawiec², Yongqiang Wang⁴ and Rachel S. Goldman²; ¹Materials Science and Engineering, University of Michigan—Ann Arbor, Bellevue, Washington, United States; ²Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, Wrocław, Poland; ³National Institute for Research and Development in Microtechnologies, Bucharest, Romania; ⁴Los Alamos National Laboratory, Los Alamos, New Mexico, United States; ⁵Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States.

Due to the significant bandgap narrowing induced by the incorporation of dilute fractions of N and Bi in compound semiconductors, emerging dilute nitride-bismide alloys are of significant interest for optoelectronic devices operating in the near- to mid-infrared range.^{1,2} For GaAsNBi, it has recently been shown that Bi promotes the formation of (N-As)_N interstitial complexes,³ which are not accounted for in typical analyses of x-ray diffraction data. Furthermore, it has been proposed that Bi behaves as an isoelectronic impurity in GaAs. However, there are conflicting reports regarding the energetic position of the Bi impurity state either 0.18 eV

above¹ or 0.08 – 0.4 eV below^{4,5,6,7,8,9} the valence band maximum. Here, we have examined the alloy composition dependence of the energy bandgap and electronic states in GaAsNBi alloys. Using direct measurements of N and Bi mole fractions, via ion beam analysis, in conjunction with direct measurements of the out-of-plane misfit via x-ray rocking curves, we determine a new “magic ratio” for lattice-matching of GaAsNBi alloys with GaAs substrates. In addition, using a combination of photoreflectance and photoluminescence spectroscopy, we determine a new map of the composition- and misfit-dependence of the energy bandgaps, along with revealing the energetic position of Bi-related states at approximately 0.18 eV above the valence band maximum. These findings offer a predictive guide to bandgap engineering using GaAsNBi alloys and provide insight into the combined influence of Bi and N on electronic structure that may be extended to other emerging dilute nitride bismide alloys, such as GaPNBi and InAsNBi. We gratefully acknowledge support from the National Science Foundation (Grant No. DMR 1410282 and DMR 1810280). ¹A. Janotti, S.-H. Wei, and S.B. Zhang, *Phys. Rev. B* 65, 115203 (2002). ²S.J. Sweeney and S.R. Jin, *J. Appl. Phys.* 113, 043110 (2013). ³J. Occena, T. Jen, E.E. Rizzi, T.M. Johnson, J. Horwath, Y.Q. Wang, and R.S. Goldman, *Appl. Phys. Lett.* 110, 242102 (2017). ⁴Y. Zhang, A. Mascarenhas, and L.-W. Wang, *Phys. Rev. B* 71, 155201 (2005). ⁵S. Francoeur, S. Tixier, E. Young, T. Tiedje, and A. Mascarenhas, *Phys. Rev. B* 77, 085209 (2008). ⁶K. Alberi, O.D. Dubon, W. Walukiewicz, K.M. Yu, K. Bertulis, and A. Krotkus, *Appl. Phys. Lett.* 91, 051909 (2007). ⁷C.A. Broderick, M. Usman, and E.P. O’Reilly, *Semicon. Sci. Tech.* 28, 125025 (2013). ⁸C.-Z. Zhao, H.-Y. Ren, T. Wei, S.-S. Wang, and K.-Q. Lu, *J. Electron. Mat.* 47, 4539 (2018). ⁹V. Virkkala, V. Havu, F. Tuomisto, and M.J. Puska, *Phys. Rev. B* 88, 235201 (2013).

4:30 PM J09

(Student) Modeling and Measurement of Carrier Trapping and Tunneling in Al_xIn_{1-x}As_ySb_{1-y} Digital Alloys Stephen D. March¹, Andrew Jones², Ann K. Rockwell¹, Min Ren², Maddison Woodson², Scott J. Maddox¹, Joe Campbell² and Seth Bank¹; ¹Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas, United States; ²Electrical and Computer Engineering, University of Virginia, Charlottesville, Virginia, United States.

Low-noise, high-gain avalanche photodetectors (APDs) for telecommunication-wavelength sensing are difficult to realize due to the stochastic nature of the impact ionization gain mechanism, which leads to variation in the gain, parameterized by excess noise. Staircase APDs proposed by Capasso [1] mitigate this noise source by localizing impact ionization at deterministic locations within the device. We recently demonstrated the successful growth of digital alloy $\text{Al}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$ materials [2] that provide the necessary band offsets, and used these materials to realize the first single-step staircase APD [3]. However, scaling to higher staircase step counts has been hampered due to anomalous gain arising from conduction band carrier trapping and valence-to-conduction band-to-band tunneling [4]. A simple set of design parameters derived from modeling and measuring carrier trapping is needed before multi-step staircase APDs can be produced. In this work, we address this need by combining modified, self-consistent rate equation modeling [5,6] with capacitance-voltage and current-voltage measurements to parameterize these materials. Two-step staircase APD structures were grown using molecular beam epitaxy on (001)-oriented n-GaSb substrates with different varied conduction band profiles to modulate carrier trapping, such that depletion-width resolution of C-V is not limited by the Debye length [7]. Differences in light versus dark C-V measurements indicate a large spike in the electron carrier concentration of $1.1 \times 10^{12} \text{ cm}^{-2}$ at a depletion depth of $\sim 240 \text{ nm}$, which corresponds well with the anticipated position of the trapped carriers. Furthermore, it agrees well with modeled carrier pile-up values between 0.9 – $1.2 \times 10^{12} \text{ cm}^{-2}$. Additional intensity-dependent C-V measurements are underway to further clarify the carrier trapping and to rule out absorption at the staircase steps. We also demonstrate the predicted performance for future devices to show that the minimum thermionic barrier to effectively trap carriers is $\sim 0.3 \text{ eV}$ and the minimum tunneling distance necessary to mitigate band-to-band tunneling in devices with these digital alloy materials is approximately 60 nm. Additional temperature-dependent tests are in progress to further qualify and quantify thermionic barrier and tunneling. This work was supported by the Army Research Office (W911NF-17-1-0065) and DARPA. References: [1] F. Capasso, *IEEE Trans. Nucl. Sci.* 30, 424 (1983). [2] S.J. Maddox, et al., *57th Electronic Materials Conf. (EMC)*, Columbus, OH (2015) [3] M. Ren, et al., *73rd Device Research Conf. (DRC)*, Columbus, OH (2015) [4] S.J. Maddox, et al., *74th Device Research Conf. (DRC)*, Newark, DE (2016) [5] D. J. Moss, et al., *IEEE J. Quant. Elec.*, 30, 4, (1994) [6] K. Toprasertpong, et al., *Phys. Rev. B* 96, 075441 (2017) [7] E. F. Schubert, et al, *Appl. Phys. Lett.* 57, 497 (1990)

4:50 PM J10

(Student) Externally Applied Strain on GaSb Based GaInAsSb Quantum Well Membranes Andrew F. Briggs¹, Scott D. Sifferman², Kenneth Underwood³, Juliet Gopinath^{3,4} and Seth Bank⁵; ¹Electrical and Computer Engineering, University of Texas at Austin, Austin, Texas, United States; ²Microelectronics Research Center and ECE Dept., The University of Texas at Austin, Austin, Texas, United States; ³Department of Physics, University of Colorado Boulder, Boulder, Colorado, United States; ⁴Department of Electrical, Computer and Energy Engineering, University of Colorado Boulder, Boulder, Colorado, United States; ⁵The University of Texas at Austin, Austin, Texas, United States.

Understanding the ultimate strain limits of mid-infrared (mid-IR) semiconductor emitters, as well as how it affects the optical properties and recombination dynamics, is essential for continued research in mid-IR photonics. GaSb-based GaInAsSb alloys are an important alloy system for 3-4 μm emission; however, the small bandgap of GaInAsSb leads to significant Auger recombination and free carrier absorption that compromise device performance [1]. Increasing the compressive strain of GaInAsSb quantum wells (e.g. by changing the group-V composition) breaks the heavy-hole light-hole degeneracy and increases emission efficiency [2]. Characterizing the effect of strain on recombination and emission properties is a laborious process that typically requires the growth of numerous samples of varying compositions. Here, we report a nanomembrane-based platform that permits the continuous adjustment of the strain state of emitters via applied stress. The applied uniaxial strain change was as large as 2.3%, comparable to the 2.5% compressive biaxial strain built in by the molecular beam epitaxy growth process. With this technique we can vary strain over the entire range of what is possible through epitaxial growth and characterized strain-dependent recombination processes. Previous work on III-V based flexible electronics has demonstrated the fabrication of flexible solar cell junctions based on InP [3] and GaAs [4]. Those materials systems are ideal for nanomembrane fabrication because the AIAs epitaxial lift-off technique employed has nearly infinite selectivity. No such analog exists for the GaSb material system so a direct etching method using a solution of 1M CrO_3 and HF (8:1) and an $\text{InAs}_{0.91}\text{Sb}_{0.09}$ etch stop layer are used [5]. Membranes were bonded onto flexible PTFE substrates using a Au-Au cold welding approach used previously for flexible materials transfer [3]. Samples were then mounted onto a 1D sample stretcher to vary the uniaxial strain. Samples were characterized with Raman spectroscopy and photoluminescence (PL) as a function of applied strain. We observed a PL shift from the original 3.25 μm emission wavelength to 3.4 μm with the highest strain applied. This PL shift corresponds to an energy shift of 17 meV in the bandgap and a calculated applied pressure to the quantum well of $5 \times 10^9 \text{ dyn/cm}^2$. Raman measurements were performed in a similar fashion. A Raman shift of 1.8 cm^{-1} was observed which corresponds [6] to an applied pressure of $\sim 6 \times 10^9 \text{ dyn/cm}^2$, in agreement with the PL spectra. From the applied pressure, we calculated the uniaxial tensile strain applied to the quantum wells to be 2.3%. Further optical and material studies including X-ray diffraction as a function of strain will be presented at the conference. This work was supported by the National Science Foundation (Award No. DMR-1508603 and DMR-1508783). [1] L. Shterengas, et al., *Novel In-Plane Semiconductor Lasers XV*, 2016. [2] M. E. Flatté, et al., *Physical Review B*, vol. 59, no. 8, 1999. [3] K. Lee, et al., *Applied Physics Letters*, vol. 97, no. 10, 2010. [4] Y. Lee, et al., *Applied Physics*, vol. 15, no. 11, 2015. [5] M. Grzesik, et al., *Journal of Electronic Materials*, vol. 42, no. 4, 2013.

SESSION K: Epitaxial Materials on Si Session Chairs: Kurt Eyink and Emma Renteria Wednesday Afternoon, June 26, 2019 Michigan League, 3rd Floor, Koessler

1:50 PM K01

SiGe Growth on a Sapphire Substrate Using UHV-CVD Technique Abbas Sabbar¹, Joshua M. Grant¹, Perry Grant¹, Wei Dou², Aboozar Mosleh³, Zhong Chen² and Shui-Qing Yu¹; ¹Electrical, University of Arkansas-Fayetteville, Betonville, Arkansas, United States; ²Department of Electrical Engineering, University of Arkansas, Fayetteville, Arkansas, United States; ³Electrical Engineering, Arkansas Tech University, Russellville, Arkansas, United States.

Silicon germanium (SiGe) alloys are important semiconductors due to the use of these materials in many applications such as metal-oxide semiconductor field-effect transistor (MOSFET), modulation doped field

effect transistors (MODFETs) heterojunction bipolar transistor (HBT), high electron mobility transistor (HEMT), high-temperature thermoelectric devices, photovoltaic solar cells, and photon detectors. However, electronic components and circuits fabricated on conventional bulk Si substrates are not suitable for space communications due to the limitations of device bandwidth, circuit performance, operating temperature, and radiation hardness. Therefore, silicon-on-insulator (SOI) technology started and it is widely utilized in RF communication circuits. However, the need of high mobility devices made NASA Langley Research Center (NASA LaRC) developing silicon germanium on insulator SiGe). Previously, epitaxial growth patterns of SiGe on sapphire substrates are reported using rapid thermal chemical vapor deposition, MBE, and sputtering systems. Previous growth methods were either using wafer bonding or a complicated method by implanting Si to achieve an amorphous layer and crystallizing solid-phase regrowth of the amorphized silicon and then using the top silicon layer as a seed to grow Si or SiGe. Therefore, the CVD growth using commercial precursors of germane (GeH_4) and silane (SiH_4), is desired and has not been fully developed. In this work, we present growth results from SiGe growths using an Ultra-High Vacuum Chemical Vapor Deposition (UHV-CVD) reactor with the commercially available germane (GeH_4) precursor. The samples were characterized using spectroscopic techniques such as ellipsometry, Raman, and X-ray diffraction (XRD). The samples were grown in a custom-built cold walled UHV-CVD deposition described by Mosleh, et al. The backside of sapphire substrates was coated with 1 μm -thick titanium layers using an electron beam evaporator. Due to the transparency of sapphire, titanium layers were used to absorb the infrared radiation from the heater to raise the substrate temperature needed for the epitaxy of SiGe. The sapphire was then cleaned using methanol and loaded directly into the load lock after drying with nitrogen. The growth temperature was kept at 500-600°C while the chamber pressure at 1 T. Flow rates for the germane and silane precursors were 10 and 2-8 standard cubic centimeters per minute (sccm). The argon was used as a carrier gas with a flow rate of 25 sccm. SiGe samples were first characterized using Raman spectroscopy to explore the material crystallinity. The typical sample was grown at 600°C with flow rates of 10 and 4 sccm for the germane and silane precursors. The Raman shift shows the Ge-Ge (LO) phonon at 297 cm^{-1} from the Ge-Ge LO phonon peak of 300 cm^{-1} for the film. A peak attributed to the Si-Ge LO phonon is observed at 396 cm^{-1} . The narrow width of the Ge-Ge mode peak of the Raman spectroscopy plot shows that the material has high crystallinity. The spectroscopic ellipsometry was used to investigate the absorption properties and thickness of samples. The absorption cutoff wavelength is $\sim 1050 \text{ nm}$. The growth rate for the film remained $\sim 70 \text{ nm/min}$ with total thickness of a 750 nm. High-resolution X-ray diffraction (HRXRD) was used to further investigate the material quality and optimize growth recipes. The peak position is 27.44 degree. The rocking curve plots of the $2\theta - \omega$ scans were fitted using Gaussian methods. The d-spacing and lattice constant were calculated using Bragg's Law with values of 3.24 and 5.624 Å, respectively. After that, Vegard's law was used to determine the mole fraction of Si. The calculated mole fraction of incorporated Si was 0.13. In conclusion, the SiGe is grown using commercial gas precursors using a CVD system. The material characterization shows that crystalline growth is achieved. The details of the results will be presented at the conference.

2:10 PM K02

A Growth Model Leading to Larger-Area, High-Quality, Laterally Grown Ge Films on Si Weizhen Wang and Nate Quitoriano; McGill University, Montreal, Quebec, Canada.

We have recently reported a new relaxation mechanism grown Ge thin films on Si using a metal-catalyzed, lateral growth technique at 380 °C in microfabricated, micro-crucibles. There were two surprising results; first, the films are fully relaxed, despite the low growth temperature and, second, the cross-sectional transmission electron micrographs suggest high-quality (low threading dislocation density) films. Standard planar growth of Ge on Si involves the nucleation and glide of dislocations to relax the 4% lattice mismatch between the two materials; the nucleation of dislocations implies highly defective films, which is why the high-quality state of the lateral films is surprising. Dislocation glide is a thermally activated process and so, at these low temperatures, it would be greatly impeded and should result in a strained film, which is why the fully relaxed nature of our laterally grown Ge on Si is surprising. In this work, we discuss the growth evolution of the films, with varying Au catalyst size, flow rate and growth time and develop a model to understand and predict the size of the Ge films. Using this understanding, we were able to engineer larger-area, laterally grown films through variations in growth time as well as micro-crucible geometry.

2:30 PM K03

(Student) Progress Towards B-III-V Optoelectronic Devices on Silicon
Kyle M. McNicholas¹, Rasha El-Jaroudi², Jan Kopaczek³, Andrew Jones⁴, Daniel J. Ironside⁵, Robert Kudrawiec³, Joe Campbell⁴ and Seth Bank¹;
¹Microelectronics Research Center and Department of Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas, United States; ²Electrical Engineering, University of Texas at Austin, Austin, Texas, United States; ³Institute of Physics, Wroclaw University of Science and Technology, Wroclaw, Poland; ⁴Department of Electrical and Computer Engineering, The University of Virginia, Charlottesville, Virginia, United States; ⁵University of Texas at Austin, Austin, Texas, United States.

Highly-mismatched semiconductor alloys, in which the constituent elements have substantial differences in size and/or electronegativity, have been broadly pursued to capitalize on the significant changes in both the band structure and crystal lattice. The disparity in size/electronegativity of the constituent elements often substantially increases the alloy enthalpy of mixing, typically limiting the stable composition range to only dilute concentrations. We recently reported progress on the growth of highly-mismatched BGaAs alloys and showed that B concentrations large enough to enable coherent growth of direct-gap BGaAs on Si can be accessed using a highly kinetically-limited growth regime,¹ potentially enabling a new approach to the incorporation of direct bandgap optoelectronic devices on Si. However, because of the traditional challenges in the growth of boron-containing alloys, many fundamental properties necessary for the integration of these materials with optoelectronic devices remain unexplored. For example, there are few reports addressing reliable dopant activation and the electrical properties of these materials; a precise understanding the effects of B composition on the alloy band structure remains to be experimentally verified; and virtually no investigations of heterojunction band alignments have been performed. Our efforts here aim to address these issues through continued investigation of the growth and properties of BGa(In)As. In the dilute B regime, we demonstrate for the first time, both n and p-type doping of BGaAs alloys using Te and Be, respectively, enabling the first BGaAs p-n and p-i-n junction devices. Outside the dilute regime, we present our continued efforts to improve the growth of BGa(In)As on GaP and GaP-on-Si templates and probe the optical properties of these materials. BGaAs and BGaInAs films with thicknesses ranging from 30 to 1000 nm were grown on (100) oriented GaAs, GaP, and GaP-on-Si substrates by solid-source molecular beam epitaxy. Hall measurements in the van der Pauw configuration show that Be readily incorporates as an active p-type with measured hole concentrations ranging from $\sim 2 \times 10^{16}$ to 1×10^{18} cm⁻³ and corresponding hole mobility ranging from 178 to 114 cm²/V-s. We observed no evidence of n-type conductivity in Si-doped BGaAs, however, we found that Te readily incorporates as an active n-type dopant in BGaAs, with measured electron concentrations ranging from $\sim 1 \times 10^{18}$ to 6×10^{18} and corresponding electron mobility ranging from 1313 to 683 cm²/V-s. At fixed Te doping levels of $\sim 5 \times 10^{18}$ cm⁻³, a significant decrease in electron mobility was observed as the B concentration was increased, with the electron mobility decreasing from 1991 cm²/V-s at 0% B to 617 cm²/V-s at 2.7% B. It is unclear if the decreased mobility is the result of defect scattering, alloy disorder, or distortion of the conduction band edge predicted to arise through interactions with isolated and clustered B states in BGaAs.² Homojunction BGaAs p-n and p-i-n diodes exhibited rectifying behavior and photoresponse measurements show an apparent blue shift in cut off wavelength with increasing B, consistent with our previous observations.¹ Efforts are underway to further characterize the photoresponse and emission of these devices, as well as to translate to GaP and GaP-on-Si substrates; progress towards these goals will be reported at the conference. This work was supported by the National Science Foundation (ECCS-1838984) and performed at the National Science Foundation supported Texas Nanofabrication Facility (NNCI award 1542159). [1] McNicholas et al., Electronic Materials Conference (2018) [2] Lindsay and O'Reilly, Phys. Stat. Sol. 5 (2008)

2:50 PM K04

CBRAM Based on Single Crystalline Si Thin-Films Grown by Solid Phase Epitaxy Inho Kim; Korea Institute of Science and Technology, Seoul, Korea (the Republic of).

Low dimensional defects such as dislocation in single crystal Si serve as fast diffusion path of Ag ions. Recently, efforts have been made to employ dislocations in single crystal based oxide and silicon as reliable Ag filaments in CBRAM (Conductive Bridging Random Access Memory). Conductive Ag filaments are reported to be well confined in one dimensional dislocation defects in nanometer scale and exhibit promising device performances in terms of retention time, endurance, linearity and on/off ratio. However, there has been a rare study of controlling the

location of the low dimensional defect formation, which is a key factor to device production. In this study, we performed research to create the low dimensional defects on the active region of the epitaxially grown Si thin films for CBRAM by our proposed approach. The single crystal Si thin films were grown by solid phase epitaxy. We fabricated CBRAM devices by sandwiching the epitaxial Si thin films between the active metal of Ag and highly conductive Si substrate. We investigated the device performance of CBRAM including intentionally controlled defects in the epitaxial Si thin films and discuss the effect of the low dimensional defects on the resistive memory device performances. Furthermore, we performed the feasibility study on the use of the epitaxial Si based CBRAM for artificial synapse for neuromorphic computing. The fundamental device parameters of the epitaxial Si CBRAM were extracted, and we propose the future research direction to optimize the device parameters for the artificial synaptic device applications.

3:10 PM REFRESHMENT BREAK

SESSION L: Epitaxial Devices Session Chairs: Charles Lutz and Kunal Mukherjee Wednesday Afternoon, June 26, 2019 Michigan League, 3rd Floor, Koessler

3:30 PM L01

High-Mobility (> 700 cm²/V-s) Helical Tellurium Field Effect Transistors Enabled by Transfer-Free, Low-Temperature (120 °C) Direct Growth Guanyu Zhou¹, Rafik Addou¹, Qingxiao Wang¹, Shahin Honari¹, Chris Cormier¹, Lanxia Cheng¹, Ruoyu Yue¹, Christopher Smyth¹, Akash Laturia¹, Jiyoung Kim¹, William G. Vandenberghe¹, Moon J. Kim¹, Robert Wallace¹ and Chris Hinkle^{2,1}; ¹Materials Science and Engineering, University of Texas at Dallas, Dallas, Texas, United States; ²Department of Electrical Engineering, University of Notre Dame, Notre Dame, Indiana, United States.

The realization of high-performance semiconductor devices directly grown and processed at low temperatures would greatly impact future electronic technologies and applications. For example, 3D vertical monolithic integration is strictly limited by the thermal budget (< 450 °C) imposed to safeguard the underlying metal interconnects or devices. Flexible electronics fabrication processing needs to remain below 200 °C to protect commonly used polymers. As a result, materials for flexible electronics typically have very low carrier mobilities, limiting the prospects for high-performance flexible technologies like wearable electronics and bendable displays. We find a promising avenue to achieve high-mobility, low-temperature grown semiconductors in tellurium (Te), whose crystalline structure contains atoms that are covalently bonded into a 1D helical chain, and the 1D chains are van der Waals (vdW) bonded into a hexagonal lattice. The vdW interaction allows high-quality crystal growth at much lower temperatures than for semiconductors with covalent interactions. Te has thickness tunable bandgaps, from 0.33 eV for "bulk" films increasing to 1.4 eV for a 2D monolayer. We carried out the Te growth in an MBE system, and have realized high quality Te film growth on a wide range of technologically relevant substrates, e.g., SiO₂/Si, PET, ALD-HfO₂, GaN, Al₂O₃ and SiC. At the growth temperature of 120 °C, the Te growth on all substrates exhibits the form of compact, needle-like structures. The advantage of transfer-free direct growth of Te nanostructures is demonstrated by the back-gate FETs that were fabricated using Te needle-like structures directly grown on SiO₂/Si at 120 °C. The room-temperature I_D-V_G curve of the FET exhibits excellent hole conduction. The field-effect mobility was extracted using $\mu_{FE} = L / (WV_D C_G) (\partial I_D / \partial V_G)$, giving a room-temperature mobility of 707 cm²/V-s. The temperature dependent mobility over 170 K can be fitted by a T^{-α} power law, indicating the mobility is phonon limited. This Te device performance is significantly higher than other low-temperature grown materials such as poly-Si and ZnO. This performance is also much higher than or comparable to other synthetic vdW materials like MoS₂ or black phosphorus on SiO₂/Si, with Te having the significant advantage of utilizing a low-temperature, scalable growth technique, compatible with heterogeneous 3D integration and flexible devices. The transfer-free direct growth avoids the device degradation that occurs from the transfer process. For comparison, we fabricated FETs out of Te needle-like structures grown at 120 °C on HOPG and then transferred them to SiO₂/Si. The best device exhibited a mobility of 420 cm²/V-s, which is significantly degraded relative to the transfer-free device. We also demonstrate FETs made out of Te films grown at 20 °C on HOPG and transferred to SiO₂/Si, exhibited a mobility of only 41 cm²/V-s, that was unchanged as a function

of measurement-temperature, indicating a likely grain boundary scattering mechanism. The mobility difference between the Te films grown at different temperatures can be explained by differences in the morphology of the thin films. AFM and RHEED images reveal that, as the growth temperature is increased from -70 to 120 °C, the Te films evolve from in-plane textured sheet-like structures to needle-like single crystals. STEM of the Te films grown at -70 °C and 120 °C clearly reveal the same hexagonal, helical atomic structure within a given grain for all of the samples. Therefore, the low mobility for the Te sheet-like structures grown at 20 °C is indeed caused by grain boundary scattering from the criss-cross morphology (Fig. 2b). In conclusion, we achieved a room temperature hole field effect mobility of 707 cm²/V-s using transfer-free, low-temperature direct growth of Te needle-like structures on SiO₂/Si. Helical Te nanostructures offer a promising route forward for low temperature fabrication of high-mobility FETs.

3:50 PM L02

(Student) Epitaxial Regrowth for Photonic Crystal Surface Emitting Lasers (PCSELS) Kevin J. Reilly¹, Sadvikas J. Addamane⁴, Connor Dix¹, Seuongwon Yeom³, Akhil Kalapala³, Ganesh Balakrishnan² and Weidong Zhou³; ¹Center for High Technology Materials, The University of New Mexico, Albuquerque, New Mexico, United States; ²University of New Mexico, Albuquerque, New Mexico, United States; ³Department of Electrical Engineering, The University of Texas at Arlington, Arlington, Texas, United States; ⁴Center for High Technology Materials, University of New Mexico, Albuquerque, New Mexico, United States.

Molecular beam epitaxy (MBE) regrowth is investigated as a fabrication method for photonic crystal surface emitting lasers (PCSELS). We demonstrate an edge emitting laser operating at the design wavelength and identify an appropriate substrate cleaning method to use before regrowth. Lastly, electron beam lithography (EBL) exposure dose is varied to obtain a desired photonic crystal (PhC) dimension post-regrowth. Surface emission from semiconductor lasers offers advantages of 2D integration, freedom from catastrophic optical damage, and narrow circular beam shapes. Still, edge emitting lasers (EELs) dominate high power applications since it is challenging to realize single mode emission from high power surface emitting lasers (SELs). PCSELS produce high power single mode output by employment of a 2D PhC resonant cavity embedded within an EEL device structure. The PhC isolates a single optical mode and diffracts it vertically, thereby enabling high power coherent lasing in-line with the growth direction. Additionally, because of the variability afforded in PhC design, PCSELS promise a host of other functionalities not easily attained by other types of lasers, such as on-chip control of beam shape, direction, and polarization. The described MBE regrowth begins with an initial growth containing a bottom cladding layer, active region, and PhC region. In a second step, the PhC layer is patterned by EBL and reactive-ion etch. Lastly, the patterned surface is regrown with top cladding and a top contact layer. Initial efforts have been directed towards the fabrication of PCSELS with a mature active region technology, specifically 980 nm InGaAs quantum wells (QW), so that focus can be placed on laser cavity design and thermal engineering related issues. These advances will later be translated to an ultimate objective, the development of mid-wavelength infrared devices. The 980 nm laser design consists of an In_{0.15}Ga_{0.85}As QW active region, Al_{0.38}Ga_{0.62}As cladding layers and Al_{0.25}Ga_{0.75}As waveguides on a GaAs substrate. The growth is carried out using MBE on a Semicon VGV80H reactor and devices are fabricated into dimensions of 100µm x 1mm. The PhC region is part semiconductor and part void. GaAs substrates are patterned by EBL and reactive ion etch and the subsequent regrowth creates pockets of air beneath the surface. The design dimensions, determined by 3D coupled wave theory simulations, dictate a radius of 66 nm, a depth of 304 nm (after regrowth), and a lattice constant of 292 nm for a 980nm emission wavelength. PhC quality is dependent on cleaning and oxide removal before regrowth. To identify a successful cleaning method, multiple techniques were explored including: (1) in-situ oxide desorption at 610°C for 20 mins, (2) a HF dip followed by oxide desorption at 610°C for 20 mins, (3) a H₂SO₄ (95%) soak for 5 min and a thermal cleaning at 550°C for 20 mins. The third cleaning technique (H₂SO₄) produced regrowths with the most uniform hole shape and minimal surface defects. To achieve PhCs of proper dimension, a single pattern was written several times over a range of EBL exposure doses and cross-sectional images were analyzed post regrowth. Future experiments will investigate the variation of hole shape via regrowth controls. Interrupting PhC hole symmetry, either in-plane or about the z-axis, has been shown to benefit PCSEL efficiencies. There are two primary ways that MBE regrowth can be used to introduce variation in hole symmetry, namely tilt and taper. PhC feature shape in early PCSELS, fabricated by wafer bonding, could be influenced only through the initial patterning. By implementation of epitaxial regrowth, tilt and taper can be effectively influenced with purposeful manipulation of growth rates,

overpressures, MBE irradiation direction, and relative crystal orientation. This work was supported by the High Energy Laser Joint Technology Office (HEL-JTO). Contract number: N00014-17-1-2557

4:10 PM L03

Etch and Surface Passivation Study of AlSb Diodes Grown on GaSb Substrates Emma J. Renteria¹, Sadvikas J. Addamane¹, Eduardo Padilla^{2,3}, Adam A. Hecht², Ganesh Balakrishnan¹, John Klem³, Anthony Rice³, Gregory W. Pickrell³ and Paul Sharps³; ¹Center for High Technology Materials, University of New Mexico, Albuquerque, New Mexico, United States; ²Department of Nuclear Engineering, The University of New Mexico, Albuquerque, New Mexico, United States; ³Sandia National Laboratories, Albuquerque, New Mexico, United States.

Common detectors for gamma radiation are sodium-iodide (NaI) scintillators, or semiconductor devices of either germanium (Ge) or cadmium-zinc-telluride (CZT). However, most of these detectors do not exhibit optimal performance and suffer one or more shortcomings including cooled operation, lower energy resolution, poor spectral performance, reduced photopeak efficiency and limitations in detector size. Aluminum antimonide (AlSb) has been identified as a promising candidate for high resolution, room temperature gamma detection due to its wide energy bandgap, high carrier mobilities and high atomic number. Nonetheless, the use of AlSb for the fabrication of gamma detectors has been limited by the difficulties of growing bulk AlSb in single crystal form with low enough defect levels for gamma-ray detection. Traditional bulk crystal growth techniques are not effective for the growth of bulk AlSb due to the rapid oxidation of aluminum, high volatility of antimony, and the reaction of molten AlSb with most crucible materials. Although still challenging, epitaxial growth is a more promising technique to grow high quality AlSb materials. The biggest limitation of epitaxial growth is the achievable thickness of the deposited layer. After growth and fabrication of AlSb detectors, the rapid oxidation of aluminum once again becomes a problem since the AlSb sidewalls are exposed to air when the devices are electrically isolated by mesa etch. The conductive oxides and dangling bonds on the sidewalls allow high leakage currents which in turn affects the detection of radiation. In this work, we investigated the effect of etching and passivation of etched mesa sidewalls on the electrical behavior of AlSb detectors. The AlSb detector is a 3 µm thick p-n diode grown on a (001) GaSb substrate using molecular beam epitaxy. After top and bottom contacts are deposited, the samples are patterned for mesa etch. Mesa etch is done either by dry-etch using an inductively coupled plasma reactor with BCl₃ gas or by wet-etch using a solution of HF:H₂O₂:H₂O with a ratio of 2:1:20. Then, after current-voltage measurements are performed, the samples are passivated with an ammonium sulfide treatment and re-measured again. Before passivation, devices isolated by dry-etch show approximately 2 orders of magnitude lower dark current density than devices isolated by wet etch. However, after passivation, devices isolated by wet-etch showed equal or better performance than dry-etch. Although passivation improves the performance of all devices, passivation has a greater effect on the devices isolated by wet-etch. After passivating the mesa sidewalls with ammonium sulfide, the turn on voltage of wet-etch devices increased from ~0.5 V to ~1 V, making these diodes suitable to radiation detection applications. The presentation will provide extensive characterization data including morphology characteristics of sidewalls, current-voltage measurements, and radiation response of the diodes.

4:30 PM L04

All Solution-Processed MAPbI₃ Perovskite Crystal with 2D Ruddlesden-Popper Coating for Low-Cost, High-Resolution Radiation Detectors Suneel Joglekar¹, Mark D. Hammig² and Lingjie J. Guo¹; ¹Electrical and Computer Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Nuclear Engineering & Radiological Sciences, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

Organic-inorganic hybrid perovskites, a class of intrinsic semiconductor materials known for their high mobility, low defect density, use of earth-abundant elements, and ability to be solution-processed at low temperatures have been intensively investigated, yielding optoelectronic devices with performances on par with those using far more expensive material, especially for photovoltaic (PV) cells. The composition contains heavy elements with high radiation absorption cross-sections, making perovskites also useful as the active material for both intensity-based and spectroscopic x-ray and gamma ray detectors. However, inter-device variability and long-term stability of perovskite devices are major drawbacks, especially for spectroscopic gamma ray detectors. Using methylammonium lead iodide perovskite single crystals (PSCs) grown using solution-based inverse temperature crystallization, we demonstrated a facile, solution-based post-processing method to coat the bulk perovskite

crystal with a layer of a 2D Ruddlesden-Popper (R-P) hybrid perovskite, passivating the MAPbI₃ crystal surface and increasing the carrier lifetime by over 55% by reducing the density of near-surface trap states. The passivated MAPbI₃ surface and higher-bandgap R-P surface coating greatly improved the device yield and consistency of perovskite room-temperature gamma ray detectors. When using a combination of a R-P surface treatment and large-area conformal metal contacts, the average energy resolution for the 81 keV peak from a ¹³³Ba source is improved from 39.9 % to 24.9 %. Furthermore, the yield (percentage of measured PSCs with a distinct gamma peak or peak edge) improved from 43.8 % to 100 %, and the repeatability was greatly improved, with the standard deviation dropping from 22.6 % to just 6.58 % energy resolution. In this study, we demonstrate not only the highest energy resolution from all solution-grown perovskite gamma ray detectors, but also one of the first extensive investigations into inter-device variability, greatly improving upon previously-reported results. In addition to improving the energy resolution of perovskite-based gamma ray detectors, to under 15 % (12.0 keV) for 81 keV gamma rays, this solution-based technique could pave the way for low-cost, scalable perovskite surface passivation for improvement of other perovskite-based semiconductor devices.

4:50 PM L05

Epitaxial AlAsSb for Spectroscopic Gamma Detectors John Klem¹, Jin Kim¹, Gregory W. Pickrell¹, Anna Tauke-Pedretti¹, Michael Wood¹, Quinn Looker¹, Donald Bethke¹, Eduardo Padilla¹ and Preston Webster²; ¹Sandia National Laboratories, Albuquerque, New Mexico, United States; ²Air Force Research Laboratory, Albuquerque, New Mexico, United States.

AlSb has potential advantages relative to current state-of-the-art materials as a charge-based detector for spectroscopic gamma radiation measurement. Relative to high-purity Ge, AlSb has both higher effective atomic number and bandgap energy, which should reduce the required detector volume and increase the allowable operation temperature. In contrast to CdZnTe, AlSb has improved electron/hole mobility symmetry, which may allow dual-carrier transport that will improve gamma energy resolution. Bulk growth of AlSb has been proposed and attempted as a route toward detector realization, but the highly reactive nature of this material makes synthesis, fabrication, and characterization of detectors difficult. In contrast, epitaxial growth allows for effective in-situ encapsulation to avoid oxidation, and additionally allows examination of similar ternary and quaternary alloys. The low carrier concentration, high mobilities, and long lifetimes that this material system may provide are essential to detector performance. In this work, we have grown and characterized thick, lattice-matched AlAsSb grown by molecular beam epitaxy on GaSb substrates, and demonstrated a technique for fabricating heterostructure diodes while avoiding oxidation by using epitaxial surface passivation. Heterostructure diodes were characterized using capacitance-voltage measurements to relate AlAsSb net dopant concentrations to beryllium doping levels. Beryllium-doped AlAsSb structures with net dopant densities of $1\text{-}5 \times 10^{15} \text{ cm}^{-3}$ were obtained, tracking the intended beryllium doping concentrations and thereby demonstrating net acceptor behavior. Unintentionally doped AlAsSb exhibited a net doping concentration of less than $1 \times 10^{15} \text{ cm}^{-3}$. Diodes with AlAsSb absorber layer thicknesses of up to 10 microns exhibited AlAsSb x-ray rocking curve full-width half-maxima of 30 arcseconds and crosshatch-free surface morphologies, demonstrating excellent composition and strain control. Characteristics of bipolar heterostructure diodes with GaSb surface passivation were measured near room temperature. Diodes with unintentionally doped AlAsSb showed net doping concentrations near $5 \times 10^{14} \text{ cm}^{-3}$, with depletion widths of 4 microns at an applied bias of 5 V. Devices showed strongly asymmetric current-voltage characteristics typical of p-n diodes. Although reverse-bias leakage current was voltage dependent, there was no apparent breakdown for reverse bias as high as 100 V. At zero bias, AlAsSb diodes with 10-micron absorber layers displayed a 17.5 keV x-ray responsivity similar to a reference Si diode with a fully depleted 25-micron absorber. Further improvements to the epitaxial design should reduce reverse leakage current, allowing demonstration of improved responsivity with significant reverse bias. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

SESSION M: Characterization of Defects and Interfaces Session Chairs: Geoffrey Foster and James Gallagher Wednesday Afternoon, June 26, 2019 Rackham Building, 4th Floor, Amphitheatre

1:30 PM M01

Atom Probe Tomography Study of Dopant and Impurity Distributions Near Planar and Non-Planar GaN Homo Junctions Alexander Chang¹, Mohsen Nami², Bingjun Li², Jung Han² and Lincoln Lauhon¹; ¹Northwestern University, Evanston, Illinois, United States; ²Yale University, New Haven, Connecticut, United States.

Beyond its successful implementation in lighting and RF applications, GaN is promising for the next generation of power devices. Fast switching with low energy loss can be realized through nonplanar vertical diode structures with active regions formed by selective area etching and regrowth. To maximize breakdown voltage and minimize leakage current, it is essential to minimize impurity incorporation and precisely control dopant distribution in the active region. During selective area growth, different facets evolve with different growth velocities and impurity incorporation rates. Thus, tomographic analysis with high spatial resolution and chemical sensitivity becomes necessary to characterize dilute species near non-planar interfaces. We describe atom probe tomography (APT) characterization of planar and non-planar p⁺/n-GaN structures, with emphasis on detection sensitivity of intentional and unintentional impurities. GaN homo junctions were grown by metal-organic chemical vapor deposition at Yale University and analyzed using APT at Northwestern University. For planar structures, n-GaN templates were exposed to air prior to the regrowth of p-GaN, and secondary ion mass spectroscopy (SIMS) measurements were utilized to calibrate the APT detection sensitivity. Although SIMS result revealed spatially localized Si contamination (atomic surface density of 10^{12} cm^{-2}) near the regrowth interface, detection of Si in GaN using APT was limited due to the overlapping ²⁸Si⁺ and ¹⁴N₂⁺ mass to charge ratios. The APT detection limit of Mg dopants varied from $0.5 \times 10^{18} \text{ cm}^{-3}$ to $2 \times 10^{18} \text{ cm}^{-3}$, depending on the specimen geometry and APT run conditions. The APT detection limits of C and O impurities were typically $5.0 \times 10^{18} \text{ cm}^{-3}$ and $1.0 \times 10^{19} \text{ cm}^{-3}$, respectively. To investigate the Mg dopant distribution after thermal activation, continuously grown planar p⁺/n-GaN diodes were thermally annealed at 800 °C and 820 °C. Clustering analyses were performed on reconstructed APT data from annealed samples as well as as-grown sample described above, which was exposed to air before p-GaN regrowth. Although carbon contamination may complicate the clustering analysis due to the overlapping peaks of ¹²C⁺ and ²⁴Mg⁺⁺ ions, SIMS measurement on all samples indicate C levels less than $2 \times 10^{16} \text{ cm}^{-3}$, which is below the detection limit of Mg dopants. Our clustering analyses on 820 °C annealed sample suggest formation of limited number of small Mg clusters (< 2nm) during dopant activation process. On the other hand, random Mg distribution was observed in as-grown sample and 800 °C annealed sample. Furthermore, we discuss our efforts to extract the built-in field near planar p/n junctions correlated to dopant distribution using spatial variations in charge states of evaporated Ga ions, a proxy to surface electric field. For non-planar structures, p⁺-GaN was regrown on n-GaN trenches approximately 10 μm wide and 300 nm deep. The trenches were oriented parallel either to the a-axis or m-axis of the hexagonal crystal structure. During selective area regrowth, five to seven ~3 nm thick (6ML) Al_{0.05}Ga_{0.95}N layers were grown, evenly distributed temporally, as marker layers to trace the regrowth facet evolution. APT specimens were fabricated from lateral p/n junctions along either a-axis or m-axis. We report the 3D impurity distributions near non-planar homo junctions, as well as the facet-dependent impurity incorporation and growth rates.

1:50 PM M02

(Student) Neutron and Gamma Radiation of Gallium Nitride with Varying Growth Orientations Sam C. Sprawls¹, Joshua Gallagher², Farnood Mirkhosravi³, Matthew Durbin³, Azaree Lintereur², Daniel Feezell³, Michael Scarpulla¹ and Emily Mace⁴; ¹Materials Science and Engineering, University of Utah, Salt Lake City, Utah, United States; ²Nuclear Engineering, The Pennsylvania State University, State College, Pennsylvania, United States; ³University of New Mexico, Albuquerque, New Mexico, United States; ⁴Pacific Northwest National Laboratory, Benton County, Washington, United States.

Gallium nitride has great potential in radiation-hard high-power electronic devices due to its wide bandgap and strong atomic bonding. However, still little is known on how GaN's growth direction affects radiation damage.

This study aims to understand how growth direction affects where damage occurs in GaN electronic devices. We grew GaN in three orientations: nitrogen face, gallium face, and m-plane non-polar. The N face was grown on sapphire, while the m-plane nonpolar was grown on free standing GaN, and the Ga face was grown on both substrates. To make PN junctions, organometallic vapor phase epitaxy (OMVPE) film growth was used with silicon as our n-type dopant and magnesium as our p-type dopant. N-contacts are composed of gold over nickel, while p-contacts are gold over palladium. A photolithography and a wet chemical etch were used to create PN diodes and circular transmission line measurements (CTLMS). Samples were irradiated at Penn State University using their TRIGA neutron reactor. Samples received doses of 10E14, 10E15 and 10E16 neutrons per cm². A control sample was also kept to ensure that damage was not due to degradation over time. We analyzed the diodes behavior by calculating the turn-on voltage of 12 irradiated diodes from each radiation dose. The turn-on voltage was calculated by extrapolating the current versus voltage (IV) curve to the x-axis once the IV curve transitioned from exponential to linear behavior. A change in turn-on voltage indicates the radiation damage has affected the overall device performance. We analyzed 3 N-type and 3 P-type CTLM sets from each radiation dose. Using the CTLMS, we were able to calculate the resistivity of P and N-type GaN as well as specific contact resistance for each sample. This locates where damage is occurring in our PN diodes. We observed a large increase in diode turn-on voltage for devices that had been irradiated to 10E16 neutrons per cm² (n/cm²). We believe this change in turn-on voltage is due to voltage being dropped over an increased series resistance in the device. To understand where the voltage drop was occurring, we found the change in resistivity of the bulk P-type and N-type GaN, and the change in the specific contact resistance. We measured this using our CTLMS, finding both the nitrogen and gallium face orientation increased in P-type resistivity below an order of magnitude from 10E14 to 10E15 n/cm². However, the N-type GaN resistivity and specific contact resistance increased by over an order for the nitrogen face orientation while the gallium face did not show a large difference between 10E14 to 10E15 n/cm². We will be examining the 10E16 n/cm² radiation dose in the coming weeks. From these initial results, it appears that the gallium face orientation is resistant to increases in device resistance compared to the nitrogen orientation mainly due to N-type resistivity and specific contact resistance showing less change. To understand what defects the neutron radiation damage is creating in our samples, we will be examining the Ga face and N face samples grown on sapphire using a transmission electron microscope (TEM). By comparing the 10E16 n/cm² dosed samples to the control samples, we hope to understand changes in the crystal structure due to neutron radiation damage. We will also be making photocapacitance measurements of our samples to verify the defects we see in the crystal structure from our TEM analysis are not an anomaly that is only found on the atomic scale, but are consistent throughout the electronic devices and are the reason for the increase in turn-on voltage.

2:10 PM M03

(Student) Properties of Oxide Reconstructions in AlN and GaN Kelsey J. Mirrieles¹, Joseph H. Dycus^{1,2}, Jonathon N. Baker¹, Joshua Harris¹, Pramod Reddy³, Ramón Collazo¹, Zlatko Sitar^{1,3}, James LeBeau¹ and Douglas L. Irving¹; ¹Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina, United States; ²EAG, Raleigh, North Carolina, United States; ³Adroit Materials, Inc., Raleigh, North Carolina, United States.

Properties of AlN/GaN surfaces are important for realizing the tunability of AlN/GaN devices, as the presence of surface states contribute to Fermi level pinning. This pinning can influence the performance of high electron mobility transistors (HEMTs) and are also important to passivation of the surface when developing high-power electronic devices. It is widely understood that both AlN and GaN surfaces oxidize. There are many possible reconstructions for each surface. It is therefore a challenge to identify relevant surface reconstructions in advance of detailed simulation. Because of this, different approaches are often employed to select initial structures to reduce the computational load. These approaches usually rely on either electron counting rules or oxide stoichiometry, as both of these models tend to lead to structures that are believed to be the most energetically favorable. Electron counting rule structures are believed to have a lower energy because there are sufficient electrons to fully saturate each covalent bond. In turn, oxide stoichiometry models seek structures based on the requirement that every two Al atoms must have three O atoms so as to maintain the 2/3 Al/O ratio as found in Al₂O₃. In this study, we explore models from these approaches, but also explore a reconstruction of the (0001) surface directly observed using scanning transmission electron microscopy (STEM) and supplemented with predictive density functional theory (DFT) simulations. The stability of the observed surface reconstruction is compared to these models and previous

work. This comparison is done on a relative energy scale due to the lack of inversion symmetry for this surface. Relative surface energies are calculated as a function of relevant chemical potentials. For example, the chemical potential of oxygen was extended to finite temperature and various partial pressures to explore changes in stabilities of surfaces as external conditions are varied. Furthermore, surface states are calculated directly using hybrid exchange-correlations functionals that correct for the underestimation of the bandgaps in AlN (6.1 eV) and GaN (3.5 eV) and improve the predicted positions of surface states within the gap. Additional small stoichiometry deviations from the proposed model are also explored. Based on all of these results, we propose driving forces for oxide reconstructions which fall outside the conventional oxide stoichiometry and electron counting rules, such as (0001) polarity mitigation in AlN and GaN. Additionally, surface states for selected models will be discussed and their implications to device performance will be presented.

2:30 PM M04

(Student) Effects of Forming Gas Anneal on the Structure of Al₂O₃/GaN Interface Benjamin McEwen¹, Isra Mahaboob¹, Kasey Hogan¹, Emma Rocco¹, Vincent E. Meyers¹, Sean A. Tozier¹, Aivars Lelis², Ronald Green², Franklin Nouketcha² and Fatemeh (Shadi) Shahedipour-Sandvik¹; ¹Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, Albany, New York, United States; ²U.S. Army Research Laboratory, Adelphi, Maryland, United States.

AlGaN/GaN-Based High Electron Mobility Transistors (HEMTs) have been shown to be excellent candidates for high power, high frequency switching applications due to the high breakdown field of GaN and low on-resistance. The low on-resistance is a result of the formation of a two-dimensional electron gas (2DEG) at the AlGaN/GaN interface, allowing conduction with minimal impurity scattering. One issue with conventional HEMT devices is high gate leakage current. Reduction of gate leakage has been achieved by inserting a dielectric layer between the gate and the semiconductor to create a metal-insulator-semiconductor HEMT (MISHEMT). However, device reliability issues associated with the dielectric, namely, threshold voltage (V_{th}) instability, have yet to be fully resolved [1]. In MISHEMT devices the dielectric/semiconductor interface is largely responsible for V_{th} instability as a result of a high density of interface states (D_{it}) that act as electron traps with a wide distribution of time constants [1]. Reduction of this D_{it} is the subject of ongoing research. An Al₂O₃ gate dielectric is commonly used in AlGaN/GaN MISHEMT devices. The dielectric layer is deposited via atomic layer deposition (ALD), which forms a smooth interface with GaN, even after high temperature annealing under nitrogen ambience [2]. However, it has been shown that annealing Al₂O₃ on GaN in forming gas (5% H₂/95% N₂) ambience results in lower D_{it} , compared to as-deposited and N₂-annealed Al₂O₃ on GaN [3]. While it is believed that hydrogen passivates defects at the Al₂O₃/GaN interface [3], it has not been reported how the forming gas anneal affects the structure of the materials near this interface. In this work, the effect of forming gas anneal on the Al₂O₃/GaN interface is studied using transmission electron microscopy (TEM) and energy-dispersive X-ray spectroscopy (EDS). 8 nm of Al₂O₃ was deposited using thermal ALD, with the substrate held at 300 °C. Alternating pulses of trimethylaluminum (TMA) and water were used as the Al and O precursors, respectively to grow Al₂O₃ layer-by-layer. Al₂O₃/GaN/AlGaN/GaN MISHEMTs were fabricated; the Al₂O₃ was subjected to a 750 °C N₂ anneal for 30 s, and TEM imaging shows minimal interdiffusion between the Al₂O₃ and GaN. Furthermore, EDS mapping shows that Al and O are evenly distributed in the Al₂O₃, clearly separated from the AlGaN layer by the GaN cap. These observations indicate that the Al₂O₃ is of good quality (constant composition and thickness) and uniformity. Although MISHEMT devices were fabricated and measured, a simpler device structure will more effectively associate device characteristics with dielectric/semiconductor interface. For this, Al₂O₃/GaN metal-insulator-semiconductor capacitors (MISCAPs) are being fabricated and subjected to different forming gas annealing conditions. I-V and C-V characteristics of the fabricated devices will be presented and correlation with structural and compositional differences observed in TEM/EDS mapping will be given. [1] Ostermaier, C., Lager, P., Reiner, M., & Pogany, D. (2018). Review of bias-temperature instabilities at the III-N/dielectric interface. *Microelectronics Reliability*, 82(December 2017), 62–83. [2] Chang, Y. C., Huang, M. L., Chang, Y. H., Lee, Y. J., Chiu, H. C., Kwo, J., & Hong, M. (2011). Atomic-layer-deposited Al₂O₃ and HfO₂ on GaN: A comparative study on interfaces and electrical characteristics. *Microelectronic Engineering*, 88(7), 1207–1210. [3] Long, R. D., Jackson, C. M., Yang, J., Hazeghi, A., Hitzman, C., Majety, S., ... McIntyre, P. C. (2013). Interface trap evaluation of Pd/Al₂O₃/GaN metal oxide semiconductor capacitors and the influence of near-interface hydrogen. *Applied Physics Letters*, 103(20), 2–7.

2:50 PM M05

(Student) Native Point Defects of MOCVD-Grown ZnGeN₂ and Their Substrate Dependence Micah Haseman¹, Md Rezaul Karim², Benthara Hewage Dinushi Jayatunga³, Kathleen Kash³, Hongping Zhao^{2,4}, Walter R. Lambrecht² and Leonard Brillson^{1,2}; ¹Physics, The Ohio State University, Columbus, Ohio, United States; ²Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ³Physics, Case Western Reserve University, Cleveland, Ohio, United States; ⁴Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States.

ZnGeN₂ is a member of the heterovalent ternary II-IV-nitride family now attracting increased attention worldwide. Closely related to the technologically important III-nitrides, ZnGeN₂ consists of more earth-abundant and environmentally friendly elements with potential for more versatile optoelectronic lattice matching. Key to their device application is the control of native point defects and affecting doping and carrier compensation. The identification of native point defects in ternary semiconductors such as ZnGeN₂ can be challenging. Whereas most thermodynamically stable defects in wide band gap binary semiconductors such as GaN or ZnO are cation or anion vacancies, stable defects in ternary allows may include antisites, interstitials, and their complexes. The presence of hydrogen during growth may introduce H interstitials and complexes as well. We have begun to use depth-resolved cathodoluminescence spectroscopy (DRCLS) to measure native point defect densities and their nanoscale spatial distributions at ZnGeN₂ surfaces, interfaces, and epitaxial layers versus metalorganic chemical vapor deposition growth, substrate type, and processing conditions. The defect distributions of MOCVD-grown ZnGeN₂ films on GaN, c-, and r-sapphire were studied using depth-resolved cathodoluminescence and supplemented by Monte Carlo simulations to provide excitation depths for varying incident beam energies. CL spectra of films grown on c-sapphire revealed numerous optical transitions in the 1.7-4.6 eV range and mirrored CL spectra typically seen in GaN, suggesting a similar band structure to group III nitrides. A film grown on r-sapphire, which is more closely latticed matched to ZnGeN₂ than c-sapphire, and the film grown on GaN had a high degree of uniformity in the z-direction with fewer defect centers than the c-sapphire film. We find a strong dependence of defect distribution and density on substrate type, with fewer, but more intense, emission centers in films on r-sapphire and GaN, while ZnGeN₂ grown on c-sapphire revealed a greater distribution of defects but with an order of magnitude drop in luminescence. The observations made here with DRCLS can be combined with theory to help identify the nature of these defects and develop methods to guide epitaxial growth. The authors gratefully acknowledge support from NSF grant DMR-19-00130 and DMREF 1533957.

3:10 PM REFRESHMENT BREAK

SESSION N: III-Nitride Materials and Devices
Session Chairs: W. Alan Doolittle and Christian Wetzel
Wednesday Afternoon, June 26, 2019
Rackham Building, 4th Floor, Amphitheatre

3:30 PM N01

(Student) Ultra-High Temperature Annealing of Aluminum Nitride Grown by Molecular Beam Epitaxy Eric T. Reid¹, David A. Laley², Ping Wang³ and Zetian Mi⁴; ¹Electrical and Computer Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ³University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ⁴Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

Aluminum nitride (AlN) epitaxially grown on sapphire and silicon substrates is critically important for a broad range of applications, including ultraviolet optoelectronics, high power/frequency electronics, and the emerging quantum photonics. To date, however, the quality of AlN is severely limited by the presence of large densities of dislocations, undesired impurity incorporation (e.g., carbon and oxygen) and poor current conduction. In this context, we have investigated the epitaxy and characteristics of AlN directly on sapphire and silicon substrates by utilizing ultra-high temperature (up to 1850 °C) molecular beam epitaxy (MBE). AlN epilayers were grown under slightly metal-rich conditions with a substrate temperature near 900 °C. The resulting AlN epilayers

were characterized using atomic force microscopy (AFM), scanning transmission electron microscopy (STEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), and photoluminescence spectroscopy (PL). The as-grown AlN samples exhibit relatively large dislocation densities, evidenced by the broad (102) linewidths (~1100 arcsec). We subsequently performed *in situ* high-temperature annealing of AlN/sapphire in the MBE chamber, with the annealing temperature in the range of 1400 to 1700 °C. Drastically improved quality was measured after annealing. XRD measurements show the annealing process can yield (002) linewidths of 60 arcsec, and (102) linewidths of 880 arcsec, which are significantly narrower compared to the as-grown AlN samples, suggesting much reduced dislocation densities. In addition, AFM measurements show a root mean square (RMS) roughness of 0.25 nm, indicating smooth epilayers that are ideal for fabrication of devices and waveguides. The resulting AlN epilayers grown on sapphire substrate have quality comparable or better to that grown by metal-organic chemical vapor deposition (MOCVD). Our studies have further shown that Al(Ga)N grown by MBE can exhibit significantly improved p-type conduction, due to the hydrogen-free growth environment and the minimization of carbon and oxygen impurity incorporation, compared to the conventional MOCVD process. Further studies of XRD spectra during high-temperature annealing allow us to optimize the time and temperature of the annealing cycle. Significantly, the PL emission was increased by nearly five-fold after high-temperature annealing, due to the significantly reduced defect distribution. The epitaxy of AlN on Si wafer with both Al and N polarity is currently in progress and will be reported.

3:50 PM N02

(Student) Demonstration of High Quality Aluminum Indium Nitride with High Indium Content Grown via Metal Modulated Epitaxy Zachary Engel, Evan Clinton and W. Alan Doolittle; Georgia Institute of Technology, Atlanta, Georgia, United States.

AlInN has been a topic of recent study due to its ability to be lattice matched to GaN at a composition of 18% indium, making it a strong candidate for power electronic and optoelectronic applications. An area that has been largely unexplored thus far is the application of AlInN towards photovoltaic applications. AlInN has a tunable bandgap range from 0.7 to 6.1 eV spanning from the infrared to the ultraviolet range. More specifically at a composition of about 70% indium AlInN has a bandgap of 1.7 eV, making it perfect for tandem solar cells with silicon. Many challenges exist with the growth of AlInN. As a result of the large lattice parameter mismatch between the binaries AlN and InN a large miscibility gap exists for the ternary. In addition, the growth regimes of InN and AlN are significantly different in MBE. At the low temperatures required for the growth of AlInN the aluminum adatoms have a low mobility, often leading to lateral phase separation in the film. Metal Modulated Epitaxy offers a good solution to the growth issues of AlInN. This flux modulated technique allows for growth to initiate and proceed under metal rich conditions which increases surface diffusion lengths of the Aluminum even at low temperatures while limiting droplet formation and terminating in a dry surface. For comparison ~100 nm thick high indium content AlInN samples were grown using traditional nitrogen rich (0.8 III/V ratio) MBE and MME using a III/V ratio of 1.3 with a dose designed to prevent surface segregation (details supplied at the conference). Both films were grown cold at 375 degrees C to limit phase separation. The 100 nm MME AlInN showed high crystal quality in XRD with a FWHM of 184 arcsec for the (0002) reflection, a FWHM of 1421 for the (105) reflection, and a composition of 73% indium, as well as AFM surface roughness of 0.882 nm rms. The composition of the 110 nm MBE sample was found to be 72% indium with the FWHM of the (0002) AlInN peak being 783 arcsec and the FWHM of the (105) peak being 2456 arcsec. The AFM surface roughness of this sample was found to be 1.52 nm. The MME technique produced higher quality material of similar composition compared to the traditional nitrogen rich growth method. The sample grown via MME displays lower XRD peak widths, indicating a higher degree of crystallinity than the non-modulated, nitrogen rich growth method as well as a smoother surface morphology in AFM. Optical and electrical results will be presented at the conference.

4:10 PM N03

Strain-Balanced Nonpolar InGaN/AlGaIn Heterostructures for Infrared Intersubband Devices Alexander Senichev, Brandon Dzuba, Trang Nguyen, Yang Cao, Rosa Diaz, Michael Manfra and Oana Malis; Purdue University, West Lafayette, Indiana, United States.

The III-Nitride materials have the potential to enable novel intersubband devices for modulation, emission, and detection of light in the near-infrared and far-infrared ranges. The material properties of the III-nitride system essential for practical applications were extensively studied in the

past for polar c-plane orientations due to the availability of high-quality GaN substrates. However, growth on polar orientations of GaN introduces fundamental design limits related to built-in polarization fields. The fabrication of nitride heterostructures on semipolar and nonpolar GaN planes reduces or eliminates the built-in polarization fields leading to simplified design of intersubband devices, enhanced accessible spectral range, reduced distortion of electronic wavefunctions and increased confinement for high energy states. Previously, we have demonstrated terahertz intersubband absorption in non-polar m-plane AlGaIn/GaN superlattices [1]. However, the development of nonpolar m-plane intersubband devices in a broad spectral range has been hampered by challenges to grow high Al-composition AlGaIn on m-plane GaN [2]. Moreover, the lattice mismatch between GaN and AlGaIn limits the total thickness attainable in intersubband devices before the structure relaxes introducing dislocations and defects. To expand the spectral range of nonpolar nitride heterostructures and mitigate the impact of lattice mismatch, we studied InGaIn/AlGaIn superlattices grown by plasma-assisted molecular beam epitaxy on nonpolar GaN (1-100). InGaIn quantum wells provide an additional degree of freedom to tune intersubband transitions to the near-infrared region without increasing the Al-composition in AlGaIn barriers. Moreover, the combination of InGaIn and AlGaIn layers having opposite strain sign in a single superlattice period can effectively alleviate strain issues in infrared heterostructures [3]. The vastly different optimal growth temperatures for Al- and In-containing alloys limit the growth of InGaIn/AlGaIn heterostructures. The thermal InN decomposition at growth temperatures required for AlGaIn alloys substantially reduces the indium incorporation into InGaIn. In an attempt to provide a descriptive model, we studied indium incorporation as a function of the growth temperature in m-plane InGaIn layers grown under effectively indium-rich conditions. We found that indium incorporation can be well described by an Arrhenius dependence of InN decomposition at high temperatures, and low indium compositions. At lower growth temperature, deviation of indium incorporation from this dependence was associated with gradual deterioration of the surface morphology. The m-plane InGaIn layers with indium composition up to 20% grown under effectively indium-rich conditions show smooth morphology with low RMS roughness comparable with low-temperature GaN. Subsequently, a strain-balanced InGaIn/AlGaIn superlattice structure was designed and grown. The XRD analysis shows the thickness and composition of quantum wells and barriers in close agreement with the structure design. The well-pronounced thickness fringes indicate exceptional layer thickness uniformity and low interface roughness. The low-temperature photoluminescence has a narrow bandwidth that supports the expected low density of strain-related dislocations. InGaIn/AlGaIn superlattices with Si-doped barriers were designed and grown to reveal the impact of growth conditions, structural properties, and doping scheme on near-infrared intersubband absorption properties. The measured near-infrared intersubband absorption spectra will also be discussed. We acknowledge support from the National Science Foundation (NSF award DMR-1610893). AS and BD were supported from NSF award ECCS-1607173. TN, YC, and OM acknowledge partial support from NSF grant ECCS-1253720. [1] C. Edmunds et al., *Appl. Phys. Lett.* 105, 021109 (2014) [2] T. Nguyen et al., *Phys. Status Solidi* 215, 1700828 (2018) [3] M. N. Fireman et al., *J. Appl. Phys.* 122, 075105 (2017)

4:30 PM N04

Epitaxial Growth and Optically Pumped Stimulated Emission in AlGaIn/InGaIn Ultraviolet Multi-Quantum-Well Structures [Ping Chen](#), Youngjae Park, Yuh-Shiuan Liu, Theeradetch Detchprohm, P. Douglas Yoder, Shyh-Chiang Shen and Russell Dupuis; Georgia Institute of Technology, Atlanta, Georgia, United States.

A series of AlGaIn/InGaIn ultraviolet (UV) multiple quantum wells (MQWs) were grown in a metalorganic chemical vapor deposition (MOCVD) system, and their performance under optically pumped stimulated emission were experimentally investigated. During the MOCVD epitaxial growth of the AlGaIn/InGaIn MQWs, the ramping rate from a lower temperature for InGaIn quantum wells (QWs) to a higher one for AlGaIn quantum barriers (QBs) was intentionally changed from 1.0 degree/s to 4.0 degree/s. Atomic force microscopy (AFM) images showed that AlGaIn QBs have a smooth surface with clear step flow patterns. The surface morphology of InGaIn QWs was improved by a thermal annealing effect during the growth temperature ramping and varied with different temperature ramping rates. The results of optically pumped stimulated emission indicated that the threshold pumping power density of MQWs was decreased with increasing temperature ramping rate from 1.0 degree/s to 3.0 degree/s, and then slightly increased when the ramping rate was 4.0 degree/s. Then two AlGaIn/InGaIn MQW structures with optical confinement layers on both the n- and p-sides were designed. The threshold power density of optically pumped stimulated emission for sample A was determined to be 168 kW/cm².

cm². The sample B with a larger quantum well thickness and a smaller period number was designed to reduce the negative effect of the interface roughness between AlGaIn QBs and InGaIn QWs. The optical investigation of sample B showed a threshold pumping power density of 124 kW/cm², which is 26% lower than sample A. These AlGaIn/InGaIn MQW structures have been applied to the MOCVD growth and device fabrication of our 369 nm vertical-cavity surface-emitting lasers (VCSELs).

4:50 PM N05

(Student) Epitaxial Growth of Relaxed InGaIn Films on Zn-Face ZnO Substrate by Plasma-Assisted Molecular Beam Epitaxy [Kamruzzaman Khan](#), Sandra M. Diez Pinzon, Zhe (. Jian and Elaheh Ahmadi; EECS, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

InGaIn based structures are attractive for different optoelectronic and electronic applications e.g., long wavelength light emitters, solar cells with broad absorption spectrum and tunnel junctions with low barriers. Simulating ongoing quest has been going on for last two decades in this direction. (In,Ga)N alloys allow bandgap energy from 0.7 eV to 3.4 eV with band gap engineering. However, achieving In incorporation larger than 0.3 is still challenging because of large mismatch between InGaIn and GaN. Due to the large lattice mismatch, the critical thickness of InGaIn films grown on GaN decreases and after the critical thickness InGaIn film relaxes by forming defects. Besides, InN and GaN have very different thermal stabilities. InN starts decomposing at 500 °C whereas the GaN growth temperature is ~700 °C by plasma-assisted molecular beam epitaxy (PAMBE). Because of the challenges mentioned above, different research has initiated different methods to develop a relaxed InGaIn as pseudo-substrate. Growing In_zGa_{1-z}N on relaxed In_xGa_{1-x}N pseudo-substrate (z>x) is a much reliable option because of having less lattice mismatch resulting in larger critical thickness. Several groups have studied the growth of relaxed InGaIn films on GaN substrates. Compositional grading [1] and complex multi-step procedure [2] have been proposed as options to grow relaxed InGaIn on GaN. However, it has been proved that partial or full relaxation of InGaIn films on GaN substrates introduces high density of V-defects and pits. These kinds of defects deteriorate the structural and optical quality of the InGaIn films. Besides, compositional grading technique introduces the formation of threading dislocations during relaxation. In this work, we have studied the growth of InGaIn on ZnO substrates using plasma-assisted molecular beam epitaxy (PAMBE). InGaIn and ZnO are isomorphic and, therefore, have same stacking order. Moreover, according to Vegard's law In_{0.2}Ga_{0.8}N is lattice matched to ZnO in c-plane. In addition, utilizing PAMBE, which is a relatively low-temperature growth technique, will suppress the formation of unwanted In₂O₃ interlayers in the InGaIn and ZnO interface. Here, we will present the impact of various growth conditions, including growth temperature, In/Ga fluxes and InGaIn thickness on InGaIn film quality and composition. We have also investigated various surface pretreatments such as annealing in different environments, HF etching, and UV ozone to improve the surface morphology of ZnO and achieve terrace-like surface morphology. A terrace-like morphology is shown to facilitate step-flow growth and improve the surface morphology of InGaIn. The impact of ZnO surface pre-treatment on InGaIn quality will be presented. *References: [1] Hestrofferr K. et al physica status solidi (b) vol 253 (2016) [2] Kobayashi A. et al. Scientific Reports vol 7, 12820 (2017)*

SESSION O: Gallium Oxide Devices and Transport
Session Chairs: Masataka Higashiwaki and Marko Tadjer
Wednesday Afternoon, June 26, 2019
Rackham Building, 4th Floor, Assembly Hall

1:30 PM O01

(Student) β -Ga₂O₃ Delta-Doped Field Effect Transistors with Cutoff Frequency of 27GHz Zhanbo Xia¹, Hao Xue¹, Chandan Joishi¹, Joe McGlone¹, Nidhin Kurian Kalarickal¹, Shahadat H. Soheli¹, Mark Brenner¹, Aaron R. Arehart¹, Steven A. Ringel^{1,2}, Saurabh Lodha³, Wu Lu¹ and Siddharth Rajan^{1,2}; ¹Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ²Material Science and Engineering, The Ohio State University, Columbus, Ohio, United States; ³Electrical Engineering, Indian Institute of Technology Bombay, Mumbai, India.

In this work, we discuss the growth and fabrication of delta-doped Gallium Oxide (β -Ga₂O₃) field effect transistors with current gain cut-off frequency of 27 GHz. β -Ga₂O₃ is the largest bandgap (~4.5 eV) semiconductor with controllable doping that can be grown directly from

the melt in single crystal form. The predicted breakdown electric field of $\beta\text{-Ga}_2\text{O}_3$ (6-8 MV/cm) [1] is higher than that of GaN or SiC (~3 MV/cm), which when combined with electron mobility (predicted ~250-350 cm²/Vs) and electron velocity (predicted ~2×10⁷ cm/s[2]) yields amongst the best figures of merit for power electronic and high frequency devices. Delta doped field effect transistors are one possible approach to enable high sheet charge density in a scaled device. In this work, we report Ga₂O₃ delta doped MESFET with the highest reported cutoff frequency (f_T) of 27 GHz, which is the highest reported to date for $\beta\text{-Ga}_2\text{O}_3$. The device structure used in this work was grown on (010) Fe-doped semi-insulating $\beta\text{-Ga}_2\text{O}_3$ substrates by O₂ plasma MBE. One silicon delta doped layer with Si concentration of 1.3 × 10¹³ cm⁻² capped with 20 nm undoped Ga₂O₃ was grown on 450nm undoped buffer layer. Source and drain regions were patterned and etched for heavily doped n-type Ga₂O₃ contact regrowth. Electron beam lithography was used to define a 120nm Ni T-shaped gate on PMMA/MMA/PMMA resist stack. Hall measurements indicate 1.13×10¹³ cm⁻² channel charge density with electron mobility of 70 cm²/Vs. A maximum DC drain current $I_{D,MAX}$ of 0.26 A/mm was measured at $V_G = 2$ V and $V_D = 12$ V, and a maximum transconductance $g_{m,max}$ of 44 mS/mm was measured at gate bias of -2.5 V. Using a drain current level of 0.1 mA/mm for breakdown, a breakdown voltage (V_{BR}) of 150 V was estimated in a 1.4 μ m gate-drain spacing device. Peak f_T and f_{MAX} of 27 GHz and 16 GHz were obtained at $V_G = -3$ V and $V_D = 12$ V. To estimate the device source resistance, source current was swept while the gate was forward biased reference to keep a 1 μ A/mm forward current. The source resistance was estimated as the differential of the gate voltage with respect to source current. Based on this method, source resistance of 7.4 Ω mm was extracted. This resistance is significantly higher than that estimated from TLM measurement (3 Ω .mm), possibly due to surface depletion in the source access region. To understand the small signal performance of the device, we simulated the same structure using Silvaco ATLAS for comparison. Maximum drain current density of 0.6 A/mm and extrinsic f_T of 40 GHz were obtained from simulation. Both measured and simulated S parameters were de-embedded using the same small signal circuits model [3], and an intrinsic f_T of 30 GHz was extracted from measurements. This value is lower than the corresponding value from simulation (75 GHz). We attribute the discrepancy to the large source resistance, which leads to depletion of the charge at the source edge of gate. This causes drain current saturation while electron velocity under the gate is still below saturation velocity. The extracted gate-source capacitance (C_{gs}) is 260 fF/mm which is much lower than simulated value, and the value from large-area C-V measurements. In addition, the extracted channel resistance (R_{gs}), is also significantly higher than the simulated R_{gs} . These results also support our hypothesis that the large source resistance are limiting the performance of the devices. In summary, we demonstrated delta doped $\beta\text{-Ga}_2\text{O}_3$ MESFET with cutoff frequency of 27 GHz, and discuss the principal limiting factors for the device. This result demonstrates the potential of $\beta\text{-Ga}_2\text{O}_3$ for future millimeter wave device applications. The project depicted was funded by National Science Foundation ECCS-1809682 and AFOSR GAME MURI (Grant FA9550-18-1-0479, Program Manager Dr. Ali Sayir). **References:** [1] M. H. Wong, et. al., *IEEE EDL*, vol. 37, no. 2, pp. 212-215, 2016. [2] K. Ghosh, et. al., *JAP* 122, 035702 (2017).[3] B. Hughes, *IEEE TED*, vol. 36, no. 10 (1989)

1:50 PM O02

High Electron Density $\beta\text{-(Al}_{0.23}\text{Ga}_{0.77})_2\text{O}_3/\text{Ga}_2\text{O}_3$ Modulation Doped Heterostructures Nidhin Kurian Kalarickal², Zhanbo Xia², Joe McGlone², Yuewei Zhang², Wyatt Moore², Siddharth Rajan^{2,1} and Aaron R. Arehart²; ¹Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States; ²Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States.

We report on the design and demonstration of $\beta\text{-(Al}_{0.23}\text{Ga}_{0.77})_2\text{O}_3/\text{Ga}_2\text{O}_3$ modulation doped heterostructures to achieve high sheet charge density. To achieve high sheet charge density without parallel conduction we investigated the use of a low spacer thickness between the delta doping and heterojunction interface. We find that that this strategy enables higher 2DEG sheet charge density up to 5.3×10¹² cm⁻² with mobility of 145 cm²/Vs. The presence of a 2DEG channel was confirmed by measurement of low temperature field effect mobility (μ_{FE}) of 765 cm²/Vs. The electron density of 5.3×10¹² cm⁻² is the highest reported sheet charge density obtained without parallel conducting channels in an (Al,Ga)₂O₃/Ga₂O₃ heterostructure system. With a high breakdown field strength of 8 MV/cm, $\beta\text{-Ga}_2\text{O}_3$ has the potential to be useful in several high frequency and power switching applications. The availability of native $\beta\text{-Ga}_2\text{O}_3$ substrates enables high quality epitaxial growth using techniques like MBE, MOCVD, HVPE and PLD. Lateral devices like $\beta\text{-Ga}_2\text{O}_3$ MESFETs for high frequency application have been demonstrated with high on/off ratio and breakdown voltage[1], but the performance of these devices are

mainly limited by the low mobility (50-90 cm²/V-s). (Al,Ga)₂O₃/Ga₂O₃ MODFETS are attractive in this aspect since they can enable 2D electron gas with excellent transport properties. (Al_{0.18}Ga_{0.82})₂O₃/Ga₂O₃ MODFETS with mobility as high as 180 cm²/Vs have been demonstrated but these devices are mainly limited by the low conduction band offset (0.3- 0.4 eV) resulting in low sheet charge density (~2×10¹² cm⁻²)[2]. Since parallel conduction occurs due to a potential drop in between the heterojunction interface and the barrier layer, minimizing this distance (spacer layer) is a promising strategy to increase the sheet charge density. The effect of this aggressive scaling of the spacer layer thickness is not expected to be very significant since it is phonon scattering that is dominant in limiting room temperature mobility. The (Al,Ga)₂O₃/Ga₂O₃ modulation doped structure was epitaxially grown on Tamura (010) Fe-doped substrate in a Riber/ MBE Solutions M7 system. The epitaxial stack consists of a Ga₂O₃ buffer of 150 nm and (Al_{0.23}Ga_{0.77})₂O₃ cap of 25 nm. Si source heated to 950 °C (open 2.5s) is used for delta doping the (Al,Ga)₂O₃ layer 1nm away from the heterojunction interface. The HRXRD scan of the sample shows 23% Al composition based on the peak separation. Field effect mobility (μ_{FE}) and C-V measurements were used to probe the 2DEG channel at 300 K and 15K. Field effect mobility was estimated using C-V and transconductance measurement on fat FET devices with large gate lengths (100 μ m). Room temperature μ_{FE} measurements show a peak mobility of 145 cm²/V-s, and the mobility of the 2DEG remains above 100 cm²/Vs up to a charge density of 4×10¹²cm⁻². C-V characteristics show a weak temperature dependence with a slight decrease in charge from 5.5×10¹² cm⁻² to 5.3×10¹² cm⁻². This is in contrast to samples with thicker spacer layers (4.5 nm), which showed significant freeze-out from 3.6×10¹² cm⁻² to 1.8×10¹² cm⁻² at low temperature indicating the inability of thick spacers to support a 2DEG density in excess of ~2×10¹² cm⁻². The field effect mobility shows significant enhancement at low temperature with the peak value increasing from 145 to 765 cm²/V-s indicating the absence of ionized impurity scattering present in a parallel channel. In summary we have investigated scaling of the spacer layer thickness as a strategy to increase the sheet charge density in (Al_{0.23}Ga_{0.77})₂O₃/Ga₂O₃ heterostructures. We show that sheet charge density greater than 5×10¹²cm⁻² can be achieved with mobility in excess of 140 cm²/Vs. This work was funded by AFOSR GAME MURI (Grant FA9550-18-1-0479, Program Manager Dr. Ali Sayir). **References:** [1] Xia, Zhanbo, et al." *IEEE Electron Device Letters* 39.4 (2018): 568-571. [2] Zhang, Yuewei, et al." *Applied Physics Letters* 112.17 (2018): 173502

2:10 PM O03

(Student) Ternary Orthorhombic (InxGa1-x)2O3 and (AlxGa1-x)2O3 Thin Films—Growth and Material Properties Anna Hassa, Daniel Splith, Max Kneiß, Holger von Wenckstern and Marius Grundmann; Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, Leipzig, Germany.

Gallium oxide is a wide bandgap semiconductor appearing in various polymorphs, with the monoclinic β -polymorph being the most studied phase up to now. In the last years, the orthorhombic κ -phase is of increasing interest because of its predicted large spontaneous polarization P of 23 μ C/cm² along its c-axis [1]. At the interface of heterostructures P will change abruptly. The resulting charge accumulation render heterostructures in the orthorhombic phase well suited for the fabrication of high power devices such as high electron mobility transistors. Therefore, the stabilization of the κ -phase within the ternary alloy system with In or Al is of interest. During growth of the orthorhombic modification by molecular beam epitaxy [2] or pulsed-laser deposition [3], it is necessary to offer tin. Besides this, the stabilization of the κ -phase sensitively depends on other growth parameters, such as growth temperature and oxygen pressure [3]. We present material properties of a $\kappa\text{-(In}_x\text{Ga}_{1-x})_2\text{O}_3$ and a $\kappa\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ thin film with continuous composition spread [4] grown by pulsed laser deposition on (00.1) Al₂O₃. As target segments we used Ga₂O₃/In₂O₃ as well as Ga₂O₃/Al₂O₃ doped with tin to facilitate formation of the orthorhombic phase, which was observed for an indium content up to 35 at.% [5] and an aluminum content up to 49 at.% enabling band gap engineering between 4.3 [5] and 5.6 eV. Further, we show how the growth conditions affect the phase formation in ternary thin films. Resulting samples were investigated by means of X-ray diffraction, transmission, energy-dispersive X-ray spectroscopy, and atomic force microscopy. [1] Maccioni et al., *Appl. Phys. Express* 9, 04102 (2016) [2] Kracht et al., *Phys. Rev. Appl.* 8, 054002 (2017) [3] Kneiß et al., *APL Materials* 7, 022516 (2019) [4] von Wenckstern et al., *CrystEngComm* 15, 10020 (2013) [5] Hassa et al., *APL Materials* 7, 022525 (2019)

2:30 PM O04

(Student) Observation of the Franz-Keldysh Effect in β -Ga₂O₃ Schottky Diode Darpan Verma¹, Nidhin Kurian Kalarickal², Siddharth Rajan² and Roberto C. Myers^{1,2}; ¹Department of Material Science and Engineering, The Ohio State University, Columbus, Ohio, United States; ²Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States.

Beta gallium oxide (β -Ga₂O₃) has emerged as an attractive material candidate for high power electronic devices due to its high breakdown field (8 MV cm⁻¹), electron saturation velocity, and Baliga figure of merit. Additionally, the large band gap (4.9 eV) makes β -Ga₂O₃ an attractive material for applications in power electronic devices, optoelectronic devices as well as gas sensors and solar blind UV detectors [1-4]. Here we present observations of the Franz-Keldysh effect in Schottky diodes of β -Ga₂O₃. The device structure consists of 1 μ m thick UID layer of β -Ga₂O₃ grown on Sn doped (100) β -Ga₂O₃ substrates by plasma-assisted molecular beam epitaxy (PAMBE). A Ni/Au (30nm/100nm) stack is deposited ex-situ by e-beam evaporation to form the Schottky diodes. A bottom ohmic contact was made with Ti/Au (30nm/130nm) stack which completely covers the back side. Photocurrent spectroscopy is performed as a function of reverse bias voltage and we observe a decrease in absorption edge of β -Ga₂O₃ with increasing reverse bias. β -Ga₂O₃ Schottky Barrier Diodes (SBD) investigated in this study are illuminated from the top. Light reflected from the backside contact gets absorbed in the active region and is measured as photocurrent. The devices showed a characteristic exponential increase in photocurrent with the reverse bias for above bandgap illumination. Sweeping the wavelength range at different reverse bias voltages shows a shift in band edge with reverse bias. Increasing the reverse bias voltage from -5 to -39 V resulted in a decrease in the absorption edge of β -Ga₂O₃, while the peak values of photocurrent get shifted from 245 nm to 261 nm, respectively. Franz Keldysh effect causes sub-bandgap absorption under the applied electric field indirect bandgap semiconductors. Measuring the photocurrent due to the sub-bandgap thus serves as a tool to quantify the electric field profile in the active region of the device. Understanding the electric field distribution within the device structure will be immensely powerful for the design of field terminations in ultra-wideband gap materials like β -Ga₂O₃. In conclusion, we have investigated Franz Keldysh effect-based shift of absorption edge in β -Ga₂O₃ Schottky Barrier Diodes. This would enable the estimation of electric field profiles in β -Ga₂O₃ based devices. Acknowledgment NK and SR acknowledge support from AFOSR GAME MURI (Grant FA9550-18-1-0479, Program Manager Dr. Ali Sayir). References [1] Q. He, W. Mu, H. Dong, S. Long, Z. Jia, H. Lv, Q. Liu, M. Tang, X. Tao, M. Liu, Appl. Phys. Lett. **110**, 093503 (2017). [2] S.J. Pearton, J. Yang, P.H. Cary IV, F. Ren, J. Kim, M.J. Tadjer, M.A. Mastro, Appl. Phys. Rev. **5**, 011301 (2018). [3] G. Franssen, P. Perlin, T. Suski, Phys. Rev. B **69**, 045310 (2004). [4] T. Maeda, T. Narita, M. Kaneshika, T. Uesugi, T. Kachi, T. Kimoto, M. Horita, J. Suda, Appl. Phys. Lett. **112**, 252104 (2018).

2:50 PM O05

(Student) Deep Depletion and Hole Generation in β -Ga₂O₃ MOS Capacitors Hannah N. Masten, Jamie Phillips and Rebecca L. Peterson; Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

The excellent material properties and availability of high-quality single-crystalline substrates has made β -Ga₂O₃ a great candidate for high power electronics and wide-bandgap optoelectronics. Controllable n-type doping of β -Ga₂O₃ has been demonstrated in a wide range of concentrations, but p-type doping has not yet been demonstrated, and there is debate over whether or not p-type material may even be achievable. Holes have been predicted to be self-trapping and have a very low mobility in β -Ga₂O₃. A better understanding of holes within β -Ga₂O₃ is necessary to evaluate the feasibility of bipolar devices. Previously we have demonstrated a ternary alloy rare earth scandate, (Y_{0.6}Sc_{0.4})₂O₃, as a potential dielectric insulator for β -Ga₂O₃ metal - oxide - semiconductor (MOS) devices. (Y_{0.6}Sc_{0.4})₂O₃/ β -Ga₂O₃ (010) MOS capacitors (MOSCAPs) showed a low total interface charge density (< 1 × 10¹² cm⁻²) and high dielectric breakdown fields (4.3 - 6.0 MV×cm⁻¹). Here, we observed from current - voltage (*J-V*) measurements that leakage increases significantly as the MOSCAP is biased into accumulation (positive bias), while low leakage is maintained in depletion (negative bias) until a large negative voltage bias is reached. We investigated the differences in the leakage mechanisms using illumination and temperature - dependent measurements, and we observed thermal and photo-generation of holes while the MOSCAP was in deep depletion. Specifically, *J-V* measurements were obtained while the MOSCAP was illuminated with a 265 nm LED. The leakage during negative bias increased by approximately an order of magnitude due to the photo-generation of electron-hole pairs. (Y_{0.6}Sc_{0.4})₂O₃ is expected to have a

negative valence band offset with β -Ga₂O₃ of -0.9 eV and therefore there is no barrier to impede the transport of holes to the top metal contact. In contrast, during positive bias, illumination did not have a significant effect on leakage. Deep depletion was observed using capacitance - voltage (*C-V*) measurements: the capacitance at large negative bias continues to decrease instead of saturating due to reaching a maximum depletion width. Temperature-dependent *J-V* measurements were performed in the dark from 200K to 300K. The depletion leakage showed a weak electric field dependence, and a low thermal activation energy of 0.16 eV was extracted from the Arrhenius plot. Based on these results, we hypothesize that the leakage current in the dark under negative bias is due to thermal generation of holes assisted by a deep level trap near the valence band of β -Ga₂O₃.

3:10 PM REFRESHMENT BREAK

3:30 PM O06

Unintentional Incorporation of Si and N Atoms in Ga₂O₃ Films Grown by Plasma-Assisted Molecular Beam Epitaxy Yoshiaki Nakata, Takafumi Kamimura, Man Hoi Wong, Phuc H. Than and Masataka Higashiwaki; National Institute of Information and Communications Technology, Tokyo, Japan.

Nitrogen (N) is an element theoretically predicted to behave as a deep acceptor in Ga₂O₃ [1]. Recently, we experimentally investigated the electrical properties of a N-doped Ga₂O₃ layer formed in an *n*-Ga₂O₃ substrate by ion-implantation doping [2]. Annealing of the N-doped Ga₂O₃ layer at temperatures higher than 1100°C, which was the temperature required for activation of the implanted N atoms, gave rise to a large energy barrier in the *n*-Ga₂O₃ and effectively blocked current flow, suggesting that N-doped Ga₂O₃ acts as a *p*-type material. In this study, we investigated the material and electrical properties of unintentionally-doped (UID) Ga₂O₃ epitaxial layers grown by plasma-assisted molecular beam epitaxy (PAMBE), in which Si and N atoms were automatically doped. UID Ga₂O₃ layers were grown on β -Ga₂O₃ (010) substrates by PAMBE with four different O₂ fluxes of 0.5, 1.0, 2.0, and 3.0 sccm. A standard effusion cell was used for Ga, and activated oxygen radicals/ions were generated by decomposing high-purity O₂ gas (>99.99995%) with an RF-plasma cell at 250 W. The substrate temperature during the growth was fixed at 630°C. Growth rates of the epitaxial Ga₂O₃ films were 0.05, 0.27, 0.30, and 0.30 μ m/h for the O₂ fluxes of 0.5, 1.0, 2.0, and 3.0 sccm, respectively. Note that based on the MBE growth diagram proposed by Vogt and Bierwagen [3], the O₂=1.0 sccm condition was estimated to be near stoichiometry. Depth profiles of Si and N atom concentrations in the UID Ga₂O₃ films were analyzed by secondary ion mass spectrometry. All the PAMBE-grown films contained UID Si and N atoms. The Si concentration normalized by growth rate was almost constant for all the samples. On the other hand, the N concentration decreased from 1 × 10¹⁸ to 7 × 10¹⁶ cm⁻³ with increasing O₂ flux from 1.0 to 3.0 sccm. At O₂=1.0 sccm, the N concentration was about ten times larger than that of Si. It can be considered that the UID Ga₂O₃ layer grown at O₂=1.0 sccm acted as a *p*-type material, if all the Si and N dopants were fully activated as shallow donors and deep acceptors, respectively. Note that we have never observed unintentional doping of Si and N atoms in Ga₂O₃ epitaxial films grown with ozone as an O source, and that the unintentional Si and N incorporation was confirmed for Ga₂O₃ layers grown in a different MBE machine equipped with the same type of O plasma cell. Therefore, we consider that autodoping of Ga₂O₃ with Si and N is a unique phenomenon caused by the O plasma cell. It is highly possible that Si was supplied from a plasma bulb made by quartz in the O-plasma cell, as had been observed in ZnO growth [4]. The source of N atoms is still unclear; however, it is likely due to the N₂ impurity (<0.2 ppm) incorporated in the high-purity O₂ source gas. Similar unintentional co-doping of Si and N was also observed in halide vapor phase epitaxial β -Ga₂O₃ films [5]. We also succeeded in fabricating normally-off Ga₂O₃ MOSFETs by using the PAMBE-grown unintentionally N-doped Ga₂O₃ layer as a channel. The device process and characteristics will be presented at the conference. This work was partially supported by Council for Science, Technology and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), "Next-generation power electronics" (funding agency: New Energy and Industrial Technology Development Organization). [1] H. Peelaers *et al.*, APL Mater. **7**, 022519 (2019), [2] M. H. Wong *et al.*, Appl. Phys. Lett. **113**, 102103 (2018), [3] P. Vogt and O. Bierwagen, Appl. Phys. Lett. **108**, 072101 (2016), [4] S. Akasaka *et al.*, Jpn. J. Appl. Phys. **50**, 080215 (2011), [5] M. J. Tadjer *et al.*, Appl. Phys. Lett. **113**, 192102 (2018).

3:50 PM O07

Novel P-Type Oxides of Corundum-Structured α - Ir_2O_3 for Gallium Oxide Electronics Kentaro Kaneko¹, Shu Takemoto¹, Shin-ichi Kan¹, Takashi Shinohe² and Shizuo Fujita¹; ¹Electronic Science and Engineering, Kyoto University, Kyoto, Japan; ²FLOSFIA Inc., Kyoto, Japan.

Gallium oxides (Ga_2O_3) has been gathering much attentions for their huge band gaps of 5.61 eV (α - Ga_2O_3) [1] and 4.48 eV (β - Ga_2O_3) [2]. Ga_2O_3 takes 5 types of crystal polymorph, among these, corundum-structured α - Ga_2O_3 is attractive in view of bandgap tuning from 3.7 to ~9.0 eV by alloying with corundum-structured α - In_2O_3 and α - Al_2O_3 accompanying high crystallinity[3][4]. Besides highly crystalline α - Ga_2O_3 thin films are grown on sapphire (α - Al_2O_3) substrates by mist CVD technique [5], followed by evolution of Schottky barrier diodes with extremely low on-resistance [6] and normally-off operations [7]. However, the lack of p-type oxide semiconductors acting as a counterpart of both α - Ga_2O_3 and β - Ga_2O_3 has obstructed high-performance power devices based on Ga_2O_3 . We have been focusing on corundum-structured p-type α - $(\text{Rh,Ga})_2\text{O}_3$ [4] and α - Ir_2O_3 . Typically, α - Ir_2O_3 has a bandgap of 2.6 eV[8], and a possibility to widen a bandgap up to 5 eV by alloying with α - Ga_2O_3 . However, these are metastable phase and there are few reports on synthesis of single-phased crystals. Making of single-phased α - Ir_2O_3 thin films is a key to control bandgaps and hole concentrations. Single-phase α - Ir_2O_3 thin films were fabricated on c-plane sapphire (α - Al_2O_3) substrates by mist CVD method. The $2\theta/\theta$ scanning profiles of X-ray diffraction (XRD) showed obtained thin films were single-phased α - Ir_2O_3 thin films their XRD peaks were derived from only 0001 diffractions. No other peaks from other crystal polymorphs were detected. To determine the crystal structure of obtained α - Ir_2O_3 thin films, cross-sectional transmission electron microscope (TEM) observation was conducted. All the diffraction spots from the α - Ir_2O_3 are situated slightly inside of those from the α - Al_2O_3 , due to the different lattice constants. This is a strong evidence that the Ir_2O_3 thin film takes corundum structure with longer lattice constants along a- and m- axes than α - Al_2O_3 . Within the experimental accuracy, it was estimated to be 5.0-5.1 Å. Then the lattice mismatch between α - Ir_2O_3 and α - Ga_2O_3 is under 1% along the a-axis. The most promising property we expect for α - Ir_2O_3 is p-type conductivity. For this purpose, the Hall effect measurement using Van der Pauw method was conducted. The α - Ir_2O_3 showed clear p-type conductivity with the positive Hall coefficient. The hole density and mobility calculated using the obtained Hall coefficient were $1.0 \times 10^{21} \text{cm}^{-3}$ and $2.3 \text{ cm}^2/\text{Vs}$, respectively. For α - Ir_2O_3 , X-ray photoelectron spectroscopy (XPS) measurements were conducted to determine the electrical orbitals which consist valence bands. The XPS spectra clearly indicates that the valence band is consisted with Ir 5d orbitals, whose energy levels were situated upper than the 2p orbitals of oxygen atoms. The origin of p-type conductivity is attributed to that the top of valence band of α - Ir_2O_3 is formed by the Ir 5d orbitals rather than 2p orbitals of oxygen atoms. [1] A. Segura *et al.*, Phys. Rev. Mat. 1, 024604 (2017). [2] T. Onuma *et al.*, Jpn. J. Appl. Phys. 54, 112601 (2015). [3] K. Kaneko *et al.*, J. Appl. Phys. 113, 233901 (2013). [4] K. Kaneko *et al.*, Jpn. J. Appl. Phys. 57, 02CB18 (2018). [5] D. Shinohara *et al.*, Jpn. J. Appl. Phys. 47, 7311 (2008). [6] M. Oda *et al.*, Appl. Phys. Express 9, 021101 (2016). [7] News release from FLOSFIA INC. ; <http://flosfia.com/20180713/> [8] R. K. Kwar *et al.*, Appl. Surf. Science, 206, 90 (2003).

4:10 PM O08

The Effects of Bi on the Electronic Structure of In_2O_3 and Ga_2O_3 Anderson Janotti and Fernando P. Sabino; Materials Science and Engineering, University of Delaware, Newark, Delaware, United States.

In_2O_3 and Ga_2O_3 are wide-band gap semiconductors that are important for a wide range of technological applications, such as transparent contacts in solar cells and LEDs, liquid crystal displays, and high power transistors. Their highly dispersive conduction bands are composed of the metal s orbital and lie relatively low with respect to the vacuum level, making it easy to dope n -type. Their valence bands are composed mainly of $O p$ orbitals, leading to high ionization potentials, making it difficult to achieve p -type doping; acceptor impurities tend to create deep levels. One way to overcome this limitation is to raise their valence bands. Using first-principles calculations we explore different approaches to lift the valence band in these oxides by alloying. We discuss the effectiveness of different alloying elements, both on oxygen and metal sites. We compute the formation enthalpy of these alloys, and their stability with respect to phase separation. We calculate band gaps, and analyze the effects of alloying on the position of the valence and conduction bands, determining the band alignment between the alloys and the parent compounds. Finally, we address their optical properties by calculating absorption coefficients as a function of alloy composition.

4:30 PM O09

Magneto-Transport Studies of β - Ga_2O_3 Adam T. Neal¹, Said Elhamri^{1,2} and Shin Mou¹; ¹Materials and Manufacturing Directorate, Air Force Research Laboratory, Dayton, Ohio, United States; ²Department of Physics, University of Dayton, Dayton, Ohio, United States.

Recent developments in the epitaxy of β - Ga_2O_3 have yielded significant improvements in carrier transport properties, resulting in the first observations of Landau level formation in high magnetic field and low temperature via Shubnikov de Haas (SdH) oscillations [1]. However, aspects of the magneto-transport properties of β - Ga_2O_3 , including the nature of spin-splitting in SdH oscillations and the isotropy of the cyclotron effective mass, remain to be explored experimentally. In this work, we study the magneto-transport of β - Ga_2O_3 to better understand topics such as Landau level spin-splitting, the role and strength of spin-orbit coupling, and cyclotron effective mass in the material. Studies of SdH oscillations as a function of parameters such as temperature, magnetic field, and applied gate voltage will be presented. [1] Y. Zhang *et al.* "Demonstration of high mobility and quantum transport in modulation-doped β - $(\text{Al,Ga})_2\text{O}_3/\text{Ga}_2\text{O}_3$ heterostructures" *Applied Physics Letters*, vol. 112, 173502 (2018).

4:50 PM O10

(LATE NEWS, Student) Thin-Film Thermophotovoltaic Device Fabricated by Non-Destructive Epitaxial Lift Off Tobias Burger, Deju Fan, Stephen R. Forrest and Andrej Lenert; University of Michigan—Ann Arbor, Ann Arbor, Michigan, United States.

Thermophotovoltaic (TPV) generators offer scalable, solid-state energy conversion, well suited for implementation in decentralized applications such as residential co-generation and high-temperature applications such as grid-scale thermal energy storage. State-of-the-art TPV systems, however, have been demonstrated with devices comprised of the InGaAsSb quaternary alloy system, making these technologies prohibitively expensive in comparison to conventional generators. Here, we demonstrate, for the first time, fabrication of a thin-film $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ TPV device by non-destructive epitaxial lift off, such that the epitaxial film is separated from the host InP substrate without damaging either surface. This advancement will enable reuse of the expensive InP substrate for additional film growths, drastically reducing material costs for TPV device fabrication. Our thin-film device features a selective spectral response, with high sub-bandgap reflectance well suited for enhancing photon recycle and improving conversion efficiency in TPV systems. Additionally, the device's thin-film architecture is expected to offer improved luminescence efficiency compared to conventional devices. We characterize the device's power conversion efficiency by calorimetric measurement of heat rejection in the device under illumination (1500K spectrum) in a vacuum setting. Further, we describe contributions to performance enhancement and identify limiting loss pathways through computational simulation and outline how further optimization may facilitate improved conversion efficiency on par with centralized power plants. This study serves to demonstrate the feasibility of thin-film TPV fabrication by non-destructive epitaxial lift off and substantiate claims of optical and electronic performance enhancements offered by thin-film device architecture. Enhanced conversion efficiency and reduced fabrication cost, enabled by non-destructive epitaxial lift off, may make thin-film TPV technologies accessible for power generation and storage applications

SESSION PS: Poster Session
Wednesday Evening, June 26, 2019
6:00 PM - 8:00 PM
Michigan League, 2nd Floor, Ballroom

PS01

(Student) Effect of Deposition Pressure on Electrical Properties in Electron Selective La:BaSnO₃ Thin-Films Akash Kumar, Sushobhita Chawla, Sandeep K. Maurya, Suren Patwardhan and Balasubramaniam Kavaipatti; Energy Science and Engineering, Indian Institute of Technology Bombay, Thane, India.

Thin films of La_{0.01}Ba_{0.99}SnO₃ were deposited on single crystal Lanthanum Aluminate – Strontium Aluminate Tantalate (LSAT) substrates at different oxygen partial pressure (Po₂) between 0.02 to 18 mTorr. X-ray diffraction of the films reveal that relative intensity ratio [$I_{(002)}/I_{(011)}$] increases from 0.03 to 166.67 as the Po₂ is increased, suggesting that higher Po₂ is essential for oriented growth. Room temperature resistivity of the films first decreases from 260 to 0.77 mΩ-cm for 0.06 to 6 mTorr respectively, and finally increases to a value of 3.42 mΩ-cm for the film deposited at 18 mTorr proposing that either extremities of are unfavourable for the electrical properties. Films show n-type degenerate semiconducting behaviour with all the donors readily ionized and their carrier concentrations remains constant throughout the temperature range (10 – 300K). For the given carrier concentration range, the ionized impurity and grain boundary scattering are temperature independent thus the mobility of the films deposited at 0.06 and 6 mTorr remains constant throughout the temperature range (10 – 300K). However, the film deposited at 6 mTorr exhibits phonon scattering and a reduction in mobility at higher temperatures is observed. Low temperature resistivity data reveals that the film deposited at 0.06 mTorr shows highly disordered behaviour and resistivity reduces monotonically throughout the temperature range. However, the films deposited at 0.6 and 6 mTorr undergo a metal to semiconductor transition (MST) at 65 and 35 K respectively, indicating that the transition temperature shifts towards the lower values for the films deposited at higher. The resistivity values were examined with the help of semi-classical Boltzmann's equation with quantum correction to conduction at low temperatures and it is observed that the conduction is majorly governed by electron-electron interaction rather than the weak localization effect.

PS02 WITHDRAWN

Semi-Empirical Model for ZnO Quantum Dot, Graphene Channel Photodetector Amelia Peterson and Shayla Sawyer; Electric, Computer and Systems Engineering, Rensselaer Polytechnic Institute, Troy, New York, United States.

A semi-empirical model for ZnO Quantum Dot (QD), Graphene channel photodetector is developed to predict the effect of scaling, channel composition and material, and environmental conditions on device performance. A previously fabricated version of this device had a photoresponsivity of 10⁸A/W, phototransistor gain of 3x10⁹, and a UV to visible light rejection ratio of 10³ [1]. However, the photoresponsivity of the device is limited by its large dark current due to the high conductivity of the Graphene in the absence of illumination, and the device response time is limited by the relatively slow O₂ adsorption process on the surface of the ZnO QDs. To improve upon these aspects of the device, the O₂ adsorption process must be controlled, and a new channel material must be chosen. To aid in redesigning the device, our device model produces the current-voltage characteristics and transient response of the device for a given illumination, device geometry, channel material, and ambient O₂ concentration and pressure, and from this data performance metrics such as dark current, photodetectivity, signal-to-noise ratio, and response time are calculated. The conductivity of various 2D channel materials such as Graphene, MoS₂, and BN as well bilayer Graphene and Carbon Nanotubes are modeled via the Landauer formula as a function of applied bias and injected charge. Results are compared to experimental results and data obtained from Non-Equilibrium Green's function (NEGF) simulations. The effect of the adsorption process on the lifetime of photogenerated electrons is determined through a finite difference simulation of the Elovich isotherm coupled with a 1D diffusion equation and interfacial boundary condition which provides the adsorbed surface density of O₂ over time. From this, we predict optimal channel materials, device dimensions, and O₂ concentration for specific applications such as microbial detection, communications, and missile plume detection. [1] D. Shao et al., "Organic-Inorganic Heterointerfaces for Ultrasensitive Detection of Ultraviolet Light," *Nano Lett.*, vol. 15, pp. 3787-3792, 2015.

PS03

(Student) Sputter-Instigated Plasmonic Excitations in Ultra-Thin NMZO Thin Film—For Ultra-Thin Solar Cell Applications Vivek Garg, Brajendra S. Sengar, Gaurav Siddharth, Amitesh Kumar and Shaibal Mukherjee; Electrical Engineering, Indian Institute of Technology Indore, Indore, India.

CuInGaSe (CIGSe) solar cells have recently set a new record efficiency of 22.9 %, thus demonstrating a continuous improvement of this technology. Currently, the standard thickness for the CIGSe absorbers is 2-3 μm. Reduction in material consumption will help to further reduce the cost. When approaching the material reduction by reducing the absorber thickness to below 700 nm leads to increase in production quantity but, on the other hand, it considerably reduces light absorption in absorber layer causing in strongly enhanced recombination at the back contact. Additionally, alkali metals (Na, K, Rb, etc.) have been extensively acknowledged as beneficial dopants that contribute to improving the p-type conduction in the absorber layers. In general, Na diffuses into the CIGSe layers from the soda-lime glass (SLG) substrates. Use of soda lime glass is the major obstacle towards the realization of flexible solar cell devices. Here, we will focus on a novel approach to tackle both the above-mentioned issues by a) investigating a novel means to generate broadband plasmonic generation in ultrathin NMZO layers for backscattering of light towards absorber for enhanced absorption in ultra-thin solar cells. b) removal of the rigid soda-lime glass substrate by introducing NMZO layer in between back-contact and absorber as the source of Na. We report a novel approach to excite plasmons in Na-doped MgZnO (NMZO) thin films in the wide spectral range. In this work, a new methodology to generate plasmons in the NMZO thin film using dual-ion beam sputtering (DIBS) system is reported. Sputtering of material during growth by utilizing secondary DC-ion source present in the DIBS system leads to the generation of different metallic and metal oxide nanoclusters of its constituent elements. Moreover, the formation of nanoclusters and generation of plasmons are verified by electron energy loss spectra obtained by UPS analysis, FESEM, and spectroscopic ellipsometry. Additionally, calculation of valence bulk, valence surface, and particle plasmon resonance energies are performed, and indexing of each plasmon peaks with corresponding plasmon energy peak of the different nanoclusters are done. Moreover, SIMS measurement is performed to verify the diffusion of Na towards the absorber layer. Therefore, this approach offers a convenient method to produce plasmon resonance across the broad spectral range spanning 1.31-9.75 eV. Further, use of this dual ion beam sputter instigated plasmon enhanced NMZO thin film can be a novel mean to improve the p-type conduction of the absorber and increase the absorption within the absorber through backscattering phenomenon to enhance the performance of ultrathin photovoltaic devices.

PS04

MBE-Grown Self-Powered β-Ga₂O₃ Schottky Solar Blind UV Detector with Rectification > 10⁷ Anamika S. Pratiyush², Zhanbo Xia³, Sandeep Kumar², Yuewei Zhang³, Chandan Joishi^{3,5}, Rangarajan Muralidharan¹, Siddharth Rajan⁴ and Digbijoy N. Nath¹; ¹Centre for Nano Science and Engineering, Indian Institute of Science, Bangalore, Bengaluru, India; ²Centre for Nano Science and Engineering (CeNSE), Indian Institute of Science (IISc), Bengaluru, India; ³Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ⁴Ohio State University, Columbus, Ohio, United States; ⁵Indian Institute of Technology Bombay, Mumbai, India.

We report on self-powered Schottky deep-UV detector on homoepitaxial β-Ga₂O₃ grown by plasma-assisted MBE on Fe-doped semi-insulating (010)-oriented β-Ga₂O₃ substrate. The Schottky detectors with vertical device geometry exhibited more than 7 orders of rectification at 2 V with an external quantum efficiency of 3% and 11% at zero bias and a reverse bias of 8 V respectively. The detectors also exhibited ~3 orders of UV-to-visible rejection ratio in conjunction with ~2 orders of photo-to-dark current ratio at zero bias with no persistent photoconductivity in transient response. Solar-blind UV detectors sensitive to wavelengths below ~290 nm are of great interest for a plethora of applications. There are several reports of metal-semiconductor-metal (MSM) deep-UV detectors based on epitaxial β-Ga₂O₃ and on bulk β-Ga₂O₃; however, a few reports on vertical Schottky detector on epitaxial or bulk β-Ga₂O₃ substrate exist [1-5]. In this work, devices were realized on plasma-assisted MBE-grown β-Ga₂O₃ unintentionally doped layer (UID) (Thickness ~100 nm) on top of heavily Si-doped (Doping concentration ~2 X 10²⁰ cm⁻³ (Thickness~60 nm) β-Ga₂O₃ on (010)-oriented Fe-doped β-Ga₂O₃ substrate. Oxygen plasma power of 300W with a chamber pressure of 1.5 x 10⁻⁵ Torr, and Ga flux of 8x 10⁻⁸ Torr, were used during β-Ga₂O₃ growth. The substrate temperature was 700 °C. The root mean square (RMS) roughness was ~ 1.0 nm for a scan area of 5 X 5 μm² (from AFM). Ni/Au (30/100 nm) metal stack was

e-beam evaporated on the top undoped layer to form Schottky contact and Indium dot was used to form the bottom Ohmic contact to the n++ doped layer. The peak responsivity values of 4 mA/W (corresponding EQE ~ 3%) and 21 mA/W (EQE ~ 11%) were measured at zero bias and -8 V respectively, indicating the self-powered nature. The cut-off was observed at 253-255 nm (4.9 eV). The UV-to-visible rejection ratio was found to be ~ 3 orders at zero bias, indicating true solar blind nature. The detectors exhibited an asymmetric dark current-voltage (I-V) characteristic with > 10⁷ of rectification at a bias of 2 V. The ideality factor was extracted from the linear fitting of dark I-V characteristics, which comes out to be 1.31. The extracted Schottky barrier height at Ni/β-Ga₂O₃ junction was found to be 1.4 eV, which is close to reports in the literature [6]. A photo-to-dark current ratio of ~ 2 orders at zero bias and in reverse bias regions was measured. Photocurrent remained almost the same as dark current in forward bias region, which is typical of Schottky detectors. The detectors showed gain at biases higher than -10 V. The transient response showed no persistent photoconductivity in transient response measurements. The rise and fall times (10% - 90 %) were found to be 0.41 s and 0.45 s (at zero bias) respectively. Temperature-dependent current-voltage characteristics agree with the thermionic emission model. [Funding: This work was funded by Space Technology Cell (STC) and Joint Advanced Technology Program (JATP), Department of the Defense, Defense Threat Reduction Agency (Grant HDTRA11710034), ONR EXEDE MURI program, and the OSU Institute for Materials Research Seed Program.] **References:** [1] Oshima et al, APL 1, 11202 (2008). [2] Guo et al, Opt. Mat. Exp. 4, 1067 (2014). [3] Pratiyush et al, APL 110, 221107 (2017). [4] Alema et al, Proc. Of SPIE, 10105 (2017) [5] Chen et al, 8, 4185 (2016) [6] Farzana et al, APL 110, 202102 (2017)

PS05

(Student) Relationship Between Basal Plane Dislocation Distribution and Local Basal Plane Bending in PVT-Grown 4H-SiC Crystals
 Tuerxun Ailihumaer¹, Hongyu Peng¹, Balaji Raghothamachar¹ and Michael Dudley²; ¹Stony Brook University, Stony Brook, New York, United States; ²State University of New York at Stony Brook, Stony Brook, New York, United States.

Efforts to improve the quality and size of 4H-SiC wafers have resulted in size of 6" and dislocation densities of the order of 10³ cm⁻². The presence of significant quantities of crystallographic defects in bulk 4H-SiC crystals continues to be a major obstacle for achieving high-quality 4H-SiC substrates. Of particular note is the nucleation and distribution of basal plane dislocations (BPDs). BPDs are deformation-induced and are mostly generated during post-crystal growth cooling or high temperature annealing processes. BPDs have been associated with the formation of Shockley stacking fault leading to an increase in forward voltage degradation and are undesirable. Depending on the PVT growth conditions, internal stresses due to non-uniformity of temperature field cause lattice plane bending. During cooldown, this bending is accommodated by the inhomogeneous distribution of BPDs in a PVT grown 4H-SiC boule and persists in wafers sliced from the boule. Crystal bending affects subsequent wafer processing especially polishing and device fabrication. Therefore, analysis of the BPD distribution (sign and density) enables us to better understand basal plane bending, which provides insight into further improvement of the crystal growth process. Synchrotron Monochromatic Beam X-ray Topography (SMBXT) studies in grazing incidence geometry reveal the appearance of black and white contrast of BPDs which are associated with opposite sign of Burgers vectors. Based on the principle of ray tracing, black contrast BPDs are generated by focusing of diffracted X-rays when the extra half plane is extending away from the imaged surface, while defocusing of X-rays contribute to the generation of white contrast BPDs due to the extra half plane extending towards the surface [1]. The inhomogeneous distribution of the two types of BPD contrast will thus result in concave/convex shape of the basal planes. In our study, we have evaluated the ratio of the black/white contrast of BPDs along 11-20 direction across multiple 6-inch diameter 4H-SiC substrates sliced from the same and different boules and predicted how the lattice is tilted in different substrate wafers. High resolution X-ray diffraction measurements are currently underway to investigate the variation of rocking curve peak shift along 11-20 direction and thus to further verify our result. [1] X. Huang, D.R. Black, A.T. Macrander, J. Maj, Y. Chen, M. Dudley, Appl. Phys. Lett. 91 (231903) (2007).

PS06

(Student) Structural, Thermoelectric and Magnetic Properties of Mn_{1-x}Zn_xSb₂Se₄ (x = 0, 0.01, 0.03, 0.04, 0.05, 0.06, 0.08, 0.1, 0.15)
 Brandon A. Buchanan¹, Juan S. Lopez², Yiqiao Huang³ and Ferdinand Poudeu⁴;
¹MSE, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; ³Materials Science & Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ⁴University of Michigan, Ann Arbor, Michigan, United States.

Abstract: An exciting new class of magnetic semiconductors given by the parent structure M_{1-x}M'_xPn₂Se₄ (M = Fe, Mn; M' = Sn, Zn; Pn = Sb, Bi) have garnered much research attention recently since the system has been shown to exhibit separate and precise magnetic/electronic tunability.^{1,2} The compound series crystallizes isostructurally in the low-symmetry monoclinic space group C2/m (#12). The structure allows decoupling at the atomic-scale of the magnetic and semiconducting sublattices, giving the ability to separately tune the electronic and magnetic properties of the system.^{1,2} The magnetic behavior can be selected by using Fe/Mn (ferromagnetic or antiferromagnetic) and the carrier type can be chosen with Sb/Bi (p-type or n-type). Due to the tunability of the electronic and magnetic properties, M_{1-x}M'_xPn₂Se₄ has shown promise in thermoelectric and spintronic materials. In this study, Mn_{1-x}Zn_xSb₂Se₄ (x = 0-0.15) was synthesized via a conventional solid-state synthesis route. Zinc (a nonmagnetic atom) was substituted at the magnetic site (Mn), and the effects of the substitution was studied. Successful single-phase synthesis was confirmed using powder X-ray diffraction for x = 0-0.03, and for x = 0.04-0.15 a small binary peak of ZnSe was also noticed. Rietveld refinement was utilized to extract the lattice parameters of the ternary and binary structures. For the ternary structure, lattice parameter shifts were seen across the Zn range, suggesting Zn incorporation within the lattice was successful. For the binary phase, a lattice parameter shift was also seen, indicating the formation of Zn_{1-x}Mn_xSe. With differential scanning calorimetry, a small Se melting peak was observed for all samples, and the melting point was T_m ~ 677-680°C for the ternary compound. After the first melting, the samples decomposed. X-ray photoelectron spectroscopy elemental analysis confirmed that all elements were in their anticipated oxidation states (Mn²⁺, Zn²⁺, Sb³⁺, and Se²⁻). Thermoelectric properties of this material were also taken: for x = 0.01 at T = 323.15 K, the electrical conductivity was found to be ~0.53 S/m; the Seebeck coefficient was found to be ~-896 μV/K, indicating a p-type material; the total thermal conductivity (κ_T) was found to be ~0.68 W/m²K; the maximum figure of merit (zT) occurred for x = 0.01 at T = 623.15 K, with zT = 0.02. The electrical conductivity data was fit using the Arrhenius equation to extract bandgap and activation energy, and κ_T was fit using the Wiedemann-Franz law to decouple the electronic and lattice contributions to κ_T. Finally, temperature-dependent magnetic susceptibility data was taken and fit using the Curie-Weiss law in the paramagnetic region. The Néel temperature (T_N) was consistently around 20 K. From the fit, the Weiss constant was found to be large and negative, indicating an antiferromagnetic material. Throughout the series, the effective magnetic moment (μ_{eff}) calculated using the fit and the Langevin theory of paramagnetism was consistently larger than the magnetic moment predicted for Mn²⁺ (d⁵, high-spin, octahedral coordination) using Hund's rules. So, an additional magnetic contribution must be enhancing the magnetic moment. Based on an AFM-coupled bound magnetic polaron configuration, the individual magnetic moments would be enhanced, giving a proposed magnetic lattice to explain the increased moments. **References:** 1. Djieutedjeu, H.; Olvera, A.; Page, A.; Uher, C.; Poudeu, P. F. P. High-Tc Ferromagnetism and Electron Transport in p-Type Fe(1-x)Sn(x)Sb₂Se₄ Semiconductors. *Inorganic chemistry* **2015**, *54*, 10371. 2. Ranmohotti, K. G. S.; Djieutedjeu, H.; Poudeu, P. F. P. Chemical manipulation of magnetic ordering in Mn(1-x)Sn(x)Bi₂Se₄ solid-solutions. *Journal of the American Chemical Society* **2012**, *134*, 14033.

PS07

(Student) Binarized Neural Networks Enabled by Forming-Free Memristor
 Yong Kim¹, Won Hee Jeong¹, Kyeong-Sik Min² and Byung Joon Choi¹; ¹Materials Science and Engineering, SeoulTech, Seoul, Korea (the Republic of); ²School of Electrical Engineering, Kookmin University, Seoul, Korea (the Republic of).

Memristor crossbar arrays were fabricated based on a Ti/HfO₂/Ti stack that exhibited electroforming-free behavior and low device variability in a 10 x 10 array size. The binary states of high-resistance-state and low-resistance-state in the bipolar memristor device were used for the synaptic weight representation of a binarized neural network using a two-column scheme. The electroforming-free memristor was confirmed as being suitable as a binary synaptic device because of its higher device yield, lower variability, and less severe malfunction (for example, hard break-

down) than the electroformed memristors based on a Ti/HfO₂/Pt structure. The feasibly working binarized neural network adopting the electroforming-free binary memristors was demonstrated through simulation. Eight input patterns were applied to the CBAs with pre-trained synaptic weights, which resulted in the corresponding pattern recognition by maximizing the current summation. This simple memristor crossbar array with the absence of the selector device or multi-level operation could significantly reduce the burden for fabrication.

PS08

(Student) EPR and Optical Studies of Extrinsic (Fe, Cr, Ir, Mg) and Intrinsic Point Defects in β -Ga₂O₃ Crystals Christopher Lenyk and Nancy C. Giles; Engineering Physics, Air Force Institute of Technology, Wright-Patterson AFB, Ohio, United States.

Experimental studies of acceptors and donors in bulk single crystals of gallium oxide are presented. Ga₂O₃ is an ultrawide band gap oxide semiconductor with large device breakdown voltages and promising radiation resistance for electronics in space applications. Unintentionally doped bulk crystals typically are *n*-type with free carrier concentrations near 10¹⁷ cm⁻³ due to Group IV shallow donors [1]. Electron paramagnetic resonance (EPR) is uniquely suited to identify and study both extrinsic and intrinsic defects in this material. EPR allows determination of hyperfine and *g* matrices for the paramagnetic defects. Since Ga₂O₃ has two crystallographically inequivalent Ga sites (one tetrahedrally bonded and one octahedrally bonded), the EPR technique is especially important to determine the specific environments for impurities incorporated on cation sites. The characteristic EPR spectra, i.e., their “fingerprints”, for several extrinsic defects (neutral Mg acceptors, Fe³⁺, Cr³⁺, and Ir⁴⁺) and intrinsic defects (Ga vacancies and self-trapped holes) have been reported [2-5]. We have extended these studies to investigate the transfer of charge between Ir donors, Fe acceptors, and Mg acceptors. Special attention is given to the role of Cr in Ga₂O₃. We correlate the EPR results with optical data obtained using temperature-dependent absorption, thermoluminescence (TL), and photoluminescence (PL). A Bruker EPR spectrometer with capability to orient the sample relative to the magnetic field provides complete spectral dependence in the a-b, b-c and c-a planes. Samples were obtained from Northrop Grumman Synoptics (Charlotte, NC) and Kyma Technologies (Raleigh, NC). Anisotropy of the hyperfine associated with gallium ions (Ga has two isotopes with nuclear spin I = 3/2) often allows one to distinguish between various defects. An Oxford Instruments helium flow system (4-300 K) allows us to establish optimum monitoring conditions for the paramagnetic centers. For above-band-gap excitation, we use x-rays or uv sources. For below bandgap excitation, we used light sources extending from 250 nm to 3.39 microns. By investigating the thermal stability of changes in the charge states of defects under different illumination conditions, we use EPR to explore the interplay between donors and acceptors. We find that Cr impurities are an effective TL center and play a role in charge transfer from deep levels. 1. “Donors and deep acceptors in β -Ga₂O₃”, Adam T. Neal, Shin Mou, *et al.*, Applied Physics Letters **113**, 062101 (2018). 2. “Gallium vacancies in β -Ga₂O₃ crystals”, B.E. Kananen, L.E. Halliburton, *et al.*, Applied Physics Letters **110**, 202104 (2017). 3. “Electron paramagnetic resonance study of neutral Mg acceptors in β -Ga₂O₃ crystals”, B.E. Kananen, L.E. Halliburton, *et al.*, Applied Physics Letters **111**, 072102 (2017) 4. “Self-trapped holes in β -Ga₂O₃ crystals”, B.E. Kananen, L.E. Halliburton, *et al.*, Journal of Applied Physics **122**, 215703 (2017). 5. “Ir⁴⁺ ions in β -Ga₂O₃ crystals: An unintentional deep donor”, C.A. Lenyk, N.C. Giles, *et al.*, Journal of Applied Physics (2019, in press).

PS09

Stimulated Anti Stokes Raman Scattering in Silicon Nanowires Daksh Agarwal and Ritesh Agarwal; University of Pennsylvania, Sunnyvale, California, United States.

Silicon photonics has been an active area of research in the past two decades due to ever increasing demand for more computational power and faster device speeds. Since photoluminescence based lasers cannot be built from Si because of its indirect bandgap, Raman processes have been investigated as a possible source for laser. While cm scale Stokes Raman lasers have been built, it has been impossible to realize anti Stokes based Raman in bulk or at the nanoscale because of difficulty in achieving stimulated upconverted Raman. Anti Stokes Raman laser would open up new avenues for wavelength conversion as well as mitigate issues related with heat generation since it would naturally consume phonons (heat) during its operation. We report, for the first time, stimulated Anti Stokes Raman scattering (SARS), a precursor for anti Stokes Raman laser, in Si nanowire cavities. At cavity mode resonance, light is confined into low mode volume-high intensity electromagnetic modes inside the Si nanowire cavities because of which SARS is observed at sub mW pump powers.

This is the first time SARS has been observed in Si and is a significant first step in realizing a nanoscale low powered upconverted Si laser for applications in the next generation of nanoscale devices.

PS10 WITHDRAWN

Predicting Chromaticity Shift Behavior of Phosphor Converted LEDs Using Differential Chromaticity Analysis Eric Bretschneider^{1,2}; ¹EB Designs & Technology, Grapevine, Texas, United States; ²QuarkStar, Las Vegas, Nevada, United States.

To date, lifetime estimates of LEDs used for solid-state lighting have been based on modeling luminous flux behavior as an exponential decay in time. Accurate predictions of long term lumen maintenance behavior can be made using as little as 6,000 hours of reliability data. Chromaticity shift constitutes another parametric failure, but the lack of a general method for predicting chromaticity shift over time has resulted in a test to failure methodology which may result in products with unacceptably short lifetimes being introduced into the market. The typical chromaticity shift behavior of LEDs is characterized by a short term rapid increase in chromaticity shift followed by an incubation period during which the chromaticity shift is essential constant for a period of a few thousand to tens of thousands of hours. At the end of the incubation period, the chromaticity shift behavior shifts to a linear increase with respect to time increases as a linear function of time. As if predicting a step change in a formerly stable variable isn't complicated enough, the direction of terminal chromaticity shift may be towards blue, green, yellow or red. Differential Chromaticity Analysis is a simple mathematical framework that is able to predict the duration of the incubation period and the terminal chromaticity shift behavior without prior knowledge of the LED package format, materials of construction or phosphor system. Details of the model and calculation results will be discussed.

PS11

(Student) Mesostructural Visualization of Single-Crystal Diamond Irradiated by GeV Sn and Zr Erik Vyhmeister and Elias Garratt; Materials Science, Michigan State University, East Lansing, Michigan, United States.

Within the next 5 to 10 years, radiation levels in high energy physics facilities like the Large Hadron Collider and the Facility for Rare Isotope Beams are expected to exceed 2x10¹⁶ n_{eq}/cm² per year. In such environments breakdown of detectors leads to loss of data, lack of accurate particle detection, and increased operational costs. Single crystal diamond (SCD) has shown promise as a particle radiation detector material, demonstrating superior charge collection efficiencies at 10¹⁴ n_{eq}/cm² compared to silicon and the ability to self-repair leading to prolonged lifetime and increased reliability as radiation sensors. Radiation damage mechanisms in diamond are relatively well understood, with primary knock-on collisions constituting the majority of point-like defects in diamond. In harsh radiation environments these point-like vacancies are expected to be relatively well-distributed in the diamond sensor material. However, the expected performance of diamond relative to charge collection efficiency of holes or electrons is inconsistent, indicating induced vacancies and other defects within the diamond lattice interact during irradiation and self-repair leading to a complicated microstructure. We present the characterization of the type and extent of lattice damage caused in high purity (~1 ppb N) CVD grown single-crystal diamond subjected to GeV Sn and Zr irradiation. High-precision, spatially resolved X-ray diffraction methods are used generate a spatial map of the underlying structural changes (damage) induced by ion bombardment. These maps of damage distribution are expected to inform on the interactions and behavior of distributed defects before and after repair by annealing. By codifying the structural state of diamond as function of location, localized changes to the lattice can be tracked and repair methodologies developed to increase repair efficiency relative to their observed behavior.

PS12

(Student) Synthesis of Ferrite-Ferroelectric Coaxial Nanofibers by Electrospinning and Studies on Magneto-Electric Interactions Ying Liu, Peng Zhou, Mitchell Harshfield and Gopalan Srinivasan; Physics, Oakland University, Rochester, Michigan, United States.

Composites of ferromagnetic and ferroelectric phases are of interest for studies on the nature of coupling between the electric and magnetic subsystems and for useful applications such as sensors of magnetic fields and high frequency signal processing devices [1]. The coupling between the ferroic phases is mediated by mechanical strain. In an applied magnetic field H, for example, magnetostrictive strain in the ferromagnetic phase when transferred to the ferroelectric phase will result in an electrical

response due to piezoelectric effect in the ferroelectric phase. Composites of ferromagnetic oxides, alloys or metals and ferroelectric lead zirconate titanate (PZT) or barium titanate (BTO) are reported to show very strong magneto-electric (ME) coupling. Very recent efforts on enhancing the ME coupling in multiferroic composites have focused on nanocomposites. Since the ME coupling originates from strain transfer at the interface between the ferroic phases, nano-composites with surface area-to-volume ratios that are orders of magnitude higher than bulk or layered systems are expected to show very strong ME coupling. This work in on the synthesis of coaxial nanofibers of nickel ferrite (NFO)- barium titanate (BTO) and NFO-PZT by electrospinning, assembly of the fibers into 2D and 3D superstructures in a magnetic field and measurements on ME interactions [2]. Electrospinning techniques were used to prepare core-shell fibers of 0.5-1.5 micron in diameter. Fibers were annealed at 700-800 C and characterized in terms of structure and ferroic order parameters by scanning electron microscopy, X-ray diffraction, and scanning probe microscopy. Fibers free of impurities with uniform core and shell structures were evident from these studies. Ferromagnetic and ferroelectric order parameters for the fibers compare favorably with parameters for bulk NFO and BTO or PZT. The fibers were assembled into discs and films in a uniform magnetic field or a field gradient. Studies on ME coupling in the assembled films and discs were done by magnetic field H induced polarization, magneto-dielectric effects at low frequencies and at 16-24 GHz, and low frequency ME voltage coefficients (MEVC). We measured ~ 7 -32% change in remnant polarization for $H = 7$ kOe, and a MEVC of 0.4 mV/cm Oe at 30 Hz. Strong ME interactions were evident from H -induced variation in permittivity at 20-22 GHz. A model was developed for low-frequency ME effects in an assembly of fibers and took into account dipole-dipole interactions between the fibers and fiber discontinuity. Theoretical estimates for the low-frequency MEVC have been compared with the data. 1. Srinivasan, Gopalan, Shashank Priya, and N. Sun. *Composite magnetolectrics: materials, structures, and applications*. Elsevier, 2015. 2. Sreenivasulu, Gollapudi, Jitao Zhang, Ru Zhang, Maksym Popov, Vladimir Petrov, and Gopalan Srinivasan. "Multiferroic Core-Shell Nanofibers, Assembly in a Magnetic Field, and Studies on Magneto-Electric Interactions." *Materials* 11, no. 1 (2018): 18.

PS13

(Student) Fabrication and Characterization of Ag Nanowires Integrated with ITO Nanodots for a Transparent Conductive Electrode in Ultraviolet Light-Emitting Diodes Gun Hee Lee¹, Tran Viet Cuong^{1,2}, Beo Deul Ryu^{1,2}, Hyungtae Yeo¹, Eun-Kyung Suh¹ and Chang-Hee Hong¹; ¹School of Semiconductor and Chemical Engineering, Chonbuk National University, Jeonju, Korea (the Republic of); ²LED Agri-bio Fusion Technology Research Center, Chonbuk National University, Jeonju, Korea (the Republic of).

GaN-based ultraviolet light emitting diodes (UV-LEDs) has attracted much attention in recent years due to their potential application in biological agent identification, chemical sensing, instrumentation, and fluorescence excitation. However, the optical output efficiency of UV-LEDs is still limited by several factors, including high threading dislocation, and high resistivity of p-GaN due to Mg doping difficulties. In addition, a high optical absorption characteristic of indium tin oxide (ITO) in the UV region making it difficult to be used as a transparent conducting oxide in UV-LEDs. In this context, silver nanowire (AgNWs) has been considered as a substitution for ITO due to its outstanding properties such as high flexibility, optical transmittance, and high electrical conductivity. However, post-coated AgNWs results in a random arrangement that gives rise in high contact resistance. In order to overcome this problem, we herein demonstrate a high quality of transparent conductive electrode based on AgNWs integrated with ITO nanodots. A typical diameter of ITO nanodots and distribution density in optical conditions were about 150 nm and 5×10^9 cm⁻², respectively. Consequently, the optical transmittance of AgNWs integration with ITO nanodots was found to be higher than 90% in UV and visible range. For the application, UV-LEDs with a transparent conducting oxide layer of AgNWs integrated with ITO nanodots, ITO nanodots, and ITO were fabricated, respectively. The device performances of the UV-LEDs with three different electrodes were compared. The electroluminescence intensity of UV-LED with AgNWs-ITO nanodots indicated significant improvement as compared to those of other electrodes because of the effective current spreading and optical transmittance. In the other hand, the highest electroluminescence intensity was attributed to the effective current spreading path and surface texturing effect of AgNWs and nanodots.

PS14 WITHDRAWN

Fabrication of Flexible Energy Storage Device Using MnO₂@Graphene Composite Synthesised by Electrochemical Exfoliation Method Himadri T. Das, Sreejith P. Babu and Elumalai Perumal; Green Energy Technology, Pondicherry University, Kalapet, India.

Conventional energy storage devices have relied upon the ability of the electrochemically active materials to store the charge in the wide potential region with high Coulombic efficiency. Transition metal oxides are considered as ideal electrode materials in various energy storage devices, owing to their unique features, namely, high theoretical specific capacity; pseudocapacitive nature and ability to deliver large energy and power density. However, it suffers from many drawbacks, such as low electronic conductivity and capacity fading with the number of cycles. To address these shortfalls metal oxides are, usually, embedded within a conductive carbon-based matrix (for example graphene). The use of graphene would afford easy pathway for electron movement and increases the surface area for higher interaction of active electrode materials with electrolyte. Subsequently, graphene-based transition metal oxides composites have attracted active research pursuits in synthesizing the low-cost effective electrode materials for energy storage devices. In this work, we report a facile and economic approach to produce manganese oxide nanorods amalgamated on the graphene sheets (MnO₂@G) powders with an aim to achieve improved electrochemical activity. This electrochemical exfoliation strategy demonstrates a synthesis scheme from the graphite sheets at a constant voltage of 10 V in the MnSO₄ bath solution, the outcome of which is the black shiny flaky powders. The crystallinity MnO₂@G powders' was confirmed by XRD analysis. The TEM reveals the incorporation of MnO₂ nanorods on the exfoliated few layers of graphene nanosheets. The physiochemical and electrochemical properties were tuned by varying concentrations of MnSO₄ solutions. Interestingly, it was found that the yield of graphene as well as the performance of MnO₂@G governed by the concentrations of salt solution. The degree of graphitization in the as-prepared materials was investigated by depth analysis in the Raman spectroscopy. Further, the electrochemical performances of MnO₂@G were examined by cyclic voltammetric, charge-discharge and electrochemical impedance spectroscopy studies in a three-electrode set-up. It was discovered that the MnO₂@G composite prepared using 0.1 M MnSO₄ solution has a delivered better electrochemical performance. To realize the practical applicability of the MnO₂@G composite, flexible light-weight solid-state prototype asymmetric supercapacitor was fabricated using MnO₂@G as positive and graphene as the negative electrode. The fabricated devices exhibited ample storage capacity along with high energy density and power density which were capable of powering consumer electronics applications. Thus, in the present work, we have developed a cheap and effective electrochemical preparation of exfoliated MnO₂@G composites in high yield. This scheme could serve as a precedent to the development of potential electrode materials for energy storage devices. References: H. T. Das, K. Mahendraprabhu, T. Maiyalagan, P. Elumalai, *Sci. Rep.*, **2017**, 7, 1-14. M. Huang, F. Li, F. Dong, Y. X. Zhang, L. L. Zhang, J. Mater. Chem. A, **2015**, 3, 21380-21423. K. Ghosh, C. Y. Yue, M. S. Moniruzzaman, R. K. Jena, S. Bi, *Sustainable Energy Fuels*, **2018**, 2, 280-293. M. F. El-Kady, Y. Shao, R. B. Kaner, Graphene for batteries, supercapacitors and beyond, *Nat. Rev. Mater.*, **2016**, 1, 1-14. E. Duraisamy, H.T Das, A. S. Sharma, P. Elumalai, *New J. Chem.*, **2018**, 42, 6114-6124.

PS15

Interfacial Characteristics of Thermal Atomic Layer Deposited AlN on n-GaN Hogyoung Kim, Hee Ju Yun and Byung Joon Choi; Seoul National University of Science and Technology, Seoul, Korea (the Republic of).

Because of large band gap, high electron saturation velocity, and high breakdown field, gallium nitride (GaN) and related materials have gained much attraction for fundamental studies as well as device applications such as light emitting devices, high-power, high-temperature, high-frequency devices. High performance GaN based devices can be realized when metal/GaN interfaces are controlled with a low interface state density and removal of native oxide. Atomic layer deposited aluminum nitride (AlN) has been researched as a passivation layer, which were found to effectively compensate the high-density slow-response acceptor-like interface traps, with the smaller frequency dispersion. However, AlN can be easily oxidized during the air exposure, requiring a protection layer. In this work, we investigated the interfacial properties of Pt/GaN diodes with different dielectric layers such as Al₂O₃/AlN, HfO₂/AlN and HfO₂/Al₂O₃/AlN. Here, oxide layers were also acted as an AlN protection layer. According to conductance-voltage characteristics, there existed two types of traps (interface and border traps) for Al₂O₃/AlN and one type of traps (interface traps) for HfO₂/AlN and HfO₂/Al₂O₃/AlN. The border traps were

found to be located at 0.33~0.35 eV below the GaN conduction band. Most of all, the lowest interface traps density was observed for $\text{HfO}_2/\text{Al}_2\text{O}_3/\text{AlN}$. The reverse leakage current was explained by Fowler-Nordheim (FN) for HfO_2/AlN and $\text{HfO}_2/\text{Al}_2\text{O}_3/\text{AlN}$ and trap assisted tunneling (TAT) for $\text{Al}_2\text{O}_3/\text{AlN}$. X-ray photoelectron spectroscopy (XPS) analysis showed that the formation of Ga-O bonds near the AlN/GaN was suppressed effectively. Our work suggests that $\text{HfO}_2/\text{Al}_2\text{O}_3$ bilayer is a beneficial AlN protection layer. Further investigation using XPS and transmission electron microscopy (TEM) is in progress and will be discussed later.

PS16

(Student) Tuning Infrared Transmittance of ITO-Based Multilayer Films by Using Ag Disc Array Hyeon-Seop Im and Tae-Yeon Seong; Korea University, Seoul, Korea (the Republic of).

The development of high-quality transparent conducting electrodes (TCEs) is essential for enhancing the performance of photonic and optoelectronic devices such as photovoltaic cells, photodetectors, and LEDs. Currently, ITO has been commonly employed as TCE because of its high transparency (over 85% at 460 nm) and low resistivity ($\sim 10^{-4} \Omega\text{cm}$). However, there is a need for creating alternative TCEs that have higher figure of merit (FOM) than ITO to further improve the efficiency of devices. Thus, in this study, we first used Ag disc array (200 and 300 nm in diameter) to realise the high-infrared-transmittance of ITO-based multilayers. The electrical and optical properties of the ITO/Ag disc array/ITO samples were compared with ITO-only and ITO/Ag/ITO samples. Unlike the ITO/Ag/ITO sample, the transmittance of Ag disc array multilayer samples exhibited undulation in the visible region and large depression in the infrared spectral region. At 982 nm, the 300-nm Ag disc, ITO/Ag/ITO, and ITO-only samples had a transmittance of 95.1%, 32.5% and 86.8%, respectively. This implies that the transmittance in the IR region can be tuned by controlling size of the Ag discs. The sheet resistances of the Ag disc array, ITO/Ag/ITO, and ITO-only samples were 75.7-79.7, 4.77 and 147.96 $\Omega/\text{sq.}$, respectively. The Ag disc array samples showed mobilities of 32.11 – 33.91 cm^2/Vs , while the ITO/Ag/ITO sample gave 17.45 cm^2/Vs . The 200-nm Ag disc array sample exhibited higher Haacke's figure of merit (FOM) than the ITO/Ag/ITO sample. Finite-difference time-domain (FDTD) simulations were performed to understand the measured transmittance behaviour and the undulating transmittance of the Ag disc array samples was attributed to localised surface plasmon resonance effect. These results show that the transmittance in the IR region can be tailored by controlling size of the Ag discs and the Ag disc multilayers could act as a potentially important TCE or optical filter for IR devices.

PS17

(Student) Seebeck and Hall Coefficient Measurements on ZnSnN_2 and MgSnN_2 —Estimating the Density of States Effective Mass James R. Millard¹, John W. Cenker¹, Jeffrey Dyck¹, Krystal R. York⁴, Robert Makin³ and Steve Durbin²; ¹Physics, John Carroll University, University Heights, Ohio, United States; ²Western Michigan University, Kalamazoo, Michigan, United States; ³Electrical and Computer Engineering, Western Michigan University, Kalamazoo, Michigan, United States; ⁴Electrical and Computer Engineering Department, Western Michigan University, Kalamazoo, Michigan, United States.

There has been significant interest in the family of heterovalent ternary nitrides, in particular ZnSnN_2 and MgSnN_2 , as alternatives to InGaN for some optoelectronic applications. The II-IV-nitride compounds can be thought of as derived from the parent III-nitride compounds, where pairs of column III atoms are replaced with a Sn and either Zn or Mg atom. Key advantageous distinctions with both ZnSnN_2 and MgSnN_2 include the property that disorder on the cation sublattice affects the band gap (through essentially the entire visible spectrum), and they are composed of earth-abundant and nontoxic elements. Research into the basic electronic and optical properties of these materials are still at the early stages. For example, there have been no experimental reports of the effective mass of oxygen-free material to offer comparison to theoretical studies that predict a value of $m^* \sim 0.1 m_e$. [1-3] In this work, we present temperature dependent electrical resistivity, Hall effect and Seebeck coefficient (S) data on thin films of MgSnN_2 and ZnSnN_2 grown on (111) YSZ by plasma-assisted MBE. Samples represent a range of cation ordering, and recently we have succeeded in synthesizing cubic ZnSnN_2 . The electron concentration of typical samples is in the 10^{19}cm^{-3} range and independent of temperature, which indicates a degenerate carrier gas. Hall mobility is also independent of temperature. Seebeck coefficient data of ZnSnN_2 show a roughly linear dependence on temperature from 30 K – 300 K, which is expected for a degenerate carrier gas. Comparisons of the carrier concentration and Seebeck data to a Boltzmann transport model in the

relaxation time approximation allow for a determination of the density of states effective mass. This analysis on the room temperature data provide an effective mass of $\sim 0.08 m_e$ in the case of ZnSnN_2 ; measurements on MgSnN_2 are in process. A discussion of the dependence of this value on a range of carrier concentration values will be provided. References: [1] A. Panya, W.R.L. Lambrecht, and M. van Schilfgaarde, Phys. Rev. B **84**, 165204 (2011). [2] L. Lahourcade, N. C. Coronel, K. T. Delaney, S.I.K. Shukla, N. A. Spaldin, and H. A. Atwater, Adv. Mater. **24**, 2562 (2013). [3] T. D. Veal, N. Feldberg, N. F. Quackbush, W. M. Linhart, D. O. Scanlon, L. F. J. Piper, and S. M. Durbin, Adv. Energy Mater. **5**, 1501462 (2015).

PS18

Variable Field Hall Measurements and Multi-Carrier Analysis for Low Mobility Material with FastHall™ Jeffrey Lindemuth; Lake Shore Cryotronics, Westerville, Ohio, United States.

Variable field Hall measurements determine the resistivity and Hall coefficient of a material at various magnetic fields. For multi-carrier analysis, this data is fit to models of the conduction to extract the number of carriers, the type, the mobility, and the carrier concentration of each carrier. In traditional DC field Hall measurements, these quantities are measured at both positive and negative field for each magnetic field. The resistivity and Hall coefficient are calculated as the sum (resistivity) and difference (Hall coefficient) of the two field measurements. Due to offset and temperature drifts in the measurements, this DC method is limited to materials with mobility 10 $\text{cm}^2/(\text{Vs})$ or greater. Methods such as AC field Hall are useful to measure lower mobility samples; however, since the measured Hall coefficient is a weighted average (rms) of all fields swept out by the AC magnetic field, the data is not useful for multi-carrier analysis. FastHall™ is a method for Hall measurements that uses the reverse-field reciprocity theorem instead of physical field reversal to remove unwanted offsets in the Hall measurement. The field reversal is obtained by interchanging the current source connections to the sample, with the voltage measurement connections. This reversal can be accomplished at relatively high frequencies (100s of Hz) so the advantage of AC field is achieved, and low mobility material can be measured. With the FastHall™ protocol, the field applied to the sample is a DC field, so the FastHall™ data can be used for variable field Hall measurements and multi-carrier analysis. The data only needs to be acquired at positive fields, so the measurement time is at least twice as fast as standard DC methods. Also, the FastHall™ method can be used with superconducting magnet systems as well as electromagnet systems. To test the feasibility of using the FastHall™ method for multi-carrier analysis, a GaAsSb sample was measured using both the FastHall™ method and the standard DC field method. The mobility of the GaAsSb sample was low enough (about 20 $\text{cm}^2/(\text{Vs})$) to show the usefulness of FastHall™ for low mobility materials, but not so low that the sample could not be measured with standard DC methods. The DC field Hall measurement was performed using a Lake Shore Model 9709 HMS system, which allows measurements to magnetic fields of 9 T. The FastHall™ measurements were completed using a prototype Lake Shore Model M91 FastHall™ measurement controller and a 9 T superconducting magnet. In each case, the resistivity and Hall coefficient were measured at 30 different fields between 0.01 T and 9 T. The data was fit to the standard two carrier conductivity model; the mobility and resistivity of each carrier is derived from this fit. In each case, one of the carriers was a hole, the other was an electron. For the DC Hall method, the mobility of the hole was 48, and the mobility of the electron was 56. For the FastHall™ method, the mobility of the hole was 46, and the mobility of the electron was 68. The conductivity of the hole was 4 times lower than the conductivity of the electron in both methods. The fit to the data was better with the FastHall™ protocol. The FastHall™ method provides a Hall measurement protocol to obtain variable field Hall data for multi-carrier analysis. Of course, for low mobility materials, the conduction methods may not be band conduction, so care must be used to analyze the data.

PS19

(Student) Wide Bandgap and Uniform Nanocrystalline Zinc-Oxide for Nanocrystalline Inorganic Perovskite-Based LEDs Jihun Lim¹, Orlando Trejo², Carli Huber³, Neil P. Dasgupta² and Lingjie J. Guo^{1,2}; ¹Electrical Engineering and Computer Science, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Mechanical Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ³Materials Science and Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

Over the last few years, halide inorganic perovskite materials have attracted much attention due to their optoelectronic properties. Here, we introduce atomic-layer-deposition (ALD) of high quality nano-crystalline

Zinc-oxide (ZnO) as the electron transport layer for light-emitting-diodes (LED) using nano-crystalline inorganic halide perovskites of CsPbBr₃. X-ray photoelectron spectroscopy analysis showed that the ALD ZnO films contained a high density of oxygen-vacancies acting as donors, leading to an electron carrier concentration of $\sim 10^{19}/\text{cm}^3$. These properties were shown to be independent of thickness and time dependent electrical characteristics. Additionally, atomic force microscopy (AFM) analysis shows that the ZnO surface roughness was below 2nm. The large valence-band offset of the junction due to ZnO's wide bandgap facilitated emission from the green LED, despite the charge imbalance in the LED structure. In conclusion, the facile deposition of wide bandgap and uniform nano-crystalline ZnO charge transport layers by ALD could be promising as perovskite-based emission layers to suppress the non-radiative states at the interface for future optoelectronic devices.

PS20

(Student) Surface Encapsulated β -Ga₂O₃ Nanomembrane Field-Effect Transistor with Atomic-Layer Deposited Al₂O₃, Jiyeon Ma¹, OukJae Lee² and Geonwook Yoo¹; ¹School of Electronic Engineering, Soongsil University, Seoul, Korea (the Republic of); ²Center for Spintronics, Korea Institute of Science and Technology, Seoul, Korea (the Republic of).

β -Ga₂O₃ with a wide bandgap of 4.9 eV has attracted much attention as promising materials for next power devices applications due to its superior electrical properties allowing high temperature and high voltage operation [1]. As its monoclinic structure allows a facile cleavage into nanomembrane along [100] direction using mechanical exfoliation, several studies are investigated based on the nanomembrane preserving the intrinsic electrical properties [2, 3]. However, the superior electrical properties are degraded by surface defect states and adsorbates such as water and oxygen molecules inducing channel depletion effect [4]. Hence, surface passivation is imperative to maintain and improve the electrical properties. Here, we report the effect of ALD Al₂O₃ encapsulation on β -Ga₂O₃ nanomembrane FETs. Mechanically exfoliated β -Ga₂O₃ flakes from a (-201) surface β -Ga₂O₃ bulk with unintentional doping n-type doping (UID) concentration of $4.8 \times 10^{17} \text{ cm}^{-3}$ were transferred onto a heavily doped p-type Si substrate with thermally grown 300nm SiO₂. Source and drain electrodes were defined by photolithography, thermal evaporation n of Ti/Au (20nm/120nm), and lift-off process. Then, the top surface of β -Ga₂O₃ was passivated with the 20 nm thick Al₂O₃ layer deposited by ALD at 200 °C. Lastly, source/drain (S/D) contact was open by reactive-ion etching (RIE) using CF₄/O₂ gases. Fig. 1 illustrates a schematic of the fabricated β -Ga₂O₃ FET, and Fig. 2(a) shows its representative SEM image. Fig. 2(b) shows cross-sectional high resolution transmission electron microscopy (HR-TEM) of β -Ga₂O₃ without defect and strain. Lattice plane of (200) and (002) were confirmed by using d-spacing calculation as shown in the selected-area electron diffraction pattern of Fig. 2(c), which β -Ga₂O₃ indicates flakes were exfoliated in direction of [100]. Fig. 3 (a) and (b) shows that STEM image of the interface of Al₂O₃/ β -Ga₂O₃(100) and EDX compositional mapping of different layers, confirming achievement of a uniform Al₂O₃ deposition on the β -Ga₂O₃ surface. Fig. 4 and Fig. 5 show transfer and output characteristics of the fabricated β -Ga₂O₃ FET before and after Al₂O₃ passivation, respectively. After the passivation, electrical parameters including maximum transconductance (g_m), hysteresis (ΔV), contact resistance (R_c) and subthreshold slope (SS) were improved, as summarized in Table 1. These results are associated with alleviation of surface defects and adsorbates by Al₂O₃ encapsulation, which leads to minimized surface channel depletion and negative voltage threshold voltage shift (V_{th}). Fig. 6 shows comparison of three-terminal off-state breakdown measurement between unpassivated and passivated β -Ga₂O₃ FET with Al₂O₃. Although the unpassivated β -Ga₂O₃ FET shows the breakdown voltage (BV) of 123 V, no destructive breakdown of the Al₂O₃ passivated β -Ga₂O₃ FET was not observed in the sweep range. In summary, we have investigated the effects of ALD Al₂O₃ passivation on β -Ga₂O₃ FETs. By the passivation, electrical parameters are improved, and no electrical breakdown is observed in sweep range at three-terminal off-state breakdown measurement. Therefore, the results substantiate that ALD Al₂O₃ passivation layer plays a key role to improve and sustain performance of β -Ga₂O₃ FETs. This work was supported by the NRF grant (2017R1C1B5017470) and by the MOTIE (2000030), Korea. The EDA tool was supported by the IC Design Education Center (IDEC), Korea. Reference: [1] M. Higashiwaki, et al., *Applied Physics Letters*, 2013. **103**(12). P. 123511. [2] H. Zhou, et al., *IEEE Electron Device Letters*, 2017. **38**(1) p. 103-106. [3] H. Bae, et al., *IEEE Electron Device Letters*, 2018. **39**(11) p. 1708-1711. [4] S. Song, et al., *Applied Physics Letters*, 2008. **92**(26). p 263109.

PS21

Laser Seeding for the Preparation of Conductive Features on Glass Substrates Joel N. Schrauben; Central Research, Electro Scientific Industries, Portland, Oregon, United States.

This talk will describe a novel process for the preparation of conductive features on glass substrates. In this process, an ultrafast green laser is utilized to remove material from a transparent glass substrate, and a second laser source deposits Cu droplets through the laser-induced forward transfer of a donor film into the laser-etched features. Electroless plating methods that employ the laser-deposited Cu droplets as autocatalytic sites for plating (i.e., "seeds") are then used to fill in the laser-etched features. This methodology has been applied to prepare highly transparent conductive networks of Cu wires. The geometry and connections of the wires are completely determined by the laser processing parameters, which offers great flexibility for tuning the electrical and optical properties of the transparent conducting electrode. Honeycomb and crosshatched patterns comprising 10 micron wide wires with variable pitch were plated on borosilicate glass substrates. The crosshatched patterns have sheet resistances less than 1 Ohm/square and transmittance over 90% across the visible, surpassing typical ITO performance. Microscopic imperfections were observed in the plated material, which, in addition to shrinking the size of the plated features, represent fruitful space for further optimization of the process. Using the same methods toward the preparation of printed circuit boards that utilize bulk glass as a dielectric medium, we have demonstrated fine pitch wires, variable diameter through holes and blind vias and a multilayer stack. The deposits have a resistivity less than a factor of 1.5x that of bulk copper for 5-10 mm long wires. For PCB manufacturing, the process presents the potential for significant material savings in terms of base materials, process chemicals, and waste disposal/recycling costs, e.g., glass is on the order of 100-fold less expensive than some current high-frequency dielectrics, and wet processes account for a large part of standard PCB/substrate manufacturing.

PS22

(Student) Impact of Organic and Chlorine Based ALD Precursors on Hafnium Dioxide Based Nanoscale RRAM Devices Jubin Hazra¹, Maximillian Liehr¹, Karsten Beckmann², Christopher Hobbs², Martin Rodgers² and Nathaniel Cady²; ¹Nanoscale Engineering, SUNY Polytechnic Institute, Albany, New York, United States; ²College of Nanoscale Science & Engineering, SUNY Polytechnic Institute, Albany, New York, United States.

Resistive Random Access Memory (RRAM) is a novel form of non-volatile memory expected to find applications in neuromorphic computing, artificial intelligence, and memory. Its advantages include simple structure, small area, low power consumption, compatibility with CMOS processing technology, and high switching endurance. In this work, fully integrated nanoscale CMOS/RRAM structures were implemented on a 300 mm wafer platform using a custom RRAM module within SUNY Polytechnic Institute's 65nm CMOS process technology. The RRAM device stack is comprised of a TiN bottom electrode, a HfO₂ mem-resistive switching layer, a Ti oxygen exchange layer (OEL), and a TiN top electrode. This stack is implemented between the M1 and M2 metallization layers, using a FEOL-compatible process flow. In an effort to improve device performance, the impact of the HfO₂ atomic layer deposition (ALD) precursor on the threshold voltages, resistance levels, endurance, and yield was investigated. A two-wafer split was executed between two 6.3 nm thick HfO₂ films, one with an organic based precursor and the other with a chlorine based precursor. Secondary ion mass spectroscopy (SIMS) characterization was used to quantitatively differentiate the relative amount of C and Cl content in these two different HfO₂ films. For electrical characterization, a pulse-based approach was adopted to apply pulses in the orders of tens of microseconds for set/reset operation of ReRAM devices. A read pulse of -0.2 V with a 10 us pulse width was applied after each set/reset operation, to read out the high resistance state (HRS) and low resistance state (LRS). To gain a statistically significant comparison, 50 RRAM devices were tested on similarly positioned dies for each wafer. Based on those 50 tested devices, we demonstrated an overall yield of 86% for Cl based HfO₂ precursor, as compared to 52% for the organic HfO₂ precursor wafer, resulting in significant yield improvement. Higher forming voltages and memory window were also observed for devices fabricated using the Cl based precursor. Ongoing compositional and structural analysis of the deposited HfO₂ films via TEM and electron energy loss spectroscopy (EELS) are expected to reveal distinct differences which contribute to the differences in yield, memory window and forming voltage for the Cl vs C based HfO₂ precursors.

PS23

Resources for Uncertainty Analysis [Kris Bertness](#); National Institute of Standards and Technology, Boulder, Colorado, United States.

It can be argued that science is not the pursuit of what we know with certainty, but rather that pursuit in which we evaluate how well we know what we assert is true. Uncertainty analysis thus becomes a key component in the evaluation of scientific “truth.” This poster will describe resources made available by the National Institute of Standards and Technology (NIST) and other world-wide national metrology institutes to aid technologists in the evaluation of uncertainty in their data. These resources include the NIST Uncertainty Machine, a free on-line Monte Carlo simulator <https://uncertainty.nist.gov/>, NIST Technical Note 1297, <https://www.nist.gov/pml/nist-technical-note-1297>, and the more comprehensive Guide to the Expression of Uncertainty in Measurement, the “GUM”, <https://www.bipm.org/en/publications/guides/gum.html>. We will illustrate several examples and address the concepts of systematic vs. random error and statistical independence. Student attendees of the Electronic Materials Conference are encouraged to use this information in applications for the NIST-sponsored Student Uncertainty Analysis award.

PS24 WITHDRAWN

(Student) NSF Hurricane Harvey—Ultrasensitive Photodetector Development for High Throughput Bacteria Detection in Floodwater [Lauren Brady](#)¹, [Dali Shao](#)¹, [Debjit Ghoshal](#)², [Valencia Koomson](#)³ and [Shayla Sawyer](#)¹; ¹Electrical and Computer Systems Engineering, Rensselaer Polytechnic Institute, Troy, New York, United States; ²Chemical and Biological Engineering, Rensselaer Polytechnic Institute, Troy, New York, United States; ³Electrical and Computer Engineering, Tufts University, Medford, Massachusetts, United States.

Flooding after major hurricanes such as Hurricane Harvey can have long term consequences on water quality and human health. Pathogenic bacteria found in floodwaters present unique dangers as significant quantities of these pathogens can remain active for several months after a catastrophe happens, posing a hidden threat to those affected by natural disasters. By improving the synergistic properties of nanocomposites to create an ultrasensitive ultraviolet (UV) detector, the goal is to identify and quantify bacteria in floodwaters in real time. Intrinsic fluorescence serves as our detection mechanism for optical analysis, as these microbes will fluoresce when excited in the UV range. Our previous ultrasensitive UV light detector was created using a highly conductive graphene channel and a ZnO quantum dot (QD) layer, with a 10-decyltrichlorosilane organic self-assembled monolayer (SAM) interface, to reduce the impacts of charged impurity scattering and other scattering mechanisms on the carrier mobility. Experimental results from our device show a high photoresponsivity of 10^8 A/W, an increase in the carrier mobility to $10,800$ $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$, and a gain of 3×10^9 in the UV region. To improve device performance, alternatives to the SAM layer are explored to trade-off ultrahigh responsivity for improved dark current and faster time response. Devices with different absorption wavelengths are created by changing the QDs layer with materials such as cadmium sulfide (CdS). These devices are integrated into a frequency domain spectrometer circuit architecture that will allow for the creation of a sensor network that can be deployed real time.

PS25

(Student) Electronic Characteristics of $\text{Cu}_3(\text{BTC})_2$ Metal-Organic Framework Based Capacitors [Liz M. Montanez Huaman](#)^{1,2}, [Ina Strauss](#)³, ²Jürgen Caro³ and ¹Jörg Osten¹; ¹Institut für Materialien und Bauelemente der Elektronik (MBE), Gottfried Wilhelm Leibniz Universität Hannover, Hannover, Germany; ²Laboratory of Nano and Quantum Engineering, Gottfried Wilhelm Leibniz Universität Hannover, Hannover, Germany; ³Institute of Physical Chemistry and Electrochemistry, Gottfried Wilhelm Leibniz Universität Hannover, Hannover, Germany.

Metal Organic Frameworks (MOF) have been emerged as promising candidates for sensing applications due to its high porosity nature and large surface area which are tailored by changing the functionality of the linkers [1,2]. Particularly, the synthesis of thin MOF films on silicon substrates opens the possibility to integrate them easily into electronic devices such as capacitors and transistors. High density of defects can limit the reliability of electronic devices, therefore, characterization of interfacial defects are of great importance. Here, we present a detailed defect characterization in ultra-thin $\text{Cu}_3(\text{BTC})_2$ films incorporated within metal-insulating-semiconductor (MIS) capacitor structures. $\text{Cu}_3(\text{BTC})_2$ were deposited on thermally growth silicon dioxide surfaces by the spray-coating method. The crystal structure of the MOF was verified by X-ray diffraction (XRD) experiments. The results demonstrated a crystalline structure mainly oriented along the (222) diffraction plane. The

functionality of MOFs within MIS capacitors has been investigated through impedance measurements by sweeping the gate voltage from inversion to accumulation and back. We observed the formation of hysteresis which clearly indicates the presence of border traps. On the other hand, the conductance curve exhibits a peak as a signature of interface traps. It was found that the $\text{Cu}_3(\text{BTC})_2/\text{SiO}_2$ stack based MIS capacitor shows improved density of interface and border traps and better insulating qualities than non-annealed SiO_2 alone. The relatively low density of interfacial defects demonstrates the potential of MOFs in capacitors devices. [1] W.J. Li, J.L., Z.H. Sun, T.F. Liu, J. Lü, S.Y. Gao, C. He, R. Cao, J.H. Luo, Nat. Commun. 7 (2016) 11830. [2] L. Montañez, K. Müller, L. Heinke, H.J. Osten, Microporous and Mesoporous Mater. 265 (2018) 185–188.

PS26

(Student) Formation and Characterization of the $\text{Sm}_x\text{Mg}_{1-x}\text{Mg}_2\text{Sb}_2$ System [Mack M. Marshall](#), [Sevan Chanakian](#) and [Alexandra Zevalkink](#); Michigan State University, East Lansing, Michigan, United States.

In recent years there has been renewed interest in Mg_2Sb_2 , which forms in the CaAl_2Si_2 crystal structure, due to its high performance as an *n*-type thermoelectric material. Motivated by reports of superstructuring, and in an effort to explore the Mg_2Sb_2 system further, Samarium was substituted on the cation site. $(\text{Mg},\text{Sm})\text{Mg}_2\text{Sb}_2$ is the only material with the CaAl_2Si_2 structure reported to form a superstructure. While the traditional CaAl_2Si_2 structure is formed by layers of cations sandwiching $[\text{Mg}_2\text{Sb}_2]^{2-}$ slabs, the superstructure alternates between ordered Mg^{2+} and Sm^{2+} cation sheets, thus increasing the number of atoms per unit cell by a factor of two. Increased number of atoms per unit cell is associated with decreased thermal conductivity due to increases in the number of phonon modes. Understanding why this superstructure forms will provide insight into bonding in analogous materials and a possible avenue into engineering the thermal properties of the CaAl_2Si_2 crystal family. Interestingly, the lattice parameters of the $(\text{Mg},\text{Sm})\text{Mg}_2\text{Sb}_2$ superstructure deviate from the expected values following Vegard's Law. In order to explore the bonding nature in the superstructured CaAl_2Si_2 crystal system and understand the effects of superstructuring on the thermal and mechanical properties, the series $(\text{Mg}_{1-x}\text{Sm}_x)\text{Mg}_2\text{Sb}_2$ ($x = 0.25, 0.5, \text{ and } 0.75$) has been synthesized. Here the chemical characterization, thermal properties, and elastic moduli of this series are presented. Furthermore a discussion into the lattice distortions is provided by accounting for bond lengths between cation sheets.

PS27

(LATE NEWS) Surface Plasmon Wave Sensor Based on Graphene-TMD van der Waals Heterostructure [Partha Goswami](#); Deshbandhu College, University of Delhi, New Dehli, India.

Based on earlier works, it was shown that the dispersion of the van der Waals heterostructures (vdWHs) of graphene monolayer on 2D transition metal dichalcogenide (GrTMD) substrate comprises of the spin-split, gapped bands involving the $q^{2/3}$ (unconventional) behavior and not the well known $q^{1/2}$ behavior for strongly incarcerated intra-band plasmon dispersion at finite doping and the long wavelength limit. In this paper it is also found that (inter-band) acoustic plasmons for electron doping is possible if the system is surrounded by negative dielectric constant (NDC) materials. The intra-band absorbance is found to decrease with the frequency at a given gate voltage and increase with the gate voltage at a given frequency; the inter-band transmittance, however, is found to be a decreasing function of frequency and the gate voltage. The notable outcome of this work is the identification that the graphene-transition metal dichalcogenide (TMD)-graphene hybrid nanostructures is a plasmonic meta-surface for ultra-sensitive bio-sensing. The exponentially decaying fields of a surface plasmon wave (SPW) propagating along interface is highly sensitive to the ambient refractive index variations. For a SPW sensor with excellent performance, the full width at half maximum (FWHM) should be as small as possible. It is shown that FWHM is smaller at high photon energy and low gate voltage. In fact, in Figure 1, one can see a 3 D plot of FWHM as a function of the photon energy and the gate voltage. The reciprocal of FWHM is an important sensor performance parameter. It may be noted that though the metal-dielectric based SPW has been widely employed for sensing applications such as gas sensing, temperature sensing, and bio-sensing, due to its high sensitivity and reliability a SPW sensor based on the Gr-TMD heterostructure, however, has greater advantage as it is likely to have good (tunable) performance.

PS28

Crystal Growth and Lattice Dynamics of AMg_2Sb_2 ($X=\text{Ca, Mg, Sr}$) Zintl

Phases **Mario Calderon Cueva**; Chemical Engineering and Materials Science, Michigan State University, East Lansing, Michigan, United States.

In recent years, the low intrinsic lattice thermal conductivity of layered materials has been studied in an effort to increase the energy conversion efficiency for thermoelectric materials. MgMg_2Sb_2 has been found to have surprisingly low lattice thermal conductivity compared to heavier members (CaMg_2Sb_2 and SrMg_2Sb_2) of the same structure type. However, a detailed understanding of the mechanisms responsible for this behavior remains unclear. In this work, the anharmonic character of optical phonons is evaluated as a method to clarify the influence of bonding on the thermal conductivity. For that purpose, single crystal samples were obtained via self-flux growth technique for each compound. Additionally, spark plasma sintering (SPS) was used to obtain polycrystalline samples. For each compound phase purity was confirmed by powder XRD. Temperature-dependent Raman spectroscopy and inelastic neutron scattering measurements were conducted to characterize the anharmonicity behavior of the different compounds. Raman spectra were collected for single-crystalline and polycrystalline samples. The results obtained confirm the large anharmonic behavior of MgMg_2Sb_2 compared with isostructural compounds.

PS29

(Student) **Optoelectronic Excitations on the Nanoscale** **Markus Borsch**, Eric Martin, Steven T. Cundiff and Mackillo Kira; University of Michigan, Ann Arbor, Michigan, United States.

The ongoing miniaturization of electronic and optoelectronic devices can make quantum effects become more important, potentially leading to non-classical behavior. At the same time, the exceptional properties of bound electron-hole complexes/clusters, such as excitons and dropletions [Nature **506**, 471 (2014)], could yield a new class of excitonic and clustronic devices. Clearly, a deep understanding of the formation, interaction, and transport of carriers, excitons, and other quasiparticles in semiconductor nanostructures is necessary for advancing such quantum devices. We present a new cluster-expansion-based approach to include spatially local excitations up to two-particle correlations. The resulting theoretical framework is applied to quantitatively explain experiments producing a decreasing excitation-spot size when the optical excitation spot approaches nanoscale. The simplest form of the cluster expansion yields the semiconductor Bloch equations (SBEs) [Kira & Koch, *Semiconductor Quantum Optics*, (Cambridge, 2012)] that systematically and nonperturbatively describe the influence of many-body effects on optical properties. For homogeneous excitations the SBEs can be solved very efficiently. However, when spatially inhomogeneous excitations or structures are considered, the numerical effort grows exponentially. We derive the full kinetics of clusters up to doublets based on a Wigner-function approach paired with the cluster expansion. At this level, we not only describe polarization-density dynamics within the SBEs but also the decay of polarization into incoherent excitons. The approach replaces spatially homogeneous clusters of the SBEs by local microscopic clusters that has a macroscopic spatial dependence. For example, a microscopic polarization $P_{\mathbf{k}}$ becomes $P_{\mathbf{k}}(\mathbf{R})$ at position \mathbf{R} where \mathbf{k} refers to relative momentum at the nanoscale. In addition to the homogeneous contributions, the cluster dynamics is influenced by kinetic contributions producing a ballistic expansion of the excitation, a Hartree potential that tries to push the system towards local charge neutrality, and additional gradient terms from the exciting optical field, Coulomb renormalizations, and two-body correlations. We apply this new theory to study an experiment where gallium arsenide quantum-wells are excited by an ultrafast and tightly focused laser pulse, that is resonant with the 1s exciton. A second time-delayed probe pulse, which is spatially scanned across the optically excited region, is used to measure the spatially resolved nonlinear response. As a result, the excitation dynamics can be studied with both a spatial and temporal resolution. We find that the width of the created excitation spot changes after the initial excitation. A transient decrease of the spot size by about 2 % within the first 2-3 ps after the excitation is observed, followed by a slow diffusive expansion. We find that the conversion of polarization to incoherent excitons is essential to explain the reduction of the excitation spot size. If excitons are not included in the calculation, we only find a fast ballistic expansion of the excitation spot because electrons and holes are not bound to each other if the system does not contain either polarization or excitons. Only when two-body correlations are included to the calculation, we find a transient decrease of the spot size followed by an expansion, similar to the experiment. This shows that the observed reduction of the excitation spot size is a true many-body effect that is mediated by the Coulomb

interaction. In summary, we have developed a new cluster-expansion approach for spatially localized excitations in nano-optoelectronics. As a new effect, our experiment-theory comparison identifies a narrowing excitation spot as a result of polarization-to-population conversion. The developed approach can be extended to study quantum optoelectronic devices.

PS30

(Student) **Epitaxial Stabilization of $\kappa\text{-Ga}_2\text{O}_3$ and $\kappa\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ Thin Films for Heterostructure Device Applications by Tin-Assisted PLD on Different Substrates** **Philipp Storm**¹, **Max Kneiß**¹, Anna Hassa¹, Daniel Splith¹, Holger von Wenckstern¹, Thorsten Schultz², Norbert Koch², Michael Lorenz¹ and Marius Grundmann¹; ¹Faculty of Physics and Earth Sciences, Felix Bloch Institute for Solid State Physics, Universität Leipzig, Leipzig, Germany; ²Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany.

Due to the high expected breakdown field of $\beta\text{-Ga}_2\text{O}_3$ of 8 MV/cm [1], $\beta\text{-Ga}_2\text{O}_3/\beta\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ heterostructure devices are a promising alternative for power electronics. Recently, first modulation-doped field-effect transistors based on heterostructures on $\beta\text{-Ga}_2\text{O}_3$ substrates [2] featuring high mobilities in the $\beta\text{-Ga}_2\text{O}_3$ channel material have been reported. However, doping of $\beta\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ is still an issue. A feasible solution would be polarization doping, where a 2DEG can be created solely by polarization jumps at heterostructure interfaces. In contrast to the monoclinic β -phase, the metastable orthorhombic κ -phase of Ga_2O_3 is expected to exhibit a high spontaneous electrical polarization of $23 \mu\text{C}/\text{cm}^2$ along its c -direction [3]. However, for the application of this modification in $\kappa\text{-Ga}_2\text{O}_3/\kappa\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ heterostructure devices, the $\kappa\text{-Ga}_2\text{O}_3$ template as well as the $\kappa\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ barrier layers need to be grown with high crystalline quality on suitable substrate materials. The growth mechanism of the κ -phase is currently still under debate, especially in pulsed laser deposition (PLD). It was found, however, that the presence of tin is required for the formation of this phase [4]. Little is also known about the growth of the $\kappa\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ alloy system or important material parameters necessary for device design such as the variation of band gap, lattice constants or electrical polarization. Until now, only one report deals with the growth of $\kappa\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ by mist CVD on AlN templates [5]. In this work, we first show the PLD-growth of binary $\kappa\text{-Ga}_2\text{O}_3$ from a Sn-doped Ga_2O_3 target on different substrates ($c\text{-sapphire}$, $\text{STO}(111)$, $\text{YSZ}(111)$ and $\text{MgO}(111)$). (001)-oriented growth in the κ -phase with three rotational domains, well-defined in-plane epitaxial relationships and high crystalline quality was verified by XRD. Reciprocal space maps were utilized to determine the out-of-plane and in-plane lattice constants. AFM measurements reveal smooth surface morphologies with a RMS roughness below 1 nm, rendering these layers excellent growth templates for heterostructures. We performed depth-resolved XPS-measurements and found a tin enrichment at the surface. From this, we propose surfactant-mediated epitaxy as possible growth mechanism. The homogeneous $\kappa\text{-(Al}_x\text{Ga}_{1-x})_2\text{O}_3$ layers in this work were grown employing radially-segmented Sn-doped $\text{(Al}_x\text{Ga}_{1-x})_2\text{O}_3/\text{Ga}_2\text{O}_3$ targets with $x = 0.2$ or 0.4 . The Al-content in the layers was varied by a change in the position of the laser spot on the target, a technique extensively described in [6]. As substrate materials, $c\text{-sapphire}$ without miscut, or with 3° as well as 6° miscut, conductive Nb-doped STO(111) substrates and PLD-grown MgO(111) templates were used. Epitaxial growth and smooth surface morphologies were obtained with similar in- and out-of-plane orientations as for the binary layers. Further, composition-dependent lattice constants and bandgaps were evaluated. [1] Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012) [2] Zhang *et al.*, Appl. Phys. Lett. **112**, 173502 (2018) [3] Maccioni *et al.*, Appl. Phys. Expr. **9**, 041102 (2016) [4] Kneiß *et al.*, APL Materials **7**, 022516 (2019) [5] Tahara *et al.*, Appl. Phys. Lett. **112**, 152102 (2018) [6] Kneiß *et al.*, ACS Comb. Sci. **20**, 643 (2018)

PS31

(Student) **All-Semiconductor Selective Metamaterial Emitter at 3.45 μm with Larger Feature Sizes for Thermophotovoltaic Energy Conversion Applications** **Minsu Oh**, Emily Carlson and Thomas E. Vandervelde; Electrical Engineering, Tufts University, MEDFORD, Massachusetts, United States.

Thermophotovoltaic (TPV) systems are similar to photovoltaic systems except that they convert heat (infrared light) into electricity instead of focusing more on the visible. The efficiency of TPV energy conversion can be improved with a selective emitter that emits photons at just above the bandgap energy towards the TPV photodiode. Some metamaterials (MMs) have been reported for their selective absorption/emission properties for TPV applications. However, many of these selective MM emitters are made of a number of metallic and dielectric layers and have nanometer scale feature sizes where fabrication is difficult and can lead to pattern

imperfections that lower the performances. Additionally, with smaller feature sizes in nanometer scales, the MM emitter's performances may be more likely to decrease in time with more materials used or more interfaces between materials owing to optical property variation, compound formation, and phase transformation at elevated temperatures. This provides motivation to develop larger feature sized, simpler-structured selective MM emitters with fewer different materials used. One of the benefits of utilizing a semiconductor as the constituent material of a MM is that they offer more degrees of freedom in tailoring the MM's optical properties by a means of doping. For these reasons, we are interested in all-semiconductor selective MM emitters with larger feature sizes for TPV applications. In this work, we built a single layer of cylindrical structures of p-type Si. The electromagnetic responses of our selective MM emitter were simulated via CST Microwave Studio 2018 with a plane wave excitation at normal incidence. The software's Frequency Domain Solver was used to more precisely generate simulation meshes for circular structures. The optical dispersion curves of the p-type Si were generated using the Drude model. By optimizing the dimensions of the simulated MM structures, a peak emissivity of 92.4% was obtained at 3.45 μm with a FWHM of 400 nm. The peak emission wavelength of 3.45 μm here corresponds to the peak wavelength of blackbody radiation approximately at 840 K. The smallest dimension on the xy-plane of our structure is 0.7 μm , and the smallest-dimension-to-peak-emission-wavelength ratio (SDPW) of the structure is 0.203. We define the SDPW as the smallest dimension on the xy-plane of the structure divided by the peak emission wavelength to indicate relative fabrication ease compared to the peak emission wavelength. The selective MM emitter structure we propose here will be significantly easier to fabricate than previously reported selective MM emitters for TPV applications. We believe that our work demonstrates a path forward for future research on all-semiconductor selective MM emitters that will have relative fabrication ease with a variety of peak emission wavelengths and bandwidths for TPV applications. Fabrication and absorption/emission test results are forthcoming.

PS32

(Student) Plasma Density Impact on the Polycrystalline Diamond Growth on GaN Mohamadali Malakoutian¹, Matthew Laurent¹ and Srabanti Chowdhury^{1,2}; ¹Electrical and Computer Engineering, University of California, Davis, Davis, California, United States; ²Electrical Engineering, Stanford University, Stanford, California, United States.

GaN-based field effect transistors (e.g. HEMTs) exhibited an extremely high-power output at high frequencies. However, there are some significant limiting factors of the performance in the GaN HEMTs, which lead to a reduced channel mobility and large leakage current due to the self-heating. Therefore, it is necessary to dissipate the generated heat from the device. Owing to the excellent heat conductivity of diamond (~20 W/cm.K), a layer of polycrystalline diamond (PCD) on GaN can be used to spread the heat from the top of the device [1]. As hydrogen plasma is the main species in diamond growth, it can damage the GaN and change the properties of the 2-dimensional electron gas (2DEG). Also, it can prevent a uniform PCD deposition on the surface, as it is etching in the same time. In this work, a PCD layer was grown on Ga-polar, N-polar, and SiN/N-polar GaN, to compare the properties of the grown layer and the GaN-diamond interface. For all the samples, a polymer-assisted seeding technique has been used for the nucleation of diamond [2]. Then a low power growth recipe with different pressures (40, 60, and 80 torr) has been utilized for the growth (2% CH₄/H₂, ~650 °C, 1300 W microwave plasma, 1 hr). The interface of the GaN/diamond on N-polar and SiN/N-polar GaN exhibits no etching or decomposition of the GaN, while for the Ga-polar GaN, it shows an extensive etching sign in the interface. It can be concluded that the Ga-face of the GaN has a poor chemical stability in the H₂ plasma and may need to deposit diamond in Ar-rich plasma. The other important parameter is the uniformity of the PCD layer. SiN/N-polar GaN substrate shows a uniform layer of diamond with no delamination, while in the case of N-polar GaN without SiN, the diamond layer delaminates from >50% of the substrate. The delamination happens during the cooling down process, as the sapphire exhibits a large compressive stress. Formation of the SiC in the interface improves the adhesion of the diamond to SiN interlayer. Also, as the coefficient of thermal expansion for SiN is less than GaN and is closer to diamond, it makes a graded heterostructure (diamond/SiN/GaN/sapphire::1.1/3.3/4.1/5.3 $\mu\text{m}/\text{m.K}$) to compensate the difference in the thermal expansion between materials. Therefore, we have selected the SiN/N-polar GaN substrate for pressure study of the diamond growth. According to the top-view SEM micrographs, by increasing the pressure from 40 to 60 torr, there is a slight change in the grain size (130 to 180 nm), while at 80 torr the grain size increases by a factor of ~2 from 60 torr case (180 to 350 nm). PCD with 130, 180, or 350 nm grain size corresponds to a thermal conductivity of

40, 58, or 110 W/m.K, respectively. From the cross-sectional view of SEM micrographs, it can be seen that the thickness and the growth rate of the PCD are increasing by elevating the pressure (or the plasma density). The PCD thickness is ~170 nm for 40 torr, ~250 nm for 60 torr, and ~400 nm for 80 torr pressure. The grain size determines the surface to volume ratio, which corresponds to the sp² and hydrogen content. So, to have more sp³ bonding less grain boundaries or larger grain sizes are desired. It can be clearly seen that, by increasing the pressure the Raman spectra exhibits a reasonably sharper diamond peak around 1332 cm⁻¹, which confirms lower surface to volume ratio and higher sp³ bonding. In the Raman spectra, there is also some signs of sp² bonding and the hydrogen from the grain boundaries at around 1120, 1450, and 1560 cm⁻¹, which changes slightly with pressure. According to the results, the larger grain size of the PCD is desired for heat spreading purposes, as the thermal conductivity increases by the grain size. To have a larger grain size and higher sp³ bonding ratio, a higher growth pressure is needed. [1] Y. Zhou et al., Appl. Phys. Lett. 111, 041901 (2017). [2] H. A. Girard et al., ACS Appl. Mater. Interfaces, 1 (12), 2738–2746 (2009).

PS33

(Student) Evaporation of Ba and Sc from Scandate Cathode Surfaces Mujan Seif¹, Qunfei Zhou^{2,3}, John Balk¹ and Matthew Beck¹; ¹Department of Chemical and Materials Engineering, University of Kentucky, West Bloomfield, Michigan, United States; ²Materials Science and Engineering, Northwestern University, Evanston, Illinois, United States; ³Center for Nanoscale Materials, Argonne National Laboratory, Evanston, Illinois, United States.

Thermionic cathodes are key components in a wide range of vacuum electron devices (VEDs), including traveling wave tubes, microwave devices, thermionic energy converters, and more. A high performance subset of these, scandate cathodes, are fabricated by impregnating porous Sc₂O₃-doped W matrices with xBaO-yCaO-zAl₂O₃. The lifetime of these high performance cathodes is thought to depend on the rate at which evaporated surface Ba is replenished by Ba from within the porous bulk. To compute this rate, an understanding of the mechanisms by which Ba moves through porous W is critical. These mechanisms likely include surface diffusion and vapor flow, the latter being our focus. Previous work has calculated surface energies of a number of configurations of adsorbed Ba and O on the dominant facets present in the W grains. Currently, we use first-principle calculations to investigate conditions that instigate Ba desorption from the aforementioned surface configurations. The role of Sc is not yet known. It has been suggested that its role is similar to that of Ba, but little has been done to test this hypothesis. Here, Sc is examined with the same approach as Ba.

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(Student) Surface Passivation of III-Nitride Nanowires for Enhanced Solar Water-Splitting Nick Pant^{1,2}, Srinivas Vanka^{3,2}, Baowen Zhou², Alexa Roberts², Krishnamurthy Kulkarni² and Zetian Mi²; ¹Applied Physics, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Electrical Engineering and Computer Science, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ³McGill University, Montreal, Quebec, Canada.

Artificial photosynthesis sees the marriage of water and sunlight, two highly abundant resources, for a carbon-neutral and sustainable source of energy. Using only sunlight to split water into its constituents hydrogen and oxygen with high efficiency and long-term stability has been a long-endured challenge. Photocatalytic and photoelectrochemical water-splitting are two viable approaches for producing solar hydrogen. III-nitride nanowires grown on silicon by plasma-assisted molecular beam epitaxy (MBE) offer a promising platform for studying these reactions due to their excellent optical and electronic properties, large surface area to volume ratio, and long term stability. Efficient solar-to-hydrogen conversion requires excellent interfacial charge kinetics and transfer; dangling bonds and defect states on surfaces can act as electron traps and recombination centres that stymie this process. In this work, we show that surface passivation of III-nitrides by atomic layer deposition (ALD) of Al₂O₃ (~2 nm) can drastically increase both the solar-to-hydrogen (STH) efficiency of photocatalytic water-splitting and the photocurrent density of photoelectrochemical water-splitting by nearly one order of magnitude. The photocatalytic reaction proceeded on p-GaN and p-InGaN/GaN nanowire surfaces with photodeposited Rh/Cr₂O₃ as the hydrogen evolution co-catalyst. A 350 W Xenon lamp with an AM1.5G filter simulated 28 suns to create nearly flat-band conditions that allowed for electrons and holes to be extracted from the surface. With Al₂O₃ surface passivation, the photocatalytic hydrogen evolution rate for p-GaN increased by 54% and for p-InGaN/GaN by 22%, corresponding to STH efficiencies of 1.96% and 1.79%, respectively, which are among the best

reported values for direct solar water splitting. Moreover, photoelectrochemical water-splitting occurred spontaneously under AM1.5G (1 sun) on two photocathodic heterostructures: (1) *p*-InGaN nanowires linked by tunnel junctions to *n*-type silicon and (2) *p*-InGaN nanowires linked by tunnel junctions to *n*⁻*p*-*p*⁺ silicon solar cell. We platinized these structures using a previously reported photodeposition method and tested their performance in 0.5 M H₂SO₄ in both two-electrode and three-electrode configurations. Remarkably, under the two-electrode setup, the single junction structure (*p*-InGaN/TJ/*n*-Si) demonstrated an order of magnitude greater photocurrent with surface passivation and an STH of 1.17% at 0 V vs. IrOx. Similar results held for the double junction structure (*p*-InGaN/TJ/*n*⁻*p*-*p*⁺-Si) in the two electrode setup where Al₂O₃ yielded nearly a factor of two improvement in device performance. We believe surface passivation plays a critical role in these reactions by reducing unwanted surface recombination that depletes the photogenerated charge carriers available for water-splitting. Optimization of the surface passivation process is currently under progress to yield photocatalytic devices with STH >5% and double junction devices with STH >15%. Further investigations are ongoing to enable us to better understand the surface mechanisms that allow for such remarkable enhancement in performance.

PS35

(Student) Influence of Oxygen Deficiency on the Rectifying Behavior of Transparent Oxide Semiconductor-Metal Interfaces—Case Study of Amorphous Zinc-Tin-Oxide Oliver Lahr¹, Sofie Vogt¹, Thorsten Schultz², Peter Schlupp¹, Holger von Wenckstern¹, Norbert Koch², Marius Grundmann¹ and Anna Hassa¹; ¹Faculty for Physics and Earth Science, Felix Bloch Institute for Solid State Physics, Universität Leipzig, Leipzig, Germany; ²Institut für Physik, Humboldt Universität zu Berlin, Berlin, Germany.

Transparent amorphous oxide semiconductors (TAOS) have superior electronic transport properties compared to amorphous silicon. Further, their transparency in the visible spectral range makes TAOS promising for applications within bendable transparent circuits. Amorphous indium gallium zinc oxide metal-semiconductor field-effect transistors are already used as pixel drivers in OLED displays. To fabricate high performance electronic devices, the formation of rectifying contacts is required. The important role of oxygen for the formation of highly rectifying contacts to crystalline oxide semiconductors has been discussed in literature. A prominent example is zinc oxide, where a non-reactive deposition of the metal contact leads to a Schottky barrier height of 0.75 eV, independent of the used metal and its work function [1,2]. This is attributed to a high oxygen vacancy density at the interface [1]. For many other oxide semiconductors, such as SnO₂, In₂O₃ and indium-gallium-zinc-oxide, it is known that a reduction of interface near oxygen vacancies is required to achieve rectifying contacts [3-5]. For non-reactive metal depositions, ohmic or weakly rectifying behavior is observed [2,4-6]. We investigate the influence of the amount of (active) oxygen offered during the formation of rectifying contacts on the properties of Schottky barrier diodes comprising amorphous zinc-tin-oxide (ZTO) [7]. The ZTO thin films were deposited by pulsed laser deposition at room temperature. All metal and metal oxide contacts were deposited by de-sputtering. A comparative study of a ZTO/platinum (ZTO/Pt) Schottky contact (SC) and a ZTO/platinum oxide/platinum (ZTO/PtO_x/Pt) SC is performed. The samples were investigated by current-voltage measurements and x-ray photoelectron spectroscopy (XPS). A significant difference was measured in the current rectification of the two kinds of contacts. The ZTO/Pt SC does not exhibit rectification, whereas the ZTO/PtO_x/Pt SCs have rectifications of one order of magnitude or higher. We demonstrate with depth-resolved XPS measurements that a diffusion of oxygen takes place and leads to the vastly different current-voltage characteristics. For amorphous ZTO based devices an improvement of the characteristics over time has been reported [8]. XPS and current-voltage measurements were performed on as deposited and stored samples. We observe an improvement of the ZTO/PtO_x/Pt SC and constant performance of the ZTO/Pt SC. We provide evidence that a diffusion of oxygen causes the improvement of the ZTO/PtO_x/Pt SC and propose a recipe to enhance the oxygen diffusion and therewith the device optimization. [1] S. Müller *et al.*, J. Appl. Phys. **116**, 194506 (2014) [2] M. W. Allen *et al.*, Appl. Phys. Lett. **92**, 122110 (2008) [3] O. Bierwagen *et al.*, Appl. Phys. Lett. **98**, 172101 (2011) [4] O. Bierwagen *et al.*, Appl. Phys. Express **2**, 106502 (2009) [5] A. Chasin *et al.*, Appl. Phys. Lett. **101**, 113505 (2012) [6] H. von Wenckstern *et al.*, APL Mater., **2**, 046104 (2014) [7] T. Schultz *et al.*, Phys. Rev. Appl., **9**, 064001 (2018) [8] S. Bitter *et al.*, ACS Appl. Mater. **9**, 26574 (2017)

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(Student) Electrical Properties of Different Dopants in κ -(In_xGa_{1-x})₂O₃ Thin-Films Grown by CCS Catharina Krömmelbein, Anna Hassa, Max Kneiß, Daniel Splith, Holger von Wenckstern and Marius Grundmann; Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, Universität Leipzig, Leipzig, Germany.

The wide bandgap semiconductor gallium oxide has potential application in electronic devices, because of its large breakdown fields and high Baliga figure of merit [1]. Further application fields of gallium oxide can be quantum well infrared photodetectors, UV-photodetectors, touch panel displays, solar cells or optical communication systems [2]. Besides the monoclinic β -polymorph of Ga₂O₃, being up to now the most investigated one, the orthorhombic modification is of increasing interest, because of its predicted large spontaneous polarization of 23 $\mu\text{C}/\text{cm}^2$ [3]. At the interface of κ -Ga₂O₃-based, ternary heterostructures a discontinuous change of the polarization occurs, leading to a charge accumulation that can potentially be exploited in high-electron mobility transistors. Therefore, it is crucial to determine deposition conditions allowing growth of ternary layers with tailored material properties. First conducting ternary thin films based on κ -(In_{0.01}Ga_{0.99})₂O₃:Zr were demonstrated recently [4]. The upcoming challenge will be to improve the electronic properties of such thin films to realize a broad field of electronic devices. In the present study, we show differently doped κ -(In_xGa_{1-x})₂O₃ thin films prepared on (00.1) Al₂O₃ substrates by pulsed laser deposition with combinatorial composition spread approach to create samples with defined lateral variation of the cation composition [5]. Each of the PLD-target used segments consists of a similar proportion of Ga₂O₃/In₂O₃ and 4.75 wt.% tin to facilitate the formation of the κ -modification [6]. Additionally, one segment was doped with zirconium or silicon to induce n-type conductivity, since nominally undoped Ga₂O₃ possesses insulating properties [7]. Pt-Schottky barrier diodes were fabricated by photolithography, reactive sputtering, and investigated at RT by current-voltage measurements revealing an increase of rectification ratios with decreasing Zr. The best contact based on a Zr doped κ -(In_xGa_{1-x})₂O₃ thin films exhibits a rectification ratio of about six orders of magnitude. The best κ -(In_xGa_{1-x})₂O₃:Si based contact of about four orders of magnitude. Further, the surface morphology was measured by means of atomic force measurements to deduce the root mean square surface roughness as e.g. 4 nm for a Si content of 4.2 at.%. [1] Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012) [2] von Wenckstern, Adv. Electr. Mat. **3**, 1600350 (2017) [3] Orita *et al.*, Thin Solid Films **411**, 134-139 (2002) [4] Hassa *et al.*, APL Materials, accepted (2019) [5] von Wenckstern, CrystEngComm **15**, 10020 (2013) [6] Kracht *et al.*, Phys. Rev. Appl. **8**, 054002 (2017) [7] Varley *et al.*, Appl. Phys. Lett. **97**, 142106 (2010)

PS37

Theoretical Prediction of Intercalation Compounds Formed by Co-Intercalation of Mg Ions with Diamine into Graphite Anodes for Mg-Ion Batteries Pegah S. Mirabedini¹ and P. Alex Greaney²; ¹Material Science and Engineering Program, University of California, Riverside, Riverside, California, United States; ²Department of Mechanical Engineering, University of California, Riverside, Riverside, California, United States.

Reliable reversible batteries that use Mg working ions would have the advantages of carrying a charge greater than +1, besides being abundant, inexpensive, nontoxic and promising a low reduction potential and high specific capacity. However, Mg-metal is strongly passivated and so makes a poor anode and thus there is currently an effort to identify suitable anode materials for Mg storage. One approach in this effort has been to examine the co-intercalation into graphite anodes of Mg with Ethylenediamine [1]. Incorporation of co-intercalates such as diamine can greatly enhance the onset potential and lead to forming new GICs. In this paper, we present the results of a series of density functional theory calculations examining the likely structure, packing, and energetics of these co-intercalation compounds of ethylenediamine with a series of alkaline earth metals. To this end, we examine the energy differences between a variety of possible *cis* and *trans* ethylenediamine polymorphs to find candidate structures for forming co-intercalation packing with Mg. Armed with this library of structures planer tiling permutations with alkali earth ions were examined – including structures in which the metal ions dimerize. In the final step, the energy and electronic structure of geometrically permissible tessellation interleaved into graphene bilayers were examined. The results will potentially contribute to achieving a fundamental understanding of intercalation energetics, compositions, and structures which will lead to the fabrication of GICs with enhanced properties including improved capacity and battery performance. I Xu, W., Zhang, H., & Lerner, M. M. (2018). Graphite Intercalation by Mg Diamine Complexes. *Inorganic chemistry*, *57*(14), 8042-8045.

PS38

(Student) Density Functional Theory Calculations of ZnO Nanopyramids—Crystal Growth and Improved Performance in Water Splitting Pegah S. Mirabedini², Taehoon Lim¹, Alfredo A. Martinez-Morales^{1, 2, 4} and P. Alex Greaney^{3, 2}; ¹Center for Environmental Research and Technology, University of California, Riverside, Riverside, California, United States; ²Material Science and Engineering Program, University of California, Riverside, Riverside, California, United States; ³Department of Mechanical Engineering, University of California, Riverside, Riverside, California, United States; ⁴Department of Chemical and Environmental Engineering, University of California, Riverside, Riverside, California, United States.

ZnO semiconductors are known as excellent materials for photocatalytic applications because of their high photosensitivity, nontoxic nature, and large bandgap. A variety of morphologies containing polar and non-polar surfaces can be achieved by controlling the crystal growth condition. Energetic stability and efficiency are two important factors in determining the feasibility of a photocatalyst for oxygen evolution reactions in water splitting applications. Polar surfaces generally are known to have higher photoelectrochemical activity increasing water splitting efficiency. However, a key question is whether these surfaces are also stable. ZnO pyramidal nanostructures are deposited through chemical vapor deposition (CVD). Herein, we perform a set of Density Functional Theory (DFT) calculations to compare the stability and electronic structure of the surfaces formed during different stages of the growth process. Although these pyramidal structures are generally not stable due to their relatively high surface energy, our calculations prove that under specific growth conditions, these morphologies are stable. These structures have been successfully synthesized via CVD, and their enhanced photocatalytic activity is consistent with the differences in the electronic structure of the surfaces computed with DFT.

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PS39

(Student) Coherent Magnetic Nano-inclusions Induce Charge Localization Leading to High-Tc Ferromagnetism and Enhanced Thermoelectric Performance in Half-Heusler Alloys Ruiming Lu; Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States.

Performance improvement traditionally realized through a combination of power factor optimization via electronic doping and lattice thermal conductivity reduction using nanostructuring have reached their optimal limits in many leading thermoelectric materials, making further enhancement in the thermoelectric figure of merit extremely challenging. Here, we demonstrate a novel approach to electronic transport engineering using coherent magnetic nano-inclusions. We found that the incorporation of coherent magnetic nano-inclusions with full-Heusler (FH) structure $(\text{Ti}(\text{Ni}_{4/3}\text{Fe}_{2/3})\text{Sn})$ into a half-Heusler (HH) matrix $(\text{Ti}_{0.25}\text{Zr}_{0.25}\text{Hf}_{0.5}\text{NiSn}_{0.975}\text{Sb}_{0.025})$ with optimal doping level and lattice thermal conductivity leads to high Curie temperature ferromagnetism ($T_c \sim 650$ K) along with a large reduction in the effective carrier density within the HH matrix. It is believed that the embedded magnetic FH nano-inclusions interact with the spin of itinerant carriers, leading to charge localization and the formation of overlapping bound magnetic polarons (BMPs). This gives rise to significant enhancements of both carrier mobility and thermopower, which minimizes the reduction in the overall power factor, simultaneous with a large drop in the total thermal conductivity owing to the reduction of the electronic contribution to the thermal conductivity. We anticipate that the implementation of magnetic secondary phases will pave the way towards even larger figures of merit in a variety of state-of-the-art thermoelectric materials.

PS40

(Student) Low-Angle Grain Boundaries Effect on the Conversion Efficiency of Single-Crystal-Like GaAs Thin-Film Solar Cells on Flexible Metal Foil Sara Pouladi¹, Monika Rathi¹, Pavel Dutta¹, Shahab Shervin¹, Jie Chen², Weijie Wang³, Venkat Selvamannickam¹ and Jae-Hyun Ryou¹; ¹Mechanical Engineering, University of Houston, Houston, Texas, United States; ²Materials Science and Engineering Program, University of Houston, Houston, Texas, United States; ³Mechanical Engineering, University of Houston, Houston, Texas, United States.

The effects of low-angle grain boundaries (GB) in single-crystal-like GaAs thin-film on its photovoltaic performance is studied using a numerical simulation. Here, 1D and 2D modeling are employed to simulate a solar cell device based on the properties of single-crystal-like GaAs thin films grown on metal tape including their minority carriers' mobility, lifetime, and diffusion length. The 1D model by incorporating a uniform biaxially textured GaAs compared to single crystal GaAs predicts efficiencies $\sim 21\%$

for average carrier lifetimes of 1 ns which is not consistent with experimental results with an efficiency of 4.3%. 1D simulation generally works well for I-V characteristics prediction of conventional crystalline SCs, but it fails for newly-developed single-crystal-like GaAs SC devices with different material property and non-vertical device geometry. Hence, we develop a 2D model to study the effect of localized recombination centers in the material by defining different regions of defective low-angle grain boundaries and single crystalline intra-grains. The 2D model shows very well matched result with experiment mainly due to its capability to consider localized material inhomogeneity and lateral carriers dynamic. The amount of grain boundary density on the SC performance is studied by the 2D model. Increasing the grain size of GaAs from 2 μm to 50 μm can improve the efficiency of solar cells from 4.8% to 12.3%. The Voc of devices shows more sensitivity to the amount of grain boundary densities than other SC characteristic factors. The 2D model is also employed to study bulk passivation of GBs which shows that thin film single-crystal-like GaAs solar cells with an efficiency of $\sim 19.7\%$ can be achieved even at a small grain size of 2 μm if effective grain boundary passivation is applied.

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(Student) Structural and Electrical Property Control Through Varied Cation Ratio in Zinc-Tin Oxides Sebastian Husein¹, Julia Medvedeva² and Mariana I. Bertoni³; ¹School of Engineering for Matter, Transport, and Energy, Arizona State University, Tempe, Arizona, United States; ²Missouri University of Science and Technology, Rolla, Missouri, United States; ³School of Electrical Computer and Energy Engineering, Arizona State University, Tempe, Arizona, United States.

In this study, we use a combinatorial sputtering approach for deposition of zinc tin oxide (ZTO) spanning 100% SnO₂ to 100% ZnO with compositional libraries containing a large set of varied Zn:Sn ratio, sputtered at 300 °C, 400 °C, and 450 °C substrate temperatures (T_s). The as-deposited films grown at $T_s = 300$ °C exhibit a clear transition from crystalline to amorphous at approximately 37 % $[\text{Zn}]/([\text{Zn}]+[\text{Sn}])$, revealed by x-ray diffraction. For $T_s = 400$ °C, a similar transition occurs at 45%. For both T_s , a transition from amorphous to crystalline exists near 70 % $[\text{Zn}]/([\text{Zn}]+[\text{Sn}])$. Films grown at $T_s = 450$ °C are currently under evaluation. The electrical properties, obtained by Hall effect at room temperature, of the amorphous phase films are of particular interest, and a significant peak in conductivity is observed near the transition from amorphous to crystalline at the three T_s . Amorphous oxide semiconductors (AOS) have been increasingly studied the past decade, especially for photovoltaic (PV) devices and display technologies. Materials receiving the most attention are ternary and quaternary oxides consisting of post-transition metals, e.g., Zn-Sn-O, Zn-In-O, Zn-In-Sn-O, or In-Ga-Zn-O. Interest in AOS alternatives to their more established crystalline counterparts (e.g., Sn-doped indium oxide, Al-doped ZnO) is due to their extremely smooth surfaces, greater chemical and thermal stability, mechanical flexibility, and mobilities an order of magnitude greater than hydrogenated amorphous Si [1, 2]. These properties are attainable with large area, low temperature deposition conditions without compromising optical and electrical properties [3, 4]. A particularly attractive AOS is amorphous zinc tin oxide (a-ZTO), a non-toxic and scalable material (due to high elemental abundance) which has shown a Hall-effect carrier mobility of up to 35 cm² V⁻¹ s⁻¹ with good thermal stability [5]. However, understanding of the composition-structure-property relationship in ZTO is wanting, and in particular, a complete exploration of the ZnO-SnO₂ tie-line and resulting amorphous phases is lacking. For films in the present study, the maximum conductivity (σ) increases with increasing T_s . A shift to higher Zn content for the location of the maximum σ is also observed with increasing T_s , as seen in Fig. 1(a) of the extended abstract. For $T_s = 300$ °C, 400 °C, and 450 °C, the maximum σ were ~ 233 S/cm, ~ 322 S/cm, and ~ 420 S/cm respectively. These occurred at $[\text{Zn}]/([\text{Zn}]+[\text{Sn}]) = 37.4\%$, 47.5%, and 85.2% respectively. Further evaluation of the compositional characteristics of the amorphous phase is needed to make an accurate determination of the underlying origin of the carrier density and carrier mobility, leading to such trends of σ . To obtain such information, *ab initio* molecular dynamics liquid-quench and density functional theory simulations were performed. Simulations of the amorphous ZTO structures were created using a quench rate of 200 K/ps. By inspecting the coordination of each cation species, it is readily seen that the Zn-O coordination varies significantly compared to Sn-O coordination. More in-depth analysis revealing the coordination of the cation species with varied cation ratio, the number of face, edge, and corner-sharing metal-oxygen polyhedra, and the metal species contribution to the Bader charge near the Fermi energy level will be presented. However, findings reveal two crucial factors: (1) zinc cations control the morphology and crystallization of the system, which determines the carrier mobility; whereas (2) tin cations govern the carrier generation in the system. [1]: T.

Kamiya, H. Hosono, *NPG Asia Mater.*, vol 2, no. 1, 2010. [2]: H. Hosono, *J. of Non-Cryst. Solids*, vol. 352, 2006. [3]: X. Yu, T. Marks, A. Facchetti, *Nature Mater.*, vol. 15, 2016. [4] J. Medvedeva et al., *Adv. Electron. Mater.*, 3, 2017. [5]: M. Morales-Masis et al., *Adv. Funct. Mater.*, 26, 2016.

PS42

Self-Standing ZnO Nanotube/SiO₂ Core-Shell Arrays for High Photon Extraction Efficiency in III-Nitride Emitter Semi Oh^{1,2}, Seong-Ju Park² and Kyoung-Kook Kim³; ¹University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Gwangju Institute of Science and Technology, Gwangju, Korea (the Republic of); ³Korea Polytechnic University, Siheung, Korea (the Republic of).

One-dimensional (1D) nanostructures have been intensively studied over the past few years due to their special properties and potential applications in nanoscale electric and optoelectronic devices. An important issue in this field is how to realize the controllable growth of a 1D nanostructure to obtain the desired functionality and put it into practice. ZnO ($n = 2.1$) is a wurtzite structure, wide band gap ($E_g = 3.37$ eV), large exciton binding energy (60 meV) and high transmittance above near-ultraviolet wavelength. Therefore ZnO is an exceptionally important oxide semiconductor material, particularly in nanotechnology due to the ease with which its diverse 1D nanostructures can be grown. Over the last few years, 1D-ZnO nanorods (ZNRs) have considerable interest because such nanostructures exhibit extraordinary structural, surface, electrical, optical, magnetic, mechanical, and thermal properties different unlike bulk ZnO material. Many groups have tried to fabricate the ZNR arrays on emitters for enhancing photon extraction efficiency (PEE) of emitters by decreasing the difference of refractive index between GaN ($n = 2.4$) and air ($n = 1$). However, conventional GaN-based emitters use an indium tin oxide (ITO) layer ($n = 2.1$) as a p -type transparent conducting electrode. Therefore, a greater increase in the PEE of the emitter with ITO layer means that the refractive index of the ZnO nanostructures must be lower than the ITO layer. Compared to other 1D counterpart nanorods, obtaining a tubular nanostructure has been highly desirable for special recent technological applications due to its superior optical, electrical, thermal, and mechanical properties. In addition, the tubular structure has the high efficiency and activity caused by its high porosity and large surface area. Most importantly, ZnO nanotubes (ZNTs) have a photon or electrical wave guideline through the surface of the wall and relatively lower refractive index than ZNRs. In this study, we report the synthesis of vertically self-standing ZNTs on emitters for increasing the photon extraction efficiency (PEE) by catalyst-free hydrothermal method at low temperature (~ 90 °C). In addition, the SiO₂ layer ($n = 1.46$) was coated on the ZNTs array for a greater increase in the PEE of the emitter by increasing the antireflection effect between the ZNTs and air. The optical output intensity of self-standing ZNT arrays on the emitter is increased by up to 31.5% and 8% at an injection current of 100 mA compared to those of conventional emitter (C-emitter) with ITO layer and ZNR arrays on the C-emitter without the degradation of the electrical properties. Furthermore, we fabricated the ZNT/SiO₂ core-shell nanostructure arrays on the C-emitter for further increase the antireflection effect in a manner that showed an approximately 55.9% enhancement for PEE at an injection current of 100 mA compared with C-emitter.

PS43

(Student) Development of Pico-Watt Heat Resolution SThM Probe to Investigate of Heat Transfer in Atomic Scale Seunghoe Koo, Jaehye Park and Kyeongtae Kim; Mechanical Engineering, Incheon National University, Incheon, Korea (the Republic of).

As the thermo-physical properties at the nanoscale are key characteristics that determine the operation of nanoscale devices (nano electronics, nano photonics, nano energy conversion etc.), measuring and analyzing them have been considered important with the development of nanotechnology. In addition, with recent advances in nanotechnology the measurement and verification of thermal properties at molecule- and atomic-scale are required. Among the technologies to measure nanoscale thermal properties, scanning thermal microscopy has been well known what can measure the thermal and energy transfer phenomena with the highest spatial resolution. It is necessary to develop a new probe capable of measuring a smaller heat than that of the current scanning thermal microscope probe in order to measure pW~nW heat level at the molecular or atomic scale. In this study, we developed a pico-Watt scanning thermal microscopy probe that can measure the pico-watt level heat transfer. The 'pico-watt calorimeter', which can measure the heat transfer with the pico-watt level, is integrated to the probe over the cantilever fabricated through the MEMS process. A thermo-resistive probe was fabricated with a platinum serpentine line with a width of sub 1 μ m, and a tip was formed

by dry etching the silicon nitride thin film. The developed probe has ~ 100 uK temperature resolution and thermal resistance of $\sim 10^7$ W/K, which can measure ~ 10 pW heat. The pico-watt scanning thermal microscopy combined with the probes is expected to identify the energy transfer phenomenon and contribute to the measurement technic at the atomic scale.

PS44

(Student) N-Type Zintl Thermoelectric Compounds in the Eu-Ga-Sb Phase Space Sevan Chanakian¹, Francisco Suarez², Sabah Bux² and Alexandra Zevalkink³; ¹Materials Science, Michigan State University, East Lansing, Michigan, United States; ²Thermal Energy Conversion Technologies Group, Jet Propulsion Laboratory, Pasadena, California, United States; ³Michigan State University, East Lansing, Michigan, United States.

In order to develop efficient thermoelectric couples capable of generating electricity from a heat gradient, both p and n -type thermoelectric materials are necessary. Zintl phases are strong contenders for high temperature thermoelectric applications due to their inherently low thermal conductivity, tunable electrical resistivity, and high temperature stability. Because thermoelectric generators operate at high temperatures, ranging between 200°C and 1000°C, the chemical compatibility of the materials used in devices is an important consideration. Thus there is large incentive to develop an all Zintl thermoelectric couple. However, historically Zintl phases exhibit p -type behavior due to compensating vacancy defects which negate efforts to engineer n -type materials. In recent years a handful of n -type Zintl phases have come to light including Mg₃Sb₂ and KAlSb₄. Here we explore the thermoelectric properties of new n -type Zintl phases in the Eu-Ga-Sb phase space, notably Eu₇Ga₈Sb₈ and its Ga deficient superstructure Eu₆Ga₈Sb₈. Eu₆Ga₈Sb₈ has previously been reported to have a small bandgap and a large crystal structure making it an interesting material system to study for thermoelectrics. Our preliminary results suggest that these structurally related crystal systems exhibit extremely low thermal conductivity, 0.45 W/mK at 575 K, and can be doped n -type with the substitution of La on the cation site.

PS45 WITHDRAWN

Conformal Epitaxy of ZnO/III-Oxides Superlattices—Experiment vis-à-vis First-Principles Calculations Che-Min Lin², Wan-Chen Hsieh³, Chun Fu Chang¹, Hui Chun Huang³, Wei-Jhen Ciou¹, Ming-Chen Chou¹, Po-Hung Lin¹, Tai-Siang Lin¹, Sung-Wei Yeh⁵, Chih-Hsiung Liao⁴, Paritosh Wadekar⁶, New-Jin Ho³, Li-Wei Tu¹, Tsan-Chuen Leung⁸, Quark Y. Chen¹ and Wei Kan Chu⁷; ¹Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan; ²Physics, National Sun Yat-sen university, Kaohsiung, Taiwan; ³National Sun Yat-sen University, Kaohsiung, Taiwan; ⁴Physics, ROC Military Academy, Kaohsiung, Taiwan; ⁵Mold and Die Engineering, National Kaohsiung University of Science and Technology, Kaohsiung, Taiwan; ⁶Physics, National Sun Yat Sen University, Kaohsiung, Taiwan; ⁷Physics and TeSUH, University of Houston, Houston, Texas, United States; ⁸Physics, National Chung-Cheng University, Chiayi, Taiwan.

Inspired by a previous work on the ZnO/AlO superlattices of conformal epitaxy successfully grown on the also c-oriented sapphire substrates, which exhibited white luminescence because of the energy states existing in the mid-bandgap of ZnO, we ask whether Ga, the Group-III element following Al, can also be made into ZnO/GaO superlattices of conformal structures. Here, we assessed such possibilities via first-principles calculations. From the Bader charge analysis and charge density differences, we found that the Ga atoms would transfer electrons to the O atoms at interfaces to form stronger chemical bonding. The d-orbitals of the Zn atom at interface is closer to the Fermi level as compared to those of the Zn atoms in the bulk. From the d-band model, this upshift of the d-orbital states of Zn enhances the catalytic activities at interface. The overall results point to the stability of the conformal epitaxial structure. Comparisons will be made between the AlO and GaO counterparts in regards to their crystal and energy band structures.

PS46

High Hardness and Transparent Organic-Inorganic Hybrid Thin-Film for Antistatic Film Young Ki Hong¹, Donghyuk Park² and Sunjong Lee³; ¹Gyeongsang National University, Jinju, Korea (the Republic of); ²Inha University, Incheon, Korea (the Republic of); ³Korea Institute of Industrial and Technology, Cheonan, Korea (the Republic of).

The antistatic films are indispensable in touch screen industry to prevent electrostatic effects. Conductive polymers have been studied for promising antistatic agents because of its simple process on sheet resistivity and cheap price, although a low hardness and poor adhesivity. Among them, PEDOT:PSS films have been attractive for decades due to its remarkable

electrical and optical properties, which are controllable through the synthetic parameters. For example, as the ratio of PSS increases, the sheet resistance of PEDOT:PSS increases. However, it is a laborious task to increase the durability and hardness of PEDOT:PSS in thin film using the conventional method. In this report, we demonstrate an organic-inorganic hybrid thin film of PEDOT:PSS with silica nanoparticles (Si-NPs) showing high hardness and transmittance. The inorganic Si-NPs with various particle size were synthesized at low temperature by sol-gel process. Without using polysilsesquioxane, hardness of Si-NPs were significantly enhanced. SEM, FT-IR and XPS experiments show the average particle size of Si-NPs controlled from 19nm to 35nm. The addition of additives reduced the capillary force that occurred during the drying process of the homogeneously mixed PEDOT:PSS/Si-NPs solution. The spin-coated thin film which has a thickness of ~100nm showed appropriate resistance ($10^7 \Omega/\text{sq}$) and high hardness (6H) for antistatic coating. While preparing the hybrid film, extra UV and thermal treatments were skipped, which made the synthetic process to be simplified and the total process time was significantly reduced. Moreover, this hybrid thin film achieved a high transmittance (92%) and stabilized durability for 100 hours under the constant temperature and humidity test (85°C, 85%). This result suggests that the hybrid thin film of PEDOT:PSS/Si-NP has a high potential to the various antistatic applications.

PS47 WITHDRAWN

(Student) Variable Range Hopping and Relaxation Dynamics of Charge Carriers in Graphene and Graphene Wrapped V_2O_5 Nanoparticles Surya B. Duvvuri and Govindaraj Gurusamy; Physics, Pondicherry University, Kalapet, India.

Since the advent of graphene, it has embarked its applicability in various domains of science and technology. Based on applicability and yield there are plenty of graphene synthesis techniques available. When high yield and cost-effectiveness are a major concern, the most promising way to synthesize graphene is via reduction of graphene oxide. The product obtained by such a method is widely known as reduced graphene oxide (RGO). RGO is widely used in the energy storage industry, electrochemical sensors, biosensors, electronics, optoelectronics and catalysis applications. Carrier transport studies in RGO shows variable range hopping type conduction of free carriers. This kind of transport is defect dependent and can be probed using Raman spectroscopy. Quantification of the hopping mechanism can be done using I_D/I_G ratio obtained from the Raman spectrum. The precursor of RGO, graphene oxide also shows a variable range hopping conduction mechanism. Graphene oxide consists of sp^2 conducting channels and sp^3 insulating islands. Relaxation current in such kind of materials can be explored using Cole-Cole type combined conduction and dielectric model for relaxation currents. It is observed that hybrids of RGO have better and feasible applicability than RGO alone. Amongst graphene hybrids, RGO composite with metal oxide has gained immense momentum. Many metal oxides along with RGO has been studied. Oxides of vanadium find application in energy storage and conversion devices, various sensors, catalysts, and field effect transistors. Graphene V_2O_5 composite has been extensively used to study fundamental physics and electronic applications. The high yield alternative to graphene- reduced graphene oxide has been explored in the composite form with V_2O_5 in the field of energy storage. Vanadium pentoxide has been used as anode and supercapacitor electrode material due to its various merits such as layered structure and multiple stable oxidation states. In this work, we have synthesized RGO wrapped V_2O_5 using hydrothermal synthesis. Wrapping of RGO on V_2O_5 particles enhances latter's conductivity, surface area and strength. This composite is a heterogeneous conductor. The ac and dc electrical measurements have been performed from 143 to 323K. To analyze electrical properties $\sigma(\omega)$ has been fitted using Cole-Cole type conduction and dielectric model. In this model, current contribution from free conduction electron, relaxation of pinned dipole leading to conduction current and relaxation of free dipoles leading to dielectric current have been accomplished using a single equation. Dc conductivity and relaxation timescales were obtained from the fit and it is observed that σ_{dc} and conduction and dielectric timescales follow $T^{1/2}$ dependence. This is a sign of Variable range hopping. In bare V_2O_5 Arrhenius type conduction is observed in this temperature regime. How the wrapping of V_2O_5 with RGO affects the conduction dynamics will be discussed.

PS48

(Student) Effect of Oxygen Plasma-Treatment on the Electrical Characteristics of Ni Schottky Contact on n -GaN Tae Ju Lee and Tae-Yeon Seong; Korea University, Seoul, Korea (the Republic of).

Because of the wide band gap, high breakdown field, and high electron saturated velocity, GaN-based semiconductors are regarded to be promising for the fabrication of electronic devices including high electron mobility transistors, heterojunction bipolar transistors, and UV Schottky barrier photodetectors. To improve the efficiency of these electronic devices, the formation of high-quality Schottky contacts is essential. In particular, MSM photodetectors are suitable for field-effect-transistor (FET)-based optoelectronic integrated circuit applications because they have extremely low intrinsic capacitance and the compatibility of the fabrication process of FET-based electronics. Therefore, for the fabrication of high-efficiency electronic devices, it is vital to develop high-barrier Schottky contacts and to understand their electrical and interfacial characteristics. Thus, in this study, we investigated the effect of oxygen plasma treatment on the electrical and interfacial characteristics of Ni Schottky contacts on n -GaN for high-performance electronic devices. The Ni contacts were annealed at 600 °C for 6 min in N_2 ambient before and after oxygen plasma treatment. Calculations using the thermionic emission model-based current-voltage characteristics of the samples showed relatively small Schottky barrier heights (SBHs) of 0.55–0.82 eV and ideality factors of 1.50–2.34. Conventional activation energy plot showed much smaller Richardson constant than the theoretical value. To comprehend such anomaly, the modified Richardson plot, inhomogeneous model, and capacitance-voltage method, were adopted, where their SBHs were measured to be in the range 0.80–1.25 eV. The temperature-dependent SBHs and ideality factors indicate that barrier characteristics could be explained in terms of barrier inhomogeneity at the interfaces. The X-ray photoemission spectroscopy (XPS) and scanning transmission electron microscopy (STEM)-energy dispersive X-ray spectroscopy mapping results were performed to understand the mechanism for the improved Schottky barrier. Based on the electrical, XPS and STEM results, the annealing temperature dependence of the SBHs is described and discussed.

PS49

Si Quantum Dots and Light Emission in Nd Doped Si-Rich HfO_2 Films Prepared by Magnetron Sputtering Tetyana V. Torchynska[†], Leonardo Gabriel Vega Macotella[‡], Larysa Khomenkova^{3,5} and Fabrice Gourbilleau⁴; ¹ESFM, Instituto Politécnico Nacional, Av. IPN., Mexico City, Mexico; ²ESIME, Instituto Politécnico Nacional, Av. IPN., Mexico City, Mexico; ³Photoelectronic, V. Lashkaryov Institute of Semiconductor Physics at NASU, 45 Pr. Nauky., Kyiv, Ukraine; ⁴CIMAP, UMR CNRS/CEA/ENSICAEN/UNICAEN, 6 Boulevard Marechal Juin, 14050, Caen, France; ⁵National University "Kyiv-Mohyla Academy", 2 Skovorody str., Kyiv, Ukraine.

The impact of phase varying on emission properties of Nd-doped Si-rich HfO_2 films obtained by RF magnetron sputtering has been investigated by means of scanning electron microscopy, energy dispersive X-ray spectroscopy, X-ray diffraction, X-ray photoelectron spectroscopy and photoluminescence techniques. It was observed that thermal treatment of the films at 950 and 1100°C governs a phase separation process. The formation of small HfO_2 nanocrystals (3nm) of the tetragonal phase together with the Si quantum dots (QDs) occurs at 950°C. Upon annealing at 1100°C, the larger tetragonal SiO_2 and HfO_2 nanocrystals (\approx 8nm) appeared. The appearance of bright emission in the visible-near-infrared spectral range related to the optical transitions in the 4f intra shell energy levels of Nd ions has been detected. The investigation of annealing effect on luminescent properties revealed that the enhancement of Nd^{3+} ion emission occurs due to an effective energy transfer from Si QDs towards Nd ions. The energy transfers into the Nd ions from some native host defects, such as oxygen vacancies, has been detected as well. It was shown using XPS that the oxidation of Si-QDs at high temperature annealing (1100°C) lead to intensity decreasing the Nd ion related emission. The later effect can be stimulated as well by decreasing the oxygen vacancy contents in the HfO_2 matrix. Since hafnia-based materials have high density and very sensitive to high-energy excitation, our results offer multifunctional applications of doped hafnia films, such as the luminescent materials for traditional phosphors.

PS50

Reflectance and Raman Characterisation of Mechanically Exfoliated ReS₂ Flakes Tim Batten¹, Tim Prusnick² and Sarah C. Shidler³; ¹Renishaw plc, Wotton-under-Edge, United Kingdom; ²Renishaw Inc., Chicago, Illinois, United States; ³Renishaw Inc., West Dundee, Illinois, United States.

In this work, we use a combination of reflectance measurements and Raman spectroscopy to quickly locate and characterise the thickness of mechanically exfoliated flakes of ReS₂. Mechanical exfoliation is a very common production technique for 2D materials used in research. Generally, this technique produces only small amounts of thin (few layers of material) and it is a very labour intensive task to locate and identify these thin flakes. Typically flakes are deposited on a Si/SiO₂ substrate, which allows flakes to be visualised using optical microscopy, the user then scans the sample with a high magnification objective lens which is both time consuming and arduous. Raman mapping is an alternative method to find and characterise the flakes, but Raman measurements typically take on the order of seconds and it is very time consuming to map cm² areas at sub micrometre resolution. To speed things up we perform a prescan reflectance measurement using the Raman laser to find suitable flakes for additional raman analysis, such scans are very quick with collection speeds in excess of 1000 spectra/s. Figure 1 illustrates a reflectance image of ReS₂ flakes on a Si/SiO₂ substrate, along with flake thickness determined using the low wavenumber Raman bands. Here it can be seen that for thin flakes (<4 layers) the reflected laser intensity is less than that from the substrate. For thicker flakes the reflectance is higher than the substrate.

PS51

Correlated Photocurrent and Raman Spectroscopy Mapping Measurements of Single Crystalline Silicon Solar Cells Tim Batten¹, Tim Prusnick², Sarah C. Shidler², Hubert Seigneur⁴, Asif Mahmud³ and Parag Banerjee³; ¹Renishaw plc, Wotton-under-Edge, United Kingdom; ²Renishaw Inc., Chicago, Illinois, United States; ³Department of Materials Science & Engineering, University of Central Florida, Orlando, Florida, United States; ⁴Florida Solar Energy Center, University of Central Florida, Orlando, Florida, United States.

In this work we demonstrate how simultaneous photocurrent and Raman spectroscopy measurements can be used to locate and identify defect regions in single crystalline silicon solar cell modules. We also utilise Raman spectroscopy to look at the stress distribution in individually encapsulated silicon solar cells laminated under varied conditions (encapsulant material, encapsulant layer thickness, interconnect soldering). Raman spectroscopy is a non-contact, non-destructive analytical technique that provides sub-micrometre information on the vibrational, crystal and electronic structure of materials. It is the ideal method for investigating solar cell materials including the different forms of silicon and perovskites and can be used to determine, crystal quality, stress/strain and electronic properties. Recent advances in instrumentation has made characterisation of these materials easier and more comprehensive, adding features such as ultrafast mapping (>1000 spectra/s) and automatic sample focus tracking capabilities. When collecting Raman spectroscopy data a laser source is shone on the sample surface, which in electronically connected devices may create a photocurrent. When collecting a Raman map of a sample the laser is scanned across the sample surface and by continuously measuring the photocurrent we can create a corresponding photocurrent map to go with the Raman map. This photocurrent map allows defected areas, where the current is lower than average to be visualised, and the corresponding Raman data can be used to better understand the root cause.

PS52

(Student) High Performance Organic Electrochemical Transistors—Working Mechanism and Future Applications as a Biosensor Vikash Kaphle; Physics, Kent State University, Kent, Ohio, United States.

Organic Electrochemical Transistors (OECTs) are seen as a key device for the field of bioelectronics [1]. OECTs are mainly used to detect ions, metabolites, hormones, DNA, Dopamine, lactic acid. Furthermore, they are used to record brain activity, the activity of electrically active cells or tissues, or to drive an active matrix display. OECTs operate in an aqueous environment and at low voltages, they can be flexible, and they are bio-compatible [2-4]. In the standard model of OECTs [5] switching is described by straightforward electrostatic arguments using an ionic gate capacitance. Despite the success of the model, the precise nature of this capacitance is missing. Here, we discuss the working mechanism of OECT and show that not only the gate capacitance depends on the applied potential, but depletion capacitances at source and drain electrodes have to be included into the model as well. In particular, we show that the potential

profile inside the transistor channel can only be fitted by a modified Bernard's model accounting for a non-uniform hole mobility inside disordered materials [6], if the voltage dependence of the capacitances is taken into account. For their intended use in implanted devices, OECTs have to show a superior stability in harsh environments. Here, we study the origin of gate bias stress and hysteresis of OECTs and propose approaches to minimize these instabilities [7]. A compact device model is proposed that includes these instabilities and can lead to new ways to optimize the stability of OECTs. Based on this improved understanding of the working mechanisms of OECTs, devices with a transconductance greater than 2 mS and on/off ratios in excess of 10³ using a gel-type electrolyte, which has the potential to be integrated into wearable clothing. References [1] Xenophon Strakosas, Manuelle Bongo, Roisin M. Owens, J Appl Polym Sci 2015, 41735,1. [2] Jonathan Rivnay, Sahika Inal, Alberto Salleo, Roisin M. Owens, Magnus Berggren, and George G. Malliaras, Nat. Mater. 2018, 3,1. [3] P. Leleux, J. Rivnay, T. Lonjaret, J. M. Badier, C. Benar, T. Herve, P. Chauvel, G. G. Malliaras, Adv. Healthcare Mater. 2015, 4, 142. [4] D. Khodagholy, V. F. Curto, K. J. Fraser, M. Gurfinkel, R. Byrne, D. Diamond, G. G. Malliaras, F. B. Lopez, R. M. Owens, J. Mater.Chem. 2012, 22, 4440. [5] Daniel A. Bernardis, George G. Malliaras, Adv. Fun. Mater. 2007, 17, 3558. [6] Jacob T. Friedlein, Sean E. Shaheen, George G. Malliaras, Robert R. McLeod, Adv. Electron. Mater. 2015, 1, 1500189. [7] Vikash Kaphle, Shiyi Liu, Chang Min Keum, Bjorn Lussem, Physica Status Solidi A 2018, 215, 1800631.

PS53

(Student) Temperature-Dependent Bond Strength and Sound Velocity in (GeTe)_mSb₂Te₃ Alloys Wanyue Peng; Chemical Engineering and Materials Science, Michigan State University, East Lansing, Michigan, United States.

(GeTe)_mSb₂Te₃ alloys have been previously shown to be excellent thermoelectric material with a figure of merit >2 when fully optimized. The (GeTe)_mSb₂Te₃ superlattice can be visualized as *m* layers of GeTe inserted into the center of each Sb₂Te₃ slab, which expands the initial unit cell of Sb₂Te₃ to include long-range ordered 3D blocks with vacancies between the blocks. The (GeTe)_mSb₂Te₃ superlattice exhibits a phase transition from rhombohedral (*R*- $\bar{3}m$) to cubic rock salt (*Fm*- $\bar{3}m$) at high temperature, similar to GeTe. This reversible phase transition is accompanied by abrupt changes in electrical and optical properties, enabling applications in phase-change memory devices. However, even though the structural and thermal properties of these materials have been studied in some depth, the effect of the phase transition on bond strength and phonon transport properties has not been studied. In this study, we combine high-temperature X-ray diffraction and high-temperature resonant ultrasound spectroscopy to measure the lattice parameters, elastic moduli and sound velocity in (GeTe)_mSb₂Te₃. We find that the elastic moduli and speed of sound increase gradually with increasing temperature up to the phase transition, then exhibit a final sharp increase upon transforming to the rock salt structure after which the elastic moduli begin to decrease. Our results suggest that with increasing temperature, the ordered vacancy layers diffuse gradually into the surrounding distorted rock salt matrix, increasing the interlayer bond strength, thus leading to the anomalous temperature-dependence of the thermal conductivity.

PS54

(Student) Ultrafast Nonperturbative Switching of Carbon Nanotube Excitons Weiwei Jiang¹, Kankan Cong², Bryan Anthonio², Junichiro Kono² and Mackillo Kira¹; ¹University of Michigan—Ann Arbor, Ann Arbor, Michigan, United States; ²Rice University, Houston, Texas, United States.

Unlike pristine graphene, carbon nanotubes (CNTs) can be designed to become direct-gap semiconductors. Since most of the field lines of the Coulomb interaction reside outside the effectively one-dimensional structure, CNTs can produce extremely strongly Coulomb bound electron-hole pairs, i.e. excitons detectable even at room temperature. This extremely strong Coulomb coupling also introduces other many-body features, such as excitation-dependent lifetime of coherences and Coulomb renormalizations. We present comprehensive theory–experiment investigations, that identify nonperturbative strong-field and many-body effects that can be exploited to optically switch CNT properties on an ultrafast time scale. We start by demonstrating that strong light–matter interactions can transiently shift excitonic absorption during the presence of an ultrafast pulse while it returns to its original position after the excitation. In this configuration, we apply a 200fs-long pump pulse that is tuned well below the exciton resonance to avoid significant carrier generation due to excitonic absorption. In this situation, optical field transiently generates optical polarization that ideally and adiabatically follows the pulse. The main mechanism for switching stems from the

presence of the field that moves the exciton resonance due to the optical Stark effect. At the same time, there will also be some amount of scattering of coherences even from the transiently generated densities, which induces dephasing and broadening for the excitonic polarization. This absorption can create residual excitation after the pulsed excitation, which would be detrimental for a reversible Stark-effect switching because the exciton response would change after the excitation. However, such scattering takes some time to build up such that polarization at a given time depends on polarization and densities created at an earlier time. We perform systematic quantum-kinetic many-body computations and compare the results quantitatively with experiments to demonstrate that quantum-memory effects can indeed be utilized to realize a sizable switching that is essentially reversible on ultrafast timescales. Using the same predictive quantum theory, we also investigate light-matter interactions for a pump that is resonant with the exciton state, characterized via pump-probe spectroscopy. This regime can simultaneously exhibit multiple nonperturbative effects such as Rabi splitting and nonlinear mixing. Since we use a pulsed excitation, we do not expect to see a constant splitting of the exciton resonance into two because the Rabi splitting is proportional to the *pulsed* field amplitude of the pump. Nevertheless, our detailed theory-experiment analysis reveals that this setup can produce strong wave-mixing that appears as coherent oscillations when probe pulse arrives before the pump, and a nearly constant spectral splitting after the pulse. In particular, a resonant excitation produces strong optical switching which is irreversible due to carriers accumulated after the pump pulse. We also have verified that the switching changes its character when the CNT configuration itself eliminates wave mixing altogether. Our results show that all switching and nonlinear features stem from spectral hole burning in this situation. In other words, only those CNTs that are resonant with the field produce irreversible switching while the nonresonant ones show an unaltered response. In summary, we demonstrate clear conditions to realize reversible ultrafast switching vs. irreversible switching due to strong light-matter and Coulomb effects in CNTs.

PS55

(Student) Electrically Probing and Tuning of Molecular Physisorption on Graphene [Wenzhe Zang](#)¹, Girish S. Kulkarni¹, Karthik Reddy², Hongbo Zhu², Kyunghoon Lee¹, Xudong Fan² and Zhaohui Zhong¹;

¹Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Ann Arbor, Michigan, United States;

²Department of Biomedical Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

Nanoelectronic systems are perfect testbeds to study and mimic the physicochemical nature of noncovalent interactions which, though weak in nature (~ 100s of meV), form the bedrock of most biological and cellular processes. Furthermore, the ability to electrically tune the charge density (hence the chemical potential) in nanomaterials via electrostatic gating provides another knob to control such interaction. Unfortunately, nearly all existing electronic sensing methodologies are based on charge transfer (covalent interactions) which does not fully represent the interaction between the adsorbed vapor molecules and a pristine nanosurface. Here we present results of electrical probing and tuning of the noncovalent physisorption of both polar and nonpolar molecules on graphene surface by using two different sensing techniques – heterodyne sensing and μ ColumnFET sensing. Temperature-dependent molecular desorptions for six different polar molecules and five non-polar species were measured in real-time to study the desorption kinetics and extract the binding affinities. Furthermore, we demonstrate, for the first time, electrical tuning of molecule-graphene binding kinetics via electrostatic gating of graphene; the molecular desorption can be slowed down nearly three times within a gate voltage range of 15V. Our results not only provide insight into the non-covalent interaction dynamics between graphene and both polar and non-polar molecules, but also pave the way to electrically tailor physisorption dynamics at nanoscale interfaces.

PS56

(Student) Nitrogen, Sulfur Co-Doped Reduced Graphene Oxide/Hexagonal Tungsten Trioxide (WO₃) Nanorods Nanocomposite as High-Performance Anode Materials for Lithium-Ion Batteries [Yiqiao Huang](#)¹ and Ferdinand Poudeu²;

¹Materials Science & Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States;

²University of Michigan, Ann Arbor, Michigan, United States.

Tungsten trioxide (WO₃) is a promising anode material for lithium ion battery due to its environmental friendliness and high theoretical specific capacity (693 mAh g⁻¹). In this study, WO₃ nanorods with hexagonal crystal structure are anchored on nitrogen and sulfur co-doped reduced graphene oxide matrix to form nanocomposite (NSG/WO₃). The synthesis is achieved by a facile hydrothermal reaction at 180 °C for 12 hours.

Scanning transmission electron microscopy (STEM) images reveal that the tiny WO₃ nanorods with length ranging from 40 nm to 100 nm and diameter ranging from 5 nm to 15 nm are wrapped by doped reduced graphene oxide (RGO) matrix. X-ray photoelectron spectroscopy (XPS) results confirm that the nitrogen and sulfur atoms are successfully doped into the RGO matrix through the formation of chemical bonding with carbon atoms in the RGO structure. Thermogravimetric analysis (TGA) indicates that the nanocomposite contains ~46 wt. % of WO₃. The nanocomposite is made into anodes for coin cell tests, and it shows an excellent specific discharge capacity of 1030 mAh g⁻¹ at the first cycle and high rate capacities of 513.0, 384.1, 268.9, 200.6 and 150.4 mAh g⁻¹ at the current density of 100, 200, 500, 1000 and 2000 mA g⁻¹, respectively. Additionally, the nanocomposite also exhibits superior cycle stability sustaining a high discharge capacity of 196.1 mAh g⁻¹ at a large current density of 1500 mA g⁻¹ for 200 cycles. This result is superior to previously reported data on hexagonal WO₃-based materials. The high performance of NSG/WO₃ materials can be attributed to synergistic contributions from (1) the small size of WO₃ nanorods which, effectively shorten the diffusion length of Li⁺; (2) the structural support from doped RGO matrix, which alleviates the huge volume change of WO₃ nanorods during Li⁺ insertion/extraction; and (3) the nitrogen and sulfur co-dopants, which provide large numbers of surface defects, as proven by Raman spectroscopy, serving as channels to improve the Li⁺ diffusion. In addition, the electrochemical impedance spectroscopy (EIS) measurement demonstrates that nitrogen, sulfur co-doped RGO can reduce the electrochemical impedance of the electrode, further improving the electrochemical performance of the anode. This research provides some significant strategies of future anode materials design for lithium ion battery.

SESSION P: Printed and Flexible Materials and Devices
Session Chairs: Sarah Swisher and William Wong
Thursday Morning, June 27, 2019
Michigan League, 2nd Floor, Kalamazoo

8:20 AM P01

Inkjet Printed Graphene and Composite Graphene-Graphene Aerosol Gel for Enhanced Charge-Transfer Studies Wenjun Xiang, Arjun Nepal, Christopher Sorensen and Suprem Das; Kansas State University, Manhattan, Kansas, United States.

Flexible printed electronics represent an emerging class of technology with broad applications due to their relatively simple fabrication (such as mask-less technology and multi-layer integration) and economically competitive advantages. Printed devices and circuits such as touch screens, environmental and biological sensors, logic circuits, radio frequency transmitters, photovoltaic cells, and electronic textiles could be widely integrated in IoT platforms to be used in day-to-day life¹⁻³. For high spatial resolution, leading to high sensitivity of the devices the inkjet printing provides one of the most promising route when compared to other printing methods.⁴ After a decade and half of graphene research, mostly fundamental understanding of graphene's unique properties, there have been great interest for scalable manufacturing of graphene devices and circuits for various novel applications⁵. Solution-phase ink formulation and inkjet printing of graphene and related materials for printed electronics has shown considerable potential due to graphene's high electrical and high thermal conductivities, mechanical flexibility and chemical robustness⁶. However, manipulating the surface nanostructure and functionalities remains challenge for practical printed circuits, in conjunction with the above properties. Our research focuses on improving the properties of Ink-jet printing graphene-based devices by combining graphene ink with graphene aerosol gels (GAGs) that could provide larger surface area due to its highly porous structure. Inks with graphene nanosheets (GNs ink) and with composite of graphene nanosheets and graphene aerosol gels (GN-GAGs ink) were formulated where a stable suspension of GNs and GAGs were confirmed. Subsequently they were ink-jet printed on flexible polyimide substrates with interdigitated electrode (IDE) geometry to study their electrochemical activities by analyzing their charge transfer processes between the carbon atoms interfaced with the solution samples in an electrochemical cell. Post-printing processes such as inert gas annealing were exploited to mechanically strengthen the printing layer on flexible substrate as well as chemically reduce the oxygen and organics attached to the carbon lattice. The porous structure as well as the network distribution of the GAGs in the GNs matrix in the printed IDEs were conformed from the transmission electron microscope (TEM) studies. Finally, cyclic voltammetry (CV) studies were conducted with potassium ferricyanide and hexa-ammine-ruthenium(III) chloride probes to reveal the enhanced electron transfer properties of the GN-GAGs as compared with pure GNs. The emergence of well-defined oxidation-reduction peaks in GN-GAGs printed surface as compared with printed surface with pure graphene is correlated to the porous network structure. References: [1] IEEE Sensors Journal 2015, 15(6), 3164-3185 [2] Small 2014, 10(17), 3515-3535 [3] Adv. Mater. 2016, 28(22), 4397-4414 [4] ACS Nano, 2012, 6 (4), 2992-3006 [5] Critical Reviews in Solid State and Materials Sciences, 2010, 35(1), 52-71 [6] Nature Nanotechnology 2008, 3, 563-568

8:40 AM P02

(Student) Inkjet Printing of Inorganic Films and Nanomaterials for Optoelectronic Applications Brent Cook¹, Maogang Gong¹, Daniel Ewing², Matt Casper², Alex Stramel², Alan Elliot² and Judy Wu¹; ¹Physics and Astronomy, The University of Kansas, Lawrence, Kansas, United States; ²Department of Energy's Kansas City National Security Campus, Kansas City, Kansas, United States.

Inkjet printing offers a simple, scalable, and low-cost approach for fabrication of devices based on nanomaterials with the goal to integrate them with CMOS. Currently, most nanomaterials and precursor inks require post-treatment at high temperatures, chemical vapor deposition, high vacuum and controlled gaseous environments to form crystalline phases. However, quantum dots (QDs) such as crystalline PbS, ZnO, and nanocube FeS₂, can be synthesized directly into inks for on-chip printing of high-performance optoelectronic devices without post heat treatments. In this work, we report our recent progress in addressing several critical issues that arise from inkjet printing of optoelectronic devices on SiO₂ and graphene including: 1) the poor QD-QD linkage and interface that arises

from printed QDs having a Van der Waals contact when printing multi-layer quantum dots and 2) ink coagulation of precursors that occurs from printing on a hydrophobic surface. The first issue is approached by using a ligand exchange to remove long carbon chained molecules such as octadecylamine and 1-octadecene that are present on the FeS₂ and PbS surfaces after synthesis. However, the linkage from top layers of QDs can still remain poor as a result photoconductors have to be fabricated in a pixelated structure as opposed to tandem designs. The second issue concerning precursor inks was resolved a couple of ways. One method utilizes surface heat treatment which was varied from 22-80 °C to find the best printing conditions and the other method utilizes QDs to assist interlinking droplets that form naturally from printing on a hydrophobic silicon dioxide surface. This was achieved two ways, one, by incorporating the QDs into the precursor to form a nanocomposite ink, and two, treating the surface with QDs to alter the surface roughness and hydrophobicity. Performance for UV-IR detection has achieved a photoresponsivity up to 10⁸ A/W and 10⁷ A/W for printed ZnO QDs and PbS/FeS₂, on graphene field effect transistors. In addition, precursor inks such as ZnO and WO₃ can also be printed and annealed in air without need of vacuum or controlled gas environments. The inkjet printing of ZnO/ZnO QDs composites and WO₃ precursor inks for photoconductor applications have achieved responsivities of up to 10² A/W and ~2 A/W respectively. These results indicate that the applicability of inkjet printing of nanostructures for UV-IR detection and thin films is viable and has room for more improvement including better precursor synthesis and solution based techniques.

9:00 AM P03

High Performance and Air-Stable Polymeric Thin-Film Transistors Sunghwan Lee¹ and Grant Drewelow²; ¹School of Engineering Technology, Purdue University, West Lafayette, Indiana, United States; ²Mechanical Engineering, Baylor University, Waco, Texas, United States.

Although unsubstituted polythiophene (PT) has several promising properties such as high electrical conductivity as well as excellent environmental and thermal stability, its insoluble nature makes it challenging to be processed using conventional solution-based techniques. Therefore, the implementation of unsubstituted PT in organic electronic and optoelectronic devices has been quite limited. However, the volatility of thiophene monomer enables the use of oxidative chemical vapor deposition (oCVD) to readily synthesize and deposit PT films. Organic TFT devices utilizing oCVD-processed polythiophene as the channel material show excellent on and off states, drain current saturation behavior, and low threshold voltages (between -1 V and 0.3 V). The maximum measured field effect mobility was approximately 0.02 cm²/Vsec. The PT-TFTs present consistent device performance for more than 90 days, confirming superior device stability over time in air. Photo-conductivity studies reveal that charge carrier density increases with increasing light intensity and the field effect mobility enhances as a result of an increase in carrier density. The specific contact resistance between oCVD PT channel and metallization was evaluated using TLM measurements. The TFT/TLM investigation shows an improvement in contact resistance with increasing gate bias which is attributed to an effective modulation of channel conductivity as a function of gate bias. The TLM study enable the estimation of channel carrier density, which has been challenging to measure via conventional 4-point probe and Hall Effect measurements, and therefore the establishment of carrier transport mechanism that operates in polythiophene thin films. oCVD PT shows an increase in carrier mobility with increasing carrier density at the regime lower than approximately 5x10¹⁷ /cm³ where the carrier transport is governed by the charge screening effect while at higher carrier density regime, weak ionized impurity scattering dependence is observed. The low-temperature processed oCVD PT exhibiting great air-stability and promising photo-conductivity behavior may have important application in, for example, flexible displays and organic photovoltaics that require superior ductility, air-stability and photo-responsibility. The performance of oCVD PT materials and devices may be further enhanced by decreasing defects in the polymer structure and improving relatively high contact resistance of the channel and metallization interface.

9:20 AM P04

Carbon Fiber Electronics—Creating Multifunctional Materials Using Low-Cost Fabrication Gerd Grau¹, Jiefeng Qiu², Mohamad K. Idris¹ and Luis Pinto³; ¹Electrical Engineering and Computer Science, York University, Toronto, Ontario, Canada; ²Mechanical Engineering, York University, Toronto, Ontario, Canada; ³Physics and Astronomy, York University, Toronto, Ontario, Canada.

Carbon fiber composites are a promising class of structural materials that are becoming increasingly prevalent in many high-tech applications

ranging from airframes to high-performance bicycle frames to prosthetics. Freeform shapes can be manufactured in an automated fashion by braiding or weaving fiber bundles into a tight mesh and encasing it in a resin matrix. Depending on the resin, the material can be hard or flexible. Mechanically, these materials combine high strength with light weight. Electrically, carbon fibers act as conductors. This means carbon fibers can be used to additively manufacture large-area electronic systems with 3D geometry. One potential application is structural health monitoring (SHM). The carbon fibers themselves can act as sensors of mechanical strain and damage giving direct information on the structural integrity of composites. This information can be difficult, expensive or impossible to obtain using classical approaches such as discrete strain gauges, especially for complex geometries. In order to apply carbon fibers in this new way, they need to be understood as electronic materials. In this talk, I am going to describe our group's recent progress in fabricating and characterizing electronic carbon fiber materials and devices. Carbon fiber composites are hierarchical structures that are made up of individual fibers (diameter on the order of 10 μ m), fiber bundles of thousands of fibers and weaves or braids of fiber bundles. Weaves can be understood as regular, anisotropic 2D conductors consisting of a matrix structure. The key parameters of this matrix are the resistance of the orthogonal fiber bundles, the junction resistance between crossing fibers, the weaving pattern and the orientation of fibers relative to the contacts. The effect of these parameters on electrical response can be modulated by different strain and damage states enabling structural health sensing. We have developed printed electronics techniques as a low-cost and facile method to make reliable contacts to carbon fiber sheets and will present electrical characterization results of such printed carbon fiber composites. More complex devices can be fabricated by functionalizing carbon fibers with other functional materials. We will demonstrate this concept with an electroluminescent (EL) carbon fiber composite. The strain state of the structure can be read out easily by visual inspection of changes in the EL light output. EL phosphor particles are dispersed in an elastomeric matrix and a thin film is applied to a carbon fiber weave back-electrode. The front electrode needs to be transparent to allow the generated light to escape. A sparse carbon fiber electrode has several advantages over other transparent electrodes. Carbon fibers offer superior mechanical properties combined with simple fabrication, very low cost and good sheet resistance depending on fiber grade. Sparse carbon fiber electrodes were fabricated by different methods. Chopped fibers were dispersed in a solvent to create a random network. Sparse carbon fibers can also be aligned in a particular direction to interact only with strain in that direction. We will present electrical, optical and mechanical characterization of carbon fiber-based electroluminescent devices. In conclusion, carbon fibers are a promising electronic material complementing their traditional use as a structural material. Applications include structural health monitoring of carbon fiber composite structures as well as the low-cost integration of electronic functionality into 3D composite systems, especially in conjunction with printing and other solution-processing methods.

9:40 AM P05

(Student) Lead-Free Tactile Sensors and Energy Harvesting Devices for Wearable and Flexible Electronics Rajinder S. Deol, [Nitika Batra](#), Henam S. Devi, Bhaskar Mitra and Madhusudan Singh; Electrical Engineering, Indian Institute of Technology Delhi, New Delhi, India.

Lead-free, bio-conformable and lightweight piezoelectric materials used in sensors and actuators are expected to address a capability gap in wearable electronics applications[1]. Conventional methods of production of an attractive lead-free material, potassium sodium niobate (KNN) using physical vapor deposition, thermomechanical methods, accompanied with high temperature (600-1100°C) sintering[2] result in high thermal budget processes incompatible with flexible substrates needed, and retention of synthesized compositions due to the known volatility of potassium[3]. In contrast, sol-gel methods provide excellent stoichiometric control over the final product. In this work, we have used a previously reported KNN sol[4] with some process improvements to deposit thin films for electromechanical characterization of the film and fabricated a tactile sensor on a flexible substrate. To estimate the electromechanical performance of the material, a thin film (~60-70 nm) of KNN was deposited on a tungsten-coated Si substrate and studied using piezoresponse force microscopy (PFM, Bruker Dimension Icon). Using different excitation voltages between 2V and 8V, a d_{33} value of ~70pC/N was estimated, which may contain electrostatic tip interaction artifacts[5,6]. Tactile sensors were fabricated on an indium tin oxide coated polyethylene terephthalate (PET) substrate in the form of large area (~5cm x 1 cm) strips with a drop-casted KNN film dried at 90°C (to minimize any warping of the substrate) followed by a thermally evaporated top electrode (Ag, 3 x 10⁻⁷Torr, Angstrom Engineering). A thick drop-casted active film was intentionally chosen to increase the size

of the measured signal under flexion. The device is connected to an oscilloscope (Tektronix MDO3054) through a full wave bridge rectifier to mimically mimic likely operational conditions for an energy harvesting circuit. The device shows a fast response on the application of variable pressure with a human hand. The magnitude of the voltage signal generated (~40 mV) is over and above the rectification drop of approx. 1.4 V expected through the rectifier. The yield of sensors was fairly low (~20%) due to this high rectification loss. This loss of signal for the sensor can be recovered by signal processing and the loss of energy in the harvester can be partially mitigated by the use of a Schottky or a fast action diode. Further work for charge recovery and signal processing is underway. KNN-based flexible devices can be thus used for sensing as well as energy harvesting applications for Internet of Things (IoT) devices in a wearable form factor. [1] A. Khan, Z. Abbas, H. S. Kim, and I.-K. Oh, *Smart Mater. Struct.*, vol. 25, no. 5, p. 053002, 2016. [2] J.-F. Li, K. Wang, F.-Y. Zhu, L.-Q. Cheng, and F.-Z. Yao, *Journal of the American Ceramic Society*, vol. 96, no. 12, pp. 3677–3696, Nov. 2013. [3] A. Kupec, B. Malic, J. Tellier, E. Tchernychova, S. Glinsek, and M. Kosec, *J Am Ceram Soc*, vol. 95, no. 2, pp. 515–523, Feb. 2012. [4] R. S. Deol, M. Mehra, B. Mitra, and M. Singh, *MRS Advances*, vol. 3, no. 5, pp. 269–275, 2018. [5] Y. Ivry, N. Wang, D. Chu, and C. Durkan, *Phys. Rev. B*, vol. 81, no. 17, p. 174118, May 2010. [6] S. Kim, D. Seol, X. Lu, M. Alexe, and Y. Kim, *Scientific Reports*, vol. 7, p. 41657, Jan. 2017.

10:00 AM REFRESHMENT BREAK

SESSION Q: Electronic Materials for Bio Session Chairs: Suprem Das and Curt Richter Thursday Morning, June 27, 2019 Michigan League, 2nd Floor, Kalamazoo

10:20 AM Q01

Biosensor Array Using CVD-Grown Graphene for Influenza Virus Detection Takao Ono¹, Shota Ushiba², Yasushi Kanai¹, Naruto Miyakawa², Ayumi Shinagawa², Kaori Yamamoto¹, Masami Tanioku¹, Yasuhide Ohno³,¹ Kenzo Maehashi⁴, Koichi Inoue¹, Yohei Watanabe⁵, Shin-ichi Nakakita⁶, Toshio Kawahara⁷, Masahiko Kimura², Yasuo Suzuki⁷ and Kazuhiko Matsumoto¹; ¹ISIR, Osaka University, Osaka, Japan; ²Murata Manufacturing, Nagaoka, Japan; ³Tokushima University, Tokushima, Japan; ⁴Tokyo University of Agriculture and Technology, Koganei, Japan; ⁵Kyoto Prefectural University of Medicine, Kyoto, Japan; ⁶Life Science Research Center, Miki, Japan; ⁷Chubu University, Kasugai, Japan.

In recent years, highly pathogenic avian influenza is attracting global attention in poultry farming. Moreover, when the influenza virus (IFV) achieves human infectivity through mutation, severe pandemic is predicted. In the early stage of infection, IFV attaches to cell surface using its hemagglutinin. Avian or human infectivity of IFV is determined by binding affinity of hemagglutinin to sialoglycan on avian or human cell surface, respectively. Based on this infection process, the authors have developed high-sensitive detection method for emergence of human-infectious avian IFV by using sialoglycan-modified graphene FET (G-FET). Graphene is favorable for electrical biosensing, because it is two-dimensional material having ideally high surface-to-volume ratio and it has the highest carrier mobility in known materials resulting in effective transduction of contact of charged target into large drain current change in G-FET. The authors have reported that G-FET specifically detected human-infectious IFV in concentration of patient's saliva. However, in the report the authors used exfoliated graphene, which is inadequate for real use, due to its low production efficiency. In this study, the authors synthesized CVD graphene and applied it to G-FET array for IFV sensor. Also, they developed portable G-FET system and applied it to on-site measurement of avian influenza sample obtained in Alexandria, Egypt, where avian influenza runs rampant. Graphene was grown on copper foil using methane in vacuum furnace at 950°C. In Raman spectra, sharp G-peak (~1580 cm⁻¹) and 2D-peak (~2700 cm⁻¹) was observed and D-peak (~1350 cm⁻¹) was hardly observed. It shows high quality of graphene. The CVD-grown graphene was then transferred to Si/SiO₂ substrate, connected to Au/Ti electrodes and etched to form G-FET channel. 82 G-FETs were arrayed on a chip. For portable G-FET system, 32 G-FETs were arrayed on a chip. Sialoglycan was modified on G-FET via π -stacking linker. The modification was confirmed by the shift of Dirac point, current minimum in ambipolar transfer characteristics of G-FET, toward positive voltage direction. It is owing to negative charge of sialoglycan, which induces hole carrier to graphene. All measurements were carried out in pH 7.4. First, 82 G-FETs on a chip was separated into two areas and samples with and

without IFV were simultaneously introduced to each area. Position of Dirac point and its shift were diverse in G-FETs, but by averaging the response among G-FETs in each area and comparing to G-FETs without IFV, positive Dirac-point shift in G-FETs with IFV were clearly observed. The quality of graphene is not uniform so far, but by averaging among G-FET array, accurate response was elicited. Next, 32 G-FETs on a chip for portable system was separated into three areas for human sialoglycan, avian sialoglycan and no sialoglycan. Then the whole system was transported to Egypt and applied to clinical sample obtained there. The sample was H9N2 avian IFV extracted from chicken and amplified in allantoic fluid. After IFV binding, Dirac point was positively shifted in all G-FETs. It can be attributed to nonspecific adsorption of the protein in allantoic fluid. By comparing three areas, positive Dirac-point shift was larger in sialoglycan-modified G-FETs, but was not different between G-FETs with avian and human sialoglycan. Meanwhile, fluorescent immunostaining clearly visualized IFV particles on G-FET. Particles were dense only on avian sialoglycan modified G-FET. The conflict between results of electrical and fluorescent measurements may be due to contamination of other kind of virus such as Newcastle disease virus. Toward practical and commercial use of G-FET system, the authors constructed G-FET biosensor array and portable G-FET system. The portable G-FET system will open up a new possibility of on-site diagnosis to prevent oncoming influenza pandemic. [Acknowledgement] This work was supported by JST-CREST (JPMJCR15F4).

10:40 AM Q02

Novel Drug Delivery System Prepared by Coaxial Electrospinning—Local Cancer Therapy, Multiple Drug Cocktail Therapy and “On-Demand” Therapy Daewoo Han and Andrew Steckl; Nanoelectronics Laboratory, Electrical Engineering and Computer Science, University of Cincinnati, Cincinnati, Ohio, United States.

Core-sheath fibers formed by coaxial electrospinning have emerged during last decade as extremely versatile materials, because they can (a) integrate two or more material properties into a single fiber structure, (b) provide controlled release rates of drugs encapsulated in the fiber core, (c) protect incorporated drugs from harsh ambient. In another important medical application non-woven fiber network of randomly aligned electrospun fibers are intrinsically very similar to the natural extracellular matrix (ECM), which is especially useful for tissue engineering and treatment. In addition to the sustained release, current research trend for controlled drug delivery is moving forward to (a) “cocktail” therapy releasing multiple drugs in controlled manner to obtain synergistic effects and (b) “on-demand” reactions which release the selected functional molecules upon detecting the targeted stimulus. Here, we present different materials strategies for drug delivery involving (a) anti-cancer drug incorporated nanofiber disc implants for local cancer therapy against malignant glioblastoma multiforme (GBM), (b) dual drug delivery using triaxial fibers, (c) stimuli-triggered release using self-immolative sheath, and tri-phasic pH responsive release (“no release; sustained release; burst release”) within physiological pH range. GBM is one of most aggressive cancers, presenting a 5-year survival rate of 5.1% with extremely high recurrence rate (> 90%) and very short mean survival time (< 15 months). Carmustine (bis-chloroethyl-nitrosourea - BCNU) loaded core-sheath fibers have been successfully fabricated, and formed into densified fibrous discs for implantation and local treatment directly into the brain. Sustained release of incorporated BCNU over an extended period (> 150 days) resulted in very promising in-vivo results with much higher median survival time of 63 days and long-term survival (LTS) rate of 50% at 150 days compared to the control group with mean survival time of 11 days and 0% LTS. For multiple drug delivery with different kinetics, a tri-layered fiber structure (core-intermediate-sheath) was adapted. Two drugs are incorporated either in the core or the sheath individually, and the intermediate hydrophobic layer acts as a barrier between the layers. This compound fiber structure provides abrupt burst release of one drug from the sheath while a 2nd drug from the core is released gradually. The sheath thickness and coaxial nozzle dimensions can adjust the sustained release rate from the core. Stimuli-triggered release from the core of coaxial fibers was also demonstrated using self-immolative polymers (SIP) in the sheath. Once triggered by target stimuli, the sheath polymer is depolymerized revealing the core fiber surface, which initiates the release from the core material. Due to the high surface area of electrospun membranes, depolymerization rate is ~ 25x faster than that of the equivalent cast films, leading to much higher responsiveness to external stimuli. Another stimuli-responsive release is demonstrated using core-sheath fibers made of two different pH responsive Eudragit polymers. Due to different pH dissolving range of core (pH => 6) and sheath (pH => 7), tri-phasic pH response is obtained: (a) no release at pH 5, (b) sustained release of core in pH 6, and quick release of core and sheath in pH => 7. Ultimately, it is hoped that in the near future, all of these features can be combined into a

single delivery system which initiates the drug release by external stimuli, and then controls the release rates of multiple drugs to deliver synergistic drug effects over a long-term period.

11:00 AM Q03

(Student) Optimization of Organic Electrochemical Transistor Media for Bacterial Characterization Eric Frantz, Ashkan Tirgar and Andrew Steckl; Nanoelectronics Laboratory, Electrical and Computer Engineering, University of Cincinnati, Cincinnati, Ohio, United States.

Ion generation in bacteria cells is a central component in their life cycle. Therefore, understanding bacterial ion-generation can lead to a better understanding of bacterial responses to stimuli, and the mechanisms that regulate ion transport. Ion-based communication both within and between bacteria colonies is also of importance in detecting the presence of various bacterial species and controlling their development [1]. Optical measurements with fluorescent dyes are commonly used to detect and quantify ion concentrations both within and outside of individual cells or cultures. Electronic measurements of bacterial ions are typically done using ion-selective electrodes and ion-sensitive field effect transistors. Unlike fluorescent measurements, electronic measurement of ions is limited to extra-cellular ions but does not require the use of dyes or fluorescent microscopes. We have used organic electrochemical transistors (OECTs) to measure ion concentrations in traditional electrolyte solutions and in bacteria growth media. OECTs have become popular in whole-cell characterization and detection [2] due to their high transconductance, biocompatibility, low cost, small size, ease of integration into measurement systems, and functioning ability in aqueous environments. OECT operation is driven by ions from either liquid or semi-solid ion source. Electrolytes and bacterial broth media are commonly used as ion sources for OECTs. Cell culture media contain a wide variety of non-ion species, such as peptides and yeast. Understanding the effect non-ion species have on OECT performance is essential for understanding bacterial cell interaction and optimizing detection sensitivity. We have studied key parameters of PEDOT:PSS-based OECT operation, including transconductance, ON/OFF ratio, and optimal gate voltage, for several liquid and gel ion sources: KCl, NaCl, PBS, LB broth, YT broth, and water solutions. Peak transconductance was achieved using a 0.1M KCl solution. Transconductance values for both YT and LB broth were found to perform at only 84% and 57% compared to that of 0.1M KCl. On/Off ratios, however, increased 300% and 224% for LB and YT broth when compared to 0.1M KCl. A shift in optimal gate voltage from ~0.6V to ~0.3V was measured for both broth solutions compared to pure electrolyte solutions (KCl, NaCl, etc.). Our results show that broth solutions perform noticeably different than traditional pure-electrolyte solutions. 1. Humphries, J., et al., *Species-independent attraction to biofilms through electrical signaling*. Cell, 2017. **168**(1): p. 200-209. e12. 2. Strakosas, X., M. Bongo, and R.M. Owens, *The organic electrochemical transistor for biological applications*. Journal of Applied Polymer Science, 2015. **132**(15).

11:20 AM Q04

Biosynthesis of Molybdenum Disulfide Nanoparticles Using The Metal-Reducing Bacterium *Shewanella Oneidensis* MR-1 James D. Rees; Electrical, Computer and Systems Engineering, Rensselaer Polytechnic Institute, Troy, New York, United States.

The bacterium *Shewanella oneidensis* MR-1 is a dissimilatory metal-reducing bacterium capable of performing anaerobic respiration using a metal as terminal electron acceptor. Isolated from Lake Oneida in Upstate New York, *S. oneidensis* MR-1 was first noted for its manganese-reducing capability, but has now been shown to reduce a range metal ions such as Fe(III), Mn(IV), As(V) and Cr(VI), as well as sulfur anions such as thiosulfate and sulfite. In the lab, *Shewanella* has been grown anaerobically in media enhanced with sulfur and metal ions in order to produce several types of chalcogenide nanoparticles, such as zinc sulfide and arsenic trisulfide. Given the utility of chalcogenide materials for electronics and photonics applications, bacterially-synthesized chalcogenide nanoparticles present a tantalizing avenue for green chemistry. Compared to similar materials produced using traditional chemical synthesis methods, bacterially-synthesized nanomaterials can be produced at much lower temperatures and using fewer chemical reagents. This work presents a method of synthesizing molybdenum disulfide nanoparticles using *S. oneidensis* bacteria. Molybdenum disulfide is a layered semiconductor with an indirect band gap in its bulk state and a direct bandgap in its monolayer state. It also exhibits changes in its electronic properties when its surfaces are functionalized with molecules, giving it applications for both photodetection and biosensing. An anaerobic batch culture of *S. oneidensis* MR-1 was incubated at room temperature in the presence of molybdenum oxide, resulting in the

production of molybdenum disulfide crystals less than a micron in diameter. These crystals were detected using scanning electron microscopy, transmission electron microscopy, absorbance spectroscopy and X-ray diffraction. In addition to confirming that molybdenum disulfide can be produced by *Shewanella* bacteria, the data collected using these methods provide insight on the size, morphology and photoresponse of nanoparticles generated this way. The findings also allow inferences to be made about how the confluence of several mechanisms present in an anaerobic *Shewanella* culture combine to make such a synthesis possible, while providing clues about how such processes can be further improved or extended to other materials.

11:40 AM Q05

(Student) A High Speed, High Sensitivity and Universal Graphene Vapor Sensor for Both Polar and Non-Polar Molecules [Wenzhe Zang](#)¹, Girish S. Kulkarni¹, Hongbo Zhu², Kyunghoon Lee¹, Xudong Fan² and Zhaohui Zhong¹; ¹Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Ann Arbor, Michigan, United States; ²Department of Biomedical Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

The burgeoning of wearable health technology has made direct current (DC) driven nanoelectronic chemical detection one of the most attractive candidates due to its simple circuitry. To date, nearly all existing DC sensing methodologies are based on charge transfer between the sensor and the adsorbed vapor molecules. However, the high binding energy at the charge-trapped sites significantly limit those sensors' response to tens to hundreds of seconds and also makes it inherently difficult for non-polar molecule detection, of which donor and acceptor effect is quite poor. Here we report a radically different sensing mechanism by exploiting the incomplete screening effect due to the semi-metallic nature of graphene. Molecular absorption induces capacitance change on the graphene transistor, which can be amplified intrinsically by the graphene transistor's transconductance and measured conveniently as DC current change. Rapid (down to sub second) and sensitive (down to ppb) detection of a broad range of vapor analytes, including 17 polar and non-polar molecules, are achieved on a centimeter-area graphene field effect transistor covered with a microfabricated flow channel. Specifically, we demonstrated, for the first time, alkane detection based on pristine CVD graphene. Our results not only pave the way to a universal gas sensor technology which offers high speed and high sensitivity to nearly all types of analytes, but also provide an ideal test bed for probing physisorption kinetics between hydrocarbon and π system.

SESSION R: Probes for Nanoscale Phenomena Session Chairs: Rachel Goldman and Edward Yu Thursday Morning, June 27, 2019 Michigan League, 2nd Floor, Michigan

8:20 AM R01

Ferroelectricity in Binary Oxides as Studied by Electrical Scanning Probe Techniques [Umberto Celano](#); imec, Leuven, Belgium.

Ferroelectric (FE) doped-hafnia (HfO_2) holds the promise of a lead-free material system to reignite integrated ferroelectrics in microelectronics with impact on fast switching logic devices, low-power and high-density non-volatile memory and integrated sensors.^{1,2} Therefore, it does not surprise the growing interest of both academic and industrial communities. This yielded to extensive studies on planar and vertical HfO_2 -based capacitors, including the demonstration of aggressively scaled ferroelectric field effect transistors (FeFET) and random access memory (FeRAM) in planar and vertical architectures.³⁻⁵ The monoclinic phase in hafnia can be reduced by incorporation of doping, capping layers and thermal annealing, thus increasing the presence of non-centrosymmetric orthorhombic phase that determines the appearance of a bi-stable, non-volatile electrical polarization. Although the abundance of reports on FE- HfO_2 , understanding and probing the ferroelectric effects at the material level remains a key challenge. In particular, it is not well established how to sense piezoelectric and ferroelectric properties without interfering with the intrinsic dielectric behaviors of ultrathin doped- HfO_2 (e.g. leakage, trap-charging or surface potential modifications) or without inducing electrochemical effects such as nanoscale redox processes.^{6,7} For the reasons listed here, the direct observation of ferroelectric effects on doped- HfO_2 layers remains complicated, with limited nanoscopic details to interpret (a) the appearance of intrinsic ferroelectric properties, (b) the local mechanisms of domains formation and polarization reversal. Here,

we select Si:HfO₂ as a model system (8 nm thick film). First, we review the possible methods to investigate ferroelectric properties using scanning probe microscopies (SPM). Second, standalone capacitors are characterized electrically using conventional polarization-voltage (P-V) hysteresis extracted by current-voltage (I-V) characteristics. Finally, in the attempt to isolate the intrinsic properties of Si:HfO₂, state-of-the-art SPM analysis techniques are used on the same films that underwent electrical characterization. In contrast with the electrode averaged electrical characterization, the SPM-based measurements are generally performed with the probe in direct contact with the oxide layer, applying the bias directly to the bottom electrode with the tip grounded. Thanks to their nanometric spatial resolution and sensitivity for variation in surface potential, leakage current and converse piezoelectric effects, various SPM methods have proved themselves among the best analysis techniques for FE effects. This offers the possibility to extract information from the FE- HfO_2 while disentangling the ferroelectric effects from other common processes in ultrathin oxides (e.g., leakage current, charge-trapping, and dielectric breakdown). References 1. Börske, T. S., Müller, J., Bräuhaus, D., Schröder, U. & Böttger, U. Ferroelectricity in hafnium oxide thin films. *Appl. Phys. Lett.* **99**, 0–3 (2011). 2. Park, M. H. *et al.* Ferroelectricity and Antiferroelectricity of Doped Thin HfO₂-Based Films. *Adv. Mater.* **27**, 1811–1831 (2015). 3. Breyer, E. T., Mulaosmanovic, H., Mikolajick, T. & Slesazek, S. Reconfigurable NAND / NOR logic gates in 28 nm HKMG and 22 nm FD-SOI FeFET technology. *IEDM Tech. Dig. IEEE Int. Electron Devices Meet.* 669–672 (2017). 4. Nardi, F. *et al.* Switching of nanosized filaments in NiO by conductive atomic force microscopy. *J. Appl. Phys.* **112**, 064310 (2012). 5. Florent, K. *et al.* T12-4 First Demonstration of Vertically Stacked Ferroelectric Al Doped HfO₂ Devices for NAND Applications T158 T159. 158–159 (2017). 6. Starschich, S., Menzel, S. & Böttger, U. Evidence for oxygen vacancies movement during wake-up in ferroelectric hafnium oxide. *Appl. Phys. Lett.* **108**, (2016). 7. Waser, R. & Aono, M. Nanoionics-based resistive switching memories. *Nat. Mater.* **6**, 833–40 (2007).

8:40 AM R02

Modeling Scanned Probe Microscopy of Organic and Perovskite Semiconductors [Ryan Dwyer](#)², Lee Harrell¹ and John A. Marohn¹;

¹Chemistry and Chemical Biology, Cornell University, Ithaca, New York, United States; ²Chemistry and Biochemistry, University of Mount Union, Alliance, Ohio, United States; ³Physics and Nuclear Engineering, US Military Academy, West Point, New York, United States.

Scanning probe microscopy is often extended beyond simple topographic imaging to study electrical forces and sample properties, with the most widely used experiment being frequency-modulated Kelvin probe force microscopy. The equations commonly used to interpret this frequency-modulated experiment, however, rely on two hidden assumptions: (1) the tip charge oscillates in phase with the cantilever motion to keep the tip voltage constant; and, (2) any changes in the tip-sample interaction happen slowly. One or both of these assumptions is violated in experiments. In many scanned probe studies of functional materials including organic and perovskite solar cell films and ion conductors. Starting from an electro-mechanical model of the cantilever-sample interaction, we use Lagrangian mechanics to derive coupled equations of motion for the cantilever position and charge. We solve these equations analytically using perturbation theory, and, for verification, numerically. This general approach rigorously describes scanned probe experiments even in the case when the usual assumptions of fast tip charging and slowly changing samples properties are violated. We develop a Magnus-expansion approximation to illustrate how abrupt changes in the tip-sample interaction cause abrupt changes in the cantilever amplitude and phase. We show that feedback-free time-resolved electric force microscopy cannot uniquely determine sub-cycle photocapacitance dynamics. We then use first-order perturbation theory to relate cantilever frequency shift and dissipation to the sample impedance even when the tip charge oscillates out of phase with the cantilever motion. Analogous to the treatment of impedance spectroscopy in electrochemistry, we apply this approximation to determine the cantilever frequency shift and dissipation for an arbitrary sample impedance in both local dielectric spectroscopy and broadband local dielectric spectroscopy experiments. The general approaches we develop provide a path forward for rigorously modeling the coupled motion of the cantilever position and charge in the wide range of electrical scanned probe microscopy experiments where the hidden assumptions of the conventional equations are violated or inapplicable.

9:00 AM R03

(Student) Surface Potential Imaging of High-Aspect-Ratio Si Microwires Fabricated by Metal-Assisted Chemical Etching Process Erfan Pourshaban¹, Seokmin Jeon², Yohan Yoon³, David J. Magginiti⁴ and Heayoung P. Yoon³; ¹Electrical and Computer Engineering, University of Utah, Salt Lake City, Utah, United States; ²U.S. Naval Research Laboratory, Washington, DC 20375, USA, Washington, District of Columbia, United States; ³Materials Science and Engineering, University of Utah, Salt Lake City, Utah, United States.

High-aspect-ratio silicon (Si) microwires have shown excellent optical and electrical properties than in their planar counterparts, representing an attractive device architecture for low-cost optoelectronic devices, biological and chemical sensors, and solar energy harvesting applications. Among various 3-dimensional etching approaches, metal-assisted chemical etching (MacE) is the most cost-effective and versatile method that is based on simple electrochemical reactions. With the presence of a noble metal catalyst film (e.g., gold), a pair of redox reactions are promoted at the liquid/catalyst/Si interfaces. Hydrogen peroxide (H₂O₂) is reduced by the catalyst film, and a hole (h⁺) is injected from the catalyst into Si. The oxidized Si is then etched out by the reaction with hydrofluoric acid (HF) forming a soluble silicon hexafluoride (H₂SiF₆). However, this complex interfacial interaction often alters the surface and sub-surface electronic properties of as-synthesized Si microwires. The structure-property relationships are not presently well understood. Here, we report the chemical, topological, and electronic properties of Si microwires fabricated by MacE process. We use frequency-modulated Kelvin probe force microscopy (FM-KPFM) to measure the surface potential of as-synthesized Si microwires in comparison to that of Si planar control and HF treated samples. Prior to the measurements, high-aspect ratio Si microwire arrays were fabricated by the MacE process. Arrays (2.5 mm x 2.5 mm) of microwire were patterned on a bare Si wafer using double-layer lithography ($\approx 1 \mu\text{m}$ LOR10B / $\approx 1.7 \mu\text{m}$ S1813). Following oxygen plasma cleaning (75 W for 20 sec), 30 nm thick Au film was evaporated with a deposition rate of $\approx 3 \text{ \AA/s}$. The Au patterned samples were then placed into the mixed solution of 10 M HF (36 ml) and 0.3 M H₂O₂ (3 ml), and chemically etched for 3 hours at room temperature. The photoresists and the Au film were washed off with photoresist remover and gold etchant, resulting in about 30 μm long Si microwire arrays. For the HF surface treatment, a part of as-prepared Si sample was cleaved out and additionally etched in HF solution for 2 min. Each set of Si microwire arrays was placed into a vial with 10 μl isopropanol and sonicated for 5 sec and dispersed onto a substrate for further characterizations. The collected FM-KPFM data show a significant high surface potential difference for as-synthesized Si microwires (611 mV) than in Si planar control (-510 mV). Presumably, it is attributed to some chemical residue from the fabrication and a thin oxide layer produced during the MacE processes. The presence of the oxide layer is evident in the energy dispersive X-ray spectroscopy (EDS), showing the peak of O-K _{α} at $\approx 0.51 \text{ keV}$. In contrast, this oxygen peak on the HF treated microwires does not present. The corresponding KPFM data also reveal that the surface potential of HF treated Si microwires of -352 mV, which is close to that of Si planar control. The surface roughness of the HF-treated sample decreases to $\approx 11 \text{ nm}$ (vs. $\approx 16 \text{ nm}$ for as-synthesized Si microwires). Overall, a short HF treatment on as-synthesized Si microwires is likely to recover their surface electronic properties. We will further discuss the strategy to restore of the surface and subsurface properties of MacE processed Si microwire arrays.

9:20 AM R04

(Student) Impact of Ar Ion Beam Milling on Surface Electronic Characteristics of Polycrystalline CdTe Solar Cells David J. Magginiti¹, Yohan Yoon², Seokmin Jeon², Erfan Pourshaban³ and Heayoung P. Yoon^{3,1}; ¹Materials Science and Engineering, University of Utah, Salt Lake City, Utah, United States; ²U.S. Naval Research Laboratory, Washington, DC, District of Columbia, United States; ³Electrical and Computer Engineering, University of Utah, Salt Lake City, Utah, United States.

With continuous improvements in power conversion efficiency, thin-film CdTe solar cells have become a leading contender for low-cost and high-performance photovoltaic technology on the market today. To further enhance the performance, considerable efforts have been devoted to understanding the role of microstructures (e.g., grain boundaries) and inhomogeneous interface properties. Given the small length scale of grains (a few μm or less), measurement techniques such as near-field scanning optical microscopy, conductive atomic force microscopy (c-AFM), Kelvin probe force microscopy (KPFM), and electron beam-induced current (EBIC) have been utilized. These local probes often require a smooth sample surface in order to reduce the artifacts arising from the surface

roughness of the samples. A low-angle Ar ion beam milling technique ($< 6 \text{ keV}$) is often beneficial in order to eliminate topographic effects and to cleanly expose the microstructures on top as well as the cross-section of the devices. However, the downside of this process is a possible surface and sub-surface modification caused by ion bombardment, bond breakage, and re-deposition of etched materials. In this work, we present surface analysis on CdTe solar cells before and after Ar ion beam milling process. Specifically, we investigate the surface potential difference of the samples at the level of individual grains and grain boundaries. A stack of *n*-CdS (200 nm) and *p*-CdTe (4000 nm) thin-films was thermally evaporated on an oxidized silicon wafer (300 nm SiO₂). By changing the substrate temperature, the size of CdTe grains ranges from $\approx 20 \text{ nm}$ ($< 200^\circ\text{C}$) to 7 μm ($> 450^\circ\text{C}$). The deposition rate for CdTe is $\approx 2.5 \text{ nm/s}$ for all samples. Surface roughness increases approximately exponentially with growth temperature, reaching to 200 nm at 540°C. For Ar ion beam milling, the samples were placed on a holder horizontally, and 3 keV ion beams were irradiated with an incline of 3° to the sample for approximately 7 minutes. The surface of the final sample for KPFM is as smooth as $< 20 \text{ nm}$. In KPFM, we directly measure the contact potential difference between the tip and the sample surface in the dark conditions. The recorded contact potential difference (CPD) values of as-deposited CdS/CdTe samples were lower at the grain boundaries (e.g., 0.775 V) than in grain interiors (e.g., 0.790 V). In contrast, the CPD variation of the Ar ion beam milled samples decreased across microstructures. The random brightness contrast in the KPFM map still remain near grain boundaries, implying that the Ar ion beam irradiation impact to electronic properties near/at grain boundaries. Further studies on the Ar ion beam milling process at different injection angles and the beam energy, as well as a possible solution of surface restoration (e.g., thermal annealing) are in progress.

9:40 AM R05

(Student) Atomic-Level Friction Imaging of Graphene and TMD Materials via Lateral Force Microscopy in Ambient Conditions Donghyeon Moon¹, Sunghyun Kim¹ and Suenne Kim²; ¹Applied Physics, Hanyang University, Yongin-si, Korea (the Republic of); ²Photonics and Nanoelectronics, Hanyang University, Ansan, Korea (the Republic of).

Atomic-level friction imaging enables the observation of the edge structure of nanoribbons, moiré patterns in stacked 2-dimensional materials, etc. The ability to obtain atomic-scale friction images via lateral force microscopy (LFM) is of particular importance because it allows non-destructive imaging at ambient conditions. We have obtained atomic-level frictional images of 2-dimensional graphene and transition metal dichalcogenide (TMD) monolayers through the LFM technique using an atomic force microscope (AFM). All measurements were conducted under ambient conditions. To overcome the problems of thermal drift, an AFM employs XY feedback control schemes. However, atomic-level LFM friction images were found to be disturbed by the feedback system. Thus, the thermal drift effect in LFM friction images needs to be compensated differently. In this work, we present experimental strategies for obtaining reliable atomic-level LFM friction images of 2-dimensional materials in the ambient environment. Additionally, we discuss the effects of scan parameters-gain, scan size, and scan rate-on the atomic LFM images. We have repeatedly obtained atomic-level LFM friction images based on our strategies and will show here the dependence of friction of 2-dimensional graphene and TMD materials on their atomic structures. *D.M., S.H.K., and S.K. were financially supported by the National Research Foundation (NRF) of Korea grant funded by the Korea Government (2014R1A1A2056555, 2017R1D1B04036381).

10:00 AM REFRESHMENT BREAK

10:20 AM R06

Extreme-UV-Assisted Atom Probe Tomography Norman Sanford¹, Paul Blanchard², Luis Miaja Avila², David Diercks³, Brian Gorman³ and Ann N. Chiaramonti²; ¹NIST, Boulder, Colorado, United States; ²National Institute of Standards and Technology (NIST), Boulder, Colorado, United States; ³Colorado School of Mines, Golden, Colorado, United States.

We have constructed and operated a prototype extreme-UV-assisted atom probe tomograph (XAPT). The XAPT was realized by replacing the vis/near-UV laser, installed on a conventional laser-assisted atom probe (L-APT), with a coherent extreme-UV (EUV) source. This approach was motivated by the hypothesis that a direct photo-ionization-assisted pathway for field evaporation of ions should offer significant improvements over conventional L-APT- which is generally regarded as a thermally-driven process [1]. Compared with L-APT, we expected (and indeed found) that the XAPT will often yield lower background counts in the mass spectra, reduced occurrences of molecular ions, and improved quantitative accuracy. Our tabletop EUV source consisted of an ultrafast,

amplified Ti:sapphire laser driving an Ar-filled glass capillary waveguide. Coherent EUV pulses are produced by a mechanism of high-harmonic generation, which has been described elsewhere [2]. The evacuated EUV beam path was coupled to the atom probe chamber with a vacuum manifold, which permitted analysis under typical UHV conditions. At the specimen tip, the EUV characteristics of pulse width, repetition rate, wavelength (energy), and pulse fluence were 10 fs, 10 kHz, 30 nm (42 eV), and $2.5\text{E-}8\text{ J/cm}^2$, respectively. Comparative XAPT and L-APT analyses were separately performed on specimens of GaN and SiO₂ (amorphous fused silica). These materials are instructive to examine because L-APT (355 nm laser) is typically unable to return the correct stoichiometry of SiO₂ under any tool operational conditions. Moreover, L-APT analysis of GaN will only return the correct, stoichiometric composition (50% Ga, 50% N) when the pulse fluence is roughly $2\text{E-}7\text{ J/cm}^2$. Higher pulse fluences at 355 nm generally yield a nonphysical, Ga-rich composition; lower fluences yield a N-rich composition. Standard FIB techniques were used to prepare specimens of GaN and SiO₂ for XAPT analysis [3]. Preliminary, comparative L-APT and XAPT analysis of SiO₂ has been reported recently [4]. L-APT returned an off-stoichiometry composition of 41% Si and 59% O; XAPT yielded 33% Si and 66% O (stoichiometry). Preliminary, comparative L-APT and XAPT analyses of GaN have also been reported [5]. XAPT found a composition of 49% Ga and 51% N; L-APT yielded pulse-fluence-dependent composition, and returned, 68% Ga and 32% N for a pulse fluence of roughly $2\text{E-}6\text{ J/cm}^2$. The estimated uncertainty of these composition measurements is 1–3 at. % depending upon such factors as dataset size and peak ranging. Specimen temperature for all comparative measurements was roughly 50 K. Additionally, XAPT-derived mass spectra show reduced occurrences of complex molecular ions and reduced “thermal tails” (persistent field emission after laser pulse has passed). Ongoing work intended for presentation at the meeting includes XAPT analysis of GaN/InGaN multilayers and Mg-doped GaN films. The overall conclusion from these early experiments is that the XAPT approach offers measurable improvements over conventional L-APT. 1. D. J. Larson, et al, Local Electrode Atom Probe Tomography (Springer, New York, 2013) 2. L. Miaja Avila, et al, Phys. Rev. Lett. 97, 113604 (2006) 3. P. Blanchard, et al, Crystals 8, 178 (2018) 4. A. N. Chiramonti, et al, Atom Probe Tomography and Microscopy (APT&M), Wash. DC, p. 296 (2018) 5. L. Miaja Avila, et al, Frontiers in Optic (FiO), Optical Society of America, Wash. DC, p. FTu5C. 3 (2018)

10:40 AM R07

(Student) Influence of QD Morphology on Photoluminescence in GaSb/GaAs Multilayers Christian Greenhill¹, Stephen Clark³, Eric Zech¹, Alexander Chang², Ganesh Balakrishnan³ and Rachel S. Goldman¹; ¹Materials Science & Engineering, University of Michigan, Ann Arbor, Michigan, United States; ²Materials Science and Department, Northwestern University, Evanston, Illinois, United States; ³University of New Mexico, Albuquerque, New Mexico, United States.

Due to the predicted composition and strain dependence of nested (type I) versus staggered (type II) band alignments, GaSb quantum dots (QDs) have been identified as promising for a variety of optoelectronic applications, including photovoltaic solar cells, photodetectors, charged-based memory, and light emitters. For GaSb/GaAs multilayers, typically used in devices, atomic structures ranging from QDs, quantum rings (QRs) and clusters have been observed with photoluminescence (PL) energies in the infrared ranging from 0.9 eV to 1.3 eV. However, the association of these emission energies with specific nanostructure types (i.e. QDs vs. QRs vs. clusters) remains elusive. Here, we investigate the morphology and optical properties of GaSb/GaAs multilayers, with and without 3D nanostructures, using cross-sectional scanning transmission microscopy (STEM), atom probe tomography (APT), and PL. For both cases, PL energies at 1.33eV and 1.48eV are observed and are attributed to the 2D GaSb layers and the GaAs, respectively. For the case with 3D nanostructures, two additional PL emissions are observed at lower energies near 1.08eV and 1.2eV. In addition, both individual QDs and circular arrangements of QDs, termed QD-rings, are observed. For the QDs and QD-rings, Sb-rich cores are apparent with Sb compositions up to 40 at. % (individual QDs) and up to 25 at. % (QD-rings). We attribute the observed PL emissions at 1.08eV and 1.2eV to emissions from the individual QDs and QD-rings, respectively. This new insight into the relationship between QD morphology and PL emission energies is important for optimizing near to far-infrared optoelectronic devices.

11:00 AM R08

(Student) Measurement of Excitation Coherence Lengths Using Multi-Spatial-Mode Four-Wave Mixing Torben L. Purz^{1,2}, Eric Martin¹, Zhaorong Wang¹, Hui Deng¹ and Steven T. Cundiff¹; ¹Physics, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Physics, University of Göttingen, Göttingen, Germany.

We develop a multi-spatial-mode four-wave mixing (FWM) experiment to determine the coherence length of excitons and exciton-polaritons in 2D-materials. In various systems, the coherence length is of great importance as it defines an upper spatial limit for coherent manipulation, fundamental to applications in quantum information processing [1] and transport in photovoltaics [2]. Here, we introduce a new method of measuring coherence length in condensed systems by performing FWM spectroscopy with excitation beams of distinct spatial modes that are sensitive to the coherence length of the excitons. This can be understood by noting that the FWM occurs in a domain determined by the coherence length of the excitons, i.e. for a vanishing coherence length, the electric fields are multiplied in the spatial domain, while for a coherence length of infinity, the mixing occurs in the spatial-frequency domain. Between these two limiting cases, a finite coherence length may be treated theoretically by the fractional Fourier transform (FrFT). The coherence length can be related to the order of the FrFT via the parameters for the step size and the spatial extent of the computation grid. When taking the intensity ratio of the FWM signal that results from using pure Gaussian spatial modes of the beams versus Gaussian and non-Gaussian modes for different beams, this yields an unambiguous relationship between intensity ratio and coherence length within the reasonable range for coherence lengths. The measured intensity ratio can be compared to the simulated intensity ratio curve which directly gives the corresponding coherence length. To easily generate tunable spatial beam modes, we have designed a phase-element that shifts a central portion of the beam by π , compared to the outer portions. At the focus, this will yield a mode with two lobes left and right of the center, giving a very high sensitivity to the mixing-domain and thus coherence length of the excitons. Tuning the thickness of the central stripe allows for changing the sensitivity range for the coherence length from 300 nm to 4 μm . By spectrally resolving the FWM signal, one can further disentangle different contributions that may arise from local and non-local states. [1] N. Bonadeo et al., “Coherent optical control of the quantum state of a single quantum dot,” Science 282, 1473–1476 (1998) [2] J.-L. Bredas et al., “Photovoltaic concepts inspired by coherence effects in photosynthetic systems,” Nat. Mat. 16, 35–44 (2016).

11:20 AM R09

(Student) Characterization of Polycrystalline Microstructure with Picosecond Ultrasonics Yuzhou Wang¹, David Hurlley², Zilong Hua², Gaofeng Sha¹, Vitaliy Gusev³, Samuel Raetz³ and Marat Khafizov¹; ¹Mechanical and Aerospace Engineering, The Ohio State University, Columbus, Ohio, United States; ²Idaho National Laboratory, Idaho Falls, Idaho, United States; ³Université du Maine, Le Mans, France.

Utilization of polycrystalline materials in electronics application offers an economic advantage over traditional single crystals at the expense of modified electronic performance caused by grain boundaries. The impact of grain boundaries on the performance of electronic materials remains an important research topic. Numerous modelling and experimental studies have been conducted to reveal the grain boundary’s influence on dopant distribution, material strength, and carrier transport. Microscale X-ray scattering methods provide necessary spatial resolution in 3D but require use of synchrotron sources. More accessible electron microscopy methods are limited to 2D characterization and characterization of subsurface structure requires destructive sectioning. In this work, we use laser-based picosecond ultrasonics to characterize the 3D microstructure in a polycrystalline cerium dioxide, as a surrogate for semiconductor material with electronic bandgap in the tunability range of pulsed lasers. Acoustic phonons are excited by an ultra-short optical pump pulse absorbed at the surface. Acoustic wave travels into the depth of the sample, sampling the local environment. A second time-delayed probe pulse experiences reflection from the sample surface and a wave front of the acoustic pulse. By analyzing the reflected signal impacted by propagation of the wave and photoelastic coupling, we are able to determine the orientation of individual grains and reconstruct the location of subsurface grain boundary. The non-destructive feature, large probing depth, and sub-micrometer resolution make this method particularly suitable for the in-situ measurement of depth-dependent properties in semiconductor materials. Further developments of this approach will provide opportunity for characterization of defect and dopant concentration profiles around decorated grain boundaries with the ultimate goal to design advanced electronic devices.

11:40 AM R10

(LATE NEWS, Student) Near-Field Coupled Thermal Transport in van der Waals Metamaterials Sean McSherry and Andrej Lenert; Chemical Engineering, University of Michigan, Ann Arbor, Michigan, United States.

Introduction: Transmitting large radiative energy fluxes, while suppressing phonon-mediated conduction, can offer unique improvements to emerging technologies such as near-field thermophotovoltaics and electroluminescent cooling. Van der Waals metamaterials (vdW-MMs), which contain periodic structures of 2D vdW - layers, transparent dielectrics, and/or highly doped metals (see Fig. 1), are good candidates to achieve these desired properties. Here, we investigate heat transfer in vdW - MMs using experimental and computational techniques. We observe that the transport of large radiative fluxes, which occurs through cascading photon emission and absorption, can be characterized as contributions to the effective thermal conductivity. **Experimental and Computational Techniques:** We have developed a high-temperature experimental 3ω method to measure and decouple the radiative and non-radiative contributions to thermal conductivity of a thin-film material (see Fig. 2). In conjunction with our experiments, we model the radiative contributions to the thermal conductivity (radiative conductivity) in vdW-HMMs using the Multilayer Electromagnetic Solver for Heat Transfer (MESH), which simulates near-field heat transfer in multilayer structures based on fluctuational electrodynamic principles. Our model simulates interlayer near-field heat transport between adjacent metamaterial periods under an imposed temperature gradient (see Fig. 3). **Results:** Our computational results suggest that radiative heat transfer in vdW-MMs, unlike conventional isotropic media, is enhanced due to the coupling of surface electromagnetic waves which support near-field radiative fluxes across mesoscopic distances. The magnitude and selectivity of the radiative flux can be manipulated by controlling the metal and/or 2D layer doping concentration and metamaterial fill fraction. In turn, this transport can be effectively captured by contributions to the thermal conductivity. For a realizable doped-graphene metamaterial with infrared plasmonic modes², the radiative conductivity is predicted to be the same order of magnitude (>0.1 W/mK) as the non-radiative counterpart (≈ 0.25 W/mK). We plan to discuss our ongoing efforts to measure the thermal conductivity at high temperatures with a customized 3ω technique. **Significance and Contribution:** Based on the understanding developed in this work, we can engineer vdW-MMs to maximize radiative conductivity and suppress phonon-mediated conduction. In turn, this approach offers a practical method for achieving near-field transport between macroscale objects without the burden of manufacturing vacuum-based nanoscale gaps. [1] K. Chen, B. Zhao, and S. Fan., *Comput. Phys. Commun.* (2018) [doi:10.1016/j.cpc.2018.04.032]. [2] Y. C. Chang et al., *Nat. Commun.* (2016) [doi:10.1038/ncomms10568].

SESSION S: 2D Devices and Interfacial Engineering
Session Chairs: Mona Ebrish and Isaac Ruiz
Thursday Morning, June 27, 2019
Michigan League, 2nd Floor, Vandenberg

8:20 AM S01

Measurement and Control of Chiral Edge States in Graphene Curt Richter¹, Son T. Le^{2,1}, Joseph A. Hagmann¹, David Newell¹ and Ji Ung Lee³; ¹Physical Measurement Laboratory, National Institute of Standards and Technology, Olney, Maryland, United States; ²Theiss Research, La Jolla, California, United States; ³CNSE, SUNY Polytechnic, Albany, New York, United States.

Many U.S. companies with efforts in quantum information science are using solid state electronic qubits, leveraging decades of semiconductor manufacturers experience in fab facilities and equipment. Superconducting (SC) qubits are currently the leading approach to quantum computing in companies, such as IBM and Google. Unfortunately, the coherence time for SC devices are remarkably short and many physical qubits for error correction are needed to encode one logic qubit. Qubits based on topologically protected systems are predicted to have orders of magnitude better coherence times which will enable quantum circuits based on topology to be scaled to large and powerful systems. To create topological quantum systems with the necessary non-abelian statistics, it is necessary to isolate and control exotic states of matter. The most promising approach involves harnessing zero mode Majorana Fermions (MFs): a type of particle that is identical to its own antiparticle. [1] One approach to forming MFs is to couple superconducting materials to the 1D edge states

in graphene in the quantum Hall regime to create Majorana zero-modes bound to vortices. These chiral Majorana modes, as they are sometimes known, are a novel and exciting approach to quantum information processing. [2,3] Initial evidence of Majorana zero-modes has been reported, but there has been no unambiguous experimental detection despite efforts from multiple groups around the world. [4-6] We present here the results of measuring and manipulating 1D chiral edge states in graphene pn-junction devices. While these channels are not yet coupled to superconductors to form vortex-bound Majorana zero-modes, the manipulation of these edge channels is analogous to performing quantum operations on chiral MFs. We experimentally investigate charge carrier transport in graphene p-n junction (pnJ) devices using independent p-type and n-type electrostatic gating which allows characterization of the junction interfaces in the quantum Hall regime. In devices with one pnJ we show that only the edge state associated with the lowest Landau level (LL) fully equilibrates across the pnJ . [7] None of the other edge states equilibrate to transmit current across the junction. In other words, a pnJ can be used to spatially and energetically separate one edge channel from the others so that it can be independently manipulated. By using a second device based on h-BN-sandwiched graphene with two $pnJs$ and a unique ring-shaped device geometry, the interactions between edge-states are probed at both the electrostatic edges defined by $pnJs$ and at the graphene physical edge. A first pnJ is used to decouple the edge-state of the energetically lowest LL from the others while the second pnJ "senses" the amount of equilibration that occurred between the lowest LL and the rest. These measurements show that all the edge-states strongly equilibrate at the graphene physical edge despite the relatively short distance that they travel along it in our device. The measurements also confirm that the lowest LL edge-state is decoupled from the other LL's along the electrostatic pnJ . Thus, we have demonstrated that chiral edge states in graphene can be spatially separated from one another at appropriate $pnJs$ and then returned and mixed together at physical graphene edges. We believe that these same techniques could be applied to Majorana zero modes bound to chiral edge vortices to separate entangled states, perform quantum gate operations, and then return and mix them for "read out." **References:** [1] E. Majorana, *Nuovo Cim.* 14, p171 (1937). [2] C. W. J. Beenakker et al., arXiv:1809.09050v2 (Nov. 2018). [3] B. Lian, et al., *PNAS* 115 (43) 10938 (Oct. 2018). [4] V. Mourik et al., *Science* 336 (6084) p1003 (2012). [5] A.D.K. Finck, et al., *Phys. Rev. Lett.* 110, 126406 (2013). [6] S. Nadj-Perge et al., *Science* 346 (6209), p602, (2014). [7] N. N. Klimov, et al., *Phys. Rev. B* 92, 241301 (2015).

8:40 AM S02

(Student) Two Terminal Devices Based on Two-Dimensional Materials Omar B. Mohammed and Sanjay Banerjee; Microelectronics Research Center, Department of Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas, United States.

Introduction The p-n junction is one of the earliest electronic devices ever made, and still considered an important and essential element in any electronic system. Various materials can be used to build a p-n junction device, and 2D materials is one of them. An important features 2D materials can offer are the ability to tune their electronic properties easily, and dangling-bonds-free surfaces of the 2D materials which allows for engineering a near-perfect interfaces between different 2D materials. In this work we will study two different structures: lateral and vertical junction, by using various 2D materials. **Global versus Local gated devices** The highly doped Si substrate serves as a global back gate which can be used to tune the carrier densities in the ReS_2 channel material. The use of SiO_2 as a gate dielectric in the global gate structure does not allow for hole accumulation, and as a result the polarity of the channel cannot be reversed. This can be ascribed to the properties of the SiO_2/ReS_2 interface as well as to the ReS_2 material itself. ReS_2 is an n-type material and this is presumably due to the S vacancies in the material. In addition, the trapped donors at the SiO_2/ReS_2 interface increase the N-doping in the channel material even further, making it extremely difficult to reverse the polarity in such structures. Add to this the very high electric field needed to accumulate holes, and it can cause a catastrophic breakdown due to the high defect density inside the SiO_2 , as is observed experimentally. On the other hand, the hBN/ ReS_2 interface has considerably lower interface states, therefore, allows hole accumulation. The p-type conductivity is less than that of electron-type material, partly due to the lower mobility of holes in ReS_2 . Nonetheless, the ambipolar characteristics of ReS_2 , in addition to its direct band gap, have potential applications in electronics and optoelectronics. **ReS_2 lateral homojunction device** The ability to accumulate electrons and holes in the ReS_2 material by using electrostatic doping make it possible to construct a lateral homojunction device. Two separate metal pads were deposited on a Si/SiO_2 substrate. One is to dope part of the ReS_2 flake n-type, while the other is to dope the other half p-type. Using the dry transfer method, we transferred a stack of ReS_2 on

top of hBN above the metal pads. The I-V characteristics of the fabricated diode show a high cut-in voltage. A possible explanation is that a Schottky barrier is connected in series with the p-n junction, and we should overcome this barrier first before significant current can pass through the device. To mitigate this problem, we annealed the samples in ultra-high vacuum at 340°C to improve the carrier injection efficiency through the interface. The I-V characteristics of the device after heat treatment shows a well-behaved diode with a cut-in voltage ~1.5V (which is comparable to ReS₂ band gap) at room temperature, and slightly increases as temperature decreases, which is consistent with the carrier density reduction and energy bandgap widening. The rectification ratio (RR) of the fabricated diode is in the range of 10⁵. **Vertical heterostructure tunnel p-n junction** We fabricated a vertical stack of p-type WSe₂, an hBN interlayer tunnel dielectric, and an n-type ReS₂, to form a type II heterojunction. Since WSe₂ has a lower electron affinity, WSe₂ acts as the p-type side, and ReS₂ as the n-type side, with a thin hBN tunnel barrier in between. The WSe₂/hBN/ReS₂ heterostructure shows a very low reverse saturation current. When forward biased, it passes a high current since the tunnel barrier is very thin. The characteristics of the fabricated device show a well-behaved diode characteristic, with RR of 10⁶. **Acknowledgment** This work is supported by the Army Research Office (ARO) Grant # W911NF-17-1-0312

9:00 AM S03

Molecularly Thin All-Solid-State Non-Volatile Memory Gated by a Monolayer Electrolyte Jerry Liang¹, Ke Xu¹, Maokun Wu², Weihua Wang², Kyeongjae Cho³ and Susan Fullerton-Shirey¹; ¹University of Pittsburgh, Pittsburgh, Pennsylvania, United States; ²Department of Electronic Science and Engineering, College of Electronic Information and Optical Engineering, Nankai University, Tianjin, China; ³Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, Texas, United States.

A non-volatile, solid-state, one-transistor (1T) memory is demonstrated based on electric double layer (EDL) gating of a WSe₂ field-effect transistor (FET) using an electrolyte that is a single molecular layer thick. The “monolayer electrolyte” consists of cobalt crown ether phthalocyanine and lithium ions, which are positioned by field-effect at either the surface of the WSe₂ channel or a h-BN capping layer to achieve ‘1’ or ‘0’, respectively. Bistability is significantly improved by the h-BN cap, with density functional theory (DFT) calculations showing an enhanced trapping of Li⁺ near h-BN due to an adsorption energy increase of 1.345 eV compared to vacuum. The threshold voltage shift between the two states corresponds to a change in sheet carrier density of ~2.5 × 10¹² cm⁻², and an *on-off* ratio exceeding 10⁴ at the back gate voltage of 0 V. The *on-off* ratio remains stable after 1000 cycles and the retention time for each state exceeds 6 hours (max measured). When the write time approaches 1 ms, the *on-off* ratio remains > 10², showing that monolayer electrolyte-gated, 2D non-volatile FET can respond on timescales similar to existing flash memory. The data suggest that faster switching times, and lower switching voltages will be achievable by top gating the device – work that is currently in progress. This research was supported by NSF under Grant No. ECCS-GOALI-1408425.

9:20 AM S04

(Student) Electric Characterization of In-Plane Few-Layer 2H-1T' MoTe₂ Homo Junction Interfaces Rui Ma¹, Youngdong Yoo³, Zachary P. DeGregorio², Lun Jin², Prafull Golani¹, James E. Johns³ and Steven J. Koester¹; ¹Dept. of Electrical & Computer Engineering, University of Minnesota, Minneapolis, Minnesota, United States; ²Dept. of Chemistry, University of Minnesota, Minneapolis, Minnesota, United States; ³Dept. of Chemistry, Ajou University, Suwon, Korea (the Republic of).

Introduction: It is known that structural phase transitions from the semiconducting (2H) phase to the metallic (1T/1T') phase in transition metal dichalcogenides (TMDCs) can be applied to make high-performance field-effect transistors (FETs) with low contact resistance [1], as well as memristors [2, 3]. Among all TMDCs, molybdenum ditelluride (MoTe₂) attracts the most interest because it requires the least energy to transform from its 2H phase to 1T' phase [4]. Due to the small energy difference, this 2H to 1T' transition has been induced by electrostatic doping [5] and laser irradiation [6], however, the phase transitions observed previously used exfoliated MoTe₂ and only one reported heterostructure FETs [6] utilizing the phase-engineered 1T' contacts. Recently, in-plane few-layer 2H-1T' MoTe₂ homo junctions have been successfully synthesized by controlling the tellurization of Mo nanoislands [7]. In this work, we demonstrate FETs with in-plane few-layer 2H-1T' MoTe₂ homo junctions achieving Ohmic contacts. We extract the energy offsets at the metal/2H and 1T'/2H interfaces and find a substantially lower energy barrier at the 1T'/2H interface compared to the metal/2H interface over the gate sweeping

window. **Device fabrication:** In-plane few-layer 2H-1T' MoTe₂ homo junctions were synthesized on 300nm SiO₂/n-Si substrates by depositing Mo nanoislands followed by reacting with Te flux at controlled rates [7]. Mesa regions were patterned and etched into the MoTe₂ on the as-grown substrates to form rectangular areas consisting of 2H, 1T', and 1T'/2H/1T' nanosheets. Next, contacts to the nanosheets were formed by patterning and lifting off Ti/Au contact metal to fabricate 2H-only, 1T'-only, and 1T'/2H/1T' devices, respectively. The phases of the channel materials were confirmed by Raman mapping. **Results and analysis:** From the transfer length method measurements, the extracted contact resistance of the metal/1T' interface was found to be 4 orders of magnitude lower than that of the metal/2H interface. From the temperature dependent transfer characteristics, the 1T'/2H/1T' device shows increasing current on/off ratio and subthreshold slope with decreasing temperature, implying a mobility-limited transport, while this improvement is not prominent in the 2H-only device, suggesting a thermionic-limited transport. The nonlinear output characteristics of the 2H-only device at both 77 K and 300 K indicate the presence of a Schottky behavior at the metal/2H interface, and the linear output characteristics of the 1T'/2H/1T' device suggest Ohmic-like behavior of the metal/1T' electrode and the 1T'/2H interface. The Schottky barrier heights for the three interfaces (metal/2H, metal/1T', and 1T'/2H) using temperature-dependent characterization. The overall barrier height for the 1T'/2H and metal/1T' interfaces is dramatically lower than that of the metal/2H interface over all backgate voltage values. The small 1T'/2H interface energy barrier and Ohmic metal/1T' contact could allow for electrical detection of the phase transition in the device channel leading to novel memory devices. Future work will include characterizing the 1T'/2H interface using TEM and improving the quality of the CVD MoTe₂. **Acknowledgement:** The work was supported by DTRA Basic Research through Award No. HDTRA1-14-1-0042. Portions of this work were carried out in the UMN Characterization Facility which receives partial support from the NSF through the MRSEC program under Award No. DMR-1420013. **References:** [1] R. Kappera, et al., Nat. Mater., 2014; [2] F. Zhang, et al., Nat. Mater., 2018; [3] X. Zhu, et al., Nat. Mater., 2018; [4] D. H. Keum, et al., Nat. Phys., 2015; [5] Y. Wang, et al., Nature, 2017; [6] S. Cho, et al., Science, 2015; [7] Y. Yoo, et al., Adv. Mater., 2017.

9:40 AM S05

(Student) Direct Visualization of the Graphene/MoS₂ Heterostructure Interface Shruti Subramanian¹, Yuanxi Wang¹, Simon Moser³, Ke Xu², Susan Fullerton-Shirey² and Joshua A. Robinson¹; ¹The Pennsylvania State University, State College, Pennsylvania, United States; ²University of Pittsburgh, Pittsburgh, Pennsylvania, United States; ³EO Lawrence Berkeley National Lab, Berkeley, California, United States.

Heterogenous combinations of two-dimensional (2D) layered materials provides us with an ability to tune several electronic and optical properties tailored for specific applications. Transition metal dichalcogenides (TMDs) are attractive 2D materials in the “beyond graphene” realm of materials. To utilize their unique electronic properties, it is important to develop low resistance contacts to these materials. Graphene is a promising candidate and has been shown to produce low-resistance contacts to a few TMDs. But this has been done by manual stacking via exfoliation or polymer-assisted transfer, which is not a scalable method. One avenue that is still in its infancy, yet could provide significant potential for scalability and be enroute “all-2D” electronics is the realization of as-grown graphene contacts to 2D materials beyond graphene. The quality of the interface of the heterostructure is of paramount importance and determines the electronic coupling and consequently the resulting contact resistance that graphene provides as a contact. Here, we discuss the properties of the heterostructure interface via several complex characterization methods and theoretical predictions. Using powder vaporization to grow the TMDs on patterned epitaxial graphene, directly yields 2D lateral heterostructure between graphene and TMDs like MoS₂, without the need for transfer of any 2D layers. Investigation of this synthetic lateral heterostructure via several advanced characterization techniques leads to an understanding of the structure of this interface. Cross-sectional transmission electron microscopy shows that the interface between graphene and MoS₂ is in fact, a pristine overlap of the MoS₂ onto the graphene for a few hundred nanometers. A nano-angle resolved photo-electron spectroscopy (ARPES) map of the system allows for being able to track the valence band in order to understand the charge transfer between the two materials constituting the heterostructure, which is supported by Kelvin probe force microscopy measurements and theoretical predictions of the depletion widths and other parameters.

10:00 AM REFRESHMENT BREAK

10:20 AM S06

Engineering Charge Trapping in Low-Dimensional Semiconductors for Optoelectronic Devices

Jack Alexander-Webber¹, Ye Fan¹, Hope Bretscher², Arelo Tanoh², Akshay Rao² and Stephan Hofmann¹;
¹Department of Engineering, University of Cambridge, Cambridge, United Kingdom; ²Department of Physics, University of Cambridge, Cambridge, United Kingdom.

Low-dimensional materials such as monolayer transition metal dichalcogenides (TMDs) and semiconductor nanowires hold exceptional promise for future optoelectronic devices due to their unique combination of optical, mechanical and electronic properties. However, the large surface-area-to-volume ratio in these materials results in an extreme sensitivity to the local electronic environment, such as the presence of interface charge traps. We develop high efficiency optoelectronic devices by combining passivation techniques to control charge trapping processes in low-dimensional materials. Charge trapping of photoexcited carriers can dominate the photoconductivity of atomically thin TMDs. The exploitation and control of naturally occurring and artificially introduced charge traps can therefore be of great importance in device development. The organic superacid, trifluoromethanesulfonimide (TFSI), has been shown to enhance the photoluminescence quantum yield of MoS₂ and WS₂ [1]. Whilst the microscopic mechanism remains controversial it has generally been attributed to a reduction in the charge trap density in sites such as sulphur vacancies within the TMD lattice. In addition to “intrinsic” charge trapping, a significant density of traps exist at the gate dielectric interface. Atomic layer deposition (ALD) of Al₂O₃ is particularly well suited to the passivation of charge traps at the SiO₂-semiconductor interface [2,3]. We describe here the effects of TFSI and ALD, both individually and in combination, on the photoconductivity of MoS₂ and WS₂ transistors. We find that the improved mobility and photocurrent provided by ALD passivation can be combined with a significantly reduced dark current by treating with TFSI prior to ALD. Using hysteresis characterisation, we decouple the observed photoexcitation-induced trapping from conventional electric field-induced trapping to gain a fundamental insight into the interface trap states. Our results highlight the significance of charge trap engineering and offer pathways towards the development of low-dimensional optoelectronic devices. [1] Amani et al. Nano Lett., vol. 350, 1065 (2015). [2] JA Alexander-Webber et al. 2D Materials, vol. 4, 011008 (2017). [3] JA Alexander-Webber et al. ACS Appl. Mat. & Inter. vol. 9, 43993 (2017).

10:40 AM S07

(Student) Photoluminescence Properties of MoS₂ Under Large Strain Gradients

Alex C. De Palma¹, Gabriel Cossio², Kayleigh Jones³, Quan Jiamin³, Xiaoqin Li^{1,3} and Edward T. Yu^{1,2};
¹Materials Science and Engineering Program, Texas Materials Institute, The University of Texas at Austin, Austin, Texas, United States; ²Department of Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas, United States; ³Department of Physics, The University of Texas at Austin, Austin, Texas, United States.

Molybdenum Disulfide (MoS₂) and other transition metal dichalcogenides (TMDs) have unique optical and electronic properties in the few-layer regime not found in their bulk counterparts. Additionally, MoS₂ exhibits unique mechanical properties, having been shown to withstand large mechanical strain before rupture¹. Strain can modify the optical and electronic properties of MoS₂, and work has been ongoing to utilize the coupling of strain and other properties to engineer novel applications. For example, single photon quantum emitters assembled into periodic arrays via localized inhomogeneous strain have been demonstrated in the TMD WSe₂². Notably, TMDs such as WSe₂ and MoS₂ are piezoelectric³, meaning that strain gradients within the material can induce a charge density, which could have implications for the optical and electronic properties beyond those of homogeneous strain. In order to realize MoS₂ and other TMDs for strain engineering applications, a thorough understanding of the effects of strain and strain gradients on the properties is necessary. In this work, we characterize the effects of large strain and strain gradients on the emission characteristics of MoS₂ during free standing indentation. MoS₂ is suspended over an array of holes etched out of SiO₂ via nanosphere lithography with dimensions of 700 nm diameter and 300 nm depth. A MoS₂ flake containing monolayer and multilayer regions was exfoliated from a bulk crystal of MoS₂, before being transferred via a polydimethylsiloxane (PDMS) substrate to the nanopatterned SiO₂ substrate. Suspended MoS₂ was then deformed by means of atomic force microscope (AFM) indentation with a Si tip of radius ~7nm. Indentation of such a small hole with a sharp AFM tip can yield not only large tensile strain, but also large strain gradients. The combination of large strain gradient with the piezoelectric nature of MoS₂ results in a spatially varying charge density depending on the strain

distribution. Calculations using an analytic model for indentation of a nonlinear membrane with a spherical indenter⁴ and the Piezoelectric coefficient e_{11} for MoS₃⁵ have shown that these charge densities could be as high as 10¹² e/cm² at the points of highest strain gradient. The photoluminescence (PL) of suspended MoS₂ was measured simultaneously during indentation as a function of indentation depth. PL measurements were performed via a 100x side objective in the backscattering geometry using a 532 nm excitation laser. With knowledge of the indentation depth and force, we were able to precisely control the mechanical deformation of the MoS₂. The PL peaks were found to decrease in energy and broaden with increasing indentation force, corresponding to the effects of increasing tensile strain on PL observed in uniformly strained MoS₂⁶. Further investigations into the effects of the piezoelectric-induced charge density on the emission properties of highly inhomogeneously strained MoS₂ will be discussed. References [1] ACS Nano, 5 (12), 9703–9709 (2011) [2] Nat. Commun. 8, 15093 (2017) [3] J. Phys. Chem. Lett. 3, 2871–2876 (2012) [4] Int. J. Non. Linear. Mech. 3 (3), 307–324 (1968) [5] Nat. Nanotechnol. 10 (2), 151–155 (2015) [6] Nano Lett. 13 (8), 3626–3630 (2013) This research was primarily supported by the National Science Foundation through the Center for Dynamics and Control of Materials: an NSF MRSEC under Cooperative Agreement No. DMR-1720595.

11:00 AM S08

(Student) Enabling High Performance 2D-TFTs on Glass Substrates via Hydrogen Silsesquioxane

Joseph R. Nasr¹ and Saptarshi Das^{1,2};
¹Engineering Science and Mechanics, The Pennsylvania State University, University Park, Pennsylvania, United States; ²Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania, United States.

Since the 1970s, the thin-film transistor (TFT) has been the backbone of light-emitting diodes and liquid crystals, which are widely used in our every-day displays technologies. Enabled by their atomistic ultra-thin body nature, two-dimensional (2D) materials like the transition metal dichalcogenides (TMDCs) have become an attractive material platform to replace the current TFT technology that suffers from relatively poor performance and expensive fabrication processes. TMDCs have already demonstrated superior electronic and optoelectronic properties compared to current state-of-the-art a-Si:H, polysilicon, organic, and oxides semiconductors. For instance, TMDCs offer 100x better mobility values than a-Si:H, large ON/OFF ratio, transparency over the visible light spectrum, mechanical flexibility, and temperature stability, which are essential components to realize the aforementioned technologies. However, in order to integrate 2D-TMDCs into the TFT technology, it is imperative to fabricate and benchmark these materials on transparent insulating substrates, i.e. multicomponent flexible glass substrates. Therefore, in this study, we fabricated, characterized, and benchmarked the electronic properties of exfoliated MoS₂-based TFTs on multicomponent glass substrates provided by Corning Incorporated against similar rigid Si/SiO₂ substrates in both monolayer and multilayer form. A negative tone e-beam resist, hydrogen silsesquioxane (HSQ), was used as the top-gate dielectric yielding to ~10⁶ ON/OFF ratios, and field effect mobility (μ_{FE}) extracted from the peak transconductance of ~9 cm²/V-s and ~0.8 cm²/V-s for multilayer and monolayer MoS₂, respectively. In addition, the threshold voltage (V_{TH}) extraction of these devices elucidated the fact that the electronic properties of MoS₂ are entirely substrate-dependent and elaborate on how it can be used to facilitate high performance or low power applications.

11:20 AM S09

(Student) Convergent Ion-Beam Alteration of 2D Materials and Metal-2D Interfaces

Zhihui Cheng¹, Hattan Abuzaaid¹, Yifei Yu², Fan Zhang³, Yanlong Li³, Steven G. Noyce¹, Yuh-Chen Lin¹, Jay Doherty¹, Chenggang Tao³, Linyou Cao² and Aaron D. Franklin^{1,4};
¹Electrical and Computer Engineering, Duke University, Durham, North Carolina, United States; ²Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina, United States; ³Physics, Virginia Tech, Blacksburg, Virginia, United States; ⁴Chemistry, Duke University, Durham, North Carolina, United States.

The advantageous electrical, mechanical and optical properties of two-dimensional (2D) materials have attracted tremendous research seeking to integrate them into the next generation of transistors, optoelectronics, and sensors [1]–[3]. Although many methods have been explored to modify 2D materials [4], [5], physically tailoring the properties of 2D materials and consequently tuning the carrier transport across metal-2D contact interfaces is still deficient. Here we demonstrate the alteration of MoS₂ and metal-MoS₂ interfaces using a convergent ion beam. **Different beam energies, from 60 eV to 600 eV, are shown to have distinct effects on**

the optical and electrical properties of MoS₂. The altered MoS₂ was mapped using atomic force microscopy (AFM). The height profile suggests that the 200 eV ion beam has a stronger etching effect on the 1L MoS₂ and the underlying SiO₂ compared to the 60 eV ion beam. After 60 eV Ar⁺ ion beam exposure, the 1L MoS₂ region turns dark in photoluminescence mapping, which suggests that the ion beam disrupts the crystal structure of 1L MoS₂. Defects and deformations created across different layers were investigated, revealing an unanticipated improvement in the Raman peak intensity of multilayer MoS₂ when exposed to a 60 eV Ar⁺ ion beam. Scanning tunneling microscopy (STM) was used to probe the altered 4L MoS₂ surface, showing that the MoS₂ crystallinity still remains. This largely intact crystallinity of the 4L MoS₂ surface is in contrast to the significantly diminished PL peak of 1L MoS₂, supporting the argument that the defects spread throughout multiple layers rather than concentrating at the surface. Using cross-sectional scanning transmission electron microscopy (STEM), alteration of the crystal structure after a 600 eV ion beam bombardment was observed, including generated defects and voids in the crystal. Comparing the unexposed region to the one exposed for 25 s, defects and deformations can be seen across different layers. The MoS₂ thickness decreased from 10 nm (15L) to 4 nm (5L-6L) after 25 s of ion beam exposure. After the 50 s of exposure, only 2-3L partially remains. Surprisingly, some interlayer delamination in the MoS₂ crystals is also observed. In addition, small and large gaps appear horizontally between different regions and vertically between different layers. These new effects could have profound implications for metal-2D material interfaces and other applications such as intercalation and sensing devices. We show that the 60 eV ion beam yields improvement in the metal-MoS₂ interface by decreasing the contact resistance from 17.5 kΩ*μm to 6 kΩ*μm at a carrier concentration of $n_{2D} = 5.4 \times 10^{12}$. Of special note is that we only exposed the contact region, keeping the channel region intact, by using PMMA as a mask. Compared to the 60 eV ion beam, 200 eV ion beam exposure tends to degrade the contact performance. As the ion beam energy increases to 600 eV, the device performance degrades even further. These results are consistent with the amount of damage and disorder created by the higher energy ions. In conclusion, we have uncovered the effects of different ion beam energies on MoS₂ using a variety of characterization techniques. The impact of Ar⁺ ion beam bombardment across different layers of MoS₂ is particularly interesting, as visualized in Raman mapping and STEM images. The 60 eV ion beam shows promise for improving carrier injection in metal-2D material interfaces, whereas 200 eV and 600 eV ion beams degrade the contact performance. This work is supported in part by NSF ECCS-1508573, ECCS-1542015, ECCS-1508856, and U.S. Army Research Office Grant W911NF-15-1-0414.

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11:40 AM S10 **WITHDRAWN**

The Effects of Gamma-Ray and Proton Radiation on hBN Encapsulated Graphene Field Effect Transistors Maya Narayanan Kutty¹, Ozhan Koybasi², Øystein Dahl³, Takashi Taniguchi⁴, Kenji Watanabe⁴, Eduard Monakhov¹ and Branson D. Belle³; ¹Centre of Materials Science and Nanotechnology, Department of Physics, University of Oslo, Oslo, Norway; ²SINTEF DIGITAL, Oslo, Norway; ³SINTEF INDUSTRY, Oslo, Norway; ⁴Advanced Nanomaterials Laboratory, High Pressure Group, National Institute for Materials Science, Tsukuba, Japan.

Graphene-based devices have exhibited an enormous potential for various technological applications owing to the unique electrical, mechanical and optical properties of graphene. It is essential to thoroughly study the effects of radiation on graphene field effect transistors (GFETs) in order to assess the reliability of these devices when they operate in a radiation harsh environment. The field effect mobility and charge neutrality (Dirac) point of GFETs are highly sensitive to unintentional doping from surrounding environment traps and fixed charges at oxide/substrate interface. Prior studies have shown that high energy photons of Gamma radiation on GFETs can cause electrically active defects in the substrate, increase trap density at the interfaces, and possibly modify the lattice of graphene making it exhibit p-doped behavior [1-2]. Encapsulation of graphene with a lattice-matched hexagonal boron nitride (hBN) can isolate it from moisture rich ambient air and the dielectric environment thereby preserving the high quality electronic transport of graphene. Here we report on the radiation induced defects by evaluating the material and electrical responses of hBN encapsulated exfoliated GFETs and non-encapsulated CVD grown back-gated GFETs under irradiation by ⁶⁰Co (Gamma rays) with cumulative doses of 5, 30, 105, 305kGy. The Raman spectrum (at 532nm) of non-encapsulated CVD grown graphene before and after gamma irradiation shows an upshift of both G and 2D peaks.

This upshift can be attributed to an increase in doping. On the other hand, hBN encapsulated exfoliated graphene shows no significant changes in G peak and 2D peak, indicating that hBN encapsulated GFETs experiences less effects of gamma radiation. The transport characteristics of hBN encapsulated exfoliated GFETs measured at RT indicate shift in the Dirac voltage from 0.01V pre-irradiation to 1.36V at post 5kGy irradiation, -6.91V at 30kGy and back to 1.33V post 105kGy irradiation. This deviation of Dirac voltages at incremental doses can be attributed to both the formation of additional defects and to the movement of charges in the oxide/substrate interface at each dose. Both CVD grown GFETs and hBN encapsulated exfoliated GFETs show drastic mobility degradation with increasing radiation dose. In hBN-encapsulated exfoliated GFETs, the electron mobility decreases by ~80% while the hole mobility decreases by ~70% after gamma irradiation of 305kGy. This asymmetric mobility degradation is consistent with theory [3] where in electron mobility degrades more rapidly due to coulomb-scattering by positive trapped charges. We infer that the energy deposited by radiation creates electrically charged defects in the substrate and substrate/oxide interfaces, thereby negatively affecting device performance. Furthermore, we expand our study to compare the effects on graphene lattice between high energy photons in gamma radiation to the ion induced damage by proton irradiation. To that effect, we will present the electrical and material study of the effects of 1.9MeV proton radiation at different fluences on hBN encapsulated exfoliated GFETs compared to the non-encapsulated CVD grown graphene. **References** [1] R.C. Walker II, T. Shi, E.C. Silva, I. Jovanovic, and J.A. Robinson, *Phys. Status Solidi A*, 213 (12), 3057 (2016). [2] K. Alexandrou, A. Masurkar, H. Edrees, J.F. Wishart, Y. Hao, N. Petrone, J. Hone, and I. Kymissis, *Appl. Phys. Lett.*, 109, 153108 (2016). [3] C.D. Cress, J.G. Champlain, I.S. Esqueda, J.T. Robinson, A.L. Friedman and J.J. McMorrow, *IEEE TRANSACTIONS ON NUCLEAR SCIENCE*, 59 (6), 3045 (2012).

SESSION T: Materials for Memristors and Computation

Session Chair: Angel Yanguas-Gil

Thursday Morning, June 27, 2019

Michigan League, 3rd Floor, Room D

8:20 AM T01

(Student) High Quality Lithium Niobite Grown by Liquid Phase Electroepitaxy for Use as a Memristor Timothy M. McCrone¹, Aheli Ghosh³, Bill Zivasatienraj², Alex S. Weidenbach² and W. Alan Doolittle²; ¹Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States; ²Georgia Institute of Technology, Atlanta, Georgia, United States; ³ECE, Georgia Tech, Atlanta, Georgia, United States.

High quality crystals of lithium niobite (LiNbO₃) have been grown using liquid phase electroepitaxy (LPEE). LPEE is a combination of Liquid phase epitaxy and electroplating technologies that allows a) rapid (up to ~100 μm / hour) deposition of high quality crystalline films and b) reduced oxidation state sub-oxides not possible without the electrical bias. It is found that at varying voltages and relative chemical precursor concentrations the crystal quality changes. LiNbO₃ is a material of interest due to the high mobility lithium atoms in the material's structure. Applying a bias on these materials causes the intercalated lithium ions to be disturbed, flowing to the anode and altering the resistance of the electrical channel. Having access to high quality bulk material allows for a better understanding of the amount of delithiation that can be achieved in future devices. The large amount of delithiation without structural change of the material also produces the opportunity for this material to be studied as a potential complement to LiCoO₂, a common battery cathode, due to LiNbO₃'s relatively higher conductivity and similar crystal structure. In addition the change in resistance caused by delithiation opens up the opportunity for this material to be used as a memristor, a device type of increasing interest due to its use in neuromorphic computing. Initial results were from samples grown at 900°C and allowed to grow for 24 hours using niobium wire as a seed for random nucleation. The resulting structure consists of an apparent "boule" of approximately 2.1 cm length and 1.2 cm radius. The grown boules were cleaned in deionized water by sonication allowing the boule to be reduced by the removal of residual niobium oxide dissolved in lithium metaborate exposing large 5x5mm crystallites originating from the niobium wire. Larger crystallites were selected to create devices, while smaller samples were used for powdered XRD analysis confirming the material phase and later used for battery applications. Volatile and nonvolatile memristive characteristics in lithium niobite are studied. A large hysteresis "bowtie" curve is observed with a

hysteresis window of 1.2 volts at 180-113mA. This hysteresis rotates clockwise with successive cycles as expected. These electrical properties were compared to other published material including samples of lithium niobite created through MBE and sputtering. Prospects for controlled nucleation and seeded growth will be discussed.

8:40 AM T02

(Student) Evidence of Lithium Doping Gradients in Sputtered Lithium Niobite Memristors Resulting in Modification of Vertical Conductivity Alex S. Weidenbach¹, Bill Zivasatienraj¹, Aheli Ghosh¹, Timothy M. McCrone¹, Joshua Shank², M. Brooks Tellekamp³ and W. Alan Doolittle¹; ¹Georgia Institute of Technology, Atlanta, Georgia, United States; ²Sandia National Laboratories, Albuquerque, New Mexico, United States; ³National Renewable Energy Laboratory, Golden, Colorado, United States.

Lithium niobite (LiNbO₂), a sub-oxide of the highly studied optical material lithium niobate (LiNbO₃), is a layered semiconductor consisting of planes of niobium oxide and loosely bound lithium ions. Once studied as a low temperature superconducting material, LiNbO₂ has shown promise as a battery material as well as shown hysteretic behavior due to its mobile planes of lithium making it promising for use as a memristor in neuromorphic computing applications. Both volatile and nonvolatile mechanisms can be seen in sputtered LiNbO₂ memristors. The conductivity of LiNbO₂ is set through the lithium vacancies found in the film. Sputtered LiNbO₂ nonvolatile memristors showed a non-linear change in resistivity in relation to thickness implying a possible change in crystal structure as the film is being deposited. LiNbO₂ was sputter deposited in an RF/DC sputter through co-deposition of lithium oxide (Li₂O) and niobium (Nb). Argon was used as the working gas and no reactive species were introduced during the deposition. Films of varying thicknesses of 70 nm, 115 nm, 190 nm, 310 nm, 390 nm, and 460 nm were deposited to study changes in the structure of the film throughout the deposition process. The films were characterized with x-ray diffraction (XRD) and resistivity of the films was measured. Memristive devices were fabricated in linear geometries of 200 μ m by 700 μ m. These devices showed resistivities of 0.60 ohm*cm, 0.089 ohm*cm, 0.062 ohm*cm, 0.075 ohm*cm, 0.078 ohm*cm, and 0.012 ohm*cm for films of thicknesses 70 nm, 115 nm, 190 nm, 310 nm, 390 nm, and 460 nm respectively. The significant change in resistivity from the 70 nm film to the 115 nm film was investigated through x-ray diffraction to check for any changes in crystal structure in the films. Symmetric 2 θ - ω XRD scans of the varying thickness LiNbO₂ sputtered films were taken. A peak shift of 0.56 degrees can be seen between the 70 nm film and the 390 nm film. While a shift can be seen the overall shape of the x-ray peak remains unchanged implying no significant change in the crystal structure of the films as the thickness increases. This shift could be caused by a difference in incorporated lithium in each of the films. A decrease in incorporated lithium in the crystal structure would correlate to a shift x-ray peak as the crystal structure expands with the loss in lithium. To investigate both the 70 nm and 460 nm films were placed in ~37% HCl for 22 hours to deintercalate lithium from each of the films. A shift in the x-ray peak of the 70 nm film after soaking in HCl of 0.119 degrees shows that as lithium is removed from the system the crystal structure moves toward that of the more conductive films. The 460 nm film showed negligible changes in its x-ray peak implying that there was little lithium left in the crystal available to be deintercalated by the HCl soak. The shift of the 70 nm film after deintercalation of lithium in HCl shows the resistivity of sputtered LiNbO₂ memristors can be tuned through controlled removal of lithium through chemical deintercalation.

9:00 AM T03

A Green Synthetic Pathway to V(IV) Oxide-Based Resistive Switching Devices Henam S. Devi, Akshita Mishra, Samim Reza, Madhusudan Singh and Nitika Batra; Electrical Engineering, Indian Institute of Technology Delhi, New Delhi, India.

Vanadium is a transition metal with a number of distinct oxidation states that occur in technologically relevant oxides [1]. VO₂, in particular, is deposited using physical vapor deposition, PLD, and epitaxy [2,3]. In this work, we report a green chemical synthetic approach for production of pure phase VO₂, using a two-step process employing ammonium metavanadate (NH₄VO₃), formic acid, citric acid, and distilled water. In contrast to conventional expensive and cumbersome [4,5,6] methods, these precursors are derivable from natural sources – formic acid from ants (genus *formica*), and citric acid from a microbial process (*Penicillium* mold on sugar). NH₄VO₃ (0.02 gm) and 1 ml of formic acid were added to 10 ml DI water at 75°C under constant stirring prior to addition of 0.01 g of citric acid to the reaction mixture, which underwent a color change to blue indicating formation of vanadium(IV) oxide. After vacuum drying,

the product was washed with methanol to remove residues. The powder was annealed at 700°C under an inert atmosphere prior to material analysis. Powder X-ray diffraction (PXRD, Rigaku Ultima IV using Ni-filtered Cu-K α radiation) reveals the formation of pure monoclinic phase (VO₂(M), PDF:969009090). Elemental composition (1:1 V:O weight ratio with trace carbon) was confirmed using energy dispersive X-ray analysis (EDAX, RONTEC Quantax 200). The high surface energy of particles is suggested by agglomeration observed using scanning electron microscopy (SEM, Zeiss EVO 50). Inks of VO₂ in DI water are found to be very stable over 30 days for a few formulations. To fabricate the resistive memory device, shadow masked bottom contacts consisting of sputtered Cr (adhesion layer, ~1mTorr, 200Å) and thermally evaporated Au (3x10⁻⁷ Torr, 400Å) were deposited (Angstrom Engineering) on a silicon dioxide (SiO₂) wafer (University Wafers) without breaking the vacuum. The ink was spin-coated and dried (60°C) multiple times[7] on these substrates to form a reasonably uniform 1 mm layer. Top electrodes (Ag, 1000Å) were thermally evaporated in a cross-bar geometry with respect to bottom contacts to form metal-insulator-metal (MIM) structures. Upon dual-sweep mode characterization (Keithley 4200-SCS), a repeatable pinched hysteresis (over a [-6V,2V] range) characteristic was obtained, which is characteristic of filament type resistive switching[8]. Inducement of metallic filaments is expected to be facilitated by the low redox potential (~0.34V) of VO₂ [8], thereby lowering the configurational barrier between low- and high resistive states. This green synthetic pathway, coupled with the above low-temperature fabrication process, is expected to enable the production of low-switching threshold resistive memory devices suitable for low power memory circuits. 1. M. Liuet al., *Adv. Energy Mater.* 2017, 7: 1700885-34. doi: 10.1002/aenm.201700885. 2. J. Nag et al., *J. Phys.: Condens. Matter* 2008, 20: 264016-15. doi:10.1088/0953-8984/20/26/264016 3. T. Slusar et al., *APL Mater.* 2016, 4: 026101-8. doi: 10.1063/1.4940901 4. S.R. Popuriet al., *Inorg. Chem.* 2013, 52: 4780–4785. doi: 10.1021/ic301201k 5. Y Choi et al., *Sol. Energy Mater. Sol. Cells*, 2018, 176: 266-271. doi:10.1016/j.solmat.2017.12.008 6. Y. Li et al., *J. Colloid Interface Sci*, 2016, 462:42-47. doi: 10.1016/j.jcis.2015.09.056. 7. A. Mishra et al., *Journal of Elec Materi*, 2019. doi:10.1007/s11664-019-06975-4. 8. F. Pan et al., *Mat.Sci Eng.R*, 2014, 83:1-49. doi:10.1016/j.mser.2014.06.002.

9:20 AM T04

Effect of Grain Surface Area on Yttria Based Resistive Switches Mangal Das¹, Amitesh Kumar², Sanjay Kumar¹ and Shaibal Mukherjee¹; ¹HNRG, Electrical Engineering, Indian Institute of Technology Indore, Indore, India; ²IIT Indore, Indore, India.

The effect of interface and film roughness on the RS parameters for yttrium oxide-based devices have been discussed in this report. Our device has shown synaptic functions such as nonlinear transmission characteristics, long-term plasticity (LTP), short-term plasticity (STP) and learning behavior (LB). **Effect of Grain Surface Area:** Fig. 1(a-d) shows current-voltage (I-V) characteristics of the devices which are obtained by applying the triangular voltage excitation of -5 to 5 V (peak to peak). Highly crystalline devices N1 and N2 (Fig. 2(a)) do not show any consistent RS behavior. Whereas amorphous N3 (Fig. 2(b)), N4 (Fig. 2(c)) and, polycrystalline N5 (Fig. 2(d)) show RS. Fig. 1(e,f) shows endurance measurement, HRS and LRS are measured concerning the number of switching cycles at a read voltage of 0.1 V for device N3, N4, and N5. Device N3 and N4 both show switching for ~23000 cycles whereas device N5 collapses after ~7000 cycles. Endurance measurements indicate that the switching properties of the N3 and N4 (Fig. 1(e)) device are highly reproducible. SEM images of the top surface of yttrium oxide thin film have been shown in fig. 1(g,h,i). Roughness of the yttrium oxide thin film surface increases as deposition temperature increases from 300 °C (N3) to 500 °C (N5). It can be observed that top surface of device N3 (fig. 1(g)) has a very smooth surface with small GBs whereas roughness increase in the case of N4 and N5. GBs become more observable (appears as small cracks) at the top surface of device N4 (fig. 1(h)) and in N5 (fig. 1(i)). Grain boundaries (GBs) are always correlated with grain morphology, grain surface area (GSA). Fig. 2(a,b) shows mean (M) and standard deviation (SD) of GSA and set and reset voltages in devices N3, N4, and N5. Set and Reset voltages are extracted from I-V characteristics of the devices (fig 1). SEM images (fig. 1(g,h,i)) of yttrium oxide top surface show GB and GSA variations along the top yttrium oxide thin film surface. It is important to note that SD (GSA and set and reset voltages) increases as we move from N3 to N5 devices. It is a well-known fact that GBs and GSA play a significant role in RS. Synaptic functions such as LTP, STP and learning behavior (LB) are observed in our Al/Y2O3/n-Si ('N3') type device. Fig 3(b) shows the conductivity variation for Al/Y2O3/n-Si ('N3') type devices when subjected to different pulse excitation (fig 3(a)). A more substantial change in conductivity occurs when high-intensity and longer period pulses are applied to our device. Above phenomena are similar to

the nonlinear transmission characteristics of natural synapses if conductivity is considered as synaptic weight. Fig 3(c) shows the response for a sequence of 50 potentiating voltage pulses (“PO” process) followed by 40 depressing pulses (“DE” process). The device conductivity (synaptic weight) can be increased (decreased) by applying successive potentiating voltage pulses (depressing voltage pulses). Such activity of device conductivity (synaptic weight) is similar to synapses. Fig 3(d) shows the results of a test in which the device is stimulated with 40 consecutive voltage pulses; in which the synaptic weight gradually increases under continuous voltage pulses. It is interesting to observe that when the applied voltage pulses is removed, a spontaneous decay of synaptic weight can be observed (fig 3(e)). The decay rate is speedy at the initial stage which gradually decelerates and stabilizes at a value of ~28% of its first value after ~20 s. A similar trend can be observed in the “learning and forgetting behavior” of human memory. When the re-stimulation process (fig 3(f)) is initiated from the previous state, it takes only 15 pulses, comparatively very less than the number of pulses required in the first learning process as shown in fig 3(d), to recover to ~100% of the synaptic weight of device as represented in fig 3(f).

9:40 AM T05

Tunable Color Reflector Using GeTe in a Multi-Layer Structure
Mohsen Jafari, Afzaal Qamar, Lingjie J. Guo and Mina Rais Zadeh;
EECS, University of Michigan, Ann Arbor, Michigan, United States.

We show that a phase change material (PCM), Germanium Telluride (GeTe), when integrated into a sub-wavelength layered optical cavity, can produce widely tunable reflective colors. It is shown that the crystallization temperature (T_x) of GeTe is dependent on the film thickness for thin-films of less than ~20 nm, which is exploited for color tuning. Four colors from the same physical structure were demonstrated by electrical heating, through novel optical and thermal engineering of a thin film stack that includes two GeTe layers with only a single integrated joule heater element. The selective sensitivity to incident light angle and low polarization dependence, as well as the low static power consumption of this device make it a good candidate for potential consumer electronics applications. We show that a phase change material (PCM), Germanium Telluride (GeTe), when integrated into a sub-wavelength layered optical cavity, can produce widely tunable reflective colors. It is shown that the crystallization temperature (T_x) of GeTe is dependent on the film thickness for thin-films of less than ~20 nm, which is exploited for color tuning. Four colors from the same physical structure were demonstrated by electrical heating, through novel optical and thermal engineering of a thin film stack that includes two GeTe layers with only a single integrated joule heater element. The selective sensitivity to incident light angle and low polarization dependence, as well as the low static power consumption of this device make it a good candidate for potential consumer electronics applications. Tunable color filters with improved power, speed, and reliability have application in display systems which are among the most commonly used optical components in consumer market. Most modern display systems use three or more separate sub-pixels (or cells) to produce a single pixel of an image. Recent low power pixels include microelectromechanical (MEMS) based mirrors,^[1] color E-ink,^[2] etc. Having movable objects, however, has proven to be a major limitation of these devices in terms of durability, switching power consumption, and reliability in response to mechanical shocks in portable electronics. To address this, a chalcogenide based structural color is demonstrated here using a phase change material (GeTe). For the first time, an integrated tunable color reflector with multi-layers of GeTe is demonstrated utilizing the crystallization temperature dependence on the thickness of the GeTe films (for thicknesses < 30 nm).^[3] The large change in the refractive index of GeTe is used to switch the reflected color of the structure and achieve four different colors consists of: red, blue, green, and yellow. To achieve this, an integrated joule-heating approach is used to transition the GeTe film. GeTe film undergoes a crystallographic phase transition which results in large change in its optical refractive index (both real(n) and imaginary part (k)).^[4] The device consists of a two thin GeTe films sitting on top of a SiO₂ layer acting as an optical phase shifter. Apart from its color tunability, the proposed structure does not require any subwavelength lithography such as those needed in metasurface-based color filters, which results in lower cost needed for large area applications.^[5,6] There is a thick palladium/nickel chromium (Pd/NiCr) reflector under the SiO₂ layer, which serves as one of the cavity mirror surfaces. Using a refractory metal (palladium) results in higher reliability of the device during repeated heating cycles. The GeTe layers on top separated by TiO₂ serve as the other semi-Bragg reflector of the cavity. Phase transition of GeTe is controlled using the buried NiCr conductor through joule heating. T_x dependence on the film thickness is shown using in-situ X-ray diffraction (XRD).

10:00 AM REFRESHMENT BREAK

SESSION U: Low-Dimensional Structures— Quantum Dots, Wires, Wells Session Chairs: Minjoo Lee and Joshua Zide Thursday Morning, June 27, 2019 Michigan League, 3rd Floor, Room D

10:20 AM U01

(Student) InP Quantum Dots for Dislocation-Tolerant, Visible Light Emitters on Si Pankul Dhingra^{1,4}, Yukun Sun^{2,1,4}, Shizhao Fan^{1,4}, Ryan Hool^{3,4} and Minjoo L. Lee^{1,4}; ¹Department of Electrical and Computer Engineering, University of Illinois Urbana Champaign, Champaign, Illinois, United States; ²Department of Electrical and Computer Engineering, Yale University, New Haven, Connecticut, United States; ³Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Champaign, Illinois, United States; ⁴Micro and Nanotechnology Lab, University of Illinois, Urbana, Illinois, United States.

We present the first demonstration of InP quantum dots (QDs) on Si showing room-temperature, visible photoluminescence (PL) intensity nearly identical to samples grown on GaAs. The past few years have seen tremendous progress in the development of 1.3 μm InAs quantum dot (QD) lasers on Si with low threshold current density and high reliability despite threading dislocation densities (TDD) of 10⁷ cm⁻².¹ The high luminescence efficiency of InAs QDs on Si can be attributed to lateral carrier confinement of the QDs and high QD density, 3 orders of magnitude higher than the TDD. Epitaxial InP QDs embedded in (Al_xGa_{1-x})_{0.52}In_{0.48}P can also be grown on GaAs and have recently been used to demonstrate red and near-infrared lasers with low threshold current density². Here, we show that the apparent dislocation-tolerance of InAs QDs on Si also extends to InP QDs on Si, making them an ideal candidate for low-cost visible and near-infrared lasers and light emitting diodes (LEDs). We grew InP QD PL structures on bulk GaAs and GaAs/Si virtual substrates using solid source molecular beam epitaxy (MBE). GaAs/Si virtual substrates were grown on commercially available GaP/Si(001) templates using a 3.6 μm thick GaAs_xP_{1-x} step-graded buffer. The active region of the QD PL structure consisted of 3 monolayers (ML) of InP QDs buried by an 8 nm In_{0.48}Ga_{0.52}P (InGaP hereafter) quantum well (QW) and sandwiched by 200 nm (Al_{0.33}Ga_{0.67})_{0.52}In_{0.48}P barriers. InP QDs underwent self-assembly by the Stranski-Krastanov growth mode after ~1.7 ML of deposition, analogous to InAs QDs. QW PL structures were also grown to compare dislocation tolerance. Lattice-matched Al_{0.51}In_{0.49}P carrier blocking layers were grown surrounding the active region to reduce surface recombination losses. Cross-sectional transmission electron microscope (XTEM) images of samples grown on both GaAs and GaAs/Si were nearly identical, showing coherently strained InP QDs capped by a smooth InGaP QW. Planar-view cathodoluminescence (CL) maps showed essentially no dislocations for the sample grown on GaAs, as expected. In contrast, a TDD of 3.3×10⁷ cm⁻² was observed for the sample grown on GaAs/Si. Atomic force microscopy (AFM) showed a high QD density of 1.3×10¹¹ cm⁻² on both substrates, which is several orders of magnitude greater than the TDD in the active region. We performed room-temperature PL measurements to characterize the emission wavelength and intensity of InGaP QWs and InP QDs grown on both GaAs and GaAs/Si virtual substrates. We subjected the samples to rapid thermal annealing (RTA) at 700-850°C, as RTA can remove point defects in MBE-grown phosphides and thus improve optical properties.³ On both substrates, the QWs and QDs emit at 649 nm and 713 nm with a full width at half maximum of 12 nm and 31 nm, respectively, similar to values reported in previous literature. The integrated intensity of the InGaP QW sample grown on GaAs/Si is ~9× lower than the QW on GaAs due to the high TDD. In contrast, the integrated intensity of InP QDs on Si is ~16× higher than the InGaP QW on Si and within 15% of InP QDs grown on GaAs, showing the high dislocation tolerance of InP QDs. In conclusion, we show that high density InP/AlGaInP QDs can be grown on Si with similar structural and optical properties as growth on bulk GaAs, paving a pathway towards low-cost, integrated light emitters with potential applications ranging from micro-LEDs to optogenetics. ¹ D. Jung, Z. Zhang, J. Norman, R. Herrick, M. J. Kennedy, P. Patel, K. Turnlund, C. Jan, Y. Wan, A. C. Gossard, and J. E. Bowers, ACS Photonics 5 (3), 1094 (2018). ² P. M. Smowton, J. Lutti, G. M. Lewis, A. B. Krysa, J. S. Roberts, and P. A. Houston, IEEE J Sel Top Quant 11 (5), 1035 (2005). ³ M. Jalonen, M. Toivonen, P. Savolainen, J. Königäs, and M. Pessa, Appl. Phys. Lett. 71 (4), 479 (1997).

10:40 AM U02

(Student) BGaInAs/GaAs Quantum Wells for 1.3 μ m Lasers Rasha El-Jaroudi¹, Kyle M. McNicholas¹, Brent A. Bouslog¹, Jan Kopaczek², Robert Kudrawiec² and Seth Bank¹; ¹Microelectronics Research Center and Department of Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas, United States; ²Institute of Physics, Wroclaw University of Science and Technology, Wroclaw, Poland.

Here we present the first BGaInAs quantum wells (QW) emitting at 1.3 μ m grown coherently on GaAs. These telecom-range GaAs-based emitters are attractive for low-cost vertical-cavity surface-emitting laser (VCSEL) sources for LIDAR and fiber communication systems as they can be easily integrated with AlGaAs/GaAs distributed Bragg reflectors and AlOx native oxide layers. These BGaInAs alloys have the highest boron concentration (11%) and highest indium concentration (44%) in addition to the highest simultaneous boron and indium concentrations (11% boron and 40% indium) yet demonstrated for epitaxially grown BGaInAs. Prior BGaInAs investigations yielded either high indium concentrations (~35%) and low boron concentrations (~1%) or larger boron concentrations (~4%) with a reduction in indium concentration (~8%).^{1,2} BGaInAs QW's and films were grown by solid source MBE on (100) GaAs substrates. Samples were characterized by x-ray diffraction (XRD) and room temperature photoluminescence (PL). Both the films and QW's exhibit Laue oscillations indicative of good crystalline quality. BGaAs films 300nm thick and with 2.7% boron were grown with and without indium. Room temperature PL showed a 3x enhancement in PL intensity with the addition of indium and, as expected, a red-shifting in wavelength. The large lattice-mismatch between InGaAs and GaAs complicates the growth of InGaAs on GaAs substrates at telecom wavelengths. As the indium concentration increases towards 1.3 μ m, the amount of compressive strain increases and the optical quality of the material degrades. The small lattice constant of BAs offers the opportunity to continue to increase the indium concentration by strain compensating via the addition of boron. We prepared InGaAs/GaAs QWs which exhibited ~an order of magnitude decrease in PL intensity and no wavelength extension past 1.25 μ m as the indium increased from 40% to 44%. XRD of the In_{0.44}Ga_{0.56}As QW is suggestive of relaxation. With the addition of 2.2% boron into the In_{0.44}Ga_{0.56}As QW, there was both an increase in PL intensity (3x) and an extension in wavelength to the technologically important wavelength of 1.3 μ m. We attribute this wavelength extension to the reduction in strain of the BGaInAs QW compared to the InGaAs QW as the addition of boron is expected to shorten the wavelength of InGaAs.³ Increasing the boron concentration to 3.8% with the same indium concentration did not result in a significant reduction in PL intensity, suggesting that further increasing the indium and boron is a viable path to access the important telecom wavelength of 1.55 μ m on GaAs substrates. This work was supported by the National Science Foundation (ECCS-1838984). [1] Hamila et al. J. of Appl. Phys. (2012) [2] Geisz et al. Appl. Phys. Lett. (2000) [3] McNicholas et al. 60th Electronic Materials Conference (2018)

11:00 AM U03

(Student) Spatially and Spectrally Controlled InAs Quantum Dot Molecules Lauren McCabe¹, Henry Carfagno¹, Joshua Zide² and Matthew Doty²; ¹University of Delaware, Newark, Delaware, United States.

We present on patterned InAs quantum dot (QD) growth in conjunction with quantum dot molecules (QDMs) for built in spectral tuneability. InAs QDs have long been considered as possible qubits, and numerous proof-of-concept quantum operations have been performed. However, the random nucleation for these self-assembled QDs and the spectral inhomogeneity that arises from variations in size, composition, and shape have made it impossible to produce arrays of identical QDs that are desired for scalable production of devices. Most other prospective material platforms for quantum device technologies face similar problems with inhomogeneity. To overcome these challenges we are engineering a new, molecular beam epitaxy (MBE) grown III-V QD material platform with built-in spectral tunability and site control. To do this we are combining patterned QD growth [1, 2, 3] with QDMs, where the energy levels of these QDMs can be tuned to a target wavelength with an applied electric field [4]. An advantage of the patterned growth is that through the use of lithographically defined markers, the patterned QDMs can be processed after growth for optical devices. However, typical patterned growth produces low optical quality QDs [5]. To address this we are implementing a column of QDs in between the patterned GaAs surface and the QDM. This maintains the spatial location but creates a buffer layer away from defects at the growth interface. The patterned nano-holes are defined by electron beam lithography and etched with an acid solution. Various nano-hole spacings and sizes have been investigated and found that a 10 μ m spacing between nano-holes has the highest QD occupancy so far of 89%. We hope to tune the growth parameters to achieve 100% QD occupancy in

the pattern. The initially patterned QD serves as a tracer to grow a column of QDs by strain-based growth. We are investigating the growth of the tracer columns and the optical quality of the QDs in the columns as they get further from the patterned growth interface. [1] *App. Phys. Lett.* 92, 18 (2008) [2] *App. Phys. Lett.* 87, 24 (2005) [3] *Phys. Rev. Lett.* 91, 196103 (2003) [4] *App. Phys. Lett.* 89, 23 (2006) [5] *Rep. Prog. Phys.* 72, 046502 (2009)

11:20 AM U04

Anomalous Stranski-Krastanov Growth Mode of Tensile-Strained (111)-Oriented GaAs Quantum Dots Christopher F. Schuck¹, Simon Roy¹, Trent Garrett², Qing Yuan³, Ying Wang³, Carlos I. Cabrera⁴, Kevin Grossklaus⁵, Thomas E. Vanderveide⁵, Baolai Liang³ and Paul Simmonds^{1, 2}; ¹Micron School of Materials Science and Engineering, Boise State University, Boise, Idaho, United States; ²Physics Department, Boise State University, Boise, Idaho, United States; ³College of Physics Science & Technology, Hebei University, Baoding, China; ⁴Center for Research in Sciences, Research Institute in Basic and Applied Sciences, Autonomous University of the State of Morelos, Cuernavaca, Mexico; ⁵Department of Electrical and Computer Engineering, Tufts University, Medford, Massachusetts, United States.

We present evidence of self-assembled quantum dots (QDs) with anomalous Stranski-Krastanov (SK) growth – whose WL thickness is tunable. The SK growth mode is a commonly-used method for the strain-driven epitaxial growth of dislocation free quantum dots (QDs) with tunable optoelectronic properties. [1] SK growth proceeds in three stages with increasing material deposition: (i) a 2D wetting layer (WL) forms and grows thicker; (ii) at some critical thickness, 3D QDs begin to self-assemble on the WL; and (iii) the QDs grow while the WL thickness remains fixed at the critical thickness. [1] We grow GaAs tensile-strained QDs (TSQDs) embedded in In_{0.52}Al_{0.48}As(111)A for optical analysis, and on the surface for structural analysis, by molecular beam epitaxy. These GaAs TSQDs exhibit unique properties that derive from their (111)-orientation and their residual tensile strain. [2,3] Growth proceeds via the initial formation of a 2D WL, followed by a transition to 3D TSQD self-assembly, consistent with the SK growth mode. However, in contrast with traditional SK growth, additional deposition leads to *both* the QDs and the WL increasing in size. This unique result is of interest both in its fundamental physics as well as its potential device applications. By tuning both TSQD size and WL thickness, we can modify the QD-QW interactions in this hybrid quantum system. [4] Benefits will include accurate control over TSQD and WL band structure for infrared optoelectronic applications. Since growth of the WL ceases once the critical thickness is reached, varying the WL thickness for a given QD system is not typically possible. Therefore, researchers have found creative approaches to sidestep this constraint on WL thickness. However, the ability to tune WL thickness in one simple SK growth step, without additional processing or growth parameter constraints, would be preferable, opening the door to future applications looking to harness WL/QD interactions. We provide evidence for this tunable WL thickness with atomic force microscopy, photoluminescence spectroscopy, high resolution cross-section transmission electron microscopy, electron energy loss spectroscopy, and computational modelling. [1] B.A. Joyce and D.D. Vvedensky, *Mater. Sci. Eng. R* 46, 127 (2004). [2] C.F. Schuck, R.A. McCown, A. Hush, A. Mello, S. Roy, J.W. Spinuzzi, B. Liang, D.L. Huffaker, and P.J. Simmonds, *J. Vac. Sci. Technol. B* 36, 031803 (2018). [3] P.J. Simmonds and M.L. Lee, *J. Appl. Phys.* 112, 054313 (2012). [4] M. Shahzadeh and M. Sabaeian, *AIP Adv.* 4, 067113 (2014).

11:40 AM U05

(Student) Mechanisms of GaN Quantum Dot Formation During Nitridation of Ga Droplets Hongling Lu¹, Caleb Reese¹, Sunyeol Jeon¹, Yaming Fan², Emily Rizzi¹, Yuqun Zhuo³, Qi Liang² and Rachel S. Goldman²; ¹Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; ²Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; ³Key Laboratory for Thermal Science and Power Engineering of the Ministry of Education, Dept. of Energy and Power Engineering, Tsinghua University, Beijing, China.

GaN-based quantum dots (QDs) have been proposed for a variety of optoelectronic devices. Typically, QD formation is driven by a Stranski-Krastanov growth mode transition. Alternatively, the nucleation and conversion of metal droplets to QDs via nitridation, known as droplet epitaxy (DE), has emerged as a promising approach to achieve strain-free QDs. To date, conflicting results have been reported regarding the formation mechanisms of DE GaN QDs. GaN DE has been described as a liquid-phase epitaxy-like and/or a surface-diffusion driven process. Here, we investigate the formation mechanisms for DE GaN QDs using a

combined computational-experimental approach. Our first-principles calculations of activation barriers suggest that N is immobile while Ga has a relatively high surface diffusivity, independent of the starting surface structure and chemistry. We consider the temperature and substrate dependence of the size distributions of droplets and QDs, and report on two competing mechanisms mediated by Ga surface diffusion, Ga droplet coarsening with QD formation via impinging N atoms and Ga droplet out-diffusion with QD nucleation at adsorbed N surface sites. We also discuss the relative roles of nucleation and coarsening dominant growth, as well as the phase selection, on various substrates. The new insights provide an opportunity for tailoring QD size and phase distributions for a wide range of III-N semiconductor QDs.

SESSION V: Oxide Doping and Composites
Session Chairs: Leonard Brillson and Rebecca Peterson
Thursday Morning, June 27, 2019
Michigan League, 3rd Floor, Henderson

8:40 AM V01

Role of Lithium and Sodium in InO-Based Amorphous Oxide Semiconductors from First Principles Ivan Zhuravlev and Julia Medvedeva; Physics, Missouri University of Science and Technology, Rolla, Missouri, United States.

Oxides of post-transition metals provide a rich parameter space for exploring diverse electronic and optical properties. Among them, transparent conducting oxides, such as tin doped indium oxide or aluminum doped zinc oxide, are known for a unique combination of high electrical conductivity and optical transparency in the visible range[1]. Complex multi-cation oxides have recently become competitive with silicon as the active transistor layer in LCD displays. The amorphous phase of the oxides is favored both for flexible and high resolution display applications because the low deposition temperature opens up a possibility to use polymer substrates, while low internal stresses and good etchability allow production of large-area uniform films. Amorphous oxide semiconductors (AOSs) were shown to exhibit optical, electrical, thermal, and mechanical properties that are comparable or even superior to those possessed by their crystalline counterparts[2]. One of the central technological advantage of an AOS is its tunable electrical conductivity. Although amorphous materials lack grain boundaries and periodicity, the electron transport in AOSs is more complex than in the crystalline phases: strong distortions of the metal-oxygen polyhedra and intricate structural morphology in AOSs determine the carrier generation and mobility which is limited by electron scattering associated with nano-crystallinity, composition, defects, thermal vibrations, and lattice strain[3,4]. According to the earlier works, incorporation of pre- or post-transition metals, such as Sc, Y, La, or Ga, Sn, Zn, into the amorphous In_2O_3 may significantly affect the local structure and reduce the medium-range ordering [4,5]. From the theory of glass formation, it is known that alkali metal oxides such as Li₂O and Na₂O serve as structural modifiers, controlling the polyhedra network of the host and increasing the materials density. In this work, we employ *ab-initio* molecular dynamics liquid-quench simulations and accurate density-functional calculations to understand how addition of Li or Na to amorphous indium oxide affects (i) the nearest-neighbor In-O distances, coordination, and the local O-In-O angles; (ii) the In-O polyhedra sharing and distribution, i.e., the medium-range structure that governs the morphology of the amorphous semiconductor; and (iii) the defect formation, number of carriers, and electron velocities that determine the carrier generation and carrier transport. We have performed a thorough systematic analysis of how density, quench rate, cation composition, and oxygen stoichiometry affect the resulting structural and electronic properties. In order to obtain correct band gap and optical properties, a hybrid functional was used. The calculated pair correlation function of a-InO:Li is similar to that for a-InO with a clearly defined first-shell peak (that corresponds to the nearest In-O bonds) and suppressed structural features at a longer range. A small shoulder in front of the In-O peak is attributed to the shortest Li-O bonds. The calculated effective coordination number (ECN) distribution shows that addition of Li increases the amount of fully-coordinated (ECN>5.5) In atoms and, at the same time, introduces a fairly large amount of highly under-coordinated In atoms (ECN<4.5). The results suggest that Li, unlike the conventional pre- and post-transition dopants, may facilitate carrier generation governed by under-coordinated In atoms and enhance carrier mobility via the formation of low-dimensional InO_6 polyhedra chains. [1] D.S. Ginley, H. Hosono, D.C. Paine, Eds., *Handbook of Transparent Conductors*, Springer, Boston, MA, 2011 [2] X. Yu, T.J. Marks, A. Facchetti, *Nat. Mater.* **15**, 383 (2016)

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9:00 AM V02

(Student) Investigating Doping Effects of Hydrogen in Indium Oxide Through Electrochemical Capacitance-Voltage Profiling and UV-Irradiation Studies Sebastian Husein¹, William Weigand², Mathieu Bocard³, Zachary C. Holman², Julia Medvedeva⁴ and Mariana I. Bertoni²; ¹School of Engineering for Matter, Transport, and Energy, Arizona State University, Tempe, Arizona, United States; ²School of Electrical Computer and Energy Engineering, Arizona State University, Tempe, Arizona, United States; ³Institute of Microengineering, Photovoltaics and Thin Film Electronics Laboratory, Ecole Polytechnique Fédérale de Lausanne, Neuchâtel, Switzerland; ⁴Department of Physics, Missouri University of Science and Technology, Rolla, Missouri, United States.

We investigate the various effects of hydrogen incorporation in hydrogenated indium oxide (IO:H) thin films. First, we show that electrochemical capacitance-voltage (ECV) profiling can be used for IO:H films to characterize the doping concentration as a function of depth through the layers. Then, concerning morphology of these films, we observe a grain-size decrease from ~50 nm to ~10 nm as H concentration increases from ~3% to ~7 at.%, (H concentration measured by Rutherford backscattering, RBS, and elastic recoil detection, ERD) as shown in Fig. 1 of the extended abstract. Furthermore, by comparing the average number of grain boundaries in the actively etched area of ECV to the depth-dependent carrier density (N_e), we determine whether H preferentially segregates to grain boundaries, and calculate the doping efficiency of H (i.e., ratio of active to inactive H donors). Lastly, to determine stability of the electrically active H donors, films were subjected to intense UV-irradiation, with on-going observation of decay rate of active carriers through use of both Hall effect and ECV occurring over the course of several months. Hydrogen as an impurity in semiconductors is well known, due to its pervasiveness coupled with difficulties in removing it entirely from growth chambers. Applying density functional theory (DFT) calculations, Van de Walle et al. has shown that interstitial and substitutional H acts as a donor in *n*-type zinc oxide (ZnO) and indium oxide (IO), with the H⁺ charge state being stable for all Fermi level positions within the band gap. Consequently, H could be a cause of conductivity in these transparent conducting oxides (TCOs)—rather than acting as a compensating defect center as observed in conventional semiconductors—which may explain the measured increases in conductivity observed in TCOs with H incorporation. However, further experimental studies confirming the donor nature of H in oxides is warranted to supplement the theoretical work. In the present study, H is incorporated in the indium oxide films two ways: during sputtering deposition, and post-deposition by diffusion. For sputtering, the chamber is evacuated to varied vacuum levels, thereby varying partial pressure of water vapor, $p(\text{H}_2\text{O})$ in the chamber during deposition. Using glow discharge emission spectroscopy (GDOES) in collaboration with HORIBA Scientific, H content in the films is currently under evaluation to determine how H at.% relates to increasing $p(\text{H}_2\text{O})$. For diffusion, intrinsic, hydrogenated amorphous Si (a-Si:H(i)) layers are first deposited by PECVD on glass or Si substrates. IO thin films are sputtered as an overcoat, and the IO/a-Si:H(i)/Si or IO/a-Si:H(i)/glass stacks are annealed at 150, 200, and 250 °C in ambient. Typically, Hall effect is used to inspect doping levels of TCO thin films. Electrochemical capacitance-voltage (ECV) profiling is an alternative method used extensively on Si, III-V semiconductors such as GaAs and InP, and II-VI materials such as CdTe or ZnSe. A major advantage of ECV over Hall is its ability to profile N_e vs. depth and even characterize complex multilayers with varied doping concentrations, including p-n junctions. ECV results shown in Fig. 2 of the extended abstract reveal N_e vs. depth in two IO:H films sputtered with differing $p(\text{H}_2\text{O})$. Prior reports of ECV profiling of IO layers are lacking in part due to the large band gap (~3.3 eV) of IO, as conventional C-V profilers cannot generate a photocurrent in wide gap *n*-type material, which is required for photoelectrochemical etching. Furthermore, IO is highly reactive to the usual electrolytes, making accurate depth profiling difficult. We show these problems can be overcome and demonstrate that ECV can provide accurate, reproducible carrier concentrations in IO layers, with average concentrations comparable to Hall measurements: 3.9 at.% H = $2.22 \times 10^{19} \text{ cm}^{-3}$ (ECV) vs. $5.06 \times 10^{19} \text{ cm}^{-3}$ (Hall) and 5.2 at.% H = $7.85 \times 10^{19} \text{ cm}^{-3}$ (ECV) vs. $1.05 \times 10^{20} \text{ cm}^{-3}$ (Hall).

9:20 AM V03

(Student) Improved P-Type Conductivity and Thermal Stability of Oxygen-Rich Nickel Oxide by Li Doping Kingsley Egbo¹, Chaoping Liu^{1,2} and Kin Man Yu^{1,3}; ¹Physics, City University of Hong Kong, Hong Kong, Hong Kong; ²Physics, Shantou University, Shantou, China; ³Material Science and Engineering, City University of Hong Kong, Kowloon, Hong Kong.

NiO is one of the few p-type wide-gap oxides and hence is a widely used p-type transparent conducting oxide and hole transport layer in optoelectronic devices [1]. The p-type conductivity in NiO was believed to come from Ni vacancy (V_{Ni}) or O interstitial (O_i) acceptors in Oxygen-rich NiO_{1+ δ} while stoichiometric NiO is typically an insulator. However, NiO_{1+ δ} has limited conductivity in the range of s~1-10 S/cm (resistivity ρ ~0.1-1 W-cm) with transmittance ~40-60% in the visible range [2]. Moreover, because V_{Ni} and O_i acceptors are unstable even at room temperature, gradual degradation of the p-type conductivity of NiO_{1+ δ} has been observed over time. Extrinsic dopants such as Li and Cu can act as acceptors by substituting Ni and enhance the p-type conductivity of NiO [3]. In this study, we investigate the effect of Li doping in NiO_{1+ δ} and demonstrate that with Li doping, stable highly p-type NiO_{1+ δ} can be achieved. Nanocrystalline thin films of undoped and Li doped oxygen-rich NiO_{1+ δ} were deposited at room temperature on glass substrate with different oxygen partial pressure by RF magnetron sputtering using a pure NiO and NiO with 2wt% Li₂O targets, respectively. Oxygen flow ratio $r(O_2) = f(O_2)/[f(Ar) + f(O_2)]$ in the sputtering gas was varied to control the oxygen stoichiometry in the film. Variable temperature Hall measurement, spectroscopic Ellipsometry, Seebeck measurement and x-ray photoelectron spectroscopy were used to investigate the electrical and optical properties of the films. The effect of lithium doping on the thermal and ambient stability is also studied systematically by rapid thermal annealing (RTA). Room temperature Hall effect measurement shows that the p-type conductivity increases from s=0.25 S/cm to 4.96 S/cm with increasing oxygen content in NiO_{1+ δ} by varying the O₂ flow rate in the sputter gas from 1.4% to at 6.6%. Further increase in $r(O_2)$ show no corresponding increase in the conductivity, likely due to the saturation of O-rich native defects in the film. Compared to undoped NiO_{1+ δ} , Li doping at a given $r(O_2)$ dramatically increases the p-type conductivity. For instance, with 6.0% Li doping NiO_{1+ δ} increases the conductivity for samples grown at $r(O_2) = 1.4%$ from 0.25 to 2.9 S/cm while the sample grown at $r(O_2) = 6.6%$ increased from 4.96 S/cm to 7.7 S/cm. The hole conduction mechanism in all the samples was found to be dominated by small polaron hopping (SPH) conduction in the temperature range of 180K to 450K. Optical characterization results show a slight decrease of transmittance in the visible range with increasing $r(O_2)$. The relatively low transmittance of undoped and Li doped NiO_{1+ δ} samples comes from a strong sub-gap absorption with a broadening of the Urbach edge as the $r(O_2)$ increases. This suggests that the sub-gap absorptions originate from O-related native defects, V_{Ni} , O_i and their complexes. An apparent correlation between the obtained Urbach energy of these sub-gap states and film conductivity is also observed. Annealing study show that while the resistivity of undoped p-type NiO_{1+ δ} increases drastically at annealing temperature > 200°C, the resistivity of Li doped samples increase only slightly. From Arrhenius plots of conductivity versus annealing temperatures the activation energies for the decrease in the conductivity for samples grown with $r(O_2) = 1.4%$ were estimated to be ~0.32 and 0.23 eV for Li doped and undoped NiO_{1+ δ} samples, respectively. Our results suggest that both the conductivity and thermal stability of oxygen-rich NiO_{1+ δ} can be improved by Li doping and hence Li doped NiO_{1+ δ} is an effective p-type transparent material for various optoelectronic applications. This work is supported by the General Research Fund of the Research Grants Council of Hong Kong under Project No. CityU SRG 7005106. **References** [1] Z. Wang *et al.*, *Adv. Mater.*, vol. 28, no. 20, May 2016 [2] H. Sato *et al.*, *Thin Solid Films*, vol. 236, Dec, 1993 [3] J.Y. Zhang *et al.*, *J. Mater. Chem. C*, vol. 6, 2018

V04 WITHDRAWN

(Student) CuO-rGO Composite Sensor for Room Temperature NO₂ Sensing—Role of Morphology Jyoti Jyoti and Ghanshyam D. Varma; Physics, I.I.T. Roorkee, Roorkee, India.

9:40 AM V05

Carbon/Cobalt-Based Nanohybrids for Solar-Driven Hydrogen Generation Fabiola Navarro-Pardo^{1,2}, Ana C. Tavares¹, Haiguang Zhao³, Zhiming M. Wang² and Federico Rosei^{1,2}; ¹Institut National de la Recherche Scientifique, Varennes, Quebec, Canada; ²University of Electronic Science and Technology of China, Chengdu, China; ³Qingdao University, Qingdao, China.

Due to their outstanding catalytic, optical and electronic properties, nanohybrids based on transition metal oxides and transition metal

chalcogenides are attractive materials for the development of earth-abundant electrodes in a variety of renewable energy technologies. We have strategically designed hybrid nanostructures with properties that can challenge the most important constraints for the progress in solar-driven energy conversion devices, such as high efficiency and long-term stability. We particularly focused this investigation on the development of hybrid electrodes with potential applications in devices for hydrogen generation. We first optimized the interaction of graphene oxide (GO) to improve the electrical properties within cobalt oxide nanoribbons. We obtained these one-dimensional nanostructures via electrospinning technique using a cobalt-based precursor solution, including different concentrations of GO. We evaluated the performance of these cobalt nanohybrids (CoNHs) in Na₂S/Na₂SO₃ aqueous electrolyte (pH=13) due to its wide application in photocatalytic and photoelectrochemical (PEC) devices. We demonstrated that the addition of GO noticeably reduced the charge transfer resistance of the electrodes, decreasing from 4.4 Ω to 2.5 Ω for the 0wt% GO/CoNHs and the 12wt% GO/CoNHs, respectively. Furthermore, the CoNHs displayed outstanding electrochemical long-term stability, as the overpotential required to keep a current density of -10 mA cm⁻² is invariable for over 42 h. The structural characterization of the nanohybrids indicated that during continuous operation, the CoNHs rebuilt and regenerated *in situ* leading to the formation of two-dimensional nanostructures comprising a mixture of cobalt chalcogenides (Co₃S₄ and CoS₂). The integration of the CoNHs in a quantum-dot based PEC cell and an alkaline electrolyzer (1M KOH) demonstrates the versatility and viability of these alternative electrodes toward active and solar-driven fuel generation. These findings motivated us to obtain similar electrodes with another graphitic nanomaterial, i.e. carbon nanotubes (CNTs). In this associated work, we used non-covalent functionalization to lower at least 10 times the content of carbon nanomaterial. Further modifications of these electrodes were achieved by electrodeposition and phosphorous doping of the nanoribbons resulting in promising electrocatalytic performance, similar to that of the platinum electrode and outstanding long-term stability performance (for over 48 hours). With these findings, we have demonstrated a cost-efficient and scalable approach to develop high performance and stable hybrid nanostructures based in carbon/cobalt compounds. Due to their intrinsic properties, these advanced materials could be applied not only in photoelectrochemical cells but also in other devices such as capacitors, fuel cells or li-ion batteries.

10:00 AM REFRESHMENT BREAK

SESSION W: Materials for THz, Plasmonics and Polaritons
Session Chairs: Seth Bank and Stephanie Law
Thursday Morning, June 27, 2019
Michigan League, 3rd Floor, Koessler

8:20 AM W01

(Student) Mid-Wave Infrared Filtering via Subwavelength Dielectric Zero-Contrast Gratings Michael Barrow and Jamie Phillips; Electrical Engineering and Computer Science, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

Subwavelength dielectric gratings provide narrowband optical filtering based on guided mode resonance. They can utilize a compact, readily fabricated platform requiring few layers, and may be tuned by varying the grating dimensions lithographically. Infrared applications including thermal imaging, spectroscopy, and hyperspectral imaging, have helped fuel interest in subwavelength gratings. Previously, we have demonstrated infrared filtering in the long-wave IR (8 - 12 μm) using high index contrast dielectric gratings based on suspended silicon/air. A zero-contrast grating (ZCG) scheme, wherein a high-index dielectric grating is positioned atop a slab of the same material and surrounded by a low-index medium, offers another degree of tuning guided mode resonant behavior and possible improvement in filter performance. In this work, we investigate mid-wave infrared (MWIR, 3 - 6 μm) ZCG filters based on air/Si/SiO₂ structures fabricated on commercial silicon-on-insulator wafers. Using conventional microfabrication techniques, we demonstrate ZCG filters with quality factors (Q) ranging up to 175 at a wavelength of 4.4 μm when operating at near-normal incidence. The background high-reflectivity window extends from about 4 to 5.5 μm . Experimental results agree with optical mode coupling simulated by finite element methods. While the filters are designed for light polarized with magnetic field parallel to the gratings (transverse magnetic, TM), we demonstrate coupling to transverse electric (TE) modes when the incident light is azimuthally oblique. These TE modes have weaker coupling than TM modes of the same order, enabling narrower resonance linewidths when experimental conditions prohibit normally-incident collimated light, such as typically configured during FTIR characterization. By using a strongly-coupled TM mode to provide the background rejection and a weakly-coupled TE mode to furnish narrowband transmittance, we demonstrate a ZCG with a Q of 175. Furthermore, the introduction of periodic notches along the length of the grating lines may enable TE coupling at normal incidence. For light that is TM-polarized with respect to the grating periodicity, the electric field is orthogonal to the direction of notch periodicity, allowing normal-incidence TE-coupling. Further two-dimensional ZCG grating designs based on square and hexagonal lattices will be presented in the goal of offering polarization-independent filtering.

8:40 AM W02

(Student) Nanoscale Mapping and Spectroscopy of Non-Radiative Hyperbolic Modes in Hexagonal Boron Nitride Joseph R. Matson¹, Lisa V. Brown^{2,3}, Georg Ramer², Marcelo Davanco², Zhiyuan Sun⁴, Andrey Kretinin⁵, Yiguo Chen^{6,7}, Igor Vurgaftman⁸, Nicholas Sharac⁸, Alexander Giles⁸, Michael Fogler⁴, Takashi Taniguchi⁹, Kenji Watanabe², Kostya Novoselov⁵, Stefan Maier⁶, Andrea Centrone² and Joshua Caldwell¹; ¹Vanderbilt University, Nashville, Tennessee, United States; ²National Institute of Standards and Technology, Gaithersburg, Maryland, United States; ³University of Maryland, College Park, Maryland, United States; ⁴University of California San Diego, La Jolla, California, United States; ⁵University of Manchester, Manchester, United Kingdom; ⁶Imperial College London, London, United Kingdom; ⁷National University of Singapore, Singapore, Singapore; ⁸U.S. Naval Research Laboratory, Washington D.C., District of Columbia, United States; ⁹National Institute for Materials Science, Tsukuba, Japan.

Polaritons are quasiparticles consisting of a coupled photon with a coherent charge oscillation. These coupled modes enable deeply sub-diffractive confinement of light, for applications ranging from sub-diffractive imaging to enhanced chemical sensing. The most studied polaritons are surface plasmon polaritons (SPPs), in which light couples to free carrier oscillations. SPPs offer broad tunability through carrier manipulation, but are limited by the optical losses caused by high carrier scattering rates. An alternative to SPPs are surface phonon polaritons (SPhPs), where light couples to the optic phonons, with much lower losses due to slower phonon scattering. Hexagonal boron nitride (hBN) is a polar semiconductor that supports phonon polaritons within the Reststrahlen band, the spectral range between the transverse and longitudinal optic

phonon frequencies of the material. The anisotropy in the crystal structure of hBN causes the material to support two Reststrahlen bands (between ~ 6.2 - 7.3 and ~ 12.1 - 13.2 μm) with hyperbolic behavior - behaving as a dielectric along at least one axis, and as a metal along the orthogonal axes. Such hyperbolicity offers potential applications in areas from sub-diffractive imaging through hyperlensing, remarkable confinement of light, exceptionally large optical density of states for controlling the spontaneous emission rates of local emitters, etc. Compared to previous hyperbolic metamaterials, hBN has significantly lower loss, and does not need rigorous fabrication steps. The hyperbolicity of hBN allows the phonon polaritons to propagate through the *volume* rather than along the surface of the material. Within deeply subwavelength optical cavities, these hyperbolic PhPs (HPhPs) exhibit several sets of polaritonic modes, each offering distinct near-field modal profiles. HPhPs have been observed in far-field measurements, and mapped using scattering type scanning near-field optical microscopy (s-SNOM). However, these measurement techniques only access a subset of the full polariton dispersion of the material. The higher order, non-radiative modes were therefore unobserved, only theoretically predicted. Here, we measure and image both the radiative and non-radiative HPhPs using photothermal induced resonance (PTIR). In PTIR, the modes are excited using a scattering, metallized AFM tip similar to s-SNOM. However, instead of measuring the scattered optical fields, PTIR measures the local thermal expansion via the mechanical tip deflection. Thus, the PTIR signal is proportional to the absorption of the material or structure. Through careful resonance lineshape analysis and comparison with far-field and nano-FTIR spectra, we have identified ~ 20 resonant dispersive modes not observed using s-SNOM and far-field measurements. These resonances were confirmed as HPhP resonances by their spectral dispersion and through comparison with analytical predictions of these modes. Our results show the first clear observation of these predicted, but previously unreported "dark" HPhPs. These higher-order modes exhibit a range of angular and radial momenta distinct from the radiative modes - which could provide control over field concentration, orbital angular momenta and polarization with nanoscale precision. In contrast to s-SNOM, our PTIR data indicate a strong spatial dispersion in the HPhP resonant intensities as the tip moves across the surface of the structure. These results suggest that PTIR is not only useful for observing dark HPhP modes, but also provides information on the propagation of these volume-confined modes that is inaccessible to other near-field measurements such as s-SNOM.

9:00 AM W03

(Student) Multilayer Dielectric Metasurfaces for Multiwavelength Metaoptics You Zhou and Jason Valentine; Vanderbilt University, Nashville, Tennessee, United States.

Metasurfaces provide a versatile platform for manipulating the wavefront of light using planar nanostructured surfaces. Despite wide applications for thin and flat optics, metasurfaces are restricted by their operational bandwidth and limitations in achieving independent control over multiple properties of light. Here, we propose a multilayer metasurface platform for increasing the design landscape of metaoptics. As a proof of concept, we experimentally demonstrate this approach for multiwavelength metaoptics, including multiwavelength metalenses and holograms.

9:20 AM W04

(Student) All-Dielectric Metasurfaces for Narrow-Band Near-Unity Thermal Emissivity Austin Howes, Joshua R. Nolen, Joshua Caldwell and Jason Valentine; Vanderbilt University, Nashville, Tennessee, United States.

Metasurface optics often use dielectric nanostructures for Mie-type modes that are low-loss and spectrally narrower than their plasmonic counterparts. Mie dipolar resonances are well-studied in many traditional materials but have not yet been explored in cases of extremely high permittivity, dispersion, and loss. We investigate the effects of each of these parameters and design 3C-SiC nanostructures with two orthogonal Mie resonances at the same wavelength, a composite known as a Huygens mode. While Huygens modes are typically used for achieving unity transmission in dielectric metasurfaces, we observe that such modes under the correct conditions are useful as narrow-band thermal absorbers. We experimentally realize 3C-SiC devices with 78% absorptance amplitude and a quality factor of 170 at a working wavelength of 13 μm . This unique absorber design benefits from a higher quality factor than other works at this wavelength range, a large absorption amplitude with a single pass-through of the structure, transmissive operation, insensitivity to angle of incidence, and as a result serves as a unique and strong candidate for the future of ultrathin narrow-band thermal sources.

9:40 AM W05

Quantum Confinement, Finite-Size and Anisotropy Effects in Ultrathin Plasmonic Films Igor V. Bondarev¹, Hamze Mousavi¹ and Vladimir M. Shalaev²; ¹Mathematics and Physics, North Carolina Central University, Durham, North Carolina, United States; ²Electrical and Computer Engineering, Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana, United States.

We report on the recent progress in the theoretical understanding of the quantum optical properties of quasi-2D plasmonic nanostructures (metasurfaces and films) of controlled finite thickness [1-4]. While being constant for relatively thick films, the plasma frequency of ultrathin plasmonic films acquires the spatial dispersion typical of 2D materials, gradually shifting to the red with film thickness reduction [1]. This explains recent experiments done on ultrathin TiN films of controlled variable thickness [5]. The confinement induced plasma frequency spatial dispersion and associated dielectric response nonlocality can result in the new attractive features of the magneto-optical response of the film [3]. Specifically, the magnetic permeability exhibits a sharp resonance structure shifting to the red as the film aspect ratio increases. When tuned appropriately, the ultrathin films of finite lateral size can be negatively refractive in the IR frequency range. Compared to the thick film a dipole emitter near the ultrathin film shows a two-order-of-magnitude radiative decay rate enhancement, which can be qualitatively understood in terms of the interacting image dipoles, and can even be enhanced unidirectionally using ultrathin, periodically anisotropic metal-dielectric plasmonic nanostructures [4]. We show that the overall light-matter interaction in close proximity to plasmonic films can be controlled not only by varying the chemical composition and material quality of the film but also by adjusting its thickness and aspect ratio as well as by choosing the deposition substrates and coating layers appropriately. We believe our findings open up entirely new avenues for potential applications of ultrathin plasmonic films in modern optoelectronics. Acknowledgments: NSF-DMR-1830874 (I.V.B.), DOE-DE-SC0007117 (H.M.), ONR-N00014-16-1-3003 (V.M.S.) References: [1] I. V. Bondarev and V. M. Shalaev, Universal features of the optical properties of ultrathin plasmonic films, *Optical Mater. Express* 7, 3731 (2017). [2] I.V. Bondarev and V.M. Shalaev, Quantum electrodynamics of optical metasurfaces, 2018 International Applied Computational Electromagnetics Society Symposium (ACES), 1-2. [3] I. V. Bondarev, H. Mousavi, and V. M. Shalaev, Optical response of finite-thickness ultrathin plasmonic films, *MRS Commun.* 8, 1092 (2018). [4] I. V. Bondarev, Finite-thickness effects in plasmonic films with periodic cylindrical anisotropy [Invited], *Optical Mater. Express* 9, 285 (2019). [5] D. Shah, H. Reddy, N. Kinsey, V.M. Shalaev, and A. Boltasseva, Optical properties of plasmonic ultrathin TiN films, *Adv. Optical Mater.* 5, 1700065 (2017).

10:00 AM REFRESHMENT BREAK

10:20 AM W06

(Student) Approaching Ultra-Strong Polaritonic Coupling within CdO Bilayers Joshua R. Nolen¹, Evan L. Runnerstrom², Kyle P. Kelley², Thomas G. Folland¹, Angela Cleri³, Joseph Nordlander³, Nader Engheta⁴, Jon-Paul Maria³ and Joshua Caldwell¹; ¹Vanderbilt University, Nashville, Tennessee, United States; ²North Carolina State University, Raleigh, North Carolina, United States; ³The Pennsylvania State University, State College, Pennsylvania, United States; ⁴University of Pennsylvania, Philadelphia, Pennsylvania, United States.

Epsilon-near-zero (ENZ) modes are supported in films of polaritonic materials with vanishing permittivity values and deeply sub-wavelength thicknesses. These novel optical excitations are associated with extreme electric field confinement, enabling control over light-matter interactions such as resonant perfect absorption and strong nonlinear interactions. Recent studies have demonstrated ENZ phenomena in doped transparent conducting oxides (TCOs). Unlike traditional metals that are not tunable in the IR and THz due to fixed, high carrier densities, TCOs allow for tuning of both carrier density and electronic mobility. One highly promising TCO is highly-doped CdO, which has been shown to achieve electron mobilities extending upwards to 500 cm²/V-s with carrier densities ranging from 10¹⁹ to 10²⁰ cm⁻³. Unique to this material is a range of carrier densities where increasing values result in *increasing* mobilities. ENZ modes are unique for their strong absorption/emission and narrow resonant linewidths that can be achieved without the need for nanostructuring. This behavior has been utilized to achieve perfect absorption in thin films as well as thermal emissivity control. These modes are attributed with a nearly-flat spectral dispersion that consequently results in low group velocities and short propagation lengths, diminishing their utility. However, these limitations may be mitigated through hybridization with other polaritonic modes, such as surface plasmon

polaritons (SPPs) which are also supported in doped CdO films. Unlike ENZ modes, SPP modes propagate at a much higher group velocity but are hindered by carrier scattering losses and highly sensitive to surface morphology. Careful control over the carrier concentration during film growth has opened the door to achieving multilayer CdO films. Here we show that epitaxially-grown bilayer stacks of CdO, with bottom and top layers supporting SPP and ENZ modes respectively, exhibit cavity-free strong coupling between the ENZ and SPP modes and overcome the deficiencies of each constituent mode. The combined ENZ-SPP dispersion of these bilayer films displays a prominent anti-crossing with a separation that is on the order of the mode frequency, giving clear evidence of strong coupling. The degree to which these modes are strongly coupled together is partially dependent on the spectral overlap of the modes. By carefully controlling the plasma frequency of the two individual CdO layers, this spectral overlap and thus the ENZ-SPP dispersion, can be tuned. We also show that tuning the oscillator strength of the individual modes is another approach towards manipulating the ENZ-SPP dispersion. This is controlled geometrically, by tuning the ENZ layer thickness. In more recent work we have extended our focus to other geometries, such as trilayer CdO films where an undoped middle layer acts as a dielectric spacer between the SPP and ENZ layers. Controlling the thickness of the undoped middle layer is another method of tuning the ENZ-SPP coupling. We also examine this ENZ-SPP hybridization within three-dimensionally confined cavities to monitor the impact of nanostructuring upon this strong coupling phenomena and how this can be used as independent knobs for tuning the resonant absorption, and alternatively thermal emission, of the structures. By fabricating such hybrid materials into nanostructure arrays, direct control of the emission polarization, spatial coherence and divergence is also engineered through careful design of nanostructure geometry and periodicity. This approach may lead to the realization of spectrally tunable thermal emitters for narrow-band, polarized and spatially coherent IR sources.

10:40 AM W07

Near-Monochromatic Multimode Optical Antennas on Epsilon-Near-Zero Thin Films Owen Dominguez¹, Leland J. Nordin², Junchi Lu¹, Daniel Wasserman³ and Anthony Hoffman⁴; ¹Electrical Engineering, University of Notre Dame, South Bend, Indiana, United States; ²ECE, The University of Texas at Austin, Austin, Texas, United States; ³University of Texas at Austin, Austin, Texas, United States; ⁴University of Notre Dame, Notre Dame, Indiana, United States.

The spectral response of optical antennas is often controlled via the geometry of the antenna. For example, the frequency of the fundamental mode scales linearly with the length of the antenna. While the influence of the substrate is often overlooked, it plays an important role in determining the optical modes supported by the antennas because it constitutes a significant component of their local dielectric environment. For antennas fabricated on low-loss, epsilon-near-zero (ENZ) substrates, the response of the optical antennas can be drastically altered. Here, we demonstrate a near-monochromatic response for mid-infrared multimode optical antennas fabricated on ENZ materials. We show how the vanishing index of the substrate, arising from the ENZ permittivity of the substrate, results in pinning of the fundamental antenna mode and the next two higher harmonics into a narrow wavelength range. We also demonstrate the coupling of multiple antenna modes to the ENZ Berreman mode supported on thin ENZ films. We fabricate arrays of optical antennas on 1.2 μm thick AlN films on a Mo groundplane using electron beam lithography and Ti/Au (5/85 nm) metal deposition. AlN exhibits an ENZ region around 885 cm⁻¹ (11.3 μm). In total, we fabricate 15 4x4 mm² arrays comprising antennas of different lengths, ranging from 2.73 to 20.58 μm, as measured via scanning electron microscopy. We characterize the arrays using polarization-, angle-, and wavelength-dependent reflection measurements on the external port of a Fourier transform infrared spectrometer with a cooled HgCdTe detector, ZnSe lenses, and a KRS-5 linear polarizer. Coupling between the modes of the optical antenna and the Berreman mode is controlled via the polarization of the incident light. For the longest antennas (20.58 μm), when only the antenna modes are excited, we observe a pinning of the fundamental antenna mode and the next two harmonics within a spectral bandwidth of approximately cm⁻¹, about 3.5% of the frequency of the fundamental mode. This pinning of multiple antenna modes into a narrow spectral region is a significant departure from the typical spacing of harmonics of an optical antenna by integer multiples of the fundamental frequency. Furthermore, when we simultaneously excite the Berreman mode and the optical antennas by rotating the polarization of the incident light, coupling between the Berreman mode and each antenna mode is observed, further altering the dispersion of the system. The experimental measurements agree well with numerical

simulations in COMSOL Multiphysics and a coupled oscillator model. The results of this work could open new paths towards engineering optical antennas and light-matter interactions between confined optical modes and ENZ materials.

11:00 AM W08

(Student) Modeling and Characterizing Far-Infrared Optical Modes in ZnO Nanoparticles [Irfan Khan](#)¹, Evan P. Gies², Ryan K. Roeder² and Anthony Hoffman¹; ¹Department of Electrical Engineering, University of Notre Dame, Notre Dame, Indiana, United States; ²Department of Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, Indiana, United States.

Recently, there has been growing interest in confined optical modes on polar crystals for the long-wavelength infrared ($\lambda \sim 10 - 60 \mu\text{m}$). These modes that are often excited at the surface of a bulk material or thin film are called surface phonon polaritons (SPhPs), and they couple electromagnetic radiation to vibrations of the crystal lattice. SPhPs have been used to demonstrate enhanced emission and absorption in the long-wavelength infrared. The vast majority of this work has been carried out on thin films or bulk materials of dielectrics or semiconductors—all of which are amenable to standard nanofabrication techniques. Localized SPhPs (non-propagating surface modes) in polar nanoparticles (PhNPs) could be useful for developing a far-infrared optical infrastructure similar to that of plasmonic nanoparticles that are used in the visible and near-infrared; however, demonstrating localized SPhPs in polar dielectric nanoparticles is challenging due to the random shape, orientation and imperfect distribution of the PhNPs. In this work, we identify and characterize these localized modes for ZnO nanoparticles using both simulations and experiment. We also study and discuss the effects of anisotropy, random orientation, and agglomeration of the nanoparticles on the surface modes. We model the absorption and scattering of ZnO PhNPs analytically using Mie theory and numerically using the Discrete Dipole Approximation (DDA) method. In both approaches, we use a harmonic oscillator approximation with Lorentzian broadening to model the real and imaginary parts of the dielectric permittivity. The model incorporates anisotropy along the c-axis of ZnO. Mie theory predicts localized surface modes for ZnO spherical nanoparticle at 515 cm^{-1} and 531 cm^{-1} . We use DDA method to calculate the absorption efficiency for a 500 nm ZnO nanoparticle for both isotropic and anisotropic cases. The DDA method agrees well with Mie theory, predicting a redshift of 3 cm^{-1} . Comparing the absorption for isotropic and anisotropic PhNPs, the absorption peak is broadened from 15.7 to 30.7 cm^{-1} . We demonstrate the effects of agglomeration by comparing the calculated absorption of 16 randomly oriented anisotropic nanoparticles clumped together. We observe reduced absorption efficiency and significant broadening of the absorption peaks for agglomerated nanoparticles. Similarly, to show the effect of disorder, we calculate absorption for 16 randomly-arranged non-touching nanoparticles with anisotropic permittivity in a monolayer. We observe a broadening of 22 cm^{-1} , a 40% increase for this case as compared to the single nanoparticle with anisotropic permittivity. We perform optical measurements on ZnO PhNPs and compare the measurements with the predictions of our models. ZnO PhNPs with an average diameter of 500 nm were prepared in a pressed KBr matrix (1:200 concentration) and as a self-assembled monolayer (SAM) on a double-side polished GaAs substrate. We characterize the samples via transmission measurements using a Bruker 80v Fourier transform infrared spectrometer. We observe a single broad peak in the measured transmission spectra of the pressed KBr matrix samples at 523 cm^{-1} , which we attribute to the localized SPhP. The presence of a single peak is due to broadening that arises from the random orientation of the anisotropic PhNPs and agglomeration. This work could be useful for developing a nanoparticle platform for the long-wavelength infrared.

11:20 AM W09

Possibilities of p-Diamond as a Plasmonic Material for Terahertz Applications [Sergey Rudin](#)¹, Greg Rupper¹, Tony Ivanov¹ and Michael S. Shur²; ¹U.S. Army Research Laboratory, Adelphi, Maryland, United States; ²Rensselaer Polytechnic Institute, Vienna, Virginia, United States.

The gate-controlled hole gas at the hydrogenated diamond surface was predicted to have a plasmonic response to a terahertz and sub-terahertz electric field, making p-diamond field effect transistors (FETs) promising candidates for implementing room temperature plasmonic devices [1]. The predicted performance of diamond plasmonic detectors shows their potential for high temperature, high voltage, and radiation hard applications and for THz communications and spectroscopy [2] in the atmospheric windows from 0.2 to 0.6 THz. The hole mobilities in our samples range from 30 to $250 \text{ cm}^2/\text{Vs}$, approaching the values ($\sim 300 \text{ cm}^2/\text{Vs}$) that allow for a room temperature resonant plasmonic response in this

communication window. This makes p-diamond a unique material for Beyond 5G THz communications, since a resonant plasmonic response makes also possible the realization of p-diamond based emitters in terahertz and sub-terahertz range, using strong current driven plasma instability in gated channels. Toward the optimal design of p-diamond plasmonic devices we simulated the response using the complete set of hydrodynamic equations, including the thermal transport and accounting for effects of viscosity and pressure gradients. The response of a p-diamond FET is measured as a dc voltage shift at the drain contact, induced by a time-varying electric field with voltage amplitude U_a in a channel with the gate voltage swing U_0 . We computed response as a function of the signal frequency and input signal voltage amplitude for a weak signal ($U_a \ll U_0$) where the response is proportional to U_a^2 , and for a strong signal ($U_a > U_0$) where the response is proportional to U_a . The key parameters used in the simulations are channel length, hole mobility, viscosity, hole effective mass, and gate-to-channel capacitance. In the strong signal regime we find that a shock wave develops in the charge density and drift velocity profiles. This causes spikes in the electric field values in the channel. Due to high value of the dielectric breakdown field in diamond (over 10 MV/cm) the diamond plasmonic device can operate in the strong signal regime, when a shock wave propagates in the channel. This makes the p-diamond an especially attractive material for terahertz emitters based on current-driven plasma instability, including the “plasmonic boom” design of emitters [3]. [1] M. Shur, S. Rudin, G. Rupper, and T. Ivanov, *Appl. Phys. Lett.* **113**, 253502 (2018). [2] I.V. Gorbenko, V. Kachorovskii, and M. Shur, *Optics Express*, **27**, No. 4, 4004 (2019). [3] G. R. Aizin, J. Mikalopas, and M. Shur, *Phys. Rev. B* **93**, 195315 (2016).

11:40 AM W10

(LATE NEWS, Student) Temperature Dependence of Defect Luminescence in Semiconductor $\text{Mn}_2\text{V}_2\text{O}_7$ [Pramod Ravindra](#)¹, Raghav Chaudhary², Kausik Majumdar² and Sushobhan Avasthi¹; ¹Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India; ²Department of Electronics and Communication Engineering, Indian Institute of Science, Bangalore, India.

Metal oxides are a prolific class of materials for solar energy conversion due to their low toxicity, high stability, abundance and low cost of synthesis and thin film deposition. Vanadates are of special interest due to their unique electronic structure. However, interest in oxides for solar energy has traditionally been focused on photoelectrochemical energy conversion. The steep improvement in the organic-inorganic perovskite solar cells in the past decade has reinvigorated the interest in all-oxide-photovoltaics, encouraging the search for oxide-based solar absorbers. $\text{Mn}_2\text{V}_2\text{O}_7$ (MVO) was recently identified as a potential candidate for solar water splitting which served as the motivation to employ it as an oxide absorber. Understanding the defect dynamics is essential to control and engineer defects in materials. Optical properties are a good probe of defects. In this work, we present an investigation of the temperature dependence of sub-bandgap photoluminescence from MVO, and their relevance to MVO as a solar absorber. Polycrystalline thin films of MVO were deposited using pulsed laser deposition on SrTiO_3 substrates. XRD and XPS analysis indicate reasonable phase pure and stoichiometric MVO films were obtained. UV-visible spectroscopy measurements at room temperature reveal a primary indirect bandgap of 1.62 eV and a higher direct bandgap of 1.75 eV. A high absorption coefficient was observed for wavelengths below 675 nm, suggesting strong blue and green absorption. A steep fall in the absorption coefficient below the absorption onset was observed, suggesting low defect absorption. This is also corroborated by a low value Urbach energy of 76 meV. This is comparable to high quality ZnO and is lower than typical oxides, where structural defects act as recombination centres. This suggests that structural defects like grain boundaries might not be a significant detriment to solar performance. Photoluminescence measurements were performed using a 532 nm laser excitation. No band-to-band recombination was observed due to the indirect nature of the primary bandgap, but sub-bandgap peaks were observed, including two sharp emissions near 1.56 eV, with linewidths close to 400 meV and a separation of 380 meV. Most of the analysis in this work is reported for these two most intense peaks. The peak intensities reduced as the temperature was increased from 10 K. Beyond 160 K, were indistinguishable from noise - a characteristic of exciton dissociation into free carriers. The peak intensity followed a power law dependence with the excitation power, with an exponent of 0.6, confirming the defect-based excitonic origin of the sharp peaks. The exciton binding energy was calculated to be 26.1 meV, which is remarkably low for an oxide, and comparable to other solar absorbers. This means the thermal energy at room temperature is sufficient to induce exciton dissociation into free carriers which can then be collected using an electric field. This also shows that luminescent defects in MVO are shallow. The increase in

linewidth with temperature was modeled by incorporating the effect of exciton-phonon interactions. The inhomogeneous broadening, and interaction parameters for acoustic and optical phonons were found to be comparable to III-V nitrides and ternary oxides. Further, one and two phonon emission sidebands were observed at separations equal to the optical phonon energy predicted by the model. The energy peak positions showed an anomalous monotonic blueshift with increasing temperature, which is opposite to the trend in semiconductors. From 10 K to 160 K, the peak position increased by 5 meV. While this can be attributed to defects in the material, further investigation is needed to establish the mechanism. In summary, the optical luminescence properties of MVO have been investigated and results show MVO is a potential solar absorber.

SESSION X: III-Nitride Materials for Power Electronics
Session Chairs: Kenneth Jones and Jae-Hyun Ryou
Thursday Morning, June 27, 2019
Rackham Building, 4th Floor, Amphitheatre

8:20 AM X01

Development and Characterization of GaN Photoconductive Switches
 Andrew D. Koehler¹, Geoffrey Foster¹, Ani Khachatrian¹, Paul D. Cunningham¹, James C. Gallagher¹, Travis J. Anderson², Karl Hobart¹ and Fritz J. Kub¹; ¹U.S. Naval Research Laboratory, Washington, District of Columbia, United States; ²Naval Research Laboratory, Washington, District of Columbia, United States.

The high critical electric field strength and direct bandgap of GaN makes it a well-suited material for a high power photoconductive semiconductor switch (PCSS). This work focuses on development of semi-insulating GaN, with high electric field strength to be used as a PCSS. Carbon incorporation in GaN epitaxial layers is used to suppress off-state leakage current while maintaining high on-state photoconductivity with breakdown field strength of 1.26 MV/cm. Annealing the GaN:C films in a nitrogen overpressure, up to 1200C results in an improvement in breakdown field strength of ~2.86 MV/cm. Characterization of the GaN PCSS devices are performed by singulating and mounting the PCSSs onto a 50 Ohm microstrip transmission line. The turn-on transient of the GaN PCSS are recorded by triggering the PCSS with a 100 fs laser at 335 nm and 1 kHz repetition rate. The laser illuminates the entire active device area between the two electrodes (1 mm wide and 30 um gap between pads). A 25 GHz oscilloscope was used to acquire the fast rising transient, and a 62.3 ps rise time was measured. The fall time is significantly slower, 20.5 ns, due to charge trapped in mid-gap states, likely a result of the midgap carbon states used make the GaN semi-insulating. Further optimization of GaN epitaxial layers, contact formation, passivation materials, and encapsulation materials will be discussed.

8:40 AM X02

(Student) MOCVD Growth of Low Background Doping GaN on GaN Substrate Yuxuan Zhang¹, Md Rezaul Karim², Hyunsoo Lee¹, Mohammad Wahidur Rahman¹, Siddharth Rajan³ and Hongping Zhao¹; ¹Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ²Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ³Ohio State University, Columbus, Ohio, United States.

Gallium nitride (GaN) has been considered as a promising wide band gap semiconductor material for vertical high power device applications, due to its high thermal conductivity ($1.5 \text{ W} \cdot \text{cm}^{-1} \cdot \text{K}^{-1}$), high electric breakdown field ($E_{br} \sim 3.5 \text{ MV/cm}$), high electron mobility (phonon limited mobility $>2000 \text{ cm}^2/\text{Vs}$), and high electron saturation velocity ($1.5 \times 10^7 \text{ cm/s}$). Thus, GaN possesses Baliga figure of merit (FOM) at least 5X better than SiC and 1000X better than Si. In contrast to the efforts on development of lateral power switching transistors, pursuing GaN vertical power devices is still at an early stage. Among several challenges to achieve true avalanche breakdown vertical GaN power devices, the existence of impurities and intrinsic defects in the epi GaN drift layer is one major contributor for premature breakdown. For MOCVD grown unintentional doped (UID) GaN, the typical background doping is at low- 10^{16} cm^{-3} , which has significantly limited the breakdown voltage that can be achieved. Therefore, it is critical to develop MOCVD growth process to achieve high purity GaN drift layer with low background doping. In this work, GaN films were grown on top of free standing GaN substrate, using Trimethylgallium (TMGa) and NH_3 as precursors, H_2 as carrier gas, and V/III ratio of 3500. The growth temperature was optimized at 975 °C with a growth rate of $\sim 1.7 \mu\text{m/hr}$. A series of material characterization was

performed for the as-grown GaN epilayer grown on GaN substrate. The secondary ion mass spectroscopy (SIMS) depth profile revealed that the hydrogen and the oxygen concentrations are at the detection limit (10^{16} cm^{-3} , $1\text{-}2 \times 10^{16} \text{ cm}^{-3}$, respectively), while the uniform concentration of carbon and silicon are $1 \times 10^{16} \text{ cm}^{-3}$ and $1\text{-}2 \times 10^{16} \text{ cm}^{-3}$, respectively (the detection limit of carbon and silicon are $5 \times 10^{15} \text{ cm}^{-3}$, and $2 \times 10^{15} \text{ cm}^{-3}$, respectively). The low trace amount of impurities in the MOCVD grown GaN epilayer is key to prevent premature breakdown. Surface roughness for both GaN substrate and GaN epilayer was characterized via atomic force microscopy (AFM). The measured root mean square (RMS) for GaN substrate was 0.21 nm, while the RMS for the as-grown GaN epilayer was 0.095 nm for the scanning area of $1 \mu\text{m} \times 1 \mu\text{m}$. The epilayer thickness is about 7.7 μm . Capacitance-voltage (C-V) measurements were carried out to probe the free carrier concentration. CV curves at 1 MHz and 1 kHz were both obtained. The CV curve at 1 MHz kept relatively flat, which indicates the low level of free carrier concentration. The net carrier concentration was extracted from the CV curve at 1 kHz. The estimated free carrier concentration $N_A - N_D$ was at $\sim 1 \times 10^{15} \text{ cm}^{-3}$. This result indicates a low level of compensation exists in the as-grown GaN epilayer. More characterization of the films will be performed to understand the fundamental defects in the GaN epi-layer. In summary, high quality MOCVD GaN homoepitaxy on free standing GaN substrate was achieved with low background doping. Smooth surface with RMS $< 0.1 \text{ nm}$ was measured for an as-grown GaN epilayer. The results from this work promise the great potential of MOCVD GaN for high voltage vertical power device applications.

9:00 AM X03

(Student) AlInN for Vertical Power Electronic Devices Matthew R. Peart, Damir Borovac, Wei Sun, Nelson Tansu and Jonathan J. Wierer; Electrical and Computer Engineering, Lehigh University, Bethlehem, Pennsylvania, United States.

The benefits and challenges of AlInN as a next generation power electronic semiconductor using a theoretical analysis is presented. Initial device simulated and experimental data are also presented. $\text{Al}_x\text{In}_{1-x}\text{N}$ has many attractive properties for power devices such as being lattice matched to GaN at $x=0.82$, available GaN substrates, a wide bandgap ($\sim 4.4 \text{ eV}$), and high experimental mobility ($\sim 450 \text{ cm}^2/\text{Vs}$). To determine the figure-of-merit (FOM) of $\text{Al}_{0.18}\text{In}_{0.82}\text{N}$ analytically, the values of the critical electric field (E_c) and electron mobility (μ_n) are taken from Monte Carlo simulations [1] and experimental data [2]. For the $\text{Al}_{0.18}\text{In}_{0.82}\text{N}$ theoretical values two extreme data sets are used from Ref. [1] that assume full alloy scattering or no alloy scattering. This provides two sets of ionization rates and mobilities where alloy scattering results in lower mobilities and lower ionization rates. For experimental values $\mu_n \sim 450 \text{ cm}^2/\text{Vs}$ [2], and the E_c is estimated using the measured bandgap (E_g) and an equation based on a least squares fit of the known E_c and E_g for various semiconductors [3]. Fig. 1 shows a plot of R_{on} versus breakdown voltage for the measured and theoretical (with and without alloy scattering) values of AlInN as well as other wide bandgap semiconductors for comparison [3], [4]. The AlInN FOM spans from 18% - 130 % times greater than GaN, and the highest possible values are comparable to Ga_2O_3 and $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$. A vertical $\text{Al}_{0.82}\text{In}_{0.18}\text{N}$ power diode (Fig. 2a) is simulated using the Silvaco Atlas technology computer aided design (TCAD) software to reveal unique challenges of AlInN power devices using the measured E_c and μ_n values shown in Table 1. The TCAD model can account for the conduction band discontinuity and polarization fields across the GaN/AlInN heterointerface. These effects create band bending over long distances, a resulting thick depletion layer, and a large on-resistance. This depletion layer and resistance is reduced closer the analytical values by using a doping grade from 10^{19} cm^{-3} to 10^{16} cm^{-3} over 200 nm near the interface. The current versus voltage characteristics for the graded structure is shown Fig. 3 where $R_{on} \sim 14 \text{ m}\Omega\text{-cm}^2$ and breakdown voltage (V_{br}) is $\sim 13 \text{ kV}$. As a comparison, a GaN power diode with the same drift layer thickness and doping has a V_{br} of $\sim 4 \text{ kV}$. Of course, this V_{br} is a function of the drift layer thickness and doping and higher V_{br} are possible. The impact of using p-GaN instead of p- $\text{Al}_{0.82}\text{In}_{0.18}\text{N}$ is investigated and the impact of the heterointerface needs to be considered in the edge termination design. $\text{Al}_{0.82}\text{In}_{0.18}\text{N}$ has a FOM that exceeds that of GaN and is competitive with $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ and Ga_2O_3 . It also has additional benefits beyond these materials such as a lattice match substrate, the ability to dope n- and p-type, and high electron mobilities. In order to realize and precisely determine these high AlInN FOM values, experimental challenges will need to be overcome such as polarization fields and bandgap discontinuities at AlInN/GaN interfaces and doping control by lowering high levels of oxygen in the films. We present some initial results for devices with 300nm thick AlInN n- drift layers with GaN p+ layers demonstrating for the first time an AlInN p-n rectifier. The advantages of AlInN elucidated here should motivate further interest to tackle the

challenges faced in this material for power electronic applications.

References: [1] S. Shishehchi, F. Bertazzi, and E. Bellotti, *J. Appl. Phys.*, vol. 113, no. 20, pp. 0–9, 2013. [2] J. Zhang, et al., *J. Appl. Phys.*, vol. 109, no. 5, 2011. [3] J. L. Hudgins, et al., *IEEE Trans. Power Electron.*, vol. 18, no. 3, pp. 907–914, 2003. [4] J. Y. Tsao et al., *Adv. Electron. Mater.*, vol. 4, no. 1, 2018.

9:20 AM X04

(Student) Rectification in Vertically Conducting Power GaN-on-Si Heterojunctions Christopher M. Matthews¹, Brendan Gunning^{2,1}, Evan Clinton¹ and W. Alan Doolittle¹; ¹Georgia Institute of Technology, Atlanta, Georgia, United States; ²Advanced Materials Sciences, Sandia National Laboratories, Albuquerque, New Mexico, United States.

Gallium nitride (GaN) on silicon (Si) heterojunction devices have been grown and fabricated as the first step toward the realization of vertically conducting GaN on Si power semiconductor devices. Power diodes need low turn-on voltages in forward bias and high breakdown strength in reverse bias. We have measured these properties in one permutation of GaN on Si. Additionally, for other applications such as III-nitride-Si tandem solar cells, achieving vertical ohmic conduction across a GaN-Si interface is crucial. GaN on Si devices typically use an insulating buffer layer, most commonly AlN, between the nitride device stack and the Si substrate because GaN is more lattice matched to AlN [2.5% mismatch] than to Si [17% mismatch]. However, the AlN buffer is significantly more insulating, with a bandgap of 6 eV, than GaN, which has a bandgap of 3.4 eV. The main difficulties when growing GaN on Si include strain engineering due to the lattice and thermal mismatch, preventing the Si substrate from forming an insulating SiN when exposed to active nitrogen species, as well as controlling the Ga-Si eutectic which can result in harmful mixed phases. For these reasons, nucleation and growth of vertically conducting GaN on Si remains a challenge, and GaN grown directly on Si is generally of lower structural quality than GaN grown on other substrates or buffers. Four different permutations of n- and p-GaN and n- and p-Si have been grown and fabricated into large area 2 mm x 2 mm heterojunction diodes. The electrical behavior of the devices was measured and found to be highly dependent on the band alignment of the doped GaN-on-Si structures. Initial measurements comparing the four structures indicate p-GaN on p-Si devices tend to show rectification, while n-GaN on p-Si devices can have ohmic behavior. Other permutations have current blocking and/or highly resistive behavior. In the p-GaN/p-Si case, the heterojunctions have a low turn-on voltage of approximately 1 V. It is noted that some large area power devices withstand large voltages up to 160 V and offer promise for future power applications. The n-GaN/p-Si ohmic contact has a resistance of 14.95 Ω (0.6 Ω -cm²). The resistance of the bulk Si has been determined to be approximately 15 ohms, indicating that the device's resistance is dominated by the Si rather than the GaN/Si interface. These ohmic contacts may enable future heterojunction solar cells. SiLENSe™ simulations of the ideal band structures support the idea that rectifying barriers exist in p-GaN on n-type silicon devices, as indicated by the I-V characteristics. However, the p-GaN/p-Si band structure suggests an initially flat valence band that could be misaligned by bias. This is consistent with the low turn-on voltage, but it is not yet clear that this supports the rectification of the experimental structure. Likewise, simulations suggest a strong barrier next to a deep interface electron well for the n-GaN/p-Si and n-GaN/n-Si devices. Simulations under bias are forthcoming.

9:40 AM X05

(Student) Polarization Edge Termination for GaN Vertical Power Devices Matthew R. Peart and Jonathan J. Wierer; Electrical and Computer Engineering, Lehigh University, Bethlehem, Pennsylvania, United States.

In order to realize maximum breakdown voltages in GaN power devices, localization of the electric field must be prevented. This field localization results from crowding of the depletion layer under reverse bias that is due to finite size of the device, and it occurs at contact discontinuities or device edges. The most successful edge terminations in GaN power devices are formed by implantation-based methods to create junction terminations extensions (JTEs), field rings, and bi-layer structures [1]-[4]. III-nitrides have high piezoelectric and spontaneous polarization, and heterointerfaces can have large amounts of charge. Here a method of edge termination utilizing this polarization induced-charge is presented [5]. The polarization edge termination is demonstrated on a vertical GaN power diode and consists of a 5nm thick n-type AlGaIn layer on top of a p-type GaN layer that is located on the periphery of the main p-n junction. The spontaneous and piezoelectric polarization present in III-nitrides result in fixed charges at the AlGaIn/GaN heterointerface and the p-GaN layer becomes depleted at this interface under reverse bias. Numerical

simulations show this AlGaIn/GaN heterointerface can be engineered to control the depletion region under reverse bias to prevent localization of electric fields and premature avalanche breakdown. The simulated vertical p-n power junction consists of a 200 nm thick p⁺-type layer with a Mg concentration [Mg] of 2×10^{18} /cm³, a 10 μ m thick n-type drift layer with a Si concentration [Si] of 2×10^{16} /cm³, and a 2 μ m thick n-type contact layer with a [Si] of 10^{19} /cm³ on the bottom. Ohmic contacts are placed on either side with the top 20 μ m wide p-contact, only contacting the left-hand side. A nearly-intrinsic i-GaN layer is added with a donor density of 10^{15} /cm³ that simulates a deadening implant and creates a simple boundary condition at the edge of the device. The edge termination consists of a 5 nm thick Al_xGa_{1-x}N layer that is 70 μ m wide on top of the p⁺-GaN layer between the p-contact and the device edge. The Al_xGa_{1-x}N edge termination layer is doped n-type with [Si] at 10^{17} /cm³. In the simulation x is varied from 0 to 0.8 and the [Mg] is varied from 1.5×10^{18} /cm³ to 3×10^{18} /cm³ to change the polarization sheet charge or depletion width in the p⁺-GaN layer. The device is simulated using Silvaco Atlas TCAD software. The simulation demonstrates that when the charge and electric field is correctly balanced at the appropriate value of x for Al_xGa_{1-x}N then nearly parallel-plate reverse breakdown performance can be achieved. Al content at this optimum point results in peaked electric fields at the edges of the device or near the p-contact with lower breakdown voltages. Also, as the doping or thickness in the p⁺ or n⁻ regions are changed, the polarization charge required to correctly balance the space charge changes and thus the optimal value of x also shifts. Finally, simple analytical models that account for charge balancing at breakdown predict the same optimum Al content as the TCAD model. **References:** [14] I. C. Kizilyalli, et al., *IEEE Electron Device Lett.*, vol. 36, no. 10, pp. 1073–1075, Sept. 2015. [28] J. J. Wierer, et al., *IEEE Trans. Electron Devices*, vol. 64, no. 5, pp. 2291–2297, March 2017. [39] J. R. Dickerson, et al., *IEEE Trans. Electron Devices*, vol. 63, no. 1, pp. 419–425, Dec. 2015. [410] I. C. Kizilyalli, et al., *IEEE Trans. Electron Devices*, vol. 60, no. 10, pp. 3067–3070, June 2013. [5] M. Peart, et al., *IEEE Electron Device Lett.*, Under Review

10:00 AM REFRESHMENT BREAK

10:20 AM X06

(In,Ga)N LEDs with Remote P-GaN:Mg Regions—Demonstration of a Novel P-Doping Approach Chirag Gupta, Yuuki Enatsu, Stacia Keller and Umesh Mishra; ECE, University of California, Santa Barbara, Santa Barbara, California, United States.

P-type conductivity in III-Nitrides is typically obtained by Mg doping. Using p-type GaN:Mg, numerous devices have been demonstrated. However, the high activation energy of Mg (in GaN ~160 meV), typically results in only ~1% ionization of Mg atoms at 295K. This problem is further exacerbated by hydrogen passivation of Mg during MOCVD growth and/or processing steps [1-4]. This severely impedes the device design space, and it is therefore desirable to develop a technique to obtain p-type layers without Mg doping. The polarization fields present in c-plane (Al,Ga,In)N can be utilized to address these concerns. By spreading the polarization fields via grading, negative charges can be created that are then neutralized by holes from a hole supplying region. Thus a p-type layer free of Mg doping can be obtained [1-4]. In our previous work, a Mg doped p-type capping layer was necessary to provide the holes in the undoped graded InGaIn layer beneath [3, 4]. In this study we demonstrate that p-GaN:Mg does not need to cover the entire graded InGaIn layer. Instead, the p-type hole supply material can be provided in a small region to serve as hole supply for the entire graded InGaIn layer. LED structures grown with graded un-doped InGaIn as p-type layer and with a selectively regrown p-GaN:Mg covering an area of 2500 μ m² demonstrated uniform light emission over an area as large as 15000 μ m², 6 times the area covered with p-GaN:Mg. The LED structures with 5 period (In_{0.15}Ga_{0.85}N/GaN) MQWs were grown by MOCVD on bulk GaN substrates. The p-type region was composed of 100 nm linearly graded undoped InGaIn with an alloy composition from 0 to 5% [3, 4]. Three LED samples were prepared. For the first sample, following the graded InGaIn layer, a 40nm thick p-GaN layer was grown *in-situ* to act as the hole supply layer. The same *in-situ* growth was performed for the second sample, however, the p-GaN was etched selectively after growth to allow for the remaining p-GaN (over an area *A*) to act as hole supply for a significantly larger area (up to 20*A*). For the third sample, to avoid dry etch damage, selective area regrowth was employed to deposit p-GaN:Mg over area *A*. Thick Ni/Au was deposited as the p-type contact on p-GaN (over area *A*) and for probing the LEDs. Thereafter, a thin Ni/Au (4nm/5nm) layer was additionally deposited over a larger area (up to 20*A*) thus defining the LED area. As expected, uniform light emission was observed for the reference sample with p-GaN deposited over the entire LED area ranging from *A* to 20*A*. The second LED sample fabricated with partially etched p-GaN

layer over the LED area ($A-20A$) demonstrated emission only at the edge of the p-GaN layer (area A) and no light emission was observed from the remaining LED area ($A-20A$). This indicates that the plasma damage was detrimental to either the MQW underneath and/or to the flow of holes from the p-GaN layer to the graded InGaN region. The third LED sample with regrown p-GaN over an area A of $50 \times 50 \mu\text{m}^2$ demonstrated the following results: LEDs up to an area of $150 \times 100 \mu\text{m}^2$, corresponding to an area 6 times larger than the area covered with p-GaN, demonstrated uniform light emission. However, for LEDs larger than the $6A$ area, non-uniform light emission was observed. Further improvements in light emission over areas larger than $6A$ can be expected with optimized regrowth and improved ohmic contacts. This experiment clearly demonstrates that graded layers in combination with a “remote” hole supply region can be utilized to obtain a p-type conductivity in III-Nitrides. This technique is particularly useful for obtaining buried active p-type layers for electronic devices and for long wavelength LEDs with limited thermal budget due to high Indium alloy composition in quantum wells. [1] J. Simon *et al* 2010 Science **327**, 60; [2] L. Zhang *et al* 2010 *Appl. Phys. Lett.* **97** 062103; [3] Y. Enatsu *et al* 2016 *Appl. Phys. Express* **9** 075502; [4] Y. Enatsu *et al* 2017 *Semicond. Sci. Technol.* **32** 105013.

10:40 AM X07

Ion Implantation and Activation in GaN James C. Gallagher¹, Travis J. Anderson¹, Andrew D. Koehler¹, Geoffrey Foster¹, Alan G. Jacobs², Boris N. Feigelson¹, Michael Mastro¹, Jennifer K. Hite³, Karl Hobart¹ and Fritz J. Kub¹; ¹U.S. Naval Research Laboratory, Washington, District of Columbia, United States; ²US Naval Research Lab, Washington, District of Columbia, United States; ³US Naval Research Laboratory, Washington, District of Columbia, United States.

Many GaN devices require selective-area n-type and p-type doping. These include n-type Si doping to reduce contact resistance in RF HEMTs and p-type Mg doping for the body and termination of vertical power switches. Use of ion implantation and activation should in theory use less steps than the selective area regrowth technique. One challenge of using the ion implantation technique is that it requires temperatures high enough to destabilize and decompose the GaN. Previous studies [1], [2] have shown that the decomposition can be minimized using a protective AlN cap, a N_2 overpressure, and a Symmetric Multicycle Rapid Thermal Annealing (SMRTA) process [3]. This study reports the effects of annealing conditions on the ion activation and defect formation in Si and Mg doped GaN. To study Si activation, ions were implanted in semi-insulating carbon doped GaN grown on SiC. The samples were capped with AlN and activated using both conventional RTA at atmospheric pressure and using a N_2 overpressure. After stripping the AlN cap and depositing ohmic Results show similar levels of Si activation using both annealing conditions; however, the atmospheric pressure annealing leads to the formation of low activation energy defects likely from nitrogen vacancies. Using a 30 atm overpressure prevents such formations from leaving the unimplanted regions semi-insulating, and preserving the breakdown voltage. We found that annealing at the ideal temperature of 1075°C yields a low contact resistivity 2×10^{-8} ohm-cm². The activation of Mg ions has been recently reported and requires in GaN using the SMRTA method in an overpressure at temperatures above 1500°C [3], [4]. Further optimization is required before this process is viable. For this project, we tested the effects of ion activation temperature, ion implantation dose, AlN cap structures, and post activation surface treatment on the electrical, optical, and structural properties of the p-type region. The results will be discussed. [1] J. D. Greenlee, T. J. Anderson, B. N. Feigelson, V. D. Wheeler, K. D. Hobart, and F. J. Kub, “Comparison of AlN Encapsulants for Bulk GaN Multicycle Rapid Thermal Annealing,” *ECS J. Solid State Sci. Technol.*, vol. 4, no. 12, pp. P403–P407, Sep. 2015. [2] J. D. Greenlee, T. J. Anderson, B. N. Feigelson, S. H. Chan, S. Keller, and M. Tahhan, “Characterization of a selective AlN wet etchant,” *Appl. Phys. Express*, vol. 8, p. 036501, 2015. [3] M. J. Tadjer *et al.*, “Selective p-type Doping of GaN:Si by Mg Ion Implantation and Multicycle Rapid Thermal Annealing,” *ECS J. Solid State Sci. Technol.*, vol. 5, no. 2, pp. P124–P127, Dec. 2016. [4] T. J. Anderson, J. D. Greenlee, B. N. Feigelson, J. K. Hite, K. D. Hobart, and F. J. Kub, “Improvements in the Annealing of Mg Ion Implanted GaN and Related Devices,” *IEEE Trans. Semicond. Manuf.*, vol. 29, no. 4, pp. 343–348, Nov. 2016.

11:00 AM X08

Topological and Electrical Effects of Annealing Capped GaN Films Michael A. Derenge, Kenneth A. Jones and Randy P. Tompkins; RDRL-SED-E, Army Research Lab, Adelphi, Maryland, United States.

It is important to be able to locally dope GaN because it can be used to lower its contact resistance; it should be particularly useful for p-type material since the acceptor depths are deep. Because it is necessary to

anneal the GaN to activate the implanted dopants, it is important to know how the process is affected by the annealing temperature, T_A , and time t_A , and the quality of the GaN film. One obvious problem is the preferential evaporation of N, which creates hexagonal pits, as well as N vacancies, N_V , that are known to be donors that could compensate the activated p-dopants. We utilize an AlN annealing cap to reduce the N escaping kinetics so we also examine how its structure, as well as the stresses generated by the lattice mismatch and differences in the thermal coefficient of expansion, TCE, between the cap and the film, as well as between the sapphire substrate and the film, affect the film’s properties. In this paper we explore the effects of varying T_A and t_A using a dual AlN cap to protect the surface of (0001) GaN films grown on sapphire. We qualitatively examine how the stresses produced by thermal cycling affect the film by making measurements near the edges and closer to the center where the stresses are larger. Changes in the surface roughness of both the AlN cap and the GaN film with the capped etched off are recorded using AFM, and changes in the electrical properties are determined using CV and iV measurements made on Schottky diodes fabricated on the samples. The surface topographs provide insight into the thermally induced movement of surface atoms and structural defects near or at the surface. Forward and reverse bias characteristics, and carrier concentration (n_0) distributions are interpreted in terms of possible electrically active point defect creation. We show that the GaN films can be annealed up to a T_A of 1300°C for a t_A as long as 8 minutes without forming large hexagonal thermal etch pits, but a detectable surface deterioration can occur even when the cap adheres well. There are substantial changes in the electrical properties of the Schottky diodes fabricated on them. In some cases the surface appears to begin to deteriorate at threading edge dislocations that form small angle grain boundaries created by polygonization during the annealing process as is suggested by the thermal etch pits aligned along $\langle 11\bar{2}0 \rangle$ directions that are observed in AFM topographs of samples annealed for shorter t_A at lower T_A . It is likely that the etch pits are formed by the preferential evaporation of N. This produces defects with donor-like properties near the surface, as is suggested by the shorter depletion layer widths in the CV measurements. These CV curves show that the n_0 increases towards the surface and increases at higher temperatures and longer times. The annealing has an initial positive effect, as the conductance, G , above the voltage knee, V_K , increases with T_A up to 1250°C with the shorter time anneals and up to 1200°C when they are longer. This is likely due to an increase in the mobility caused by the annealing out of some crystalline defects, as at the higher T_A and longer t_A G drops possibly because some of the N_V created by the annealing create N_V^- complexes. The G_K , the G below V_K , increases as T_A and t_A increase suggesting there is a donor induced forward leakage current. The effect is much more pronounced for reverse leakage currents as they increase orders of magnitude even for the lower T_A and shorter t_A are used. AFM from the center shows more deterioration than the edge. That there is considerable compressive stress in the film is shown by the positive shift in V_K of ~ 0.3 V produced by the piezoelectric induced charge. For the samples with the smooth surfaces the diodes in the center of the sample where the stresses are higher tend to have a smaller G above V_K , larger G_K below V_K , larger reverse leakage current, and larger n_0 at the higher T_A and longer t_A than those near the edge.

11:20 AM X09

Bevel Junction Termination in GaN Devices to Reduce Peak Electric Fields Using 3D Nanoprinting of Grayscale Features Geoffrey Foster^{1,2}, Andrew D. Koehler¹, James C. Gallagher^{1,2}, Joseph G. Tischler¹, Travis J. Anderson¹, Karl Hobart¹ and Fritz J. Kub¹; ¹U.S. Naval Research Laboratory, Washington, District of Columbia, United States; ²American Society for Engineering Education, Washington, District of Columbia, United States.

Electric field crowding in lateral and vertical GaN devices reduces the breakdown voltage compared to the maximum theoretical value, limiting the performance and reliability of these devices. Conventional photolithography results in binary definition of features, where square corners can cause electric field lines to crowd at the junction edge. However, grayscale lithography can define tapered features in the photoresist, which can then be transferred to the device structure to mitigate peak electric fields at the edges of features. 3D nanoprinting is used to form grayscale features on GaN devices to reduce electric field crowding, thereby extending their breakdown voltages. An example is reducing the peak electric field at the semiconductor surface of vertical GaN devices using a bevel-edge junction termination extension (JTE). The bevel-edge JTE is formed by transferring a 3D nanoprinted resist profile into the GaN using Cl_2 inductively couple plasma (ICP) reactive ion etching (RIE). Bevel-edge JTEs on GaN PN diodes will be constructed with negative bevel termination schemes. Maskless 3D nanoprinting lithography via a two-photon process allows for patterning of arbitrary 3D shapes into resist [1]. The Nanoscribe Photonic Professional GT allows for

3D micro and nano structures to be patterned in resist based on the concept of “direct laser writing”. The Nanoscribe is used for developing grayscale features to reduce peak electric fields in GaN PN diodes [2]. To demonstrate the potential of the 3D nanoprinting technology to form bevel-edge JTE for vertical GaN devices, PN epitaxy is grown on native GaN substrates. The N-type region is doped to $\sim 1 \times 10^{16} \text{ cm}^{-3}$ with a thickness of 10 μm . The P-type region is doped to 1×10^{18} . Vertical GaN PN diodes are fabricated by first evaporating Ohmic metal on the backside of the N+ GaN substrate and annealing at 800C in N₂ to form the cathode contact. Lifting off circular Ohmic contacts to the P-type region forms the anode. Then, IP-Dip photoresist is 3D nanoprinted to serve as the etch mask for Cl₂ ICP RIE. For this GaN PN diode, a bevel angle of 1.875° and length = 12.2 μm is required to reduce peak electric field by 50%. Etch selectivity between GaN and the IP-Dip photoresist was found to be 0.598 to create the bevel edge JTE with correct aspect ratios. Three structures were measured, the JTE, a 200 μm mesa, and a 150 μm mesa (same size as metal). The small mesa showed a large leakage current, while the JTE and large mesa had small leakage current. Breakdown voltages were observed to be between 90V and 140V for the large and small mesa, and between 390V and 420V for the JTE. Breakdown voltage is likely limited to defects and not surface field, but the JTE shows a clear improvement in breakdown voltage. **References** [1] N. Anscombe, “Direct laser writing” *Nature Photonics* **Volume 4**, pages22–23 (2010) [2] J. Balagia, “Power Semiconductor Devices” ISBN-13: 978-0534940980, 1995.

11:40 AM X10

Implanted Mg Activation in Ga- and N-Polar GaN Alan G. Jacobs¹, Boris N. Feigelson¹, Jennifer K. Hite¹, Cameron A. Gorsak², Lunet E. Luna¹, Travis J. Anderson¹ and Fritz J. Kub¹; ¹US Naval Research Laboratory, Washington, District of Columbia, United States; ²Physics, University of Notre Dame, Notre Dame, Indiana, United States.

Here we present a direct comparison between the activation in implanted Mg ions in N- polar and Ga- polar GaN substrates to produce p-type GaN via Symmetric Multicycle Rapid Thermal Annealing (SMRTA). Physical dopant activation was achieved by annealing in moderate nitrogen pressures (3.3 MPa), to extend thermodynamic stability by $\sim 100 \text{ K}$, with a bi-layer Si₃N₄ and AlN cap structure, and short temperature pulses ($< 5 \text{ s}$) to temperatures in excess of 1300 °C coupled with longer periods of annealing near 1000 °C. Implantation damage was fully removed during annealing as measured by Raman spectroscopy and High Resolution X-ray Diffraction. Both the Raman E₂^{HT} and the (0002) rocking curve FWHMs were reduced compared to as-grown material after implantation and annealing. Low-temperature photoluminescence (LTPL) at $\sim 80 \text{ K}$ clearly shows development of UV luminescence associated with magnesium activation but with dependence on GaN film polarity. Activation was more readily achieved for N- polar films with measured UV luminescence up to $\sim 15 \times$ as intense as yellow/green luminescence compared to $\sim 2.4 \times$ for Ga-polar films. The greater activation of N- polar material was primarily due to a higher thermal stability compared to Ga- polar films. This demonstration of implanted Mg activation by SMRTA enables a facile route toward next generation vertical devices.

SESSION Y: Gallium Oxide Defects and UV Optoelectronics Materials

Session Chairs: Sriram Krishnamoorthy and Shin Mou

Thursday Morning, June 27, 2019

Rackham Building, 4th Floor, Assembly Hall

8:20 AM Y01

Atomic Scale Characterization of Point Defects and Their Complexes in $\beta\text{-Ga}_2\text{O}_3$ Using Scanning Transmission Electron Microscopy Jared Johnson¹, Zhen Chen², Joel B. Varley³, Christine Jackson¹, Farzana Esmat¹, Aaron R. Arehart¹, Hsien Lien Huang¹, Steven A. Ringel¹, Chris G. Van de Walle⁴, David Muller² and Jinwoo Hwang¹; ¹The Ohio State University, Columbus, Ohio, United States; ²Cornell University, Ithaca, New York, United States; ³Lawrence Livermore National Laboratory, Livermore, California, United States; ⁴Materials Department, University of California, Santa Barbara, Santa Barbara, California, United States.

$\beta\text{-Ga}_2\text{O}_3$, with its unique properties and advantages, provides promising opportunities to develop new-generation ultra-wide band gap (UWBG) materials and devices. There are, however, important issues revolving $\beta\text{-Ga}_2\text{O}_3$, such as the unknown origins of intrinsic n-type doping, low doping efficiency, difficulty in p-type doping, and electronic trap states. Tackling these outstanding issues critically requires better understanding of point defects. However, what has been missing in the field is the detailed physical picture describing the exact structure of point defects, including their types, distribution, and incorporation into the lattice. Gaining such detailed information is crucial to connect the theoretical calculations to the experimentally measured properties. Here, we present the direct observation of individual cation interstitials and their complexes in $\beta\text{-Ga}_2\text{O}_3$ using high resolution scanning transmission electron microscopy (STEM). Using the atomic level spatial resolution and precision of STEM, we directly determined the preferred sites for cation interstitials, and confirmed the formation of their complexes with cation vacancies that have been predicted by density functional theory (DFT) calculations. STEM of multiple bulk $\beta\text{-Ga}_2\text{O}_3$ samples with different Sn doping level revealed that Sn doping facilitates the formation of these cation interstitial – divacancy complexes. Three-way comparison between STEM, DFT, and defect spectroscopy data confirms that the observed defect complexes must be the origin of the defect trap detected at E_c - 2.16 eV. Our STEM data therefore delivers new experimental information about the atomic scale structure of point defects that can be directly compared to the atomic scale simulations and measured physical characteristics, which brings a new powerful way to understand and control the properties of $\beta\text{-Ga}_2\text{O}_3$ to advance them to novel UWBG applications.

8:40 AM Y02

(Student) Neutron Irradiation and Thermal Anneal Impact on Ga₂O₃ Deep Level Defects Hantian Gao¹, Shreyas Muralidharan¹, Md Rezaul Karim², Susan M. White⁵, Lei Cao⁵, Kevin Leedy³, Hongping Zhao⁴, David Look⁶ and Leonard Brillson^{1,2}; ¹Physics, The Ohio State University, Columbus, Ohio, United States; ²Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ³Air Force Research Laboratory, Wright-Patterson AFB, Ohio, United States; ⁴Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ⁵Nuclear Reactor Lab, The Ohio State University, Columbus, Ohio, United States; ⁶Semiconductor Research Center, Wright State University, Dayton, Ohio, United States.

Ga₂O₃ has been considered a promising material for next generation high power devices due to its wide band gap enabling very high breakdown fields and n-type doping ranging from intrinsic to degenerate, both features of which lead to numerous solid-state electronic applications. Native point defects play important roles in changing the electronic properties of Ga₂O₃ by compensating free carriers, reducing their mobilities, “pinning” Fermi level and Schottky barriers, and forming trap states to initiate breakdown. However, native point defects and their detailed configurations have still been relatively unexplored in Ga₂O₃. In this work, we used a unique combination of surface-sensitive spectroscopy techniques, including depth-resolved cathodoluminescence spectroscopy (DRCLS), and surface photovoltage spectroscopy (SPS) together with a series of bulk/surface treatments, including neutron irradiation, thermal anneal, and gallium ion deposition to study and control point defects within the outer tens of nanometers of Ga₂O₃ grown by various methods. Moreover, with electrical Hall effect measurement, we are able to correlate changes of native point defects with donor/acceptor profiles. In DRCLS, all four growth methods

exhibit common optical features at 2.5 eV, 3.0 eV, 3.5 eV and 3.8 eV respectively. By doing a series of neutron irradiations with various dosages, we observed systematic increases of the 2.5 eV and 3.0 eV features, leading to identification of two possible V_{Ga} related energy levels in the band gap. To further study the detailed configuration of both features, forming gas (97% He and 3% H₂) anneal was performed on the LPCVD grown Ga₂O₃ sample. The effect of this forming gas anneal is to increase the intensity of the 2.5 eV feature toward the surface, suggesting such feature could be related to indiffusion of H and additional V_{Ga} -H complex formation, as previous proposed¹. Further study of Ga deposition and electron paramagnetic resonance (EPR) would provide additional microscopic evidence. In contrast, thermal anneal in N₂ increase the 3.5 eV peak intensity toward the surface, which further confirms the V_{O} -related nature of such feature we reported previously¹. With surface and bulk physical/chemical processing techniques, we are able to change native point defects in Ga₂O₃. DRCLS permits us to measure how such defect features are removed or created by those processes, leading to better understanding of their physical nature and configurations in Ga₂O₃. This study suggests a new avenue for monitoring and controlling native point for electronic applications not only in Ga₂O₃, but in other semiconductors as well. The authors gratefully acknowledge support from AFOSR Grant No. FA9550-18-1-0066 (A. Sayir)¹ H. Gao, *et al.*, *Appl. Phys. Lett.* **122**, 242102 (2018).² J. B. Varley, *et al.*, *Appl. Phys. Lett.* **97**, 142106 (2010).³ Z. Zhang, *et al.*, *Appl. Phys. Lett.* **108**, 052105 (2016).

9:00 AM Y03

Investigation of Extended Defects in 20 μ m Thick β -Ga₂O₃ Epilayer Using Ultraviolet Photoluminescence Imaging and X-Ray Topography
Nadeemullah Mahadiq¹, Robert Stahlbush¹, Marko Tadjer¹, Karl Hobart¹, Peter L. Bonnano¹ and Akito Kuramata²; ¹Naval Research Laboratory, Washington, District of Columbia, United States; ²Novel Crystal Technology, Saitama, Japan.

Interest in β -Ga₂O₃ is emerging to fabricate certain classes of power electronics such as power converters with capabilities beyond existing technologies, due to its large bandgap (4.8eV) and the availability of large diameter (6 inch), relatively inexpensive substrates grown from the melt. However, the growth technology for substrates and epilayers is relatively in early stages compared to the more mature GaN and SiC technologies, and the role of extended defects on device performance is not well known. Extended defects such as threading and basal plane dislocations influence the device performance by degradation of its breakdown voltage and can also effect on-state resistance. There have been a few reports on defect identification using microscopy techniques such as TEM and SEM [1,2]. However, identification and analysis of defects on a more global scale is required to correlate with device performance and yield. Imaging of such defects is crucial in order to investigate their origins and correlate with growth conditions, in order to mitigate them in both the substrates and epilayers. In this work, we investigate extended defects in 20 μ m thick, (001) oriented, β -Ga₂O₃ epilayers grown by halide vapor phase epitaxy on edge-defined film-fed growth β -Ga₂O₃ substrates using ultraviolet photoluminescence (UVPL) imaging technique for the first time, and correlate with high resolution synchrotron x-ray topography (HRXRT) imaging. UVPL imaging was performed by exciting the defect states with 355nm laser illumination and the imaging conditions were varied to enhance defect contrast. HRXRT was performed using 15keV x-rays, and using three Bragg diffraction conditions. Threading screw, edge, and basal dislocations were distinguished in HRXRT images using the $g \cdot b$ criterion. The threading screw type dislocations, which are in the growth direction, appeared to be large core resembling nanopipes. These defects were also observed in the UVPL images, with additional single tilted threading dislocations found that were not resolved in the HRXRT images. The dislocation density of the nanopipes were 30 cm⁻², and basal dislocations were \sim 20 cm⁻². The threading dislocation density varied greatly across the sample from 0-3000 cm⁻² as seen in the UVPL imaging. Additionally, a low angle grain boundary was also observed in the films. Using the laser excitation at high power densities, greater than 50 Wcm⁻², we also observed formation of micro-cracks in the sample, which then could be propagated throughout the sample and cause sample cleaving. Observation of possible dislocation motion was also observed in the UVPL imaging. A comparison and analysis of various extended defects and their possible origins will be presented. References: [1] Villora et. Al., *Mater Res Bull*, 37, 769, (2002) [2] Nakai et. Al., *Jpn. J. Appl. Phys.*, 54, 051103 (2015)

9:20 AM Y04

(Student) A Study of the Interface of β -Ga₂O₃ with Ti/Au Contacts
Ming-Hsun Lee¹ and Rebecca L. Peterson²; ¹Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; ²Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

Monoclinic β -Ga₂O₃, a next-generation wide bandgap semiconductor, is promising for high power and high frequency electronics applications. To develop Ga₂O₃-based power devices, it is critical to identify ohmic electrodes with low specific contact resistance as well as thermally-stable interfaces that do not suffer from degradation. To date, most reported ohmic contacts on Ga₂O₃ are based on Ti interfacial adhesion layers. From thermodynamics, the favored reactions at the interface can be predicted: the Ti/Ga₂O₃ interface is predicted to result in oxidation of Ti and reduction of Ga₂O₃. Therefore, here we investigated the interfacial reactions and interdiffusion of titanium/gold ohmic contacts with a tin-doped single-crystal β -Ga₂O₃ (010) substrate [1]. After rapid thermal annealing (RTA) at 470°C in N₂ for 1 minute to form an ohmic contact, we examined the interface via scanning/ transmission electron microscopy (S/TEM) with Energy Dispersive X-ray Spectroscopy (EDX) as well as Electron Energy Loss Spectroscopy (EELS). We demonstrate that even after a very brief (1-min) 470°C anneal, Au and Ti suffer from significant interdiffusion. After RTA, the highest Ti concentration is found in a thin (\sim 5nm) layer of Ti-TiO_x near the interface. A portion of this Ti-TiO_x layer is lattice matched with β -Ga₂O₃. The remainder of the Ti has diffused into the adjacent Au and Ga₂O₃ layers. Below the Ti-TiO_x layer, there is a 3-5 nm defective β -Ga₂O₃ layer that has non-negligible Ti incorporation, while preserving the monoclinic structure. Above the Ti-TiO_x layer, a layer of intermixed Au-Ti exists with a layer of Ti-rich nanocrystallites (radius \sim 2 nm) embedded within it. Via chemical mapping, electron microscopy imaging, and selected area diffraction patterns, we confirm the multilayer structure. The thermodynamic favorability of the observed redox processes are analyzed quantitatively by calculation of Gibbs free energies of the reactions. Based on these observations, we propose possible reasons for ohmic contact formation at the Ti/Au - β -Ga₂O₃ interface: (a) the interdiffusion of Ti and Au; (b) the formation of a thin Ti-TiO_x layer, which aids band alignment; and (c) the formation of a lattice matched defective Ga₂O₃ layer and Ti-TiO_x layers adjacent to crystalline β -Ga₂O₃, which may facilitate the transport of carriers. Such a physical understanding of Ti/Au metallization can provide insights for future materials selection for thermally- and electrically-stable contacts in β -Ga₂O₃ power devices. [1] M.-H. Lee and R. L. Peterson, "Interfacial Reactions of Titanium/Gold Ohmic Contacts with Sn-doped β -Ga₂O₃," *APL Materials* **7** (2): 022524 (2019).

9:40 AM Y05

(Student) Towards Using Ion Implantation for Controlled Exfoliation of β -Ga₂O₃
Michael E. Liao, Tingyu Bai, Yekan Wang and Mark Goorsky; Materials Science & Engineering, University of California, Los Angeles, Los Angeles, California, United States.

In this work, (010) β -Ga₂O₃ substrates were implanted with hydrogen ions (H⁺) at a dose of 1.2×10^{17} cm⁻² and subsequently annealed. Ion implantation can be used for exfoliating thin layers of a material and has been demonstrated previously with silicon,¹⁻³ III-V's,^{4,7} and II-VI's.⁸ In this method, hydrogen or helium ions are implanted in a handle substrate and then subsequently annealed. The implanted ions diffuse and agglomerate during annealing, and surface blistering or exfoliation occurs under the appropriate processing conditions. Previously, another method of exfoliating thin layers of β -Ga₂O₃ had been achieved using a mechanical approach that exfoliates material parallel to the (100) and (001) cleavage planes.^{9,10} However, this mechanical approach will be challenging to integrate in the large-scale processing setting since only millimeter-scale areas have been achieved. The ion implantation approach, on the other hand, is highly compatible with large-scale processing since large "blanket" layers can be exfoliated. Additionally, exfoliation along non-cleavage planes can be achieved, which is a degree of freedom especially important for β -Ga₂O₃ since its materials properties are anisotropic due to its low-symmetry monoclinic crystal structure. Both high-resolution X-ray diffraction (XRD) measurements and transmission electron microscopy (TEM) images were employed to study the structural evolution with annealing in the implanted β -Ga₂O₃ substrates. Since ion implantation induces strain into the implanted substrate's subsurface region, symmetric (020) ω :2 θ XRD scans were measured. The ω :2 θ scans show that annealing at temperatures of 150 °C for 8 hours and then subsequently 300 °C for 16 hours shows a slight change in the strain present in the sample. However, strain fringes were still present indicating that a substantial amount of strain had not yet been removed. Subsequently annealing the same sample at 500 °C for 1 hour was sufficient in removing this strain. ω

scans were also measured before and after each annealing step and it was observed that the peak width widens after each anneal step. This peak widening in the ω scans corresponds to subsurface diffusion of the hydrogen ions and hydrogen agglomeration. TEM images were taken at the implantation region and showed subsurface hydrogen void formation after annealing, which is consistent with the measured ω scans. Before any annealing no voids were observed while after annealing at 500 °C hydrogen voids were present and had an average size of 9 nm. The evidence thus far demonstrates that ion implantation provides a promising approach for exfoliating thin layers of β -Ga₂O₃. References 1. M. Bruel, et al., Jpn. J. Appl. Phys. 36, 1636 (1997) 2. C. M. Varma, Appl. Phys. Lett. 71, 3519 (1997) 3. C. Miclaus, et al., J. Phys. D: Appl. Phys. 36, A177 (2003) 4. S. Hayashi, et al., Appl. Phys. Lett. 85, 236 (2004) 5. S. Hayashi, et al., J. Electrochem. Soc. 153(12), G1011 (2006) 6. S. Hayashi, et al., J. Electrochem. Soc. 154(4), H293 (2007) 7. E. Padilla, et al., ECS Trans. 33(4), 263 (2010) 8. C. Miclaus, et al., J. Electron. Mat. 34(6), 859 (2005) 9. Y. Kwon, et al., Appl. Phys. Lett. 110, 131901 (2017) 10. M. J. Tadjer, et al., Mechanical Exfoliation of Large Area (100) β -Ga₂O₃ Onto Arbitrary Substrates for High Power Devices, ECS (2017)

10:00 AM REFRESHMENT BREAK

10:20 AM Y06

(Student) Effect of Hydrogen Annealing on Schottky Contacts to (-201) β -Ga₂O₃ Ryan Bunk¹ and Jerry M. Woodall²; ¹Electrical and Computer Engineering, University of California, Davis, Davis, California, United States; ²ECE, University of California, Davis, Davis, California, United States.

In the last few years there have been great strides made in β -Ga₂O₃ photonic and power devices, however due to the unipolar nature of this material many devices rely upon Schottky contacts to function. Thus, a large effort has been made to study the behavior of these contacts, such as barrier height and ideality factor of different metals, as well as their breakdown voltages. Additionally, methods of improving the quality of Schottky contacts have been explored, such as oxygen radicals or plasma, as well as some halogen-based passivation. A topic of recent interest is the use of hydrogen in passivation of Ga₂O₃, as it is found to react with open Ga and O bonds to form Ga-H and O-H bonds. Most studies of hydrogen annealing demonstrate an increase in the carrier concentration, along with a change in defect density, but few show the end result on device characteristics. Here, we demonstrate a significant improvement in the current-voltage characteristics of a Ga₂O₃ Schottky diode using a relatively low temperature annealing in hydrated forming gas (HFG). The presence of water vapor is found to further improve the characteristics of the Schottky diode, which is believed to be due to inhibiting the direct reduction of Ga₂O₃ by H₂. Further details will be presented at the conference.

10:40 AM Y07

Vacuum Ultraviolet Light Emission from MgZnO-Based Thin Films and Quantum Wells Kentaro Kaneko¹, Kyohei Ishii¹, Mizuki Ono², Kanta Kudo², Takeyoshi Onuma², Tohru Honda² and Shizuo Fujita¹; ¹Electronic Science and Engineering, Kyoto University, Kyoto, Japan; ²Department of Applied Physics, Kogakuin University, Hachioji, Japan.

Exploration of short-wavelength semiconductor light emitters is a challenging issue in order to substitute present gas-sources. III-nitride semiconductors are the promising frontier materials, but the shortest wavelength available lies in ~210 nm, corresponding to the band gap of AlN (~6.0 eV). From this point of view, our attention has been focused on MgZnO, whose maximum band gap is ~7.8 eV[1], aiming at vacuum ultraviolet luminescence (< 200 nm). Mg₂Zn_{1-x}O films with high Mg contents (x>0.7) were grown on MgO (001) substrates by the mist CVD method [2]. The x-ray and electron-beam diffraction revealed rocksalt structure without noticeable incorporation of other phases. The x-ray diffraction rocking curves tended to be narrower for the higher Mg contents in MgZnO, because of lowered lattice mismatch to MgO substrates. The growth mode was three dimensional as evidenced by the step-terrace structures with the step height of 0.21 nm, which corresponds to the mono-atomic layer height, by means of the AFM observation. The TEM observation showed that the dislocation defects in MgO substrates penetrated into the MgZnO layers but the generation of dislocation defects from the MgZnO/MgO interface was hardly seen. Optical properties of samples were characterized by optical transmission spectroscopy and CL study with the acceleration beam energy of 5 kV at 6-300 K. For Mg₂Zn_{1-x}O films with x=0.95 and 0.92, CL peaks appeared at 199 and 212 nm at 6 K and at 205 and 207 nm at 300 K, respectively, without noticeable luminescence at the longer wavelengths. For the sample of x=0.95, the spectrally integrated CL intensity at 300 K over that at 6 K (I_{300}/I_6), which

is supposed to be the internal quantum efficiency at 300 K, was about 3.2%. However, the luminescence peak energies were lower by 0.5-0.7 eV than the band gap energies. This large Stokes-like shift is attributed to the local band gap fluctuation [3] Efforts were continued to fabricate MgZnO/MgO quantum wells. In their CL spectra, the main peaks were around 200 nm, and the peak positions showed apparent blueshift with decreasing the quantum well thickness. This may be associated with quantum effects, on which our research will be focused in the future. [1] R. C. Whited and W. C. Walker, Phys. Rev. Lett. 22, 1428 (1969). [2] K. Kaneko et al., Appl. Phys. Express 9, 111102 (2016). [3] T. Onuma et al., Appl. Phys. Lett., 113, 061903 (2018).

11:00 AM Y08

(Student) UV Photodetectors Based on (Al,Ga,In)₂O₃-Alloy Films Luke A. Lyle¹, Serdal Okur⁶, Joshua Letton², Venkata S.N. Chava³, Robert F. Davis¹, Gary Tompa⁵, MVS Chandrashekar² and Lisa Porter⁴; ¹Materials Science and Engineering, Carnegie Mellon University, Youngstown, New York, United States; ²University of South Carolina, Columbia, South Carolina, United States; ³Electrical Engineering, University of South Carolina Columbia, Columbia, South Carolina, United States; ⁴Carnegie Mellon University, Pittsburgh, Pennsylvania, United States; ⁵Structured Materials Industries Inc., Piscataway, New Jersey, United States; ⁶Princeton Optronics, Hamilton Township, New Jersey, United States.

Due to its ultrawide bandgap, β -Ga₂O₃ is well suited for ultraviolet (UV) photodetectors that are solar-blind and therefore insensitive to wavelengths >280 nm. These devices are of interest for applications such as missile plume tracking, water purification, and flame detection. Furthermore, alloying with Al or In allows the potential to tune the bandgap and engineer the wavelength selectivity. In this study β -Ga₂O₃ films, unalloyed and alloyed with indium or aluminum, were grown via metalorganic chemical vapor deposition (MOCVD) on c-plane sapphire (001) substrates at temperatures between 600 and 800 °C. The films were characterized using x-ray diffraction (XRD), atomic force microscopy (AFM), optical transmittance, Raman spectroscopy, energy dispersive x-ray spectroscopy (EDX) and x-ray photoelectron spectroscopy (XPS). The films were found to be (-201) oriented, textured nanocrystalline with the β -phase structure for $X_{Al} = 0.54$ and $X_{In} = 0.12$ -0.21; the bandgaps estimated from Tauc plots and XPS were 5.6 and 4.0-4.2 eV, respectively. Schottky and MSM photodetectors were fabricated on the films: Ti/Au annealed at 400°C, and Ni served as the ohmic and Schottky contacts, respectively. The observed responsivities were > 10⁴ A/W at 12V for Ga₂O₃, > 10³ A/W at 12V for (Al_xGa_{1-x})₂O₃, and > 10² A/W at 12V for (In_xGa_{1-x})₂O₃, which to our knowledge are the highest reported values for Ga₂O₃-based thin film detectors. Noise equivalent powers were measured to be 1.25 and 1.58 pW for the Ga₂O₃ Schottky and MSM detectors, respectively. Both time response and noise measurements give insight into the presence of discrete defect states, which will be discussed in the presentation.

11:20 AM Y09

(Student) Hybrid β -Ga₂O₃/AlGaIn Schottky Barrier Diodes for Broadband Deep-Ultraviolet Optoelectronics Anisha Kalra¹, Shashwat Rathkantiwar², Sandeep Vura³, Srinivasan Raghavan², Rangarajan Muralidharan² and Digbijoy N. Nath²; ¹Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India; ²Centre for Nano Science and Engineering, Indian Institute of Science, Bangalore, India, Bangalore, India; ³Center for Nano Science and Engineering, Indian Institute of Science, Bangalore, India.

In this work, we report on the first demonstration of epitaxial β -Ga₂O₃/Al_{0.45}Ga_{0.55}N heterojunction-based, self-powered, vertical Schottky barrier photodiodes with a broadband spectral response in the deep-ultraviolet wavelength regime. The diodes exhibited a rectification exceeding three orders of magnitude till 200 °C and supported a vertical breakdown field exceeding 2.3 MV/cm. A broadband spectral response between 254 nm and 284 nm, corresponding to the band-edges of the active β -Ga₂O₃ and Al_{0.45}Ga_{0.55}N absorber layers was observed for the diodes, with photo-to-dark current ratio exceeding three orders of magnitude for bias voltages > 2V. Under reverse bias i.e. when Ga₂O₃ was biased positive w.r.t to Al_{0.45}Ga_{0.55}N, the zero-bias responsivity measured 4 mA/W at both 254 nm and 284 nm, with a UV-to-visible rejection ratio > 10³. The responsivity values increased exponentially with applied bias and exceeded the ideal responsivity values of 0.2 A/W (at 254 nm) and 0.22 A/W (at 284 nm) respectively beyond 3 V of applied bias, indicating the presence of an internal gain mechanism. This device design is scalable and holds promise towards enabling vertical diodes for high voltage, high power applications as well as focal plane arrays (FPA) for self-powered, broadband UV sensing. The possibility of growing monoclinic β -Ga₂O₃ epitaxially on wurtzite AlGaIn and the interesting band alignment between the two allows for exciting band engineering towards novel device designs. The

device epistack utilized in this work consisted of a typical AlGa_N Schottky detector stack consisting of a 500 nm thick n-Al_{0.45}Ga_{0.55}N epilayer and a 300 nm thick UID Al_{0.45}Ga_{0.55}N epilayer grown on c-plane sapphire using metal organic chemical vapor deposition (MOCVD), followed by pulsed laser deposition (PLD) of 100 nm thick β-Ga₂O₃. Vertical photodiodes were realized using i-line lithography and reactive ion etching based patterning for top (Ga₂O₃) and bottom (n-AlGa_N) layers and e-beam evaporated Ni/Au (30/100 nm) and Ti/Al/Ni/Au (20/120/30/100 nm) were used as the top (Schottky) and bottom (Ohmic) contacts, respectively. The depletion width was confirmed to be 420 nm using Capacitance-Voltage measurements and the devices supported voltages exceeding 100 V and thus, fields exceeding 2.3 MV/cm. Temperature-dependent current-voltage (I-V-T) characterization revealed hopping conduction through localized defect states as the dominant carrier transport mechanism contributing to the observed reverse leakage current across the devices. Studies to experimentally estimate the band-offsets at the Ga₂O₃/AlGa_N heterojunction and evaluate the temperature-response of the detectors are underway and would be presented at the conference. This research was supported by NaMPET (DeitY), JATP, DST through NNetRA, MHRD through NIEIN, and Ph.D. scheme of Media Lab Asia, MeitY.

11:40 AM Y10

(LATE NEWS, Student) Self-Aligned Sidewall Ohmic Contact to AlGa_N/Ga_N Multichannel Structure Jianan Song, Sang-Woo Han, Suzanne Mohny and Rongming Chu; Department of Electrical Engineering, The Pennsylvania State University, University Park, Pennsylvania, United States.

Due to the high breakdown field and the high 2DEG mobility, AlGa_N/Ga_N heterostructures are widely used for making high-speed and high-power electronics devices. Recently, there has been increasing interest in stacking multiple layers of the AlGa_N/Ga_N structures for making multichannel devices with reduce on-resistance, increased current density, and improved linearity [1]. In order to realize the full potential of the multichannel structure, it is important to form good ohmic contacts to all channels. It also important to maintain a sharp edge of the ohmic contact to enable device scaling. Conventionally, ohmic contacts on AlGa_N/Ga_N single channel structure are made by alloying Ti/Al based metal stack deposited on the AlGa_N surface, forming metallic spikes into the 2DEG [2]. More recently, regrowth of N⁺ Ga_N was found to be an effective approach for making low-resistance ohmic contacts [3]. For AlGa_N/Ga_N multichannel structure, the conventional spiking ohmic contact would have higher resistance to the lower channels; the N⁺ Ga_N regrowth approach would encounter problems including mass transport on the trench sidewall and cracking/voids at the trench corner. In this paper, we report successful demonstration of ohmic contacts directly formed on the sidewall of the AlGa_N/Ga_N multichannel structure in a self-aligned fashion. We designed the AlGa_N/Ga_N multichannel structure and acquired it from Enkris Semiconductor. It has 10 periods of AlGa_N/Ga_N 2DEG structure grown on a nominally undoped Ga_N buffer on Sapphire substrate. Each period consists of: (1) a 0.5-nm-thick AlN spacer layer to reduce alloy scattering; (2) a 5-nm-thick AlGa_N layer with an Al composition of 25%; (3) a Si delta doping with nominal doping density of 7.5×10¹² cm⁻³ on the AlGa_N top surface to provide electrons to the 2DEG channel; and (4) a 20-nm-thick Ga_N channel/cap layer. Contactless measurement of the structure shows of an electron density of 5.11×10¹³ cm⁻³, an electron mobility of 1477 cm²/V-sec, and a sheet resistance of 83.4 ohm/sqr. The fabrication process includes: (1) PECVD deposition of SiO₂ etch stop layer; (2) formation of ohmic contact trench; (3) deposition of Ti/Al (20nm/100nm) ohmic metal by Sputtering; (4) surface planarization using PMGI; (5) etching back PMGI exposing metal on the top of the mesa structure by O₂ plasma; (6) etching of Ti/Al metal on the top of the mesa structure by ICP; (7) stripping the remaining PMGI in the trench region; and (8) rapid thermal annealing at 550 °C for 1 minute in N₂ ambient. IV measurement of the circular TLM structure was performed before and after the annealing, using the Kelvin configuration. The annealing process significantly reduced the resistance. The edge of the ohmic contact remained sharp after the annealing, thanks to the low annealing temperature. From the measured and fitted resistance as a function of ohmic contact spacing, we extracted a sheet resistance of 117 ohm/sqr and a contact resistance of 0.58 ohm-mm, considering geometric correction factors. It is noteworthy that the annealed Ti/Al layer has a nonnegligible metal resistance. IV measurement shows a resistance of about 1~4 ohm when probes are landed on the same metal pad, with the probing distance similar to those during the circular TLM measurements. Future work is needed to thicken up the metal and minimize the effect of metal resistance, for example, by electroplating. [1] Howell, Robert S., et al. "The super-lattice castellated field effect transistor (SLCFET): A novel high performance transistor topology ideal for RF switching." 2014 IEEE International Electron Devices Meeting. IEEE, 2014. [2] Dora, Y., et al.

"Effect of ohmic contacts on buffer leakage of Ga_N transistors." IEEE electron device letters 27.7 (2006): 529- 531. [3] Shinohara, K., et al. "Self-aligned-gate Ga_N-HEMTs with heavily-doped n⁺-Ga_N ohmic contacts to 2DEG." 2012 International Electron Devices Meeting. IEEE, 2012.

SESSION Z: Organic/Hybrid Materials and Devices
Session Chairs: Adrienne Stiff-Roberts and William Wong
Thursday Afternoon, June 27, 2019
Michigan League, 2nd Floor, Kalamazoo

1:30 PM Z01

(Student) Highly Reliable Organo-Compatible Superhydrophobic Self-Cleaning Protection for Organic Field Effect Transistors

Daekyoung Yoo¹, Youngrok Kim¹, Misook Min¹, Geun Ho Ahn², Der-Hsien Lien², Jingon Jang¹, Hyunhak Jeong¹, Younggul Song¹, Seungjun Chung³, Ali Javey² and Takhee Lee¹; ¹Seoul National University, Seoul, Korea (the Republic of); ²Electrical Engineering and Computer Sciences, University of California, Berkeley, CA 94720, USA, UC Berkeley, Berkeley, California, United States; ³Photo-Electronic Hybrids Research Center, Korea Institute of Science and Technology, Seoul, Korea (the Republic of).

Organic semiconductors have attracted significant interest for realizing next-generation electronics due to their fast, low-cost, and low-temperature processabilities [1]. Nevertheless, it is widely reported that they could be drastically degraded by water-based hindrances. Although some efforts to address this issue by encapsulating with various materials have been reported, novel approaches to introduce an effective protection layer directly on organic components are highly desirable. In this regard, the introduction of a superhydrophobic protection layer onto the organic semiconducting layers can be a promising approach to realize reliable and practical organic semiconductor applications. The materials and processes for the superhydrophobic protection layer formation need to be organo-compatible, so that they do not damage physically or chemically when placed on the organic layers, and thus their electrical characteristics would not be degraded. In this presentation, we report a facile method to deposit an organo-compatible superhydrophobic protection layer on organic semiconductors under ambient conditions. The superhydrophobicity was achieved by simply dipping organic devices in a highly fluorinated solution dispersed with fluoroalkylsilane-coated titanium-dioxide nanoparticles [2]. Furthermore, the uniform protection layer could be deposited using a simple dipping process without any physical damages by optimizing the solvent system to match surface energy with underlying organic semiconductors. The proposed protection layer had good resistance against mechanical-stress, light-stress and water-based threats. Moreover, protected organic devices exhibited reliable electrical properties even exposed to strong solvents while maintaining self-cleaning properties from extreme water repellency and showing good thermal stability. This study provides a practical solution to enhance the reliability of organic devices in the natural environment. References: [1]. H. Sirringhaus, *Adv. Mater.* 26, 1319 (2014). [2]. D. Yoo, Y. Kim, M. Min, G. H. Ahn, D. H. Lien, J. Jang, H. Jeong, Y. Song, S. Chung, A. Javey, T. Lee, *ACS Nano* 12 11062 (2018).

1:50 PM Z02

(Student) Improving Charge Injection Properties of Organic Field Effect Transistor by Molecular Implantation Doping

Youngrok Kim¹, Seungjun Chung¹, Kyungjune Cho¹, David Harkin², Wang-Taek Hwang¹, Daekyoung Yoo¹, Jae-Keun Kim⁴, Woocheol Lee⁴, Younggul Song⁴, Heebeom Ahn⁴, Yongtaek Hong³, Henning Sirringhaus², Keehoon Kang⁴ and Takhee Lee⁴; ¹Korea Institute of Science and Technology, Seoul, Korea (the Republic of); ²University of Cambridge, Cambridge, United Kingdom; ³Electrical and Computer Engineering, Seoul National University, Seoul, Korea (the Republic of); ⁴Physics and Astronomy, Seoul National University, Seoul, Korea (the Republic of).

Organic semiconductors (OSCs) have been widely studied due to their merits such as mechanical flexibility, solution processability, and large-area fabrication. However, because of the Schottky contact at the metal-OSC interfaces, a non-ideal transfer curve feature often appears in the low drain voltage region. Considering large operation voltages required for OFETs, improving contact properties of organic/metal interface is an essential step for practical applications of OSCs. In silicon-based semiconductor industry, selective implantation doping technique is widely used to enhance the charge injection properties, and similar approach can be applied in OSCs to enhance the charge injection from electrodes to organic channel material. In this presentation, I will report the demonstration of a selective contact doping of 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F_4 -TCNQ) by solid-state diffusion in poly 2,5-bis(3-hexadecylthiophen-2-yl)thieno [3,2-b] thiophene (PBTTT) to enhance carrier injection properties in bottom-gate PBTTT OFETs [1,2].

Furthermore, the effect of post-doping treatment on diffusion of F_4 -TCNQ molecules will be discussed in order to improve the device stability. In addition, the application of the doping technique to the low-voltage operation of PBTTT OFETs with high-k gate dielectrics will be presented, demonstrating a potential for designing scalable and low-power organic devices by utilizing doping of conjugated polymers. References: [1] K. Kang, S. Watanabe, K. Broch, A. Sepe, A. Brown, I. Nasrallah¹, M. Nikolka, Z. Fei, M. Heeney, D. Matsumoto, K. Marumoto, H. Tanaka, S. Kuroda and H. Sirringhaus, *Nat. Mater.* 15, 896 (2016). [2] Y. Kim, S. Chung, K. Cho, D. Harkin, W.-T. Hwang, D. Yoo, J.-K. Kim, W. Lee, Y. Song, H. Ahn, Y. Hong, H. Sirringhaus, K. Kang and T. Lee, *Adv. Mater.*, in press (2019).

2:10 PM Z03

Modulating Chain Conformations of Polyvinyl Alcohol Through Low Cost and Nontoxic Glyoxal Crosslinker—Application in High-Performance Organic Transistors

Debdatta Panigrahi, Sujit Kumar and Achintya Dhar; Physics, Indian Institute of Technology Kharagpur, Kharagpur, India.

High leakage current and presence of numerous polar hydroxyl groups have often appeared as severe performance obstacles for polyvinyl alcohol (PVA) on its application in organic field effect transistor devices. Herein, we report a facile, yet efficient functionalization and chain structure modification technique to enhance its efficacy as a gate insulating layer. In this work, we have used glyoxal as a cross-linking agent of PVA to modulate its chain conformation and performed a detailed analysis to explore the role of glyoxal crosslinking on the electrical and structural properties of PVA. Applying various amount of glyoxal solution we have properly optimized the dose of the crosslinker to be used in the crosslinking reaction so that minimum amount of leakage can be achieved. Substantial improvement in the insulation properties as well as surface characteristics was observed after the structural modification of the polymer. Correspondingly, organic FETs were fabricated using crosslinked PVA to gauge the effect of crosslinking on the device performance of the transistors. Post-crosslinking improvements in the polymer bulk and surface characteristics were clearly emulated in the device performance parameters. Field-effect mobility as high as 5.4 cm²/V-s and 1.7 cm²/V-s were achieved employing crosslinked PVA as gate dielectric layer in Dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNTT) and pentacene based devices, respectively. Thus, our study illustrates the viability of crosslinking PVA using glyoxal and hence, can catalyze the limited use of PVA in electronic applications.

2:30 PM Z04

(Student) Towards Metallic-Type Transport in Polymers—

Establishing Structure/Property Interrelationships Hongmo Li¹, David Valverde², Andre Zeumault², Stephen Barlow², Lee Richter³, Seth Marder², Carlos Silva² and Natalie Stingelin¹; ¹School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States; ²School of Chemistry & Biochemistry, Georgia Institute of Technology, Atlanta, Georgia, United States; ³National Institute of Standards and Technology, Gaithersburg, Maryland, United States.

Current organic electronics research aims at exploiting the unique property matrix of “plastic” semiconductors, including their chemical tunability, straight-forward processability and mechanical flexibility, to create new applications. While much knowledge has been developed in the synthesis of semiconducting conjugated organic materials, there is still an immense need for establishing broadly applicable design guidelines towards highly conductive macromolecular matter. [1,2] Moreover, the multitude of possibilities for “plastic” semiconductors and dopants to assemble together over different length scales creates a daunting task to establish comprehensive and relevant correlations between structure, processing and properties. We will present here a multidisciplinary approach towards a framework to predict such structure/property interrelations. We will focus on polythiophene derivatives as model systems, including poly[2,5-bis(3-tetradecylthiophen-2-yl)thieno[3,2-b]thiophene] (PBTTT), [3] and discuss how the spatial arrangement, manipulated through intercalation and co-crystal formation with dopants, affects charge transport. We will conclude with providing a tentative picture of the complex correlation of structure and electronic landscape for the understanding of conducting “plastics” of metallic type transport. [1] Lee, K., Lee, S. et al. *Nature* 441.7089 (2006): 65. [2] Kang, K., Sirringhaus H., et al. *Nature Materials* 15.8 (2016): 896. [3] Buchaca-Domingo, E., Stingelin N., et al. *Materials Horizons* 1.2 (2014): 270-279.

2:50 PM Z05

Thermodynamics of Complexation in Donor-Acceptor Conjugated Polyelectrolyte Networks Showing Ultrafast Electronic Energy Transfer William R. Hollingsworth and Alexander L. Ayzner; Chemistry and Biochemistry, University of California, Santa Cruz, Santa Cruz, California, United States.

Conjugated polyelectrolytes (CPE) – semiconducting polymers bearing ionizable pendant sidechains – present an attractive class of materials for light harvesting due to their tunable band-gaps, low-cost solution processability, and tendency towards self-assembly in aqueous media. Our previous work has shown that conjugated polyelectrolyte complexes (CPECs) composed of oppositely charged polyfluorene and polythiophene derivatives participate in donor-acceptor electronic energy transfer on timescales of approximately 240 fs, on par with natural photosynthesis. This ultrafast energy transfer highlights the promise of these materials to be used as photoactive scaffolds in an artificial light harvesting array. However, there is relatively little information about how CPECs form, and what the thermodynamic and kinetic driving forces for complexation are, especially as compared to traditional polyelectrolytes. Using a combination of steady-state spectroscopy, time-resolved fluorescence anisotropy, and isothermal titration calorimetry, we find that the complexation rate is controlled by the strength of the *intra*chain pi-pi interactions of a CPE in its native state. Further, based on the strength of these interactions, we characterize CPEs as falling on a spectrum between protein-like (strong π - π interactions) and polyelectrolyte-like (weak pi-pi), with a strong heat input required to form complexes with the former. The necessity of heating distinguishes CPEs from traditional polyelectrolytes and adds another means of directing complexation beyond solution ionic strength and solvent quality. Moreover, the strength of *intra*-chain pi-pi interactions can be modulated by both the sidechain density and degree of regioregularity of a CPE, effectively tuning CPE temperature response. Our findings show that CPE the driving forces in CPE complexation differ significantly from that of traditional polyelectrolytes and point towards additional avenues for controlling complexation, and ultimately the formation of self-assembled artificial light harvesting assemblies.

3:10 PM REFRESHMENT BREAK

3:30 PM Z06

(LATE NEWS, Student) Stretching-Insensitive Pressure Sensor Using Strain Engineering with Rigid Film Spacer Jaeyoung Yoon, Hayun Kim and Yongtaek Hong; Department of Electrical and Computer Engineering, Inter-University Semiconductor Research Center (ISRC), Seoul, Korea (the Republic of).

Tactile and pressure sensors for electronic skin (E-skin) or wearable health care systems have recently attracted considerable interest because they are the most important and fundamental components to mimic the sensing abilities of human receptors. In order to realize the aforementioned techniques, flexible or stretchable pressure sensors that have a softness and skin-like conformability are required. Furthermore, for the body attachable pressure sensors and an imperceptible mode of wearing of them, the components of the sensors (i.e. electrodes, substrate, and dielectric layers, etc.) need to be highly thin and deformable. A great deal of body-attachable soft pressure sensors that meet the requirements has been reported. Even though most of these soft pressure sensors were demonstrated on the skin, there have been few reports in which the change or degradation of the sensor characteristics due to the dynamic deformation of the human body was investigated. One of the approaches to alleviate the change of the sensors due to body deformation can be a calibration process and signal processing using electrical circuits. However, eliminating performance degradations through structural engineering on the sensors can be a more fundamental breakthrough. Recently, a bending-insensitive pressure sensor using a nanofibre electrode sandwiched between very thin thermoplastic films (< 2 μ m) has been published. This sensor can detect pressure with the almost same performance without degradations even under the extremely small bending radius (<80 μ m). These sensors are applicable only on the bending deformation, but they are not applicable to body-attached sensors that require the stretchability of the device. Furthermore, few pressure sensors that can maintain their performance under stretching deformation have been reported. Here, we have developed a body attachable capacitive type pressure sensor of which the performance is maintained even under stretching deformation through strain engineering. Both electrodes of the sensor are composed of silvernanowires -embedded PDMS (AgNWs/PDMS composite), and the insulation layer is also composed of a thin PDMS layer, enabling the sensor device to be thin and conformable to the body deformation. In addition, rigid thermoplastic film spacers between both electrodes allow the sensing area to be protected from external

deformation by forming a strain-free area (<2% strain) under the stretching deformation. The irreversible bonding between the spacer and both electrodes maintains even at 30% biaxial deformation; analyzing the strain distribution of sensor with a digital image correlation (DIC) method, the mechanical properties were investigated. The initial capacitance value is one of the most decisive factors for the sensitivity of the sensor and that value of our sensor with strain engineering is maintained almost constant. As a result, our sensor exhibited constant sensitivity (0.2 kPa⁻¹), which is unchanging even under a biaxial 30% strain. In addition, the robustness was investigated while maintaining the performance of the sensor even at 1000 repetitions of pressure and showed fast response time and recovery time within 0.2ms. We demonstrated a wearable pulse monitoring sensor capable of detecting almost same pulse signals even with wrist movement using our pressure sensor and we have presented the usability of our sensor as E-skin or wearable health care devices.

3:50 PM Z07

(Student) Charge-Transport Networks via Small-Molecule Self-Assembly in Conjugated Polymer Bulk Heterojunctions Michael Roders^{1,3}, Matthew Kolaczowski², Reilly Seban¹, Yi Liu² and Alexander L. Ayzner¹; ¹Chemistry and Biochemistry, University of California Santa Cruz, Santa Cruz, California, United States; ²Organic Synthesis, Molecular Foundry, Berkeley, California, United States; ³Chemistry, University of California, Berkeley, Berkeley, California, United States.

Recent progress and record power conversion efficiencies in bulk-heterojunction based organic photovoltaic devices have utilized anisotropic non-fullerene small molecules in conjugated polymer blends. Despite the dramatic progress in device performance, there is a fundamental gap of knowledge in relating the small-molecule chemical structure and intermolecular interactions to the hierarchical device morphology and corresponding optoelectronic processes. In this work, we have interrogated small-molecule derivatives with the same peripheral chromophores linked by different central core motifs, leading to significantly different frontier orbital geometries and intermolecular packing. Using a combination of scanning transmission electron microscopy and resonant X-ray scattering, we find that a derivative with a triphenylamine core and propeller -shape leads to self-assembled molecular nanowires that percolate through the conjugated polymer matrix. The formation of nanowires does not lead to overly phase-separated blends, thereby retaining efficient exciton harvesting. In contrast, an alkylfluorene-based core motif results in drastically different small-molecule network that is highly branched and tortuous. In the same polymer blend. We further find that this mesoscale morphological difference appears to qualitatively transcend the molecule details of the polymer matrix. Our results demonstrate that the nanowire-based morphology leads to substantially more efficient charge transport along the percolated small-molecule network. These findings have significant implications for the design of next-generation, self-assembling small-molecule organic semiconductors in polymer-based solar cells.

4:10 PM Z08

Growth and Fluorescence Sensitization of Wide-Bandgap Organic Single Crystals Co-Doped with Emissive and Assistant Dopants Keita Takeuchi, Ryogo Abe, Asuka Suzuki, Kosuke Watanabe and Akihiko Kikuchi; Engineering and Applied Sciences, Sophia University, Tokyo, Japan.

In organic light-emitting devices, molecular doping of organic semiconductors is an important method enabling adjustment and improvement of the light emission characteristics. In a combination of host and guest materials with low energy transfer efficiency, the method of doping two types of guest materials of an assistant dopant and an emissive dopant has been extensively studied. On the other hand, organic semiconductor single crystals with regular molecular arrangements have characteristics including high charge mobility and large transition dipole moments. However, there are few examples of organic single crystal growth by solution method in which several molecules are doped with high controllability. The organic semiconductor co-doped with two different molecules was grown using a plate-like single-crystal growth technique in which a low-vapor-pressure liquid thin film was used as a two-dimensional crystal growth field and a solute was precisely and uniformly supplied by electrospray deposition (ESD). We confirmed high-efficiency energy transfer from the host to red dye via green dye by co-doping green and red dye in the host of a wide-bandgap organic semiconductor with singlet transition energy in the ultraviolet region. The fluorescent green dye 3-(2-Benzothiazolyl)-7-(diethylamino)coumarin (C6) and the fluorescent red dye 4-(Dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4H-pyran (DCM) were used as the assistant and emissive dopants, respectively. The dopants were doped in a plate-like

single crystal of 2-(4-Biphenyl)-5-phenyl-1,3,4-oxadiazole (PBD), which is a wide-bandgap fluorescent material. In experiments, molecular doped PBD single crystals were grown using a spray solution in which the solutes were dissolved with weight ratios of only PBD and PBD:DCM = 90:10. Dioctyl sebacate (DOS) was used as the low-vapor-pressure liquid for the thin-film crystal growth field. The DOS solution was saturated with each solute at room temperature. The solutions containing the solutes were sprayed from above the liquid thin film with 5 mm formed on the ITO-coated substrate by ESD. Hexagonal plate-like single crystals are precipitated and no significant effect is observed with the presence or absence of the dopants. The crystals precipitated by spraying the PBD solution and DCM-added PBD solution emit blue-violet and yellow, respectively. The peak wavelength of the non-doped PBD single crystal is about 391 nm. The DCM-doped PBD single crystal emits both the emission of PBD and the emission of DCM at ~567 nm. Next, we grew PBD single crystals co-doped with DCM and C6. The DOS solution almost saturated with each solute was used as the liquid thin film. A solution of 5 wt% C6 was prepared. Then, mixed solutions with 0–20 wt% DCM added to the C6-added PBD solution were prepared. Hexagonal plate-like single crystals are precipitated and no significant effect on the crystal shape is observed with co-doping. The fluorescence color is changed from green to yellow as the concentration of DCM is increased. In the co-doped single crystal, the emission of PBD remains very low despite the presence of DCM within the crystal. In addition, as the DCM concentration is increased, the emission intensity I_{C6} attributed to C6 is decreased and the emission intensity I_{DCM} from DCM is increased. At 10 wt% DCM, a slight C6 peak remains, but a yellow PL spectrum mostly from DCM is obtained. At the DCM concentration of 20 wt%, the I_{DCM} begins to decrease. It is considered that the DCM concentration in the single crystal increased, inducing concentration quenching. In addition, the emission intensity ratio from DCM in the co-doped crystal grown by using the spray solution with the DCM concentration of 10 wt% is 87.6%. The luminescence intensity of the co-doped single crystal is 1.73 times that of the single crystal doped with only DCM; therefore, C6 functions as an assist dopant and the luminous efficiency from DCM is greatly improved.

4:30 PM Z09

(Student) Effect of β -PFO Concentration on Device Performance in LEDs Fabricated by RIR-MAPLE Spencer Ferguson¹, Buang Zhang¹ and Adrienne Stiff-Roberts^{1,2}; ¹Electrical and Computer Engineering, Duke University, Durham, North Carolina, United States; ²University Program in Materials Science and Engineering, Duke University, Durham, North Carolina, United States.

Poly(9,9-di-n-octylfluorenyl-2,7-diyl) (PFO) is a strong candidate as the blue light source in modern organic light emitting diodes (OLEDs) due to its high color purity and luminance efficiency, but it has several challenges to overcome before implementation. Critical among these is device improvement through promotion of crystalline domains. PFO exists in at least two distinct phases, amorphous (α) and crystalline (β), the latter of which exists as a planar zigzag structure within the amorphous polymer. β -PFO exhibits greater charge-carrier mobility and color purity [1], allowing superior LED performance. While standard spin coating techniques can easily deposit the α -phase, β -phase deposition is more challenging to achieve. Whether β -PFO is promoted by solvent annealing [2] or spin-casting using poor PFO solvents [3], the surface roughness increases as the β -PFO concentration increases. In previous work, we demonstrated that emulsion-based, resonant infrared, matrix-assisted pulsed laser evaporation (RIR-MAPLE) can maintain the film surface roughness while the β -PFO concentration increases [4]. RIR-MAPLE uses an “oil-in-water” emulsion that comprises PFO dissolved in trichlorobenzene, phenol to provide low vapor pressure, and water as the continuous phase of the emulsion (with a nominal amount of surfactant). This emulsion is flash frozen and ablated with an infrared Er:YAG laser under vacuum. The laser energy resonates with the hydroxyl bond vibrational mode in water and transfers emulsified polymer particles to the substrate without degradation. Thus, the consistent surface roughness of films with higher β -PFO results because PFO crystallization is confined to emulsified particles that are transferred to the substrate as opposed to the macroscale crystallization that occurs across the substrate in solution-based deposition [3,4]. In order to clearly demonstrate the structure-process-property relationships unique to RIR-MAPLE deposition of PFO, in this work, we will determine the impact of different emulsion conditions on the emulsified particle morphology, the concentration of β -PFO and corresponding surface roughness of deposited films, and the device performance of LEDs fabricated from these films. The most relevant emulsion parameters for this study are the total PFO concentration, the primary solvent:water ratio, and the phenol:water ratio. Cryogenic transmission electron microscopy and atomic force microscopy will be

used to characterize the emulsified particle and film surface roughness, respectively. Photoluminescence and UV-Vis absorbance spectroscopy will be used to compare the β -PFO concentration for different emulsion conditions. PFO-based LEDs will be fabricated using an ITO/PEDOT:PSS/PFO/LiF/Al structure with varying β -PFO concentration and characterized using electroluminescence, current-voltage, and brightness measurements. We hypothesize that: i) PFO devices fabricated by RIR-MAPLE will exhibit higher brightness at a lower current density because β -PFO crystallinity increases, and ii) such performance improvements would be difficult to achieve using other thin-film deposition techniques to achieve β -PFO due to poor film roughness. References [1] Zhang, X. et. al., Appl. Phys. Lett., 2013 [2] Wan, H., et. al., J. Lumines., 131(7), 1393–1396, 2011. [3] Peet, J., et. al., Adv. Mat., 20(10), 1882–1885, 2008. [4] Ferguson, S., et. al, Elec. Mats. Conf., Santa Barbara, CA, June 2018.

4:50 PM Z10

Environmentally Benign Highly Luminescent Colloidal Quantum Dots, $\text{In}_{1-x}\text{Ga}_x\text{P}@ZnS$ and Their Application in QLEDs with Inverted Structure Yujin Kim and Seonghoon Lee; Chemistry, Seoul National University, Seoul, Korea (the Republic of).

Ever since 1980s, the time when colloidal quantum dots (CQDs) were first noticed by Ekimov, Brus, and Efros with the concept of quantum confinement effect, CQDs have begun to gain the spotlight. CQDs’ advantageous optical properties such as facile color tunability—ranging from near ultraviolet to visible to near infrared—, narrow spectral bandwidth, and high photoluminescence quantum yield (PL QY) have been known, their applications to light emitting diodes, photovoltaic devices, lasers, and biological markers, have been achieved. Most of them were made out of toxic elements such as Cd, Pb, and Hg. Those toxic elements are limited by the restriction of hazardous substances (RoHS) directive. Environmentally benign and highly luminescent colloidal quantum dots (CQDs) have been sought. Among them, environmentally benign InP-based CQDs have been the most widely studied as the next-generation luminescent materials. Environmentally benign III-V quantum dots were synthesized with bis(trimethylsilyl)phosphine, our newly-developed P precursor with controllable reactivity and new metal complex precursors (Indium-trioctylphosphine, In-TOP; Ga-TOP; Zn-TOP). To achieve high photoluminescence quantum yield (PLQY), the surface states associated with surface atoms on CQDs should be passivated. They are nonradiative trap states lying in between the gap. ZnS shell was overcoated as a type-I layer for the aid of electron funneling on the alloy-core $\text{In}_{1-x}\text{Ga}_x\text{P}$ to enhance photoluminescence quantum yield. In this way, $\text{In}_{1-x}\text{Ga}_x\text{P}@ZnS$ (alloy-core@outer shell) structure is generated. Furthermore, we apply those CQDs to fabricate blue-emitting quantum dot light-emitting devices (QLEDs) with the external quantum efficiency of 0.20 % which is the best among the III-V-based blue-emitting QLEDs reported so far. The synthetic scheme and $\text{In}_{1-x}\text{Ga}_x\text{P}@ZnS$ based blue-emitting QLED with inverted structure are shown in Figure below.

SESSION AA: Electron Microscopy
Session Chairs: Mark Goorsky and Heayoung Yoon
Thursday Afternoon, June 27, 2019
Michigan League, 2nd Floor, Michigan

1:30 PM AA01

(Student) Scanning Electron Nanodiffraction Based High Resolution Strain Mapping on Semiconductor Devices—From 2D to 3D Renliang Yuan¹, Jiong Zhang² and Jian-Min Zuo¹; ¹Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, United States; ²Intel Corporation, Hillsboro, Oregon, United States.

Strain is introduced to enhance the performance of MOSFETs by boosting carrier mobility [1]. High resolution strain mapping is required as a part of device metrology. While high resolution can be achieved using transmission electron microscopy, however, new challenges are also raised by new devices, such as the Intel’s new 3D tri-gate architecture, which contains multiple overlapping layers of different materials that makes strain mapping difficult using high resolution electron microscopy (HREM) or scanning transmission electron microscopy (STEM) [2]. Electron nanodiffraction (END) thus becomes the best choice in this case as it provides both high spatial resolution and high sensitivity, as contributions from different overlapping materials can be separated in reciprocal space. A large field of view can be achieved by combining scanning with END for scanning electron nanodiffraction (SEND) [3]. In SEND, the electron beam is focused into a nano-sized probe and

controlled by built-in STEM deflection coils to scan across a region of interest where diffraction patterns are acquired at each probe position. Spatial resolution is defined by electron probe size, which is typically tens of nm for a parallel beam. The resolution can be improved to unit-cell level (sub-nm) using a convergent beam. Diffracted beams form disks; their intensities are strongly affected by dynamic effects, making disk detection non-trivial. In this study, we propose a new method to identify diffraction peak positions by applying circular Hough transform to Sobel-filtered disks. The resulting image is then fitted by a Lorentzian peak to determine the position of disk center with sub-pixel accuracy. When all diffraction disks are measured, a 2D reciprocal lattice can be fitted to calculate the strain tensor. We evaluate the accuracy of this method by analyzing theoretical diffraction patterns generated by multislice simulations. Precision is also estimated from experimental patterns in multiple ways to compare different experimental conditions. With 2D strain mapping method established, we explored the possibility of measuring strain distribution in 3D. Unlike traditional tomography, diffraction reveals average strain of the illuminated sample volume rather than the integral. Hence, additional restriction is needed to make 3D reconstruction possible. We show the preliminary results of 3D strain mapping on a typical lamella sample of finFET devices, which was successfully reconstructed from several 2D strain maps scanned at different tilt angles. This technique promises a new way to study 3D strained structures in semiconductor devices as well as other strained crystalline materials at nanoscale. [1] T. Ghani *et al.*, *IEDM*, pp. 978–980, 2003. [2] J. M. Zuo *et al.*, *Ultramicroscopy*, vol. 136, pp. 50–60, 2014. [3] K. Kim *et al.*, *Micron*, vol. 71, pp. 39–45, 2015.

1:50 PM AA02

Imaging of Dopant Complexes and Strain Relaxation in Wide Bandgap Semiconductors with Scanning Transmission Electron Microscopy Tim B. Eldred¹, Joshua S. Harris¹, Jonathon N. Baker¹, Mostafa Abdelhamid¹, Douglas L. Irving¹ and James LeBeau²; ¹MSE, North Carolina State University, Morrisville, North Carolina, United States; ²North Carolina State University, Raleigh, North Carolina, United States.

As device and feature size continues to decrease in modern semiconductor applications, the need to control film growth and material composition drives analytical methods. Furthermore, understanding compensation mechanisms and defects is key to effective composition and dopant control. Scanning transmission electron microscopy (STEM) has become an important tool to directly interrogate local composition and strain. Here, we will present two methods of analyzing compensation mechanisms in film growth: detection and mapping of dopant-vacancy complexes formed to compensate Si dopants in AlN/AlGa_nN, and strain mapping along dislocations and v-pits in InGa_nN. In AlN and AlGa_nN systems, Si is a promising shallow dopant. Previous studies have shown complications due to a drop-off in charge carrier concentration as Si concentration reaches relevant concentration for device development. Theory suggests that the cause for this is the formation of dopant-vacancy complex consisting of 3 Si replacements neighboring an Al vacancy as a compensation mechanism. [1] We will present our progress detecting and mapping these dopant complexes, allowing further characterization and classification of point defects in electronic materials as a function of dopant concentration. We compare atomic-resolution STEM images from experiment to a statistical model derived from simulated images to locate dopant vacancy complexes in atomic columns. High angle annular dark field (HAADF) is used along with integrated differential phase contrast (iDPC)-STEM to increase the precision of column position and intensity measurements. From the simulated datasets, iDPC-STEM and HAADF-STEM images are generated and column intensity/location are measured with high precision using template matching. We find that the use of iDPC-STEM increases the visibility of nitrogen, allowing higher precision in measuring their positions. Based on simulations for thin (< 10 nm) samples, the defect complexes introduce > 2% change in the intensity of the Al atom column containing a vacancy and a > 4 pm shift in the projected nitrogen locations, both of which are within the detectable range for RevSTEM. We will also discuss how comparing HAADF-STEM and iDPC-STEM images with the model allows determination of defect location and orientation. Finally, we also will show how 4D-STEM (a 2D diffraction point stored at every point in the STEM image) can be used to evaluate strain relaxation across larger areas of the TEM sample. We will discuss results from In_xGa_{1-x}N, where the bandgap can be tailored across a broad range by adjusting the In content. The In content is limited by strain and subsequent phase separation and defect formation, leading to the so-called 'green gap'. We will discuss results of strain analysis for a layered growth used to relax the strain through periodic deposition of InGa_nN and GaN layers. We will discuss how this strain can be analyzed using 4D-STEM in order to correlate local strain with EDS compositional data.[2,3] By analyzing the diffraction patterns at

each scan location (x,y) we directly calculate d-spacing and strain in the sample. We will demonstrate to what extent the compensation mechanisms such as V-Pitting, threading dislocations, stacking faults and inclusion allow the relaxation of local strain. [1] A. Uedono, K. Tenjinbayashi, S. Ishibashi, Native cation vacancies in Si-doped AlGa_nN studied by monoenergetic positron beams, *J. Appl. Phys.* 111 (2012) 013512. doi:10.1063/1.3675270. [2] Y. Han, K. Nguyen, D.A. Muller, Strain Mapping of Two-Dimensional Heterostructures with Subpicometer Precision, *Nano Lett.* 18 (2018) 3746–3751. doi:10.1021/acs.nanolett.8b00952. [3] M.J. Hÿtch, A.M. Minor, Observing and measuring strain in nanostructures and devices with transmission electron microscopy, *MRS Bull.* 39 (2014) 138–146. doi:10.1557/mrs.2014.4.

2:10 PM AA03

Direct Determination of Atomic Scale Structure and Properties of Point Defect Complexes in β -Ga₂O₃ Jared Johnson¹, Zhen Chen², Joel B. Varley³, Christine Jackson¹, Farzana Esmat¹, Aaron R. Arehart¹, Hsien-Lien Huang¹, Steven A. Ringel¹, Chris G. Van de Walle⁴, David Muller² and Jinwoo Hwang⁵; ¹The Ohio State University, Columbus, Ohio, United States; ²Cornell University, Ithaca, New York, United States; ³Lawrence Livermore National Laboratory, Livermore, California, United States; ⁴Materials Department, University of California, Santa Barbara, Santa Barbara, California, United States; ⁵Materials Science, The Ohio State University, Columbus, Ohio, United States.

β -Ga₂O₃ has emerged as a promising candidate material for high performance ultra wide band gap (UWBG) electronic, optical, and power device applications, due to its unique advantages as a transparent conductive oxide including a high breakdown voltage and its availability as inexpensive high quality bulk grown single crystals. Despite these advantages, its basic properties are not fully understood, resulting in the inability to be properly controlled. In β -Ga₂O₃, the lack of understanding of its intrinsic n-type behavior, difficulty in p-type doping, low doping efficiency, and impurity contribution to electronic/optical properties can be directly linked to the point defects present. Understanding the unique properties of β -Ga₂O₃ thus requires the detailed experimental information describing the exact structure of point defects and their role on determining the important properties. Here, we will present the first direct observation of individual interstitial point defects and vacancy – cation interstitial complexes within the atomic scale structure of bulk β -Ga₂O₃ using high resolution scanning transmission electron microscopy (STEM). Using high-angle annular dark field and integrated differential phase contrast modes in STEM, we observed that cation interstitials occupy several different interstitial sites and cluster amongst themselves. Our experimentally identified point defect structures correlate directly with DFT calculations predicting the formation of divacancy – interstitial complexes that act as compensating acceptors in β -Ga₂O₃. A comparison between STEM data and deep level optical spectroscopy (DLOS) results further validate the formation of these complexes through the identification of a corresponding deep trap within the band gap of β -Ga₂O₃. By integrating the effects of Sn doping to STEM, DLOS, and DFT results, we confirm that the development of the observed point defect complexes is facilitated by Sn doping.

2:30 PM AA04

(Student) Four-Dimensional Scanning Transmission Electron Microscopy Characterization of Molecular Ordering of Organic Semiconducting Polymers Gabriel A. Calderon Ortíz¹, Menglin Zhu¹, Letian Dou² and Jinwoo Hwang³; ¹Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States; ²Davidson School of Chemical Engineering, Purdue University, West Lafayette, Indiana, United States; ³Materials Science, The Ohio State University, Columbus, Ohio, United States.

Organic photovoltaics (OPVs) have been widely studied as promising candidates for affordable and easy to produce organic photovoltaic devices. The main obstacle so far is the relatively low efficiency of these devices compared to their inorganic counterparts. In order to improve their photovoltaic efficiency, thorough characterization of these materials is required to establish new structure-property relationships and potential ways of improving their performance. We studied Poly(3-hexylthiophene-2,5-diyl) (P3HT) and P3HT: Phenyl-C61-butyrac acid methyl ester (PCBM) (P3HT:PCBM) heterojunction thin films via fluctuation electron microscopy (FEM) using a scanning transmission electron microscope (STEM), coupled with a fast pixel array STEM detector. The main goal of our approach is to characterize the details of the molecular ordering which is important to understand and control the properties of OPVs, but has remained elusive due to the difficulty of the characterization. FEM is a nano-diffraction based technique that allows for collection of diffraction patterns at the nanoscale, the beam used of this study had a diameter of 2 nm, which provides much higher resolution than commonly used techniques, such as X-ray diffraction.

Intensity variance among thousands of diffraction patterns collected in this experiment can be correlated to the expected Alkyl and π - π stacking of P3HT. This technique also provides information on type, size, volume fraction, spatial and orientation distribution of the molecular ordering at the nanoscale. To complement fluctuation data, angular correlation analysis was performed, resulting mainly on a 2-fold symmetry which is expected for these kinds of polymers. Moreover, with the addition of the new generation pixelated detector, real space reconstruction of the nanoscale ordered regions can be easily achieved at different scattering vectors (k), which provides further information of the type or ordering and orientation of the polymer.

2:50 PM AA05

(Student) Accelerated Electromigration Study of Cobalt Thin Films by *In Situ* TEM Brent Engler and Robert Hull; Rensselaer Polytechnic Institute, Troy, New York, United States.

Cobalt has been studied in the interconnect field for years based on its utility as a capping layer for Copper interconnects but only recently as the primary material in local interconnects, as dimensional scaling limits the effectiveness of traditional Cu interconnects. Compared to Cu, Co suffers from a higher bulk resistance but requires less liner material, has a higher resistance to stress voiding, a higher resistance to Electromigration (EM) failure, and better resistance scaling in low dimensions due to a longer electron mean free path. The combination of the mean free path and decreased liner requirements result in a critical dimension where Co interconnects have a lower total resistance than Cu of the same dimension. Cobalt has a complex EM behavior, and while it is generally known to be significantly more resistant to EM than Cu, there is little data on the failure mechanisms at low dimensions. Because Co has a sign change in the normal Hall resistance, R_H , above 400C, the direction of EM, indicated by the sign of the effective charge Z^* , also changes. The quantities R_H and Z^* do not change sign at the same temperature, as electron induced EM has been observed above 600C. *In-Situ* TEM allows for unique insight into the mechanisms of EM with high temporal and spatial resolution and independent control over temperature and current density within a large range of operating conditions. In this work the conducting structures are fabricated over an electron transparent window of amorphous silicon nitride and proximal heat sink structures act to mitigate the effects of Joule heating. Many lines can be tested in parallel under nominally identical or varied thermal and geometrical parameters, and finite element modelling is used to calculate the temperature distribution over the sample geometry. The *in-situ* technique allows for real time observation of resistance change and microstructural evolution to monitor EM in bulk and record the nucleation and growth/migration of voids. In this work we show observations of *in-situ* Co electromigration under accelerated testing conditions with a focus on the microstructural origins and morphological evolution of EM voids. Our experimental parameter space covers the range of temperature from 30°C to 1000°C and current density up to 1×10^7 A cm⁻². This will contribute to a microstructural understanding and model of EM in low dimension Co structures across a wide range of temperature, current, and geometric conditions. Acknowledgements: This work was supported by the NYSTAR Focus Center at RPI, C150117 (not sure if this is current), and made extensive use of cleanroom and characterization facilities in the Center for Materials, Devices and integrated Systems (cMDIS) at RPI.

3:10 PM REFRESHMENT BREAK

SESSION BB: Nanofabrication

Session Chairs: Daniel Ewing and Patrick Shea
Thursday Afternoon, June 27, 2019
Michigan League, 2nd Floor, Michigan

3:30 PM BB01

(Student) Simple and Cost-Effective III-V Compound Semiconductor Nanofabrication via Metal-Assisted Chemical Etching Thomas S. Wilhelm^{1,2}, Alex P. Kolberg³, Zihao Wang¹, Cody W. Soule⁴, Mohadeseh A. Baboli^{1,2}, Jian Yan⁵, Stefan F. Preble^{1,4} and Parsian Katal Mohseni^{1,4,2}; ¹Microsystems Engineering, Rochester Institute of Technology, Rochester, New York, United States; ²NanoPower Research Laboratories, Rochester, New York, United States; ³Physics, Rochester Institute of Technology, Rochester, New York, United States; ⁴Microelectronic Engineering, Rochester Institute of Technology, Rochester, New York, United States; ⁵Matrix Opto Co., Ltd., Suzhou, China.

Metal-assisted chemical etching (MacEtch) techniques are solution-based semiconductor processing methods, capable of revolutionizing wafer-scale III-V nanofabrication towards overcoming many difficulties that arise

from commonly incompatible or inefficient top-down etching, or expensive bottom-up growth approaches. MacEtch and inverse-MacEtch (I-MacEtch) combine many attractive processing advantages, including the simplicity and cost-efficiency of conventional wet-chemical etching, and the ability to yield high aspect-ratio structures that are typically generated via reactive-ion etching. Moreover, MacEtch is not hindered by many common fabrication limitations, such as the isotropic or crystallographic tendency of traditional wet etching, and the detrimental sidewall damage and lattice defects that stem from high energy ion bombardment during dry etching. MacEtch samples consist of a thin metallic catalyst layer (e.g., Au, Ag, or Pt) in intimate contact with a semiconductor. The metal-interfaced semiconductor is then submerged in an etching solution containing an acid (e.g., hydrofluoric acid or sulfuric acid) and an oxidant (e.g., hydrogen peroxide or potassium permanganate). Fundamentally, MacEtch mechanisms are modelled after a galvanic cell; that is, cathodic and anodic half reactions occur at the solution/catalyst and catalyst/semiconductor interfaces, respectively. The metal catalyzes the reduction of oxidant species within the solution, thereby locally injecting holes into the interfaced substrate. Preferential dissolution of the selectively oxidized material realizes high aspect-ratio structures using solution-based processing. While this process is most commonly utilized for Si processing, MacEtch fabrication of two key ternary compound III-V material systems is demonstrated here, including Au-enhanced InGaP and AlGaAs. Firstly, I-MacEtch of heteroepitaxial InGaP/GaAs is presented, and differential etch rates between epilayer and substrate are exploited as a viable method to produce suspended III-V nanofoils. Secondly, I-MacEtch of AlGaAs is reported for fabrication of ordered nanopillar arrays, whose aspect-ratio is shown to be tunable with Al fraction (x) and etching temperature (T). Finally, an entirely solution-based and lithography-free MacEtch process is demonstrated for fabrication of black GaAs composed of sub-wavelength-dimension nanostructures yielding less than 5% reflectance. The work detailed here provides simple, low-cost, and efficient means to customize nanofabrication processes for specific needs. It is anticipated that these methods can be utilized for adaptable and versatile processing of nanomaterials for LEDs, lasers, HEMTs, and solar cells.

3:50 PM BB02

(Student) Silicon Waveguide Fabrication by Metal-Assisted Chemical Imprinting Aliaksandr Sharstniou¹, Stanislaw Niazorau¹, Michael Gregory¹, Neil Krueger², Matthew Puckett² and Bruno Azeredo¹; ¹Arizona State University, Mesa, Arizona, United States; ²Honeywell Aerospace, Plymouth, Minnesota, United States.

Si waveguides are routinely fabricated by direct-write lithography techniques followed by reactive plasma etching. Delivering sub-100 nm resolution, 3D patterning capabilities and sub-5 nm sidewall roughness to meet the stringent requirements for waveguide performance has been a challenge for most lithographical routes. Metal-assisted chemical imprinting (MAC-Imprinting) [1] is a novel silicon patterning method developed by the authors to enable 3D patterning of silicon with nanoscale resolution. In this method, a large-area catalytic stamp possessing 3D features and a silicon wafer are brought in contact while immersed in an aqueous mixture of hydrofluoric acid (HF) and hydrogen peroxide (H₂O₂) as in the well-known metal-assisted chemical etching process (MACE). After enough time in contact, the stamp's 3D shape and nanoscale features are carved into the silicon substrate. In this work, we demonstrate for the first time the fabrication of Si waveguides by MAC-Imprinting. Stamps for MAC-Imprinting were fabricated of SU-8 photoresist using replica molding [2] of an e-beam written mold followed by UV nanoimprint lithography of SU-8 thin-films and magnetron sputtering of the catalyst thin film onto it. MAC-imprinting of prepatterned silicon-on-dioxide (SOI) wafers was carried out in solutions of HF and H₂O₂ with different etchant ratios. The imprinted waveguide features have width of 960 nm and an embedded on-axis sinusoidal grating with a period of 264 nm which is evidence that nanoscale features can be manufactured with reproducibility by MAC-imprinting. The overall implementation of MAC-Imprint as wet chemistry-based solution to patterning silicon will be discussed in the context of critical manufacturing challenges such as stamp wear, substrate damage, reproducibility and diffusion limitations. The high resolution along with a high throughput associated with MAC-Imprint can be a solution for scaling production of silicon waveguides and related 3D silicon photonic devices. **REFERENCES** [1] B. P. Azeredo, Y.-W. Lin, A. Avagyan, M. Sivaguru, K. Hsu, P. Ferreira. *Adv. Funct. Mater.*, 26, 2929 (2016). [2] K. Kwapiszewska, K. Zukowski, R. Kwapiszewski, Z. Brzozka. *AIMS Biophysics*, 3, 553 (2016).

4:10 PM BB03

(Student) Novel Vapor-Phase Passivation of (100) Germanium Surfaces with HBr Alex Molina², Jeffery Shallenberger¹ and Suzanne Mohney²; ¹Materials Research Institute, Pennsylvania State University, University Park, Pennsylvania, United States; ²Pennsylvania State University, State College, Pennsylvania, United States.

Germanium (Ge) has received attention as an alternative p-type channel material for metal oxide semiconductor field effect transistors due to its high hole mobility. To fabricate high-performance devices, the interface between Ge and the gate dielectric must be carefully prepared, with minimal etching/roughening and unintended interfacial contaminants.¹ Moreover, novel nanostructures of Ge also require careful treatment of the surface (or passivation) to allow us to interrogate their size-dependent electronic and optical properties. Due to its superior ability to remove the native oxide SiO₂ from Si, treatment of Ge in aqueous hydrofluoric acid (HF) has been studied extensively.²⁻⁴ However, treating the Ge surface with HF leaves residual Ge oxides or suboxides on the surface, and the H-terminated surface is not stable in air. This situation is undesirable for device integration. Germanium wafers treated with concentrated HCl, another hydrohalic acid, exhibited some removal of oxides from the surface, but the Ge reoxidized within 10 minutes in ambient air.³ Onsia *et al.*⁴ compared several treatments (H₂O₂, HF, HCl, HBr, and HI) and found that HBr and HI were the most effective for removing the native oxides. However, wet processing can be destructive when working with three-dimensional nanostructures; rather, vapor-phase processing allows for easier sample handling and reduced hazardous waste.⁵ In this investigation, hydrobromic acid (HBr) was used to remove the native oxide and passivate an undoped (100) Ge wafer with n-type conductivity and a resistivity of 50 Ω•cm. First, the Ge wafers were degreased and rinsed in deionized (DI) H₂O, which dissolves GeO₂. Next, the wafers were exposed to vapors above solutions with 20% and 48% HBr concentrations. Once treatment was complete, samples were immediately introduced into the x-ray photoelectron spectroscopy (XPS) load lock, then transferred into the analysis chamber with a base pressure of 3.75 x 10⁻¹⁰ Torr. The XPS system has a monochromatic Al Kα x-ray source, and samples were inclined at an angle of 45° with respect to the spectrometer. For exposures of at least 20 min above the 48% HBr solution, we found a clear reduction in the amount of oxide present compared to only degreasing and rinsing with DI H₂O. On the other hand, treatment in Br₂ vapor alone was ineffective at reducing the amount of native oxide on the Ge surface. Interestingly, stability against reoxidation in air was greatly improved for longer exposures to HBr vapor, and XPS reveals that bromine is adsorbed onto these surfaces. Although we have discovered that HBr vapor is effective at passivating Ge from reoxidation, the small amount of residual oxide initially remaining after treatment might be removed by eliminating water present during vapor-phase processing, suggesting that gaseous anhydrous HBr could be even better for our process. Future research will also focus on understanding the long-term stability of passivated surfaces in air.

4:30 PM BB04

A New Fabrication Method for Self-Inflating Floating Nanofiber Membranes Serdar Tort^{1,2}, Daewoo Han¹ and Andrew Steckl¹;

¹Nanoelectronics Laboratory, Electrical Engineering and Computer Science, University of Cincinnati, Cincinnati, Ohio, United States;

²Faculty of Pharmacy, Gazi University, Ankara, Turkey.

Electrospinning is a versatile method for producing nanofibers from synthetic or natural polymers. Recently, many nanofiber-based devices were developed in different areas such as filtration, sensor, energy storage/generation, paper-based devices and pharmaceutical applications. Oral drug delivery is very convenient and useful approach for treating chronic diseases, but it requires frequent dosage consumption because of the short effective period. Floating drug delivery systems (FDDS), which enables sustained oral drug delivery, can be developed by effervescent system. When effervescent FDDS is in contact with the acidic gastric contents, CO₂ gas is generated and becomes entrapped within swollen hydrocolloids, providing buoyancy to the dosage forms. Electrospun nanofiber membrane have a porous structure, but these micro-pores are sufficiently small to trap large gas bubbles inside. Therefore, electrospun nanofibers are a good candidate to develop an effervescent FDDS. In this study, we have investigated nanofiber-based floating drug delivery systems with different Eudragit polymers. Sodium bicarbonate (NaHCO₃) is incorporated into thin PEO films to generate gas bubbles when reacting with acidic stomach fluid. A polymer solution, containing 6 % PEO and 2 % NaHCO₃ in water, was mixed in rotating shaker for 24 h. After homogenizing the polymer solution, it was casted on a glass slide and allowed to evaporate for 24 h. The dried cast films were cut with a circular metallic die with 3 mm diameter. This cast film is sandwiched between electrospun nanofiber membranes incorporating Keyacid Red XB

(KAR) dye as a model drug. Electrospinning solution was formed using Eudragit RL and RS and KAR dye dissolved in ethanol:DMAc mixture for 24 h. In order to eliminate the effect of process parameters on nanofiber properties, formulations with different Eudragit polymer ratio were produced with the same electrospinning parameters of a 14 kV applied bias, a needle-tip to collector distance of 18 cm, and a flow rate of 0.15 mL/h. After electrospinning 200 μL of dye-polymer solution, PEO/NaHCO₃ cast films were placed on electrospun nanofiber membrane and the electrospinning process was continued with an additional 200 μL of dye-polymer solution. In this process, NaHCO₃ films were embedded within nanofiber membranes without requiring a molding process. For the characterization of dye loaded floating the electrospun membranes were characterized using SEM to obtain the surface morphology and to measure mean nanofiber diameter. Nanofibers have uniform and smooth surfaces with no beads. The mean nanofiber diameter increased from 162 to 291 nm by decreasing Eudragit RL concentration. The water contact angle of the membranes was measured using an optical tensiometer. Increasing of Eudragit RS concentration increased the contact angle of formulations from 114° to 127° which is related to the relatively more hydrophilic nature of Eudragit RL compared to Eudragit RS. In vitro release studies of dye were conducted in acidic medium (pH 1.2) to mimic gastric conditions. The released dye concentration was measured spectrophotometrically using Nanodrop One UV-Vis spectrophotometer. As expected, increasing the Eudragit RS concentration slowed the release of the dye. Floating lag times and total floating times of the combined fiber/film structure with various formulations were measured visually and ranged from zero second and more than 24 hours, respectively. In conclusion, floating nanofibers are promising controlled drug delivery systems. Further studies are needed to show the performance of this system with different hydrophilic or hydrophobic drugs.

4:50 PM BB05

(Student) Graphene Self-Folding by AFM Scanning Sunghyun Kim¹, Jegyeong Yeon¹, Ha-Jun Sung², Kee Joo Chang², Xiaoqin Li³, Jee Soo Chang⁴ and Suenne Kim⁴; ¹Applied Physics, Hanyang University, Ansan, Korea (the Republic of); ²Physics, KAIST, Daejeon, Korea (the Republic of); ³Physics, The University of Texas at Austin, Austin, Texas, United States; ⁴Photonics and Nanoelectronics, Hanyang University, Ansan, Korea (the Republic of).

Folded graphene nanostructures have been proposed to exhibit unique electrical, mechanical, and optical properties. Their overall characteristics can vary dramatically with the number of folds or rotational misalignment between adjacent layers. What if one could draw a straight line on a graphene monolayer and induce a self-fold along the line? In this presentation, we introduce such an extraordinary type of self-folding occurred in monolayer graphene¹. The graphene self-folding can be achieved by AFM scanning under a sufficient normal force large enough to overcome the interfacial adhesion between the substrate and graphene. This simple folding method does not require multiple processing steps or any polymerization that could affect the electronic properties of graphene. In addition, with the method, the self-folding occurs along the armchair or zigzag direction in the presence of cracks in the vicinity. The resulted folded graphene nanostructures (nanoribbons) are on the order of tens of nanometers with atomically sharp edges. This new folding method can be applied to other 2-dimensional van der Waals materials and lead to nanostructures that exhibit novel electronic properties. [1] J. S. Chang, S. H. Kim, H.-J. Sung, J. Yeon, K. J. Chang, X. Li, S. Kim, *Small*, 14, 1803386 (2018). *This work was supported by National Research Foundation (NRF) of Korea grant funded by the Korea Government (2017R1D1B04036381).

SESSION CC: 2D Material Heterostructures and Optical Properties

Session Chairs: Soaram Kim and Rachel Koltun

Thursday Afternoon, June 27, 2019

Michigan League, 2nd Floor, Vandenberg

1:30 PM CC01

Functional van der Waals Heterojunctions by Low-Temperature Epitaxial Growth of SnS on MoS₂ Jack Olding¹, Alex Henning¹, Qunfei Zhou¹, Jason Dong¹, Michael Moody¹, Pierre Darancet^{1,2}, Emily Weiss¹ and Lincoln Lauhon¹; ¹Northwestern University, Evanston, Illinois, United States; ²Argonne National Laboratory, Lemont, Illinois, United States.

It is well established that two dimensional or van der Waals (vdW) materials can be combined arbitrarily by mechanical stacking to produce completely new classes of atomically thin devices and materials. Indeed,

mechanical stacking provides a convenient way to explore single devices on the laboratory scale, creating a wealth of opportunities for condensed matter physicists. For vdW materials to gain wider relevance and application, however, scalable approaches to both materials and heterojunctions are needed. Furthermore, considering the scale and leverage that might be gained by integrating vdW materials and devices with existing technologies including silicon based CMOS and organic flexible electronics, it is important to develop growth processes that are well tested in industry and do not require extreme temperatures. To that end, p-type tin sulfide (SnS) was grown epitaxially on n-type molybdenum disulfide (MoS₂) by pulsed metal-organic chemical vapor deposition at 180 °C. Despite the dissimilar crystal structures, orthorhombic SnS grows on hexagonal MoS₂ by “rotationally commensurate epitaxy”. Electron backscatter diffraction measurements show the existence of two equivalent crystal orientations, and density functional theory calculations provide insight into how certain orientations of the crystals maximize (minimize) the occurrence of local favorable (unfavorable) interactions between atoms in the layers across the interface. Studies of the influence of precursor pulse and purge times on film morphology establish growth conditions that favor layer-by-layer growth of SnS, which is critical for materials with layer-dependent electronic properties. To confirm the formation of a functional *p-n* junction, Kelvin probe force microscopy measurements (KPFM) were conducted on bare MoS₂ and SnS on MoS₂ both in the dark and under illumination. In the dark, the built-in potential is as high as 0.9 eV, though the influence of atmospheric adsorbates on this value needs to be considered. Illumination results in the generation of a surface photovoltage across what is proposed to be a type-II heterojunction. DFT calculations of monolayer heterojunctions agree with the band structure derived from KPFM measurements.

1:50 PM CC02

Encapsulation Narrows and Preserves the Intrinsic Exciton Linewidth in MoSe₂ Semiconducting Monolayer Eric Martin^{1,2}, Jason Horng¹, Hanna G. Ruth¹, Eunice Paik¹, Michael-Henr Wentzel¹, Hui Deng¹ and Steven T. Cundiff¹; ¹University of Michigan, Ann Arbor, Michigan, United States; ²Monstr Sense Technologies, Ann Arbor, Michigan, United States.

Semiconducting monolayer transition metal dichalcogenides (TMDCs) are a new class of materials with the potential to transform future electronics and optoelectronics. However, they are known to have widely varying excitonic linewidths that are dependent on the local environment, excitation source, and sample history (i.e. temperature cycles and exposure to laser radiation). Many of these inconsistencies seem to have been remedied by encapsulation of the monolayer in hexagonal boron nitride (hBN), which both controls the dielectric environment and protects the TMDC. Encapsulation has also led to photoluminescence linewidths that approach previous homogeneous linewidth measurements of non-encapsulated samples [1]. We fully characterize the excitonic linewidths that determine the functionality of TMDCs for use in light absorption and light emission. Specifically we use multidimensional coherent spectroscopy (MDCS) to measure the homogeneous excitonic linewidth of exfoliated monolayers of MoSe₂, and we show that MDCS is much more sensitive to material changes than conventional optical measurements. The MDCS instrument, which has micron spatial resolution, enables characterization of the optical and coherence properties of new materials. The measurements of encapsulated MoSe₂ indicate that it has an enhanced coherence time and would be useful in high optical power applications, where non-encapsulated samples would not. The linewidth is 0.26 +/- 0.02 meV, corresponding to a dephasing time T₂ ~ 2.5 ps, which is almost half the narrowest reported values for non-encapsulated MoSe₂ flakes. Measurements of encapsulated and non-encapsulated monolayers demonstrate that encapsulation reduces the sample inhomogeneity. However, the inhomogeneous linewidth, which limits photoluminescence and linear absorption spectroscopic measurements, is roughly 5 times larger than the homogeneous linewidth in even the highest-quality encapsulated materials. The homogeneous linewidth of non-encapsulated monolayers is very sensitive to temperature cycling, whereas encapsulated samples are not modified by temperature cycling. The nonlinear signal intensity of non-encapsulated monolayers is degraded by high-power optical excitation, whereas encapsulated samples are very resilient to optical excitation with optical powers up to the point of completely bleaching the exciton. We have therefore used a very sensitive spectroscopy to indicate that non-encapsulated samples are more strongly affected by radiation and temperature cycling than previously thought. Encapsulated samples are sufficiently robust to the point that these materials may be used in laser and photovoltaic applications. REFERENCES [1]. E. Cadiz *et al.*, *Phys. Rev. X* **7**, 021026 (2017).

2:10 PM CC03

Indirect Transition and Opposite Circular Polarization of Interlayer Exciton in a hBN Encapsulated MoSe₂/WSe₂ van der Waals Heterostructure Hsun Jen Chuang, Aubrey Hanbicki, Matthew R. Rosenberger, C. S. Hellberg, Saujan Sivaram, Kathleen McCreary, Igor I. Mazin and Berend T. Jonker; Materials Science & Technology, U.S. Naval Research Laboratory, Washington, District of Columbia, United States.

An emerging class of heterostructures involves monolayer semiconductors such as many of the transition metal dichalcogenides (TMDs) which can be combined to form van der Waals heterostructures (vdWHs). One unique new heterostructure property is an interlayer exciton (ILE), a spatially indirect, electron-hole pair with the electron in one TMD layer and the hole in the other. Here, we use state-of-the-art preparation techniques to create MoSe₂/WSe₂ heterostructures encapsulated in hBN. We observe ILE emission around 1.35 eV at room temperature and resolve this emission into two distinct peaks (ILE1 and ILE2) separated by 24 meV at zero field at 5 K. Furthermore, we demonstrate that the two emission peaks have *opposite* circular polarizations with up to +20% for the ILE1 and -40% for ILE2 when excited by circularly polarized light. *Ab initio* calculations provide an explanation of this unique and potentially useful property and indicate that it is a result of the indirect character of *both* electronic transitions. These peaks are *double indirect* excitons. *i.e.* indirect in both real and reciprocal space, split by relativistic effects.

2:30 PM CC04

(Student) Topological Insulator/Hexagonal Boron Nitride/Topological Insulator Epitaxial van der Waals Heterostructures for Tunneling Spectroscopy Between Topological Surface States Joon Young Park¹, Young Jae Shin², Janghyun Jo³, Jeacheol Shin¹, Jehyun Kim¹, Hyobin Yoo², Jaeun Eom¹, Kenji Watanabe⁴, Takashi Taniguchi⁴, Dohun Kim¹, Miyoung Kim³, Philip Kim² and Gyu-Chul Yi¹; ¹Physics and Astronomy, Seoul National University, Seoul, Korea (the Republic of); ²Physics, Harvard University, Cambridge, Massachusetts, United States; ³Materials Science and Engineering, Seoul National University, Seoul, Korea (the Republic of); ⁴National Institute for Materials Science, Tsukuba, Japan.

Van der Waals (vdW) heterostructures composed of various two-dimensional (2D) materials serve as novel platforms to explore a wide variety of interesting physical properties and device applications. One of the most intriguing systems is a highly crystalline and atomically thin insulating barrier sandwiched between 2D vdW layered materials, since tunneling spectroscopy applied to the heterostructure provides a powerful tool to probe the density of states of the materials and vertical transport across the vdW interface. For example, precisely aligned two graphene layers separated by a hexagonal boron nitride (hBN) barrier layer made it possible to detect and manipulate energy-, momentum-, and chirality-conserved tunneling of Dirac fermions in graphene. (Bi, Sb)₂(Te, Se)₃ topological insulators (TIs), on the other hand, have vdW layered structures with topologically non-trivial surface states which possess great potential for applications in spintronics and topological quantum computations. TIs brought into close proximity with each other across only a few atomic barriers and tunneling spectroscopy on the system would be highly attractive in this regard. Here, we present the fabrication and measurement of vertical tunnel junctions in which two epitaxially aligned TIs are separated by a few-atom-thick hBN tunnel barrier. Ultrathin hBN layers were transferred using micromanipulation to pre-patterned sub-micrometer holes in SiN_x membranes to expose both surfaces. Subsequently, Bi₂Se₃ and Sb₂Te₃, *n*- and *p*-type TIs, respectively, were grown on both sides of the suspended hBN using molecular beam epitaxy, naturally forming vertical tunnel junctions whose interfaces were sealed under ultrahigh vacuum. High-resolution transmission electron microscopy revealed an atomically abrupt and epitaxial interface formation between the hBN substrate and top- and bottom-TIs. We performed magneto-tunneling spectroscopy of Sb₂Te₃/hBN/Bi₂Se₃ (*p*-TI/hBN/*n*-TI) and Bi₂Se₃/hBN/Bi₂Se₃ (*n*-TI/hBN/*n*-TI) junctions under in-plane and out-of-plane magnetic fields to investigate energy-momentum-spin resonance between the topological surface states (TSSs). We believe the results presented in this work paved a new way to investigate intrinsic momentum-space tunneling selection of electrons in the TSSs and to design new topological devices.

2:50 PM CC05

Highly Valley-Polarized Singlet and Triplet Interlayer Excitons in van der Waals Heterostructure Long Zhang¹, Rahul Gogna², G. W. Burg², Jason Horng¹, Eunice Paik¹, Yu-Hsun Chou¹, Kyoungwan Kim², Emanuel Tutuc² and Hui Deng¹; ¹Physics, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²The University of Texas at Austin, Austin, Texas, United States; ³Applied Physics, Univ of Michigan - Ann Arbor, Ann Arbor, Michigan, United States.

Two-dimensional semiconductors feature valleytronics phenomena due to locking of the spin and momentum valley of the electrons. However, the valley polarization is intrinsically limited in monolayer crystals by the fast intervalley electron-hole exchange. Hetero bilayer crystals have been shown to have a longer exciton lifetime and valley depolarization time. But the reported valley polarization was low; the valley selection rules and mechanisms of valley depolarization remains controversial. Here, we report singlet and brightened triplet interlayer excitons both with over 80% valley polarizations, cross- and co-polarized with the pump laser, respectively. This is achieved in a high-quality WSe₂/MoSe₂ hetero-bilayers with precise momentum valley alignment and narrow emission linewidth. The high valley polarizations allow us to identify the band minima in a hetero structure and confirm unambiguously the direct band-gap exciton transition, ultrafast charge separation, strongly suppressed valley depolarization. Our results pave the way for using van der Waals semiconductor heterostructures to control valley selection rules for valleytronic applications.

3:10 PM REFRESHMENT BREAK

3:30 PM CC06

Quantum Calligraphy—Writing Single Photon Emitters in a Two-Dimensional Materials Platform Berend T. Jonker¹, Matthew R. Rosenberger^{1,2}, Chandriker K. Dass^{3,5}, Hsun Jen Chuang^{1,4}, Saujan Sivaram^{1,2}, Kathleen McCreary¹ and Joshua Hendrickson³; ¹Materials Science & Technology, U.S. Naval Research Laboratory, Washington, District of Columbia, United States; ²Postdoctoral Fellow, National Research Council, Washington, District of Columbia, United States; ³Sensors Directorate, Air Force Research Laboratory, Wright-Patterson AFB, Ohio, United States; ⁴Postdoctoral Fellow, American Society for Engineering Education, Washington, District of Columbia, United States; ⁵KBRwyle, Beavercreek, Ohio, United States.

Single photon emitters (SPEs), or quantum emitters, are key components in a wide range of nascent quantum-based technologies, including computing, communications, sensing and metrology [1]. A solid state host offers many advantages for realization of a functional system, but single photon emission often originates from defects such as vacancy complexes whose existence and position are difficult to control with the reliability and nanoscale precision requisite for technological implementation. Recent work has identified SPE behavior from seemingly random sites in single monolayer transition metal dichalcogenides (TMDs) such as WSe₂. Subsequent work has demonstrated scalable array formation using a prefabricated pillar template over which a WSe₂ monolayer is mechanically draped, inducing a strain field in the TMD at the peak of each pillar to localize the SPE [2]. We describe here a novel paradigm for encoding strain into two dimensional materials (2DM) to create and deterministically place SPEs in arbitrary locations with nanometer-scale precision [3]. We demonstrate the direct writing of quantum emitters in two dimensional semiconductors using a materials platform consisting of a TMD layer on a deformable substrate. We use an atomic force microscope (AFM) to form nanoindentations in monolayer WSe₂ on a poly(methyl methacrylate) (PMMA) / SiO₂ / Si substrate with positioning accuracy limited by the AFM and the width of the nanoindent. We demonstrate the ability to control the depth of indentation by controlling the applied load and achieve good process repeatability. We show that quantum emitters are created and localized at these nanoindentations, and exhibit single photon emission up to 60K, the highest temperature reported for SPEs in TMD materials. These emitters are bright, producing photon rates of 10⁵/sec at low laser pump powers (~10 mW / μm²) with low spectral wandering. This *quantum calligraphy* allows deterministic placement and real time design of arbitrary patterns of SPEs for facile coupling with photonic waveguides, cavities and plasmonic structures. In addition to enabling versatile placement of SPEs, these results present a general methodology for imparting strain into 2DM with nanometer-scale precision, providing an invaluable tool for further investigations and future applications of strain engineering of 2D materials and devices. Our results also indicate that a nano-imprinting approach will be effective in creating large arrays or patterns of quantum emitters for wafer scale manufacturing of quantum photonic systems. [1] Aharonovich, I.; Englund, D.; Toth, M.; *Nat. Photonics* **2016**, *10*, 631. [2] Li, H. et al, *Nat. Commun.* **2015**, *6*, 7381. [3] Rosenberger, M.R. et al; *ACS Nano* **2019**, *13*, 904.

3:50 PM CC07

(Student) Lightwave Driven Valleytronic Qubit Flip Markus Borsch¹, Benjamin J. Girodias¹, Johannes T. Steiner², Stephan W. Koch², Christoph P. Schmid³, Stefan Schlauderer³, Fabian Langer³, Rupert Huber³ and Mackillo Kira¹; ¹University of Michigan, Ann Arbor, Michigan, United States; ²University of Marburg, Marburg, Germany; ³University of Regensburg, Regensburg, Germany.

Transition metal dichalcogenide monolayers show extraordinary properties, such as strongly bound excitons that can be pseudo-spin selected over a direct band gap. More specifically, a circularly polarized optical light dominantly excites one of the two (+K or -K) valleys, yielding valley-dependent pseudo-spin selection. We present comprehensive theory–experiment investigations demonstrating that an additional strong terahertz (THz) field can flip the pseudo-spin by moving the electron-hole excitation from one valley to the other [Nature **557**, 76 (2018)]. In particular, the resulting qubit flip can be realized on a sub-5fs timescale and be detected in polarization-direction changes in the harmonic sideband emission. This not only brings lightwave driven electronics to a new level but additionally reveals intriguing many-body Coulomb effects modified by interferences [Nature **523**, 572 (2015)]. Specifically, we study a tungsten-diselenide (WSe₂) monolayer where optically generated coherent excitons are driven by a strong THz field. In this setup, a pseudo-spin can be used as a qubit for quantum information applications only if it can be flipped faster than the pseudo-spin relaxation time (around 100 fs) and the coherent-exciton lifetime. Our microscopically computed coherent-exciton lifetimes indicate that the THz field must flip the coherent excitons faster than about 10 fs to be efficient. To provide precise predictions, we combine two first principles approaches. A density functional theory produces the electronic bands and matrix elements that we use in a dynamic cluster-expansion approach [Kira & Koch, *Semiconductor Quantum Optics*, (Cambridge, 2012)] to solve the THz-driven, extremely nonperturbative, many-body quantum kinetics *exactly* up to a desired particle number. While coherences and the qubit flip involve transporting single-particle clusters, the effect of two-body clusters and resulting many-body modifications is demonstrated to be decisive. Our calculations show that coherent excitons created in the +K valley can be moved almost completely to the -K valley by a strong THz field within 5 fs. This is clearly faster than any relevant decoherence or relaxation mechanism, making lightwave electronic switching of the qubit possible. Comparing excitonic momentum distributions before and after the transfer reveals intricate changes induced by the transfer. Specifically, the transported coherent exciton wave packet spreads, which indicates that initially generated 1s states become excited to many other excitonic states. Due to excitation induced effects, these new components will have a very different life time than the initially generated excitons. We will discuss how these yield distinct and detectable signatures in harmonic sideband emission. Especially, we will demonstrate that the Coulombic many-body interaction not only determines the exact change and transfer details, but that it strongly influences the harmonic sideband emission as well. Compared to harmonic sideband generation in bulk WSe₂ [Nature **533**, 225 (2016)], our theory–experiment comparison identifies distinct emission delays and quantum interferences with a direct link to strong Coulombic binding and scattering details. In conclusion, despite the fast dephasing and relatively fast relaxation in WSe₂ monolayers, we demonstrate that strong THz fields can be used to transfer electron-hole pairs efficiently from one valley to another, flipping the valley pseudo-spin. This elementary process may be used as a basis for lightwave driven quantum information technology at petahertz clock rates. We will also discuss how the resulting emission of harmonic sidebands assigns distinct features to directly measure novel many-body effects in strongly interacting two-dimensional materials.

4:10 PM CC08

(Student) Hyperspectral Absorbers with Semiconductor Monolayer Crystals Qiannan Wen¹, Xiaoying Lu², Ping Wang², David A. Laleyan², Eric T. Reid², Dylan Bayerl³, Emmanouil Kioupanis³, Zetian Mi² and Mackillo Kira²; ¹Applied Physics Program, University of Michigan, Ann Arbor, Michigan, United States; ²Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ³Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States.

Atomically thin semiconductors, such as transition metal dichalcogenide monolayers, are relatively new quantum materials with many demonstrations of strongly bound excitons [Nature **557**, 76 (2018)] and other quasiparticles [Nature **506**, 471 (2014)] due to only weakly screened Coulomb interaction. Recent theoretic computations [Appl. Phys. Lett. **109**, 241102 (2016)] also predict that monolayer gallium nitride can produce exciton binding energy in the excess of 200 meV, which implies

yet another intriguing quantum material with a strong excitonic absorption. Since GaN heterostructures can be grown with atomic precision, e.g. by using molecular beam epitaxy (MBE), one can directly expand experimental efforts to explore exciton coupling effects between multi-monolayer systems. We will present experimental evidence that MBE-grown GaN monolayers indeed have strong excitonic features, verified by our theory. We also discuss theoretical design results of assembling multiple monolayers into a period stack yielding monolayer 1D crystals with unique properties. Our computations show that the collective coupling between excitons can be designed to produce hyperspectral absorbers which harvest nearly 100% of light over the spectral range of the Sun. We will outline how such quantum materials could be utilized for artificial photosynthesis. Technically, we solve monolayer's optical response using semiconductor Bloch equations (SBEs) [Kira & Koch, *Semiconductor Quantum Optics*, (Cambridge, 2012)] coupled self-consistently to the Maxwell's equations. The approach systematically includes the relevant many-body effects, and allows us to make detailed predictions for monolayer absorption. As is well known, the maximum absorption of a single monolayer is 50% when the system is antireflection coated. This is under an ideal condition where many-body scattering induced nonradiative decay of polarization is equal to its radiative decay. Due to collective coupling between monolayers, we find that the absorption grows from 80% for two monolayers to above 95% for more than eight monolayers, all placed at a quarter-wavelength distance from one another for ideally matched radiative and nonradiative decay. Besides providing improved absorption, increasing monolayer number makes the peak absorption less sensitive to dephasing. Thus, our results show that high absorption levels could be reached for a large range of operational conditions with multilayer structures. Despite its high absorption peak, a stack consisting of identical monolayers has a relatively narrow absorption bandwidth. We demonstrate that a hyperspectral absorber can be realized by having multiple monolayer stack with different, chirped, energy centers. We will show that the found designs are robust against key operational parameters, and find above 90% absorption can be obtained from near infrared to ultraviolet spectral range. We will also show the possibility to minimize the size of the monolayer stacks by considering different stacking orders, monolayer spacing, and using the mirror to enhance the absorption by as few monolayers as possible. We also analyze the effect of sample imperfections by randomly changing properties of individual monolayers using a Monte Carlo method. We identify which configurations are stable against reasonable levels of imperfections. In summary, our results introduce the concept of compact hyperspectral absorber, built of monolayer crystals, that achieve nearly perfect flatband absorption robust to device imperfections.

4:30 PM CC09

(Student) Impact of H₂O Intercalation on Methyl Germanane Band Gap Luminescence Brenton A. Noesges¹, Thaddeus J. Asel¹, Warren Huey², Shishi Jiang², Kevin Krymowski³, Yaxian Wang³, Wolfgang Windl³, Josh E. Goldberger² and Leonard Brillson^{1,4}; ¹Physics, The Ohio State University, Columbus, Ohio, United States; ²Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio, United States; ³Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States; ⁴Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States.

Since the isolation of monolayer graphene, two-dimensional van der Waals materials persist as an exciting research area due their large surface-to-volume ratio, high free carrier mobility and ease of stacking with other 2D materials for modular device design. However, many of these materials are not air-stable which complicates characterization and device construction. Additionally, impurities between van der Waals layers can act as scattering centers and cause additional doping. Germanane, an air-stable germanium analogue to graphene, which unlike transition metal dichalcogenides (MoS₂, MoSe₂, WS₂...) always has a 1.6 eV direct bandgap that can be tuned by varying modifying the ligand group attached the Ge scaffold making germanane attractive for optoelectronic purposes [1]. Germanane, made by washing CaGe₂ with an acid chosen to leave behind the desired ligand termination, is sensitive to intrinsic and extrinsic factors which affects the electronic properties of the material. Point defects in the germanium scaffold and incomplete synthesis reactions can create electronically active states within the band gap [2]. Environmental factors like humidity, ambient pressure, and interlayer contamination will also modify observed electronically active states. We used a combination of bulk and surface-sensitive optical spectroscopies guided by density functional theory (DFT) calculations to identify defect states and observe how atmospheric conditions affect the electronic properties of germanane. Depth-resolved cathodoluminescence spectroscopy (DRCLS) collected in the near-infrared to near-ultraviolet range (0.7 eV to 5.5 eV) identified four mid-gap defect levels

while a complementary measurement, surface photovoltage spectroscopy (SPS), determined relative position of the defect level to the conduction and valence bands. The defect features do not vary with ligand indicating defects reside in the Ge scaffold. DFT confirms germanium mono- and divacancies with varying hydrogen termination induces defect levels at the observed transition energies. Pressure and humidity-controlled photoluminescence spectroscopy (PLS) also identifies how background pressure and inclusion of moisture significantly changes the measured electronic structure of germanane. PLS measurements collected in low vacuum are virtually identically to DRCLS collected in ultra-high vacuum (UHV) conditions [2]. Upon exposure to pressure above a few hundred millitorr, the original PL signal is altered until pumping is resumed. If the germanane is in a water-free gas (N₂, O₂, Ar...) the luminescence is quenched no new states forming. However, once H₂O is introduced by simply using air or bubbling the venting gas through water, a new hydrated state emerges with energy around 1.8 – 1.9 eV, larger than the original bandgap. The induced hydrated state can be removed by putting the germanane back into vacuum. Changes in the PL spectra are continuous as the system is vented/pumped making this germanane a candidate for humidity or pressure sensing. DFT calculations can again be combined with experimental results to provide a consistent explanation for water intercalation in germanane. This work supported by NSF MRSEC under award number DMR-1420451. [1] S. Jiang, K. Krymowski, T. Asel, M.Q. Arguilla, N.D. Cultura, E. Yanchenko, X. Yang, L.J. Brillson, W. Windl, J.E. Goldberger, *Chem. Mater.* **28**, 8071-8077 (2016). [2] T.J. Asel, E. Yanchenki, X. Yang, Shishi Jiang, Kevin Krymowski, Y. Wang, A. Trout, D.W. McComb, W. Windl, J.E. Goldberger, L.J. Brillson, *Appl. Phys. Lett.* **113**, 061110 (2018).

4:50 PM CC10

Band Alignment in Black-Violet Phosphorous Heterostructures Daniel Hashemi¹, Michael Snure² and Stefan C. Badescu¹; ¹Air Force Research Laboratory, Wright-Patterson AFB, Ohio, United States; ²Air Force Research Lab, Wright Patterson AFB, Ohio, United States.

Two-dimensional (2D) materials including graphene and phosphorene are attracting extensive attention due to their outstanding properties and wide range of applications in electronic and optoelectronic devices. In particular, the 2D phosphorus family provides a potentially exciting system to build devices from consisting of multiple semiconductors with a range of band gaps (0.3 to 3 eV). This materials system allows the unique opportunity to build van der Waals heterostructures using a single element, P. Heterostructures composed of black (BLK-P) and violet (V-P) phosphorous, which can be formed during bulk synthesis [1, 2] or through decomposition of BLK-P can be formed, which may exhibit unique physical properties important to various applications. Accurate modeling tools can help predict and assess the band alignment in these novel systems and at their interfaces with encapsulating materials like Boron nitride (BN), protecting the conduction channel via encapsulation with wide-bandgap quasi-2D materials. Understanding of band alignment in these heterostructures is of great importance to their electronic properties and potential applications in the field of nanoelectronic devices. Here, we investigate the bandgaps of several materials and their band alignments using accurate density functional theory (DFT) with the Heyd-Scuseria-Ernzerhof (HSE) XC functional and added Van der Waals interactions. The method is validated using known bandgaps for BLK-P, phosphorene, and other wide-bandgap 2D materials such as hBN. The bandgaps vary widely between allotropes. Their band alignment is modeled, offering insights into tunneling barrier heights in prospective devices. [1] Z. Zhang, D.H. Xing, J. Li, Q. Yan "Hittorf's phosphorus: the missing link during transformation of red phosphorous to black phosphorus" *CrystEngComm*, 2017, 19, 2017. [2] M. Snure "Violet/black phosphorus van der Waals heterojunction emitters", in preparation.

SESSION DD: Thermoelectrics and Thermal Transport Session Chairs: Alexandra Zevalkink and Joshua Zide Thursday Afternoon, June 27, 2019 Michigan League, 3rd Floor, Room D

1:30 PM DD01

Interplay Between Chemical Bonding and Thermal Transport in Layered Zintl Phases Alexandra Zevalkink; Michigan State University, East Lansing, Michigan, United States.

Layered AMg₂Pn₂ Zintl compounds have received a great deal of attention recently due to their excellent thermoelectric properties. In particular, the binary compound MgMg₂Sb₂ exhibits zT values up to 1.6,

due to its n-type dopability, high band degeneracy, and anomalously low lattice thermal conductivity. Here, we explore the role that the cation plays in determining the elastic moduli and thermal properties in AMg_2Pn_2 compounds (Pn = Sb or Bi and A = Mg, Ca, Sr, Ba, Yb, Eu, Sm). Temperature-dependent resonant ultrasound spectroscopy, inelastic neutron scattering, and Raman spectroscopy were used to investigate the bond strength and rate of bond softening, while phonon calculations within the quasi-harmonic approximation were used to obtain the mode Grüneisen parameters. Our results show that the binary compounds MgMg_2Sb_2 and MgMg_2Bi_2 stand out as having anomalously soft shear moduli and large mode Grüneisen parameters, which we attribute primarily to the size of the Mg cations. Mg is too small for the 6-fold octahedral coordination with Sb or Bi, leading to weak interlayer bonds, highly anharmonic transverse acoustic phonon modes, and high rates of Umklapp phonon-phonon scattering. The consequence is that, despite its low mass, the small Mg cation on the A site leads to lattice thermal conductivity drastically lower than that of heavier isostructural compounds.

1:50 PM DD02

Thermoelectric Properties at Near Room Temperature on Mg_2Sn Thin Film Co-Doped with Ag and Cobalt Mikihiko Nishitani and Yukihiro Morita; Engineering, Osaka University, Suita, Japan.

The thermoelectric battery for wearable device working at near RT has been reviewed with the arrival of the Internet of Things (IoT) society. For such applications, thin film materials and devices without toxicity are suitable due to the easy contact to the heat source, especially human body. The Mg_2X (X = Si, Sn) is one of promising material to make such a device of thermoelectric energy generation and to replace the Bi-Te material system since it is made of abundant and low-cost elements without toxicity [1]. We have already presented on the thin film Mg_2X (X = Si, Sn) deposited by conventional magnetron sputtering system [2-3]. Although it is limited to p-type thin film materials, we found that by coating a Ag thin film on a substrate in advance, the quality of the Mg_2Sn thin film can be improved due to liquid phase layer created by the interaction with Ag and incident Sn flux on the substrate. When the Mg_2Sn thin film with the thickness of 2-3micron m is formed at a substrate temperature of 550 °C on a substrate on which an Ag thin film of about 100 nm is formed in advance, the crystallinity is improved as compared with the case where the Ag precoat film is absent, and Ag doping evenly in the Mg_2Sn thin film can be carried out. The maximum value of the PF factor at 300 K is 221 $\text{mWm}^{-1}\text{K}^{-2}$ obtained from the Ag-doped thin film at Mg / Sn ratio 2 (near the stoichiometric composition). In this study, we report the results that we try to make further improvements on the thermoelectric properties, based on the successful results. To improve the performance of p-type thermoelectric materials, we considered the addition of elements that can contribute to the electronic state near the top of the valence band with 3d orbital electron. So, we studied the dependency of DOS on the valence band of the Mg_2Sn thin film as a function of the amount of Cobalt added. We have confirmed experimentally that adding Cobalt to Mg_2Sn contributes to DOS in its valence band. That means that there is a possibility of improving the Seebeck coefficient according to Mott's formula. Based on the above experimental information, we moved to next step to try to further improve the thermoelectric characteristics of the Mg_2Sn thin film by combining the process of precoating the Ag thin film (which can improve the crystallinity of the Mg_2Sn thin film) and Cobalt addition. Experimentally, we have the graphs which are shown the Seebeck coefficient, the electric conductivity and the PF with the Ag amount (abscissa) and the Cobalt amount (ordinate) in the Mg_2Sn thin film obtained from the XPS measurement, respectively. All Mg_2Sn : Ag, Co thin films prepared by the process used in this study showed p-type conduction, and the PF, which is important for thermoelectric properties, is relatively higher in the region where the Ag content is 0.5-1.5 atomic% and the Cobalt content is 5-6 atomic %. So far, in our Mg_2Sn :Ag thin film, the highest PF at RT is 221 $\text{mWm}^{-1}\text{K}^{-2}$, but as a result of further attempting to add Cobalt, 481 $\text{mWm}^{-1}\text{K}^{-2}$ is obtained as the highest value in the Mg_2Sn :Ag,Cobalt thin film. We speculate that Cobalt addition to the Mg_2Sn thin film greatly increased the hole concentration but at the same time it suppressed the decrease in the Seebeck coefficient. To compare our data with data from other research institutions, we add our data in Fig.1 which is edited by quoting Figure 5(c) shown in reference 4. References 1. V.K.Zaitsev, M.I.Fedorov, E.A.Gurieva, I.S. Eremin, P.P. Konstantinov, A. Yu. Samunin, M.V. Vedernikov, Phys.Rev. B74,045207 (2006). 2. Y. Morita, Y.Hayashi, H.Tsuchiura, M.Nishitani, Material.Res.Soc.Symp. Proc.1642 (2014) | DOI:10.1557/opl.2014.544. 3. Mikihiko Nishitani, Katsuki Yokoyama, Yukihiro Morita, Tetsui Kurashiki, MRS advances, 1(60) 3977 (2016). 4. Chunlei Wan, Ruoming Tian, Mami Kondou, Ronggui Yang, Pengan Zong, and Kunihito Koumoto, NATURE COMMUNICATIONS | DOI: 10.1038/s41467-017-01149-4.

2:10 PM DD03

(Student) Plasmonic Multicomponent Aerogels for Solar Thermal Energy Conversion Zachary Berquist¹, Ashley R. Bielinski², Andrew Gayle², Hannah Kim¹, Neil P. Dasgupta² and Andrej Lenert¹; ¹Chemical Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Mechanical Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

Visibly-transparent silica aerogels are a promising alternative to vacuum insulation in solar thermal applications such as concentrated solar power (CSP). However, they are characterized by undesirable thermal radiative transmission in the mid-infrared. Here, we experimentally and computationally investigate multicomponent aerogels which selectively enhance infrared absorption and, in turn, suppress outgoing radiative losses at high temperatures. We incorporated aluminum-doped zinc oxide (AZO) into silica aerogels using Atomic Layer Deposition (ALD). ALD facilitated conformal deposition of the film into the nanoporous template, enabling tunable AZO thickness and composition within the bulk of the aerogel. The effect of the AZO on the optical and thermal properties of the aerogels were characterized using UV-Vis-NIR, ellipsometry, FTIR, and hot-disk techniques. We demonstrate that these multicomponent aerogels absorb more broadly in the infrared. Moreover, the addition of the AZO component leads to a plasmon resonance in the mid-infrared. We also experimentally demonstrate a significant decrease in heat losses at CSP-relevant temperatures (500-700 °C) with the use of multicomponent (AZO/SiO₂) aerogels. The measurements agree with our simulations of coupled radiative and conductive heat transfer. These results suggest that plasmonic multicomponent aerogels have the potential to significantly improve the performance of low-irradiance, high-temperature solar receivers.

2:30 PM DD04

(Student) Thermal Transport in Sapphire Irradiated by Swift Heavy Ions Vinay S. Chauhan¹, Azat Abdullaev², Zhandos N. Utegulov² and Marat Khafizov¹; ¹Mechanical and Aerospace Engineering, The Ohio State University, Columbus, Ohio, United States; ²School of Science and Technology, Physics Department, Nazarbayev University, Astana, Kazakhstan.

Ion implantation has been extensively used as a method to introduce dopants into semiconducting materials to tailor their electronic properties. The impact of accelerated particles causing displacement damage on structural and electronic properties have been extensively studied. Very few studies have considered the impact of the displacement damage on thermal conductivity, primarily due to difficulty in measuring thermal conductivity in thin damaged layers limited to few hundreds of nanometers if the energy of the implanted particle is below 1 MeV. Irradiation by swift heavy ion (SHI) with energies on the order of 100 MeV derived from high energy accelerators has been used to emulate the structural damage caused by the energetic particle in a nuclear reactor environment. It can also be used to tailor material properties over several microns thick layers owing to their much larger penetration depth. In the case of SHI, the bombarded particle interacts with the electrons of the target atoms. This leads to intense localized thermal spikes causing displacement of lattice atoms around a cylindrical core (ion track) along the ion path. The ordered structure of ion tracks is expected to result in properties not previously observed. In this work, we are particularly interested in the impact of SHI irradiation on thermal properties of insulating aluminum oxide (sapphire) as a model system where thermal transport is governed by lattice vibrations. Aluminum oxide is considered as a window transparent to electromagnetic wave across a broad range in extreme environments that are subject to irradiation by energetic particles. Therefore, the impact of radiation damage on its dielectric and optical properties and structural stability have been widely studied. This makes it an attractive candidate for studying thermal transport. Sapphire was irradiated by 167 MeV Xe SHI at $10^{12} - 10^{14}$ ions/cm² fluences. Stopping and Range of Ions in Matter (SRIM) simulations were performed to identify different damage regions associated with electronic and nuclear stopping of ions. The thickness of damaged region was calculated to be ~11 μm. The thermal conductivity was measured using the modulated thermoreflectance techniques such as time-domain thermoreflectance (TDTR) and spatial-domain thermoreflectance (SDTR). These techniques are based on optical pump-probe configuration where pump laser heats the sample and reflectivity change of probe is used to monitor temperature changes on the surface. Limited penetration of thermal waves in these thermoreflectance approaches makes them useful for studying the impact of ion beam damage on thermal transport properties. Especially when these approaches are coupled with Raman spectroscopy the defects in the material can be identified and quantified. Our measurements revealed a notable reduction in thermal conductivity. Depth-resolved measurements

achieved by varying the modulation frequency of the pump laser beam allowed us to extract the thermal properties of different damage layers. Low dose (10^{12} ions/cm²) irradiations reduced thermal conductivity by ~50% in the damaged zone. In the case of high dose samples, a more complex damage profile was observed characterized by an amorphous layer of 85 nm and 165 nm for ion dose of 5×10^{13} and 1×10^{14} ions/cm², respectively. The conductivity of the amorphous layer was found to be 1.4 W/mK, a value comparable to theoretical estimated of minimum conductivity in sapphire. The changes in the thermal conductivity of the damaged layer were analyzed quantitatively using the classical thermal transport model to understand the impact of ion-tracks on thermal transport.

2:50 PM DD05

(Student) Pressure Tuning of Thermal Properties Measured by Transient Thermoreflectance in Diamond Anvil Cell Xianghai Meng¹, Tribhuwan Pandey⁵, Jihoon Jeong², Suyu Fu⁶, Jing Yang⁷, Ke Chen³, Akash Singh⁸, Feng He⁹, Xiaochuan Xu¹⁰, Jianshi Zhou⁹, Wen-pin Hsieh¹¹, Abhishek K. Singh⁸, Jung-Fu Lin⁶ and Yaguo Wang⁴; ¹Mechanical Engineering, The University of Texas at Austin, Austin, Texas, United States; ²Department of Mechanical Engineering, The University of Texas at Austin, Austin, Texas, United States; ³ME, MIT, Boston, Massachusetts, United States; ⁴University of Texas, Austin, Texas, United States; ⁵Oak Ridge National Laboratory, Oak Ridge, Tennessee, United States; ⁶The University of Texas at Austin, Austin, Texas, United States; ⁷Carnegie Geophysical Laboratory, DC, District of Columbia, United States; ⁸Indian Institute of Science, Bangalore, India; ⁹TMI, The University of Texas at Austin, Austin, Texas, United States; ¹⁰Omega optics, Austin, Texas, United States; ¹¹Institute of Earth Sciences, Academia Sinica, Taipei, Taiwan.

The transport properties of mineral materials at high pressure are the critical components in planetary interior models. The invention of diamond anvil cell (DAC) makes it possible to simulate the hydrostatic pressure condition under the earth mantle and core in geophysics field. High pressure can drastically reduce the atomic volume thus increase the electronic density, in turn resulting in novel and special behaviors due to the modified electronic and phononic dispersion. Recent years, with the incorporation of DAC and a wide variety of functional materials, new features discovered at high pressure start to bring more research interest into high-pressure condensed matter physics, such as semiconductor to metal transition, high T_c superconductors, band-gap opening. However, probing the thermal transport under high pressure is always challenging with traditional methods due to the compact cell size. Here we incorporate DAC device into our recently developed picosecond transient thermoreflectance system to study the thermal conductivity tuning under extreme strain. Due to the optically transparent feature of diamond over a wide electromagnetic wavelength range, we are able to resolve the thermal conductivity of materials at high pressure over tens of GPa. In our study on multilayer vdW 2D semiconductor-MoS₂, a significant enhancement of thermal conductivity by a factor of 7 is observed, which results from the pressure-modified phonon dispersion. Our approach combining optical TTR technique and DAC could also be utilized to study broader types of materials and could find impact in geophysical studies of heat conduction in the earth's mantle.

3:10 PM REFRESHMENT BREAK

SESSION EE: Characterization of Epitaxial Materials

Session Chairs: Ganesh Balakrishnan and Mark Wistey

Thursday Afternoon, June 27, 2019

Michigan League, 3rd Floor, Room D

3:30 PM EE01

(Student) Ray Tracing Simulation of Images of Dislocations and Precipitates on X-Ray Topographs of GaAs Epitaxial Wafers Hongyu Peng¹, Tuerxun Ailihu², Balaji Raghothamachar¹ and Michael Dudley³; ¹Stony Brook University, The State University of New York, Stony Brook, New York, United States; ²Stony Brook University, Stony Brook, New York, United States; ³State University of New York at Stony Brook, Stony Brook, New York, United States.

Synchrotron X-ray topography has been widely utilized to characterize defects in crystals such as SiC, GaAs, GaN and etc, providing us with the guidelines to study the formation mechanism of the defects such as dislocations, grain boundaries and inclusions. In this study, we have

applied this technique to study AlInGaP epitaxial layers grown on GaAs substrates. This system is promising for high-brightness light emitting diodes. However, the formation of defects such as (interfacial)dislocations and inclusions during epi growth can reduce the efficiency of the device. To have a better understanding of the nature of these dislocations and inclusions formed during epitaxial growth, we have used ray tracing simulations of defects to compare and characterize the defects in X-ray topography. The use of ray tracing simulations has been particularly useful in readily identifying and characterizing Burgers vectors of dislocations using only one reflection instead of the traditional method of recording at least 3 reflections and applying $g \cdot b = 0$ and $g \cdot b_l = 0$ criteria. This technique has been widely used in characterization of threading dislocations in SiC wafers [1]. In this study, we have similarly used ray tracing simulations to characterize dislocations in GaAs epitaxial layers by using well-known expressions for displacement field around expected dislocations and comparing the calculated images with observed images on grazing incidence topographs. At the same time, X-ray topographs of these wafers also reveal precipitates. Recently, the dynamical image of precipitates showing dark and white contrast on opposite sides of g vector has been simulated by Okunev, Verozubova and coworkers[2][3], the result of which matches well with the experimental images. On grazing incidence X-ray topographs, precipitate images consist of a series of dark circles corresponding to the series of angular steps used to image the entire wafer, novel observation observed for the first time. These dark circles are larger in size for regions away from the precipitate while smaller when it is approaching the center of the precipitates. To have a better understanding of the relationship between the strain field and the size and depth of the precipitates, we carried out ray tracing simulation to relates the strain field model to the contrast in grazing-incidence X-ray topographs. The simulated images and the experimental images will be discussed in this paper, and detailed information of the precipitates and dislocations in GaAs epitaxial wafers will be provided. Ref. [1] X. R. Huang, M. Dudley, W. M. Vetter, W. Huang, W. Si and C. H. Carter Jr. *J. Appl. Cryst.* (1999). 32, 516-524 [2] A. O. Okunev and G. A. Verozubova. *J. Appl. Cryst.* (2015). 48, 1228-1233 [3] A. O. Okunev, G. A. Verozubova, E. M. Trukhanov, I. V. Dzjuba, P. R. J. Galtier and S. A. Said Hassani. *J. Appl. Cryst.* (2009). 42, 994-998

3:50 PM EE02

Punctuated Growth of ErAs Nanoparticles on GaAs(001) Surfaces Kurt Eyink, Yuanchang Zhang, Madelyn Hill, Lawrence Grazulis and Krishnamurthy Mahalingam; AFRL/RXAN, Wright-Patterson AF, Ohio, United States.

ErAs is a semimetal that grows epitaxially on GaAs and has been researched since it was initially proposed as a high quality contact to GaAs in the 70's. More recently research has focused on use in thermoelectrics, ultrafast detectors, and for use as a plasmonic component in GaAs based devices. Molecular beam epitaxially grown ErAs has been formed mainly by two different approaches. One involving co-deposition of the Er during GaAs growth and the other as a separate deposition on a GaAs surface. In this effort, we study the ability to control the size and density of the ErAs nanoparticles (NPs) deposited on a vicinal GaAs(001) surface through a punctuated growth technique. In particular, we have studied the nucleation of ErAs at one temperature (580C, 600C, and 620C) followed by the growth with a reduced Er Flux at an elevated temperature of 640C. This approach was taken to prevent additional nucleation. We have analyzed the structures with transmission electron microscopy (TEM) and atomic force microscopy (AFM) and spectroscopic ellipsometry (SE). TEM and AFM were used to characterize the structural quality of the nanostructure. TEM showed high quality ErAs NP. AFM was able to clearly see the ErAs nanoparticles and clearly demonstrated our ability to control the density of the particles with the initial seed growth. The size was then adjusted through the additional growth at the higher temperature lower flux condition. We will discuss this punctuated growth in terms of an excluded volume deposition where the low flux conditions produce a roughening morphology and the high flux conditions allow the nucleation of NPs. Depending on the density of the NPs this eliminates roughening from the low flux conditions.

4:10 PM EE03

(Student) Mesostructural Visualization of Boundary Effects on Continuous Step-Flow Growth of CVD Diamond Shengyuan Bai¹, Ramón D. s. Díaz², Yun Hsiung¹ and Elias Garratt¹; ¹Chemical Engineering and Materials Science, Michigan State University, East Lansing, Michigan, United States; ²Electrical and Computer Engineering, Michigan State University, East Lansing, Michigan, United States.

Diamond has shown superior properties that make it desirable as high frequency/high power solid state circuit breakers in electric grid or as sensor materials in harsh environments such as automotive and aerospace

engines. The implementation of diamond in such fields requires the growth of large area crystals. However, in over 60 years of diamond research, the growth of electronic grade large area diamond remains elusive. Lateral outgrowth and mosaic growth of CVD diamond is a promising avenue for large size diamond wafers to be realized, however mesoscale effects arising from evolving boundary conditions during growth impede scaling of diamond to 2-inch diameters due to breakdowns in continuous step-flow growth. To overcome this limitation, the fundamental mechanisms governing these mesoscale effects must be characterized and understood. Understanding the fundamental mechanism of step-flow breakdown within certain boundary conditions requires an approach accounting for microstructural changes over large length scales. Mesoscale characterization arises as a promising approach to understand the step-flow mechanism. Characterization by micro x-ray diffraction (μ -XRD) mapping presents an ideal measurement platform for this type of understanding. In this work, we examine the step-flow behavior at the mesoscale, contrasting lateral outgrowth edge effects between the center and outer rim of the single crystal diamond (SCD) plate.[GE1] By understanding how crystal structure evolves relative to these conditions, we can understand the mechanisms leading to breakdowns in crystal growth step-flow. SCD, cut into two identical sections A and B, was grown by MPACVD and scanned using a microbeam of x-rays to examine the structural state of growth at center and edges. Results demonstrate after growth and regrowth by MPACVD, continuous step-flow growth from the edges of the SCD plate at the center remains continuous, in contrast to the edge where we observe a typical breakdown in continuity. This indicates the boundary conditions between the two are under the influence of unique forces. Local lattice structure, or structural states, were visualized by mapping the (400) phase at the edge vs. center of grown samples with 500-micron spot-size scanning x-ray rocking curve (μ -XRC) and 2θ - ω . μ -XRC mapping results show the local structural state of the (400) phase at the center retains low mosaicity (FWHM 0.032), indicating good crystalline quality. As growth is repeated this condition evolves; the growth front from crystal block A begins to dominate B, leading to continuous step-flow overgrowth and increasing homogenization from 0.092° to 0.035[GE2] ° FWHM at the interface. Furthermore, misorientation of the (400) lattice planes tends to reduce after successive regrowth. This suggests boundary conditions for merging edges at the center of diamond plates suppress the rotation of crystal planes leading to the formation of polycrystalline grains commonly observed at the outer edges. We hypothesize similar boundary conditions (spatial) may be realized at the outer edges of SCD, promoting continuous step-flow lateral growth leading to larger diamond plates.

4:30 PM EE04

(Student) Efficient Room Temperature Photoluminescence (PL) from MBE ZnSe Sandwiched Between Low-Temperature Migration Enhanced Epitaxy (LT-MEE) Grown GaAs [Zongjian Fan](#)¹, Krishna Yaddanapudi², Ryan Bunk¹, Subhash Mahajan² and Jerry M. Woodall¹; ¹Department of Electrical and Computer Engineering, University of California, Davis, California, United States; ²Department of Materials Science and Engineering, University of California, Davis, California, United States.

The ZnSe-GaAs digital superlattice system (DSS) is predicted to have tunable effective bandgaps between 1.4 eV and 2.7 eV, i.e. from infrared to blue^[1-3]. If experimentally verified this DSS could provide a path to true RGB light emission with optimal chromaticity, including improved RGB displays, LEDs, and lasers, in a single lattice-matched, direct bandgap materials system. However, the non-compatible optimal epitaxy temperature^[2] of ZnSe (about 300 °C) and GaAs (about 580 °C) inhibits a practical way to integrate those two materials with tolerable interface defect density. Therefore, being able to fabricate the GaAs component of high quality DSS at the same substrate temperature for optimized ZnSe epilayers would be desirable. It has been previously shown that low defect density ZnSe/GaAs interface can be fabricated by MBE of ZnSe on Ga-terminated GaAs(100) surfaces, and models have been proposed to explain the structure of the interface^[4-7]. It usually requires growth and annealing of GaAs at a relatively high temperature. A low temperature(LT) GaAs growth technique is more favorable for DSS. MEE has been shown to form GaAs epilayers at temperatures as low as 200 °C with good quality^[8-9]. Therefore, LT-MEE could be a promising technique to realize high optical quality DSS. Previous work has studied this method and superlattices with flat interfaces were fabricated. However, they only exhibit desirable PL at 10 K^[3]. We have investigated the optical and structural interface properties of ZnSe/LT-MEE GaAs structures through a series of ZnSe epilayers on different GaAs buffers: LT-MEE GaAs, LT-MBE GaAs and regular MBE GaAs with post-annealing to obtain Ga-terminated surface for unpinned interface formation. The ZnSe/LT-MEE GaAs structure has a significantly improved ZnSe room temperature PL responses compared to ZnSe/LT-MBE GaAs. Furthermore, its intensity is

nearly the same level as the ZnSe with an ideally unpinned ZnSe/GaAs interface. Also, the peak PL intensity of ZnSe versus incident 405 nm laser power has a more linear relationship from the ZnSe/LT-MEE GaAs structure than the other two, indicating a lower nonradiative trap density. Furthermore, LT-MEE of GaAs on top of as-grown ZnSe was also investigated. Since theory and experiment showed that the unpinned ZnSe/GaAs interface has a transition structure instead of being atomically abrupt, the first monolayer used in MEE growth might play a key role for interface formation. Ga- and As-started MEE growths were both studied. Reflective high energy electron diffraction(RHEED) patterns appeared to be streaky during both growths. The PL responses of ZnSe and bottom GaAs layer could still be seen at room temperature for both, suggesting the top thin MEE GaAs did not significantly alter the properties of underneath ZnSe/GaAs structure. Peak PL intensity of ZnSe versus incident power from sample with As-started top MEE GaAs layer showed slightly larger nonlinearity than for the Ga-started one. We are currently trying to understand why our GaAs MEE process results in higher room temperature ZnSe PL efficiencies compared to [3]. In summary, we have shown that LT-MEE of GaAs is a promising way to fabricate both GaAs/ZnSe and ZnSe/GaAs interfaces with low defect density by achieving efficient room temperature PL of ZnSe sandwiched between LT-MEE GaAs. Detailed high-resolution transmission electron microscopy(HRTEM) work will be present at the conference. References: [1] S. Agarwal et al., *Electrochem. Solid-State Lett.* 13, H5 (2010). [2] N. Kobayashi et al., *Jpn. J. Appl. Phys.* 29, L236 (1990). [3] S. Ramesh et al., *Appl. Phys. Lett.* 57, 1102 (1990). [4] D. Li et al., *Appl. Phys. Lett.* 57, 449 (1990). [5] R. L. Gunshor et al., *Appl. Phys. Lett.* 50, 200 (1987). [6] Q-D. Qian et al., *Appl. Phys. Lett.* 54, 1359 (1989). [7] S. Zhang et al., *Appl. Phys. Lett.* 60, 2499 (1992). [8] Y. Horikoshi et al., *Jpn. J. Appl. Phys.* 27, 169 (1988). [9] Y. Horikoshi et al., *Jpn. J. Appl. Phys.* 28, 200 (1989).

4:50 PM EE05

(Student) Epitaxial Integration of Arbitrarily Patterned Metal Nanostructures for Photonic Applications [Alec M. Skipper](#)¹, Daniel J. Ironside¹, Yihao Fang², Jorik van de Groep³, Jung-Hwan Song³, Pankul Dhingra², Minjoo L. Lee⁴, Mark Brongersma³, Mark Rodwell¹ and Seth Bank¹; ¹University of Texas at Austin, Cedar Park, Texas, United States; ²Electrical and Computer Engineering, University of California, Santa Barbara, Santa Barbara, California, United States; ³Stanford University, Stanford, California, United States; ⁴Micro and Nanotechnology Lab, University of Illinois, Urbana, Illinois, United States; ⁵Electrical and Computer Engineering, University of Illinois Urbana Champaign, Champaign, Illinois, United States.

While the epitaxial integration of semiconductors and dielectrics has progressed rapidly in recent years, the monolithic integration of patterned metal structures with crystalline semiconductors has been comparatively underexplored. Epitaxially-embedded patterned metals could be useful in a wide variety of photonic and electronic devices to introduce both passive (e.g. polarizers or plasmonic waveguides), and active (e.g. buried Ohmic contacts) functionality. However, the integration of metals with semiconductor epitaxy presents a number of metallurgical challenges. At the elevated temperatures necessary for growth, metals can diffuse into the semiconductor, distorting the crystal structure and forming unintentional contact spikes. Furthermore, during the semiconductor overgrowth, the growth parameters must be carefully tailored to prevent polycrystalline deposition, as well as voids and dislocations which could introduce optical scattering and recombination sites that reduce the efficiency of epitaxially integrated devices. To date, the most successful approach to integrate metals into epitaxial layer stacks has focused on rare earth pnictide (e.g. ErAs) films [1] and nanostructures [2]. However, the self-assembled growth of rare earth pnictides makes the integration of arbitrary shaped metals challenging. Prior work on the integration of patterned metals focused on applications to electronic devices such as metal base transistors [3], leaving the optical properties of such structures largely unexplored. We present proof-of-concept patterned tungsten gratings embedded in molecular beam epitaxy (MBE) grown GaAs to study metal-semiconductor epitaxial integration for photonic devices. Tungsten was chosen as the metal due to being nonreactive with GaAs and stable at high temperatures making it ideal for overgrowth by MBE [4]. Lateral overgrowth of patterned tungsten features was achieved by using III-flux modulated periodic supply epitaxy to seed selective growth from a GaAs (001) substrate. By tailoring the crystal plane orientation of the patterned tungsten, this results in lateral epitaxial overgrowth that can be integrated into a III-V layer stack. Successful lateral epitaxial overgrowth is confirmed by scanning electron microscopy (SEM). Polarization resolved photoluminescence (PL) and Fourier transform infrared spectroscopy (FTIR) studies of metal nanostructures integrated with prototype quantum well emitters are underway and progress will be reported at the

conference. This material is based upon work supported by the National Science Foundation the Quantum Leap Big Idea under Grant No. DMR-1839175 and CCF-1838435. References: [1] C.J. Palmstrom et al., *Appl. Phys. Lett.*, 53, 2608-2610 (1988) [2] C. Kadow et al., *Appl. Phys. Lett.* 75, 3548-3550 (1999) [3] M.A. Hollis et al., *Advanced Processing of Semiconductor Devices*, 797, 335-347 (1987) [4] J.P. Harbison et al., *Appl. Phys. Lett.*, 47, 11, 1187-1189 (1985)

SESSION FF: Oxide Growth and Devices
Session Chairs: Shayla Sawyer and Sarah Swisher
Thursday Afternoon, June 27, 2019
Michigan League, 3rd Floor, Henderson

1:30 PM FF01

(Student) ZnO TFTs on Curved Substrates Using Optical Lithography
Mohit Tendulkar, Tianning Liu and Thomas N. Jackson; Electrical Engineering, The Pennsylvania State University, State College, Pennsylvania, United States.

Curved substrate lithography provides a means for integrating electronics on non-planar surfaces and enables the fabrication of sensors and circuits directly on such surfaces. Most reports demonstrating techniques for fabrication on curved substrates can be divided into two groups. The first group uses direct write fabrication techniques such as e-beam lithography and direct laser writing. These techniques can be good at defining fine dimensions, but are time consuming, expensive, and not scalable for large area high volume production. The second group uses polymeric stamps to transfer features to the curved substrate. Layer-to-layer alignment is often difficult for stamps and both pattern distortions and stamp life can be problematic. We present a curved substrate lithography method by combining conventional lithography and flexible masks. A Hybrid Technology Group (HTG) aligner was modified to accommodate our curved substrates. A substrate holder for curved substrates was designed that positions the substrate in proximity to the mask during alignment and provides vacuum contact between mask and substrate during exposure. Flexible polyester masks are held by a frame that surrounds the curved substrate holder and micrometers allow 3-axis alignment with typical alignment error less than 10 μm over a 10 cm \times 10 cm substrate. A UV LED source provides for fast and uniform exposure of the curved substrate. To fabricate ZnO TFTs on curved substrates, a 100 nm thick chromium layer was deposited by sputtering onto cleaned curved glass substrates. The chromium layer was patterned using curved substrate lithography with a conventional DNQ-Novolac photoresist and wet etching to form gates for the TFTs. Next, 30 nm thick aluminum oxide (Al_2O_3) and 12 nm thick zinc oxide (ZnO) were deposited using plasma enhanced atomic layer deposition. The Al_2O_3 and ZnO were patterned using curved substrate photolithography and wet etching in hot phosphoric acid and dilute hydrochloric acid respectively. Next, 100 nm thick titanium source and drain contacts were deposited by sputtering and patterned using curved substrate photolithography and liftoff. Finally, the devices were passivated using 30 nm thick Al_2O_3 , deposited by atomic layer deposition. ZnO TFTs fabricated on curved substrate have good uniformity and linear region mobility of 20 cm^2/Vs . The device characteristics are similar to devices fabricated on flat glass. This approach for vacuum contact lithography on curved substrates enables fabrication of devices and circuits directly on non-planar substrates with high throughput. ZnO TFTs fabricated on curved substrates using this technique have performance similar to devices fabricated on planar substrates.

1:50 PM FF02 WITHDRAWN

Seeking Conformal Epitaxy of Heterostructures—Growth of ZnO/MoO₃ Superlattices by Atomic Layer Deposition and Characterization of Their Physical Properties Wei-Jhen Ciou¹, Wan-Chen Hsieh³, Yu-Suan Hong¹, Hui Chun Huang¹, Ming-Chen Chou¹, Tai-Siang Lin¹, Po-Hung Lin¹, Che-Min Lin⁷, Chun Fu Chang¹, Sung-Wei Yeh⁴, Paritosh Wadekar⁵, Li-Wei Tu¹, Chih-Hsiung Liao⁶, New-Jin Ho⁸, Quark Y. Chen^{2, 1} and Wei Kan Chu²; ¹Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan; ²Physics and TeSUH, University of Houston, Houston, Texas, United States; ³National Sun Yat-sen University, Kaohsiung, Taiwan; ⁴Mold and Die Engineering, National Kaohsiung University Of Science and Technology, Kaohsiung, Taiwan; ⁵Physics, National Sun Yat Sen University, Kaohsiung, Taiwan; ⁶Physics, ROC Military Academy, Kaohsiung, Taiwan; ⁷Physics, National Sun Yat-sen university, Kaohsiung, Taiwan.

Superlattices of ZnO/MoO₃ have been prepared by atomic layer deposition (ALD) on a-oriented sapphire substrates at 177 °C. The electrical

properties were studied via measurement of resistivity as a function of temperature (T) from T=15 K to 300 K and magnetic field (B). T and B are set as complementary quantities, either a variable or a fixed parameter while the other varies. The superlattice structures comprise multiple periods of ZnO/Mo₃ bilayers that are hoped to incur new physical properties not seen in their pristine form. Careful data analysis by brute-force data fitting based on thermally activated processes of band conduction resulted largely in four midgap states responsible for the measured functional dependence of resistivity on T and B. Except for the shallowest state that is at ca. 5 meV from the band edge, the other three states consistently follow the linear relation of over the whole studied temperature range, hence demonstrate negative magnetoresistance. The shallowest state, however, follows a positive B-square dependence in revelation of a cyclotron effect for free carriers moving along a spiraling path. The countering magnetoresistive behaviors make the magnetoresistance exceedingly small and difficult to measure despite meticulous effort. Analysis of the charge carrier mobilities, according to the simple power law of temperature, suggest that impurity charge scattering and lattice vibration scattering mechanisms are both at play. The significances of the findings in association with the heterojunctions, whether within the layers or with the junction interfaces will be discussed.

2:10 PM FF03

(Student) Electrical Performance of Annealed Zinc-Tin-Oxide Thin-Film Transistors Made by H₂O-Based Thermal Atomic Layer Deposition Christopher Allemang¹, Orlando Trejo², Neil P. Dasgupta² and Rebecca L. Peterson¹; ¹Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ²Mechanical Engineering, University of Michigan, Ann Arbor, Michigan, United States.

Fabrication of active devices on top of existing complimentary metal-oxide-semiconductor (CMOS) substrates is being studied as a way to increase device density and continue Moore's law. Zinc tin oxide (ZTO), an amorphous oxide semiconductor, is a strong candidate for 3D-IC heterointegration of thin film devices on CMOS owing to its wide bandgap (~3 eV), high electron mobility, and large area uniformity. BEOL integration of ZTO on CMOS requires fabrication of high-performance devices using low temperature deposition techniques to preserve the underlying CMOS device performance. Among the potential thin film deposition techniques, atomic layer deposition (ALD) is a promising low temperature process that allows precise control of film interfaces, stoichiometry, and thickness. Previous work of ALD ZTO using H₂O₂ as the oxidant resulted in conducting behavior as-deposited and annealing at 350 °C or above was required for semiconducting behavior [1], [2]. Here, using an H₂O-based ALD ZTO process, bottom-gate top contact thin film transistors (TFTs) were fabricated and show semiconducting behavior as-deposited. Annealing to 300 °C results in high performance semiconducting behavior. Approximately 50 nm of ZTO was deposited at a substrate temperature of 130 °C using diethylzinc (DEZ), tetrakis-dimethyl-amine-tin (TDMASn), and H₂O precursors. With a 1:1 Zn:Sn cycle ratio, a supercycle consisted of one Zn cycle followed by a Sn cycle before the supercycle was repeated. The samples were then annealed at 300, 400, or 500 °C in an air ambient for 1 hour. Surface and depth profile x-ray photoelectron spectroscopy (XPS) was used to study the Zn:Sn ratio and oxygen-related components as a function of annealing. The electrical properties of ZTO TFTs were studied as a function of annealing temperature. Films annealed at 300 °C result in enhancement mode devices with an electron mobility of 0.69 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$, subthreshold slope (SS) of 0.44 V/dec, and $I_{\text{on}}/I_{\text{off}} > 10^7$. Mobility is strongly dependent on gate insulator/semiconductor interface surface treatment and was measured up to 1.25 $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$. Both mobility and SS increase with increased annealing temperature above 300 °C. This work thus presents a novel pathway towards scalable nanomanufacturing of high-performance electronics on a wide range of temperature-sensitive substrates. This work was supported by a National Science Foundation Scalable Nanomanufacturing award #1727918. Portions of this work were performed using the LNF and (MC)² facilities, which are supported by the College of Engineering at the University of Michigan. [1] J. Heo, S. Bok Kim, and R. G. Gordon, "Atomic layer deposited zinc tin oxide channel for amorphous oxide thin film transistors," *Appl. Phys. Lett.*, vol. 101, no. 11, p. 113507, Sep. 2012. [2] B. D. Ahn, D. Choi, C. Choi, and J.-S. Park, "The effect of the annealing temperature on the transition from conductor to semiconductor behavior in zinc tin oxide deposited atomic layer deposition," *Appl. Phys. Lett.*, vol. 105, no. 9, p. 092103, Sep. 2014.

2:30 PM FF04

Preparation and Characterization of Zinc Oxide Glasses Through Kinetic-Control Andre Zeumault¹, Carlos Silva^{2,3} and Natalie Stingelin^{1,4};

¹Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States; ²Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia, United States; ³Physics, Georgia Institute of Technology, Atlanta, Georgia, United States; ⁴Chemical Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States.

In a conventional physical vapor deposition process used to deposit metal oxide thin films, the distance between target and substrate allows for film stoichiometry and crystallinity to be separately controlled. In contrast, solution processing of metal oxides involves coupled chemical and structural transformations in which the stoichiometry and crystallinity vary simultaneously throughout the annealing process and are not easily controlled¹⁻³. Although correlations exist relating device electrostatics and electronic transport to stoichiometry and crystallinity⁴, current processing methods do not allow control of the latter, thereby limiting the degree to which film electronic properties can be engineered to meet application-specific needs. To improve versatility of these materials, this work exploits the drying-kinetics of sol-gels to achieve independent kinetic control of stoichiometry and crystallinity in solution-deposited metal oxide films. Using a zinc oxide sol-gel solution consisting of zinc acetate dihydrate, monoethanolamine and 2-methoxyethanol as solute, stabilizer and solvent respectively, we demonstrate the control of crystallinity in zinc oxide films simply by varying the drying rate. In doing so, we find that amorphous films are obtained at high drying rates, whereas crystalline films are obtained at low drying rates. The amorphous content was determined by in-situ heat capacity measurements using fast scanning chip calorimetry⁵ on films inkjet-printed directly onto calorimeter chips⁶. This allowed for the unambiguous identification of amorphous content, including the direct observation and characterization of the glass-transition in amorphous zinc oxide films for the first time. Thus, our contributions are two-fold: first, we establish a method of preparing solution-processed metal oxide films having precise crystallinity using kinetic control, and second, we outline a method for unambiguous characterization of amorphous content in solution-deposited metal-oxide films through combination of inkjet printing and chip calorimetry. We outline our primary findings in Figure 1, which compares the specific heat capacity for two samples dried at different rates: slowly, at room temperature for 24 hours (Fig. 1a) and quickly, from 22°C to 150°C at 100°Cs⁻¹ (Fig. 1b). The specific heat capacity is measured at different heating rates from 100°Cs⁻¹ to 10,000°Cs⁻¹. For samples subjected to fast drying, the specific heat capacity exhibits a clear and pronounced glass transition, indicating the presence of a large amorphous content in the films. A glass transition was not observed for samples subjected to slow drying, although these samples showed evidence of crystalline domains, visible under polarized light microscopy as shown in the inset of Figure 1a. By contrast, samples subject to fast drying were not visible, as expected for amorphous films. We note that XPS chemical analysis indicates the formation of carbon-free zinc oxide films with a zinc hydroxide to zinc oxide ratio of 21%, suggesting that zinc oxide formation is complete at just 150°C, consistent with reports elsewhere⁷. The establishment of an initial amorphous phase allows for the film crystallinity to be adjusted through subsequent annealing. We illustrate this in Figure 2. As shown, the initial amorphous state (Fig. 2a) is stable until 250°C, and gradually crystallizes with increased annealing temperature. Based on these observations, we envision this technique of preparation and characterization of semiconducting oxide glasses via chip calorimetry to be especially useful in the development of low-cost, efficient thermoelectric materials, due to the ability to tune lattice thermal conductivity by controlling crystallinity, in addition to the favorable *phonon-glass electron-crystal* properties and solution processability of metal oxides.

2:50 PM FF05

(Student) New CVD Based Growth Method for Highly Crystalline Epitaxial ZnO Layers on Various Substrates Raphael Müller¹, Florian Huber¹, Okan Gelme¹, Matthias Töws¹, Manfred Madel¹, Ulrich Herr² and Klaus Thonke¹; ¹Institute of Quantum Matter / Semiconductor Physics Group, University Ulm, Ulm, Germany; ²Institute for Functional Nanosystems, University Ulm, Ulm, Germany.

A chemical vapor deposition (CVD)-based growth process for high temperature growth of zinc oxide (ZnO) bulk material is presented, which uses methane (CH₄) as precursor to reduce commercially ZnO powder at temperatures above 900°C, instead of the established carbo-thermal growth recipe which uses carbon powder as reducing agent. The resulting zinc vapor is transported by an argon carrier gas to the substrate (~830°C) along a temperature gradient in a three-zone furnace, and is then re-

oxidized with pure oxygen, forming a ZnO layer. By the use of CH₄ as the reducing agent, the II-V ratio – as well as the growth duration – can be controlled very precisely and growth rates of several micrometers per hour can be realized. This scheme was used to grow a series of samples with increasing supply of zinc vapor in order to monitor the resulting layer formation on c-plane sapphire with aluminum nitride (AlN) nucleation layer (grown by MOVPE). We show that the ZnO heteroepitaxial layer is growing in c-plane direction right from the start of the growth process and forms a closed, smooth high-quality single crystalline layer after a growth time of ten minutes only. By further increasing the growth time, very high crystalline and extremely pure ZnO layers can be grown. The same process with slight adjustments concerning temperature and gas flows also works for the heteroepitaxial growth on other substrates like gallium nitride (GaN) or Si (111) w/o AlN nucleation layer. For growth on GaN or c-plane sapphire with AlN nucleation layer homogeneous, fully c-oriented, monolithic layers with smooth surface and no rotated domains are achieved. On GaN a full width at half maximum (FWHM) in an omega scan for the (0002) reflex of less than 100 arcsec can be realized, and slightly higher values are found for the growth on c-plane sapphire with aluminum nitride nucleation layer. All layers show excellent properties in low temperature photoluminescence (PL) measurements, with a line width for donor bound exciton emission of about 200 μeV and additionally iron doped samples show a line width of 28 μeV only for the related emission at 1.787 eV. The carrier concentration of the layers is in the range of 10¹⁵ cm⁻³, which is a prove for the high purity of the layers and provides a good base for doping experiments or optical investigations. Furthermore, such high quality ZnO layers have great potential for a broad range of optoelectronic applications, or can be used as sacrificial layers for the growth of free-standing gallium nitride (GaN), as we also demonstrated.

3:10 PM REFRESHMENT BREAK

3:30 PM FF06

(Student) Atomic Layer Deposition of Bismuth Vanadate Photoanodes

Ashley R. Bielinski¹, Sudarat Lee¹, James Branco², Samuel L. Esarey², Andrew Gayle⁴, Eric Kazayak¹, Kai Sun³, Bart M. Bartlett⁴ and Neil P. Dasgupta¹; ¹Mechanical Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ³Materials Science and Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ⁴Chemistry, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

Solar water splitting using semiconductor photoelectrodes provides a route for storing renewable energy from sunlight as chemical bonds. However, many common semiconductors such as Si and GaP photocorrode in aqueous conditions. One solution is to use stable electrode materials such as metal oxide semiconductors. Bismuth vanadate (BVO) is a promising mid-bandgap semiconductor for solar water oxidation. Its 2.4 eV bandgap enables visible light absorption and it has appropriate valence band alignment for the oxygen evolution reaction. In the typical planar architecture, BVO is limited by charge carrier transport, surface recombination, and slow water oxidation kinetics. Core-shell nanowire architectures can be used to improve charge carrier separation and light absorption by decoupling carrier diffusion lengths and light absorption depths onto orthogonal directions. The light can be absorbed along the length of the nanowire, but the carriers only have to diffuse along the radius. Synthesizing complex 3D architectures at the nanoscale is challenging with common solution deposition techniques for BVO. Atomic layer deposition (ALD) is a thin film deposition technique using gas-phase, self-limited surface reactions that enables conformal coverage of 3D nanostructures with sub-nanometer thickness control. In this study, we developed a process of depositing BVO using ALD to create core-shell nanowire photoanodes. The ALD BVO was deposited using a nanolaminate of bismuth and vanadium oxides using Bi(OCMe₂Pr)₃ as the bismuth source, vanadium(V) oxytriisopropoxide as the vanadium source, and water as the oxidant. The samples were then post annealed to achieve the photoactive monoclinic BVO phase. The BVO stoichiometry was tuned from Bi-rich to V-rich by changing the relative thickness of the initial binary oxide layers. The composition and phase of the BVO films were investigated using x-ray photoelectron spectroscopy (XPS) and grazing incidence x-ray diffraction (GIXRD). The as-deposited nanolaminate was shown to mix fully during the annealing process by scanning transmission electron microscopy (STEM). BVO film light absorption, as measured by UV-vis spectroscopy, and photocurrent, measured in a 3-electrode cell with 1-sun illumination were optimized as a function of composition and thickness. Sulfite oxidation was used to study the optoelectronic properties of the BVO films independent of the water oxidation surface kinetics. A planar electrode with a BVO film thickness of 42nm achieved a photocurrent of 2.24 mA/cm² at 1.23 V vs. RHE.

Core-shell nanowire photoanodes were also constructed using a ZnO nanowire array coated first with an ALD SnO₂ interlayer and then the ALD BVO film. The 3D photoanodes showed a 54% increase to 3.45 mA/cm² at 1.23 V vs. RHE. This is the highest photocurrent reported to date for any photoanode using an ALD film as the primary light absorber.

3:50 PM FF07

Enhancement Mode Perovskite Oxide BaSnO₃ MOSFETs with Current On/Off Ratio of 10⁸ Hao Yang¹, Junao Cheng¹, Caiyu Wang¹, Christopher Freeze², Omor Shoron², Nicholas G. Combs², Wangzhou Wu², Susanne Stemmer², Siddharth Rajan¹ and Wu Lu¹; ¹Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ²Materials Department, University of California, Santa Barbara, Santa Barbara, California, United States.

Perovskite oxides with two cation sites own appealing properties such as superconductivity, photoconductivity, high permittivity, ferroelectricity, and so on. Among perovskite oxide materials, BaSnO₃ (BSO) with wide bandgap (~3eV), wide visible-to-near-IR transmittance, and high conductivity above 10⁴ S/cm has great potential for high-power and transparent devices. BSO can be easily doped at the two cation sites despite of its large bandgap. At room temperature, high mobility up to 320 cm²/Vs and high charge density of 8 × 10¹⁹ cm⁻³ have been demonstrated in La-doped BSO thin films [1], due to the smaller electron effective mass and small electron-phonon interaction compared with other perovskite oxide materials. So far the research attention has been paid on photovoltaic applications. Here we show n-type enhancement mode MOSFET based on BSO channel with a high current on/off ratio. The epitaxial layer structure consists of a 5.3 nm La-doped BSO layer and a 15.7 nm unintentionally doped BSO buffer layer grown on a DyScO₃ (DSO) substrate. The Hall mobility and sheet resistance of the doped BSO material are 4 cm²/Vs and 65 kΩ/square, respectively. A 10 nm HfO₂ gate dielectric layer was deposited by atomic layer deposition. Ti/Au ohmic metal for BSO MOSFET was optimized at various annealing conditions yielding a contact resistance of 0.1-0.24 ohm-mm. The BSO MOSFET with a gate length of 2 μm exhibited an I_{on}/I_{off} ratio of 8.3 × 10⁸, a maximum transconductance of 13 mS/mm, and a saturation current of 21.6 mA/mm at V_{ds} = 6 V. To our knowledge, the current on/off ratio is the highest value ever reported on perovskite field effect transistors, in spite of the large density of threading dislocations in BSO on DSO substrates. With linear extrapolation of transfer curves, the threshold voltage was found to be 3 V, indicating the enhancement operation mode for this BSO MOSFET. By fitting the linear region of the transfer curve, we extract the field effect mobility 4.8 cm²/Vs. The subthreshold swing, defined by ΔV_g , is 680 mV/decade. The poor subthreshold swing value is attributed to the high thread dislocation density in BSO layer. The effective trap density N_t can be extracted from the subthreshold swing with ΔV_g , which is found to be 5.9 × 10¹³ cm⁻²eV⁻¹. Though better device performance can be expected through further material and device engineering, the BSO MOSFETs reported here demonstrate their potential in oxide electronics. Reference: 1. H. J. Kim, U. Kim, T. H. Kim *et al.*, *Phys. Rev. B: Condens. Matter Mater. Phys.* **2012**, 86, 165205.

4:10 PM FF08

Velocity Saturation in BaSnO₃ Thin Films Hareesh Chandrasekar¹, Junao Cheng¹, Nicholas G. Combs², Patrick B. Marshall², Susanne Stemmer², Wu Lu¹ and Siddharth Rajan³; ¹Electrical Engineering, The Ohio State University, Columbus, Ohio, United States; ²University of California, Santa Barbara, Santa Barbara, California, United States; ³Ohio State University, Columbus, Ohio, United States.

Perovskite oxides, due to their sheer diversity of electronic properties, offer an attractive platform for integrating disparate device functionalities. Unfortunately most perovskites have poor electron mobilities which makes them less attractive for electronic switching. BaSnO₃, a wide bandgap semiconductor (E_g=3.1 eV) with reported mobility of 320 cm²/Vs,[1] is a notable exception to this rule. Such high mobility, allied with high doping densities (10²⁰ cm⁻³) achievable in BSO films, makes this material of considerable interest from a device perspective. However, in addition to low-field transport parameters such as carrier mobility, the operation of highly-scaled electronic switches and RF amplifiers depends critically on high-field transport, i.e saturation velocity of carriers. While the mobility of BSO thin films have been studied and modeled,[2] there are no reports on high-field transport in this material. In this work, we measure the saturation velocity of electrons in highly-doped BSO thin films for the very first time and model its density dependence due to the dominant optical phonon scattering process. BSO films of ~30 nm total thickness (10 nm undoped-BSO followed by 20 nm La-doped BSO – n_s=2.65 × 10¹⁴ cm⁻², μ=96 cm²/Vs) capped with 20 nm of BaTiO₃ (BTO) were grown on DyScO₃ substrates using MBE (Fig. 1). Saturation velocity

was measured on I-shaped test structures (Fig 2) having wide source-drain contacts with a narrow mesa-defined constriction between them.[3] This geometry reduces any voltage drop due to the contact regions and confines the applied potential and current within the channel. Device fabrication commenced with ICP-RIE etching of BTO followed by ohmic contact deposition (Ti/Al) and then ICP-RIE etch of BSO to define the I-shaped structures (Fig. 3). Pulsed I-V measurements (1μs width, 1ms duration) using G-S probes on various device dimensions (Fig. 4) was used to extract saturation velocity, v_{sat} = J/nq, where J and n_s are current density (A/mm) and sheet carrier concentration (cm⁻²). Saturation was observed for electric fields ranging from 60-75 kV/cm with saturated current densities of 17-42 A/mm (Fig. 4). We extract a saturation velocity of (7.3±2.38) × 10⁶ cm/s from measuring multiple devices of different dimensions. Given the strong optical phonon modes predicted in BSO,[2] it is very likely that carrier back-scattering due to LO-phonon emission at the source acts as the velocity “clamping” mechanism leading to saturation, analogous to that observed in 2DEGs in GaN and layered materials.[4,5] Briefly, at higher electric fields the carrier distribution at the source injection point shifts to higher energies in k-space making LO-phonon emission more favorable (Fig. 5). However, in this case the 20 nm of doped BSO more closely resembles a 3-D electron gas rather than a 2-D case. Hence we reformulate the LO-phonon model to account for 3-D confinement in La:BSO (Fig. 6) with a net LO phonon energy of 120 meV. [5] The observed v_{sat} of 7.3 × 10⁶ cm/s fits remarkably well with that predicted by the 3-D model. Both models also show a density-dependent saturation velocity with a maximum values of 1.8 × 10⁷ cm/s (for 2-D) and 2.15 × 10⁷ cm/s (for 3-D). Better control over doping in La:BSO films is necessary to validate these predictions and indicate an area for further research. [1] H. J. Kim *et al.*, *Appl. Phys. Express* **5**, 061102 (2012). [2] K. Krishnaswamy *et al.*, *Phys. Rev B* **95**, 205202 (2017). [3] S. Bajaj *et al.*, *Appl. Phys. Lett* **107**, 153504 (2015). [4] T. Fang *et al.*, *IEEE Electron Device Lett.* **33**, 709 (2012). [5] H. Chandrasekar *et al.*, *IEEE Trans. Electron Devices* **63**, 767 (2016). [6] T.N. Stanislavchuk *et al.*, *J. Appl. Phys.* **112**, 044108 (2012). The authors acknowledge funding from DARPA DREaM program (ONR N00014-18-1-2034, Program Manager Dr. Young-Kai Chen, monitored by Office of Naval Research, Program Manager Dr. Paul Maki), and Office of Naval Research Grant N00014-18-1-2704 (Program Manager Dr. Brian Bennett).

4:30 PM FF09

(Student) Phase Evolution During Solution Processing of BaSnO₃ Nanoparticles—Towards Low Temperature Synthesis of Transparent Conducting Oxides Sushobhita Chawla, Akash Kumar, Sandeep K. Maurya and Balasubramaniam Kavaipatti; Department of Energy Science and Engineering, Indian Institute of Technology Bombay, Mumbai, India.

The effect of reaction kinetics and annealing conditions on the phase evolution of BaSnO₃ nanoparticles (NPs) synthesized *via* solution processing is studied. In the initial phase of the study annealing was done under ambient conditions and annealing temperature and time were varied from 200 °C to 600 °C and 2 h to 6 h respectively. Annealing under ambient conditions led to a secondary phase of BaCO₃ which is a result of carbonation due to atmospheric CO₂, as confirmed by X-ray diffraction pattern. Further, it was concluded that this secondary phase formation is an interplay of annealing time and temperature. Phase pure BaSnO₃ is obtained only after annealing at 600 °C for 6 h. Curbing the formation of secondary phases leads to the synthesis of phase-pure crystalline BaSnO₃ NPs at a temperature as low as 130 °C, as confirmed by X-ray diffraction pattern. The d-values obtained from HRTEM images are 2.895 Å and 2.38 Å which are close to the ones found from the X-ray diffraction pattern corresponding to BaSnO₃₍₁₁₀₎ (d = 2.91 Å) and BaSnO₃₍₁₁₁₎ (d = 2.383 Å) peaks respectively. The lattice parameter calculated from the most prominent peak of BaSnO₃, i.e. (110) is found to be 4.11 Å, equal to the lattice parameter of bulk BaSnO₃. HRTEM images also reveal that the size of synthesized NPs is in the range of 10-20 nm. Moreover, a 100 nm thick spin-coated film shows a transmittance of around 70-80 % in the visible range (400–800 nm). To this date this is the lowest reported temperature at which BaSnO₃ NPs are successfully synthesized which, in future, will expand the horizons for its optoelectronic applications in numerous structures. Importantly, such low synthesis temperatures make BaSnO₃ available for use in devices, which have a temperature limitation during device processing, such as perovskite-based solar cells in a *n-i-p* architecture or heterojunction Si solar cells.

4:50 PM FF10

(LATE NEWS, Student) Direct Growth of Crystalline III-Vs on Amorphous Dielectrics Using a Combination of Epitaxial and Non-Epitaxial Methods Debarghya Sarkar¹, Yunpeng Xu¹, Sizhe Weng², Mitchell Dreiske¹, P. Daniel Dapkus¹ and Rehan Kapadia¹; ¹Ming Hsieh Department of Electrical and Computer Engineering, University of Southern California, Los Angeles, California, United States; ²Department of Chemical Engineering and Materials Science, University of Southern California, Los Angeles, California, United States.

Integration of III-V compound semiconductor devices with Si electronic and photonic systems in a scalable and cost-effective method, remains a holy grail in semiconductor research and development. Direct growth on an amorphous buffer above the first active layer, using traditional III-V growth methods like MOCVD or MBE, gives polycrystalline films with grain sizes typically much less than a micron. State-of-the-art approach to integrate III-V active layers with Si, involves wafer bonding or epitaxial growth and transfer. Although the devices made on the substrates using these approaches are of excellent quality, this approach is limiting based on cost, time, limited materials, and scalability perspectives. Here we use a non-traditional growth approach, using a newly developed non-epitaxial process called Templated Liquid Phase (TLP) to create a single crystalline mesa (10 μm diameter) followed by epitaxial selective area growth by MOCVD on the initial III-V mesa. We envision this approach as a potential method to integrate crystalline electronic materials on amorphous dielectric surfaces, and the preliminary results of this process is presented here. MOCVD InP grown on TLP InP is used as a representative demonstration to lay the groundwork. However, this approach is quite general to expand to other families of III-V materials to efficiently harness the rich advancement made in the epitaxial growth literature to be integrated on amorphous dielectrics on the back-end of silicon. Briefly, TLP is a growth approach to directly grow single crystalline III-V (InP, InAs, GaP, InGaP, etc.) mesas on non-epitaxial substrates like metals, oxides and nitrides [1-7]. The process involves first depositing a group III mesa with SiO₂ capping layer on the substrate, then performing a liquid-solid phase transformation to the desired III-V material by heating in presence of the respective group V vapor. By tuning the growth conditions, each mesa is ensured to have a single nucleation, which gradually grows with time to transform the entire group III to the III-V compound. Importantly, this process allows the monolithic growth of a single crystalline III-V material with optoelectronic quality similar to that of commercial single-crystal wafers, in the desired geometry and location on various substrates. Using single-crystal InP templates as the seed layer, InP is then epitaxially grown selectively on the mesas using MOCVD. Briefly, the process involves first selectively etching extraneous InP growths around the intended mesas using a self-aligned RIE, then etching away the SiO₂ capping layer, followed by MOCVD growth. Faceted crystalline geometries of the mesas after MOCVD growth indicates the single crystal nature of the seed template. Growth parameter (temperature, precursor flux, V/III ratio) variations are studied to obtain the best MOCVD InP-on-TLP InP morphology and optoelectronic properties. This potentially opens up a new scalable and cost-effective method of integrating high electronic and optoelectronic quality III-V materials and devices with silicon integrated circuits. References: [1] R. Kapadia et al., Scientific Reports, vol. 3, 2013. [2] R. Kapadia et al., Chemistry of Materials, vol. 26, no. 3, pp. 1340-1344, 2014. [3] K. Chen et al., Nature Communications, vol. 7, 2016. [4] Q. Lin et al., ACS Nano, vol. 11, no. 5, pp. 5113-5119, 2017/05/23 2017. [5] D. Sarkar et al., ACS Nano, vol. 12, pp. 5158-5167, 2018. [6] D. Sarkar et al., ACS Nano, vol. 12, pp. 1656-1668, 2018. [7] D. Sarkar et al., Journal of Vacuum Science and Technology B, vol. 36, pg 031204, 2018.

SESSION GG: SiC and Related Materials, Characterization and Devices
Session Chairs: MVS Chandrashekhara and Nadeemullah Mahadik
Thursday Afternoon, June 27, 2019
Michigan League, 3rd Floor, Koessler

1:30 PM GG01

Towards Precise Control of Hetero-Polytypic Structures During Synthesis of SiC for Scalable Quantum Information Platforms Matthew Highland¹, David J. Mandia², Angel Yanguas-Gil², Joseph Heremans¹, David Awschalom^{3,4} and Stephan Hruszkewycz¹; ¹MSD, Argonne National Laboratory, Argonne, Illinois, United States; ²Energy Systems Division, Argonne National Laboratory, Lemont, Illinois, United States; ³Institute for Molecular Engineering, The University of Chicago, Chicago, Illinois, United States; ⁴Institute for Molecular Engineering & Materials Science Division, Argonne National Laboratory, Argonne, Illinois, United States.

SiC has been studied, developed, and utilized as a wide bandgap semiconductor for a number of applications such as solid state lighting and high power electronics. In these efforts one of the key considerations has been controlling which of the many possible structural polytypes of SiC is formed during the synthesis process. There has been recent interest in utilizing the polytypes of SiC to create well controlled heteropolytypic structures for use as quantum information materials. This has been driven by the observation that 4H-SiC crystals have displayed optically active point defects with long life times that are well suited for quantum information applications. Photoluminescence spectra measured from SiC samples have shown emission lines labeled PL5 and PL6 which correspond to defect states with long lifetimes that persist up room temperature making them well suited for quantum information applications. Though the origin of these is not yet known, computational studies have indicated that they may originate from 6H-SiC nano-inclusions in a 4H-SiC matrix. As such, synthesizing heteropolytypic SiC structures that mimic the properties of these 6H-SiC nano-inclusions may be a pathway for forming suitable quantum information materials. However, precisely controlling polytype formation during the synthesis of SiC is extremely challenging given the number of processes and synthesis conditions that affect their formation. To better understand these complex interactions we seek to construct a high temperature chemical vapor deposition system (HT-CVD) compatible with the synthesis of SiC and real-time in-situ x-ray scattering measurements. High energy synchrotron x-rays are capable of penetrating the HT-CVD environment and sensitive to structural polytypes, surface transformations, and thin film growth modes. The realization of such a synthesis system presents a number of significant engineering challenges. We will describe a proposed design for a HT-CVD system capable of forming SiC, with the required stability for in-situ x-ray scattering measurements, that is compatible with recent advances in halide assisted growth chemistry. We will also discuss the potentially unique insight that the realization of this system will give into the formation and control of heteropolytypic structures in SiC for quantum information.

1:50 PM GG02

Doping Dependence of Stacking Fault Expansion in 4H-SiC Peter L. Bonanno, Nadeemullah Mahadik and Robert Stahlbush; Naval Research Laboratory, Washington, District of Columbia, United States.

SiC-based power devices have captured a small but steadily growing share of the power electronics market due to the material's advantages over Si. Among these are a 3-times higher bandgap, which allows a 10-times thinner device for the same breakdown voltage, granting lower switching losses, higher frequency switching, and the possibility for higher blocking voltages without excessive on-resistance. SiC also has 3-times larger thermal conductivity, making device cooling easier. SiC's viability is owed to the suppression in the active layer of basal plane dislocations (BPDs) that dissociate into Shockley stacking faults (SSFs) that expand throughout the material during device operation. The SSFs degrade the operation of SiC devices by decreasing on-state conductivity and increasing off-state leakage. From a commercial point of view, the solution to the SSF problem is to suppress the presence of BPDs in the device active area. From a materials point of view, the faulting of BPDs during device operation to form SSFs is a complex process that is still not completely understood. The current work aims to develop a more complete model of this process by investigating the effect of epilayer doping and by

extension, misfit strain, on stacking fault expansion rate due to localized carrier recombination, which is the process responsible for expansion during device operation [1]. Early models relied either on mechanical stress [2-4] or lowering electronic energy by expanding the conduction-band quantum well due to the SSF [5-7]. Ha et al. [7] showed that the former is insufficient to explain observed SSF expansion. While the electronic energy lowering is the dominant factor in SSF expansion, in this work we examine the effects of doping concentration and strain on the expansion. A 10^{18} cm⁻³ Nitrogen-doped 8°-offcut 4H-SiC substrate was diced and used to grow 3 different 20 μm-thick epilayers, each identical except for their doping levels, which were 10^{17} , 10^{16} and 10^{15} cm⁻³, which correspond to elastic misfit epilayer strains of -2.75, -3.03 and -3.05×10^{-5} , respectively. Carriers were injected at the stacking fault sites using a 355 nm laser, and photoluminescence images of the stacking faults were collected through a 655 nm low pass filter using a cooled CCD camera. The stacking fault expansion was tracked by recording the movement of the Si-core partial dislocations, which luminesced strongly. As expected, the Si-core partial displacement in each sample was linear with total energy injected. The displacement per injected energy (“velocity”) for each epilayer depended on the doping level, with the lower doped (and thus more highly strained) epilayers exhibiting more velocity. Specifically, compared to the 10^{17} cm⁻³-doped epilayer, Si-core displacement was twice as much in the 10^{16} cm⁻³-doped epilayer and 4 times as much in the 10^{15} cm⁻³-doped epilayer for the same injected energy. This trend suggests that doping concentration and resulting strain does have an enhancing effect on the rate of SSF expansion. We interpret this effect in the context of electronic energy balance to create a more complete model. [1] J. D. Weeks, J.C. Tully, and L.C. Kimerling, *Phys. Rev. B* 12, 3286 (1975) [2] J.Q. Liu, M. Skowronski, C. Hallin, R. Söderholm, and H. Lendenmann, *Appl. Phys. Lett.* 80, 749 (2002). [3] M. E. Twigg, R. E. Stahlbush, M. Fatemi, S. D. Arthur, J. B. Fedison, J. B. Tucker, and S. Wang, *Appl. Phys. Lett.* 82, 2410 (2003). [4] P. O. Å. Persson, L. Hultman, H. Jacobson, J. P. Bergman, E. Janzén, J.M. Molina-Aldareguia, W. J. Clegg, and T. Tuomi, *Appl. Phys. Lett.* 80, 4852 (2002). [5] M. S. Miao, Sukit Limpijumng, and Walter R. L. Lambrecht, *Appl. Phys. Lett.* 79 4360 (2001). [6] A. Galeckas, J. Linnros, and P. Pirouz, *Appl. Phys. Lett.* 81, 883 (2002). [7] S. Ha, M. Skowronski, J. J. Sumakeris, M. J. Paisley, and M. K. Das, *Phys. Rev. Lett.* 92, 17 (2004)

2:10 PM GG03

Electrical Characterization of Single Crystal Boron Carbide Metal-Semiconductor Diodes MVS Chandrashekar¹, Michael Straker², Abdulganiyu Ajilore⁴, William A. Phelan³ and Michael Spencer⁴;
¹University of South Carolina, Columbia, South Carolina, United States;
²Physics, Morgan State University, Baltimore, Maryland, United States;
³Chemistry, Johns Hopkins University, Baltimore, Maryland, United States;
⁴ECE, Morgan State University, Baltimore, Maryland, United States.

We report on the current-voltage (I-V) and capacitance-voltage (C-V) characteristics of Ti/Au/B4C metal/semiconductor diodes grown using a laser-diode float zone technique. Such ultra-hard, highly conductive, refractory borides melt congruently, and are lattice matched to the wide and ultra-wide bandgap (UWBG) III-Nitrides, of interest for power electronics, and other extreme applications. In addition, B4C (lattice matched with GaN) is used in military armor, where single crystals will aid in characterizing the mechanical properties of such armor, and clarify the failure mechanisms in this anisotropic icosahedral material. Finally, we also note that while B4C is ideally supposed to be a wide-bandgap semiconductor, and therefore transparent [1], it presents as black due to its polytypic nature, which leads to point defects. In this study, we demonstrate the high concentration of electrically active intrinsic defects partially responsible for this black color. Experimental: The B4C single crystals were grown using a 1kW 985nm laser diode in a float-zone configuration from commercially purchased high-purity B4C hot-pressed ceramic rods, at an estimated temperature of ~2400°C. After growth, 2mm thick crystals were oriented into the <101>-h plane using Laue white-beam x-ray technique (Fig 1), cut, and polished with diamond grit down to 0.1μm to an RMS roughness <5nm. Powder x-ray diffraction, and electron dispersive spectroscopy (EDS) both showed B/C~4, as expected. Glow discharge mass spectroscopy showed purity in the ppm range. Ti/Au contacts were evaporated on the as-polished surface using a shadow mask to eliminate the need for lithography. Results and discussion: The I-V curves were linear below 0.05V (Fig. 1a). Analysis of the nonlinear symmetric I-V's above this voltage suggested trap-related tunneling into the B4C from the metal, manifesting as a 104x increase in current over 0.5V. This was supported by weak temperature dependence down to 80K (Fig. 2b). Our presentation of the first ever C-V measurements of B-4C (Fig. 2c) showed the clear presence of holes as the charge carriers, at a concentration ~1020cm-3 at a depletion depth ~3nm, again supporting

tunneling transport across the metal/semiconductor junction. Given that the impurity concentration is in the ppm range, we attribute the origin of these carriers to intrinsic point defects. Unpolished as-cut surfaces showed very non-uniform characteristics ranging from ohmic to non-linear as for a polished surface. We reconcile these measurements with previously reported defect levels within the bandgap of B4C, and discuss the implications of these results on the engineering of B4C for mechanical applications. Given that these metal-semiconductor devices are strongly rectifying, they may be used for high temperature thermoelectrics [2], as well as neutron detection [3], as has been suggested in the literature. References: 1. Anwar Hushur et. al, *J. Phys. Cond. Matter*, 28, 045403 (2016) 2. I. Gunjishima et. al, *Mat., Trans.*, 42, 1445 (2001) 3. B.W. Robertson et. al, *Appl. Phys. Lett.*, 80, 3644 (2002)

2:30 PM GG04

(LATE NEWS, Student) Extreme Confinement Characteristics of Deep-UV Emission from Monolayer GaN/Al(GaN) Nanowire and Planar Heterostructures Anthony Aiello¹, Yuanpeng Wu¹, Ayush Pandey¹, Ping Wang¹, Woncheol Lee², Jiseok Gim², Kai Sun², Robert Hovden², Emmanouil Kioupakis², Zetian Mi¹ and Pallab Bhattacharya¹;
¹Department of Electrical Engineering and Computer Science, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States;
²Department of Materials Science and Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States.

Emission in the deep-UV wavelengths can be obtained from GaN layers of thickness ~1-2 monolayers sandwiched by AlN or AlGaN barrier layers. The extreme quantum confinement greatly increases the electronic gap into the deep-UV range and leads to a very large exciton binding energy, ~100-200meV at room temperature¹. A large exciton binding energy, which has not been borne out experimentally, may be useful for excitonic light sources and for experiments in cavity quantum electrodynamics. In the present study we have investigated the luminescence from 1 monolayer (ML) GaN disks embedded in AlN nanowires on silicon substrates, which are known to be relatively free of extended defects, and a planar sample wherein the 1ML GaN is embedded in Al_{0.65}Ga_{0.35}N barriers. The samples were characterized by temperature-dependent and time-resolved photoluminescence (TRPL) measurements. We measure a PL peak energy ~5.2eV and an exciton binding energy, E_{BX}, 160-260meV at room temperature in the nanowire samples, in agreement with theoretical calculations. Similar results are obtained from the planar ML GaN sample. The ML GaN/AlN disk-in-nanowire (NW) arrays were grown on (111)Si by MBE. Self-assembled catalyst-free 60nm GaN NW is first grown under nitrogen-rich conditions at 810°C, followed by ~150nm AlN NW grown at 900°C. Three GaN quantum disks (nominally 1ML thick) separated by 10nm AlN barriers were next grown at 850°C. A nitrogen flow rate of 0.33sccm and plasma power of 350W were maintained, corresponding to a III/V ratio of ~0.3, during the ML GaN growth. The average NW diameter is 35nm and the area density is 6x10⁹cm⁻². MBE growth of the planar heterostructures was carried out on AlN/sapphire templates. 50nm of an AlN buffer layer is first grown at 750°C, followed by 350nm of Al_{0.65}Ga_{0.35}N at 690°C. A short growth interruption (~10s) under nitrogen plasma results in the formation of the ML GaN layer, on which 60nm of Al_{0.65}Ga_{0.35}N is finally grown. HRTEM measurements indicate that the GaN layer in both NW and planar samples is ~1ML thick. Macro-PL measurements made on the NW samples with an excitation (hν=6.2eV) spot size of ~20μm show an inhomogeneous-broadened spectrum at all temperatures in the 4-300K range. The peak energy follows the Varshni equation with E_{peak}=5.18eV at 300K. An S-type behavior at low temperatures indicates the presence of localized states in and around the ML GaN and redistribution of carriers amongst them. A distinctly different temperature dependence of E_{peak} is observed in microphotoluminescence measurements with a 5μm pinhole. Peaks and shoulders with narrower linewidths (~3-80meV) are observed. The value of E_{peak} of a particular transition remains constant at a relatively low energy up to ~50K, after which a pronounced blue-shift is observed up to 200K, followed by a decrease of E_{peak} with increasing temperature. At 300K, E_{peak} is again ~5.28eV. We attribute this behavior to carriers in a highly localized state subjected to a large internal field and the quenching of this field with increasing temperature by carriers released from surrounding defects. The value of E_{peak} remains unchanged, and the PL intensity varies almost linearly, with incident excitation intensity, indicating the excitonic nature of the PL. The room temperature value of E_{peak} is close to the theoretically calculated optical gap of the 1ML GaN, from which a value of E_{BX}~260meV is derived for these transitions. A recombination lifetime of 3ps is measured at cryogenic temperatures, confirming extreme confinement and strong overlap of the electron and hole wavefunctions. With increase of temperature, the lifetime increases due to broadening of the wavefunctions. A similar trend in the results is

observed from the planar ML GaN sample. These novel measured characteristics under extreme confinement will be presented and discussed. 1) D. Bayerl, et al. *Appl. Phys. Lett.* **109** 241102 (2016)

2:50 PM GG05

(LATE NEWS, Student) Negative Differential Resistance and Sequential Resonant Tunneling Transport in GaN/AlGaN Heterostructures

Jimmy Encomendero¹, S.M. Islam¹, Vladimir Protasenko¹, Anthony Hoffman³, Debdeep Jena^{1,2} and Huili Grace Xing^{1,2}; ¹School of Electrical and Computer Engineering, Cornell University, Ithaca, New York, United States; ²Department of Materials Science and Engineering, Cornell University, Ithaca, New York, United States; ³Department of Electrical Engineering, University of Notre Dame, Notre Dame, Indiana, United States.

From ultra-fast resonant tunneling diodes (RTDs) to quantum cascade lasers (QCLs), III-Nitride heterostructures hold the promise for the development of high-power terahertz sources of radiation. With a wide and tunable band gap spanning several electron-volts, III-Nitride heterostructures represent a highly versatile platform for tailoring electronic levels via quantum confinement. This advantage, coupled with their high breakdown electric-fields, high thermal conductivity, and high electron saturation velocity, make III-Nitride semiconductors an unmatched material system for the development of highpower electronic and photonic devices. These outstanding material properties have prompted considerable research efforts aiming at the engineering of resonant tunneling transport within this revolutionary family of wide bandgap semiconductors. Recently, breakthroughs in III-Nitride epitaxial growth, device fabrication, and polar heterostructure design have allowed us to demonstrate reliable room-temperature negative differential conductance (NDC) in GaN/AlN RTDs. In addition, the first nitride-based RTD oscillators have been demonstrated last year, attesting to the robustness of the resonant tunneling phenomena enabled by III-Nitride tunneling heterostructures. In the present work, we engineer sequential resonant tunneling transport in GaN/AlGaN heterostructures composed of multiple stages of GaN quantum wells coupled by AlGaIn tunneling barriers. Vertical transport is studied in these devices under both bias polarities, revealing a region of robust NDC under forward bias with a peak tunneling current of ~ 15 kA/cm². Numerical simulations of the overall device structure indicate that because of the internal polarization fields, the groundstates of the multiple GaN wells give rise to a Wannier-Stark ladder at equilibrium conditions. We employ temperature-dependent tunneling spectroscopy to study quantum transport over a wide temperature window spanning from 80 K up to 400 K. Under low forward bias (< 1 Volt), the current-voltage characteristics exhibit a weak temperature dependence, showing that charge transport occurs via tunneling injection. In contrast, the reverse bias current is dominated by thermionic emission, therefore it exhibits a considerable temperature dependence. At high temperatures, the forward conductance-voltage curve exhibits a single peak at ~ 1 Volt, as a result of the flattening of the Wannier-Stark ladder. At cryogenic temperatures, this single conductance peak breaks into multiple conductance peaks and valleys, consistent with the picture of sequential resonant tunneling transport across the device active region. Under high-forward bias, the bound states on the emitter are aligned into a resonant configuration at ~ 3.2 Volts, in reasonable agreement with the experimental onset of NDC, measured at ~ 3.5 Volts. These results constitute the first demonstration of negative differential conductance and sequential tunneling transport in a GaN/AlGaIn heterostructure, thus showing the great potential of nitride-based resonant tunneling injection for achieving population inversion in III-Nitride quantum cascade structures.

3:10 PM REFRESHMENT BREAK

3:30 PM GG06

Spin Dependent Trap Assisted Tunneling Measurements on Hot Carrier Injection-Induced Leakage Currents in SiO₂ on 4H-SiC James P. Ashton¹, Patrick M. Lenahan¹, Daniel J. Lichtenwalner² and Aivars Lelis³; ¹Engineering Science and Mechanics, The Pennsylvania State University, University Park, Pennsylvania, United States; ²Power R&D, Wolfspeed, A Cree Company, Research Triangle Park, North Carolina, United States; ³United States Army Research Laboratory, Adelphi, Maryland, United States.

4H-SiC metal-oxide-semiconductor field effect transistors (MOSFETs) have great potential in high power and high temperature applications. However, the performance of these transistors is, as yet, somewhat limited by several factors. Effective carrier mobility at the 4H-SiC/SiO₂ interface is fairly low, generally around 30 cm²/Vs. Passivation techniques involving nitric oxide anneals, and more recently with the addition of a

barium interfacial layer (IL)^{1,2}, have been utilized to increase the channel mobility, but the physical mechanisms involved in the improvements are, as of yet, not fully understood. In addition, reliability issues related to defects within the gate oxide, such as gate leakage resulting from stressing, create additional performance limitations in MOSFETs based on 4H-SiC. In this work, for the first time, we utilize electrically detected magnetic resonance (EDMR) via spin dependent trap assisted tunneling (SDTAT) to detect deep level defects within the SiO₂ involved in oxide leakage currents. These currents are caused by hot carrier stressing. We believe our work may be of interest for at least two reasons: first, the work provides atomic scale information about a reliability issue in 4H-SiC MOSFETs and also suggests that SDTAT may be of widespread usefulness in studies of stress-induced leakage currents in other MOS systems. The work utilized two EDMR spectrometers. One spectrometer operates at approximately 9.5 GHz with magnetic fields of about 340 mT. The second spectrometer operates at approximately 141 MHz with magnetic fields of about 5.0 mT. In our measurements, we utilize 4H-SiC MOSFETs that have a barium IL. The EDMR measurements involved both spin dependent recombination (SDR) via the bipolar amplification effect (BAE), which is primarily sensitive to near-mid gap states in the SiC, and EDMR detected through SDTAT observed through oxide gate leakage generated by hot carrier stressing of the gate oxide. Before hot carrier oxide stressing, the BAE response we observe is consistent with a SiC near interface defect, a silicon vacancy³. After stressing, we observe a change in the BAE response which is due to an additional spin dependent current, a stress-induced leakage current in the oxide. By stressing, we can induce quite high gate leakage currents; the spin dependent response in the gate currents is large enough to substantially alter the BAE response. After stressing, the apparent BAE response is actually a combination of SDTAT and SDR. This combination yields an EDMR response with two lines, one corresponding to the SiC silicon vacancy defect and the other corresponding to the tunneling defect. The g corresponding to the silicon vacancy defect is approximately 2.0030³ and the g corresponding to the tunneling defect is 2.0038. As yet, the physical nature of the defect involved in tunneling has not been identified. We demonstrate directly that the altered response is due to EDMR of leakage current in the oxide by disconnecting the source and drain and measuring the spin dependence of the current through the oxide by applying a gate bias and monitoring the gate to substrate current as a function of the magnetic field. In these measurements, the silicon carbide defect, the silicon vacancy signal corresponding to a g of 2.0030, disappears but the tunneling signal corresponding to g = 2.0038 remains. The work at Penn State was supported by the U.S. Army Research Laboratory. Any opinions, findings, conclusions, or other recommendations expressed herein are those of the authors and do not necessarily reflect the views of the U.S. Army Research Laboratory. ¹ D.J. Lichtenwalner, L. Cheng, S. Dhar, A. Agarwal, and J.W. Palmour, *Appl. Phys. Lett.* **105**, 1 (2014). ² J.H. Dycus, W. Xu, D.J. Lichtenwalner, B. Hull, J.W. Palmour, J.M. Lebeau, and J.M. Lebeau, **201607**, (2017). ³ C.J. Cochrane, P.M. Lenahan, and A.J. Lelis, *Appl. Phys. Lett.* **100**, (2012).

3:50 PM GG07

(Student) Gate Oxide Reliability Assessments of Commercial 4H-SiC

MOSFETs Tianshi Liu¹, Susanna Yu², Diang Xing¹, Minseok Kang¹, Arash Salemi¹, Marvin White¹ and Anant Agarwal¹; ¹ECE, The Ohio State University, Columbus, Ohio, United States; ²Electrical Computer Engineering, The Ohio State University, Dublin, Ohio, United States.

4H-SiC MOSFETs for high-voltage applications are now commercially available in a fast-growing market. Since the cost of manufacturing SiC MOSFETs is still high, most device vendors have to make trade-offs between device cost and reliability/ruggedness. Despite considerable advancement in device performance of commercial 4H-SiC MOSFETs, gate oxide reliability is still an important issue. In order to have long-time reliability of the gate oxide of 4H-SiC MOSFETs, two major concerns should be investigated: Fowler-Nordheim (F-N) tunneling current and Time-Dependent Dielectric Breakdown (TDDB). It is worth noting that these measurements, have so far been performed on small area SiC MOS capacitors and no study on commercial 4H-SiC MOSFETs, to the author's knowledge, has been reported. Therefore, it is critically important to analyze the F-N tunneling current and TDDB on relatively large area commercial SiC MOSFETs at different temperatures to evaluate the current status of the gate oxide reliability of these devices and predict their ruggedness under realistic operations. Due to a lower effective barrier height and a higher gate oxide electric field at the interface of SiC/SiO₂ compare to the Si/SiO₂, electron tunneling probability into the gate oxide of 4H-SiC MOS devices is higher than the Si MOS devices. Furthermore, the F-N injection of electrons into the gate oxide increases at elevated temperatures. Agarwal et al showed that as temperature increases, the magnitude of the tunneling current increases, thus lowering the electric

field at which the dielectric breaks down in small area 4H- and 6H-SiC MOS capacitors [1]. It has also been reported that the intrinsic mean-time-to-failure (MTTF) of n-type 6H-SiC MOS capacitors exhibits a higher acceleration factor for both higher electric fields and elevated temperatures [2]. These studies indicate that the gate oxide reliability issue can become more significant when these devices operate under extreme conditions. This work focuses on the ruggedness of the gate oxide of commercially available 4H-SiC MOSFETs from several vendors. We investigated the F-N tunneling current as a function of gate bias by measuring the gate leakage current with the device under positive or negative gate voltage and source and drain terminals grounded. The gate leakage current is monitored until the gate oxide approaches its breakdown. In order to study the temperature dependence of the F-N tunneling current, the gate leakage current is measured at different temperatures up to 300°C. For TDDB measurements, due to the statistical nature of dielectric breakdown, several commercial devices are tested at each gate oxide voltage and temperature to obtain an accurate failure distribution. First, a fairly high gate bias, close to the breakdown of the gate oxide, is applied to the devices at room temperature with source and drain terminals grounded. The time to fail is recorded when the gate current reaches a pre-determined value. This test is repeated for several values of gate bias. These measurements are repeated for higher temperatures (175 °C and 300 °C). Then, the mean time to Failure (MTTF) is extrapolated back to recommended operating voltage and temperature of the device to predict the lifetime. [1] A. K. Agarwal, et al., *IEEE Electron Device Letters* 18, no. 12 (1997): 592-594. [2] M. M. Mathur, et al., *IEEE Transactions on Electron Devices* 46, no. 3 (1999): 520-524.

4:10 PM GG08

(Student) Time-Dependent Bias-Stress-Induced Threshold Voltage Instability of 4H-SiC MOSFETs Susanna Yu, Tianshi Liu, Xing Diang, Arash Salemi, Minseok Kang, Marvin White and Anant Agarwal; Electrical Computer Engineering, The Ohio State University, Dublin, Ohio, United States.

Thanks to its unique properties such as wide bandgap, high electric field, and high thermal conductivity, Silicon Carbide (SiC) semiconductor devices are being developed to replace the conventional Silicon (Si) power devices that are approaching the fundamental material limits in power electronic applications [1]. However, MOS-based SiC devices that are currently commercially available in the market may lack ruggedness in certain aspects. In order to reduce device cost, some tradeoffs between device size and ruggedness have to be made. In recent years, a number of potential reliability issues for SiC MOSFETs have been reported including very low short-circuit times, threshold voltage instability, body-diode robustness, and gate leakage currents at high temperatures. Threshold voltage instability, studied in this work is caused by a high density of traps and trapped charges at or near the interface of SiC/SiO₂ [2, 3]. It is worthwhile to study the threshold voltage instability of the commercial devices in order to evaluate whether the devices are robust enough for the applications such as automotive requiring stringent reliability requirements. Due to the existence of these traps, when a positive DC bias is applied to the gate over a long period of time, the threshold value shifts in the positive direction due to the capture of electrons by traps. Conversely, when a negative bias is applied to the gate over a long period of time, the threshold voltage shifts in the negative direction resulting in a significant increase in leakage current in the off-state. Furthermore, a negative shift of threshold voltage can cause devices to turn on unexpectedly and lead to failures. In this work, the results of threshold voltage instability measurements of 1200 V 4H-SiC DMOSFETs from different vendors are reported. We investigate this particular trap-induced device degradation on commercially available devices by applying a positive and negative DC voltage stress on the gate over a long period of time, with source and drain grounded. Both positive (20 V, 25 V, and 30 V) and negative (-15 V, -20 V, -25 V) bias stresses were applied for 10, 20, 50, and 100 hours at room temperature. At the end of each stress, transfer characteristics (I_D - V_G) were measured to determine the threshold voltage shifts. After the completion of positive gate stress up to 100h, -10V was applied for 5 mins to release the electrons captured at or near the SiC/SiO₂ interface during the positive bias stress. Likewise, after completing the negative bias stress measurements, +10V was applied for 5 mins to restore devices to initial condition. Considerable variance between devices from different vendors was observed implying that while some vendors have been able to significantly reduce the near interface traps in the gate oxide, the others may still be far behind. [1] J. A. Cooper, Jr. and A. K. Agarwal, "SiC power-switching devices—The second electronics revolution?" *Proc. IEEE*, Vol. 90, No. 6, pp. 956–968, 2002. [2] A. K. Agarwal and S. Haney, "Some critical Materials and Processing Issues in SiC Power Devices", *Journal of Electronic Materials*, Vol. 37, No. 5, pp. 646–654, 2008. [3] A. J. Lelis, R. Green, D. B. Habersat, and M. El, "Basic mechanisms of

threshold-voltage instability and implications for reliability testing of SiC MOSFETs," *IEEE Trans. Electron Devices*, Vol. 62, No. 2, pp. 316–323, 2015.

4:30 PM GG09

Effects of Deposition Temperature of Ti and Mo Schottky Contacts on Ti/SiC and Mo/SiC Schottky Diodes Tom Oder, Sai B. Naredla and Krishna C. Kundeti; Physics and Astronomy, Youngstown State University, Youngstown, Ohio, United States.

Molybdenum (Mo) and titanium (Ti) have been recognized as metals with high melting points, high tensile strength and high corrosion resistance. In this investigation, silicon carbide (SiC) Schottky diodes have been fabricated using Mo and Ti as the Schottky contacts. The contacts were deposited by magnetron sputtering on the n-type 4H SiC at different temperatures from 25 °C to 900 °C. The electrical properties of the diodes were determined by current-voltage, capacitance voltage and current-voltage-temperature measurements. The diodes fabricated with Mo contacts showed energy barrier heights ranging from 1.04 - 1.58 eV. While the ideality factors vary from 1.03 to 1.44, there maintain values at or below 1.1 for contacts deposited above 200 °C. The diodes with Ti contacts deposited at 200 °C and annealed had the optimum current-voltage characteristics consisting of large barrier height of 1.13 eV and ideality factor of 1.04. These diodes in addition had very low leakage current of 6.6×10^{-8} A at a reverse voltage bias of 400 V. The X-ray diffraction analysis of the contacts revealed the formation of carbides and silicides at the interface. The improved properties for diodes with contacts deposited at elevated temperatures could be related to formation of interfacial alloys possessing higher work functions. These improvements could provide means to further improve the performance of 4H-SiC Schottky diodes where these metals are used as contacts.

4:50 PM GG10

(LATE NEWS, Student) High Quality N-Polar GaN Epilayer Grown Directly on Si Through Controlled Nanowire Coalescence Kishwar Mashooq¹, Srinivas Vanka^{1,2}, Ping Wang¹, David A. Laleyan¹, Ayush Pandey¹ and Zetian Mi¹; ¹Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ²Department of Electrical and Computer Engineering, McGill University, Montréal, Quebec, Canada.

High quality N-polar GaN that can be epitaxially grown on low cost, large area Si wafer is of tremendous importance for application in power electronics, LED lighting, avalanche photodiodes, and artificial photosynthesis. For example, N-polar GaN has demonstrated superior performance for mm-wave power amplifiers, compared to conventional Ga-polar devices. To date, however, it has remained extremely challenging to grow GaN epilayers directly on Si, due to the meltback etching of GaN with Si, ~17% in-plane lattice mismatch, and large difference in thermal expansion coefficients between Si and GaN. In addition, the achievement of N-polar GaN often relies on the growth of a thick AlN buffer layer or heavy Mg-doping to flip the polarity, which, together with the very large densities of dislocations, pose significant limitations on the device performance and reliability as well as their integration on Si. In this work, we have overcome these fundamental challenges by combining conventional planar epitaxy with GaN nanowire epitaxy. Through controlled coalescence of N-polar GaN nanowire arrays, we have demonstrated high quality N-polar GaN grown directly on Si substrate. N-polar GaN nanowires are first grown directly on Si (111) substrate using plasma-assisted molecular beam epitaxy under N-rich conditions. To promote the formation of uniform GaN nanowire arrays, a Ga seeding layer is deposited prior to growth initiation, which also ensures the formation of a Ga basal plane and therefore N-polar GaN. The growth temperature is ~750°C. The Ga flux was carefully optimized to achieve uniform and densely packed nanowire arrays. Due to the efficient surface stress relaxation, such GaN nanowires are nearly free of dislocations. After the uniform nucleation and formation of GaN nanowire arrays, the growth conditions are switched to a nearly Ga-rich condition to enhance the lateral growth and hence promote the coalescence of GaN nanowires, which is achieved by decreasing N₂ flow rate and optimizing the growth temperature and Ga flux. The growth rate is ~170 nm/hr, which can be further increased by varying the growth conditions. Such a two-step growth mode has found to be essential to achieve high quality N-polar GaN grown directly on Si wafer. The growth conditions have been carefully monitored and adjusted by *in-situ* reflection high-energy electron diffraction (RHEED) to ensure that a smooth and flat surface can be achieved during the epilayer growth. To confirm the polarity of GaN, the sample was etched with 10% TMAH at 45°C for 3 minutes. Significant roughness was seen on the surface morphology confirming the N-polarity of GaN samples.

Structural and optical properties of N-polar GaN epilayers grown on Si wafer are characterized. The samples are free of cracks, which is in direct contrast of the presence of large densities of cracks for GaN epilayers grown directly on Si using conventional methods. This is because the tensile stress is effectively released through the underlying GaN nanowires. The samples exhibit smooth surface, with a root mean square roughness of ~ 0.5 nm. The presence of pits is also negligible under optimized growth conditions. Photoluminescence emission of N-polar GaN grown on Si is comparable to that of commercial GaN template grown on sapphire wafer. Yellow luminescence, that is commonly measured in GaN epilayers, is absent for N-polar GaN grown on Si in this study, suggesting a significantly lower level of defect densities. Work is currently in progress to achieve nearly dislocation-free N-polar GaN on on-axis Si and SiC substrate. A detailed investigation of their structural, electrical, and charge carrier transport properties will be performed and reported.

SESSION HH: III-Nitride Growth

Session Chairs: Karl Hobart and Andrew Koehler

Thursday Afternoon, June 27, 2019

Rackham Building, 4th Floor, Amphitheatre

1:30 PM HH01

Preparation of Gallium Nitride via High Pressure Confined Chemical Vapor Deposition Ian Campbell¹, Kayla Cooley¹, Alex Molina¹, John Badding² and Suzanne Mohney¹; ¹Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania, United States; ²Chemistry, The Pennsylvania State University, University Park, Pennsylvania, United States.

High-pressure confined chemical deposition techniques have been used to fill optical fibers that are meters long with silicon without porosity,¹ as well as to fill three-dimensional nanostructures that have repeat units on the order of tens of nanometers with nickel.² To explore the potential of this technique for gallium nitride, high pressure confined chemical vapor deposition (HPcCVD) was used to prepare centimeters-long gallium nitride samples in hollow silica fibers. Trimethylgallium and ammonia were used as precursors at V/III ratios ranging from ~ 2 -1300 with nitrogen acting as a carrier gas. Temperatures from 350-650 °C and pressures of 20-45 MPa were tested in fibers with inner diameters of 20 μ m. The densest, most uniform film was obtained at a V/III precursor ratio of ~ 1300 , starting pressure of ~ 45 MPa, and temperature of 650 °C. Selected area electron diffraction in the transmission electron microscope offers definitive evidence of the synthesis of wurtzite gallium nitride. The material has grains on the order of 10 nm with some nanoscale porosity. While future work will include identifying conditions that reduce or eliminate nanoscale porosity, such a nanostructure may also be beneficial for certain applications. For example, gallium nitride with similarly sized pores prepared using a top-down approach has recently been investigated for stem cell engineering.³ REFERENCES 1. Sparks, J. R., Sazio, P. J. A., Gopalan, V. & Badding, J. V. *Annual Review of Materials Research* **43**, (2013). 2. Liu, Y., Kempinger, S., He, R., Day, T. D., Moradifar, P., Yu, S., Russell, J. L., Torres, V. M., Xu, P., Mallouk, T. E., Mohney, S. E., Alem, N., Samarth, N. & Badding, J. V. *Nano Lett.* **18**, 546–552 (2018). 3. Han, L., Zhou, J., Sun, Y., Zhang, Y., Han, J., Fu, J. & Fan, R. J. *Nanotechnol. Eng. Med.* **5**, 1–9 (2015).

1:50 PM HH02

(Student) Role of Ga Supersaturation on Facet Formation in GaN Epitaxial Lateral Overgrowth Ke Wang¹, Felix Kaess¹, Shun Washiyama¹, Seiji Mita², Will Mecouch², Yan Guan¹, Ronny Kirste², Ramón Collazo¹ and Zlatko Sitar^{1,2}; ¹Material Science and Engineering, North Carolina State University, Raleigh, North Carolina, United States; ²Adroit Materials, Raleigh, North Carolina, United States.

Facet-controlled epitaxial lateral overgrowth (FACELO) is a technique to produce GaN films with planes inclined from the c-plane substrate surface. These films can be used as templates to grow crack-free low Al content AlGaIn for applications such as UV-A emitters. Although facet formation in ELO-GaN has been experimentally controlled by growth parameters such as temperature, pressure, and precursor flows, the mechanism behind facet formation is not properly described in terms of general crystal growth concepts such as vapor supersaturation. In general, vapor supersaturation describes the driving force for crystal growth, and determines possible growth modes such as step flow and 2D nucleation. This study will establish the general relationship between supersaturation

and the growth of FACELO GaN, providing a systematic framework for structure designed as required for relaxation engineering. The ELO-GaN was grown by MOCVD on patterned c-plane GaN/Sapphire templates that consist of 2 μ m-wide SiO₂ mask alternating with 2 μ m-wide opening. The stripe direction was along $\langle 1-100 \rangle$ direction of GaN. Growth condition with 900 °C, 80 Torr, 132 μ mol/min TEG, 1.5 slm NH₃, and 5.7 slm H₂ was chosen as our reference growth condition. Starting from the reference growth condition, growth temperature, total pressure, and metalorganic flow were varied to investigate the role of Ga supersaturation on facet formation. The Ga supersaturation at a given growth condition was estimated from the corresponding thermodynamic system in GaN MOCVD¹. Surface and cross section of ELO-GaN were characterized by scanning electron microscope. As calculated, the vapor Ga supersaturation (σ_{Ga}) above GaN increased by decreasing the growth temperature and/or increasing the total pressure. Under the base growth condition, σ_{Ga} was estimated to be 17000, 1900, and 725 at 900°C, 1000°C and 1050°C, respectively. SEM images showed that the inclined facet {11-22} appears as σ_{Ga} increases by decreasing temperature, and the shape of ELO GaN islands changed from rectangle to triangle. These results suggest that a high σ_{Ga} (≈ 17000) is necessary to obtain triangular shaped islands with enhanced vertical growth rate along c-direction. To separate the influence of growth temperature, ELO-GaN growth under different growth condition but at a fixed temperature of 900°C was demonstrated. Similar σ_{Ga} (≈ 17000) was realized by reducing total pressure to 40 Torr and increasing Ga precursor flow rate to 193 μ mol/min. GaN ELO exhibited the same triangle-shaped islands composed of {11-22} facets. Consequently, it was found that σ_{Ga} governs the facet formation in ELO and not any specific growth parameter. The detailed mechanism of supersaturation-controlled facet formation along with its relationship to facet surface energy will be presented. [1] Mita *et al.*, *J. Appl. Phys.* **104** (2008) 013521

2:10 PM HH03

Growth and Characterization of Graded AlGaIn/GaN HEMT Structures on SiC for High Linearity Transistor Technologies Fevzi E. Arkun, Jeong-Sun Moon, Joel Wong, Michael Antcliffe, Clayton Jackson, Isaac Khalaf, Robert Grabar and Andrea Corrión; HRL Laboratories, LLC, Malibu, California, United States.

Transistor technologies based on the AlGaIn/GaN hetero-structure are used in a wide variety of applications such as RF communications, radar systems, electronic warfare (EW) and power electronics. The ever-increasing number of military and commercial RF signals has created a very complex electromagnetic spectrum, and the demand for more RF signals will require greater number of devices to operate in a given band. In addition, advantages such as smaller antenna sizes and unallocated bandwidth are driving a push towards high frequency operation in the mmW region (30GHz and above). RF transceivers operating in a crowded electromagnetic spectrum with large signal to noise ratios are fundamentally limited by the intrinsic linearity vs power density tradeoff of the transistor technology. The high breakdown field, high electron saturation velocity and large charge density in the 2DEG channel of GaN-based transistor technologies is a unique combination that enables operation of devices at high power and high frequencies, however, the power requirements for the linearity performance is limited by the design of the transistor device. Realization of highly linear transistor technologies operating at high power and high frequencies is required to efficiently process RF signals in a large bandwidth and high fidelity. These linearity requirements can be fulfilled by developing new materials and device structures to improve the linearity of the transistor technology. In this paper we present the epitaxial growth and characterization of engineered GaN/Graded AlGaIn/AlGaIn structures designed to improve the linearity vs output power trade-off in transistor devices. Band structure calculations for conventional AlGaIn/GaN heterostructures show that the electron wavefunction is confined to a region close to the barrier whereas similar device structures incorporating a 6 nm 0a27% AlGaIn graded region above the conventional channel results in the spatial distribution of the electron wavefunction over the graded region of the channel. The spatial distribution of charge in the graded region of the channel minimizes non-linearities in transistor transconductance (g_m) and C_{gs} while maintaining the high mobility of carriers. Epitaxial growth of the structures was performed by using an Aixtron CCS MOCVD reactor on 100mm SI-SiC substrates. Contactless Hall mobility measurements of unpassivated device structures resulted in field-effect carrier mobility and density of 1413 cm²/V.s and 7.88 $\times 10^{12}$ /cm² respectively. Capacitance-voltage measurements of the conventional channel devices show abrupt decrease in capacitance as a function of bias confirming the presence of a sheet charge in the channel. In the case of scaled and graded channels, the decrease in capacitance is gradual due to the spatial distribution of charge in the channel region, confirming the intended spatial distribution of the electron wavefunction in the channel. Structural characterization of composition profiles for

graded active regions that are vertically scaled for mmW operation is challenging, as composition gradients are approaching the resolution limits of many small-area sampling analytical techniques, while layers are too thin to be resolved using conventional x-ray diffraction. In order to mitigate this challenge, graded superlattices were grown to generate XRD patterns representative of the active region. X-ray diffraction simulations were carried out to determine the optimum structures for evaluating scaled graded AlGaIn layers. Scaled and graded AlGaIn layers as thin as 3.5 nm were characterized by the X-ray analysis method developed. In this talk, we will present our latest data on the growth of graded channel device structures, characterization results along with modelling of X-ray diffraction patterns, and experimental results of X-ray measurements performed on scaled graded structures used in the device technologies we are currently developing.

2:30 PM HH04

(Student) Structural Differences Between Al-Rich and Ga-Rich AlGaIn Grown on (0001) Sapphire Substrates Michael E. Liao¹, Kenny Huynh¹, Tingyu Bai¹, Yekan Wang¹, Hsuan Ming Yu¹, Mohammad M. Abdullah², Kamal Hussain², Asif Khan² and Mark Goorsky¹; ¹Materials Science & Engineering, University of California, Los Angeles, Los Angeles, California, United States; ²Electrical Engineering, University of South Carolina, Columbia, South Carolina, United States.

In this study, epitaxial layers of AlGaIn with different compositions were investigated – an Al-rich ($\text{Al}_{0.60}\text{Ga}_{0.40}\text{N}$) composition and a Ga-rich ($\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$), both deposited on $\sim 2\ \mu\text{m}$ AlN buffer layers on (0001) sapphire using metalorganic vapor phase epitaxy. Asymmetric X-ray diffraction reciprocal space maps (RSMs) were generated for each sample and the 10 $\bar{1}$ 4 AlGaIn peak shapes (i.e. scattered intensities around the AlGaIn reciprocal lattice point) were examined. The RSM's showed that both AlGaIn samples were fully strained (pseudomorphic) to the AlN buffer layer. More interestingly, the AlGaIn peak shapes were different: the $\text{Al}_{0.60}\text{Ga}_{0.40}\text{N}$ sample exhibited a more circular shape while the $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$ sample exhibited a more tilted, elliptical shape. This difference in peak shapes corresponds to a difference in the defect formation for the Al-rich AlGaIn on AlN vs Ga-rich AlGaIn on AlN. In fact, elliptical RSM peak shapes had also been observed for Ga-rich AlGaIn (Ga compositions ranging from 0.69 to 0.81) grown on sapphire with a GaN buffer layer¹ and for GaN grown on (0001) sapphire.² Two-beam condition scanning transmission electron microscopy (STEM) images^{3,4} identified the types of dislocations present in the layers. Edge and screw dislocations were present in the $\text{Al}_{0.60}\text{Ga}_{0.40}\text{N}$ sample while edge, screw, and mixed dislocations were present in the $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$ sample. The higher Al-content AlGaIn contained predominately edge dislocations ($\sim 97\%$ of all observed dislocations) that were oriented 60° away from the surface, along the $[11\bar{2}1]$ direction. The lower Al-content AlGaIn also contained mostly edge dislocations ($\sim 79\%$ of all observed dislocations), but most of these made a smaller angle (39° to 49°) from the surface, along the $[22\bar{4}1]$ and $[33\bar{6}2]$ directions. Another interesting finding from the RSMs is that the 10 $\bar{1}$ 4 AlN buffer layer peak exhibited a strong lateral intensity profile. ω scans of the (10 $\bar{1}$ 2) AlN and AlGaIn reflections were also measured and the width of the AlN peaks for both samples was $\sim 410^\circ$. On the other hand, the ω scans of the (10 $\bar{1}$ 2) reflection for the AlGaIn layers have widths of 410° for the $\text{Al}_{0.60}\text{Ga}_{0.40}\text{N}$ and 550° for the $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$. Along with the difference in the RSM peak shapes, the widths of the Al-rich AlGaIn matches that of the AlN layers while the Ga-rich AlGaIn exhibits a larger peak width, supporting the STEM results. This suggests that the $\text{Al}_{0.44}\text{Ga}_{0.56}\text{N}$ sample has more of a GaN-like defect structure while the $\text{Al}_{0.60}\text{Ga}_{0.40}\text{N}$ exhibits a dislocation distribution more like the underlying AlN. References 1. M. Tsuda et al., Phys. Stat. Sol. (B) 243(7), 1524 (2006) 2. V. Darakchieva et al., Appl. Phys. Lett. 91, 031911 (2007) 3. B.H. Kong et al., Appl. Surf. Sci. 258, 2522 (2012) 4. C.J. Gu, et al. CS Mantech Conf., (2011)

2:50 PM HH05

Molecular Beam Epitaxy of High-Quality GaN and AlN on Monolayer Graphene Ping Wang, David A. Laleyan, Eric T. Reid, Dehui Zhang, Zhaohui Zhong and Zetian Mi; Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

Van der Waals epitaxy of III-nitrides on two-dimensional (2D) materials has attracted significant attention, as it promises significantly reduced dislocation densities compared to conventional heteroepitaxy on lattice mismatched substrates. The resulting epilayers can also be readily exfoliated and transferred to various substrates for subsequent device processing and integration. To date, however, controlled nucleation of adatoms on the sp²-hybridized 2D surfaces has remained difficult, due to the extremely low surface energy, which limits the formation of large-area

single-crystalline epilayers. Here, we have investigated the epitaxy and characteristics of GaN, AlN, and their heterostructures on monolayer graphene by using plasma-assisted molecular beam epitaxy (MBE). The graphene grown on Cu by chemical vapor deposition (CVD) was first transferred on different substrates (sapphire, GaN template, and AlN template) for the subsequent epilayer growth. After the transfer of graphene, the atomic steps of the underlying substrate remain clearly observable except for the grain boundaries and wrinkles of graphene. However, even with single monolayer graphene, the epitaxy of GaN and AlN is distinctly different compared with the conventional sp³ substrates, such as sapphire, SiC, and Si. By carefully optimizing the growth conditions, we have demonstrated that single-crystalline GaN and AlN with an atomically smooth surface can be achieved on monolayer graphene. We have further demonstrated that, by utilizing a post-growth stressor layer, the epilayers can be peeled off from the substrate and transferred to other arbitrary substrates. The exfoliation process depends on the interface between the epilayer and graphene. A smooth interface is beneficial for peeling-off, while a rough interface limits the exfoliated layer size. Comparing with GaN grown on sapphire, the exfoliated GaN epilayer exhibits a blue shift in Raman scattering, indicating full strain relaxation. Signals related to cubic-GaN and yellow-band emission were also measured. These are mainly caused by the random nucleation at the initial stage of growth and can be eliminated by further optimizing the nucleation process. We further observed that the excitonic emission from AlN epilayers grown on graphene is nearly identical to that of AlN grown on commercial AlN templates on sapphire, except for a small blue shift. The epitaxy of InGaIn/GaN and AlGaIn/AlN quantum well/dot heterostructures on graphene and their device applications, including the demonstration of high efficiency ultraviolet light-emitting diodes (UV LEDs), is being investigated and will be reported. This work opens up new opportunities for the van der Waals epitaxy of III-nitride materials and devices, providing new approaches for the fabrication of scalable flexible optoelectronic devices.

3:10 PM REFRESHMENT BREAK

SESSION II: Visible Emitters
Session Chairs: Matt Brubaker and Jonathan Wierer
Thursday Afternoon, June 27, 2019
Rackham Building, 4th Floor, Amphitheatre

3:30 PM II01

High Efficiency InGaIn Nanocrystal Green and Red Micro LEDs Xianhe Liu^{1,2}, Kishwar Mashooq¹, Ayush Pandey¹, Walter J. Shin¹ and Zetian Mi¹; ¹Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ²Department of Electrical and Computer Engineering, McGill University, Montreal, Quebec, Canada.

High efficiency, micro-light emitting diodes (LEDs) that can operate efficiently in the blue, green and red spectra are in demand for a broad range of applications including mobile displays, virtual/mixed/augmented reality, bio-photonics, and communications. To date, however, GaN-based micro-LEDs exhibit very low efficiency, particularly in the green and red wavelengths, which has been limited by the presence of large defect densities, surface recombination and poor current injection. In this context, we have investigated the design, epitaxy, and optical properties of dislocation-free InGaIn nanocrystals, and have demonstrated small size ($\sim 2\text{-}5\ \mu\text{m}$) LEDs that can operate relatively efficiently in the green, yellow, and orange wavelengths. InGaIn nanocrystals are arranged in a hexagonal lattice. Self-organized InGaIn quantum dots are incorporated in the nanocrystals to serve as the active medium. Photonic nanocrystal arrays with areal sizes $2\ \mu\text{m} \times 2\ \mu\text{m}$ to $10\ \mu\text{m} \times 10\ \mu\text{m}$ are designed and investigated. Such photonic crystal structures allow for the efficient extraction of the guided modes. By adjusting the flat bands of leaky modes to match the emission wavelengths of the active region, high light extraction efficiency (up to 100% in theory) can be achieved without any surface roughening and encapsulation, which will be ideally suited for high efficiency micro-LED application. Moreover, photonic crystal structures provide the unique opportunity to shape the emission profile of a micro-LED and to enhance the radiant intensity. By varying the lattice points and/or lattice phases, the beam shape can be tuned to realize LEDs with on-demand beam characteristics. In this study, the nanocrystal LED structure consists of $\sim 500\ \text{nm}$ n^+ -GaIn, five to ten vertically aligned InGaIn/AlGaIn quantum dots (QDs), an AlGaIn electron blocking layer and $\sim 240\ \text{nm}$ p^+ -GaIn cladding and contact layer. InGaIn nanocrystals are

grown on nano-patterned substrate using the technique of selective area epitaxy by plasma-assisted molecular beam epitaxy (MBE). The epitaxy takes place on GaN template on sapphire substrate with a thin (~10 nm) Ti layer being employed as the growth mask. Openings with various sizes are created on the Ti mask by e-beam lithography and reactive ion etching techniques. Under optimum growth conditions, InGaN nanocrystals are only formed in the opening apertures, and no epitaxy takes place on the Ti mask layer. The presence of surface recombination has been identified as the major cause for the low quantum efficiency for micro-LEDs. We have developed the epitaxy of InGaN core-shell nanocrystal structures, wherein a large bandgap AlGaN shell is incorporated to suppress non-radiative surface recombination. During the epitaxy of InGaN/AlGaN quantum dots, an AlGaN shell is also spontaneously formed on the sidewall of the nanowires, due to the smaller Al adatom migration rate on the lateral surfaces. The fabrication process involves the use of standard photolithography, dry etching, and contact metallization techniques and is nearly identical to that of conventional planar quantum well devices. InGaN nanocrystal micro-LEDs exhibit excellent current-voltage characteristic, with a turn on voltage ~3 V. Strong emission in the green, yellow and orange wavelengths were measured. The realization of green and red micro-LEDs with high efficiency and high brightness by exploiting the Purcell effect of photonic nanocrystals is currently in progress and will be reported.

3:50 PM II02

(Student) Luminescent Properties of Zigzag—Graded InGaN Quantum Wells Mirsaeid Sarollahi¹, Pijush Ghosh¹, Manal Aldawsari², Yuri Mайданиuk², Yuri I. Mazur³, Andrian Kuchuk³, Greg Salamo^{2,3,4} and Morgan E. Ware^{1,3}; ¹Electrical Engineering, University of Arkansas, Fayetteville, Arkansas, United States; ²Microelectronics-Photonics (MEPH), University of Arkansas, Fayetteville, Arkansas, United States; ³Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, Arkansas, United States; ⁴Physics, University of Arkansas—Fayetteville, Fayetteville, Arkansas, United States.

Recently, compositionally graded films in the III-nitrides have been studied actively due to the realization of both n- and p-type polarization doping. Additionally, with the wide spectral range of bandgaps covered, from the near UV (6.2 eV for Aluminum Nitride) to the near IR (0.7 eV for Indium Nitride), alloys of the III-nitrides have the potential for wide application to optical devices which operate throughout the visible spectrum. There has been some work in applying these graded structures to electronic devices, however, only recently have any optical devices been demonstrated. The presented work is an attempt to make broadband absorbing material in a device structure which can be implemented into photovoltaic devices by utilizing both the polarization doping properties and the wide spectral coverage demonstrated in the graded films. Here, we have designed graded quantum well (QW) structures of InGaN with the In composition increasing then decreasing in a zigzag pattern. The structures are designed by varying the maximum In composition, but maintaining a constant QW thickness. This is both in order to test the limits of the Molecular Beam Epitaxy growth control in terms of the deposition source ramping rates and to determine the limits of the maximum In composition with a narrow QW. The composition of In is varied for all structures starting from a minimum of ~3%, and increased to various maxima (17.5 to 22.5%), then finally decreased back to ~3%. These are chosen to achieve different emission energies. The samples are characterized for their structural and luminescent properties. Generally, the samples have strong X-ray diffraction symmetric reflections with well resolved thickness fringes which extend uniformly as a clear signature of graded composition growth with smooth interfaces. At the same time, the asymmetric reciprocal space maps demonstrate a characteristic tail showing mostly complete coherence of the growth with the substrate for all compositions studied. The results of extensive temperature and excitation power dependent photoluminescence studies demonstrate extremely broadband emission covering wavelengths between 380 and about 650nm. Additionally, although the general emission of structures with increasing maximum In composition shifts to lower energy, the luminescent band is comprised of several individual peaks which are currently being investigated as to the recombination mechanism of their origin. The power law dependence of all emission appears to be exciton-like. These results will be presented and explained within the scope of quantum confinement along with a varying bandgap and the associated polarization doping which is inherent in the wurtzite, III-nitride system.

4:10 PM II03

(Student) Room Temperature Luminescence of Passivated InGaN Quantum Dots Formed by Quantum-Sized-Controlled Photoelectrochemical Etching Xiongliang Wei, Syed Ahmed Al Mueyed, Matthew R. Peart, Wei Sun, Renbo Song, Nelson Tansu and Jonathan J. Wierer; Electrical and Computer Engineer, Lehigh University, Bethlehem, Pennsylvania, United States.

A large decrease in efficiency at high operating currents, or efficiency droop, is a well-known problem of InGaN-based emitters and is primarily caused by non-radiative Auger recombination.¹ One way to overcome Auger recombination is to use quantum dots (QD) instead of quantum wells for the light-emitting active layer. Theoretically, QD active layers will have higher spontaneous recombination rates and optical gain, translating into higher efficiencies at high current densities for both LEDs and laser diodes.² The theoretical benefits for QDs can only be realized with a high degree of dimensional control and QD density that the widely used Stranski-Krastonov QD growth method cannot achieve. Recently, quantum-size controlled photoelectrochemical (QSC-PEC) etching has been demonstrated as a controlled synthesis method to form InGaN QDs.³ In this method, coherent light is used during PEC etching to create photo-generated holes and induce etching of an initial InGaN layer. As etching proceeds QDs are eventually formed and shrink in size. As the QDs become smaller they eventually stop absorbing the laser light and the etch stops at a precise QD energy (laser light energy). To date, QDs formed with this method only exhibit photoluminescence at 4 K, most likely because of surface recombination. In this study, InGaN QDs are formed with the QSC-PEC process^{3,4} and passivation layers are formed to enable photoluminescence (PL) at 300 K. The QSC-PEC etch uses a 0.2 M H₂SO₄ electrolyte, Ag/AgCl reference electrode, Pt counter electrode, potentiostat to bias and measure the current, and a 445 nm laser diode as etch light source. The initial samples consist of a 7.5 nm thick In_{0.20}Ga_{0.80}N layer on GaN templates grown by MOCVD. The QSC-PEC conditions are varied with a bias of either 0.9 V to 1.5 V, an average laser power density of 20 mW/cm² or 100 mW/cm², and laser operation of either continuous wave or pulsed mode (5 % duty cycle, at 20 kHz). Etch times are between 20-30 min. The QSC-PEC etching forms QDs with conditions of 1.5 V and pulsed laser operation at ~90 mW/cm². Atomic force microscope (AFM) images show the QDs have diameters of ~20 nm and heights of ~5 nm. However, the large exposed surface area of the QDs results in little to no PL. Passivation layers are grown to recover the PL. The samples are subject to IPA for 15 min and sulfuric acid for 5 min to clean and remove oxides. Next, the passivation growth is performed and consists of a 2 nm thick Al_{0.45}Ga_{0.55}N layer followed by a 11 nm thick undoped GaN layer. After regrowth AFM images shows some pitting on the surface. However, PL with an argon ion laser at of ~20 W/cm² shows that QD emission is recovered at 300K. The peak PL intensity is ~439nm and the FWHM is ~35nm. The shift in QD PL wavelength from the laser wavelength is most likely due to changes in the energy states for the QDs with the addition of the passivation layers. Work continues to integrate this QD active layer into p-n junctions for electrical operation. ¹ J.J. Wierer, J.Y. Tsao, and D.S. Sizov, Laser Photon. Rev. 7, 963 (2013). ² J.J. Wierer, N. Tansu, A.J. Fischer, and J.Y. Tsao, Laser Photon. Rev. 10, 612 (2016). ³ X. Xiao, A.J. Fischer, G.T. Wang, P. Lu, D.D. Koleske, M.E. Coltrin, J.B. Wright, S. Liu, I. Brener, G.S. Subramania, and J.Y. Tsao, Nano Lett. 14, 5616 (2014). ⁴ X. Xiao, P. Lu, A.J. Fischer, M.E. Coltrin, G.T. Wang, D.D. Koleske, and J.Y. Tsao, J. Phys. Chem. C 119, 28194 (2015).

4:30 PM II04

(Student) Flexible Inverted InGaN Micro-LEDs Addressed by a-Si:H TFTs Pixel Circuits Qing Li¹, Mohsen Asad¹, Czang-Ho Lee¹, Manoj Sachdev¹ and William Wong²; ¹Electrical and Computer Engineering, University of Waterloo, Waterloo, Ontario, Canada; ²University of Waterloo, Waterloo, Ontario, Canada.

The advancement in gallium nitride (GaN)-based micro-LEDs has enabled the possibility of next-generation flexible emissive displays with low power-consumption and high brightness characteristics compared to existing emissive display technologies based on organic-LEDs (OLEDs). One distinct advantage for using micro-LEDs for flexible display application over OLED media is the ability to create bottom cathode inverted LED structures. Unlike the conventional OLED process, where a bottom cathode structure is impractical due to the environmental instability of the electron injection layer, micro-LED devices may be integrated onto the pixel circuit with diode on the drain-side of the driving TFT. This configuration provides much higher dynamic range for the display due to the lower over-drive voltage needed to bias the micro-LED. In addition, the development of micro-LED displays is mostly focused on CMOS-based pixel circuits that have limited mechanical flexibility and are not easily scalable to large areas. A viable alternative exists with a-Si:H-

based thin-film transistors that leverages existing low-cost fabrication methodologies and large-area scalability to provide a new pathway for low-power, high-brightness flexible displays. These opportunities in a-Si:H-based pixel circuit design take advantage of the higher luminescence efficiency and integration of micro-LEDs with TFTs that may enable the next-generation flexible displays. a-Si:H TFT pixel circuits were fabricated on flexible polyethylene naphthalate (PEN) substrates at a maximum of 170°C. The pixel circuit consisted of an access TFT having a channel width-to-length ratio (W/L) = 100 μm / 20 μm, and a driving TFT (T₀), with a W/L = 1000 μm / 20 μm, to facilitate active-matrix array addressing. After the fabrication of the pixel circuits, InGaN-based micro-LED, fabricated on sapphire wafers with an area of 100 μm × 100 μm and an ON-voltage of ~ 2.5 V, were transferred onto the inverted-staggered TFT devices. The layout design was based on simulated circuits to provide a drive current of up to 60 μA to each micro-LED with a supply voltage of 20 V and a data voltage (V_{data}) range of 5 V ~ 15 V. To increase the pixel resolution, inter-digitated source-drain electrodes were used to minimize the area of the pixel circuit resulting in an equivalent resolution of 50 pixels per inch (ppi). Characterization of the TFT and the LED showed no measurable change in the electrical and optical characteristics of the TFT and the LED, respectively. A dramatic increase in the output current of the pixel circuit of 110%, was observed under the same V_{data} range for the inverted LED structure compared to the top cathode configuration. This result shows the efficacy of combing micro-LEDs with a-Si:H TFTs for high-brightness flexible displays. Moreover, under normal array scanning operation, the pixel circuit showed a measurable charge-injection (voltage feed-through) loss due to the parasitic capacitance of T₁ at the falling edge of the sampling signal. This loss of charge lowered the over-drive voltage on T₀, causing a drop in the supply current to the micro-LED. Using a more aggressive design rule, a ~ 10% reduction of the parasitic capacitance resulted in a 20% gain in the output current. Finally, we will describe the effect of mechanical bending on the electrical and optical properties of the display pixel.

4:50 PM II05

(Student) Digital Growth of Smooth, High Quality Thick (200nm) N-Polar InGaN Films by MOCVD Shubhra S. Pasayat¹, Cory Lund¹, Yusuke Tsukada¹, Massimo Catalano², Moon J. Kim², Stacia Keller¹ and Umesh Mishra¹; ¹University of California, Santa Barbara, Goleta, California, United States; ²The University of Texas at Dallas, Dallas, Texas, United States.

Thick InGaN films are of interest for a variety of applications such as efficient light absorption in solar cells or as relaxed base layers for InGaN based optoelectronic devices [1, 2]. Growing thick, high-quality InGaN films, however, has been challenging not only because of the large lattice mismatch between GaN and InN, but also due to the low growth temperatures required for sufficient Indium (In) incorporation into the layers. While the morphology of metal polar (0001) InGaN films typically deteriorates via V-defect formation [3], thicker N-polar (000-1) InGaN films exhibit hexagonal surface defects [1]. In contrast to bulk InGaN layers, in InGaN/GaN MQW structures the defect formation can be mitigated by growing parts of the GaN barrier layer in the presence of hydrogen (H₂) in the carrier gas. In the case of N-polar films, H₂ was shown to act as a surfactant enhancing the surface mobility of adsorbed species [1]. The growth process investigated in this study takes advantage of this surfactant effect by introducing short H₂ pulses during InGaN deposition, resulting in InGaN/GaN short period superlattices with individual layer thicknesses in the order of a few nanometers, referred to as digital InGaN [2]. In this study, 200nm thick N-polar InGaN films were grown by metal-organic CVD (MOCVD) on N-polar GaN-on-sapphire base layers with a misorientation of 4° at a temperature of 820 °C. During the digital growth process, the TEGa and TMIn precursor flows were kept constant at 2.8 and 28 μmol/min, respectively, while modulating the presence of H₂. 'x' nm was grown in nitrogen (N₂) carrier gas for In incorporation, and 'y' nm in a H₂/N₂ mixture and repeating this pattern until a total thickness of 200nm was reached. This resulted in a "very short"-period 'x'nm/'y'nm InGaN/GaN superlattice with a certain average In composition. In this work, the impact of varying the 'x' and 'y' superlattice parameters, e.g. **2nm/2nm (sample A)**, **2nm/3nm (sample B)** and **2nm/4nm (sample C)**, on the morphology and Indium incorporation was studied. In a second series, additional GaN interlayers of varying thickness 'z' were placed every 40 nm of digital InGaN to further improve the surface morphology. For samples A, B and C, average In mole fractions of **7.5%**, **6.5%**, and **5.8%** respectively, were determined via high-resolution X-ray diffraction (XRD) ω-2θ scans around the GaN (0002) reflection. The RMS roughness values derived from 10μm X 10μm atomic force microscopy (AFM) scans ranged between 1.85 and 2 nm. While the majority of the sample surface was smooth, sparse hexagonal hillocks were observed via optical microscopy. Their density decreased

from 277 to 90 per 100μm² with increasing 'y' and longer presence of H₂. Although sample C demonstrated the least defects on the surface, sample A exhibited the highest In incorporation. With higher In incorporation as the priority, the growth process for **sample A** was modified to have additional GaN interlayers (grown in N₂ carrier gas), of thickness **2nm (Sample D)** and **4nm (Sample E)** placed after every **40nm of digital InGaN growth**. For samples D and E, effective Indium mole fractions of **8%** and **7%** were obtained respectively, with a reduced RMS roughness of ~1.65 nm for 10μm X 10μm AFM scans for both samples, also with a sharp reduction in the hexagonal hillocks to 72 and 54 per 100μm² in comparison to sample A. Most likely, the GaN interlayers absorbed surplus In on the growing surface, thereby, suppressing the hillock formation. Sample E with 4nm of GaN interlayer introduced every 10 loops of the 2nm/2nm InGaN/GaN superlattice demonstrated a good trade-off between In incorporation and morphology. Further experiments exploring InGaN layers with even higher indium composition are underway and will be presented at the conference. [1] S Keller *et al. Semicond. Sci. Technol.* 29 113001(2014) [2] C Lund *et al. Appl. Phys. Express* 10 111001(2017) [3] Al Balushi *et al. Appl. Phys. Lett.* 110, 022101 (2017)

SESSION JJ: Doping, Point and Extended Defects in Wide Bandgap

Session Chairs: Mark Goorsky and Christian Wetzel
Thursday Afternoon, June 27, 2019
Rackham Building, 4th Floor, Assembly Hall

1:30 PM JJ01

(Student) Enhanced Doping Efficiency of Ultrawide Bandgap Semiconductors by Metal-Semiconductor Junction Assisted Epitaxy Ayush Pandey¹, Xianhe Liu¹, Zihao Deng², Walter J. Shin¹, David A. Laleyan³, Kishwar Mashooq¹, Eric T. Reid⁴, Emmanouil Kioupakis⁵, Pallab Bhattacharya¹ and Zetian Mi⁶; ¹Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Ann Arbor, Michigan, United States; ²University of Michigan—Ann Arbor, Ann Arbor, Michigan, United States; ³Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ⁴Electrical and Computer Engineering, University of Michigan—Ann Arbor, Ann Arbor, Michigan, United States; ⁵University of Michigan, Ann Arbor, Michigan, United States; ⁶Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

To date, it has remained extremely challenging to achieve efficient p-type conduction of AlN and AlGaIn with relatively high Al content, which has been identified as one of the major obstacles to realizing high performance optoelectronic devices operating in the mid and deep UV spectra. Magnesium has been established as the only viable p-type dopant of group III-nitride semiconductors. However, it exhibits very large activation energy (up to 600 meV) in Al-rich AlGaIn, severely limiting the doping efficiency and the realization of large hole concentrations at room temperature. Here, we uniquely demonstrate that with controlled tuning of the Fermi level by an in-situ metal-semiconductor junction during epitaxy, efficient p-type conduction, which would otherwise be impossible, can be achieved for large bandgap AlGaIn. We have demonstrated that Mg-doped Al_{0.9}Ga_{0.1}N can exhibit a free hole concentration ~4.5×10¹⁷ cm⁻³ at room temperature, significantly higher than that reported previously. During conventional epitaxy, with Mg-dopant incorporation, the Fermi level shifts towards the valence band edge, which significantly reduces the formation energy for carbon, oxygen, and nitrogen vacancies. These defects have a strong compensating effect and further degrade the structural, electronic, and optical properties of Mg-doped AlGaIn. To overcome these fundamental challenges, we investigated a new paradigm of epitaxial growth – metal-semiconductor junction assisted epitaxy – of ultrawide bandgap AlGaIn. The epitaxy of AlGaIn is performed in metal (Ga) rich conditions by using plasma-assisted molecular beam epitaxy (MBE). The excess Ga layer leads to the formation of a metal-semiconductor junction during the epitaxy of Mg-doped AlGaIn, which pins the Fermi level away from the valence band at the growth front. In this unique epitaxy process, the Fermi level position is decoupled from Mg-dopant incorporation, *i.e.* the surface band bending allows the formation of a nearly n-type growth front despite p-type dopant incorporation. As such, the formation energy for substitutional Mg is dramatically reduced, even when very large densities of Mg-dopant atoms are incorporated, which is accompanied by a significant suppression of the formation of compensating defects. Utilizing this unique technique, we have demonstrated that Mg

incorporation in AlGaIn can be enhanced by nearly one order of magnitude compared to the conventional growth process; a Mg concentration $\sim 2 \times 10^{20} \text{ cm}^{-3}$ was measured in $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ for a moderate Mg flux of $\sim 7 \times 10^{-8} \text{ Torr}$. A significant reduction of compensation defects and carbon impurity incorporation was also confirmed through detailed deep level transient spectroscopy (DLTS) and secondary ion mass spectrometry (SIMS) measurements. Significantly, a free hole concentration of $\sim 4.5 \times 10^{17} \text{ cm}^{-3}$ was measured for $\text{Al}_{0.9}\text{Ga}_{0.1}\text{N}$, with resistivity values $< 5 \Omega \text{ cm}$, which is nearly three orders of magnitude lower compared to previous reports. Such a unique technique can be extended for the epitaxy/synthesis of a broad range of wide bandgap semiconductors to achieve efficient current conduction that was not previously possible. With the use of this unique epitaxy process, we have further demonstrated ultraviolet 280 nm light-emitting diodes (LEDs) exhibiting nearly a factor of ten enhancement in efficiency, compared to a sample grown using the conventional growth mode. These results, together with the realization of efficient p-type conduction of AlN will be reported.

1:50 PM JJ02

(Student) Dependence of Electronic Bands and Defect Transition Energies with Varying Al Composition and Temperature in AlGaIn Ji Hyun Kim¹, Shun Washiyama¹, Ronny Kirste², Seiji Mita², Pramod Reddy², Douglas L. Irving¹, Ramón Collazo¹ and Zlatko Sitar¹; ¹Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina, United States; ²Adroit Materials, Inc., Apex, North Carolina, United States.

Further development of AlGaIn for deep-UV optoelectronics and high-power devices faces limitations due to large compensating defect concentrations, relatively poor ohmic contacts, and high dopant activation energies due to DX formation. Consequently, point defect control still proves to be a technology limiting challenge for the further development of this technology. Density functional theory (DFT) is employed to develop quantitative models for defect configurations that lead to compensation or other deleterious effects such as recombination traps that influence the internal quantum efficiencies in AlGaIn based quantum wells. However, DFT models are calculated for 0 K and extending the predicting capabilities to processing temperatures requires understanding of the relevant energy shifts for all electronics states involved. Specifically, the shifts in the conduction and valence bands and the corresponding defect thermodynamic transition levels relative to the valence band as a function of temperature and alloy composition. This work aims to experimentally demonstrate the relationship between the point defect thermodynamic transition energy and the electronic bands relative to the vacuum level as a function of Al composition and temperature. Previously, the energy position of the conduction and valence bands have been estimated with respect to the vacuum level as a function of Al composition via X-ray photoelectron spectroscopy.¹ In this work, photoluminescence spectra of identified point defects with corresponding DFT models, are employed to estimate the defect levels within the bandgap and relative to the reference vacuum level. It is observed that point defects with localized deep states (midgap energies) are at a constant energy relative to the vacuum level, independent of Al composition. This suggests that the point defect thermodynamic transition energies and the charge neutrality level are relevant reference energies instead of the vacuum level that cannot be directly measured. Further, the conduction and valence band are shown to diverge with respect to the reference energies as the Al composition increases. These shifts (as a fraction of the change in bandgap) in the conduction and valence bands are approximately 0.7:0.3, similar to the band-offsets expected in heterostructures. Finally, we have employed C_N photoluminescence emission as the reference energy in Si doped $\text{Al}_{0.7}\text{Ga}_{0.3}\text{N}$ ($\sim 3.2 \text{ eV}$ at RT) to measure each electronic band shift as a function of temperature. The observed luminescence has been attributed to the transition between C_N^{-1} and C_N^0 , thus it involves the conduction band and hence provides information about any shift in this band. This deep level luminescence was measured at temperatures ranging from 3 K to 500K. The experimental results indicate that, with respect to the vacuum level, conduction band has a gradual decrease in energy (by about $\sim 50 \text{ meV}$). From the change in the bandgap ($\sim 170 \text{ meV}$), the valence band shifts to higher energies (by about 120 meV) with increasing temperature in relation to the conduction band shift. Here, we assume a Stokes shift of 0.5 eV whose dependence on temperature is assumed to be small compared to that of the bandgap and can be confirmed via photoluminescence excitation (PLE) spectroscopy. This contrasts previously observed heterostructure band offsets and Al composition change where the energy shift is mainly in the conduction band ($0.7 \times$ change in bandgap). This information is fundamental in extending accurate DFT predictability to higher temperatures as those observed during growth. ¹ P. Reddy, I. Bryan, Z. Bryan, J. Tweedie, S. Washiyama, R. Kirste, S. Mita, R. Collazo, and Z. Sitar, Appl. Phys. Lett. **107**, 091603 (2015)

2:10 PM JJ03

(Student) Photoluminescence Characterization of High Temperature Microwave Annealed Homoepitaxially Grown Mg-Implanted GaN

Sean A. Tozier¹, Michael Reshchikov², Kasey Hogan¹, Emma Rocco¹, Vincent E. Meyers¹, Benjamin McEwen¹, Isra Mahaboob¹, Michael Shevelev³, Vlad Sklyar³, Randy P. Tompkins⁴, Michael A. Derenge⁴, Andrew C. Lang⁵, Kenneth A. Jones⁴, Mitra L. Taheri⁵, Woongje Sung¹ and Fatemeh (Shadi) Shahedipour-Sandvik¹; ¹Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, Clifton Park, New York, United States; ²Virginia Commonwealth University, Richmond, Virginia, United States; ³Gyrotron Technology, Inc., Bensalem, Pennsylvania, United States; ⁴U.S. Army Research Laboratory, Adelphi, Maryland, United States; ⁵Drexel University, Philadelphia, Pennsylvania, United States.

Significant challenges remain towards achieving highly conductive p-type GaN. Power device applications require highly conductive areas to improve contact resistivity and achieve junction termination extension (JTE) structures, which is difficult to realize by selective region epitaxial overgrowth. A common technique employed is a selective region implantation of dopant species. In order to activate acceptors in Mg implanted GaN, it is necessary to perform high temperature annealing to heal point defects that were introduced by the high energy ion bombardment while not generating further compensating defects. However, at temperatures greater than 840 C , decomposition of GaN occurs by nitrogen desorption, resulting in the formation of Ga droplets. To alleviate this issue, a combination of an AlN capping layer and high nitrogen overpressure will need to be utilized to stabilize the surface. We report on temperature and excitation energy dependent photoluminescence measurements of Mg-implanted MOCVD uGaN films overgrown on HVPE GaN and annealed using a novel Gyrotron microwave technique. Mg implanted GaN films were annealed at temperatures and nitrogen overpressures ranging from 800 C to 1300 C and 20 bar to 40 bar respectively with and without the use of an AlN capping layer. Low temperature (18 K) photoluminescence of as-Mg implanted uGaN indicate the presence of the so-called GL2 band with peak position of approximately $2.3 - 2.4 \text{ eV}$. The GL2 band has been shown to be due to nitrogen vacancies V_N [1] and present in semi-insulating GaN. Another peak at $1.7 - 1.8 \text{ eV}$ is also observed for as-Mg implanted uGaN and it may be associated with deep defects in heavily Mg-doped GaN [2, 3]. AFM measurements following implantation shows no observable changes in surface roughness. AlN capped Mg-implanted GaN sample annealed at 1300 C and 40 bar N_2 overpressure shows little change in band position in low temperature photoluminescence spectra, but a significant increase in GL2 band intensity is observed. This is likely due to the formation of additional nitrogen vacancies by high temperature Gyrotron annealing. Uncapped Mg-implanted GaN films Gyrotron annealed at 1100 C and 40 bar overpressure, which showed signs of surface decomposition due to the lack of an AlN cap, were characterized by temperature and excitation energy dependent photoluminescence. In addition to the presence of an intense GL2 band, a significant UVL band is observed at a peak position of $3.1 - 3.2 \text{ eV}$, which is indicative of the presence of substitutional Mg_{Ga} [4]. Temperature dependent measurements of this sample shows temperature quenching behavior that is observed in n-type Mg:GaN [4]. In areas where the sample surface was not decomposed, the UVL band intensity is significantly decreased. In the complete work, temperature dependent photoluminescence measurements and analysis will be presented of conventional RTA, high temperature (1300 C) RTA, and Gyrotron pulse annealing of homoepitaxially grown Mg implanted GaN. References: [1] M. A. Reshchikov, D. O. Demchenko, J. D. McNamara, S. Fernández-Garrido, and R. Calarco, "Green luminescence in Mg-doped GaN," *Phys. Rev. B*, vol. 90, no. 3, Jul. 2014. [2] M. A. Reshchikov and H. Morkoç, "Luminescence properties of defects in GaN," *J. Appl. Phys.*, vol. 97, no. 6, p. 061301, Mar. 2005. [3] M. W. Bayerl *et al.*, "Optically detected magnetic resonance of the red and near-infrared luminescence in Mg-doped GaN," *Phys. Rev. B*, vol. 63, no. 12, Mar. 2001. [4] M. A. Reshchikov, P. Ghimire, and D. O. Demchenko, "Magnesium acceptor in gallium nitride. I. Photoluminescence from Mg-doped GaN," *Phys. Rev. B*, vol. 97, no. 20, May 2018.

2:30 PM JJ04

(Student) Identifying Defects and Their Electronic Signatures in Regrown GaN Heterostructures Jiaheng He¹, Guanjie Cheng¹, Davide Del Gaudio¹, Jordan Occena¹, Fabian Naab², Rachel S. Goldman¹, Mohsen Nami³, Bingjun Li³ and Jung Han²; ¹Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; ²Michigan Ion Beam Laboratory, University of Michigan, Ann Arbor, Michigan, United States; ³School of Engineering and Applied Science, Yale University, New Haven, Connecticut, United States.

Although silicon-based electronics are used to power light-emitting diodes and electric vehicles, their utility in high power applications is limited by a low breakdown voltage. The most promising alternative power devices consist of vertical GaN devices, which often require regrown active regions. Thus, advances in high power device performance require a detailed understanding of the influence of regrowth processing steps on interfacial defects and their electronic signatures. In this work, we examine a series of GaN p-i-n structures prepared with and without ex-situ ambient exposure and/or chemical etching through a combination of ion beam analysis methods. We aim to identify and quantify native defects, as well as both intrinsic and extrinsic point defects and their complexes on dopant activation in regrown and selective-area regrown GaN. To estimate the structural perfection of the heterostructures, we measure both channeling and random Rutherford Backscattering Spectrometry (RBS) data, and analyze the min values and the densities of displaced Ga atoms, Nd. For all samples, the min values are less than 2%, with the highest value of Nd estimated as $1.6 \times 10^{20} / \text{cm}^3$ for the “ex-situ” samples. To detect the concentrations and atomic configuration of light elements, such as hydrogen with typical concentrations $< 10^{20} / \text{cm}^3$, we use Elastic Recoil Detection Analysis (ERDA) to determine the depth-dependence of the hydrogen concentration in the three samples listed above. Preliminary results suggest an enhancement in the hydrogen concentration at the “etched/regrowth” p-GaN/uid-GaN interface in comparison to the comparable interfaces in the “in-situ” and “ex-situ” samples. To identify the electronic signatures associated with the point defects and point defect complexes, we perform spatially and depth-resolved cathodoluminescence spectroscopy. For all samples, the GaN near-bandedge (NBE) luminescence at 3.35 eV and donor-acceptor pair (DAP) luminescence at 2.85 eV are apparent. The DAP luminescence is most intense for “in-situ”. It is interesting to note that the yellow luminescence (YL) at 2.19 eV is only observed in “ex-situ” and “etched/regrowth”, while the infrared luminescence (IRL) at 1.47 eV is only observed in “in-situ”. In summary, RBS data suggests that “etched” sample has the highest crystalline quality and ERDA data suggests that “in-situ” has the highest [H]. Further studies which involve spatial-resolved CL imaging using various electron energies in order to probe the electronic signatures associated with the point defects and point defect complexes in the layers and heterostructure interfaces will be discussed. This work is supported by ARPA-E AED0000191 and the Michigan Ion Beam Laboratory.

2:50 PM JJ05

(Student) Impact of Hillock Density and Mg-Clustering on Properties of N-Polar GaN:Mg Emma Rocco¹, Isra Mahaboob¹, Kasey Hogan¹, Sean A. Tozier¹, Vincent E. Meyers¹, Benjamin McEwen¹, Olivia Licata², Baishakhi Mazumder², Michael Reschchikov³ and Fatemeh (Shadi) Shahedipour-Sandvik¹; ¹SUNY Polytechnic Institute, Colleges of Nanoscale Science and Engineering, Albany, New York, United States; ²Materials Design and Innovation, University at Buffalo, The State University of New York, Buffalo, New York, United States; ³Physics, Virginia Commonwealth University, Richmond, Virginia, United States.

Polarization engineering in III-nitride materials has led to advances in high electron mobility transistors (HEMTs) with confinement of 2-D electron gas in N-polar GaN/AlGaIn HEMTs, increased detector efficiency by polarization doping, and reduction of the quantum confined stark effect in semi-polar and non-polar LEDs. For the realization of p-type III-nitrides, magnesium (Mg) is the most commonly used dopant due mainly to an established method of activation and its activation energy. However, using Mg dopant poses a challenge to achieving high conductivity p-type material due in main part to low efficiency in ionization of dopants, formation of compensating nitrogen vacancies and the formation of electrically inactive Mg clusters at high Mg concentrations. In the nitrogen polarity, an additional growth challenge exists with the formation of hexagonal hillock structures under non-optimal growth conditions, resulting in high surface roughness. In this work, N-polar GaN films were grown by metal organic chemical vapor deposition (MOCVD) on nominally on-axis sapphire substrates. N-polar GaN templates were grown to achieve both low and high hillock density UID GaN layers. Mg-doped GaN was then overgrown on these layers followed by a thin 10 nm uGaN cap layer. GaN:Mg films grown on high and low hillock density template

layers were characterized for a comparison of optical and electrical properties. Through photoluminescence spectroscopy the so-called blue band is seen at 2.8 eV for both low and high hillock density samples. The characteristic blue shift with increasing excitation intensity indicates that the band is caused by electron transitions from a deep donor to the shallow Mg acceptor. The GaN:Mg film grown on high hillock density underlying template exhibits an additional UVL band at 3.285 eV due to a transition from the conduction band to the Mg-acceptor level commonly seen in p-type GaN, as well as acceptor and donor bound exciton peaks at 3.47 eV and 3.49 eV respectively. Hg probe C-V measurement indicates a difference in electrical conductivity with extracted N_A-N_D of $8.26 \times 10^{17} \text{ cm}^{-3}$ and $1.37 \times 10^{18} \text{ cm}^{-3}$ for low and high hillock density samples respectively. Local compositional analysis by atom probe tomography (APT) studying individual hillock structures reveals decreased clustering of Mg within the hillock structure and sidewalls compared to the planar region of the film. The increased electrical and optical activity of high hillock density materials is attributed to this decrease in clustering and increased Mg incorporation into electrically active sites in the semi-polar hillock side walls.

3:10 PM REFRESHMENT BREAK

3:30 PM JJ06

Thermal Conductivity of HVPE Grown Single Crystal GaN—Impact of Doping Pegah Bagheri¹, Robert Rounds¹, Qiang Guo¹, Ji Hyun Kim¹, Tomek Sochacki³, Ronny Kirste², Pramod Reddy², Michal Bockowski³, Ramón Collazo¹ and Zlatko Sitar¹; ¹Materials Science & Engineering, North Carolina State University, Raleigh, North Carolina, United States; ²Adroit Materials, Inc., Raleigh, North Carolina, United States; ³Institute of High Pressure Physics, Warsaw, Poland.

Gallium Nitride (GaN), as a wide bandgap semiconductor, has a broad range of applications in optoelectronics and power devices. High breakdown field (3.5 MV/cm) along with possible low on-resistance makes GaN a suitable candidate for power devices. Thermal conductivity determines the ability of power devices to dissipate heat effectively. Therefore, a careful study of GaN thermal conductivity as suitable native substrate for homoepitaxial growth and methods to control it is of great importance. GaN thermal conductivity at room temperature, as reported in literature, vary over a wide range from 130 to $269 \text{ Wm}^{-1}\text{K}^{-1}$ depending on growth methods and dominant defects. As such, there is a lack of knowledge in understanding possible phonon scattering mechanisms dominating thermal conductivity in different temperature regimes. Here we investigate the effect of point defects in the GaN thermal conductivity, focusing on impurities typically added during growth to obtain semi-insulating substrates. In this work, the thermal conductivity of HVPE grown GaN crystals doped with C, Mn and Fe was measured using the three-omega method within the temperature range of 30 K to 300 K. The typical threading dislocation density for HVPE grown GaN is in the order of 10^4 cm^{-2} . Photoluminescence spectroscopy and Hall measurement under the van der Pauw geometry are implemented to further analyze the influence of these impurities along with any other point defects in the crystals. Secondary ion mass spectroscopy was employed to determine the concentrations of dopants and other impurities. A thermal conductivity of 228 ± 4 , 221 ± 4 and $213 \pm 3 \text{ Wm}^{-1}\text{K}^{-1}$ was measured for low C, high C and Mn doped HVPE GaN samples at 298 K respectively suggesting the influence of these dopants on the thermal behavior of GaN at room temperature. While samples with low concentrations of impurities show a high conductivity value, doping with Mn and C can expectedly decrease thermal conductivity. For further investigation of scattering mechanisms and role of point defects, the thermal conductivity behavior with temperature was measured. For the entire temperature range, low C-doped GaN shows a higher thermal conductivity while Mn-doped GaN exhibits the lower thermal conductivity. In addition, the Callaway model was used to describe the GaN thermal behavior and to compare with the measured trends. At high temperature, the thermal conductivity values converge to a single value and agree with the Callaway model; however, at low temperatures experimental values start deviating from the model indicating other scattering mechanisms, such as phonon resonance scattering, which are not considered in the model. Phonon resonance scattering significantly decrease the thermal conductivity at lower temperatures depending on impurity type and concentration.

3:50 PM JJ07

(Student) Reducing Unwanted Motion of Dislocations Towards Reliable III-V Devices on Silicon Eamonn T. Hughes¹, Rushabh D. Shah² and Kunal Mukherjee¹; ¹Materials, University of California, Santa Barbara, Santa Barbara, California, United States; ²Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts, United States.

The reliability of III-V optoelectronic devices grown on silicon is currently limited by the significant density of threading dislocations present in the active region [1]. By a phenomenon known as recombination-enhanced dislocation glide (REDG), threading dislocations in the active region can glide at room temperature, which increases the total dislocation length and leads to increased non-radiative recombination and eventually device failure. It is therefore essential to better understand how REDG proceeds in device structures and devise ways to counteract it. We present a method to simultaneously observe the dynamics of dislocation motion and their effects on luminescent properties in device-like lattice-mismatched heterostructures. We use this technique to investigate the potential of reducing REDG by alloying the heterostructures with indium. With no post-growth sample preparation, (In)AlGaAs double heterostructures grown on GaAs/Ge/Si are imaged in a scanning electron microscope by cathodoluminescence (CL) to reveal threading dislocations as dark spots defects. The fact that dislocations glide so freely at room temperature in AlGaAs heterostructures is quite surprising because of the large activation energies typically required for dislocation motion in semiconductors. This occurs for two reasons: (1) carriers injected by the electron beam recombine non-radiatively at dislocations and effectively lower the Peierls energy barrier (i.e. REDG) and (2) a significant driving force is present, provided by large residual stresses (~150–200 MPa) in the film which develop during post-growth cooling due to the difference in coefficients of thermal expansion between the film and substrate. We have found that by alloying the AlGaAs heterostructure with just a few percent In, the number of moving dislocations and their glide velocities are both dramatically reduced without significantly impacting the luminescent properties of the device. The mechanism behind this change is believed to be the lattice hardening induced by the larger indium atoms. This finding potentially represents a key step toward successful integration of III-V optoelectronics on silicon. Beyond revealing the indium lattice-hardening effect, this technique allows us to capture time-lapse images of gliding dislocations in CL to study their motion and luminescent properties. By measuring dislocation glide velocity across a range of temperatures, we extract activation energies for glide of different dislocation types that are significantly lower than those reported in the literature for bulk crystals [2]. We also demonstrate the feasibility of using REDG as a means of filtering a region of dislocations, showing a 30% reduction in dislocation density. Such a technique would be a natural fit for mesa structures where threading dislocations can fully exit the crystal at the edges. In all, we present a powerful technique to observe and understand threading dislocation dynamics as they impact device structures. We find that unwanted dislocation motion can be drastically reduced by alloying GaAs-based heterostructures with small amounts of indium, paving the way for commercialization of III-V optoelectronics on silicon. **References** [1] A.Y. Liu, S. Srinivasan, J. Norman, A.C. Gossard, and J.E. Bowers, *Photonics Res.* **3**, B1 (2015). [2] K. Maeda, M. Sato, A. Kubo, and S. Takeuchi, *J. Appl. Phys.* **54**, 161 (1983).

4:10 PM JJ08

(Student) The Dependence of Optical Properties on Orientation and Strain in Silicon Vacancy Centers in Diamond Matthew W. Day¹, Kelsey M. Bates¹, Christopher L. Smallwood^{1,2,3}, Ronald Ulbricht^{2,4,5}, Travis M. Autry^{2,4,6}, Rachel C. Owen¹, Geoffrey Diederich⁷, Tim Schröder⁸, Edward Bielejec⁹, Mark Siemens⁷ and Steven T. Cundiff^{1,2,4}; ¹Physics, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²JILA, Boulder, Colorado, United States; ³Physics and Astronomy, San Jose State University, San Jose, California, United States; ⁴Physics, University of Colorado Boulder, Boulder, Colorado, United States; ⁵School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore, Singapore; ⁶National Institute of Standards and Technology, Boulder, Colorado, United States; ⁷Physics and Astronomy, University of Denver, Denver, Colorado, United States; ⁸Physics, Humboldt-Universität zu Berlin, Berlin, Germany; ⁹Sandia National Laboratories, Albuquerque, New Mexico, United States.

The silicon-vacancy (SiV) color center in diamond is a defect in the diamond lattice consisting of a single silicon atom situated between two adjacent carbon vacancies. This particular color center is inversion symmetric (belonging to the D_{3d} point group) and therefore less sensitive to first-order perturbations than, for instance, the nitrogen-vacancy center. Its small Huang-Rhys factor means that the SiV exhibits enhanced

emission in the zero-phonon line (ZPL) transition manifold (a group of four optical transitions centered around 1.68 eV) relative to other color centers [1]. These two properties make SiV centers strong candidates for separated, single photon emitters [2]. Additionally, since the absolute frequency of and splittings between optical transitions depend on the microscopic strain environment [3], these color centers can be employed to optically (and therefore remotely) measure the diamond strain tensor. Realizing these applications requires understanding the dynamics, coherent coupling, and dephasing mechanisms for optical excitations of the ZPL transitions. To that end, we use collinear photoluminescence detected multidimensional coherent spectroscopy (MDCS) [4–6] to investigate an ensemble of SiV centers in mono-crystalline diamond. MDCS measurements of SiV centers in diamond reveal two distinct and uncoupled color center populations. We observe intra-population (but no inter-population) coherent coupling. Because the microscopic polarization selection rules of the optical transitions are known with respect to the silicon-vacancy axis [7], we identify these two populations as oriented in- and out-of-plane with respect to the sample surface. Knowing which optical transitions correspond to each orientation, we can directly measure the strain tensor of the diamond lattice local to our laser spot. This result has multiple implications. The observation of polarization and orientation dependence of coherent coupling between electronic transitions is an important step on the road to engineering color center-based photonic devices, as we are able to characterize dephasing times and coupling strengths of the optical transitions from the MDCS spectra as a function of color center orientation. Additionally, the optical measurement of the strain tensor points the way to new defect-based strain sensing techniques. In the future, MDCS could be employed to measure coherent coupling between distinct SiV centers in the limit of lower color center density, similar to work conducted on small numbers of interfacial quantum dots [6], or to probe color centers embedded in a diamond-based strain sensor. The focused ion implantation work to generate the SiV centers was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. **References:** [1] J. N. Becker, et al., *Nat. Commun.* **7**, 1 (2016). [2] L. J. Rogers, et al., *Nat. Commun.* **5**, 4739 (2014). [3] S. Meesala, et al., *Phys. Rev. B* **97**, (2018). [4] P. F. Tekavec, G. A. Lott, and A. H. Marcus, *J. Chem. Phys.* **127**, 1 (2007). [5] G. Nardin, et al., *Opt. Express* **21**, 28617 (2013). [6] E. W. Martin and S. T. Cundiff, "Inducing coherent quantum dot interactions," *Phys. Rev. B* **97**, 1 (2018). [7] K. D. Jahnke, et al., *New J. Phys.* **17**, 0 (2015).

4:30 PM JJ09

(Student) Ab Initio Calculations of BAs-GaAs Alloys Istvan Gulyas and Mark Wistey; Physics, Texas State University, Austin, Texas, United States.

Alloying GaAs with boron ($B_xGa_{1-x}As$) has been suggested as an alternative to nitrogen for bandgap engineering. We present electronic properties of fully relaxed BAs-GaAs alloys calculated using the Vienna Ab-initio Simulation Package (VASP) with HSE06 hybrid functionals. We find that small supercells, corresponding to alloys with higher B concentrations, exhibit band splitting and band gap bowing, and a possible anti-crossing in the conduction band, which is typical behavior for highly mismatched alloys. However, in case of a dilute $B_{0.016}Ga_{0.984}As$ alloy, a 128-atom supercell with a single B, we find a new, deep energy level deep within the band gap, 0.467 eV above the valence band maximum. Unlike the well-behaved alloy behavior above, these isolated B atoms with nearest B-B distances of at least 17.0 Å, result in a deep trap level. This trap level might act as a recombination center in laser and solar cell applications. Nevertheless, in addition to being statistically unlikely, closer B-B arrangement reduces the total system energy, which may further reduce the probability that lone B atoms will be found in the grown material. We also investigated the band structure of alloys with compositions ranging from pure GaAs to pure BAs using small 16-atom supercells, as well as larger random alloys consisting of 64 atoms. Higher B ratios show no deep levels, but instead result in a shifting from a direct band to indirect bandgap as the B ratio increases from pure GaAs to pure BAs. The band gap shows a strong dependence on the arrangement of atoms, even with different supercells of the same overall composition. It has been suggested that the effect of B added to GaAs depends on the distance between nearest neighbor B atoms. We investigate three 54-atom supercells with 2 B atoms of different B-B nearest neighbor distances and show that the shortest B-B distance of 3.82 Å yields the narrowest direct bandgap of 1.23 eV as opposed to 1.34 eV for a B-B distance of 6.86 Å.

However, the longer B-B distance is more energetically favorable by 4.84 meV per atom. These results show that BGaAs is promising for band engineering for photonic and optoelectronic devices, provided the B concentration is kept above a few percent. Conversely, very dilute B in GaAs might serve as a rapid recombination site to reduce carrier lifetimes.

4:50 PM JJ10 WITHDRAWN

(Student) Analytical Phonon-Point Defect Scattering Models for Complex Unit Cell Materials [Ramya L. Gurunathan](#)¹, Riley Hanus², Maxwell Dylla¹ and Jeff Snyder¹; ¹Materials Science and Engineering, Northwestern University, Evanston, Illinois, United States; ²Materials Science, Northwestern University, Chicago, Illinois, United States.

Analytical thermal conductivity models are routinely applied to determine the source of phonon scattering in defective crystalline solids. This study centers, specifically, on the illustrative case of phonon scattering due to a localized mass difference in the crystal, which may stem from isotopic variation or point defects. A conceptually clear formulation of the mass difference model for multiautomic lattices is presented to resolve factors of 2-10 differences in the predictions of existing models. The analytic model is then compared to experiment and first-principles calculations to demonstrate its predictive power despite simplifying approximations of a virtual monatomic crystal and Debye model dispersion. We demonstrate how the dispersion relation sensitivity is, in practice, softened, providing justification in using this model for systems with arbitrary dispersion relations. Moreover, while the mass difference model is well-defined for the case of substitutional defects, phonon scattering due to vacancies and interstitials is less intuitive, but both are shown to reduce the thermal conductivity by over 50% even in the dilute limit [1][2]. A simple explanation based on the virial theorem is shown to describe these results well in a variety of defective solids [1]. Finally, we provide model considerations for the case of associated defects, which occur in pairs or clusters rather than the assumed random distribution of defects in the lattice. **Sources:** [1] Ratsifaritana, C. A. & Klemens, P. G. Scattering of phonons by vacancies. *Int. J. Thermophys.* **8**, 737–750 (1987). [2] Pei, Y. *et al.* Interstitial Point Defect Scattering Contributing to High Thermoelectric Performance in SnTe. *Adv. Electron. Mater.* **2**, 1600019 (2016).

SESSION KK: Nanowires and Nanotubes—Growth, Processing, Characterization and Devices
Session Chairs: Matt Brubaker and Parsian Mohseni
Friday Morning, June 28, 2019
Michigan League, 2nd Floor, Michigan

8:40 AM KK01

Crystallographic Polarity Measurements in Two-Terminal GaN Nanowire Devices by Lateral Piezoresponse Force Microscopy Matt Brubaker, Alexana Roshko, Paul Blanchard, Samuel Berweger, Charles Little, Todd Harvey and Kris Bertness; National Institute of Standards and Technology, Boulder, Colorado, United States.

A key attribute of the III-N materials system is the built-in polarization field, which influences heterostructure band bending and arises from asymmetry inherent in the wurtzite crystal structure. For planar heterostructures, the crystallographic polarity (or orientation of the [0001] crystal direction) can usually be inferred from that of the underlying substrate. However, nanowires do not necessarily adopt the underlying substrate polarity and orientation uncertainty is further compounded when nanowires are removed from the growth substrate and randomly dispersed to form two-terminal electrical test structures. To address these ambiguities, we have employed lateral piezoresponse force microscopy (L-PFM) to determine the polarity of individual nanowires configured horizontally in two-terminal test structures. Polarity measurements in piezoresponse force microscopy rely on the phase response between the deflection signal of a scanned probe tip and the applied sinusoidal tip voltage bias. In previous studies, PFM measurements were made on as-grown, vertically oriented nanowires where bias and vertical deflection couple through the d_{33} piezoelectric coefficient. Here, the nanowire is horizontally oriented with respect to the tip and couples to the lateral deflection via the shear d_{15} piezoelectric coefficient. Interestingly, there does not appear to be literature consensus on the numerical sign of the d_{15} coefficient, which is required in deriving the expected phase-polarity relationships. Instead, we determined them experimentally via L-PFM measurements on a bulk m -plane GaN sample with known orientation and find that results are consistent with a negative d_{15} coefficient. L-PFM measurements were then made on dispersed n -type nanowires as part of a growth polarity study. The nanowires were grown via self-assembly techniques, dispersed onto oxidized silicon substrates, and finally contacted by metal pads. The nanowires had a characteristic taper that allowed identification of the tip and root sections and L-PFM measurements indicate that the nanowires grow in the $[000(1)]^-$ direction. Nanowires examined by transmission electron microscopy produced lattice images that confirmed the L-PFM measurement results. To demonstrate the primary utility of two-terminal L-PFM measurements (i.e. combined characterization of electrical properties and crystallographic polarity for a single nanowire) we have also fabricated isotype nanowire diodes with an n -type GaN/Al_{0.1}Ga_{0.9}N/GaN structure. According to simulations, these devices become forward biased upon application of a positive voltage to the N -face side of the nanowire. However, L-PFM and current-voltage (I - V) measurements indicate that the devices produce an inverted bias polarity, suggesting that an alternative mechanism is responsible for the rectifying behavior (likely surface related).

9:00 AM KK02

(Student) Atomic Scale Incorporation and Characterization of Bi in III-V Semiconductor Nanowire Surfaces Sandra Benter^{2,4}, Jung-Ching Liu^{2,4}, Yi Liu^{2,4}, Johan Knutsson^{2,4}, Sebastian Lehmann^{2,4}, Kimberley Dick^{3,4}, Anders Mikkelsen^{1,4} and Rainer Timm^{2,4}; ¹Physics, Lund University, Lund, Sweden; ²Department of Physics, Lund University, Lund, Sweden; ³Department of Chemistry, Lund University, Lund, Sweden; ⁴NanoLund, Lund, Sweden.

III-V-semiconductor nanostructures have been studied intensively for the past decades. Light-weight element combinations like GaAs or InAs were the main focus, however more recently bismuth-containing alloys especially for optoelectronic and thermoelectric applications has seen renewed interest. Introducing a certain amount of Bi enables band gap engineering towards very small values, up to the point of predicted inverse band gaps in the case of pure GaBi or InBi [1]. A very large spin-orbit coupling results in extended recombination times for excitons, and the introduced lattice disorder of mixed GaAsBi or InAsBi alloys additionally enhances localization effects on carriers and excitons [2],[3]. Current manufacturing methods are concentrating on growing diluted bismides by facilitating group III, light group V elements, and Bi simultaneously as

precursors. This approach generally suffers from a relatively low level of Bi incorporation [4], leading to the formation of droplets or structural defects for higher nominal Bi concentrations. Instead we suggest to incorporate Bi into the surfaces of III-V substrates (such as InAs) via thermal evaporation of Bi and annealing of the sample under ultrahigh vacuum conditions, aiming at a well-defined surface layer of high Bi content. Furthermore, we are using GaAs and InAs nanowires (NWs) as templates, which are providing additional crystal phases and surface facets to allow the synthesis of novel 2D Bi containing structures [5]. Our previous studies on surface incorporation of Sb atoms in GaAs NWs showed a distinct variation for wurtzite (WZ) and zinc-blende (ZB) structure as observed with scanning tunnelling microscopy (STM) [6]. Here, we will present a STM study of Bismuth incorporation in InAs(111)B substrates as well as WZ and ZB surface facets of GaAs and InAs NWs. For InAs(111)B substrates, we detect a change in the surface structure depending on the amount of deposited atoms and subsequent annealing steps. For the GaAs NW surfaces, single Bi atoms were observed to replace As atoms in their group-V lattice sites. By comparing Bi incorporation into different surface facets of the same NW, clear differences between the ZB (110) and WZ (11-20) structure regarding the integration of Bi atoms became evident, with a clear tendency for well-ordered terraces of high Bi content on the WZ facet. Our experiments demonstrate the potential towards the fabrication of atomically thin layers of pure InBi or GaBi. 1. Ferhat, M. & Zaoui, A. Structural and electronic properties of III-V bismuth compounds. *Phys. Rev. B - Condens. Matter Mater. Phys.* **73**, 1–7 (2006). 2. Balanta, M. A. G., Kopaczek, J., Orsi Gordo, V., Santos, B. H. B., Rodrigues, A. D., Galeti, H. V. A., et al. Optical and spin properties of localized and free excitons in GaBiAs_{1-x}/GaAs multiple quantum wells. *J. Phys. D: Appl. Phys.* **49**, (2016). 3. Polak, M. P., Scharoch, P. & Kudrawiec, R. First-principles calculations of bismuth induced changes in the band structure of dilute Ga-V-Bi and In-V-Bi alloys: Chemical trends versus experimental data. *Semicond. Sci. Technol.* **30**, 94001 (2015). 4. Wang, L., Zhang, L., Yue, L., Liang, D., Chen, X., Li, Y., et al. Novel Dilute Bismide, Epitaxy, Physical Properties and Device Application. *Crystals* **7**, 63 (2017). 5. Knutsson, J. V., Lehmann, S., Hjort, M., Lundgren, E., Dick, K. A., Timm, R., et al. Electronic Structure Changes Due to Crystal Phase Switching at the Atomic Scale Limit. *ACS Nano* **11**, 10519–10528 (2017). 6. Hjort, M., Kratzer, P., Lehmann, S., Patel, S. J., Dick, K. A., Palmström, C. J., et al. Crystal Structure Induced Preferential Surface Alloying of Sb on Wurtzite/Zinc Blende GaAs Nanowires. *Nano Lett.* **17**, 3634–3640 (2017).

9:20 AM KK03

(Student) High-Gain InGaN/GaN Disk-in-Nanowire Array Visible Photodetectors Anthony Aiello¹, Hasib Turzo², Md Zunaid Baten² and Pallab Bhattacharya¹; ¹EECS, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Department of Electrical and Electronic Engineering, Bangladesh University of Engineering and Technology, Dhaka, Bangladesh.

Applications such as combustion control, flame monitoring, fluorescence spectroscopy and biophotonics require a robust high gain visible photodetector. The III-nitride InGaN alloys have bandgaps corresponding to the visible range. In particular, InGaN/GaN disk-in-nanowire arrays, grown on (001)Si substrates by plasma assisted MBE (PA-MBE), have been utilized to fabricate top-emitting LEDs and edge emitting Fabry-Perot diode lasers [1, 2]. Very little is known about the detailed characteristics of visible photodetectors fabricated with these nanowire heterostructures arrays. In the present study we have fabricated and characterized photodetectors with the disk-in-nanowire arrays grown on (001)Si. The devices exhibit peak responsivity at 360nm of 1450A/W and gain $\sim 10^4$. Most importantly, the high temperature photocurrent spectra exhibit distinct peaks corresponding to intersubband transitions in the disks. The transient photoresponse of the devices have also been measured. The experimental results have been analyzed and there is excellent agreement between measured and calculated data. The nanowire array samples are grown on (001) Si substrates by PAMBE. 260nm of GaN nanowire, doped n -type ($2 \times 10^{18} \text{ cm}^{-3}$), is grown at 780°C and is followed by the light absorbing region consisting of 6 pairs of (3nm) In_{0.42}Ga_{0.58}N/(12nm) GaN disk/barrier heterostructures, all undoped and grown at 600°C. Following these, 100nm of n -type GaN nanowire is grown to complete the heterostructure. The entire growth cycle is accomplished under N₂-rich conditions. The nanowire array fill factor, area density and average disk diameter are 0.4, $2 \times 10^{10} \text{ cm}^{-2}$ and 50nm, respectively. Photoconductive detectors are fabricated by a combination of photolithography, reactive ion etching and contact formation. The device is planarized by parylene deposition. The top contact on the nanowires is formed by Ni/Au/ITO and the bottom contact of Al/Au is formed on the silicon. The electroluminescence of the photoconductors exhibited a peak at $\sim 570\text{nm}$. The photocurrent response was measured in the range 300nm

to 650nm as a function of bias and temperature and exhibited three distinct peaks at 383, 430, and 493nm at 300K and higher temperatures. From a self-consistent solution of the coupled Schrödinger-Poisson equation, it is determined that the peaks are possibly related to E_2 -LH₂, E_1 -HH₃ and a defect bound E_1 -HH₁ transition. The variation of the intensity of the 3 peaks and the overall photocurrent with bias and temperature have been analyzed as described in the following. The measured peak responsivity is ~1450A/W and the maximum measured photoconductive gain is 10⁴. The temporal response of the device was also measured and this response is characterized by rise and decay time constants of 200s and 160s, respectively, and these values are a measure of hole trapping and detrapping times at the surface states on the nanowire walls. The measured spectral response as a function of bias and temperature have been analyzed by a drift-diffusion model, taking into account the number of disks in the depletion and quasi-neutral regions at each bias. There is excellent agreement between measured and calculated data. The carrier capture and emission time constants are also determined. The gain of the devices is calculated by a surface depletion based model. It is found that the very large gain values are a result of the normal photoconductive gain due to hole trapping in the nanowire surface states and a larger component resulting from an increase of the conductive cross-section of the nanowires due to hole trapping in the surface states and the resulting screening effect. Our results indicate that the disk-in-nanowire arrays may be suitable for the realization of high-temperature IR detectors based on intersubband absorption in the InGaN disks. 1) *S. Jahangir et al, IEEE J. Quantum Electronics*, **50**, 530, 2014. 2) *T. Frost et al, NanoLetters*, **14**, 4535, 2014.

KK04 WITHDRAWN

(Student) Molecular Beam Epitaxial Growth of III-Nitride Nanowire Arrays on Bulk Metallic Glass and Nanocrystalline Substrates Elline C. Hettiaratchy¹, Brelon J. May¹, Camelia M. Selcu² and Roberto C. Myers^{1,2,3}; ¹Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States; ²Department of Physics, The Ohio State University, Columbus, Ohio, United States; ³Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States.

Nanowires are uniquely primed to integrate well with a large variety of substrates such as single crystalline semiconductors, amorphous ceramics, and polycrystalline metals. Due to their strain relieving properties arising from their unique structure and morphology, integration with flexible metallic foils offers a new avenue for advancement in the field of both flexible optoelectronics and high throughput manufacturing techniques. Unfortunately, nanowires grown on polycrystalline metals substrates exhibit grain-dependent morphologies. Here we demonstrate that growing on bulk metallic glass (amorphous metal) and nanocrystalline Pt metal films results in highly uniform III-Nitride nanowires. These Nanowire arrays are uniform over length scales >100 μm. Characterization of nanowires was done with photoluminescence spectroscopy and individual nanowire electrical characteristics were measured with conductive atomic force microscopy. Mesoscale LEDs fabricated from nanowires on nanocrystalline Pt films exhibited a 32x increase in overall LED efficiency compared with simultaneously grown nanowire LEDs on bare Si.

9:40 AM KK05

Nano-Wires to Film Transitions During Pulsed-Laser Deposition—Role of Ion Distribution Davide Del Gaudio¹, Carl Boone^{1,2}, Kaitlyn Sallans¹, Erica Mason¹, Andrew Williamson¹, Sneha Yarlagadda¹, John T. Heron¹, Ilan Shalish³ and Rachel S. Goldman⁴; ¹Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; ²SELFA, UCLA, Los Angeles, California, United States; ³Ben Gurion University, Haifa, Israel; ⁴Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States.

Indium-tin oxide (ITO) nano-wires (NW) have attracted interest for flexible transparent electronics and gas sensors.[1,2] Pulsed laser deposition (PLD) is increasingly used for ITO fabrication, with NW vs. film growth usually determined by the use of an inert or reactive atmosphere. Fabrication of both NW and film has been observed in inert atmosphere but a mechanism for the transition was not discussed.[3] We study the formation of nano-wires (NW) and films during PLD of ITO. We consider the role of the plasma expanding in N₂ on the growth mode switch. For lower pressure, liquid metal droplet formation and VLS growth of NW is observed. For higher pressure, a transition to film growth is observed. We hypothesize that in the presence of low pressure N₂, oxygen is strongly scattered, leaving a metal-rich plume. As the pressure increases, the plasma plume and its metal rich core are compressed. This approach is likely applicable to a wide variety of metal-oxide NW core-shell structure for nanoscale devices. NSF grant # ECCS-1610362 [1] J. Gao *et al.* *Nanotechnology* **22**, 195706 (2011). [2] Q. Wan *et al.* *Adv. Mater.* **18**, 234 (2006). [3] R. Savu & E. Joanni, *Scripta Materialia* **55**, 979 (2006).

10:00 AM REFRESHMENT BREAK

SESSION LL: 2D Material Preparation and Applications Session Chair: Susan Fullerton-Shirey Friday Morning, June 28, 2019 Michigan League, 2nd Floor, Vandenberg

8:20 AM LL01

Can Gold-Mediated Exfoliation Preserve the Integrity of Two-Dimensional Palladium Selenide? Jing Li¹, Gong Gu¹, Hao Wang¹, Zheng Liu² and David Mandrus³; ¹Electrical Engineering, The University of Tennessee, Knoxville, Tennessee, United States; ²Nanyang Technological University, Singapore, Singapore; ³Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee, United States.

High-quality, large-area mono- and few-layer two-dimensional (2D) crystals are desired for the fabrication of van der Waals heterostructures and certain characterizations. Gold-mediated exfoliation has been developed for the exfoliation of transition metal dichalcogenides, exploiting the strong affinity between Au and chalcogens [1]. Recently, group-10 transition metal dichalcogenides, with stronger interlayer interaction and thus more sensitive layer count-dependence in electronic structures compared with the group-6 metal counterparts, have gained research interest [2,3]. The strong interlayer interaction renders Au mediation necessary for the exfoliation of small layer count flakes. Here, we report dramatic degradation of carrier mobility in Au-exfoliated atomically thin PdSe₂ flakes with decreasing layer count, correlated with Raman spectroscopy and atomic force microscopy (AFM) characterization results, indicating the impact of the conventional Au-mediated exfoliation on the integrity of the resulted 2D crystal flakes. The insight gained may point to improvement to the exfoliation process, eventually resulting in high integrity chalcogenide 2D crystal samples to enable the investigation of their intrinsic properties. The mobility decreases by nearly 4 orders of magnitude as the layer count decreases from 5 to 2 for field-effect transistors (FETs) using Au-exfoliated PdSe₂ flakes as channels fabricated on SiO₂/Si substrates; the monolayer PdSe₂-based FET exhibits insufficient conductance and gate modulation for meaningful mobility extraction. The layer counts are unambiguously determined by breathing mode Raman peaks [4]. The anomalously strong dependence of the extracted FET mobility on layer count is beyond that can be explained by increased Schottky barrier height due to increased band gap. For a flake with neighboring mono-, bi-, and tri-layer regions as determined by breathing mode Raman, AFM images reveal very rough surface morphology such that the step height cannot be discerned. In contrast, thicker (~9 nm) PdSe₂ flakes exfoliated by adhesive tapes exhibit smooth surfaces. The results indicate that residues from the Au removal process employing the commonly used KI/I₂ gold etchant. Furthermore, when the ultrathin flakes are immersed in the gold etchant extended periods of time, they are unexpectedly etched by the gold etchant, to extents dependent on layer count. Monolayer PdSe₂ flakes are gradually etched by gold etchant, evidenced by the disappearance of characteristic Raman peaks. Meanwhile, the surfaces of 2-layer and 3-layer flakes remain rough, and the flakes are partially etched, indicated by the reduction of characteristic Raman peak intensities. In contrast, the top surface of thicker PdSe₂ flakes exfoliated by adhesive tapes show no signs of degradation after a few hours of immersion in the gold etchant. We infer from these results that the Au exfoliation process introduces defects and residues to the topmost layers of PdSe₂ flakes. Since most of charge carriers are confined within several atomic layers close to the channel/oxide interface in back-gated 2D semiconductor FETs, carrier scattering by the defects in and residues on the top layer is substantially more prominent in thinner channels as a result of shortened distance between carriers and scattering centers [5]. This work was supported by DARPA (grant HR0011-13-2-0016) and by NSF (grant DMR-1410940). A portion of this research was conducted at the Center for Nanophase Materials Sciences, a DOE Office of Science User Facility. References [1] S. B. Desai, *et al.*, *Adv. Mater.* **28**, 4053-4058 (2016); [2] Y. Zhao, *et al.*, *Adv. Mater.* **28**, 2399-2407 (2016); [3] A. D. Oyedele, *et al.*, *J. Am. Chem. Soc.* **139** (40), 14090-14097 (2017); [4] A. A. Puretzy, *et al.*, *2D Mater.* **5**, 035016 (2018); [5] S.-L. Li, *et al.*, *Nano Lett.* **13**, 3546-3552 (2013).

8:40 AM LL02

Mechanism of Exfoliation of Centimeter-Sized MoS₂ on Gold Matěj Velický^{1,2}, Gavin Donnelly², Héctor Abreu¹ and Fumin Huang²;

¹Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York, United States; ²School of Mathematics and Physics, Queen's University Belfast, Belfast, United Kingdom.

Achieving both material quality and production scalability is critical for future applications of two-dimensional (2D) materials. Mechanical exfoliation generally produces the highest quality 2D materials, however, their dimensions are limited. The typical lateral size of monolayer transition metal dichalcogenides (TMDCs), such as MoS₂, has been ~100 μm on insulating substrates [1], while much larger dimensions have recently been achieved on Au substrates [2]. Here we report mechanical exfoliation of centimeter-sized monolayer MoS₂ on Au, which is facilitated by strong physisorption between the two materials, and which also extends to other TMDCs [3]. Minimization of surface contamination and roughness of the Au substrates is found to be key for successful high-yield exfoliation. Microscopic and spectroscopic characterization along with the density theory functional calculations of the MoS₂/Au heterostructures confirm the existence of a strong van der Waals interaction between the two materials, resulting in a significant charge transfer without compromising the structural integrity of the monolayer MoS₂. Furthermore, electrochemical characterization reveals that the subnanometer-thick MoS₂ monolayer strongly passivates the chemical properties of the underlying Au, and that the Au significantly increases the density of electronic state of the MoS₂, turning it from semiconducting to metallic. This simple and reproducible exfoliation technique facilitates the production of large-area TMDCs, enabling studies previously limited by their small lateral size. These findings have important implications for many research areas, such as electrode modification, photovoltaics, and photocatalysis. [1] Velický, M. et al., *Nano Lett.* 16 (2016), 2023-2032. [2] Desai, S. B. et al., *Adv. Mater.* 28 (2016), 4035-4058. [3] Velický, M. et al., *ACS Nano* 12 (2018), 10463-10472.

9:00 AM LL03

A Combined Theoretical and Experimental Study of Molybdenum Sulfides for High Efficiency Photoelectrochemical Water Splitting

Baowen Zhou³, Xianghua Kong⁴, Srinivas Vanka^{2,3}, Sheng Chu², Nick Pant^{1,3}, Hong Guo⁴ and Zetian Mi²; ¹Applied Physics, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ²Electrical & Computer Engineering, McGill University, Montreal, Quebec, Canada; ³Electrical Engineering and Computer Science, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ⁴Physics, McGill University, Montreal, Quebec, Canada.

The production of hydrogen by photoelectrochemical (PEC) water splitting, so-called artificial photosynthesis, offers one promising route for transforming the abundant but intermittent solar energy into storable chemical fuel. The fabrication of an efficient, stable, and inexpensive photocathode using earth-abundant catalysts and semiconductors is crucial for the industrial-scale utilization of this charming technique. Molybdenum sulfides (MoS_x), which has received tremendous attention in recent years, is considered as a promising catalyst to accelerate the kinetics of planar silicon because of its superior hydrogen evolution reaction (HER) catalytic activity and low cost. However, the inferior interface between MoS_x and planar silicon fundamentally suppresses charge carrier extraction, thus limiting the performance. Here, we investigate the use of defect-free GaN nanowires as an ideal linker between planar Si wafer and molybdenum sulfides catalyst. Using density functional theory calculations we discover that, due to the unique electronic interaction and excellent geometric-matching structure between GaN (10¹10)-wurtzite and MoS₂, an excellent MoS₂/GaN (10¹10)-wurtzite heterointerface can be constructed, exhibiting great potential for efficient charge carrier extraction for water splitting, which has never been investigated before. Experimentally, defect-free GaN nanowire is employed as a linker of planar silicon and molybdenum sulphides by nanostructure-engineering integration of molecular beam epitaxy and electrodeposition to produce an ideal photocathode of MoS_x@GaN NWs/Si. The GaN nanowires are vertically aligned on silicon substrate with length of ~150 nm and diameters varying from 30 to 40 nm. TEM characterization showed that a high-quality shell-core heterostructure of MoS_x@GaN was produced with a MoS_x shell of 7 nm. The well-matched electronic and geometrical properties between GaN NWs and MoS_x enable an efficient channel for charge carrier transport. As a result, a large onset potential of +0.4 V vs. RHE with a benchmarking current density of 40±1 mA/cm² at 0 V vs. reversible hydrogen electrode, the highest value ever reported for a planar Si electrode without noble metals, is achieved under standard one-sun illumination in 0.5 M H₂SO₄, exhibiting a substantial improvement compared to MoS_x/Si. The applied bias photon-to-current

efficiency (ABPE) is >5%; and long-term stability of 10 hours with a nearly 100% Faradaic efficiency is also demonstrated. To explain the significantly improved performance of the device, direct calculations of electronic properties of MoS₂/GaN(10¹10) heterointerface at atomic level were further conducted. It was found there was no energy barrier between MoS₂ and GaN; and the potential of S atoms is much lower than that of Ga and N, indicating that electrons in GaN is prone to move to MoS₂. The atomic hydrogen free energy of MoS₂ was also calculated, which is very low (0.036 eV), and even comparable to that of Pt (-0.09 eV), indicating that MoS_x is intrinsically active for hydrogen evolution reaction, which is another important contributing factor for the high performance. Work is currently in progress to further improve the device performance and to achieve unassisted solar-to-hydrogen conversion efficiency >15% using silicon and MoS_x. This work presents a promising route for the practical conversion of solar energy into hydrogen fuel with high efficiency and low cost.

9:20 AM LL04

MoS₂/Graphene Heterostructure for Gas Sensing Soaram Kim^{1,4}, Jaeseo Park^{2,5}, Seunghyun Lee³, Sanjay Krishna³, Sang-Woo Kang^{2,5} and Kevin M. Daniels^{1,4}; ¹Electrical and Computer Engineering, University of Maryland, College Park, Maryland, United States; ²Advanced Instrumentation Institute, Korea Research Institute of Standards and Science, Daejeon, Korea (the Republic of); ³The Ohio State University, Columbus, Ohio, United States; ⁴Institute for Research in Electronics and Applied Physics, University of Maryland, College Park, Maryland, United States; ⁵Science of Measurement, University of Science and Technology, Daejeon, Korea (the Republic of).

Recent sensor technology is making use of gas sensors in process control, environmental monitoring and medical diagnostics, and the use of the data can analyze in the workplace, home, and hospital as safety monitoring and biomedical health care systems [1,2]. High sensitivity, fast response time, low cost, simple fabrication, and demonstration at room temperature are preferred attributes for next-generation gas sensors. In this work, we have prepared a heterostructure of vertically grown, nanoflower-structures molybdenum disulfide (MoS₂) and graphene (MoS₂/graphene) on 6H silicon carbide (SiC) substrate with different growth conditions of MoS₂ for gas sensing application. The MoS₂/graphene heterostructure make the sensor a good candidate for gas sensing due to the synergistic combinations of atomically thin nanomaterials with dissimilar physical properties (referred to as van der Waals epitaxy). Figure 1(a) shows a schematic illustration of the experimental procedure. Bilayer epitaxial graphene (EG) was synthesized by Si sublimation on 6H SiC. The thermal sublimation method for the growth of graphene is discussed in detail elsewhere [3]. MoS₂ nanoflowers were grown on graphene/SiC directly using metal organic chemical vapor deposition (MOCVD). Molybdenum hexacarbonyl (Mo(CO)₆) and hydrogen sulfide (H₂S) were used as precursor materials, with the partial pressure ratio of 1:1. Carbonaceous impurities were first randomly deposited on graphene/SiC, acting as promoters of nucleation and growth of vertically standing MoS₂ (Stranski-Krastanov growth mode) [4]. Growth of MoS₂ was performed at 350 °C with various chamber pressures and growth times as shown in Table 1. Samples were investigated by scanning electron microscopy (SEM), Raman spectroscopy, and photoluminescence (PL). Figure 2 shows SEM images of MoS₂/graphene heterostructure on SiC. The MoS₂ nanoflowers were found to grown well onto the graphene/SiC and withstand repeated cycles of characterization measurements. Figure 3 presents the (a) Raman and (b) PL spectra of the MoS₂ nanoflowers grown on graphene/SiC. From the Raman spectra, $\Delta k = A_{1g} - E_{2g}^1$ and $I_{(E_{12g}/A_{1g})}$ were calculated as shown in Table 1, indicating the synthesized structures is indeed MoS₂. The number of layers for all synthesized MoS₂ nanoflowers is expected few layers since Δk is over 23 cm⁻¹, which also correspond with PL properties. In addition, the density of MoS₂ nanoflowers was increased as the $I_{(E_{12g}/A_{1g})}$ was decreased, which matched well with SEM results. It is clearly evident that the MoS₂ nanoflowers were synthesized well on graphene/SiC by MOCVD, which is suitable for gas sensing application due to the synergistic combinations of MoS₂ and graphene. Furthermore, we plan to fabricate MoS₂/graphene based gas sensor in the form of an array and the fabricated sensors will be exposed to various greenhouse gases and volatile organic compounds (VOCs) to test sensor sensitivity and selectivity to molecules of different sizes which would provide a lot more information. That is one of the final targeted applications of the sensor, and will be pursued in the near future.

9:40 AM LL05

(LATE NEWS, Student) Scalable Synthesis of BEOL compatible 2D WSe₂, Azimkhan Kozhakhmetov¹, Joseph R. Nasr², Fu Zhang^{1,3}, Ke Xu¹, Natalie C. Briggs^{1,3}, Christopher R. Cormier⁵, Rafik Addou⁵, Saptarshi Das², Mauricio Terrones^{1,3,6}, Robert Wallace⁷, Susan Fullerton-Shirey^{4,7} and Joshua A. Robinson^{1,3}; ¹Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, United States; ²Department of Engineering Science and Mechanics, The Pennsylvania State University, University Park, Pennsylvania, United States; ³Center for Two-Dimensional Layered Materials, The Pennsylvania State University, University Park, Pennsylvania, United States; ⁴Department of Petroleum Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania, United States; ⁵Department of Materials Science and Engineering, The University of Texas at Dallas, Richardson, Texas, United States; ⁶Department of Physics, Department of Chemistry, The Pennsylvania State University, University Park, Pennsylvania, United States; ⁷Department of Electrical and Computer Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania, United States.

Relentless scaling of transistors has led to the continuous search for novel materials and designs beyond silicon for future electronic devices. Due to outstanding structural and electronic properties, recently re-discovered 2D semiconducting transition metal dichalcogenides (TMDs) are considered to be the most promising candidate for next-generation thin film transistor (TFT) technology. Among the TMDs, WSe₂ is predicted to have a high ON/OFF ratio >10⁸ and hole mobility up to 200 cm²/V-s. Commonly, a crystalline substrate as well as elevated growth temperatures (> 800 °C) are needed to synthesize high-quality, stoichiometric, and wafer-scale TMDs including WSe₂ with the excellent optical and transport performances. Moreover, successful integration of 2D materials with the current-state-of-the-art Si-based CMOS technology will demand a large-scale growth at back-end-of-line (BEOL) compatible temperatures (< 500 °C) on SiO₂ and other insulating amorphous substrates. However, to date low-temperature synthesis of electronic grade TMDs in a technological relevant scale still remains challenging. In this work, we present a scalable synthesis of layered 2D WSe₂ on SiO₂/Si and epitaxial graphene (EG) substrates via metal organic chemical vapor deposition (MOCVD) at BEOL compatible temperatures (< 500 °C). The MOCVD growth was performed in a cold-wall CVD reactor utilizing tungsten hexacarbonyl (W(CO)₆) and hydrogen selenide (H₂Se). Controlling the reaction environment in the chamber, we obtain high-quality, fully coalesced, stoichiometric WSe₂ films. X-ray photoelectron spectroscopy (XPS), selective area diffraction (SEAD), and atomic force microscopy (AFM) measurements further confirm that synthesized WSe₂ films are polycrystalline in nature and have a thickness of ~ 2 nm which corresponds to approximately 3 atomic layers. Transmission electron spectroscopy, scanning tunneling microscopy and scanning tunneling spectroscopy reveal the presence of point defects dominated by Se vacancies, the formation of Moire pattern between low-temperature WSe₂ and EG and the electronic band gap of 1.8 eV. Electric double layer gated (EDL) and back-gated field effect transistors (FETs) exhibit enhanced ON current values as high as > 10⁶ μA/μm and ON/OFF ratio of ~ 10⁶ for BEOL compatible 2D WSe₂ films on SiO₂/Si which demonstrates 100x improvement from the all previous reports.

10:00 AM REFRESHMENT BREAK

SESSION MM: 2D Materials Engineering Session Chairs: Emmanouil Kioupakis and Nate Quitoriano Friday Morning, June 28, 2019 Michigan League, 2nd Floor, Vandenberg

10:20 AM MM01

(Student) Effect of Stacking Orientation on the Electronic and Optical Properties of 2D Nitride Heterostructures Nocona Sanders and Emmanouil Kioupakis; Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States.

In atomically thin 2D nitrides, the quantum-confined Stark shift due to the strong inherent polarization perpendicular to the 2D plane counteracts the band-gap increase caused by extreme quantum confinement. We apply first-principles calculations to investigate the electronic and optical properties of 2D, H-passivated BN, GaN, AlN, and InN in various stacking orientations, such that the electric fields are either aligned or anti-parallel in two possible configurations. We employ density functional theory and

quasiparticle corrections with the GW method, as well as the Bethe-Salpeter Equation, to derive accurate band structures, exciton binding energies, and luminescence energies. Through understanding how the stacking arrangement influences the underlying electronic and optical properties, critical insight will be gained in how to improve 2D III-nitride-based optoelectronics through accessing the additional degree of freedom provided by polarization. This work was supported by the NSF ECCS-CDS&E program (1607796). Computational resources were provided by the DOE NERSC facility under Contract No. DE-AC02-05CH11231.

10:40 AM MM02

Interlayer Exciton Laser with Extended Spatial Coherence in an Atomically-Thin Heterostructure Eunice Paik¹, Long Zhang², G W. Burg³, Rahul Gogna¹, Emanuel Tutuc³ and Hui Deng¹; ¹University of Michigan—Ann Arbor, Ann Arbor, Michigan, United States; ²Physics, Univ of Michigan - Ann Arbor, Ann Arbor, Michigan, United States; ³The University of Texas at Austin, Austin, Texas, United States.

Atomically thin two-dimensional (2D) semiconductors are a promising gain media for the next generation of semiconductor lasers and nanophotonics and have advantages over the traditional III-V semiconductors because they exhibit strong light-matter interaction, are flexible and compact, and allow easy integration with various substrates. Utilizing these advantages, we engineer a lasing device with a rotationally aligned WSe₂-MoSe₂ van der Waals heterostructure integrated with a one-dimensional (1D) silicon nitride (SiN) grating resonator. Precise rotational alignment of the two layers of the heterostructure ensures maximum overlap of the momentum valleys and therefore a strong inter-layer exciton emission. The SiN grating resonator is an ultra-compact cavity whose properties can be easily tuned by the grating parameters. The grating cavity mode energy is designed to match the WSe₂-MoSe₂ inter-layer exciton emission energy and the Q-factor is between 500 and 680. The heterostructure is placed directly on top of the grating in order to maximize the field overlap. To characterize the lasing device, we perform angle-resolved micro-photoluminescence (PL) and spatial coherence measurements. PL from the ground state cavity mode brightens up with increasing pump laser power, showing a sharp non-linear increase at threshold power. This signifies the onset of stimulated scattering into the cavity mode. Furthermore, increase in phase coherence in shown by the narrowing on emission linewidth. On the other hand, inter-layer exciton uncoupled to the cavity does not show threshold behavior nor linewidth narrowing. In order to rule out localized exciton as a source of lasing, we also perform a first order spatial coherence measurement using a Michelson interferometer. Pump power-dependent mapping of the spatial coherence shows sharp increase in coherence length above threshold power, which confirms the formation of extended spatial coherence in the lasing device. This work establishes 2D semiconductor heterostructures as a promising gain medium for energy efficient, electrically injected ultrafast laser.

11:00 AM MM03

Bandgap Tuning of 2D MoS₂ by Defect Engineering and Doping Frederick Arveteey¹, Sajedeh Pourianejad², Tetyana Ignatova² and Shyam Aravamudan¹; ¹Nanoengineering, North Carolina A&T State University, Greensboro, North Carolina, United States; ²Nanosience, UNCG, Greensboro, North Carolina, United States.

Single layer MoS₂ is direct bandgap semiconductor making it useful for smaller and energy efficient field effect transistors, photodetectors and flexible optoelectronic devices. The practicability of these applications hinges on the synthesis and transfer of high quality, large area monolayer films. Large area and high-quality single layer MoS₂ samples can be produced by vapor deposition methods and transferred using wet transfer onto other substrates for wide range of applications. Single layer MoS₂ has photoluminescence properties that can vary by the transition between trions and excitons depending on the carrier concentration. In this work, we investigate the effect of molecular doping of helium ion generated sulfur vacancies in monolayer MoS₂ films on their charge density, electronic, optical and structural properties. P-type dopant of 2,3,5,6-tetrafluoro-7,8-tetracyanoquinodimethane (F4TCNQ) is used as a strong electron acceptor and this molecule is able to change the photoluminescence intensity by switching from PL trions to PL excitons depending on the carrier density calculated using the mass action model. Sulfur vacancies in Monolayer MoS₂ are created by treating flakes with different helium ion doses and F4TCNQ molecules are able to modulate the defect levels within the bandgap and control the charge density around the defect center. Finally, the substitution of the F4TCNQ molecules in the sulfur vacancy sites modulates the carrier concentration and recovers the photoluminescence degradation of the n-doped monolayer MoS₂ from the helium ion defects. Characterization techniques such as XPS, RAMAN,

HIM, PL, AFM, CAFM I-V have been used to assess the effect of doping, sulfur vacancies and doping of sulfur vacancies on electronic, optical and structural properties of monolayer MoS₂. We have further quantified the changes introduced by molecular doping and defect engineering on the monolayer MoS₂ using carrier concentration and ideality factor. In summary, this projects aims to develop efficient engineered methods to control charge carriers, electronic, optical and structural properties for optoelectronic applications.

11:20 AM MM04

(Student) Measurement of Coherent Coupling and Interlayer Exciton Binding Energy in a MoSe₂/WSe₂ Heterostructure Hanna G. Ruth¹, Eric Martin¹, Torben L. Purz^{2,1}, Pasqual Rivera³, Xiaodong Xu³ and Steven T. Cundiff¹; ¹Physics, University of Michigan, Ann Arbor, Michigan, United States; ²Physics, University of Göttingen, Göttingen, Germany; ³Physics, University of Washington, Seattle, Washington, United States.

Monolayer transition metal dichalcogenides (TMDCs) are two-dimensional materials that have garnered interest due to their vast array of novel properties; the foremost property of monolayer TMDCs is the direct bandgap because it signifies efficient light-matter coupling. The combination of efficient light-matter coupling and the other notable properties of TMDCs, which include atomic thickness, spin-valley degenerate exciton transitions, and high carrier mobility, make TMDCs an attractive candidate for use in a variety of devices such as optoelectronics, photovoltaics, and ultra-small transistors. TMDCs are frequently used in van der Waals heterostructures. Notably, a type II heterojunction emerges when different types of monolayer TMDCs are stacked which results in ultrafast charge transfer between layers and interesting temporal dynamics of states. To this end, we are interested in investigating the coupling between electronic states in separate layers of a TMDC heterostructure. For the first time, we have employed MDCS to identify coherent couplings between excitonic states in two different layers of a TMDC heterostructure. The two-dimensional spectrum of a MoSe₂/WSe₂ heterostructure displays coupling peaks which indicate that the excitonic states in separate layers of the heterostructure are coherently coupled. The absorption at the MoSe₂ exciton resonance is coupled to the emission at the WSe₂ exciton resonance, and vice versa. These coupling peaks can be tracked as a function of the time delay T between the second and third pulse in order to resolve dynamics of the exciton coupling which can be used to determine the time scales of processes that contribute to the coupling between layers, such as interlayer charge transfer. The fact that MDCS reveals correlations between states is useful for observing electronic states with weak dipole moments that would be difficult to observe with linear spectroscopic methods. When a state with a weak dipole moment is correlated with a state with a strong dipole moment, a coupling peak between the two states will become visible in the MDCS spectrum. Therefore, MDCS reveals features of weak dipole states that would not appear in linear measurements. In our two-dimensional spectrum, this effect is exhibited by the presence of a coupling peak beginning at 1638 meV and the emission energy of each exciton. Additionally, there is no coupling peak at the emission energy 1638 meV. This pattern of peaks indicates that the correlation mechanism is excitation induced dephasing of the exciton by continuum states [1]. Thus, the peak location corresponds to the band edge of the continuum and is taken as a measurement of the interlayer bandgap. Subtracting the excitation energy of the interlayer exciton [2] from the bandgap energy gives a value for the binding energy of the interlayer exciton of 283 meV, which agrees with the theoretically predicted binding energy of the interlayer exciton [3]. [1] C. N. Borca, T. Zhang, X. Li, and S. T. Cundiff, "Optical two-dimensional fourier transform spectroscopy of semiconductors," *Chemical Physics Letters* 416, 311315 (2005). [2] Schaibley, J. R. et al. Directional interlayer spin-valley transfer in two-dimensional heterostructures. *Nat. Commun.* 7, 13747 doi: 10.1038/ncomms13747 (2016). [3] R. Gillen and J. Maultzsch, "Interlayer excitons in MoSe₂/WSe₂ heterostructures from first principles," *Phys. Rev. B* 97, 165306 (2018).

11:40 AM MM05

(LATE NEWS, Student) Low Off-Current and High On/Off Ratios in Monolayer MoSe₂ and WSe₂ Transistors Connor Bailey¹, Connor McClellan¹ and Eric Pop^{1,2}; ¹Electrical Engineering, Stanford University, Stanford, California, United States; ²Materials Science and Engineering, Stanford University, Stanford, California, United States.

Two-dimensional (2D) transition metal dichalcogenides have attracted attention for electronic applications due to their superior mobility at sub-nanometer thicknesses when compared to Si [1]. An equally important property of these 2D semiconductors are their relatively large band gaps and effective masses, potentially enabling transistors with ultra-low off-current (I_{off}). Such low-leakage transistors could be used for dynamic

random access memory (DRAM) memory selectors, reducing power consumption and increasing retention time [2]. MoS₂ has received some attention in this domain [2-4], but leakage in selenide-based transistors (MoSe₂ and WSe₂) has not been carefully investigated. These materials are expected to have larger on-current (I_{on}), which is important for non-volatile memories where both low I_{off} and high I_{on} are necessary. Here, we measure record-low I_{off} and high I_{on}/I_{off} ratios in chemical vapor deposition (CVD) grown monolayer (1L) MoSe₂ and WSe₂ field-effect transistors (FETs), demonstrating their viability for ultra-low leakage applications. 1L MoSe₂ and WSe₂ were grown by CVD directly on SiO₂ [5], resulting in large-area grains up to 100s μm in size. Back-gated FETs were then fabricated using optical lithography, with metal contacts (Pd, Ag, Au, or Ni) deposited by e-beam evaporation with channel lengths (contact spacing) from $L = 1$ to 3 μm. Devices were annealed in vacuum prior to testing. Some devices were capped with ~15 nm of Al₂O₃ deposited by atomic layer deposition (ALD) in order to improve hysteresis, stability, and I_{on} [6]. Because I_{off} is so low in these 2D material devices, measurements on typical (i.e. μm-wide) FETs are limited by the noise floor of the instrumentation. To properly measure I_{off} , we used interdigitated structures to realize ultra-wide devices with widths up to $W = 1833$ μm. The FETs were measured at various drain voltages to investigate off- and on-current behaviors at both low and high lateral (drain-to-source) fields. In MoSe₂, for $L = 2$ μm, $I_{on} < 100$ aA/μm at $V_{DS} = 0.1$ V was reached with $I_{on}/I_{off} > 10^9$, a record for 1L MoSe₂ FETs. At $V_{DS} = 1$ V, $I_{on} \approx 375$ aA/μm while maintaining $I_{on}/I_{off} > 10^9$. In general, both I_{on} and I_{off} increase with higher lateral field, while I_{on}/I_{off} degrades. This effect is likely due to gate induced drain leakage (GIDL) and band-to-band tunneling (BTBT) as predicted [2]. At high drain bias ($V_{DS} = 5$ V), good I_{on} ($= 52$ μA/μm) can be achieved while maintaining excellent I_{on}/I_{off} ($= 3 \times 10^7$). After Al₂O₃ capping, hysteresis decreases and I_{on} increases, maintaining similar I_{off} and I_{on}/I_{off} . Additionally, slight n -type doping is observed, as previously reported [7]. This suggests that such ALD encapsulation provides an easy way to achieve increased performance in 2D n -type FETs without increasing I_{off} . In WSe₂, for $L = 2$ μm, I_{off} reached ~75 aA/μm and below 10 aA/μm at $V_{DS} = 1$ V and 0.1 V, respectively, while maintaining $I_{on}/I_{off} > 10^9$. Compared to MoSe₂ at equal V_{DS} and L , WSe₂ exhibits $10 \times$ lower I_{off} , likely due to its larger quasiparticle band gap of ~2.26 eV [8], vs. ~2.15 eV for MoSe₂ [9]. In conclusion, we measured record low I_{off} in CVD-grown MoSe₂ and WSe₂ FETs with high I_{on}/I_{off} up to $> 10^9$. Additionally, Al₂O₃ encapsulation is shown to improve hysteresis and n -type I_{on} without degrading I_{off} . These results could enable memory applications with long retention and low leakage. This work was supported by the AFOSR, NSF-EFRI, SRC JUMP ASCENT, and Stanford SystemX. C.S.B. acknowledges NSF-GRFP. **Refs:** [1] C. English et al., *Nano Lett.* 16, 3824 (2016). [2] J. Kang et al., *IEDM Tech. Dig.*, 32.2.1 (2017). [3] C. Kshirsagar et al., *IEEE-DRC*, 187 (2014). [4] C. Kshirsagar et al., *ACS Nano*, 10, 8457 (2016). [5] K. Smithe, C. Bailey, et al., *ACS Appl. Nano Mater.*, 1, 572 (2018). [6] Y. Illarionov et al., *IEEE-EDL*, 38, 1763 (2017). [7] C. McClellan, et al., *IEEE-DRC* (2017). [8] R. Addou et al., *2D Mater.* 5, 025017 (2018). [9] Q. Zhang et al., *Nat. Comm.*, 7, 13843 (2016)

SESSION NN: Dielectrics and Multifunctional Oxides

Session Chairs: Doug Hall and Patrick Lenahan

Friday Morning, June 28, 2019

Michigan League, 3rd Floor, Henderson

8:20 AM NN01

(Student) Flexoelectric Bending in Lanthanide Scandates—How Charging Induces Large, Reversible Mechanical Deformations Christopher A. Mizzi, Pratik Koirala and Laurence D. Marks; Materials Science and Engineering, Northwestern University, Chicago, Illinois, United States.

Although first proposed and experimentally observed in the 1960s, flexoelectricity (the electromechanical coupling of polarization and strain gradient) in crystalline solids has remained largely unexplored. In part this is because early theory predicted a small bulk effect in most materials. However, there has been a significant increase in studies on flexoelectricity in crystalline solids over the last two decades due to experiments establishing the flexoelectric effect as an important phenomenon in high dielectric constant ceramics [1]. Flexoelectricity is particularly significant at the nanoscale because intrinsic scaling leads to large strain gradients at small length scales. This can result in substantial flexoelectric responses even for materials with modest flexoelectric properties. An exceptionally enticing aspect of flexoelectricity is that it is governed by a fourth-rank tensor: applying a strain gradient inherently breaks inversion symmetry so

this phenomenon is ubiquitous, existing in both centrosymmetric and non-centrosymmetric insulators. This is a striking distinction from piezoelectricity (the electromechanical coupling between polarization and strain), which is symmetrically constrained to only exist in materials lacking inversion symmetry. The structural constraints of the piezoelectric effect have raised a significant materials selection challenge in the attempt to replace modern lead-based piezoelectric materials with lead-free alternatives. One possible solution to this issue is to leverage the ubiquity of flexoelectricity by replacing piezoelectric-based devices with flexoelectric-based devices possessing equivalent functionality. For example, flexoelectric actuators with an equivalent figure of merit to modern piezoelectric actuators have been recently demonstrated [2]. However, improving the efficacy of flexoelectric-based devices requires a significant advancement in the basic science of flexoelectricity. There is a sizable divide between the experimental and theoretical states of the field and an abundance of open questions. In this work, large, reversible bending of lanthanide scandate single crystals under electron beam illumination of a transmission electron microscope is described in terms of a flexoelectric coupling between electron beam-induced sample charging and curvature [3]. An experimental and theoretical description of the electronic structure of lanthanide scandates utilizing a combination of X-ray photoelectron spectroscopy, ultraviolet photoelectron spectroscopy, electron energy loss spectroscopy, and density functional theory demonstrates that the proclivity for charging in lanthanide scandates is an unavoidable consequence of their electronic structure [4, 5]. The maximum potential induced by this charging is found to be Zener-tunneling limited and leads to the observed inhomogeneous mechanical deformations because of an abnormally high flexocoupling voltage. This is directly confirmed by experimental measurements of the flexoelectric response of single crystal lanthanide scandates. Additional density functional theory calculations of the flexoelectric properties of lanthanide scandates are used to elucidate the origins of the abnormally high flexocoupling voltage. [1] W. Ma, L. E. Cross, *Appl. Phys. Lett.* **78** (2001) 2920–2921. [2] U.K. Bhaskar *et al.*, *Nat. Nanotechnol.* **11** (2016) 263–266. [3] P. Koirala, C.A. Mizzi, L.D. Marks, Direct Observation of Large Flexoelectric Bending at the Nanoscale in Lanthanide Scandates, *Nano Lett.* **18** (2018) 3850–3856. [4] C.A. Mizzi, P. Koirala, L.D. Marks, Electronic structure of lanthanide scandates, *Phys. Rev. Mater.* **2** (2018) 025001. [5] C.A. Mizzi, P. Koirala, A. Gulec, L.D. Marks, Charging Ain't All Bad: Complex Physics in DyScO₃, *Ultramicroscopy*, In Press (2018).

8:40 AM NN02

(Student) Near-Nanoscale Defect Tracking in Ultra-Thin Complex Oxide Films and Conducting Interfaces Brenton A. Noesges¹, Hyungwoo Lee², Neil G. Campbell³, Ja-kyung Lee⁴, Thaddeus J. Asel¹, Tula Paudel⁵, Hua Zhou⁶, Jungwoo Lee², Jinsol Seo⁴, Bumsu Park^{4,7}, Sang Ho Oh⁴, Evgeny Y. Tsybmal⁵, Mark S. Rzchowski³, Chang-beom Eom² and Leonard Brillson^{1,8}; ¹Physics, The Ohio State University, Columbus, Ohio, United States; ²Department of Materials Science and Engineering, University of Wisconsin–Madison, Madison, Wisconsin, United States; ³Department of Physics, University of Wisconsin–Madison, Madison, Wisconsin, United States; ⁴Department of Energy Science, Sungkyunkwan University, Suwon, Korea (the Republic of); ⁵Department of Physics and Astronomy, Nebraska Center of Materials and Nanoscience, University of Nebraska–Lincoln, Lincoln, Nebraska, United States; ⁶Advanced Photon Source, Argonne National Laboratory, Lemont, Illinois, United States; ⁷Department of Materials Science and Engineering, Pohang University of Science and Technology, Pohang, Korea (the Republic of); ⁸Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States.

Electronic devices size continues to shrink, with features that are only a few nanometers to sub-nanometers in size. Characterization techniques focused at improving device quality and performance must be able to resolve defects at these length scales. Effects produced by defect formation within ultra-thin layers can permeate throughout the film and alter the interface properties between adjacent layers. Complex oxide heterostructures like the conducting interface between LaAlO₃ and SrTiO₃ with layers often only a few nm thick are particularly sensitive to defect formation where missing or substituted atoms can reduce carrier mobility, act as dopants or suppress interface conductivity. The interface between STO and LAO has been widely studied due to the high mobility two-dimensional electron gas (2DEG) present at the interface between these wide bandgap materials. Oxygen vacancies (V_O) in both materials act as an electron donor donating up to two electrons which increases carrier concentration and reduces interface mobility. While the 2DEG performance is impeded by V_O formation, the complementary 2D hole gas (2DHG) won't form unless oxygen vacancies are sufficiently suppressed. V_O must be minimized near p-type interfaces otherwise the donated electrons compensates any free holes and quench the 2DHG [1]. Using

growth techniques designed to control defect formation combined with near-nanoscale depth resolved cathodoluminescence spectroscopy (DRCLS), we identify and track several electronically active defect states like oxygen and strontium vacancies, and more complexes like titanium on strontium anti-sites (Ti_{sr}) as a function of depth through 2DEG and 2DHG STO/LAO heterostructures. Density functional theory (DFT) calculations help correlate observed DRCLS transitions to defect states [2]. Defect spectroscopy feedback after tuning growth parameters allows us to systematically investigate to the role of point defects and complexes on interface properties. DRCLS is an ideal technique for probing defects in ultra-thin layers since probe depth is continually tunable on the near-nanoscale by adjusting the electron beam voltage. We can collect luminescence containing defect information from the first couple of nanometers below the sample surface, through buried interfaces and down hundreds of nanometers into the bulk. Monte Carlo simulations determine the relationship between beam voltage and probe depth. With DRCLS, we determined the role of V_O defects on the formation of the first experimentally observed 2DHG at a LAO/STO interface which was grown in high partial oxygen pressure to minimize V_O formation. We demonstrate a sharp reduction in STO V_O concentration near the 2DHG interface compared to deep in the bulk confirming the need to minimize V_O near the p-type interface. Furthermore, metal organic precursors like titanium tetraisopropoxide (TTIP) can help supply excess oxygen while also providing extra control over cation ratio. Control over metal content is important since defects like Ti_{sr} are expected to suppress oxygen vacancy defects. Using DRCLS we identified a Ti_{sr} feature in a series of STO/LAO 2DEG structures grown in varying TTIP pressures. We observed the highest concentration of Ti_{sr} in the sample with lowest V_O density and the highest mobilities. DRCLS is an extremely useful tool for investigating defect distributions in ultra-thin layers to help understand the contribution defects have on space charge layers. Precise growth combined with DRCLS mapping of defect distributions provides a powerful approach to achieve advanced electronic features and improve material quality in semiconductor systems including but not limited to complex oxide heterostructures. Support by NSF DMR-18-00130 [1] H.Lee, et al, Direct observation of a two-dimensional hole gas at oxide interfaces. *Nature Materials* **17**, 231–236 (2018) [2] D. Lee, et al, Identification of a functional point defect in SrTiO₃. *Phys. Rev. Materials* **2**, 060403(R) (2018)

9:00 AM NN03

(Student) Direct Observation of Vo Migration in Degraded SrTiO₃ by Depth Resolved Cathodoluminescence Spectroscopy Hantian Gao¹, Sulata K. Sahu², Clive Randall² and Leonard Brillson^{1,3}; ¹Physics, The Ohio State University, Columbus, Ohio, United States; ²Material Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, United States; ³Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States.

Complex oxides such as SrTiO₃ have attracted considerable attention for a broad range of potential applications, especially as capacitor dielectrics for microelectronics. Key to their performance is their stability at elevated temperature and under high electric field stress which is limited by resistance degradation. The mechanism of such degradation has been investigated extensively, where defects are believed to play an important role.¹ Specifically, the migration of oxygen vacancies, the most common point defects in oxide, is believed to be a primary reason for such degradation process. However, more direct, spatially-resolved microscopic evidence has until now not been possible. In this work, we used spatially and depth-resolved cathodoluminescence spectroscopy (DRCLS) to study the SrTiO₃ defect distributions in three dimensions with tens of nanometers depth resolution and observed direct evidence of oxygen vacancy migration in degraded SrTiO₃ together with depth-resolved effects at Pt/SrTiO₃ electrode interfaces after high temperature electric field cycling. Two SrTiO₃ samples were degraded at elevated temperature with electric field cycling at Penn State both between laterally separated electrodes as well as normal to the electrode interfaces. Their electrical measurements showed that the SrTiO₃ resistance degradation is related to migration of oxygen vacancies from anode to cathode and the resultant carrier compensation². Using DRCLS scanned between the laterally separated electrodes, we observed increases from anode to cathode of 2.6 eV and 3.0 eV features that we have previously³ correlated with oxygen vacancies V_O. This defect redistribution can now be correlated with Penn State impedance measurements that indicate defect migration and degradation. DRCLS could also probe through both anode and cathode contacts, from the Pt/STO interface to ~130 nm below the interface with a 10-nm depth resolution. In general, the 2.6/2.9 eV Vo-related defect features are higher when probing through cathode than through anode, consistent with previous electrical measurements and lateral sample results, confirming the defect migration from anode to cathode after degradation.

Furthermore, within several tens of nanometers of the cathode Pt/STO interface, these defects exhibit dramatic changes, consistent with previous distributions that appear to depend on crystal orientation. For these electrically stressed crystals, our DRCLS confirmed the migration of oxygen vacancies from anode to cathode as well as defect redistribution near the cathode. In general, our work demonstrates that spatially-resolved cathodoluminescence spectroscopy can provide direct and microscopic evidence regarding defect movement during the degradation process, which could improve our understanding of the roles defects play under electrical stress. In addition to V_o , we could also study the behaviors of other defects, including Ti^{3+} , Ti_{Sr} , and V_{Sr} and correlate them with the activation energy distributions after degradation to achieve a more complete picture of the physical mechanisms of electrical breakdown process. The authors gratefully acknowledge support from AFOSR Grant No. FA9550-18-1-0066 (A. Sayir) ¹R. Waser, *et al.*, *J. Am. Ceram. Soc.* **73** 1645 (1990) ²T. J. M. Bayer, *et al.*, *J. Appl. Phys.* **122**, 244101 (2017). ³J. Zhang *et al.*, *J. Vac. Sci. Technol. B* **26**, 1466 (2008).

9:20 AM NN04

Imaging and Crafting Dynamic Oxygen Vacancy Behaviour in a Memristive Device Huajun Liu^{2,3}, Hua Zhou¹, Dillon D. Fong³, Yongqi Dong^{4,3}, Zhonghou Cai¹ and Liliana Stan⁵; ¹Advanced Photon Source, Argonne National Laboratory, Lemont, Illinois, United States; ²Institute of Materials Research and Engineering, A*STAR (Agency for Science, Technology and Research), Singapore, Singapore; ³Materials Science Division, Argonne National Laboratory, Lemont, Illinois, United States; ⁴National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, China; ⁵Center for Nanoscale Materials, Argonne National Laboratory, Lemont, Illinois, United States.

Crystalline defects are essential to materials properties, and understanding how to control them has helped lay the groundwork for much of modern technologies. Although this has been most apparent for silicon-based electronics, the influence of point defects can be far greater in more ionic materials like the transition metal oxides. Here, defects are not merely dopants but can be used to create entirely new functionalities, and their charged nature can lead to the rapid and reversible formation of large-scale defect structures under an applied electric field. In resistive-switching memories, or memristive devices, electrically conducting channels comprised of oxygen vacancies either grow and propagate across the device or dissolve into the insulating matrix, thereby switching the memory state. Although this process is central to the operation of the device, a microscopic picture of how this occurs remains elusive, as oxygen vacancies are not easily imaged especially under working conditions. In this talk, we will present the development of a powerful X-ray technique capable of quantitatively imaging oxygen vacancy profiles *in situ*, exploiting both chemical and structural contrast mechanisms. Focusing on model heterostructures of $WO_x/SrTiO_3(001)$, we find that memristive behaviour originates from a local phase transition as the oxygen concentration is modulated above and below a threshold stoichiometry, which is quantitatively observed by X-ray imaging and substantiated by *ab initio*-based simulations. By engineering electrode configuration, furthermore, we can guide deterministic electroforming of conduction channel in memristive devices, as observed by X-ray multimodal imaging and confirmed by simulations. Moreover, this deterministic formation of conduction channel also helps to decrease the required power for electroforming, providing efficient way for thermal management and design of low power electronics. Reversible migration of oxygen vacancies is observed in early stage of pre-electroforming process, even when the I-V curve is linear. Our work shows emerging routes to control the otherwise random electroforming process in memristive devices, paving the way to develop reliable and reproducible resistive switching memories and synaptic electronics for neuromorphic computing.

9:40 AM NN05

High Energy Density Electrostatic Capacitors with Polymer-Like Hydrogenated Carbon (PLCH) Dielectric Films Sepehrdad Akbari and Marilyn Freeman; Clarkson University, Potsdam, New York, United States.

Much interest has been focused on developing and refining more efficient energy storage devices to enable smaller, lighter and cheaper energy storage for many applications. The demand to decrease the size and weight of high energy density capacitors have led to the synthesis of thin insulator materials with very high dielectric strength. Pure diamond exhibits the highest dielectric strength of known natural materials - more than 10 MV/cm. However, diamond is expensive and hard to synthesize. Diamond-like carbon (DLC) is a metastable form of carbon, comprising both sp^3 and sp^2 carbon-carbon bonds. DLC is inexpensive to make and easy to deposit on many different surfaces. DLC typically has an amorphous microstructure

and often contains some proportion of hydrogenated carbon bonds. DLC films containing 30% - 70% hydrogenated carbon bonds are called amorphous hydrogenated carbon (a-C:H) films. These a-C:H films exhibit different electrical characteristics depending on the relative concentrations of sp^3 , sp^2 and H bonds. a-C:H films deposited by RFCVD at low bias voltages are called polymer-like hydrogenated carbon (PLCH) films. PLCH films have the highest hydrogen (H) content (40-60 at. %) among different types of a-C:H films. PLCH films have the most significant band gap, lowest film density and lowest internal stresses among all the different types of DLC films, which makes it an excellent candidate dielectric to obtain breakdown strength close to diamond. Since the energy density of a capacitor is directly proportional to the applied voltage (V) squared (V^2) and inversely proportional to the dielectric thickness, it is reasonable to believe that a high energy density film capacitor made with a very thin, high breakdown strength dielectric material. The hypothesis for this work is that PLCH dielectric films will enable fabrication of very high energy density capacitors. In the present work, PLCH films were deposited by RFCVD. The PLCH films were deposited at different bias voltages and methane/argon compositions to investigate the electrical characteristic at various deposition parameters. Raman spectrometry was used to reveal the hydrogen, sp^2 carbons and sp^3 carbon content. Using these PLCH films as the dielectric material and aluminum electrodes we fabricated many high energy density capacitors with a diameter of 6 mm. Results: a) DLC films fabricated exhibited a dielectric strength of 7.2 MV/cm (near diamond). b) Best DLC deposition parameters for highest breakdown strength were 100 V bias and 50 at. % methane. c) There is a strong correlation between the DLC deposition parameters and the chemical and electrical characteristics of the dielectric films. d) Raman characterization at a wavelength of 325 nm resulted in less background noise (PL) for hydrogenated DLC than 514 nm.

10:00 AM REFRESHMENT BREAK

10:20 AM NN06

(Student) Tunable Charge Transfer and Built-In Electric Fields Across a Semiconductor-Crystalline Oxide Heterojunction Zheng Hui Lim¹, Nicholas F. Quackenbush³, Aubrey Penn², Matthew Chrysler¹, Mark Bowden⁴, Zihua Zhu⁴, James M. Ablett⁵, Tien-Lin Lee⁶, James LeBeau², Joseph C. Woicik³, Peter V. Sushko⁷, Scott A. Chambers⁷ and Joseph Ngai¹; ¹Physics, The University of Texas at Arlington, Arlington, Texas, United States; ²Department of Materials Science & Engineering, North Carolina State University, Raleigh, North Carolina, United States; ³Materials Measurement Science Division, National Institute of Standards and Technology, Gaithersburg, Maryland, United States; ⁴Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, Washington, United States; ⁵Synchrotron SOLEIL, Saint-Aubin, France; ⁶Diamond Light Source Ltd, Didcot, United Kingdom; ⁷Physical Sciences Division, Pacific Northwest National Laboratory, Richland, Washington, United States.

Charge transfer across heterojunctions between semiconducting materials and the built-in electric fields that arise therefrom underpin the functionality of virtually all semiconductor devices, ranging from transistors to light-emitting diodes. Advances in thin-film epitaxy now enable charge transfer and built-in electric fields to be explored in heterojunctions comprised of semiconductors and single-crystalline oxides. Such hybrid heterojunctions could uniquely address emerging challenges in energy harvesting and information technology, given the complementary combination of covalent and ionic materials. Here, we present tunable charge transfer and built-in fields in a heterojunction comprised of Si and the archetype oxide semiconductor $SrTiO_3$, in which the carrier density of the latter is modulated via Nb substitution x , i.e., $SrNb_xTi_{1-x}O_{3-\delta}$. Non-monotonic anomalies in the sheet resistance of the $SrNb_xTi_{1-x}O_{3-\delta}/Si$ heterojunctions are observed, accompanied by crossovers in sign of the Hall resistance, indicating the formation of a hole gas in the Si. Hard x-ray photoelectron spectroscopy measurements reveal unprecedented asymmetric features in both the $SrNb_xTi_{1-x}O_{3-\delta}$ and Si core-level spectra that we show arise from built-in fields. Analysis of the asymmetric core-level spectra enable band alignment and band bending to be mapped across the $SrNb_xTi_{1-x}O_{3-\delta}/Si$ heterojunction. The demonstration of tunable charge transfer, built-in fields and mapping of the latter lays the groundwork for the development of functional semiconductor-oxide heterojunctions that are coupled through charge transfer.

10:40 AM NN07

(Student) Molecular Beam Epitaxy Growth of LuFeO₃ on GaN Joseph Casamento¹, Megan Holtz¹, Phillip Dang¹, Debdeep Jena², Huili Xing¹ and Darrell Schlom¹; ¹Cornell University, Ithaca, New York, United States; ²Cornell University, Ithaca, New York, United States.

Traditional III-Nitride semiconductor materials GaN and AlN have shown excellent optoelectronic properties, but very little work has been done on the integration of multiferroic oxides on nitrides to enable epitaxial ferroelectric device platforms. Recent interest has been generated in novel device architectures whose materials allow for coupling between magnetic and electronic stimuli. In this work, we report the first epitaxial growth studies of single crystalline LuFeO₃ on GaN (0001) surfaces. Lu and Fe metals were supplied using Knudsen effusion cells at base temperatures of 1350C and 1157C, respectively. Lu and Fe were continuously co-deposited on the GaN surface. Oxygen was supplied using 10% distilled ozone at a chamber pressure of 1x10⁻⁶ torr. Growth temperatures ranged from 700C to 900C, measured by a thermocouple. In-situ reflection high energy electron diffraction (RHEED) was used to assess surface evolution during growth. Phase purity and epitaxial relationship was assessed using X-ray Diffraction (XRD). Oxidation states and bonding environments of Lu and Fe were confirmed using X-ray Photoelectron Spectroscopy (XPS). Films with a surface roughness of less than 1.8 nm were confirmed by atomic force microscopy (AFM). Magnetic properties of the films were assessed using vibrating sample magnetometry (VSM). Post growth XRD measurements indicate the formation of phase pure hexagonal LuFeO₃ with peak positions consistent with prior literature reports. ^[1] In-situ RHEED monitoring along the <110> azimuth indicate LuFeO₃ grows epitaxially on GaN for thicknesses ranging from 25-150 nm and at growth temperatures between 700C and 900C. AFM images indicate sample surfaces are smooth in the same thickness range. VSM measurements show magnetic hysteresis loops at 50K, which is smaller than the reported magnetic transition temperature of 147K. ^[2] This may be due to measurement sensitivity and the low saturation magnetization (~0.02 μ_B/Fe) of LuFeO₃. Too high of an Fe flux relative to Lu roughens the surface and leads to regions in AFM whose composition is potentially Fe₃O₄. No evidence of phase separation or change in epitaxial relationship is observed with RHEED even in films that have excess iron. LuFeO₃ grown on YSZ (111) substrates is electrically insulating in hall measurements and optical absorption measurements show a weak band edge near 2 eV. Future work will involve the growth optimization, structural and electrical characterization of LuFeO₃ on two-dimensional electron gas (2DEG) structures to enable epitaxial ferroelectric applications such as negative capacitance field-effect transistors (NCFETs). [1] Mundy, J et al. *Nature*. **537**, 523-527. (2016) [2] Diessler, S et al. *Phys. Rev. Lett.* **114**, 217602. (2015).

11:00 AM NN08

Epitaxial Gate Oxides for Enhancement Mode GaN and AlGaIn Power Electronics Peter Dickens¹, Brianna Klein¹, Andrew M. Armstrong², Stanley Atcity¹, Andrew Allerman¹, Brendan Gunning¹, Albert Baca¹, Erica Douglas¹, Michael Brumbach¹, Rebecca Chow¹, Jill Wheeler¹, Jon Ihlefeld³ and Elizabeth Paisley¹; ¹Sandia National Laboratories, Albuquerque, New Mexico, United States; ²Sandia National Laboratories, Albuquerque, New Mexico, United States; ³University of Virginia, Charlottesville, Virginia, United States.

The development of wide-bandgap transistors for next generation power electronics is promising owing to their higher breakdown field and saturated electron velocity over traditional silicon insulated-gate bipolar transistors. Currently however, the improvement of wide-bandgap transistors is limited by non-ideal gate performance leading to normally-on operation, high leakage currents, and frequency dispersion. Gate oxide introduction may improve the performance, but many oxides are insufficient for wide-bandgap transistors due to low conduction band offsets and/or poor chemical and structural interface quality. In this work, we will present on the development of MgCaO gate insulators for GaN and AlGaIn transistors. We will show that the oxide has sufficiently large conduction band offsets for GaN and AlN (E_c greater than 1 eV for both). We will also show that we can tailor this band offset at the nitride|oxide interfaces through the presence of subsurface oxygen in the semiconductor. Finally, we will demonstrate an enhancement-mode transistor performance on 85% Al-content AlGaIn by utilizing thin MgO gate dielectrics with a fluorine interface treatment prior to oxide growth. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. SAND2019-1384A

11:20 AM NN09

Structural and Electrical Properties of Epitaxial MgO on 4H-SiC Peter Dickens¹, Michael Brumbach¹, Rebecca Chow¹, Stanley Atcity¹, Jon Ihlefeld² and Elizabeth Paisley¹; ¹Sandia National Laboratories, Albuquerque, New Mexico, United States; ²University of Virginia, Charlottesville, Virginia, United States.

Due to the desire to design and operate power transistors at elevated temperatures, higher switching speeds, and higher voltages, wide-bandgap semiconductors are being thoroughly researched and developed for next generation power electronics. Among wide-bandgap semiconductors, SiC is positioned at the forefront owing to its manufacturability, high breakdown field, good thermal conductivity, and saturated electron velocity. However, current gate oxide performance can limit overall device performance and lead to normally-on operation, high leakage currents, and frequency dispersion. In this work, we will present our recent efforts in developing new high- k dielectrics for implementation with SiC. Gate oxide choices for SiC are limited due to low conduction band offsets and/or poor chemical and structural quality at the oxide|carbide interface. However, we will demonstrate that epitaxial, lattice-matched alloys of MgO and CaO are prime candidates for SiC gate dielectrics. We will present on the optimization of MgO/MgCaO crystal quality and growth mode by both molecular beam epitaxy and pulsed laser deposition. We will also present data on capacitance-voltage and leakage current data on 4H-SiC. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. SAND2019-1456 A

11:40 AM NN10

(LATE NEWS, Student) An Electrically Detected Magnetic Resonance Investigation of Negative Bias Temperature Instability in Tri-Gate Metal Oxide Semiconductor Field Effect Transistors Kenneth J. Myers¹, Patrick M. Lenahan¹, Brad Bittel² and Inanc Meric²; ¹The Pennsylvania State University, University Park, Pennsylvania, United States; ²Intel Corporation, Portland, Oregon, United States.

Recently, multi-gated metal oxide silicon field effect transistors (MOSFETs) have become the dominant devices in high-performance CMOS integrated circuits. Tri-gate field effect transistors (FETs) greatly reduce short channel effects, allowing improved scalability [1]. A knowledge of the mechanisms in device degradation in these transistors is key when considering overall lifetime and performance. Unfortunately, there is little literature dealing with the atomic scale defects involved in the understanding of negative bias temperature instability (NBTI) phenomena in such devices. In this study, we investigate the defects related to NBTI at the Si/dielectric interface and within the dielectric via electrically detected magnetic resonance (EDMR). We study NBTI on tri-gate FETs. These devices contain a Si fin and substrate with 40 μm channel length, 41 & 300 nm channel width, and 40 nm fin height surrounded by a high-k metal gate. The fins are structured with <110> sidewalls and a <100> top plane. Each set of contacts contains either 66 (41 nm width) or 7 (300 nm width) fins wired in parallel with the substrate electrically connected to each fin. Additional information on similar devices can be found elsewhere [1]. NBTI stressing of these devices has been carried out by biasing the gate at -1.9 V at various temperatures. In doing so, defect density at the Si/dielectric interface, as well as within the dielectric, has been increased and has been detected through EDMR. Pre-NBT-stressed devices exhibited no observable EDMR spectra with defect density is below detectable limits. Our EDMR measurements utilized a home-built EDMR spectrometer. The X-band (~9.6 GHz) spectrometer includes a 4-inch Lakeshore electromagnet with a Micro-Now microwave bridge and a TE₁₀₂ cavity. A Stanford Research Systems Low-Noise Current Preamplifier was utilized for both device biasing and current measurement. A Rigol DG1022 arbitrary waveform generator was used in the spin-dependent charge pumping (SDCP) measurements. The detection utilized a home-built virtual lock-in amplifier. Measurements were conducted at room temperature. The results from this experiment are interesting in that they yield results somewhat different from a previous study on NBTI in planar Si/SiO₂ MOSFETs [2]. In that study, it was found that P_b centers, Si dangling bonds at the Si/SiO₂ interface, are the dominant defect in NBT-stressed Si/SiO₂ MOSFETs. The g tensor components of various P_b centers range from 2.0012 to 2.0083. In the spectra observed thus far in the tri-gate devices, we find a zero-crossing g of 2.0049 ± 0.0003 for a somewhat asymmetric, otherwise featureless, 10 Gauss-wide line. The range of g tensor components and signal width in this spectrum is qualitatively consistent with that observed by Campbell *et al.* [2], suggesting the involvement of P_b-like centers in NBTI damage. For planar devices, the spectrum changes with a change in orientation of the sample

with respect to magnetic field. In the tri-gate FETs, we observe no such variation, indicating that the NBTI mechanism in fin-based devices differs from that in planar devices. Additionally, the Elliot curves pre- and post-stress exhibit only a small increase in defect density, with a large shift in peak location. This result indicates that the NBTI stress causes a significant formation of positive charge within the dielectric and, more importantly, suggests that the interface traps present before stressing are mostly not P_b -like. [1] C. Auth *et al.*, "A 22nm High Performance and Low-Power CMOS Technology Featuring Fully-Depleted Tri-Gate Transistors, Self-Aligned Contacts and High Density MIM Capacitors," *2012 Symp. VLSI Technol.*, no. 2003, pp. 131–132, Jun. 2012. [2] J. P. Campbell, P. M. Lenahan, A. T. Krishnan, and S. Krishnan, "Observations of NBTI-Induced Atomic-Scale Defects," *IEEE Trans. Device Mater. Reliab.*, vol. 6, no. 2, pp. 117–122, Jun. 2006.

SESSION OO: Semiconductors, Metamaterials and Plasmonics
Session Chair: Stephanie Law
Friday Morning, June 28, 2019
Michigan League, 3rd Floor, Koessler

8:20 AM OO01

(Student) Short-Wave Infrared Plasma Wavelength in III-V Semiconductors Achieved via Embedding Lanthanide Monopnictide Nanoparticles into GaAs Yuejing Wang¹, Dongxia Wei², Stephanie Law³ and Joshua Zide³; ¹Materials Science and Engineering, University of Delaware, Newark, Delaware, United States; ²Material Science and Engineering, University of Delaware, Newark, Delaware, United States; ³University of Delaware, Newark, Delaware, United States.

We present the optical properties of ErAs:GaAs nanocomposite materials. Metallic and plasmonic materials are interesting for a wide range of applications including waveguiding, enhanced sensing, hyperbolic metamaterial components and so forth. Unfortunately, traditional metals like gold and silver cannot be used as plasmonic materials in the short-wave infrared due to their large and negative permittivities at these wavelengths. Heavily-doped (n-type) III-V semiconductors have been demonstrated as excellent alternative plasmonic materials, but so far their shortest plasma wavelengths are limited to $\sim 5\mu\text{m}$ mainly due to Fermi level stabilization at these high doping densities. For this work, we investigated the optical properties of a new composite III-V material and demonstrated the shortest plasma wavelength in III-V based materials so far. We used molecular beam epitaxy (MBE) growth and a co-deposition method to grow films of high concentrations of ErAs nanoparticles (NPs) epitaxially incorporated into a GaAs matrix. The plasma wavelength of these nanocomposite films can be tuned across the $2.68\mu\text{m}$ – $6\mu\text{m}$ infrared window by controlling the incorporation amount of ErAs NPs. Reflection data from the ErAs:GaAs epilayers obtained using Fourier transform infrared spectroscopy (FTIR) is in good agreement with the simulations calculated using the Drude formalism. Interestingly, the growth conditions of these materials are less constrained than more conventional highly-doped semiconductors. ErAs:GaAs films grown at substrate temperatures ranging from 450°C to 600°C show comparable optical properties, though a slight growth temperature dependence was observed. The scattering rate decreases as the growth temperature increases due to better crystallinity and the formation of larger ErAs NPs at higher growth temperature, likely leading to longer electron mean free path. The plasma wavelength blueshifts gradually as the film growth temperature increases until it reaches $2.68\mu\text{m}$, the shortest reported plasma wavelength in a III-V material. Further increases in growth temperature and increases in ErAs concentration do not shift the plasma wavelength further, indicating that the optical properties are likely limited by the ErAs bulk properties such as permittivity and electron effective mass. The plasmon response tunability of this material as well as the ease of epitaxial integration with other III-V semiconductor optoelectronic structures shows great potential for creation of a new type of metamaterials as well as other novel nanophotonic applications.

8:40 AM OO02

(Student) Tunable InGaSb Emitters Coupled with InAs:Si Through Molecular Beam Epitaxy Andrew F. Briggs¹, David Silva¹, Leland J. Nordin², Daniel Wasserman³ and Seth Bank⁴; ¹Electrical and Computer Engineering, University of Texas at Austin, Austin, Texas, United States; ²ECE, The University of Texas at Austin, Austin, Texas, United States; ³University of Texas at Austin, Austin, Texas, United States; ⁴The University of Texas at Austin, Austin, Texas, United States.

Control of quantum emitters in the mid-infrared (mid-IR) is important for understanding light-matter interactions in that region. Quantum emitters embedded in an engineered metamaterial cavity, such as those built from epsilon-near-zero (ENZ) materials, could offer new avenues for controlling and enhancing light-matter interactions [1]. Unfortunately, spectrally aligning quantum emitters with ENZ materials has proven difficult particularly in an all-epitaxial platform, which is essential for future practical applications, particularly those that require direct electrical injection. Here, we report the monolithic integration of tunable InGaSb quantum dot emitters and ENZ silicon-doped InAs (InAs:Si) grown in a single molecular beam epitaxial growth step. Previous work has demonstrated mid-IR emission from InGaSb/InAs nanostructures [2] as well as the integration of ENZ materials with these same emitters as a platform to enhance and control light matter interaction on InAs substrates [3]. Here we demonstrate tunability of this material system. Since the InAs:Si plasmonic component and the InGaSb component are separate epitaxial structures, they can be independently tuned via the doping density and composition, respectively. In order to improve emission efficiency of the type-II InGaSb/InAs nanostructures, we introduced lattice-matched AlAsSb electron blocking layers and cascaded multiple InGaSb emitter layers to study their effects on the photoluminescence emission efficiency. We also investigated Sb overpressure and growth rate in order to improve InGaSb dot morphology, characterized by atomic force microscopy. By refining the InGaSb emitter growth, we achieved room temperature $5\mu\text{m}$ emission. To vary the amount of interaction the ENZ material has with the InGaSb emitters we can vary the InAs:Si doping concentration. Previous studies have shown that high growth rate, low substrate temperature and surfactant mediated growth allow for InAs:Si to be grown with a plasma wavelength as low as $4.7\mu\text{m}$ while still remaining epitaxially smooth [4]. Samples were grown with varying plasma wavelengths to study the interaction between ENZ material and emitters as either spectral overlap is increased. In photoluminescence measurements we see a shift in each sample's emission to a longer wavelength as the plasma wavelength of the ENZ material is brought closer to the emission of the InGaSb. Further optical studies that characterize the plasmonic interactions of these materials, such as polarization and angle dependent photoluminescence, will be presented at the conference. [1] I. Liberal, *et al.*, *Nature Photonics*, vol. 11, no. 4, 2017. [2] L. Yu, *et al.*, *Journal of Vacuum Science & Technology B*, vol. 35, no. 2, 2016. [3] A.F. Briggs *et al.*, *60th Electronic Materials Conf.*, June 2018 [4] S.J. Maddox *et al.*, *56th Electronic Materials Conf.*, June 2014.

9:00 AM OO03

(Student) Interrogating Hyperbolic Metamaterials with Integrated Intersubband Transitions Using Thermal Emission Spectroscopy Kun Li¹, Evan Simmons², Andrew F. Briggs³, Seth Bank⁴, Evgenii Narimanov⁵, Viktor Podolskiy² and Daniel Wasserman⁶; ¹Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas, United States; ²Department of Physics and Applied Physics, University of Massachusetts Lowell, Lowell, Massachusetts, United States; ³Electrical and Computer Engineering, University of Texas at Austin, Austin, Texas, United States; ⁴The University of Texas at Austin, Austin, Texas, United States; ⁵School of Electrical and Computer Engineering, Purdue University, West Lafayette, Indiana, United States; ⁶University of Texas at Austin, Austin, Texas, United States.

Heavily doped semiconductor materials provide a flexible material system for the investigation and demonstration of mid-IR plasmonic and metamaterial structures. The first such demonstration was the use of heavily-doped InGaAs/undoped AlInAs layers, lattice-matched to InP, to form hyperbolic metamaterials (HMMs), unique planar metamaterials with highly anisotropic permittivity capable of negative refraction at mid-IR wavelengths [1]. The InGaAs/AlInAs is also the dominant material system for quantum cascade lasers (QCLs) operating across a wide range of the mid-IR. The QCL, now the semiconductor laser of choice for most mid-IR applications, utilizes active regions consisting complex heterostructures, with quantum-engineered intersubband transitions, to generate mid-IR light. The ability to engineer both optical transitions and metamaterial response in the same material system provides a unique tool kit for engineering and investigating light matter interaction in designer materials. Both the intersubband transitions of the QCL and the negative

refraction of the HMM are observed for TM-polarized light only, which makes investigation of coupling between these phenomena difficult in high-index materials interrogated from the growth surface. Here we demonstrate that thermal emission spectroscopy can offer a potentially powerful tool for polarization dependent characterization of complex metamaterials in the infrared. Four HMM samples (4 μm total thickness) consisting of n^+ InGaAs/AlInAs layers were grown on InP substrates with varying InGaAs/AlInAs thicknesses (80 nm, 33 nm, 9.5 nm, and 5.5 nm) by molecular beam epitaxy. The ground-to-excited state intersubband transition energies in these samples were designed to include energies both much greater and much less than the frequency range of HMM behavior, as well as energies positioned in the center of the HMM bandwidth. Samples were characterized by temperature, polarization, and angle-dependent reflection and transmission spectroscopy, as well as thermal emission spectroscopy. The transmission and reflection measurement setup is shown in Fig.1(a). The thermal emission measurement setup is shown in Fig.1(b), and is similar to a previously demonstrated approach used to measure intersubband transitions in semiconductor quantum wells [2]. The samples are heated to 100 °C and polarized thermal emission is measured using an FTIR spectrometer. An InP substrate covered with black paint was chosen as the control sample (mimicking a perfect blackbody of the same geometry). A pinhole aperture is used to block the ambient thermal energy and a wire-grid polarizer is used to differentiate the TM and TE emission. Emission is modulated by an optical chopper and the FTIR detector signal is demodulated by a lock-in amplifier for amplitude modulation step-scan measurements. Fig.2 shows the measured TM and TE emission spectra of each of the four samples. Peaks associated with intersubband transitions in the multi-quantum well system are observed in the TM-polarized thermal emission. We will discuss the origin of these emission peaks, and provide modelling results showing agreement with our experimental data. In summary, we demonstrate the utility of thermal emission spectroscopy as a tool for investigating light-matter interaction in all-semiconductor infrared metamaterials with integrated designed optical transitions. [1] A.J. Hoffman, L. Alekseyev, S.S. Howard, K.J. Franz, D. Wasserman, V.A. Podolskiy, E.E. Narimanov, D.L. Sivco, and C. Gmachl, *Nature Materials*, 6, 946 (2007) [2] De Zoysa, M., T. Asano, T. Inoue, K. Mochizuki, and S. Noda, *J. Appl. Phys.*, 118, 103101 (2015)

9:20 AM OO04

Thermal Emission of Si:InAs/AlSb Hyperbolic Metamaterial Patrick R. Sohr¹, Chi Ian Sohr² and Stephanie Law²; ¹Material Science and Engineering, University of Delaware, Royersford, Pennsylvania, United States; ²University of Delaware, Newark, Delaware, United States.

Super-Planckian thermal emission refers to emission from a material that exceeds the blackbody limit. Within the past two decades or so, there has been research on the transfer of thermal radiation between two materials that are separated by only a short distance (within the near-field). These findings indicate thermal transport greater than that predicted by Stefan-Boltzmann's Law is a result of tunneling of evanescent waves between the media [1]. While this is of fundamental scientific interest, the practical applications of such designs are limited due to the small spacing requirements. It would be beneficial to observe super-Planckian thermal emission in the far-field. While there have been a few papers that report observing this effect in the far-field, the topic is still fairly contested. It has been suggested that an anisotropic material, such as a hyperbolic metamaterial (HMM), could exhibit super-Planckian thermal emission in the far-field [2-4]. Hyperbolic metamaterials (HMMs) are artificial materials composed of subwavelength metal and dielectric structures. They are extremely anisotropic with the permittivities of opposite signs in the parallel and perpendicular directions. This results in an open isofrequency surface that can support theoretically infinitely large wavevectors. The access to large wavevectors also results in a large photonic density of states (PDOS), which make HMMs of great interest for thermal emission. Traditional artificial HMMs use noble metals like gold or silver for the metallic layer, and silicon for the dielectric layers. Although these materials work well in the visible spectral range, they are not appropriate for the mid- to long-wave infrared. It is possible to create an infrared HMM using alternating layers of doped and undoped semiconductors. In this case, the doped semiconductor acts as the metallic layer while the undoped semiconductor acts as the dielectric layer. Specifically, a Si:InAs/AlSb HMM has been shown to act as a good, low-loss infrared HMM [5]. The high wavevector modes comprising the large PDOS in the HMMs are called volume plasmon polaritons (VPPs). VPPs result from the coupling of surface plasmon polaritons at the interfaces between the metal and dielectric layers in the HMM. We previously demonstrated highly efficient coupling from free space into VPP modes using gold grating couplers. To look for super-Planckian thermal emission, we heated our grating-patterned HMM samples to 185°C and measured polarized and angle-dependent thermal emission. We observed peaks in

the thermal emission spectrum due to outcoupling from the VPP modes into free space. This emission was found to be almost completely angle-independent up to 50 degrees. Despite the enhanced emission, super-Planckian emission was not observed. This is the first report of thermal emission leveraging VPP modes, which could be used as a component of engineered thermal emission devices. [1] J. B. Pendry, "Radiative exchange of heat between nanostructures," *J. Phys.* 11, 6621-6633 (1999). [2] Y. Guo, C. L. Cortes, S. Molesky, and Z. Jacob, *Appl. Phys. Lett.* 101, 131106 (2012). [3] S. A. Biehs, M. Tschikin, R. Messina, and P. Ben-Abdallah, "Super-Planckian near-field thermal emission with phonon-polaritonic hyperbolic metamaterials," *Appl. Phys. Lett.* 102, 131106 (2013). [4] I. S. Nefedov and L. A. Melnikov, "Super-Planckian far-zone thermal emission from asymmetric hyperbolic metamaterials," *Appl. Phys. Lett.* 105, 161902 (2014). [5] P. Sohr, D. Wei, S. Tomasulo, M. K. Yakes, and S. Law, "Simultaneous large mode index and high quality factor in infrared hyperbolic metamaterials," *ACS Photonics* 5, 10, 4003-4008 (2018).

9:40 AM OO05

Investigation of Microstructure and Composition of SiGeSn Metamorphic Buffer for GeSn Based Optoelectronics Nadeemullah Mahadik, Glenn G. Jernigan, Mark E. Twigg, Chaffra A. Affouda, Jill A. Nolde and Edward H. Aifer; Naval Research Laboratory, Washington, District of Columbia, United States.

GeSn based optoelectronic devices have the potential for full Si integration to fabricate monolithic lasers, on-chip optical communications, and other photonic applications [1,2]. Silicon, germanium, and their alloys have indirect bandgaps making them inefficient light sources. Theory predicts that an unstrained alloy of GeSn with greater than 8% Sn should have a direct bandgap [3]. However, this alloy has a mismatch of ~4% from Ge and ~6.7% from Si resulting in compressive strain when grown upon these substrates. Additionally, the miscibility of Sn in Ge at equilibrium conditions is less than 2%Sn [4]. Hence, non-equilibrium growth techniques are necessary to produce GeSn alloys. GeSn epilayers with up to 15% Sn have been successfully grown using chemical vapor deposition (CVD) and using molecular beam epitaxy (MBE) [5-7]. However, these films were less than 500 nm in thickness, were under compressive stress, and did not show a direct bandgap. To accommodate the lattice mismatch between a Si or Ge substrate and the GeSn alloy, we have adopted a metamorphic graded buffer approach that is grown on Si (100) using various Si, Ge, and Sn compositions to create a relaxed buffer layer. The relaxed buffer layer also serves to reduce the dislocations in the final GeSn layer by forming misfit dislocations inside the buffer. The metamorphic buffer was grown using MBE. Initially, the Si and Ge compositions were graded to achieve a $\text{Ge}_{0.9}\text{Si}_{0.1}$ alloy. This is followed by grading the Sn in the ternary alloy up to 15% Sn to achieve a particular lattice parameter. Several growths were performed to achieve a final structure that is fully relaxed. After each growth, high resolution x-ray reciprocal space maps (RSM) were obtained using a Rigaku Smartlab diffractometer equipped with a high intensity 9kW Cu rotating anode, high flux collimating mirror, a 4 bounce Ge (220) channel cut monochromator for k_{α} radiation, a vertical goniometer, and a high speed 250 channel linear detector. Using this setup, the RSMs were obtained for the entire reciprocal space of the (004) Bragg reflection from Si to $\text{Ge}_{0.88}\text{Sn}_{0.12}$ in about 2 hours. The x-ray RSMs show that the initial layers of the SiGe were only slightly relaxing until the Si composition reached 30%, after which the alloy fully relaxes to a final composition of 12.5% Si. The initial incorporation of Sn into the alloy is almost fully relaxed within 3-4 layers and reaches a Sn composition of 12%. From this point, we have grown GeSn layers up to 1 μm thick. From the Bragg peak width of the thick GeSn layers, which was ~400 arcsecs, we have demonstrated high crystalline quality of the GeSn epilayer. Initial optical absorption studies indicate that the 12% Sn alloy had an absorption at ~3.4 μm . However, we have not yet been able to measure photoluminescence spectra from the sample likely due to presence of defects. Further epilayers with optimized growth and varying alloy compositions have been grown and are being characterized. The details of the metamorphic buffer layer growths, the RSMs from various growth attempts, a few representative TEM, and optical investigations will be presented in this paper. References [1] R. Soref, *Nat. Photonics* 4, 495 (2010). [2] X. Wang et al., and J. Liu, *J. Semicond.* 39, 061001 (2018). [3] S. Gupta, et al., *Proceedings of the IEEE International Electron Devices Meeting* p. 398 (2011). [4] C. D. Thurmond, et al., *J. Chem. Phys.* 25, 799 (1956). [5] J. Margetis, et al., *Appl. Phys. Lett.*, 113, 221104 (2018). [6] C. Clausen et al., *Semicond. Sci. Technol.* 33, 124017 (2018). [7] S. Wirths, et al., *Nat. Photonics*, 9, 88 (2015).

10:00 AM REFRESHMENT BREAK

SESSION PP: III-Nitride UV Devices and Materials
Session Chair: Russell Dupuis
Friday Morning, June 28, 2019
Rackham Building, 4th Floor, Amphitheatre

8:20 AM PP01

(Student) Growth and Characterization of AlGa_xN p-i-n-i-n Separate Absorption and Multiplication Ultraviolet Avalanche Photodiodes Marzieh Bakhtiary-Noodeh¹, Mi-Hee Ji², Hoon Jeong², Eliza Gazda³, A. Nepomuk Otte³, Shyh-Chiang Shen², Theeradetch Detchprohm² and Russell Dupuis^{1,2}; ¹School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States; ²Center for Compound Semiconductors and School of Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, Georgia, Georgia, United States; ³School of Physics & Center for Relativistic Astrophysics, Georgia Institute of Technology, Atlanta, Georgia, Georgia, United States.

Aluminum gallium nitride (AlGa_xN) has a wide bandgap energy ranging from 3.5 to 6.2 eV, which makes it useful for ultraviolet (UV) optical detectors. AlGa_xN avalanche photodiodes (APDs), a special subgroup of optical detectors, have a high sensitivity in the solar-blind region. Their capability of operation in the solar-blind spectral region, high detection sensitivity, high breakdown field, high optical gain, low dark current, with structural, chemical and thermal stability, makes them an appropriate choice for operation in a harsh environment as well. Adjustable bandgap energies in AlGa_xN APDs provides controllable wavelength detection. Back-illuminated separate absorption and multiplication (SAM) APD structures have been studied for multiplication noise reduction, gain intensification, with the elimination of light blocking issues and higher hole ionization coefficient (compared to front illumination). The main challenge for wide-bandgap materials is the limited free-carrier concentration, especially for p-doped layers, which is essential for solar-blind APD operation. Back-illuminated AlGa_xN UV-APDs need to be grown on AlN templates or other UV-transparent substrates to get a maximum UV light photoresponse. Some restrictions on available UV-transparent substrates threaten the feasibility of the development of AlGa_xN APDs. AlN/sapphire templates provide better optical transparency down to 210 nm compared to currently available AlN substrates that absorb at 265 nm. However, other issues such as lattice mismatch, different thermal expansion coefficients between the layers and the substrate, and strain-induced defects act as a source of leakage current and result in the degradation of the device performance. In this study, the solar-blind back-illuminated Al_xGa_{1-x}N p-i-n-i-n SAM-APD epitaxial layers were grown by a metalorganic chemical vapor deposition (MOCVD) with a target cut-off wavelength of 250 nm at x=0.65. X-ray diffraction (XRD) was used as an analytical technique for the characterization of the quality of the crystalline structure of AlN/sapphire template and composition confirmation of Al_xGa_{1-x}N layers. Hall-effect characterization was used for the measurement of the electrical properties of the doped layers including the free-carrier concentration, resistivity, etc. Hall samples having 1×1 cm² size were prepared and after chemical preparation, metal deposition of V/Al/Ti/Au and Ni/Ag/Ni/Au used as contact points for n- and p-type doped layers, respectively. The Al_xGa_{1-x}N epitaxial layers were grown on AlN/c-plane sapphire templates, which include AlN/AlGa_xN short-period superlattice layers (SPSLs), followed by a 0.4 μm thick n-Al_{0.71}Ga_{0.29}N layer (n~8×10¹⁸cm⁻³), 0.24 μm thick u-Al_{0.65}Ga_{0.35}N layer as an absorption layer, 0.03 μm thick n-Al_{0.595}Ga_{0.405}N layer as a launcher layer (n~8×10¹⁸cm⁻³), 0.17 μm thick u-Al_{0.595}Ga_{0.405}N layer as a multiplication layer, 0.1 μm thick p-Al_{0.37}Ga_{0.63}N layer (ρ~2.8 Ω cm), 0.04 μm thick graded p-Al_xGa_{1-x}N (x=0.37->0) layer, 0.02 μm thick p⁺-Ga_{0.99}N layer as a cap layer. The higher resistivity of the p-AlGa_xN layers in this work in comparison with p-GaN layers in the previous studies may be caused by a higher activation energy of Mg at higher Al composition. The surface morphology and the corresponding root-mean-square (RMS) of the Al_xGa_{1-x}N p-i-n-i-n UV-APD epitaxial structure grown on AlN/sapphire template were studied by atomic force microscopy (AFM). The RMS value of 1×1 μm² and 5×5 μm² scan sizes are 0.25 nm and 4.98 nm respectively. All of the epitaxial layers have been precisely grown and doped to get the best properties. The details of growth, characterization, and fabrication processes, as well as preliminary device data, will be discussed later in the conference.

8:40 AM PP02

(Student) Record High Zero-Bias External Quantum Efficiency of 88% for Al_{0.40}Ga_{0.60}N-Based p-i-n UV Detectors Anisha Kalra¹, Shashwat Rathkaniwar², Rangarajan Muralidharan¹, Srinivasan Raghavan¹ and Digbijoy N. Nath¹; ¹Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India; ²Centre for Nano Science and Engineering, Indian Institute of Science, Bangalore, India, Bangalore, India.

In this work, we report on record high zero-bias external quantum efficiency (EQE) of 88% for back-illuminated Al_{0.40}Ga_{0.60}N p-i-n UV photodetectors operating at peak detection wavelength of 290 nm. Zero-bias responsivity across the detectors measured 202 mA/W, which is the highest value reported for 290 nm solar-blind UV detectors realized on III-nitrides grown using Metal Organic Chemical Vapor Deposition (MOCVD) on any substrate. After accounting for Fresnel losses at the different interfaces in the growth stack, the 88% EQE translates to an internal quantum efficiency (IQE) of 99.2%. Both, the light-to-dark current ratio and UV-to-visible rejection ratio for the detectors exceeded six-orders of magnitude, one of the highest values reported for any UV detector. The detectivity (D*) was estimated to be 3 x 10¹⁴ cmHz^{1/2}W⁻¹. The fabricated detectors exhibited a ten-orders of magnitude rectification, a low reverse leakage current density of 1 nA/cm² at 10 V and supported breakdown voltages exceeding 5 MV/cm. The transient characteristics of the detectors showed no signature of persistent photoconductivity and the rise and fall times measured < 13 ms (limit of the measurement setup). These high-performance parameters were attained through an improved crystalline quality of the absorbing AlGa_xN epi-layer, achieved using an optimized two-temperature step AlN and AlN/AlGa_xN superlattices-based buffer for the growth of the active detector epi-stack as well as through improved contacts to the p- and n-AlGa_xN layers. This is also the first report wherein a polarization-graded p-AlGa_xN layer is utilized as the p-contact layer to enhance the carrier collection efficiency. Direct, wide and tunable energy gap of AlGa_xN can be utilized for realization of photodetectors operating in the UV regime of the electromagnetic spectrum. A finite electric field in the intrinsic absorber region and a vertical device topology makes photodetectors with a p-i-n geometry an attractive candidate for self-powered UV sensors. In this work, we utilized a simple growth technique involving a 7 nm nominally thick low temperature AlN nucleation layer (LT-AlN NL) grown at 800 °C, to obtain an optimal nucleation density on the growth surface, followed by a 500 nm high temperature AlN grown at 1100 °C and 20-periods of dislocation-filtering AlN/Al_{0.45}Ga_{0.55}N superlattices (SLs). This was then used as the buffer for the growth of the active detector epi-stack, consisting of a 500 nm thick n-Al_{0.45}Ga_{0.55}N layer, a 200 nm Al_{0.40}Ga_{0.60}N absorber layer and 200 nm p-Al_xGa_{1-x}N layer in which the Al-mole fraction of AlGa_xN was linearly graded (LG) from 0.45 to 0, to achieve polarization-induced hole doping. While utilization of the optimized buffer helped achieve high crystalline quality AlGa_xN epi-layers, use of the LG p-AlGa_xN layer and an optimized n-AlGa_xN layer helped achieve low-resistance contacts. This ultimately led to the development of large-area detectors (0.1 mm²) exhibiting a high zero-bias responsivity of 202 mA/W (88% EQE) under back-illumination which is the highest reported value for AlGa_xN epi-stacks grown using a relatively simple, cost-effective and scalable growth technique. The devices had a low reverse current density of 1 nA/cm², high forward current density of 120 A/cm² and a turn-on voltage of 4.9 V (estimated at 20 mA forward current). From the forward I-V characteristics, an ideality factor of 2.2, a series resistance of 28 ohms and shunt resistance of 3.2 x 10¹⁰ ohm were estimated. Finally, an attempt to correlate the detector performance parameters to the absorber layer crystalline quality was made a series of carefully designed epi-stacks and material, electrical and optical characterization across revealed that while screw dislocations introduce localized defect states contribute to reverse leakage current across the devices, edge dislocation were found to impact the responsivity, efficiency and hence, the temporal response of the detectors.

9:00 AM PP03

(Student) Al_xGa_{1-x}N (0≤x≤0.6) Homo Junction Tunnel Diodes Exhibiting Low Voltage Negative Differential Resistance—Progress towards Tunnel Contacts Compatible with Ultraviolet Optoelectronics Evan Clinton, Ehsan Vadiiee, Zachary Engel, Christopher M. Matthews and W. Alan Doolittle; Georgia Institute of Technology, Atlanta, Georgia, United States.

Al_xGa_{1-x}N (0<x<0.6) homo junction tunnel diodes are fabricated and demonstrate negative differential resistance (NDR) at ~1.4 V and ~2.4 V for GaN and Al_{0.19}Ga_{0.81}N respectively with high reverse bias current densities necessary for tandem series connected devices and tunnel contacts. NDR was found in the Al_xGa_{1-x}N p⁺/n⁺ diodes up to x=0.19 with

depressions but no NDR up to $x=0.42$. Tunnel junctions for the III-nitrides are heavily investigated to increase design freedom and realize tandem series connected devices, simplify fabrication with less metallization and lithography, and enable substantially better contact resistances to n-type material. In some applications, the use of heterojunction tunnel contacts introduces unwanted absorption and/or may introduce defects due to the inherent lattice mismatch. Thus, when possible, tunnel homojunctions are often preferred. Utilizing an n-type tunnel contact to a p-type layer is especially beneficial for high Al content Al_xGa_{1-x}N films where ohmic contacts to p-layers are difficult as well as hole activation and injection to active layers are problematic. Unfortunately, metal-organic chemical vapor deposition (MOCVD) grown films lack the doping abruptness necessary to form small depletion width low loss tunnel junctions and require activation anneals that limit buried p-type layers. Additionally, MOCVD grown and standard molecular beam epitaxy (MBE) grown films are limited in hole concentrations. The metal modulated epitaxy (MME) growth technique performed in an MBE system enables high hole concentrations for Al_xGa_{1-x}N and the abrupt interfaces required to form tunnel junctions without polarization engineered interlayers which can limit optoelectronic device performance. Furthermore, widening the bandgap energy from Al_xGa_{1-x}N for higher Al content tunnel contacts can allow for deep UV optoelectronics with less optical absorption loss. Metal modulated epitaxy considerations for Al_xGa_{1-x}N to limit phase separation are considered, and Mg and Si doping of Al_xGa_{1-x}N ($0 < x < 0.60$) materials is compared. We demonstrate Al_xGa_{1-x}N homojunction tunnel p+/n+ diodes and tunnel contacted n+/p+/i/n devices with silicon doped n-type layers exhibiting silicon concentrations of up to $5 \times 10^{20} \text{ cm}^{-3}$ and magnesium doped p-type layers with Mg concentrations above $7 \times 10^{20} \text{ cm}^{-3}$. Reverse bias tunneling is observed for all Al_xGa_{1-x}N devices and decreases with increasing Al content in the tunnel diodes as the bandgap increases. The highest silicon doped GaN tunnel contacted diode demonstrates a low $\sim 0.14 \text{ V}$ increase in turn-on voltage when compared to a p+/i/n control diode with a turn-on voltage of $\sim 2.9 \text{ V}$. A tunnel-contacted InGaN LED demonstrates improved current spreading and light output uniformity when compared to an LED with indium tin oxide (ITO). Additionally, a tunnel-contacted InGaN solar cell is presented and can circumvent the indium tin oxide fabrication complexity and allow high temperature operation. These results are promising for improving performance of a wide array of ultraviolet and visible wavelength III-nitride devices including light emitting diodes (LEDs), lasers, and solar cells.

9:20 AM PP04

(Student) High-Quality AlN and Al-Rich AlGa_N Epilayers Grown on Sapphire by High Temperature Molecular Beam Epitaxy David A. Laleyan¹, Eric T. Reid², Xianhe Liu², Ayush Pandey³, Mohammad Soltani⁶, Gianluigi Botton⁵ and Zetian Mi⁴; ¹Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ²Electrical and Computer Engineering, University of Michigan–Ann Arbor, Ann Arbor, Michigan, United States; ³Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Ann Arbor, Michigan, United States; ⁴Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ⁵McMaster University, Hamilton, Ontario, Canada; ⁶Raytheon BBN Technologies, Cambridge, Massachusetts, United States.

Al-rich AlGa_N, with Al compositions varying from $\sim 50\text{--}90\%$ are required for light emitting diodes (LEDs) and lasers operating in the mid and deep ultraviolet spectral range, solar-blind photodetectors, integrated UV photonics, and future high-power electronic devices. For many of these applications, it is essential that relatively thick AlGa_N layers ($>0.5 \mu\text{m}$) with atomically smooth surface and with a minimal level of defects and dislocations can be epitaxially grown on foreign lattice-mismatched substrates, which are lower cost, larger size and more widely available than bulk GaN or AlN substrates. To date, most studies on the epitaxy of Al(Ga)N have been performed by metal-organic chemical vapor deposition (MOCVD), which, however, suffers severely from unwanted impurity (e.g., carbon, oxygen) incorporation, poor current conduction, and poor control of the alloy composition. In this work, with the use of high temperature molecular beam epitaxy (MBE) (up to $1850 \text{ }^\circ\text{C}$), we have demonstrated superior quality AlN and Al-rich AlGa_N grown directly on sapphire. For an ultrathin ($\sim 0.1 \mu\text{m}$) AlN grown directly on sapphire, the (002) rocking curve peak full-width-half-maximum (FWHM) is <100 arcsec, which is significantly better than that reported previously by MOCVD for samples of comparable thicknesses. In this study, by employing a careful sequence of interruption-assisted epitaxy and in situ high-temperature annealing, many of the dislocations and stacking faults generated at the AlN/sapphire interface are reduced within the first 50 nm of growth as obtained from transmission electron microscopy (TEM) studies. 100-nm thick samples exhibit an atomically smooth surface and X-ray diffraction (XRD) (002) and (102) rocking curve peaks with full

widths at half maximum (FWHM) of less than 100 and 1300 arcsec, respectively. These are the narrowest linewidths reported using MBE, and overall for samples of comparable thickness. The band-edge photoluminescence (PL) emission is twice as strong as commercial AlN epitaxial templates that are over 10 times thicker, without the presence of defect-related emissions. With increasing thicknesses, the (002) and (102) rocking curve peaks have FWHM <20 and ~ 700 arcsec, respectively, which are among the best reported for AlN epitaxially grown on sapphire. Furthermore, a detailed study of relatively thick Al-rich AlGa_N epilayers on AlN templates on sapphire substrate will be presented. We have demonstrated that the alloy composition can be precisely controlled by tuning the Al flux and N flow rate. An atomically smooth surface morphology can be achieved by carefully controlling the Ga flux and growth temperature. Under optimized conditions, Al_{0.6}Ga_{0.4}N epilayers ($>0.5\text{-}\mu\text{m}$ thick) exhibit a surface roughness $<0.4 \text{ nm}$, and strong PL emission at room temperature. High resolution TEM analysis suggests that, despite the lattice mismatch between AlGa_N, AlN and sapphire, the formation and propagation of dislocations is significantly suppressed. This work presents important insights into obtaining superior-quality wide-bandgap Al(Ga)N epilayers on lattice-mismatched substrate without the limitations of thick buffer layers, which are essentially required to break the efficiency bottleneck of deep UV optoelectronics and for emerging integrated quantum photonics.

9:40 AM PP05

Dislocation Recovery in Al-Rich AlGa_N Films by High Temperature Annealing Yan Guan¹, Shun Washiyama¹, Ke Wang¹, Pegah Bagheri¹, James Tweedie³, Seiji Mita³, Ramón Collazo² and Zlatko Sitar¹; ¹Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina, United States; ²North Carolina State University, Raleigh, North Carolina, United States; ³Adroit Materials Inc, Raleigh, North Carolina, United States.

High temperature annealing, as proposed by Fukuyama and Miyake [1], is an effective method to reduce dislocation density below 10^9 cm^{-2} in AlN on sapphire. Recently, we have suggested that this recovery is achieved by dislocation climb via vacancy bulk or core diffusion at an elevated temperature. In this study, the dislocation reduction technique is extended to AlGa_N alloys to explore the possibility of low dislocation AlGa_N templates that would facilitate strain management in AlGa_N based devices. A 300 nm -thick Al_xGa_{1-x}N layer was grown on 2-inch c-plane sapphire substrate by metalorganic chemical vapor deposition. Al mole fraction in the AlGa_N layer was varied from 0.3 to 0.85 by varying metalorganic flow rates. The AlGa_N sample was annealed for 1 hour in a nitrogen ambient (1 atm). The annealing temperature was varied from 1550°C to 1700°C . X-ray diffraction (XRD) was employed to determine the Al mole fraction and dislocation density in AlGa_N layer before and after annealing. Influence of annealing on surface morphology was characterized by atomic force microscopy (AFM). Prior to dislocation density reduction by annealing, AlGa_N alloy stability was investigated as dislocation reduction is expected to occur at a temperature above 1600°C . AFM image on Al_{0.3}Ga_{0.7}N surface revealed that a high density of nano-pits was formed after annealing at 1630°C . This could be due to decomposition of the Al_{0.3}Ga_{0.7}N layers. Thus, effective dislocation density reduction without crystal quality degradation was not observed for low Al content samples by high temperature annealing. The AFM image for Al-rich AlGa_N layers ($x=0.70$ and 0.85) showed a smooth surface composed of atomic steps after annealing at 1630°C . In addition, XRD 2θ - ω measurement revealed that the Al mole fraction was not affected by annealing at a temperature up to 1630°C . The results suggest that Al mole fraction needs to be high enough to achieve dislocation density reduction by high temperature annealing. Edge dislocation density in as-grown Al_xGa_{1-x}N layers as estimated from AlGa_N (302) XRD rocking curve FWHM is $1\text{--}3 \times 10^{11} \text{ cm}^{-2}$ on average. Dislocation density was reduced to $2 \times 10^{10} \text{ cm}^{-2}$ in Al_{0.6}Ga_{0.4}N and $4 \times 10^9 \text{ cm}^{-2}$ in Al_{0.8}Ga_{0.2}N by annealing at 1650°C . Therefore, high temperature annealing could be employed to realize low dislocation density Al-rich AlGa_N template layers for AlGa_N-based devices such as deep UV emitters and high-power devices. The role of point defects in the process of dislocation reduction will be discussed in the context of the dislocation climb mechanism. [1] Fukuyama et al., Jpn. J. Appl. Phys. 55 (05FL02) 2016.

10:00 AM REFRESHMENT BREAK

SESSION QQ: III-Nitride UV Emitters
Session Chairs: Russell Dupuis and Daniel Ewing
Friday Morning, June 28, 2019
Rackham Building, 4th Floor, Amphitheatre

10:20 AM QQ01

(Student) Growth and Characterization of III-Nitride UV Vertical Resonant Cavity Light Emitting Diodes with Hybrid Air-Gap/AlGaN and Dielectric Distributed Bragg Reflectors Hoon Jeong¹, Chaun-Wei Tsou¹, Theeradetch Detchprohm¹, Youngjae Park¹, Karan Mehta¹, Ping Chen², P. Douglas Yoder¹, Shyh-Chiang Shen¹ and Russell Dupuis¹; ¹Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, Georgia, United States; ²Institute of Semiconductors, Chinese Academy of Sciences, Atlanta, Georgia, United States.

Nitride-based vertical-cavity surface-emitting lasers (VCSELs) at wavelengths below 400 nm have drawn tremendous interest as they are potentially utilized in various applications as highly-efficient and temperature-insensitive optical sources suitable for optical storage, optically pumped solid-state lasers and compact chip-scale atomic clocks. Previously we have demonstrated optically pumped VCSELs lasing at 375 nm. The test structure consists of 5 pairs of InGaN/Al_{0.15}Ga_{0.85}N multiple quantum well active regions embedded in Al_{0.05}Ga_{0.95}N spacers with the total optical cavity thickness of a 1λ while a semiconductor-based distributed Bragg reflectors (DBR) composing of five periods of air-gap/Al_{0.05}Ga_{0.95}N and a dielectric DBR with ten pairs of ¼-wavelength HfO₂/SiO₂ were employed as bottom and top mirrors, respectively. The lowest threshold incident power density for optically pumped lasers measured at a room temperature was estimated to be ~270 kW/cm². In this work we further implemented the hybrid DBR combination in vertical resonant cavity light emitting diodes (VRCLEDs) targeting for a 370nm peak emission wavelength. The VRCLED structure comprises three distinct regions: (1) bottom DBR mirror of 5-pair 3/4-air-gap/Al_{0.045}Ga_{0.955}N, (2) 6λ-cavity LED of n-Al_{0.08}Ga_{0.92}N (n~8E18cm⁻³) spacer/InGaN-AlGaN MQW/p-AlGaN (electron blocking/p-Al_{0.08}Ga_{0.92}N (p~3E17cm⁻³) spacer/graded p⁻-AlGaN ([Mg] >1E20 cm⁻³), and (3) dielectric DBR mirror of 10 pairs of ¼-wavelength HfO₂/SiO₂. An AIXTRON 3x2" closed-coupling-showerhead metalorganic chemical vapor deposition (MOCVD) reactor with adjustable gap was employed to grow all III-N semiconductor layers. A triple-axis high-resolution X-ray diffraction technique was utilized to precisely derive composition and growth rate of each individual III-N semiconductor layer. To form a bottom DBR, five periods of n⁻-Al_{0.014}Ga_{0.986}N (n~2E19 cm⁻³) /uid-Al_{0.045}Ga_{0.955}N was grown on a GaN/sapphire template with 3 preparation layers in the sequence of n-GaN (n~1E18 cm⁻³), uid-Al_{0.014}Ga_{0.986}N, and n⁻-Al_{0.014}Ga_{0.986}N (n~1E19 cm⁻³) prior to the DBR for improving lateral electrical path in the conductivity-selection electrochemical etching. The air-gap layers were formed using optical lithography followed by deep plasma dry etching followed by laterally etching the sacrificial layers using a conductivity-selective electrochemical etching process. Once formed, this bottom DBR provides a high reflectivity of 99.9% covering from 360 to 400 nm while the top dielectric DBR is designed for slightly lower reflectivity of >97% covering from 310 to 380nm. An indium-tin-oxide layer was employed as a contact layer for the graded p⁻-AlGaN before the dielectric DBR formation. The fabricated RCLDs can be operated up to high current density up to 40 kA/cm² with a peak emission wavelength of 375 nm and a full width at half maximum of 9.3 nm at room temperature. Details of MOCVD growth, device fabrication, and characterization will be presented.

10:40 AM QQ02

(Student) Study of Optical Waveguiding Using DUV AlGaN Integrated Optical Devices Richard Floyd, Fatima Asif, Mikhail E. Gaevski, G Simin, MVS Chandrashekar and Asif Khan; University of South Carolina, Columbia, South Carolina, United States.

To date there are no reports of systematic studies of waveguiding or on-wafer monolithic integration of optoelectronic devices in the UVC spectral region. Such integrated optical components are a key requirement for miniaturization of biological agents and solar blind radiation detection systems. We present a study of optical waveguiding in UVC spectral range using monolithically integrated AlGaN optical emitters and detectors on AlN (thickness > 2 μm)/sapphire template. As seen in Figure 1a, for this study, we fabricated linearly spaced DUV LEDs with a separation of 500 μm, and an integrated pn-junction detector (see Fig. 1b). Measuring the photocurrent as a function of detector-LED spacing, we estimate the waveguide losses to be around 10 cm⁻¹. The epilayer structure for device

fabrication was grown on AlN/basal plane sapphire templates using a low pressure MOCVD system with trimethyl-aluminum (TMA) and trimethyl-gallium (TMG) as the pre-cursors. The structure consisted of a 1.5 μm thick n⁻-Al_{0.6}Ga_{0.4}N contact layer (doping density around 2 x 10¹⁸ cm⁻³) followed by a 4 pair Al_{0.4}Ga_{0.6}N/Al_{0.5}Ga_{0.5}N Multiple Quantum Well (MQW) structure. The p-side consisted of an Electron blocking AlGaN, a polarization doped graded composition p-AlGaN, and a Mg-doped hole supply p⁻-GaN cap layer. Square geometry LED and pn-junction detector structures were then fabricated using standard photolithographic procedures. The p-contact area of UVC sources were 100 μm x 100 μm and the area of the pn-junction detector was 200 μm x 200 μm. Subsequently current-voltage, electroluminescence, cathodoluminescence and photoresponsivity measurements were performed to establish the performance of fabricated devices. The source-detector distance was varied from 0.5 to 4 mm for the photoresponsivity measurements. Contribution from individual channels: air; n⁻-AlGaN; AlN; and sapphire to light transmission were studied. To exclude cross talk through the air a light-blocking coating was deposited on the top of detector, while multiple etching and/or dicing iterations were used to study contribution of the individual epilayers. At 10mA pump current the optical power transmitted through the sapphire substrate was 600μW which we estimated to be ~4% of the total emission alluding to upwards of 96% either being absorbed or trapped within the epilayers. From our measurements reported in the past we estimate the detector responsivity to be around 10⁻³ A/W and most of the absorption to take place in the MQWs (Fig. 2b). Due to the transverse-magnetic (TM) dominant-emission of AlGa_{1-x}N (x > ~0.25) [Ref.1] the light from the LED source was approximated with a 'circular' wave front giving rise to 1/distance (1/d) dependence of the detected photocurrent. We fabricated our devices with intentionally low light coupling from source to the waveguide allowing usage of multiple sources in a row without substantial absorption at any one device (see Fig. 1b). The photocurrent was measured to be significantly lower by ~1000x compared to lossless medium 1/d dependent transmission. Applying an exponential fit to the measured attenuation we estimated the waveguide losses to be 10cm⁻¹ (Fig. 3b) in reasonable agreement with early reported absorption coefficients for AlGaN layers with similar composition [2], although we note that those measurements were at normal incidence to the c-plane, while the measurement here is within the c-plane. Our experiments demonstrate that MOCVD grown AlGaN layers form a light-guiding plate with strong confinement for UV light and relatively low optical losses (~10 cm⁻¹) that makes these materials promising base for integrated optic and optoelectronic devices. Further improvement can be achieved by reducing roughness of the layers, enhancing device coupling and optimizing the cladding material.

11:00 AM QQ03

(Student) High-Efficiency Tunnel-Injected Deep Ultraviolet LEDs at 265 nm Ayush Pandey¹, Walter J. Shin¹ and Zetian Mi²; ¹Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Ann Arbor, Michigan, United States; ²Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

AlGaN ultraviolet (UV) light emitting diodes (LEDs) typically have low efficiencies, limited by the low internal quantum efficiency, poor light extraction efficiency and inefficient p-type doping. Recently polarization engineering has been used to achieve efficient tunnel injection of holes for AlGaN UV LEDs. These tunnel junctions provide better hole injection than is possible through a conventional p-contact made on p-AlGaN, resulting in higher device efficiency. The use of a tunnel junction would also allow more efficient current spreading due to the comparatively lower resistivities of n-type AlGaN than p-AlGaN. The use of Al as an n-contact will also allow for enhanced light extraction, resulting in a further enhancement of EQE. In this work, we report on the growth and fabrication of deep UV LEDs, utilizing a GaN tunnel junction. The device structures were grown using plasma-assisted molecular beam epitaxy (PAMBE). The growth was initiated with a ~50 nm thick layer of AlN grown using migration enhanced epitaxy. A ~500 nm n⁻-Al_{0.65}Ga_{0.35}N contact layer preceded the growth of the active region. The active region of the device was grown with asymmetric barrier widths to ensure a more equal injection of holes and electrons to the four quantum wells. A p-doped AlGaN followed the growth of the active region to maximize hole injection. A ~50 nm thick p⁺ AlGaN layer with ~0.7 Ω cm resistivity was immediately grown before by the tunnel junction. By utilizing highly doped AlGaN layers with high Al content, efficient tunneling current conduction through a ~3 nm thin GaN tunnel junction was achieved. The devices were fabricated such that emission could be collected from the back of the sapphire wafer, with the use of Al as the contact to the top n⁻ AlGaN. The fabricated devices exhibited a low turn-on voltage ~9 V, reaching a current density of 20 A/cm² at a voltage of only ~10 V. Efficient

collection of the light from the sample resulted in a maximum EQE ~8% with a maximum WPE ~4.5%, which are better than previously reported LEDs operating at ~265 nm. A severe efficiency droop is seen in the devices due to intense heating of the die during measurement. The electroluminescence from the devices also shows a single peak, with a spectral linewidth ~16 nm around 265 nm. Further work is being done on proper packaging of the device to further enhance device efficiency.

11:20 AM QQ04

(Student) First Principles Calculations of Alloying Boron into Group III-Nitrides for Higher Efficiency Visible and UV LEDs Logan D. Williams¹, Kevin Greenman² and Emmanouil Kioupakis¹; ¹Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; ²Chemical Engineering, University of Michigan, Ann Arbor, Michigan, United States.

InGaN based blue LEDs have flourished in the commercial lighting market due to their great efficiency advantage over traditional lighting technologies. Similarly, advances in the efficiency of AlGaIn based UV LEDs show promise to capture large market shares in water and air sterilization, food preservation, diagnostics, industrial curing, etc. However, material issues still plague both technologies. Lattice mismatch between InGaN and GaN limits the thickness of active layers in InGaN devices, exacerbating Auger losses and efficiency droop at high power. In AlGaIn devices, hole injection into p-AlGaIn is difficult while p-GaN absorbs the UV light that the LED emits. To help address these issues, we present structural, electronic, and thermodynamic properties of boron alloyed InGaN and AlGaIn alloys calculated using hybrid density functional theory. We show that wurtzite BInGaIn with a B:In ratio of roughly 2:3 are nearly lattice matched to GaN while maintaining near the same band gap as InGaN alloys with equal indium content (L. Williams and E. Kioupakis, Appl. Phys. Lett. **111**, 211107 (2017). DOI: 10.1063/1.4997601). We also explore a range of compositions around this ratio to map the composition space for both wurtzite and zinc blende phases and predict their relative stabilities, showing that the wurtzite phase is more stable roughly when the gallium and indium contents both exceed the boron content. We show that lattice matching of any composition AlGaIn to AlN can be accomplished with a few percent boron without significantly changing the band gap. This work was supported by the NSF DMREF program #1534221 and used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.

11:40 AM QQ05

(Student) Enhancement of Light Extraction Efficiency of Tunnel-Injected Deep Ultraviolet LEDs Walter J. Shin¹, Ayush Pandey¹, Kishwar Mashooq¹, Xianhe Liu¹ and Zetian Mi²; ¹Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States; ²Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

The light extraction efficiency of AlGaIn-based deep ultraviolet (UV) light emitting diodes (LEDs) is severely reduced for high Al content alloys, due to the dominantly TM-polarized light emission from these materials, which is more difficult to extract from the surface of devices. Approaches including growth on patterned substrates, surface roughening, device encapsulation and the use of nanostructures can significantly increase the collected light from UV devices, thereby improving their efficiency. Despite these advances, the external quantum efficiency (EQE) of such devices still lags far behind their InGaN visible counterparts. In this work we report on the plasma-assisted molecular beam epitaxial growth and fabrication of deep UV tunnel junction LEDs emitting at 265 nm, grown on a high reflectivity AlN/Al_{0.7}Ga_{0.3}N distributed Bragg reflector (DBR) on sapphire. The DBR was calibrated based on the measured refractive indices of the individual layers. An AlGaIn UV LED structure was grown on top, with peak emission ~270 nm. A polarization-engineered 3 nm GaN tunnel junction was incorporated to enhance hole injection. We have demonstrated such a structure can exhibit relatively high EQE, with a low turn-on voltage. The top n⁺ AlGaIn layer was grown to be ~350 nm thick to form photonic crystal nanowire arrays on the device surface to enhance light extraction through weak coupling. The nanowires patterned on the surface were defined through electron beam lithography (EBL) and the diameter varied from ~150-300 nm, with a spacing of ~320 nm and an etch depth of around 350 nm. Detailed simulations were carried out using COMSOL to design the photonic crystal array, to maximize vertical light extraction from the top of the device assuming a perfectly matched layer as the boundary condition. Finite element method (FEM) was used for the calculation assuming a mesh size smaller than the feature size of the device so as to not induce divergent electromagnetic field distribution.

These simulations suggest that it should be possible to achieve a maximum light extraction efficiency (LEE) over 80% with a lattice constant of ~320 nm and a diameter of 160 nm. It was carefully ensured that the n⁺ AlGaIn remaining on the surface after etching would not confine the light, however, it needed to be sufficient to provide current spreading for optimum device performance. A grid on the device surface was also fabricated to facilitate hole injection. Electroluminescence measurements performed on the device show strong UV emission with a single peak at ~270 nm, with no defect-related emission in the UV and visible spectra. The linewidth of the emission was ~15 nm. The device exhibit relatively good current-voltage characteristics. Further optimization of the device design, fabrication and characterization is in progress, and the realization of high efficiency deep UV LEDs will be reported.

SESSION RR: Gallium Oxide Growth Session Chairs: Shizuo Fujita and Hongping Zhao Friday Morning, June 28, 2019 Rackham Building, 4th Floor, Assembly Hall

8:20 AM RR01

Substrate Influence on Homoepitaxial Si-Doped β -Ga₂O₃ by Pulsed Laser Deposition Kevin Leedy¹, Kelson Chabak¹, David Look^{1,2}, Vladimir Vasilyev¹, Jeff Brown³, Andrew Green¹, Antonio Crespo¹, Neil Moser¹ and Gregg Jessen¹; ¹Air Force Research Laboratory, Wright-Patterson AFB, Ohio, United States; ²Wright State University, Dayton, Ohio, United States; ³KBRwyle, Beavercreek, Ohio, United States.

β -Ga₂O₃ device development motivated by potential high power and low-loss switching applications is rapidly expanding as a result of high quality native substrate availability and the ability to shallow dope epitaxial β -Ga₂O₃. Doping the full range from low to high enables devices in these application spaces: low for high voltage breakdown, middle for low loss, and high for contacts. Recent reports of n-type homoepitaxial β -Ga₂O₃ films have primarily utilized (010) substrates produced by the edge-defined film-fed (EFG) growth method. Although EFG substrates are commercially available, current limitations on crystal size, orientation and doping, as well as material cost factors, hinder more widespread and accelerated investigations of the β -Ga₂O₃ material system. The Czochralski (CZ) growth method has also been used to fabricate crystals for β -Ga₂O₃ device development but a commercial source of CZ β -Ga₂O₃ materials does not currently exist. A comparison of homoepitaxial β -Ga₂O₃ films fabricated on substrates produced from EFG and CZ methods can provide insight into the quality of the underlying substrates in addition to a direct assessment of epitaxial growth control. In this study, we report on the structural and electrical properties of Si-doped Ga₂O₃ thin films fabricated by pulsed laser deposition on Fe compensation-doped, semi-insulating (010) and (001) β -Ga₂O₃ EFG substrates (Novel Crystal Technology) and (010) CZ substrates (Northrop Grumman Synoptics). Films were deposited at 550°C from a Ga₂O₃ target with 1 wt. % SiO₂ and characterized by x-ray diffraction, atomic force microscopy, secondary ion mass spectrometry and Hall effect measurements. For (010) substrates, XRD 2-Theta scans show only the (020) peak indicative of epitaxial growth. Rocking curves of the (020) reflection further reveal higher quality structure of β -Ga₂O₃ from the EFG substrate with a FWHM of 21 arcsec compared to 89 arcsec from the CZ substrate. AFM scans display a slightly higher RMS surface roughness of 0.27 nm from films deposited on CZ substrates compared to 0.17 nm from films on EFG substrates. Degenerative Si-doped films on EFG and CZ substrates yielded similar average Hall effect mobility and concentration results: 25 cm²V⁻¹s⁻¹ and 8.61 x10¹⁹ cm⁻³ for CZ and 29 cm²V⁻¹s⁻¹ and 1.51 x10²⁰ cm⁻³ for EFG, respectively. More variability of inconsistencies in the CZ development process. Films deposited on (001) substrates exhibited a (110) preferred orientation and degraded properties, including Hall mobility < 10 cm²V⁻¹s⁻¹ and RMS surface roughness of 5.3 nm.

8:40 AM RR02

(Student) Epitaxial κ -(In_xGa_{1-x})₂O₃ and κ -(Al_xGa_{1-x})₂O₃ Thin Films and Heterostructures Deposited by Tin-Assisted VCCS-PLD from Radially-Segmented Targets Max Kneiß, Philipp Storm, Anna Hassa, Daniel Splith, Holger von Wenckstern, Michael Lorenz and Marius Grundmann; Faculty of Physics and Earth Sciences, Felix Bloch Institute for Solid State Physics, Universität Leipzig, Leipzig, Germany.

The orthorhombic κ -phase of Ga₂O₃ recently gained remarkable interest in the scientific community. Although featuring a similar high bandgap of ~5 eV as the well-known and thermodynamically stable β -phase, it further is

expected to exhibit a high spontaneous electrical polarization of 23 $\mu\text{C}/\text{cm}^2$ along its *c*-direction [1]. Polarization differences at interfaces of κ -phase heterostructures can therefore be utilized for polarization doping to localize a 2DEG. Such 2DEGs typically feature both large carrier densities as well as high mobilities and can serve as functional layer in several device applications such as quantum-well-infrared photodetectors or modulation-doped field-effect transistors. Recent reports made progress regarding the stabilization of this modification for binary Ga_2O_3 due to the presence of tin in molecular beam epitaxy [2] or pulsed laser deposition (PLD) [3] with typically high crystal quality as well as smooth surfaces and the inevitable proof of the orthorhombic symmetry of the crystal. Less is known about the alloy systems κ - $(\text{In}_x\text{Ga}_{1-x})_2\text{O}_3$ and κ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ and their heterostructures. Only few reports deal with crucial alloy properties such as the evolution of bandgap and lattice constants [4-6]. The variation of the electrical polarization or doping possibilities are completely unknown, such that the growth and characterization of high quality alloy layers is of fundamental importance. We recently reported on the stabilization of κ - $(\text{In}_x\text{Ga}_{1-x})_2\text{O}_3$ up to $x \leq 0.35$ in a thin film with lateral composition gradient (CCS) as well as conductive Zr-doped thin films and Schottky-diodes thereon [6]. Inspired by this success, in this work we utilized the recently established VCCS-PLD technique (vertical continuous composition spread [7]) intended for the creation of discrete material libraries of alloy systems to deposit laterally homogeneous thin films both for the Al- as well as the In-alloy with various x . The ternary thin films were grown by employing radially-segmented and tin-doped $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3/\text{Ga}_2\text{O}_3$ as well as $(\text{In}_x\text{Ga}_{1-x})_2\text{O}_3/\text{Ga}_2\text{O}_3$ targets with $x = 0.2$ or 0.4 on *c*-sapphire or thin film templates of PLD-grown κ - $\text{Ga}_2\text{O}_3(001)$. We demonstrate the controllable variation of the composition of the alloy layers by adjusting the position of the PLD laser spot on the target as minutely described in [7]. (001)-oriented epitaxial growth of the alloyed layers with excellent crystal quality in the κ -modification was confirmed for all radial positions by XRD. As typical for this phase on *c*-sapphire, the thin films feature three rotational domains. Still, AFM measurements reveal smooth surface morphologies suitable for the growth of functional heterostructure devices. The composition of the thin films determined by EDX-measurements or transmission spectroscopy will be compared to numerical models for the VCCS technique. We will present the evolution of the lattice constant and bandgap of the alloy thin films and heterostructures. As expected, the bandgap determined by transmission spectroscopy or spectroscopic ellipsometry is increasing/decreasing with increasing Al-/In-content in the alloy, while the *c*-lattice constant is decreasing/increasing. [1] Maccioni *et al.*, Appl. Phys. Expr. **9**, 041102 (2016) [2] Kracht *et al.*, Phys. Rev. Appl. **8**, 054002 (2017) [3] Kneiß *et al.*, APL Materials **7**, 022516 (2019) [4] Nishinaka *et al.*, CrystEngComm **20**, 1882 (2018) [5] Tahara *et al.*, Appl. Phys. Lett. **112**, 152102 (2018) [6] Hassa *et al.*, APL Materials, Accepted (2019) [7] Kneiß *et al.*, ACS Comb. Sci. **20**, 643 (2018)

9:00 AM RR03

(Student) LPCVD Growth of Si Doped β - Ga_2O_3 Thin Films with Superior Room Temperature Mobilities Zixuan Feng¹, Md Rezaul Karim¹, Adam T. Neal², Shin Mou¹ and Hongping Zhao¹; ¹Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; ²Materials and Manufacturing Directorate, Air Force Research Laboratory, Dayton, Ohio, United States; ³U. S. Air Force Research Laboratory, Dayton, Ohio, United States.

β - Ga_2O_3 , with a bandgap of 4.5-4.9 eV and predicted high critical field of 6-8 MV/cm, represents an emerging ultrawide bandgap semiconductor material promising for electronic power device and deep-UV optoelectronic device applications. The availability of high quality, low cost and scalable Ga_2O_3 bulk substrates synthesized from melt growth methods differentiates itself from GaN. Although still at the early stage, several epitaxial growth techniques have been demonstrated for β - Ga_2O_3 growth, including molecular beam epitaxy (MBE), metalorganic chemical vapor deposition (MOCVD), halide vapor phase epitaxy (HVPE) and low pressure chemical vapor deposition (LPCVD). N-type doping of β - Ga_2O_3 has been demonstrated with different dopants including Si, Sn, and Ge. P-type doping of β - Ga_2O_3 has been predicted very challenging due to the existence of self-trapped holes (polarons). On the other hand, semi-insulating β - Ga_2O_3 has been realized by using Mg, Fe, or N. Room temperature mobilities of β - Ga_2O_3 has shown to be limited by phonon scattering due to the monoclinic complex lattice structure, with two locations for Ga atoms and three different sites for oxygen atoms. It has been theoretically predicted that the room temperature mobility for bulk β - Ga_2O_3 to be limited around 200 cm^2/Vs . The current reported highest room temperature mobility for β - Ga_2O_3 was 176 cm^2/Vs with net background charge concentration of $7.4 \times 10^{15} \text{ cm}^{-3}$, from an MOCVD grown unintentional doped film on (010) Ga_2O_3 substrate [1]. In this study, we have demonstrated controllable Si-doping of β - Ga_2O_3 film grown on

native (010) Ga_2O_3 substrate with room temperature mobility of 156 cm^2/Vs and doping concentration of \sim low-mid $\times 10^{16} \text{ cm}^{-3}$ via LPCVD. The film was grown by using high purity Ga and O_2 as precursors and SiCl_4 as N-type doping source. The growth temperature was varied between 900 and 1050 $^\circ\text{C}$. Surface scanning electron microscopy (SEM) and atomic force microscopy (AFM) characterization of the as-grown homoepitaxial film has demonstrated highly uniform surface with RMS of 3 nm. The LPCVD growth of β - Ga_2O_3 films have a wide range and controllable growth rate between sub-micron per hour to 10s micron per hour. In order to investigate the dependence of LPCVD β - Ga_2O_3 on growth conditions, especially O_2 flow rate and growth temperature, a series studies were performed using off-axis *c*-sapphire substrates as growth template. The studies indicate that both growth temperature and O_2 flow rate play an important role that determines the growth rate, electron mobility and doping concentration. Secondary ion mass spectrometry (SIMS) will be characterized to identify key impurities and quantitative concentrations in the LPCVD as-grown β - Ga_2O_3 on (010) Ga_2O_3 substrate. In addition, temperature dependent Hall measurement and capacitance-voltage measurement will be performed to probe the level of compensation and net charge concentration in the as-grown film. In summary, we have demonstrated superior room temperature mobility ($\mu \sim 156 \text{ cm}^2/\text{Vs}$) of as-grown β - Ga_2O_3 on native (010) Ga_2O_3 substrate via LPCVD. The films have a wide range and controllable growth rates with good uniformity across the whole wafer. Results from this work demonstrate that LPCVD growth technique as a promising method to produce high quality and controllable β - Ga_2O_3 for device applications. [1] Y. Zhang, F. Alema, A. Mauze, O. S. Koksaldi, R. Miller, A. Osinsky, and J. Speck, APL Mater. **7**, 022506 (2019).

9:20 AM RR04

Optical and Structural Properties of Epitaxial Growth of Si-Doped β - Ga_2O_3 Thin Films on β - Ga_2O_3 (010) by Halide Vapor Phase Epitaxy Bahadır Kucukgok¹, David J. Mandia², Jacob H. Leach³, Keith R. Evans³, John Hryn¹ and Angel Yanguas-Gil¹; ¹Applied Materials Division, Argonne National Laboratory, Lemont, Illinois, United States; ²Materials Science Division, Argonne National Laboratory, Lemont, Illinois, United States; ³Kyma Technologies, Raleigh, North Carolina, United States.

The realization of gallium oxide (Ga_2O_3) as an emerging member of the wide bandgap materials has enabled future generations of high-power electronic and ultraviolet (UV) optoelectronic devices owing to advantages of its superior properties. For instance, high breakdown electric field (8 MV/cm), a wide range of electrical concentration (10^{15} - 10^{20} cm^{-3}), large bandgap (4.5-4.9 eV), which makes it transparent from the visible into the UV wavelength region, and excellent chemical and thermal stability [1]. These favorable attributes of Ga_2O_3 make it an ideal candidate for applications in electronics and optoelectronics. However, in order to enable high-performance power devices, it is inevitable to achieve high-quality bulk single crystal substrates and thick homoepitaxial films with accurate control of electrical concentration. Epitaxial Ga_2O_3 thin films were grown by various methods, such as molecular-beam epitaxy (MBE), pulsed laser deposition (PLD), mist chemical vapor deposition (mist-CVD), metal-organic chemical vapor deposition (MOCVD), and hydride vapor phase epitaxy (HVPE) [1]. Among these growth techniques, HVPE has major advantages, including superior single-crystal film quality at rapid growth rates, and higher throughput and lower-cost production. To date, few reports have been reported on the optical, structural and electrical properties of single crystalline β - Ga_2O_3 (010) thin films, particularly grown by HVPE. In this study, we investigated the room temperature (RT) structural and optical properties of Si-doped β - Ga_2O_3 epitaxial thin films grown on (010)-oriented bulk β - Ga_2O_3 single crystal with an unintentionally doped (UID) Ga_2O_3 buffer layer by HVPE method. The growth conditions of the samples are discussed in detail elsewhere [2]. The total thickness of the grown films together with the UID buffer layer was 0.6-1.07 μm . The optical properties, refractive indices and dielectric constants, crystal quality, and structure of the samples were evaluated by means of photoluminescence (PL), spectroscopic ellipsometry (SE), high-resolution X-ray diffraction (HRXRD), and Raman spectroscopy, respectively. RT PL measurements were conducted utilizing a 260 nm excitation source and reveal strong broad emission peak around 370 nm in the UV region, which is attributed to an intrinsic transition between oxygen vacancies (V_o) and nitrogen impurities (N_int) owing to the recombination of a self-trapped exciton. Less intense broadband also emerges in the range of 650-800 nm in the red emission region, which can result from the recombination of the deeply trapped exciton. The 2theta-omega HRXRD scans exhibit (010) oriented β - Ga_2O_3 thin films, and no noticeable shift in 2theta peaks is observed. Further XRD measurements, i.e., rocking curve and reciprocal space mapping (RSM) studies are currently in progress for detail analyze on crystallography, microstructure, and crystal defects of the epitaxial Ga_2O_3

thin films. RT Raman spectrum was carried out by backscattering geometry with a 532 nm laser source and shows only β -Ga₂O₃ phonon modes indicating that the nonexistence of other phases, which elucidates that the β -Ga₂O₃ homoepitaxial layer is pure and good crystal quality. Moreover, electrical properties of the epitaxial thin films were also determined by Hall effect measurements at RT using the van der Pauw method with a magnetic field of 0.51 T and a DC current of 0.1 mA. For this purpose Cr (20 nm)/Au (150 nm) electrodes were deposited on the β -Ga₂O₃ thin film by RF magnetron sputtering followed by 5min thermal annealing at ~475 C in N₂ atmosphere. Hall measurement indicates carrier concentration of $\sim 10^{17}$ - 10^{18} cm⁻³ with an electron mobility of ~ 65 - 100 cm²V⁻¹s⁻¹. References [1] M. Higashiwaki and G. H. Jessen, Appl. Phys. Lett. **112**, 060401 (2018). [2] J. H. Leach, K. Udway, J. Rumsey, G. Dodson, H. Splawn, and K. R. Evans, APL Materials **7**, 022504 (2019).

9:40 AM RR05

(LATE NEWS, Student) Microcellulose/Single Walled Carbon Nanotube Based Flexible Pressure Sensor Daesik Kim, Eunho Oh, Jiseok Seo, Byeongmoon Lee, Yaeyoung Yoon and Yongtaek Hong; Department of Electrical and Computer Engineering, ISRC, Seoul National University, Seoul, Korea (the Republic of).

Wearable flexible pressure sensors are believed to be very important in many future technologies, such as electronic skin, touch sensors, soft robots, energy harvesting, and healthcare monitoring. Recently, many research groups have implemented capacitance, piezoelectricity, or piezoresistivity type pressure sensors using various conductive nanomaterials such as metal nanoparticles, metal nanowires, CNTs, graphenes, and polymer nanofibers. Among them, piezoresistive pressure sensors are being actively studied because of their simple read-out mechanism, fast response speed, high resolution realization and the ability to sense a relatively wide range of pressure. Piezoresistive type pressure sensors often utilize changes in contact resistance caused by changes in the physical structure of the sensor when an external force is applied. Therefore, the sensitivity of the sensor depends greatly on the physical characteristics of the structure supporting the conductive material. Many research groups have attempted to create a structure that can be easily compressed to the pressure to achieve high sensitivity, and the use of pu foam or aerogels is an example. However, these methods are relatively complicated and have disadvantages in patterning or large-area processing. In this paper, we suggest a novel and facile strategy to fabricate a flexible pressure sensor using microcellulose/Single Walled Carbon Nanotube(SWCNT) fibril structure. Since entangled structure of microcellulose has a high porosity in nature, it can easily be compressed under pressure to provide high sensitivity. In addition, the carboxyl group functionalized SWCNT can form hydrogen or covalent bonds with the hydroxyl group of cellulose to produce stable piezoresistive properties. Both cellulose and SWCNT are inexpensive, easy to pattern due to the solution processability, and have ductile and flexibility, so they are suitable material for application as a flexible devices. We used microcellulose dispersion from Exilva Inc., and prepare aqueous SWCNT by directly dispersing carboxyl functionalized SWCNT powder in DI water. The microcellulose/SWCNT thin film was formed by spary coating and dispensing on a UV/O₃ treated PEN substrate. Thereafter, the fabricated cellulose / SWCNT thin film was transferred onto a PI substrate with interdigitated electrodes and whole sensor was sealed with PI tape. The fabricated sensor shows monotonically increasing current characteristics in the range of 1 kPa to 350 kPa. And it shows high sensitivity of 25.5 kPa-1 at 1 kPa ~ 80 kPa and 5.8 kPa-1 at 80 kPa ~ 350 kPa. When an external force is applied, the porous structure of the microcellulose/SWCNT is compressed, and the number of the SWCNTs contacting the lower interdigitated electrode is increased, so that the conduction path is increased and more current flows. Conversely, when the pressure is removed, the microcellulose structure is recovered to its original state, and the number of SWCNTs bridging the electrodes is reduced, thereby reducing the current. Also, the sensor showed excellent durability, even at repetitive 10000 times loading test under condition of 0.5Hz, 200kPa pressure. To verify the feasibility of microcellulose/SWCNT based flexible pressure sensors, we demonstrated a 5×5 pressure sensor array with a resolution of 4.5 dpi. We used the Kitronyx board to readout the resistances of the 25 sensors in real time at a rate of 20Hz. This sensor matrix gave a fast response about the pressing position and intensity. It could successfully detect the shape of object lying on it without any crosstalk. With the development of a high sensitive, reliable microcellulose / SWCNT pressure sensor which can easily fabricated at low-cost, we expect that it can be utilized as wearable device, medical monitoring device and user Interface for flexible electronics.

10:00 AM REFRESHMENT BREAK

SESSION SS: Processing of III-Nitrides Session Chairs: Parsian Mohseni and Jonathan Wierer Friday Morning, June 28, 2019 Rackham Building, 4th Floor, Assembly Hall

10:20 AM SS01

(Student) Plasma Control of Defects in InN—Correlation to Residual Electron Concentration and Moss-Burstein Effect Evan Clinton¹, Ehsan Vadiee¹, Zachary Engel¹, Christopher M. Matthews¹, M. Brooks Tellekamp² and W. Alan Doolittle¹; ¹Georgia Institute of Technology, Atlanta, Georgia, United States; ²National Renewable Energy Laboratory, Golden, Colorado, United States.

Plasma-assisted molecular beam epitaxy (PAMBE) is capable of growing single phase In_xGa_{1-x}N films for all indium compositions (0 ≤ x ≤ 1). It is shown that as the indium content increases and the bandgap of the material decreases, the surface becomes more sensitive to plasma-induced damage, as observed via atomic force microscopy (AFM) and reflection high energy electron diffraction (RHEED). Thus, in order to grow high indium content In_xGa_{1-x}N films, the plasma induced crystal damage must be minimized by optimizing the nitrogen plasma discharge. By properly controlling the plasma conditions, the residual electron concentration can be reduced by ~530% resulting in a strong red shift toward the fundamental bandgap of InN. *In-situ* plasma discharge monitoring and optimization can be accomplished with a combination of optical emission spectroscopy (OES) as well as utilizing a flux gauge collector pin as a Langmuir probe. OES determines a plasma's molecular and atomic nitrogen content, while the Langmuir probe current-voltage characteristics can determine the plasma discharge acceleration voltage and ion content. In this work, correlations between plasma conditions and crystal quality are established. It is shown that an optimal condition can be achieved by increasing the nitrogen flow rate and reducing the applied power to the plasma. Beyond these conditions a stable plasma was not possible. At this optimal condition the ratio of molecular to atomic nitrogen content increases, while the acceleration voltage responsible for plasma damage decreases. InN containing the weakest bond strength of the III-nitrides and thus the most sensitive to any plasma damage is utilized as a diagnostic material for optimizing the plasma discharge. 1 μm thick InN films are grown via metal modulated epitaxy at various plasma conditions. By reducing the plasma power from 550 W to 350 W and increasing the nitrogen flow from 2.5 sccm to 7.5 sccm (growth rate increase from 2.5 to 4.6 μm/hour) the background electron concentration drops from 1.8x10¹⁹ cm⁻³ to 3.4x10¹⁸ cm⁻³, likely due to a reduction in defect density. Temperature dependent photoluminescence data from room temperature down to 4 K indicates emission from both a pinned fermi level surface as well as the bulk InN with the bulk peak emission varying with electron concentration due to the Moss-Burstein effect. The lowest energy photoluminescence peak is observed at ~0.71 eV for the film with the lowest plasma damage and thus lowest background electron concentration of 3.4x10¹⁸ cm⁻³. Higher plasma damage results in increased defect density and background electron concentrations which cause a Moss-Burstein shift of the bulk InN photoluminescence peak up to ~0.83 eV. Plasma optimization for the synthesis of III-nitrides presents a roadmap towards improved performance for longer wavelength III-nitride devices, e.g. green and red light emitting diodes.

10:40 AM SS02

(Student) Alternative, Benign Chemistries for the Photogalvanic Etching of n-GaN Daniel M. Dryden^{1,2}, Lars F. Voss¹, Rebecca J. Nikolic¹ and M. Saif Islam³; ¹Materials Engineering, Lawrence Livermore National Laboratory, Livermore, California, United States; ²Materials Science & Engineering, University of California, Davis, Davis, California, United States; ³Computer and Electrical Engineering, University of California, Davis, Davis, California, United States.

Vertical device topologies in wide-bandgap semiconductors enhance the efficiency, performance, and device density of devices including electronics and optoelectronics such as solar cells, radioisotope batteries, and transistors, but require a selective, anisotropic, and low damage etch in order to attain optimal device performance. Electrochemical etching techniques provide a powerful alternative to plasma-based etching, notably in gallium nitride (GaN), which is particularly susceptible to plasma damage-induced electronic defects and leakage pathways. Current approaches to the large-area photoelectrochemical etching of GaN often result in porosity and defect selectivity, or suffer from chemical instabilities, such as bath acidification, which limit bath lifetime or result

in sample contamination. We present alternatives to the existing etching chemistries that remedy the shortcomings of current approaches, increasing bath lifetime by a factor of four, while maintaining an etch rate as high as 200 nm/min. n-GaN was etched using a photogalvanic configuration in an alkaline solution. The solution contained KOH with or without phosphate buffer, with the addition of either $K_2S_2O_8$ or $NaIO_4$ as oxidizer. A catalytic metal mask was deposited on the GaN to act as combination counter electrode and photomask, and the sample and solution were exposed to supra-band gap UV light. Where exposed to light the GaN etched readily, while regions below the metal mask did not, resulting in features with straight sidewalls and high etch selectivity. The dependence of etching depth and quality on bath pH, oxidizer concentration and chemical potential, and buffer strength were observed, with a particular focus on means to limit porosity and defect selectivity. Increased bath temperature was shown to enhance etch rate and limit defect selectivity. Both buffering salts and the replacement of $K_2S_2O_8$ with $NaIO_4$ effectively mitigated bath acidification, at the cost of increased porosity and reduced etch rate, respectively. The etch porosity and morphology showed a large dependence on etch bath stirring, with a stirred bath eliminating trenching at the cost of increased roughness. These observations are discussed in the context of both mass transfer-limited and charge carrier-limited etching regimes, with the goal of demonstrating a smooth, controlled etch for the fabrication of devices.

11:00 AM SS03

(Student) Removal of Electrically Damaged Surface Layer Induced by Dry Etching of p-GaN by Photoelectrochemical Etching Vincent E. Meyers¹, Emma Rocco², Kasey Hogan³, Sean A. Tozier⁴, Benjamin McEwen⁵, Isra Mahabooob⁶ and Fatemeh (Shadi) Shahedipour-Sandvik⁷; ¹CNSE, State University of New York Polytechnic Institute, Albany, New York, United States; ²SUNY Polytechnic Institute, Colleges of Nanoscale Science and Engineering, Albany, New York, United States; ³Nanoscale Engineering, Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, Albany, New York, United States; ⁴Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, Clifton Park, New York, United States; ⁵College of Nanoscale Science and Engineering, SUNY Polytechnic Institute, Albany, New York, United States; ⁶Nanoscale Science and Engineering, SUNY Polytechnic Institute, Albany, New York, United States; ⁷SUNY Polytechnic Institute, Albany, New York, United States.

The development and optimization of etching techniques in GaN is integral to the advancement of PN diodes, transistors, and photodetectors (among others) for structure isolation and separation. The application motivating this work is the recovery of GaN:Mg films after high temperature processing for dopant activation. MOCVD-grown UID GaN was implanted with Mg and annealed using a novel Gyrotron microwave annealing technique at temperatures of 800 C - 1300 C. In this temperature regime, the process of GaN decomposition by nitrogen desorption must be prevented by the combined use of high N₂ overpressure and of a protective cap on the GaN surface, in this case of AlN. The physical-chemical nature of the dry-etching technique ICP-RIE makes it an effective etching process for GaN and AlN because it is highly anisotropic and etches without sensitivity to dopant or structural defects. The ICP-RIE chemistry effective on GaN is also effective on AlN. However, ion bombardment during ICP-RIE induces damage by formation of electrically active nitrogen vacancies V_N at the GaN surface. This creates a layer of electrically compensated material which inhibits formation of high-quality p-type Ohmic contacts. An etching mechanism for removal of this layer of damaged material induced by ICP-RIE has been documented in n-GaN, but has not been reported for p-GaN. In this study, Ga-polar pGaN films are grown by MOCVD and exposed to a chlorine-based ICP-RIE dry etch. Photoelectrochemical (PEC) etching technique is employed in order to remove etch-face damage and recover the underlying p-type material. Here we report on the electrical, compositional, and morphological properties of the etched films. PEC etching is a type-selective wet process that allows etching of n-GaN, selectively, over p-GaN. Conditions are optimized for PEC etching of ICP-RIE-etched p-GaN with a Xe UV lamp emitting at $\lambda=365$ nm in a solution of KOH and $K_2S_2O_8$ as oxidizer and reducer, respectively. PEC etches GaN via an oxidation reaction, and the charge balance of the etched material is maintained by a reduction reaction at the etch-face contacts. Because of this, the effects of the etch reaction can be partially characterized by a simpler etch condition operating with only KOH without a reduction reaction. There is no charge-balancing redox reaction, so etching quickly halts, but a small amount of GaN material is etched initially. As a proof-of-concept, this photochemical (PC) etch was used to characterize the type-selectivity and bulk electrical effects of the etch reaction on as-grown and ICP-etched p-GaN. To compare the effect of dry etching and the effect of PC/PEC on the GaN surface, PC etch was performed on an as-grown p-GaN sample, a p-GaN

sample etched with ICP-RIE, and an n-GaN sample. AFM reveals a small increase in surface roughness of the as-grown p-GaN film after PC etch, with an RMS roughness of 0.61 nm before etching and 1.01 nm after. However the RMS roughness of the dry-etched sample increased from 1.5 nm to over 6 nm after PC etch, suggesting increased interaction of the etchant with the surface layer of compensated (or n-type) material. The roughness of the n-GaN sample increased from 0.86 nm to 3.2 nm. The relative effectiveness of PC and PEC etching on dry etched pGaN under varying etch conditions will be compared. Formation and electrical properties of p-type contacts to the PEC-etched surface will also be discussed. Hall Effect measurements were also taken on the etch-face of a sample of as-grown p-GaN before and after a 1 hr PC etch to verify the etch process does not affect the electrical properties of the bulk material. The measured electrical characteristics before (carrier concentration 1.86e17 cm⁻³; bulk resistivity 6.54 Ω cm) and after (carrier concentration 1.57e17 cm⁻³; bulk resistivity 6.71 Ω cm) the etch are largely unchanged.

11:20 AM SS04

(Student) Wet Thermal Oxidation of AlInN Matthew R. Peart, Xiongliang Wei, Damir Borovac, Wei Sun, Nelson Tansu and Jonathan J. Wierer; Electrical and Computer Engineering, Lehigh University, Bethlehem, Pennsylvania, United States.

The oxidation of semiconductors is a powerful technique and enables new device architectures and processing methods. The most well-known oxide is the oxidation of Si into SiO₂, developed by John Moll at Bell Labs in 1950's, that is used as an insulator, a protection layer, a masking layer, and a gate oxide. The low defect density of the oxide and the simplicity of its formation make it an ideal dielectric, and its development was key to the proliferation of Si semiconductor technology. Thermal oxidation of AlGaAs [1] is also a successful oxide for the AlInGaAs semiconductor system to create current and photon confinement, and passivation. This embodiment is particularly successful with AlGaAs VCSELs. A similarly successful oxidation layer does not exist for III-nitrides. Thermal oxidation of GaN has been investigated [3]-[4], and while good interface state densities have been achieved there are major drawbacks. The growth of Ga₂O₃ on GaN suffers from an insufficient conduction band offset limiting its utility as an insulator, and it also has a rough interface morphology. Both of which contribute to poor electrical and optical properties [5]. Here we show a different approach to create a thermal oxide on GaN with good thermal and electrical characteristics. Al_{1-x}In_xN at x=0.82 is lattice matched to GaN, and when exposed to conventional wet thermal oxidation at high temperatures (700-900 °C) it is converted to a stable and robust oxide. The Al_{0.82}In_{0.18}N oxidizes at a high rate and exhibits high resistivity, a low refractive index, and smooth surface morphology making it a good candidate for use in electronic and optoelectronic devices. In this presentation, we demonstrate oxides formed from wet thermal oxidation of AlInN. Samples consisting of 100 nm and 250 nm thick Al_{0.82}In_{0.18}N layers are grown on 4 μ m thick unintentionally doped GaN on sapphire templates. The lattice matched condition was verified by x-ray diffraction (XRD) ω -2 θ scans. Hall measurement using the Van der Pauw method show the Al_{0.82}In_{0.18}N layers are n-type with an electron concentration of 2x10¹⁷ /cm³. After a cleaning process the samples are placed into a quartz tube furnace at a temperature of 900 °C with 100 sccm of nitrogen flowing through a H₂O (DI) bubbler heated to 95 °C for one hour. Spectroscopic ellipsometry verified that the 100 nm and 250 nm Al_{1-x}In_xN films are completely oxidized. The oxidation rate is faster and the oxide thickness is larger compared to reports of thermally formed oxides from AlInN [6]. The stoichiometry of the oxide was verified by x-ray photoelectron spectroscopy (XPS), and the content of oxygen in the film is ~51% and nitrogen is ~1% after oxidation. Other samples for electrical characterization are fabricated by oxidizing Al_{0.82}In_{0.18}N layers grown on n-type GaN layers (n~5x10¹⁸). The oxide is removed from portion of the sample by a polishing process and aluminum contacts were evaporated by e-beam evaporation. The oxide layer is insulating with resistivities of >8x10¹⁴ ohm-cm, similar to values reported for Al₂O₃. Voltage sweeps to electrical breakdown revealed critical electric fields > 2 MV/cm. Ellipsometry of the oxide films show a refractive index of ~1.7, providing a large index contrast layer that is useful for optoelectronic applications. These promising results provide a motivation for further study of the AlInN oxide and paths towards integration in device designs. **References:** [1] J. M. Dallesasse, et al. Appl. Phys. Lett., vol. 57, no. 26, pp. 2844-2846, 1990. [2] J. J. Wierer et al. Appl. Phys. Lett., vol. 72, pp 2742-45, 1998. [3] H. Kim, et al., J. Vac. Sci. Technol., B vol. 19, no. 579, 2001. [4] Y. Nakano, et al., Appl. Phys. Lett. vol. 82, no. 218, 2003. [5] T. Yamada, et al., Appl. Phys. Lett. Appl. Phys. Lett. 110, 261603, 2017. [6] M. Eickelkamp, et al., Phys. Status Solidi C, vol. 8, no 7-8, 2213-2215, 2011.

11:40 AM SS05

Investigation of Contaminations and Damages on C-Plane GaN

Induced by Dry Etching Bingjun Li¹, Mohsen Nami¹, Jiaheng He², Guanjie Cheng², Davide Del Gaudio², Jordan Occena², Fabian Naab², Rachel S. Goldman² and Jung Han¹; ¹Electrical Engineering and Applied Science, Yale University, New Haven, Connecticut, United States; ²Materials Science & Engineering, University of Michigan, Ann Arbor, Michigan, United States.

III-nitride based materials have gained significant attentions in recent years for power electronics due to their wide-bandgap, high electric breakdown field, and high electron mobility. Lateral and vertical geometries have been proposed for high-power devices. Vertical geometry designs are preferred due to their higher breakdown voltage on a smaller chip size, lower on-resistance, and superior reliability due to less-crowded field distribution near the surface. Selective-area doping is the cornerstone of modern vertical power devices, including current aperture vertical electron transistors (CAVET), vertical junction FETs, and superjunction FETs (SJ-FETs). Selective-area doping can be performed through ion implantation or selective-area epitaxial regrowth. However, high quality p-type GaN using ion-implantation has not been achieved yet. This is due to challenges associated with ion implantation, including high temperature annealing for dopant activation and recovery from the ion-induced damages. Selective-area epitaxial regrowth, can be used to realize selective-area doping on c-plane GaN substrates. However, due to impurities and damages induced by dry etching (ICP) at the regrowth interfaces, regrown p-n junctions have shown higher reverse leakage currents compared to continuously grown junctions. This means a thorough investigation of impurities and damages induced by ICP are important to improve the performance of nitride-based power devices. Three sets of planar p-n diodes were grown using metal-organic chemical vapor deposition (MOCVD) to study the effect of impurities and plasma-induced damages on I-V characteristics. These samples consist of a 2 μm of unintentionally-doped GaN (UID-GaN) and 200 nm p-type GaN. The first sample has UID-GaN and p-GaN grown continuously, the second sample has p-GaN grown on an air-exposed UID-GaN (template), and the third sample has a p-GaN layer grown on a 300 nm ICP-etched template. The forward and reverse-bias characterizations were performed. Similar I-V characteristics were obtained for samples one and two, while sample number three exhibited significant leakage current. Secondary ion mass spectrometry (SIMS), was performed on all samples to study the impurities at the regrowth interfaces. Si spikes with the peak of $\sim 1 \times 10^{18}$, and 8×10^{19} (atom/cm³) were detected at the regrowth interface for samples two and three respectively, while sample one did not show any impurity rise at the junction. X-Ray photoelectron spectroscopy (XPS) and X-Ray fluorescence spectrometry (XRF) were employed on ICP-etched templates, a Cl_{2p} peak and a clear presence N-vacancy were detected at the surface. Scanning spreading resistance microscopy (SSRM) and scanning capacitance microscopy (SCM) revealed the fact that ICP caused damages as deep as ~ 160 nm, this results were then confirmed by Rutherford backscattering spectrometry (RBS).