High efficiency of III-Nitrides Micro-Light-Emitting Diodes by Sidewall Passivation Using Atomic Layer Deposition

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Micro-sized light-emitting diodes (µLEDs) with high energy efficiency are desired for a variety of applications, such as virtual reality and augmented reality near-eye displays. Although InGaN µLEDs have achieved outstanding performances in display applications in recent years, the peak external quantum efficiency (EQE) decreases as the µLED dimensions shrink, which is problematic. The reduction in EQE is due to the sidewall damage from the plasma-based dry etching. The influence of plasma damage is more significant in µLEDs with smaller dimensions, because the perimeter/area ratio is greater in smaller µLEDs. In this work, we demonstrate that the EQE of µLEDs can be improved by sidewall passivation using atomic layer deposition (ALD). Moreover, we compare the µLEDs passivated by ALD and plasma-enhanced chemical vapor deposition (PECVD), which shows that ALD sidewall passivation results in better optical and electrical performances. µLEDs, grown by metalorganic chemical vapor deposition, were fabricated into six sizes ranging from 10×10 to 100×100 µm² and were passivated by PECVD or ALD with SiO₂. In terms of the optical performance, the µLEDs passivated by ALD resulted in homogeneous light emission in smaller devices compared to the µLEDs without sidewall passivation, based upon the results from electroluminescence images. The µLEDs passivated by ALD had more light emission, as the EQE of the 20×20 µm² µLED was the highest of all samples. The reduced light emission of the µLEDs passivated by PECVD was due to a decreased transparency of indium-tin oxide (ITO), which served as a transparent and ohmic p-contact. From the electrical perspective, the µLEDs passivated by ALD resulted in the least amount of leakage among all sizes while the passivation by PECVD was effective in the larger µLEDs. The influence of sidewall damage became significant as the µLED dimensions shrink, which revealed ALD is a more effective method to reduce leakage. Additionally, we also show that the technique of SiO₂ removal is crucial in leakage reduction. When employing wet etching, the isotropic nature of the etch is undesired as the LED dimensions and features get smaller. However, the barbaric etch in dry etching damaged the ITO layer and caused the devices to be more resistive and have more leakage. Consequently, the wall-plug efficiency of the 20×20 µm² µLED passivated by ALD and with wet etching was the highest among all sidewall passivation techniques. The ALD sidewall passivation indicated the size-dependent influences on peak EQE can be lessen by proper sidewall treatment.

High critical field strength and saturation electron velocity of gallium nitride (GaN) makes it a promising material for mid-wave infrared, high voltage, and high-speed switches. Photoconductive semiconductor switches (PCSSs) have advantages in pulsed power applications since it is a device that turns on with fast rise time, low jitter, and allows for high repetition rate. Semi-insulating GaN doped with carbon (GaN:C) reduces the off-state leakage current and extends the blocking voltage, while still allowing for high on-state photocurrent compared to undoped GaN. However, forming a low resistance contact to highly insulating GaN:C is challenging. Our approach is to leverage ion implantation of Si followed by an activation anneal to form an N⁺ contact layer. Implantation and activation is a planar process that is promising for formation of contact regions while mitigating high electric field points within the device. In this work, we implemented a process with a depth of 14 µm into GaN:C with carbon concentrations of 5x10¹⁹ to 1x10²⁰ cm⁻³ grown on SiC substrates. Then, a sputtered AlN capping layer is introduced before annealing at various temperatures to preserve the surface from decomposition during annealing. The AlN capping layer is then selectively wet etched and Ti/Al/Ni/Au contacts are deposited and then alloyed at 850 °C. Top-to-top lateral PCSSs are fabricated and characterized to identify the impact of the Si implantation and annealing in the contact regions on the contact resistance, off-state leakage, blocking voltage, and photocurrent.
Etching behavior was investigated as a function of KOH and K$_2$SO$_4$ concentration, temperature, UV irradiance, material quality, and contact ohmicity. Previous studies on this system used non-catalytic ohmic contacts and a catalytic external electrode, or a catalytic but non-ohmic mask; we demonstrate the use of an ohmic, catalytic mask capable of smooth etching of non-uniformly isolated features, with ohmic contacts potentially improving etch quality by removing the energy barrier to charge balance. In addition, we investigate the use of elevated-temperature etching baths to increase the etching rate, which is the first use of elevated temperatures in the KOH-K$_2$SO$_4$ system to our knowledge, and observe a significant enhancement in both etch rate and surface quality. Conditions with low irradiance, high KOH concentration, and/or non-ohmic contacts produced defective etching with ultra-thin nanowires and deep porosity. Etching rate was highly dependent on UV irradiance. Using ohmic contacts with catalytic top surfaces removed the energy barrier to charge carrier transport at the metal-semiconductor interface, resulting in non-defect-selective etching. Best results were obtained in a 65 °C bath with 25 mM KOH, 150 mM K$_2$SO$_4$, and 1.25 mW/cm$^2$ UV illumination. A “reverse crown” etch profile was observed and attributed to decreased hole recombination near contacts from enhanced charge balance. Further experiments are ongoing to fabricate n-GaN-based devices and to characterize the quality of the surfaces produced by photoelectrochemical etching in terms of their morphology and electronic performance. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344, LLNL-ABS-744732. The authors would like to thank the following sources of funding: The LLNL Livermore Graduate Scholar Program, The U.S. Department of Energy (DOE), Office of Energy Efficiency and Renewable Energy (EERE), and Advanced Manufacturing Office (AMO).

**9:40 AM KK05**

Size-Controlled Photoelectrochemical Etching of InGaN Quantum Dots and GaN Nanowires

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III-nitride quantum dots (QDs) have significant potential for single-photon sources or gain media for low threshold and high efficiency visible and UV lasers, among others. "Bottom-up" Stranksi–Krastanov growth is widely used, however both the size distribution and densities are difficult to precisely control. Here, we show a top-down fabrication process that can be controlled by the evolving properties of the nanostructures being fabricated. This process, called quantum size-controlled photoelectrochemical (QSC-PEC) etching, uses laser excitation at a selected and narrowed wavelength to control the final sizes of the QDs through an etch that self-terminates when the QD band gaps increase due to quantum confinement effects until they exceed the energy of the incident photons. Beginning with epitaxially grown InGaN films, we examine the etch process from large to quantum-scale nanostructures with AFM, scanning TEM (STEM), and photoluminescence measurements. Quantitative analysis of size and density of the ensemble are made after image-processing techniques and deconvolution of the AFM tip and QD. We further investigate the fabrication of multilayers of QDs from multiple-quanmum well structures, which can potentially increase the overall QD density per device. These results show the potential for a combination of unprecedented size uniformity and areal density for InGaN QD devices. We also have investigated the extension of this process to create QDs in other semiconductor materials systems. Results will be presented on the PEC etching of GaAs/AlGaAs planar films using above-bandgap laser light (∼790-830 nm) and characterized by AFM and STEM measurements. We demonstrate purification of high-density, vertical arrays of very high-aspect ratio (e.g. > 200:1) GaN nanowires via PEC etching of thin GaN epilayers on sapphire. Cross-sectional STEM characterization of these nanowires show that they are not correlated with dislocations from the original GaN epilayer. We propose that lateral etching below a certain diameter is retarded due to carrier depletion in the nanostructure regime, which allows for continued vertical etching even for very-high-aspect ratios. Photoluminescence measurements indicate that their optical quality is equivalent or superior to the starting unetched film, despite the much higher surface area, which is typically a source of nonradiative recombination. Such nanowires could potentially benefit numerous applications such as optoelectronics (e.g. LEDs, lasers, photodetectors), nanogenerators, and gas sensors. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. 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-NA0003525.

**10:00 AM BREAK**

**SESSION LL: III-Nitride—Epitaxial Growth II**

**Session Chairs:** Elaheh Ahmadi and Srilam Krishnamoorthy

*Friday Morning, June 29, 2018*

**Location:** University Center, Corwin East

**10:20 AM LL101**

(Stduent) Kinetic Instability of AlGaN Alloys During MBE Growth Under Metal-Rich Conditions on m-Plane GaN Miscut Towards the c-Axis

Mohammad Ali Shariatzadeh, Rosa Diaz, Trang Nguyen, J. Jian, Haiyan Wang, Geoffrey Gardner, Mike Alford, and Oana Malis; Purdue University, Lafayette, Indiana, United States.

Nonpolar m-plane AlGaN/GaN heterostructures are interesting from both a fundamental material growth perspective, and for practical applications in infrared optoelectronic devices. Intersubband optoelectronic devices utilize optical transitions within the conduction band of GaN/AlGaN quantum wells to emit or detect infrared radiation. The accessible wavelength range is mainly determined by the conduction band-offset between well and barrier material, i.e. GaN and AlGaN in this case. High Al-composition AlGaN is needed to access the technologically important telecommunications range (1.55 µm). Moreover, infrared nonpolar nitride devices theoretically benefit from the absence of built-in polarization fields that allows better control of the transition energy, and enhanced optical transition strength. To date, promising experimental results have been reported for near- and far-infrared intersubband absorption and photodetection in m-plane nitride heterostructures utilizing limited Al-composition alloys (Al$_{x}$GaN/Al$_{1-x}$GaN superlattices with x<0.5). Nevertheless, to fully realize the potential of m-plane nitrides, high aluminum composition AlGaN is needed. In this work, we examined the effect of aluminum flux on the structure of high Al-composition m-plane Al$_{x}$Ga$_{1-x}$N/GaN (x>0.5) superlattices grown by plasma-enhanced MBE under metal-rich conditions and observed an unprecedented kinetic instability of high Al composition AlGaN. We found that above a critical Al flux the AlGaN growth rate is drastically suppressed to a level close to that of AlN, and the growth mode can be referred to as Al-limited growth in Ga-rich conditions. The m-plane AlGaN/GaN heterostructures were grown on free-standing m-plane GaN substrates with threading dislocation density of < 5x10$^{4}$ cm$^{-2}$, and nominal miscut of 1° towards the c-axis (no miscut towards the a-axis). The substrate temperature was measured with a pyrometer to be 720° C. The N-limited growth rate of m-plane GaN is 8.8 nm/min, and it is the same, within experimental error, as on c-plane GaN. 15-period AlGaN/GaN superlattices with fixed aluminum flux and layer thicknesses were grown and investigated using high-resolution x-ray diffraction (HRXRD) measurements. Also, two AlGaN/GaN samples were grown with varying Al flux, and AlGaN thicknesses for scanning transmission electron microscopy (STEM). Sample A was grown to examine the dependence of AlGaN structure on Al flux and to identify the transition to the instability regime. Sample B was grown to study the time evolution of the AlGaN structure in the instability regime. For Al-fluxes higher than 1.4x10$^{13}$ atoms/cm$^{2}$s, Al$_{x}$Ga$_{1-x}$N (with x=0.55 µm) growth produces a unique nanostructure characterized by Al-rich thin planar films and flat-top stripes bordered by m-type nano-facets (aligned mostly along the c-axis). A close examination of these nanostructures (visible in superlattices A-A5) using energy dispersive x-ray (EDX) spectroscopy in the STEM indicates that the AlGaN layers are also non-uniform in composition. Essentially, homogeneous growth of n-plane Al$_{x}$Ga$_{1-x}$N with an Al composition between approximately 0.6 and 0.9 is unstable under conditions corresponding to metal-rich plasma-enhanced MBE. Our experimental results support a model in which Al-N dimers promote Ga-N dimer detachment from c-type edges on the surface. The composition variation in the nanostructures can be explained by step-bunching in the direction of the a-axis, but more theoretical work is needed to substantiate our models. Experimentally, we believe that careful control of the substrate miscut in the a- and c-direction can be used to promote m-plane growth of uniform AlGaN layers.
growth was carried out in so called “wet surface N-rich” growth conditions, where GaN surface decomposes significantly and metal layers are formed due to decomposition. As it was pointed out by B.M. McSkimming et al. [3], presenting full growth diagram for Ga-polar GaN, dry surface in N-rich conditions results in rough surface, so called 3D growth. On the other hand, theoretical calculations presented by T. Zywert [1] indicate that lower diffusion barriers can be expected for N-polar surface comparing to more commonly used Ga-polar. Higher diffusivity of adatoms for N-polar surface comparing to Ga-polar one enabled the smooth growth in N-rich conditions for N-polar substrates with miscut angle close to 4 deg [4]. In this work, we investigate the growth of GaN on N-polar high quality GaN substrates in N-rich growth conditions at miscut angles ranging from 0.3 to 4 deg at temperature 750°C. Meandering atomic step edges have been observed for wide range of atomic fluxes used for the growth. Contradictory to previous reports on meandering (finger-like) morphologies for GaN and cubic crystals [5-7], wavelength of those meanders decrease with increasing miscut angle and increase with increasing growth rate. Such observation led us to form the hypothesis that, in this case, finger-like morphology cannot be explained in simple model with non-interacting adatoms. Lower wavelength of meanders for higher miscut angles indicate that diffusion over atomic steps, blocked by Ehrlich-Schwoebel barrier (ESB), is an important process that effectively leads to lower diffusion length for higher step density. Increase in meanders’ wavelength for higher growth rate, on the other hand, indicate that Ga adatoms interact with each other leading to diffusion enhancement. We postulate that this effect can be realized by lowering ESB. To prove the hypothesis, kinetic Monte Carlo simulations were used. N-polar GaN surface morphology obtained for N-rich growth conditions was studied. Simulations were performed to test the influence of Ga and N fluxes as well as miscut angle. Model that takes into account ESB at atomic steps that can be lowered by the presence of Ga adatoms at neighboring sites was able to qualitatively reproduce experimentally observed morphologies. Growth diagram indicating transitions between different growth modes for N-rich growth on N-polar surface in PA-MBE will be presented. [1] J. N. Tosja Zywert, and Matthias Scheffler, Applied Physics Letters 73, 487 (1998); [2] G. Koblmüller, F. Wu, J. Tate, J. S. Speck, S. Fernandez-Garrido, and E. Calleja, Applied Physics Letters 91 (2007); [3] B. M. McSkimming, F. Wu, T. Huault, C. Chais, and J. S. Speck, Journal of Crystal Growth 386, 168 (2014); [4] F. Krzyzewski, M. A. Zaluska-Kotur, H. Turski, M. Sawicka, and C. Skierbiszewski, Journal of Crystal Growth 457, 455 (2016); [5] A. B. McLeod, H. LaBorde, B. Hourahine, D. Martin, and N. Grandjean, Journal of Crystal Growth 433, 36 (2016); [6] M. A. Zaluska-Kotur, F. Krzyzewski, and S. Krukowski, Journal of Crystal Growth 343, 138 (2012); [7] C. Misbah, O. Pierre-Louis, and Y. Saito, Reviews of Modern Physics 82, 981 (2010). Acknowledgements: This work was supported partially by the Polish National Centre for Research and Development Grant PBS3/A3/23/2015 and LIDER/29/015/L-7/15/BR/2016.
plasma and the film. Unexpectedly, the results also illustrate that increased applied power to the plasma bulk only slightly increases positive ion content, while having a minimal effect on the floating voltage. AFM results of 1 µm thick InN grown films exhibit reduced pit densities when grown under plasma discharge conditions with low densities of positively charged ions. These show improved techniques for plasma optimization should enable improved high indium content III-nitride device performance.

II:40 AM LL05
Impact of Early Stages of InAlN Growth by Plasma-Assisted Molecular Beam Epitaxy on Honeycomb Structures Formation

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Heterostructures of III-nitride semiconductors (GaN, AlN, and InN) have unique electronic and optical properties that make them promising for fabrication novel near-infrared and terahertz emitters and detectors based on intersubband transitions. Importantly, application of III-nitride heterostructures may include frequencies that are fundamentally inaccessible by extensional absorption of radiation. One of the major limiting factors in the growth of complex nitride heterostructures is the lattice mismatch between AlN, GaN, and InN. In case of InAlN (InAlN), the lattice mismatch between AlN and GaN (GaN) is particularly challenging, as the growth of InAlN on GaN is limited by the formation of a ‘honeycomb’ microstructure [1-3]. In work by Sahonta et al., the growth of InAlN by plasma-assisted molecular beam epitaxy (PAMBE) is described by three successive steps: the formation of Al-rich InAlN dynamical platelets, their partial coalescence, and the preferential indium incorporation at platelet boundaries due to tensile strain generated between platelets [1]. Thus, the growth mechanism includes the inevitable quasi-three-dimensional stage on the onset of InAlN formation and the transient to further two-dimensional growth, which is similar to InN growth mechanism at low temperatures [4]. Recently, several groups reported on the elimination of ‘honeycomb’ microstructure in metal-polar and nitrogen-polar lattice-matched InAlN films [5-7]. It has been assumed that the homogeneous films were achieved through the N-rich PAMBE by lowering the growth rate and increasing indium to aluminum ratio [5,6]. However, understanding of the growth mechanism affecting segregation remains primitive at best, and importantly, the control of the nucleation stage on the onset of InAlN growth has not been extensively studied. In this work, we study the impact of early stages of InAlN growth on the honeycomb microstructure formation. InAlN samples were grown on GaN surface using different schemes of growth initiation: growth on a N-rich (2x2) reconstructed GaN surface, GaN surface exposed to In-flux prior to the onset of InAlN growth, and GaN surface cooled to the InAlN growth temperature under indium coverage. The ex-situ characterization of the dynamic Al-rich platelets on the onset of the InAlN growth was done on 4-nm-thick layers using atomic force microscopy, whereas plan-view scanning transmission electron microscopy was applied to analyze ‘honeycomb’ microstructures. We discuss the dependence of the platelets size on the initial growth conditions. It was found that the size of dynamic platelets can be effectively increased by initiating the InAlN growth on GaN covered with metallic indium layer. Importantly, that excess indium on the surface is consumed during the InAlN growth and does not result in a buildup of crystalline indium droplets on the surface. The correlated analysis of high-resolution AFM and plan-view STEM data provides a better understanding of the impact of earlier stages of InAlN growth on the elimination of the ‘honeycomb’ microstructures. References [1] S-I. Sahonta et al., Appl. Phys. Lett. 95, 021913 (2009); [2] S. Choi et al., Appl. Phys. Lett. 100, 232102 (2012); [3] C. Edmunds et al., Phys. Rev. B 88, 235306 (2013); [4] C. S. Gallinat et al., J. Appl. Phys. 102, 064907 (2007); [5] S. W. Kaun et al., Semicond. Sci. Technol. 29, 045011 (2014); [6] E. C. H. Kyle et al., Journal of Crystal Growth 454, 164–172 (2016); [7] M. T. Hardy et al., J. Vac. Sci. Tech., 117 (2016).

S8:20 AM MM01
(Student) Investigation of Stable Process for Atomically Flat Si(100) Surface Under Ar/H2, Annealing to Improve H-based MONOS Characteristics

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Introduction: Recently, Metal/Oxide/Nitride/Oxide/Si (MONOS) non-volatile memory (NVM) with high-k gate material is attracting much attention to achieve low voltage operation by reducing the insulator thickness. As the scaling of FinFETs, the high-k gate insulator/Si is one of the critical issues to realize the high reliability of MONOS NVM. In our previous report, the atomic steps on Si(100) surface was realized by annealing at 1050°C/60 min in Ar/4.0%H2 ambient, utilizing the clean furnace, and the degradation of leakage currents of H-based MONOS diodes after 100 program/erase cycles were decreased by flattening. However, by the annealing in Ar/4.0%H2 ambient, there is still some issues such as a periodic surface roughness with a few micrometer length. Therefore, to realize ideal atomically flat Si(100) surface, the periodic surface roughness should be decreased. In this study, the use of chemically oxidized Si(100) for stable atomically flattening and the electrical characteristics of H-based MONOS diodes were investigated. Experimental procedure: After cleaning of Si(100) substrate with off-angle less than 1°, some of the substrates were immersed in H2O/60 min at room temperature (RT) to form 0.7 nm thick chemical oxide (Ch. Ox.). After annealing at 1050°C/10 min in Ar/4.0%H2 (3 SLM) utilizing the clean furnace, the unintentional oxide layer which was formed during the annealing process was removed by wet etching (HF: HCl=1:19). Then, HN3(MH)2O(OH)2/(NH3(OH)2) gate stack with thickness of 10/10.7/2 nm, respectively, was in-situ deposited on p-Si(100) by ECR plasma sputtering at RT. After post-deposition annealing was carried out at 600°C/1 min in N2 (1 SLM), Al top and back electrodes were evaporated. Finally, the post metallization annealing was carried out at 300°C/10 min in N2/4.9%H2 (1 SLM). The Si surface roughness was observed by non-contact mode atomic force microscopy (AFM). The CV characteristics of MONOS diodes were evaluated at RT. Results and Conclusion: The scan size dependence was decreased, and uniformity was improved by using chemically oxidized Si in spite of the short flattening duration such as 10 min. Furthermore, the obtained surface RMS roughness of 10 x 10 µm2 was decreased from 0.60 nm (without Ch. Ox.) to 0.26 nm (with Ch. Ox.). Thus, this method is suppressing the periodic surface roughness probably because the unintentional oxide formation with thickness fluctuations was suppressed. Large memory window (MW) of 1.9 V was realized by the flattening of chemically oxidized Si compared to the MW of 1.7 V in the case of without flattening. In conclusion, annealing at 1050°C/10 min in Ar/40%H2 ambient with chemically oxidized Si(100) was able to decrease Si surface RMS roughness and increase the MW of H-based MONOS diodes.

8:40 AM MM02
Electrochemically Detected Magnetic Resonance on Multi-Gate Metal Oxide Silicon Transistors

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Multi-gated metal oxide semiconductor field effect transistors (MOSFETs) have recently become important in high-performances CMOS integrated circuits. Multi-gated devices, commonly called FinFETs, have reduced short channel effects, allowing for greater scalability. However, there is little in the literature about the atomic defects at the semiconductor-dielectric interface in FinFETs. This is significant, as FinFETs have recently become the dominant device in high-performances CMOS integrated circuits. In this study, we explore traps at the FinFET Si/ dielectric interface with electrochemically detected magnetic resonance (EDMR). The devices involved in this experiment are on (100) silicon-on-insulator wafers with 90nm Si layers and 125nm buried oxides. The FETs have 1nm SiO2 and 2nm HISION/TiN/polySi-capped gate stacks with an effective oxide thickness of about 1.1μm. The body of the devices are lightly doped p-type at 2x1015/cm3. Each FinFET is configured as a gated diode with
n+/p−/p+ with a fin length of 500nm, fin height of 80nm, and fin width of 50nm. For a single set of contacts, 500 fins are connected in parallel.

Extensive electrical measurements on these devices have been reported by Young et al.[2][3] In order to increase the defect density and maximize the size of the resonance response, we have irradiated the FinFETs to 1 Mrad via a Co60 gamma source. Pre-irradiated EDMR spectra are weak to below detectable limits whereas quite strong signal to noise spectra appear after the irradiation. Our EDMR measurements utilized a home-built spectrometer. The X-band (9.5 GHz) spectrometer includes a 4-inch Lakeshore electromagnet with a Micro-Now microwave bridge and a TE102 cavity. Spin dependent device current was measured with a Stanford Research Systems Low-Noise Current Preampifier. The detection utilized a home-built virtual lock-in amplifier. Measurements were conducted at room temperature. Our results are significantly different from what is observed in both conventional EPR and EDMR measurements of irradiated and unirradiated planar MOSFETs. In planar MOSFETs, the magnetic resonance due to defects at the interface is dominated by defects in the P+ family. The g tensor components of the P+ centers vary from approximately 2.0012 to 2.0083. The zero-crossing g’s of the rather broad lines that we observe are within this range; however, the breadth of the spectra, about 25 Gauss are much larger than one would anticipate for P+ centers. Assuming the full range of g values found for the P+ centers, one would anticipate an overall linewidth of about 12 or 13 Gauss. The FinFET resonance is much sharper, centered near zero field. This is consistent with the observation of a perpendicular resonant field as the magnetic field is swept through zero applied field. We study 25 nm a-Si:N:H samples with N/ Si ratios of 1, 1.35, and 1.5. High frequency and low frequency measurements provide us with information about defect structure, as they allow some separation of spin orbit coupling and electron nuclear hyperfine interactions. The measurements also directly indicate that these defects are involved in electronic transport through these films. A comparison of EDMR measurements taken at high frequency and low field and frequency and field identify the primary defect responsible for transport through these films as a Si dangling bond such as the K center. An identical central resonance condition is observed in all three stoichiometricss, consistent with this Si dangling bond. The high frequency EDMR measurements show that the Si rich samples exhibit a different response than the N rich and stoichiometric samples. A comparison of high and low field EDMR indicates that in the Si rich samples, Si replaces some P+ centers. Most significantly, this work demonstrates the potential of EDMR to study point-defects in FinFETs. Our results, although preliminary in nature, strongly indicate that although P+ like defects likely play important roles in the Si/SiO2 interface, the defect spectrum is more complex than is the case in conventional planar MOSFETs. This project is sponsored by the Department of Defense, Defense Threat Reduction Agency under grant number DTRA1-16-0008. The content of the information does not necessarily reflect the position or the policy of the federal government, and no official endorsement should be inferred.[1] Wann, C. H., Noda, K., Tanaka, T., Yoshida, M., & Hu, C. (1996). IEEE Transactions on Electron Devices, 43(10), 1742-1753.; [2] Young, C. D., Neugroschel, A., Matthews, K., Smith, C., Heh, D., Park, H., … Bersuker, G. (2010). IEEE Electron Device Letters, 31(7), 653–655.; [3] Young, C. D., Neugroschel, A., Matthews, K., Smith, C., Park, H., Hussain, M. M., … Bersuker, G. (2010). Proceedings of 2010 International Symposium on VLSI Technology, System and Application, VLSI-TSA 2010, 68–69.

9:00 AM MM03 (Student) High and Low Field Electrically Detected Magnetic Resonance in Various Stoichiometry Silicon Nitride Thin Films—A Comparative Study

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Leakage currents in dielectric thin films utilized in current day integrated circuitry are important technological issues. Amorphous hydrogenated silicon nitride (a-Si:N:H) thin films are currently utilized in passivating layers, etch stop layers, diffusion barriers, and gate dielectrics. Previous electron paramagnetic resonance (EPR) and electrically detected magnetic resonance (EDMR) studies have identified the K center, a silicon dangling bond backbonded to three nitrogen atoms, as the primary paramagnetic defect in stoichiometric (Si,N)x films. [1] However, the effects of varying N/Si stoichiometry on defect levels and defect chemistry have not been extensively studied with EDMR. In this study, we expand upon the work by Mutch et al. by comparing the EDMR and near-zero field magnetoresistance responses of stoichiometric, Si rich, and N rich films of a-Si:N:H (Si+ N) films. The magnetoresistance (MR) phenomena, [2] changes in MR with change of device current when a low magnetic field is applied, is also a current topic of interest in many materials systems. The MR phenomena is most commonly studied in “messy” organic semiconductor structures; however, a similar effect is also observed in inorganic semiconductor and semiconductor/insulator structures. Inorganic materials systems that are extensively used in integrated circuits have been very well characterized, providing advantages over organic systems for the study of the MR phenomena. The device structures under observation consist of Ta/Si:N/H/P+Si capacitors. In all measurements presented in this study, a slowly varying magnetic field is applied to the thin film under bias. For the EDMR measurements, an oscillating microwave frequency magnetic field (10–100 MHz) and radio frequency magnetic field (v=250MHz) is applied perpendicular to the quasi-static field. As in conventional EPR, energy is absorbed by paramagnetic sites when the resonance condition is met. In the simplest cases, this resonance condition is expressed by hv=gμBB, where h is Planck’s constant, v is the frequency of the applied microwave/radiofrequency field, g is an orientation dependent parameter typically close to 2, μ is the Bohr magneton, and B is the magnetic field at resonance. In EDMR, the EPR transition is observed through a change in device current. The MR response is observed without the presence of a perpendicular magnetic field and is swept through zero applied field. We study 25 nm a-Si:N:H samples with N/ Si ratios of 1, 1.35, and 1.5. High frequency and low frequency measurements provide us with information about defect structure, as they allow some separation of spin orbit coupling and electron nuclear hyperfine interactions. The measurements also directly indicate that these defects are involved in electronic transport through these films. A comparison of EDMR measurements taken at high frequency and low field and frequency and field identify the primary defect responsible for transport through these films as a Si dangling bond such as the K center. An identical central resonance condition is observed in all three stoichiometricss, consistent with this Si dangling bond. The high frequency EDMR measurements show that the Si rich samples exhibit a different response than the N rich and stoichiometric samples. A comparison of high and low field EDMR indicates that in the Si rich samples, Si replaces some P+ centers. Most significantly, this work demonstrates the potential of EDMR to study point-defects in FinFETs. Our results, although preliminary in nature, strongly indicate that although P+ like defects likely play important roles in the Si/SiO2 interface, the defect spectrum is more complex than is the case in conventional planar MOSFETs. This project is sponsored by the Department of Defense, Defense Threat Reduction Agency under grant number DTRA1-16-0008. The content of the information does not necessarily reflect the position or the policy of the federal government, and no official endorsement should be inferred.[1] Wann, C. H., Noda, K., Tanaka, T., Yoshida, M., & Hu, C. (1996). IEEE Transactions on Electron Devices, 43(10), 1742-1753.; [2] Young, C. D., Neugroschel, A., Matthews, K., Smith, C., Heh, D., Park, H., … Bersuker, G. (2010). IEEE Electron Device Letters, 31(7), 653–655.; [3] Young, C. D., Neugroschel, A., Matthews, K., Smith, C., Park, H., Hussain, M. M., … Bersuker, G. (2010). Proceedings of 2010 International Symposium on VLSI Technology, System and Application, VLSI-TSA 2010, 68–69.

9:20 AM MM04 Transition Metal Hydrogen Interactions in P-Type Silicon Under Illumination Jack Mullins1, Vladimir Markевич1,1, Ian Hawkins1, John Murphy1, Matthew Halsall1 and Anthony R. Peaker1;1; 1School of EE, University of Manchester, Manchester, United Kingdom; 2Photon Science Institute, University of Manchester, Manchester, United Kingdom; 3School of Engineering, University of Warwick, Warwick, United Kingdom.

Hydrogen treatments are used extensively in established silicon technologies to reduce surface and interface recombinations. It has been proposed that hydrogenation could also be used to improve the minority carrier lifetime of silicon when lifetime degradation is due to transition metal contamination. Such contamination is often the case for low cost "solar" silicon where purification and/or crystal growth processes are less rigorous than for electronic grade material. The problem is particularly severe for the so-called “early” transition metals (lower atomic numbers) which have low diffusivities and cannot be getters by conventional methods. Much work has been published on hydrogen in silicon and it is evident that in n-type silicon reactions between hydrogen and some TMs can result in passivation or reduced recombination rates [eq. 1]. Peaker et al Hydrogen-related defects in silicon, germanium, and silicon–germanium alloys, in: Defects in Microelectronic Materials and Devices, eds D. Fleetwood et al. (Taylor & Francis,Boca Raton, 2009), pp. 27–55. However in general, the bonding between hydrogen and the TMs is weak (~2 eV) and so the hydrogen is dissociated at temperatures well below those experienced in device processing. Hydrogen can only be very marginally retained in silicon but its reaction with TMs (and other defects) is highly dependent on the charge state relative to the defect or impurity. Predominantly, the reaction is driven by long range Coulombic interactions. Atomic hydrogen is an amphoteric impurity with negative-U ordered donor and acceptor levels at E−0.18 eV and E−0.65 eV. The neutral state is metastable. Isolated hydrogen occurs in the positive charge state in p-type Si, while it is negatively charged in n-type. As the H+1 occupancy level lies in the upper half of the band gap it would be expected that in intrinsic Si (mid-gap Fermi level) the H+ charge state will dominate. Experimentally, there is evidence that H+ is the stable form when the Fermi level is ~0.3 eV above the mid gap energy. The end result is that in n-type Si reactions between hydrogen and transition metal occur while in p-type Si, the thermodynamic field occurs under equilibrium conditions. There are no data on p-type reactions although we have published results on some TM-hydrogen reactions in the depletion region of a Schottky diode on p-type silicon … whether such a reaction occurs or not depends on the charge state of the TM with a near mid-gap Fermi level. Recently important increases of minority carrier lifetime have been demonstrated in multi-crystalline p-type silicon when hydrogenated at elevated temperatures under strong illumination [eq. B. Hallam et al, IEEE J. Photovolt. 99, 1 (2013); S. Wenham et al., Advanced hydrogenation of silicon solar cells, U.S. Patent 9,190, 556, Nov 2015]. It has been proposed that this is due to the passivation of TMs. We have undertaken a systematic study into the hydrogenation of p-type single crystal silicon after and during illumination under magnetic field conditions. We have investigated unintentionally contaminated with specific TMs, namely Mo, V, and Fe. In this report we focus on molybdenum. We have used DLTS, Laplace DLTS and capacitance-voltage measurements to study the formation of TM−H...
Niobium nitride (NbN) is a refractory compound material which undergoes a transition to the superconducting state at a temperature (~7K), significantly higher than that of elemental Niobium (9.3K). For this reason, NbN thin films are currently used in superconducting electronic applications. It has been demonstrated that NbN thin films can be grown epitaxially on silicon carbide (SiC), aluminum nitride (AlN), and gallium nitride (GaN) substrates by a variety of deposition techniques. We present here the growth of heterostructures incorporating superconducting/metallic NbN thin films with III-nitride semiconductor films by plasma assisted molecular beam epitaxy (PAMBE). The growth is performed using an electron beam evaporation source for niobium, an RF plasma nitrogen source, and an effusion cell provides the source of gallium. NbN film growth has been performed for substrate temperatures ranging between 700°C up to 1150°C on GaN substrate and above 1300°C on SiC substrate. We demonstrate optimization of structural and superconducting properties of epitaxial NbN films on GaN, and SiC substrates as a function of substrate temperature, growth rate, and the ratio of niobium and nitrogen fluxes. We conclude that the crystalline phase, stoichiometry, and electrical properties of NbN films grown by PAMBE are highly sensitive to substrate temperature and the ratio between the flux of Nb and N. Root mean squared surface roughness of optimized NbN films on GaN or SiC substrate as measured by atomic force microscopy (AFM) for 1μm² area are approximately 0.5nm. Superconducting critical temperatures in excess of 15K are demonstrated for films as thin as 20nm. The resistivity and superconducting transition are shown to be highly dependent on growth conditions, though NbN thin films reliably exhibit metallic electronic properties above the critical temperature with resistivities of approximately 150μΩ-cm, making NbN significantly more resistive than most metals commonly used in semiconductor devices. We also compare the structural and electronic properties of NbN films grown on SiC and GaN as characterized by x-ray diffraction (XRD), atomic force microscopy (AFM), transmission electron microscopy (TEM), electron back-scatter diffraction (EBSD), I-V measurements of resistivity, and Rutherford backscattering spectroscopy (RBS). Structural differences, symmetry mismatch, and lattice parameter misfit between NbN, SiC and GaN are shown to be responsible for observed differences in the properties and optimized growth parameters between NbN films grown on GaN and those grown on SiC.[DJ] The all-epitaxial nitride superconductor/semiconductor materials system composed of NbN, AlN, GaN, InN and their alloys enables novel interfaces between established semiconductor devices and superconducting devices. We demonstrate a high performance III-nitride high electron mobility transistor (HEMT) incorporating electronic transport through a buried superconducting NbN thin film. In addition, the ability to fabricate all-epitaxial semiconductor/ superconductor heterojunctions enables exploration of new phenomena and devices utilizing the interface between electrons in the superconducting state with the range of electronic phenomena possible in III-N heterostructures. Electronic transport across an epitaxial interface between NbN source and drain contacts and a high mobility two-dimensional electron gas (2DEG) state at an AlGaN/GaN interface is demonstrated and characterized in both the superconducting and normal states, utilizing the field effect to modulate the density of carriers in the 2DEG. Epitaxial all-nitride Josephson junctions utilizing novel epitaxial tunneling barrier materials are currently being explored and preliminary results will be presented.
Laterally Overgrown Inside Dielectric Templates

Araanya Goswami, Daniel J. Pennnachio, Brian Markman, Hsin Ying Tseng, Simone Tommaso Suran Brunelli, Sukgeun Choi, Aidan Taylor, Jonathan Klaiber, Mark Rodwell and Chris J. Palmstrom1. Materials Department, University of California, Santa Barbara, Santa Barbara, California, United States; Electrical and Computer Engineering Department, University of California, Santa Barbara, Santa Barbara, California, United States.

Laterally grown III-V epitaxial layers offer multiple advantages over conventional vertically grown layers for fabricating advanced semiconductor devices. Etching vertical structures to define 30nm thick fins is a challenge and leads to considerable damage of the device structure, while lateral devices with pre-fabricated templates can be easily used to achieve lower thicknesses. Growing lateral devices on top of dielectric films also eliminates leakage currents through conducting substrates. A promising approach to laterally grow epitaxial films by using dielectric templates to confine the growth and its direction. This technique was originally developed for Si[1,2] and later used for integrating III-V semiconductor device structures with conventional Si technology[3,4]. Structural properties of these epitaxial layers grown on confined structures is required for optimizing and improving device performance. Owing to the sub-micron scale of these embedded epitaxial layers, it is challenging to characterize them. Here we present scanning electron microscopic (SEM) and transmission electron microscopic (TEM) studies of InP Confined Epitaxial Lateral Overgrowth (CELO) structures grown on chemical beam epitaxy (CBE) and organic chemical vapor deposition (MOCVD) on patterned InP (001) and InP (110) substrates. We discuss the influence of growth conditions on parasitic nucleation, evolution of facets and nature of defects. The dependence of facet planes on the growth direction and substrate orientations, and the effects of patterning procedures and geometry of the confined structures on crystal quality and yield is also explored. We further show growth and characteristics of CELO heterostructures. For CBE, the growths were performed in a VG-Semicon V80H system using phosphine (PH3) and trimethylindium (TMI) as precursors with temperatures varying from 470-520 °C. The results show a clear dependence of selectivity and facet formation on growth. Etching the top oxide layer of a CBE overgrowth SEM, shows that the facets are dependent on the growth directions. Vertical facets form in structures growing in the [110]-direction, while [001] oriented overgrowths show slanted [111]B facets for a InP(110) substrate. The facets are consistent with those expected from a general zincblende structure. Cross sectional TEM images confirm these facets, while also revealing stacking faults in the [111] plane propagating throughout the growth in the structures oriented along the [100] direction. However, the growth interface at the seed hole shows excellent crystal quality and appears to be a continuous defect free crystal lattice, suggesting that the stacking faults do not form until a [111] facet forms during the growth. Preliminary analysis show both the (110) and the (001) oriented InP wafers exhibiting similar stacking fault densities, while a reduction of the fault density is observed at higher temperatures. The TEM results consistently show a depression of the CELO box above the seed hole which has been solved in subsequent fabrication by using a spin-on resist-based process. Scanning TEM imaging carried out on a MOCVD grown CELO InP/InAs heterostructures that show extremely sharp heterojunctions, up to a few micrometers thin, can be realized in a lateral direction using this template-based growth technique. This provides a path to fabricate highly efficient lateral tunnel FETs [5]. This work was supported in part by National Science Foundation and Semiconductor Research Corporation.[1] A. Ogura et al., Appl. Phys. Lett. 57, 2806[1989][2] P.J. Schubert et.al. IEEE Elec. Dev. Lett.11,181[1990][3] L. Czornomaz et al. 2015 Symp on VLSI Tech. Dig. of Technical Papers T72[4] M. Ogura et.al. IEEE Trans. Elec. Dev.63,4233[2016][5] Long et al. IEEE Electron. Dev. Lett. 37, 345 (2016)

11:00 AM NN03

(A) Self-Formed Embedded Conical-Like Air Voids in MBE-Grown Gallium Arsenide

Alic M. Skipper, Daniel J. Ironside and Seth Bank;
The University of Texas at Austin, Austin, Texas, United States.

Patterned air gaps integrated with high-quality epitaxial semiconductors have wide ranging potential applications, including high-contrast phononics, gas sensing, and opto-fluidics [1, 2]. For example, encapsulated air gratings can be exploited to replace Bragg reflectors in VCSELs, create high-resonance sensors, and/or utilize Fano resonance for all-optical switching. However, it is difficult to integrate these structures with standard III-V optoelectronic devices without compromising material quality as conventional III-V growth techniques offer limited lateral control and other techniques, such as wafer bonding of patterned structures, can introduce interfacial defects. Previous attempts to create air gaps in zincblend III-V semiconductors have been limited in shape and size [3] and silicon-based processes damage the surface of the material Recently, we showed that tailored molecular beam epitaxy (MBE) can be used to encapsulate patterned silicon dioxide structures into a high-quality crystalline III-V matrix, yielding monolithically integrated high contrast photonic structures [4]. Here, we present the successful fabrication of nanometer-scale air cavities in GaAs with scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR). Complete etching was confirmed by monitoring the silicon dioxide phonon absorption resonance at 800 cm-1. Finite-difference time-domain (FDTD) simulations were used to evaluate potential applications of these structures. This work establishes a basis for improved high-contrast photonics and opens up new potential applications, including lab-on-a-chip sensing via seamless integration of micro-fluidics with III-V semiconductor photonic devices. This work was supported by the National Science Foundation (NSF-ECCS-1408302).References[1] C. Chang-Hasnain et al., Adv. Opt. Photon., 4, 379-440 (2012)][2] M. de Boer et al., Journal of Micromechanical Systems, 9, 1, 94-103 (2000)][3] For example M. Nishimoto et al., Appl. Phys. Express, 6, 62002 (2013)][4] D. Ironside et al., 59th Electronic Materials Conference (2017).
Heteroepitaxy Using Epitaxial Lateral Overgrowth Daniel J. Ironside1, Pankul Dhingra2, Alec M. Skipper3, Minjoo L. Lee4 and Seth Bank5; 
1University of Texas at Austin, Austin, Texas, United States; 2Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, United States.

Heteroepitaxy of lattice-mismatched materials has garnered renewed interest in recent years, as new mechanisms are sought for substrate-invariant growth of high-quality epitaxial layers with repeatable, reliable device performance. Several methods of relaxed heteroepitaxy have been proposed [1] including a variety of graded buffer schemes, aspect ratio trapping, and strained superlattice dislocation filters. One technique that has demonstrated particular promise is epitaxial lateral overgrowth (ELO) [2,3], a growth approach where small openings in dielectric-patterned substrates act as seeds for heteroepitaxial growth. Using a highly selective lateral growth process, propagating defects are localized to the small seed regions resulting in large relatively defect-free regions located immediately above the patterned dielectric layers. ELO has been previously demonstrated on several III-V binaries such as GaN/Sapphire and GaAs/ Si substrates on patterned SiO2, and/or SiN dielectric masks using MOCVD and LPE crystal growth techniques, respectively. Recently, we developed ELO for all-MBE, growth of planar encapsulation of dielectric microstructures in homoepitaxial GaAs on (001) oriented substrates [4]. Drawing on this capability, we extend this work to planar encapsulation of dielectric masking layers in large lattice-mismatch heteroepitaxial III-V MBE growth. As a test bed system, we explore the defect reduction in the device regions on InAs/GaAs from ELO of silicon dioxide layers. To this end, we show the first demonstration of ELO metamorphics using an all-MBE approach, achieving in planar coalescence of ELO InAs on (001) GaAs substrates and resulting in a ~1.3x improvement in photoluminescence (PL) and ~2–3x reduction of threading defect densities (TDD) relative to an equivalent InAs/GaAs control. Samples were grown by solid-source molecular beam epitaxy (MBE) in an EPM Model Gen II system on n-doped (001) GaAs substrates. After an initial growth of 300nm GaAs, a 500nm InAs metamorphic buffer layer was relaxed using the interfacial misfit array (IMF) technique. Then, a 25nm thin silica dielectric mask was deposited and patterned in the form of gratings at a 50% duty cycle, with pitches ranging between 1.4–2.2µm. Using MBE growth under highly selective growth conditions, InAs was grown until planar coalescence was achieved, resulting in a total growth over the patterned dielectric of ~2.25µm. For comparison, an InAs/GaAs control was grown using the identical growth layer thicknesses. Under the best grown conditions, PL of the ELO-InAs showed a ~1.3x improvement in relative PL intensity compared to control. Additionally, surface TDD was estimated using electron-channelling contrast imaging (ECCI), which showed a ~2–3x reduction in dislocation density in ELO-InAs as compared to the control. This work was supported by the National Science Foundation (NSF-ECCS-1408302).References:[1] For a recent review, J.A. Ayers, Heteroepitaxy of Semiconductors: Theory, Growth, and Characterization, CRC Press, 1st Edition (2007). [2] Z.R. Zytkowski, Thin Solid Films (2002). [3] T. Nishimaga, J. Cryst. Growth (2002). [4] D.J. Ironside et al., 59th Electronic Materials Conference (2017).
Chern Insulator $\text{Bi}_2\text{Se}_3/\text{Bi}_4\text{MnSe}_3$ Multilayer Heterostructures  

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Engineering exotic topological states motivates extensive contemporary research in topological materials, including research of magnetic topological insulators as a materials platform for the study of interactions between topological surface states and symmetry-breaking magnetic ordering. We report the results of a study that identifies several topologically nontrivial phases in $\text{Bi}_4\text{MnSe}_3$ that depend on the magnetic ordering and on the number of layers in a slab configuration. In stoichiometric bulk, the material is predicted to be an antiferromagnetically ordered strong $(Z2)$ topological insulator, which transforms into a magnetic Weyl semimetal when the spins are aligned ferromagnetically. In a magnetic Weyl semimetal, 2D slices of $k$-space between the pair of Weyl points have a non-trivial Chern number, calculated from the integral of the Berry curvature over a closed manifold in the Brillouin zone, forming the material's Hall conductivity proportional to the separation between the Weyl points, as well as unusual features like surface Fermi arcs. When the material is reduced to 1–2 layers it is topologically trivial, while increasing the thickness above three layers is predicted to result in a band inversion and a 2D Chern insulating phase, which displays quantized anomalous Hall conductivity. Furthermore, the magnetic ordering and topological behavior can be modulated by, for example, adjusting the separation between $\text{Bi}_4\text{MnSe}_3$-layers by layers of $\text{Bi}_2\text{Se}_3$. $\text{Bi}_4\text{MnSe}_3$ is formed by the intergrowth of $\{111\}$ planes of rock-salt MnSe with quintuple layers of $\text{Bi}_2\text{Se}_3$, and has been previously demonstrated to grow in a self-assembled multilayer heterostructure with layers of $\text{Bi}_2\text{Se}_3$, when grown by molecular beam epitaxy (MBE), where the number of $\text{Bi}_2\text{Se}_3$ layers separating the single $\text{Bi}_4\text{MnSe}_3$ layers is approximately defined by the relative arrival rate of Mn ions to Bi and Se ions during growth [1]. The compositional, structural, and electronic properties of these $\text{Bi}_4\text{MnSe}_3/\text{Bi}_2\text{Se}_3$ self-assembled heterostructures are presented. We support a model for the epitaxial growth of $\text{Bi}_4\text{MnSe}_3$ in a near-periodic self-assembled heterostructure with $\text{Bi}_2\text{Se}_3$, with corresponding theoretical calculations of the energetics of this material and those of similar compositions. 

Computationally derived electronic structure of these heterostructures demonstrates the existence of topologically nontrivial edge states at sufficient thickness. We report optical and electronic properties of this material with different concentrations of Mn, and therefore different average separations between $\text{Bi}_4\text{MnSe}_3$ layers, to explore the physics of this topologically non-trivial material. J. A. Hagmann et al., *New J. Phys.*, 19, 085002 (2017).

9:40 AM O005  

(Student) Charge-Density-Wave Transformation Induced by Ion Doping into 1T-TaS$_2$  

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Phase transitions along with electronic property changes in two-dimensional (2D) materials demonstrate potentials in novel devices for beyond-CMOS applications. One interesting 2D material is 1T-Tantalum Sulfide (1T-TaS$_2$), which exhibits a series of charge density waves (CDW) and periodic lattice distortions. One of its phase transitions (known as multiorbital-insulator to metal, MIT) is from near-commensurate CDW (NCCDW) phase to commensurate CDW (CCDW) phase with about 10-100x resistivity increase. Harnessing the physics of electron correlation and electronic phase transitions in this material could potentially help enable field-effect devices with performances beyond the limitations of Silicon. We present our work on directly synthesizing 1T-TaS$_2$ flakes on different substrates (SiO$_2$, sapphire, graphene etc.) by ion beam deposition. With this route, we are able to directly introduce exotic dopants into the material and tune its phase transition properties. The dopants have been evidenced by a complementary characterization tools including XPS, TEM etc. We studied the effects of dopants on 1T-TaS$_2$, phase transitions by both vibrational spectroscopy (Raman) and transport measurements, and that at an optimal level, we could stabilize 1T-TaS$_2$, CCDW phase towards much higher temperatures (100°C higher than the reported transition temperature). The characteristic peak associated with its CCDW phase has been observed by Raman technique at room temperature. This dopant’s stabilization effect has been further supported by our DFT calculations.
the radius and binding energy of the indirect exciton are 3 nm and 75 meV, respectively. In order to include strong electron-hole correlation effects we use real-time Green’s functions evaluated in the self-consistent T-matrix approximation. The screening of the Coulomb interaction by the carriers in both monolayers was included in the plasmon pole approximation of RPA. The chemical potential of free carriers evaluated in the assumption of carrier density for different temperatures. As the density of the electron-hole plasma increases the indirect exciton states are formed and at lower temperatures the system of carriers consist mostly of bound pairs. At higher densities the Mott-type transition occurs as the screening and fermion statistics turn the system into electron-hole plasma. We defined the degree of the ionization as a relative density of free carriers evaluated in the assumption of the thermal equilibrium of excitons and the electron-hole plasma. At lower temperatures the degree of ionization can be as low as 10^3, and the system is the excitonic insulator. At the densities higher than the Mott density the system changes into conducting electron-hole plasma. The results can be useful for the design of novel electronic devices based on heterojunctions of the few-monolayer materials.

11:00 AM OO10
First and Innovative Direct Determination of van der Waals Bonding Energy for 2D Layered Semiconductors Tadao Tanabe, Shu Zhao, Tang Chao, Yohei Sato and Yutaka Oyama; Materials Science, Tohoku University, Sendai, Japan.

Two-dimensional (2D) layered semiconductors have attracted much interest because of their unique crystallographic structure and potential applications. For example, GaSe and InSe are promising for both optical and electronic applications [1,2]. The layered crystals combine thin sheets by out-of-plane van der Waals interactions. For practical applications that use 2D layered semiconductors, the mechanical strength needs to be high. For example, device fabrication processes, such as dicing and wire bonding, require the crystal to be mechanically strong. However, no direct experimental determination has been carried out up to now for van der Waals bonding energy. Therefore, quantitative and direct measurements of the bonding energy are urgently required in order to obtain crucial understandings of 2D semiconductor materials. In this study, a tensile testing machine was constructed for the first quantitative determination of the interlayer van der Waals bonding force, where two stainless steel L-shaped sliders were combined, with a strain gauge between them. As a result, the interplanar binding strength of layered GaSe, Te, and InSe crystals were directly determined using our tensile testing machine, respectively. These crystals were grown by a low and fixed growth temperature liquid phase method under a controlled Se vapour pressure [3]. The stoichiometry-controlled GaSe, Te crystal has the p-type structure of GaSe, where the Te atoms are occupied with some Se sublattice in the GaSe crystal. InSe crystal has the p-type structure. The effect of adding Te on the bonding strength with respect to GaSe layers was determined from direct measurements of the Van der Waals bonding energy [4,5]. The interlayer bonding strength of GaSe, Te (x = 0.106) was about 7 times larger than that of GaSe. The bonding strength was discussed for GaSe and InSe, respectively.[1] S. Takasuna, J. Shiogai, S. Matsuoka, M. Kohda, Y. Oyama, J. Nitta, Phys. Rev. B 96, 161303(R) (2017).[2] M. Suzuki, M. Kohda, S. Takasuna, S. Matsuoka, Y. Sato, T. Tanabe, Y. Oyama, J. Nitta, Jpn. J. Appl. Phys. 57, 020308 (2018).[3] S. Zhao, Y. Sato, K. Maeda, T. Tanabe, H. Ohtani, Y. Oyama, J. Cryst. Growth 467, 107 (2017).[4] T. Tanabe, S. Zhao, Y. Sato, Y. Oyama, J. Appl. Phys. 122, 161505 (2017). JAP Featured Article[5] AIP journal highlights “Opening the Van der Waals’ Sandwich” AIP Publishing in the News: 31 Oct 2017 https://publishing.aip.org/publishing/journal-highlights “Opening the Van der Waals’ Sandwich” AIP Publishing in the News: 31 Oct 2017 https://publishing.aip.org/publishing/journal-highlights/opening-van-der-waals-sandwich

8:20 AM PP01
Alloy Methods to Align ErAs/GaAs Nanoparticles to InAs/GaAs Quantum Dots During MBE Growth Kurt Eyink, Yuanchang Zhang, Krishnamurthy Mahalingam, Brittany Urwin, Madelyn Hill and Lawrence Grazulis; AFRL/RXAN, Wright-Patterson AF, Ohio, United States.

Semiconductor rich earth-V (RE-V) nanoparticles (NPs) epitaxially embedded in lattice matched III-V semiconductor materials attracted considerable research in recent years for their potential applications in thermoelectric, plasmonic, terahertz, and tunneling devices. Hybrid nanostructures are known to elicit an enhanced optical response due to plasmonic coupling effects. It was predicted that InAs quantum dots (QDs) coupled to ErAs NPs in GaAs matrix would get the emission and absorption significantly enhanced by plasmonic energy transfer. To realize the coupling, the frequency match and maximized plasmonic field overlap are both critical. Recently, progress has been made on QD-NP self-
alignment during growth where an inverted InAs QD can be located in the divot formed by GaAs overgrowth of an ErAs NP. However, it is highly desired to get a NP grown directly on top of a QD in order to independently optimize the QD and NP growth. In this work, we use a novel way to direct the alignment of ErAs metal NP and InAs QD using molecular beam epitaxy (MBE) in a GaAs matrix. Strain driven nucleation mechanism allows lightly Er doped InAs QDs self-aligned to underlying InAs QDs. Annealing uncapped Er:InAs QDs at high temperature desorbs the indium atoms in QD. However, due to much lower volatility, Er atoms condense out and nucleate as ErAs NPs that align with the underlying InAs QDs. It was found that the amount of Er incorporated into InAs QD depends on the solubility of Er in InAs, and the Er inhomogeneous distribution in QD and non-uniform indium desorption from QD surface affects NP-QD alignment, and density of ErAs NP is lower than that of InAs QD due to coarsening effects in both InAs QDs and ErAs NPs. The defects are attributed to the rock–salt structure formed by Er atoms taking interstitial sites in InAs lattice and can be eliminated by thorough indium evaporation. With further optimization, the measure opens a new path in precise control of the position of NPs or any nanostructures that starts with formation of NPs in specified locations.

8:40 AM PP02
(Student) On the Formation of ErAs Nanoparticles by Nanosecond Pulsed Laser Ablation Matthew Lewis, Bo E. Tew and Joshua Zide; Materials Science and Engineering, University of Delaware, Newark, Delaware, United States.

The production of ErAs powders via nanosecond pulsed laser ablation in an inert environment allows for the growth of nanoparticle of a desired morphology and quantity for future use in thermoelectric film growth. Targets consisting ofKeyPressed Pressed Er and As elemental powders demonstrate incongruent ablation due to differences in vaporization enthalpy of the two elemental species and mechanical removal of target material. SEM and XRD are used to monitor the elemental and crystalline composition of the powder during growth showing an As:Er ratios that initially reach at least 22:1 within the first 10 minutes of growth, before leveling off to approximately 2:1; suggesting self-limiting vaporization characteristics. The influence of target composition and collection distance are investigated as a means with which to control powder composition and crystallite size. Vapor interaction is controlled by inert gas pressure and laser pulse overlap size is shown to have a significant impact on the overall ErAs composition of the resulting powders; such that increasing vapor interaction increases overall ErAs composition. These growth conditions are then used to demonstrate improved control over nanoparticle morphology and composition.

9:00 AM PP03
Band Structure Engineering and Control of Magnetoresistive Behavior in Lutetium Monopnictides via Epitaxial Strain Shouvik Chatterjee1, Hadass Inbar2, Anderson Janotti3 and Chris J. Palmstrom4; 1Electronics & Computer Engineering, University of California, Santa Barbara, Goleta, California, United States; 2Materials Science & Engineering, University of Delaware, Newark, Delaware, United States; 3Materials, University of California, Santa Barbara, Santa Barbara, California, United States.

Epitaxial integration of rare-earth monopnictides with III-V semiconductors has been of tremendous interest over the past few decades due to their numerous potential applications including buried metallic contacts in semiconductors, infra-red and terahertz optoelectronic devices, thermoelectrics and solar cells. In recent years, these compounds have also been shown to exhibit remarkably large magnetoresistive behavior, with a pressure-temperature phase diagram that bears resemblance to other extreme magnetoresistance materials indicating a similarity in the underlying physics responsible for such a behavior in disparate material systems. Possessing a simple rock-salt structure with a lattice constant that is closely matched to a variety of III-V semiconductors, rare-earth monopnictides offers an exciting materials platform to both understand and tune their remarkable magnetoresistive properties. To that end, we have successfully synthesized (001) LuSb and LuBi thin films on (001) GaSb substrates that show large magnetoresistance (1.8×104 and 1.1×104 at 14 Tesla, 2K for LuBi and LuSb, respectively). Our films are smooth, single-phase, epitaxial and show 1×1 reconstruction in Reflection High Energy Electron Diffraction (RHEED). Using a combination of magneto-transport studies and ab-initio calculations we establish that a perfect electron-hole compensation in these semi-metallic films is the likely mechanism for their remarkable magnetoresistance behavior. Additionally, we have also synthesized epitaxially strained pseudomorphic thin films on lattice mismatched substrates that allows us to break the cubic symmetry of the rock-salt structure. By doing so, we can control the relative occupation of the electron and hole bands that brings about a dramatic change in their magnetoresistive properties. We will show how our ability to controllably tune the electronic structure via strain engineering helps us gain important insights into their emergent magnetoresistance behavior. Furthermore, our ability to synthesize these rare-earth monopnictides in a thin film form also allows us to dimensionally confine these electronic states in the out-of-plane direction that results in the formation of quantum well states with quasi 2-dimensional transport properties. Recently, it has been proposed that it is possible to bring about a band-inversion between the rare-earth d and pnictogen p states that will make these materials topologically non-trivial with strongly spin-orbit coupled surface states. We have observed strong weak anti-localization in transport that can be fitted well with expectations from Hikami-Larkin-Nagaoka theory, which has also been seen in other topologically non-trivial thin films such as Bi2Te3. We will discuss our experimental results considering the possibility of topologically non-trivial surface states in LuSb and LuBi thin films.

9:20 AM PP04
An Atomistic Approach to Studying Phonon Scattering of Embedded Nanoparticles Joseph P. Feser and Rohit K. Kakodkar; Mechanical Engineering, University of Delaware, Newark, Delaware, United States.

Nanoparticle-in-ally material systems are promising candidates for high efficiency thermoelectric materials, due to their greatly reduced lattice contribution to thermal conductivity. In this talk, we use a recently developed frequency-domain perfectly matched layer computational technique to calculate the scattering cross sections of embedded nanoparticles across the entire Brillouin zone and for all phonon modes including transverse acoustic phonons and optical phonons for the first time. For acoustic modes, we compare the computational results against previously used results from continuum mechanics and find excellent agreement so long as the Mie regime is accurately represented within the continuum framework. Interestingly, we find that the interaction of optical phonons is remarkably different compared to its acoustic counterparts, with scattering efficiencies of optical phonons in the “Rayleigh” regime scaling independent of vibration frequency and with orders of magnitude higher scattering efficiency. We are that optical phonons should be viewed in the context of zone folding to be a folded continuation of very short wavelength acoustic phonon spectrum. Furthermore, we directly show that an interdiffused nanoparticle/matrix is more effective at scattering phonons compared to solids nanoparticle with the same net impurity concentration, with scattering efficiencies 2-fold higher in the dominant heat carrying regions.

9:40 AM PP05
(LATE NEWS) GaAsNBi Alloys—Lattice-Matching and Energy Bandgaps Jordan Oceana1, T. Jen1, W. Linhart2, Robert Kudrawiec2 and Rachel S. Goldman1; 1Department of Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; 2Department of Experimental Physics, Wroclaw University of Technology, Wroclaw, Poland.

Due to their significant bandgap narrowing, dilute nitride alloys are promising for concentrating photovoltaics expected to power the next generation. However, N-related point defects often lead to degraded minority carrier transport properties and optical efficiencies. Co-allying of GaAsN with larger elements, such as indium, antimony, and/or bismuth, allows lattice-matching to GaAs or Ge substrates. Of particular interest is GaAsNb, which is expected to provide the largest bandgap reductions, with tunable valence band and spin-orbit energy level splittings, which are also promising for temperature insensitive lasers and high selectivity spin valves. In the literature, the magic ratio for lattice matching of GaAsNb with GaAs is predicted to be x=0.59, based upon a computed value of the GaBi lattice parameter. In addition, the relationship between the bandgaps and the bandgap values are most often determined using x-ray rocking curve (XRC) measurements of strain to determine the alloy compositions, assuming the computed value of the GaBi lattice parameter, with films fully strained to GaAs substrates. Here, we use a combination of direct measurements of alloy compositions, via ion beam mass analysis of the N and Bi compositions, in conjunction with direct measurements of the out-of-plane misfit via XRC measurements of “x-ray strain”, and measurements of bandgap using photoreflectance spectroscopy, to determine a new magic ratio for lattice-matching and a new map of the quaternary bandgaps. The implications of these findings on future device design will be discussed.

10:00 AM BREAK
SESSION QQ: Narrow Bandgap Materials and Devices Session Chairs: Jamie Phillips and Kunal Mukherjee
Friday Morning, June 29, 2018 Location: University Center, Lobero

10:20 AM QQ01 (Student) Understanding the Effects of Strain and Relaxation on GaAsBi for Semiconductor and Semimetal Device Applications
Manuel A. Stevens, Kevin Grossklaus, John H. McElearney and Thomas E. Vandervorst Electrical and Computer Engineering, Tufts University, Medford, Massachusetts, United States.

GaAs$_{1-x}$Bi$_x$ grown on GaAs and InP substrates is an attractive material for small band gap semiconductor and semimetal applications. Due to the valence band anti crossing effect (VBAC), the band gap of GaAs$_{1-x}$Bi$_x$ is reduced up to 84 meV/1%Bi [1], allowing for new band gap lattice constant combinations that were previously unavailable through epitaxial growth. Most work on GaAsBi has looked at fully pseudomorphic layers grown on GaAs substrates and have reached Bi incorporation up to 22% (GaAs$_{0.78}$Bi$_{0.22}$) [2]. Although high incorporation percentages have been achieved in GaAsBi, the resulting small band gap materials have a long way to go to be implemented in high quality, small band gap devices. Previous work on high Bi content GaAs$_{1-x}$Bi$_x$ has relied on samples grown on GaAs substrates to prevent strain relaxation and were plagued by surface droplets and defects that prevented high quality, thick films from being created. In this work, we explored strained and relaxed interlayers between the substrate and the epitaxial film to study the effects on the crystalline quality and bismuth incorporation in thick films of GaAsBi (>250nm). We propose that strained under-layers may affect the incorporation of bismuth atoms in GaAs by providing a way to alleviate the local strain induced by the large atomic size difference between the Bi and As atoms. We grew our samples on a Veeco GENxplor MBE using a valved As$_4$ source and an effusion cell for our bismuth source. To determine the bismuth content in our films, we used 004 and 224 HRXRD scans to analyze the lattice constant and spectroscopic ellipsometry to determine the band gap. We fit these parameters to the predicted band gap lattice constant curves determined experimentally [1,3]. We characterized the degree of strain relaxation by examining reciprocal space maps around the 224 asymmetric reflection. We additionally used TEM to identify defect centers and through-film compositional variation. We examined structures of GaAs$_{1-x}$Bi$_x$/InGaAs/GaAs with InGaAs layers of varying thickness and indium content. This allowed us to look at the effects of both tensile and compressive strain on our bismide layers. Lessons learned from these techniques can be translated to higher Bi content materials in order to achieve smaller band gap semiconductors with reduced defect densities on GaAs and InP substrates.[1] S. Adameyko, and T. Tiedje Appl. Phys. Lett. 82 14 (2003)[2] R.B. Lewis, M. Masnadi-Shirazi, and T. Tiedje Appl. Phys. Lett. 101 082112 (2012)[3] M. Masnadi-Shirazi et al. J. Appl. Phys. 116 223506 (2014)

10:40 AM QQ02 (Student) Comparison of Tensile-Strained Ge Quantum Dots and Nanowires Embedded in InAlAs Pankul Dhingra1, Daechwan Jung2, Brendan C. Eng1 and Minjoo L. Lee3; 1Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Champaign, Illinois, United States; 2Institute of Energy Efficiency, University of California, Santa Barbara, Santa Barbara, California, United States.

Theoretical calculations show that a biaxial tensile strain of 1.4-2.0% can convert Ge into a direct-gap semiconductor.[1] Large biaxial tensile strains up to 2.3% have been demonstrated by epitaxial growth of thin Ge layers on materials with larger lattice constant, such as InGaAs and GeSn.[2,3] Recently, we demonstrated a method to grow tensile-strained Ge nanowires (NWs) embedded in an In$_{0.65}$Ga$_{0.35}$As (hereafter InAlAs) matrix using surface-mediated phase separation; the lattice constant of InAlAs is 3.7% higher than Ge.[4] Here, we demonstrate that tensile-strained Ge quantum dots (QDs) can be grown through a similar growth mode. Comparing tensile Ge QDs with NWs grown under similar conditions, we find that Ge QDs are larger and more anisotropic in shape than NWs, while exhibiting a similar Raman shift and broader room-temperature photoluminescence (PL). We conducted growth of tensile-strained Ge nanostructures using a 3-IV molecular beam epitaxy (MBE) system equipped with a Ge effusion cell. All growths started with a lattice-matched InAlAs buffer grown on an InP (001) substrate. A 500 nm nanocomposite layer consisting of either Ge QDs or NWs in InAlAs was then grown by co-deposition of Ge, In, Al and As. For NW growth, all shutters were opened simultaneously, while for QD growth the Ge shutter was periodically opened and closed to form QD superlattices; the Ge content of the nanocomposite layers ranged from 1.4-10%. High-angle annular dark field scanning-transmission electron microscopy and energy dispersive x-ray spectroscopy (EDX) revealed that Ge nanostructures had phase segregated in both the NW and QD nanocomposites. Polarized single photons [2] showed a 10+ difference in the planar density of NWs and QDs at 6×10$^{10}$ cm$^{-2}$ and 6×10$^{11}$ cm$^{-2}$, respectively. The wide disparity in density can be partly explained by the fact that NWs tend to branch throughout growth, effectively multiplying their density. In contrast, QD growth is interrupted every 10 nm, which prevents such branching from occurring. For similar growth conditions, electron channeling contrast imaging (PV-ECCI) showed a 10+ difference in the planar density of NWs and QDs at 6×10$^{10}$ cm$^{-2}$ and 6×10$^{11}$ cm$^{-2}$, respectively. The wide disparity in density can be partly explained by the fact that NWs tend to branch throughout growth, effectively multiplying their density. In contrast, QD growth is interrupted every 10 nm, which prevents such branching from occurring. For similar growth conditions, QDs showed a strongly anisotropic shape lengthened along the direction, while NWs were more isotropic. Thus, QDs form lower density and more anisotropic nanostructures with a larger in-plane size compared to the NWs. Raman spectroscopy showed that both Ge QDs and NWs exhibit an identical Ge-Ge peak at 284.1 cm$^{-1}$ corresponding to a shift of 16.0 cm$^{-1}$ from the bulk Ge-Ge phonon mode at 300.1 cm$^{-1}$. The shift in the Ge-Ge mode for both types of nanostructures corresponds to a 3.6% biaxial tensile strain, which is close to the 3.7% lattice mismatch between Ge and InAlAs. The Raman signal for QDs was found to be highly polarized along the direction, which is consistent with the anisotropic shape observed in PV-ECCI. In contrast, the Raman signal from the more isotropic NWs did not show such strong polarization effects. QD and NW samples grown under similar conditions both exhibited room-temperature PL, and the integrated intensity from the QDs was ~4+ stronger than from the NWs. Along with the higher PL intensity, QDs emit at 1176 nm, which is slightly blue-shifted compared to the 1230 nm emission of NWs. By altering the growth rate and hence the size of the nanostructures, we could tune the peak emission wavelength over 100 nm. Taken together, this work expands the form of strained Ge nanostructures that can be formed by surface-mediated phase separation while providing new insight on their basic growth.[1] M.V. Fischetti, S.E. Laux, J. Appl. Phys. 80, 2234-2252 (1996)[2] Y. Hou et al., Appl. Phys. Lett. 98, 011111 (2011)[3] S. Wirths et al., Appl. Phys. Lett. 102, 192103(2013)[4] Jung D et al. Nat. Commun. 8, 14204 (2017)

11:00 AM QQ03 (Student) Investigation of Bi Induced Three-Dimensional InAs Nanostructures on GaAs(110) by Cross-Sectional Scanning Tunneling Microscopy
Pascal Farin1, 2, Robert Zielinski1, Andrea Lenz2, Christian Dähne3, Hendrik Janssen1, Pascal Grell1 and Holger Eisele1; 1Institute of Solid State Physics, Technische Universität Berlin, Berlin, Germany; 2Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany.

Three-dimensional (3D) nanostructures like InAs quantum dots grown on GaAs(001) are one of the most extensively explored semiconductor systems. In contrast, attempts to grow 3D structures on other GaAs surfaces remained without success long time: while on GaAs(001) 3D growth of InAs is preferred, on other low-index GaAs surfaces such as (110) the InAs deposition always results in a two-dimensional (2D) growth and the misfit relaxes plastically. On the other hand, [110] oriented GaAs surfaces form the sidewalls in self-assembled GaAs nanowires. The growth of 3D nanostructures like quantum dots on such sidewalls is of interest, especially for high efficiency single photon sources [1]. Recent investigations show that the presence of Bismuth (Bi) as a surfactant induces 3D growth on GaAs(110) by reducing the surface energy. Furthermore, Bi exposure on already grown 2D InAs layers can cause a morphological phase transition, resulting in a rapid re-organization of the 2D layer into 3D nanostructures. These so-called 3D islands have optical properties of quantum dots and open the possibility to generate linearly polarized single photons [2]. In this contribution Bi induced InAs 3D islands formed within InAs monolayers on GaAs(110) are investigated structurally, using cross-sectional scanning tunneling microscopy (XSTM), for the first time. Sample growth was performed using molecular beam epitaxy. The investigated sample contains four different sets of growth parameters, namely two pairs of 1.1 monolayers deposited with and without Bi and two pairs of 2.1 monolayers subsequently exposed to Bi flux for different durations. XSTM is a powerful tool for investigation with atomic resolution in order to determine the growth mechanisms and the even more possible changes during capping, the latter been necessary for device applications. For this purpose, we cleaved the samples in ultra-high vacuum perpendicularly to the growth [110] direction. The XSTM images with atomic resolution of the InAs layers show the formation of quantum dots. The XSTM images allow the characterization of geometrical structures in terms of size, density, and morphology, all depending on the presence of Bi. Furthermore, we are able to carry out stoichiometric analyses of the chemical composition by analyzing the variation of local lattice parameter [3]. In order to explore the influence of
Bi, we compare the resulting structures upon both growth regimes, mentioned above. Hence, we are able to present a correlation between the amount of Bi in the layers and the 3D island formation. This work was supported by the DFG, SFB 787, Project A4:References:[1] P. Corfdir et al. Phys. Rev. B 96, 045435 (2017)[2] R. B. Lewis et al. Nano Lett. 17, 4555-4560 (2017)[3] A. Lenz et al. J. Vac. Sci. Technol. B 29, 04D104 (2011).

11:20 AM QQ04
Influence of QD Morphology on the Electronic States of GaSb/GaAs Multilayers

Christian Greenhill
Erie Zech
Alexander Chang
S. Clark
Sadhvikas J. Addamane
Ganesh Balakrishnan
Rachel S. Goldman
Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, United States; Northwestern University, Evanston, Illinois, United States; University of New Mexico, Albuquerque, New Mexico, United States.

Due to the predicted composition and strain dependence of type I versus type II band offsets, GaSb/GaAs quantum dots (QDs) have been identified as promising for a variety of optoelectronic applications. It has been shown that the nucleation of 2D layers (i.e. wetting layers) versus 3D islands (i.e. quantum dots) can be tuned by varying the Sb/Ga beam equivalent pressure ratio during molecular beam epitaxy. For GaSb/GaAs multilayers, atomically thin ranging from dots to rings to clusters have been observed. Although photoluminescence (PL) emissions ranging from 0.9 to 1.3 eV are often reported for multi-layered GaSb/GaAs, the association of these emissions with specific nanostructures remains elusive. Here, we examine the structural and optical properties of GaSb/GaAs multilayers containing 2D GaSb layers, with and without 3D islands. We use a combination of cross-sectional scanning tunneling microscopy and scanning transmission electron microscopy, in conjunction with atom-probe tomography (APT), to determine the compositions and dimensions of the GaSb wetting layers (WLs), quantum dots (QDs), and QD rings. For both samples, ~2nm thick WLs are observed. Since the Sb fractions, x in the WLs are < 2%, we attribute the 1.32eV emissions to the GaAsSb alloy. For samples containing 3D islands, QDs and rings of smaller QDs, with typical diameter of 25nm and height of 7nm, are observed. In both cases, Sb-rich QD cores are apparent, with x up to 0.40 and 0.25 for the individual QDs and QDs within rings, respectively.

Therefore, we attribute the 1.08eV and 1.2eV emissions to the QDs and rings of QDs, respectively. Local measurements of the electronic states using scanning tunneling spectroscopy will also be presented.

11:40 AM QQ05
(Studen) III-V Digital Alloys for Mid-IR Photodetectors

Ann K. Rockwell
Min Ren
Scott J. Maddox
Joe Campbell
Seth Bank
Electrical and Computer Engineering, University of Texas, Austin, Texas, United States; Electrical and Computer Engineering, University of Virginia, Charlottesville, Virginia, United States.

We recently demonstrated the successful growth of Al In As Sb , digital alloys on GaSb with period thicknesses between 10 and 20 monolayers (ML) and Al fractions ranging from 0 to 0.25. For samples containing 3D islands, QDs and rings of smaller QDs, with typical diameter of 25nm and height of 7nm, are observed. In both cases, Sb-rich QD cores are apparent, with x up to 0.40 and 0.25 for the individual QDs and QDs within rings, respectively.

Additionally, we have successfully used the digital alloy approach on GaSb with period thicknesses between 10 and 20 monolayers. We recently demonstrated the successful growth of Al In As Sb , digital alloys on GaSb with period thicknesses between 10 and 20 monolayers (ML) and Al fractions ranging from 0 to 0.25. For samples containing 3D islands, QDs and rings of smaller QDs, with typical diameter of 25nm and height of 7nm, are observed. In both cases, Sb-rich QD cores are apparent, with x up to 0.40 and 0.25 for the individual QDs and QDs within rings, respectively.

Therefore, we attribute the 1.08eV and 1.2eV emissions to the QDs and rings of QDs, respectively. Local measurements of the electronic states using scanning tunneling spectroscopy will also be presented.

8:40 AM RR01
Two-Dimensional Hole Gas in MBE Grown Si/Al/Si System

Aruna N. RamanaNath
SadhuKumar T. K.
Sanjeev T. K.
We recently demonstrated the successful growth of Al In As Sb , digital alloys on GaSb with period thicknesses between 10 and 20 monolayers (ML) and Al fractions ranging from 0 to 0.25. For samples containing 3D islands, QDs and rings of smaller QDs, with typical diameter of 25nm and height of 7nm, are observed. In both cases, Sb-rich QD cores are apparent, with x up to 0.40 and 0.25 for the individual QDs and QDs within rings, respectively.

Therefore, we attribute the 1.08eV and 1.2eV emissions to the QDs and rings of QDs, respectively. Local measurements of the electronic states using scanning tunneling spectroscopy will also be presented.

SESSION RR: Low Dimensional Materials
Session Chairs: Sadhvikas Addamane and Michael Gerhold
Friday Morning, June 29, 2018
Location: University Center, Santa Barbara Harbor

8:40 AM RR01
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Therefore, we attribute the 1.08eV and 1.2eV emissions to the QDs and rings of QDs, respectively. Local measurements of the electronic states using scanning tunneling spectroscopy will also be presented.

8:40 AM RR02
(Students) Self-Assembly of (111)-Oriented Quantum Dots for Entangled Photon Emission

Christopher F. Schuck
Austin Mello
Aruna N. RamanaNath
SadhuKumar T. K.
Sanjeev T. K.
We recently demonstrated the successful growth of Al In As Sb , digital alloys on GaSb with period thicknesses between 10 and 20 monolayers (ML) and Al fractions ranging from 0 to 0.25. For samples containing 3D islands, QDs and rings of smaller QDs, with typical diameter of 25nm and height of 7nm, are observed. In both cases, Sb-rich QD cores are apparent, with x up to 0.40 and 0.25 for the individual QDs and QDs within rings, respectively.

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Therefore, we attribute the 1.08eV and 1.2eV emissions to the QDs and rings of QDs, respectively. Local measurements of the electronic states using scanning tunneling spectroscopy will also be presented.

8:40 AM RR02
(Students) Self-Assembly of (111)-Oriented Quantum Dots for Entangled Photon Emission
A novel class of low cost mid-IR light emitting devices for applications such as chemical sensing.

9:40 AM RR04
InP-Based Quantum Dash Lasers Emitting at 1.55 μm with Low Threshold Current Density—Chen Shang1, Daewon Jung2, Justin Norman, Yating Wan2, Arthur Gossard2, and John Bowers1 1Materials Department, University of California, Santa Barbara, Goleta, California, United States; 2Institute for Energy Efficiency, Santa Barbara, California, United States; 3University of California, Santa Barbara, Santa Barbara, California, United States.

Utilizing self-assembled InAs nanostructures as the active material for semiconductor lasers has been drawing great attentions for their unique properties. Low threshold current density, high defect tolerance, and less temperature sensitivity have granted InAs nanostructures semiconductor lasers better performance over quantum well lasers. Great results have been obtained with the InAs/GaAs quantum dots operating at 1.3 μm. On the other hand, the InAs/InP material system targeting at 1.55 μm for telecommunication is less developed due to the low lattice mismatch between InAs and InP (3.2%). Here, we demonstrate InAs quantum dash narrow ridge-waveguide lasers grown on n-InP native substrate with a low continuous-wave threshold current density of 510 A/cm² and an output power of 25 mW. InAs nanostructure photomoluminescence (PL) samples were grown on InAlAs quantum alloy buffer, lattice matched to InP substrate, to investigate the growth conditions that gave the highest PL intensity at around 1550 nm. It was determined that, for the InAs nanostructure growth, a growth temperature of 485°C, 3.25 monolayer (ML) of InAs, a growth rate of 0.4 ML/s, and a V/III ratio of 18 during the nanostructure growth result in an overall better PL characteristic. Further tuning of the PL spectrum depends on post-nucleation ripening process, where the structure was held under As pressure for a given amount of time. Due to the low lattice mismatch between InAs and InP lattice constant, the surface diffusion of In adatoms are highly anisotropic, with the first diffusion path parallel to the surface reconstruction dimer row. As a result, the nucleated islands tend to elongate along the direction, known as quantum dashes (Qdash). By holding the structure at growth temperature, it approaches the thermodynamically more stable configuration, with the As pressure adjusting the surface diffusivity by changing the surface reconstruction pattern. A combination of As pressure was used to lower the threshold and improve the output power. The difference is more prominent at wider ridges, where the side wall effect is of less importance. The laser results are very promising for entangled photon generation enabling us to optimize TSQD properties for entangled photon generation and will underpin future applications of these unique nanostructures.[1]

References:

9:20 AM RR03
Mid-IR Light Emission from IV-VI Semiconductor Multiple Quantum Wells Grown on Silicon—Patrick McCam, Khosrow Namjou, Manisha Chakraburty, Lihua Zhao and Gary Cai, ECE, University of Oklahoma, Norman, Oklahoma, United States.

This presentation describes fabrication of a mid-IR light emitting diode (LED) from IV-VI semiconductor layers grown by molecular beam epitaxy (MBE) on silicon. Device fabrication involved eutectic bonding of epilayers to copper and removing the silicon growth substrate to allow low resistance electrical contacts and improved heat dissipation. This is the first known demonstration of a IV-VI semiconductor mid-IR light emitting device fabricated using a silicon growth substrate and epi-layer transfer. IV-VI LED devices were fabricated from IV-VI semiconductor layers grown by MBE on 3 inch diameter (111)-oriented silicon substrates. PbSe, Se, Sr, and BiSe, effusion cells were used to grow the device structure, which consisted of a 1 μm thick PbSe, a 2 μm thick SrSe, and a 300 nm thick PbSe layer. The device structure was doped with PbS to achieve n-type conductivity with a carrier density in the range of 4 x 10²⁰ cm⁻³. The last 1.75 microns were grown under a Se overpressure to achieve p-type conductivity with a hole density in the range of 4 x 10¹⁷ cm⁻³. Well and barrier thicknesses along with the absence of any significant bismuth diffusion were confirmed by ex situ secondary ion mass spectroscopic (SIMS) characterization. The IV-VI semiconductor device structure was grown on a 4 nm thick CaF₂ layer, which was grown on the silicon substrate immediately following oxide desorption as confirmed by observing a 7x7 silicon surface reconstruction in the reflection high energy electron diffraction (RHEED) pattern. Following MBE growth, the wafer was cleaved into 1 x 1 cm² chips, which were flip-chip bonded to copper using InSn eutectic metallurgy. The silicon growth substrate was then removed by immersion in deionized water to dissolve the CaF₂ layer. Etched square mesas, defined by gold evaporated through a shadow mask, were contacted with a probe tip for current versus voltage characterization and wire bonded using conductive epoxy for light emission measurements. A Fourier transform infrared (FTIR) spectrometer was used to collect the light emission spectra. The FTIR spectrometer was used to collect the light emission spectra. The FTIR spectrometer was used to collect the light emission spectra. The FTIR spectrometer was used to collect the light emission spectra. The FTIR spectrometer was used to collect the light emission spectra. The FTIR spectrometer was used to collect the light emission spectra. The FTIR spectrometer was used to collect the light emission spectra. The FTIR spectrometer was used to collect the light emission spectra. The FTIR spectrometer was used to collect the light emission spectra.
SESSION SS: Nanomagnetics and Spintronics
Session Chairs: Joseph Hagmann and Suprem Das
Friday Morning, June 29, 2018
Location: University Center, Santa Barbara Harbor

10:20 AM SS01
Rashba Spin Orbit Coupling Mediated Spin Hall Effect and Emergent Phase Transition in Si
Paul C. Lou and Sandeep Kumar
University of California, Riverside, Riverside, California, United States.

The entanglement of the charge, spin and orbital degrees of freedom can give rise to emergent behavior especially in thin films, surfaces and interfaces. Often, materials that exhibit those properties require large spin orbit coupling. We hypothesize that the emergent behavior can also occur due to spin, electron and phonon interactions in widely studied simple materials such as Si. That is, large intrinsic spin-orbit coupling is not an essential requirement for emergent behavior. The central hypothesis is that when one of the specimen dimensions is of the same order (or smaller) as the spin diffusion length, then non-equilibrium spin accumulation due to spin injection or spin-Hall effect (SHE) will lead to emergent phase transformations in the non-ferromagnetic semiconductors. In this experimental reported spin mediated antiferromagnetic metal and metal insulator transition in a Pd (1 nm)/Ni$_2$Fe$_{25}$ (25 nm)/MgO (1 nm)/p-Si (~400 nm) thin film specimen. The spin-Hall effect in p-Si, observed through Rashba spin-orbit coupling mediated spin-Hall magnetoresistance behavior, is proposed to cause the spin accumulation and resulting emergent behavior. The phase transition is discovered from the diverging behavior in longitudinal third harmonic voltage, which is related to the thermal conductivity and heat capacity.

10:40 AM SS02
(Studnet) Nanometer Scale Investigations of Fe Clustering in Half-Heusler Half-Metal Candidate CoTi$_2$Fe$_{1-x}$Sb
Bastien Bonet$, Daniel J. Pennachio, James S. Speck, and Chris J. Palmstrom$: $^1$: Materials, University of California, Santa Barbara, Goleta, California, United States; $^2$: Department of Electrical and Computer Engineering, University of California, Santa Barbara, California, United States.

Half-Heusler (h-H) compounds are an exciting class of intermetallics due to their diverse electrical and magnetic properties, including semiconducting [1], half-metallic [2], and topologically insulating [3]. With a crystal structure and lattice parameters similar to III-V compound semiconductors, the possibility of h-H/III-V heterostructures with unique properties is achievable. Recent work demonstrated a semiconductor to ferromagnetic metal transition in thin films of CoTiSb substitutionally alloyed with Fe, namely Co$_{1-x}$Ti$_x$Fe$_2$Sb and Co$_{1-x}$Fe$_x$TiSb [4]. Here electrical and magnetic properties that depended strongly on the Fe concentration, as well as Fe site occupancy, were demonstrated. In addition, half-metallic behavior was predicted for films x<0.5. The quaternary Heusler compound system’s compatibility with other Heusler and III-V compounds and its expected half-metallic behavior, make it promising for the development of future spintronic heterostructures and devices. However, understanding how these distinct electronic and magnetic properties are linked to the interactions between metallic atoms at the nanometer scale will be important to utilizing these thin films in devices. In this work, atom probe tomography (APT) and scanning transmission electron microscopy (STEM) are employed to investigate the presence and distribution of nanometer scale Fe-rich domains and their dependence on Fe content in Co$_{1-x}$Ti$_x$Fe$_2$Sb thin films. Co$_{1-x}$Ti$_x$Fe$_2$Sb samples with Fe fraction (x) of 0.2, 0.3 and 0.5 were grown by molecular beam epitaxy (MBE) on lattice matched In$_x$Al$_{1-x}$As buffer layers grown on InP(001) substrates. 140 nm-thick Co$_{1-x}$Ti$_x$Fe$_2$Sb layers were grown in a dedicated VG V80 metal MBE system. The films are epitaxial and single crystalline as measured by reflection high-energy electron diffraction and X-ray diffraction. An abrupt interface between the h-H film and III-V layer is observed in STEM. For APT analysis, the samples were evaporated in a LEAP 3000X HR operated in voltage-pulse mode with a pulse to base voltage fraction of 0.25%. The 3D reconstructions were optimized to visualize the atomic planes in the Z direction [5]. Radial distribution analysis [6] was performed to obtain the self-correlation curves between Fe atoms. Clear Fe-rich domains were evidenced for x=0.2 and x=0.3 but are no longer observed for x=0.5. Cross- and self-correlation curves were also plotted in between Co, Ti, Fe and Sb which did not reveal any other clustering in any samples. These behaviors were confirmed using statistical distribution analysis [7]. For compositions x=0.2 and x=0.3, the APT experimental distributions of Fe do not follow the binomial distribution expected for random alloys. For x=0.5, a better agreement is observed suggesting a random distribution of Fe in the sample and the absence of <d>Fe-rich domains. Thus it can be inferred that the superparamagnetism observed in x=0.2 and x=0.3 samples [4] originates from the presence of Fe rich domains in these samples [1]. H. C. Kandpal, C. Felser, and R. Seshadri, J. Phys. D. Appl. Phys., 39, 5, 776–785, (2006).[2] M. I. Katsnelson, V. Y. Irkin, L. Chioncel, A. I. Lichtenstein, and R. A. de Groot, Rev. Mod. Phys., 80, 2, 315–378, (2008).[3] H. Lin, L. A. Wray, Y. Xia, S. Xu, S. Jia, R. J. Cava, A. Bansil, and M. Z. Hasan, Nat. Mater., 7, 9, 546–9, (2010).[4] S. D. Harrington, A. D. Rice, T. L. Brown-Heft, B. Bonef, A. Sharan, A. P. McDadden, J. A. Logan, M. P. Pendry, M. F. Feldman, O. A. Merch, A. G. Petukhov, A. Janotti, L. Colakol Arslan, and C. J. Palmstrom, Phys. Rev. Mater., 2, 1, 14406, (2018).[5] F. Vurpillot, B. Gault, B. P. Geiser, and D. J. Larson, Ultramicroscopy, 132, 19–30, (2013)[6] J. Zhou, J. Odygvt, M. Thuvander, and P. Hedström, Microsc. Microanal., 19, 3, 665–675, (2013).[7] M. P. Moody, L. T. Stephenson, A. V. Ceguerra, and S. P. Ringer, Microsc. Res. Tech., 71, 7, 542–550, (2008).

11:00 AM SS03
Origin of the High Intrinsic Spin Hall Angle in β Tungsten
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Using a spin Hall material to switch the spin orientation of a neighboring magnetic layer could serve as a key element in future low-power magnetoresistive random access memory (MRAM) devices. The spin Hall angle is defined as the ratio between the induced transverse spin Hall conductivity due to spin-orbit interactions and the longitudinal electrical conductivity. Recent experimental studies have shown that β-W (A15 phase, tetrahedrally close packed crystal structure) has a very large spin Hall angle (~0.30) [1]. In contrast, the common α-W (bcc phase) has a negligible spin Hall angle (~0.07) [1]. While the large spin Hall angle in β-W is thought to be an intrinsic feature of the material, so far there have been (1) no materials that have shown a direct link between the electronic structure and the high spin Hall angle and (2) few studies that even examine the electronic structure of β-W. In this work, we calculate and confirm the fully relativistic band structure (including spin-orbit coupling) and Fermi surfaces of α and β-W using several first principle approaches, including a plane wave pseudopotential formalism (VASP) [2], an ultrasoft pseudopotential (dftWise) [3], and a relativistic Korringa-Kohn-Rostoker (KKR) Green’s function approach [4]. Analysis of the band structure indicates significant band splitting near the Fermi energy due to spin-orbit interactions, including regions near the Γ point, and along the Γ-X and Γ-M high symmetry lines. The spin Hall conductivity in both α and β-W is determined using the Kubo formula based on the A15 structure [5]. We determine spin Hall angles for α-W ranging from 0.008 (bulk) to 0.021 (film), in agreement with experiment [1]. For β-W, we predict spin Hall angles ranging from 0.1 (bulk) to 0.18 (film). Since O and N are often used to stabilize the metastable β-W crystal structure, we also discuss the potential impact of these dopants on the overall electronic structure, spin Hall conductivity and spin Hall angle [1].

11:20 AM SS04
Valence Modulation Induced Ferromagnetism in TiO$_2$/TiO$_2$
Superlattices
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Alternating layers of epitaxial TiO$_2$ and TiO$_2$ superlattices of rutile structure, ~1-nm thick per layer by RF-sputtering of a TiO$_2$ target for the TiO$_2$ layers, and by DC-sputtering of another TiO target for the TiO layers at 570°C using pure argon on c-Al$_2$O$_3$ substrates. From high resolution transmission electron microscopy (HR-TEM), the periodically alternating layers are well-defined. X-ray photoelectron spectroscopy (XPS) analyses based on the binding energy of Ti 2p$_{3/2}$ peaks suggest the co-existence of Ti$^{4+}$ and Ti$^{3+}$, thus verifying the mixed-valence nature of the TiO$_x$TiO$_{1-x}$ superlattices. The M(T) curves measured at room temperature using superconducting quantum interference magnetometry (SQUID) surprisingly showed hysteretic loops typical of ferromagnetism, although none of the constituting layers showed diamagnetism. Electrical transport
measurements of such superlattices done at zero field demonstrate transition of charge ordering at low temperatures, reminiscent of what was found in Ti-rich Ti$_2$O$_3$ single-layer thin films, made by Ti ion implantation into TiO$_2$ crystals, in which randomly distributed TiO$_2$, Ti$_2$O$_3$ and TiO were found to coexist. Preliminary First-principle (ab initio) calculations to understand the roles of oxygen vacancies showed that locations and amounts of oxygen vacancies as a whole in various TiO$_2$ super-cells could indeed lead to spontaneous magnetizations. We thus argue that mixed-valence titanium ions are responsible for the ferromagnetism.

SESSION TT: Gallium Oxide Characterization and Thermal Properties

Meeting Chairs: Doug Hall and Marko Tadjar
Friday Morning, June 29, 2018

Location: Multicultural Center, MCC Theater

8:40 AM TT01

Thermal Characterization of β-Ga$_2$O$_3$ MOSFETs

James W. Pomeroy
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β-Ga$_2$O$_3$ is a wide bandgap (4.9eV) semiconductor with an electric breakdown strength of 8 MV/cm. The Baliga figure of merit (BFOM) is 4+ that of GaN[1] and availability of large single crystal Ga$_2$O$_3$ substrates, grown by using relatively low-cost melt grown methods [2], has generated interest in β-Ga$_2$O$_3$ devices. A breakdown voltage of 755V and high drain current and on/off ratio of 10$^5$ has already been demonstrated [3]. There is also increasing interest in β-Ga$_2$O$_3$ for RF applications, which would enable the monolithic integration of power switch and RF devices. Green et al. have recently demonstrated RF performance with a power output of 0.23W/mm with PAE of 6.3% [4]. However, β-Ga$_2$O$_3$ has low thermal conductivity (27 W/m.K at the [010] direction @300K) and self-heating induced catastrophic failure was observed in Ref. [4]. We assess the thermal resistance of β-Ga$_2$O$_3$ of MOSFETs using Raman thermography and simulation. Possible thermal management solutions are investigated. Single finger β-Ga$_2$O$_3$ MOSFETs with a 2 μm gate length (1 μm-long field plate), 200 μm gate width, 5 μm gate-source spacing and 25 μm gate-drain spacing were studied, having a saturated drain current of 58mA/mm and threshold voltage of ~30V. Used device structure is illustrated in Fig. 1; more details are in Ref. [3]. Raman thermography measurements were performed following a phonon temperature shift calibration of bulk β-Ga$_2$O$_3$. A 0.5 NCS objective lens was used for the Raman, with a lateral and depth resolution of 0.5μm and ~6-8 μm, respectively, as illustrated in Fig. 1. The relatively large depth resolution is due to the transparency of β-Ga$_2$O$_3$. Figure 2 shows that the highest measured temperature occurs close the gate edge, where the peak electric field and associated Joule heating occurs in the device channel. The thermal resistance measured at the hottest location was 23 W/mm²/W (Figure 3) which is a lower limit value because of the spatial averaging described above. A 3-D finite element thermal model was used to predict the device temperature using temperature dependent, anisotropic thermal conductivities of β-Ga$_2$O$_3$ reported in Ref. [5]. A peak channel temperature of >1000°C was predicted by initially assuming that all heating occurs within a 0.5μm-long region at the drain edge of gate. Such high value is unrealistic because resistive heating in the access regions will become significant as mobility decreases at high temperature. Compared to Raman, simulation overestimates the temperature by ~30% (when averaged over the same volume). This discrepancy is attributed to uncertainty in the depth probed optically. A lower channel temperature limit can be determined by assuming uniform channel heating in the simulated peak temperature of 465°C. More accurate channel temperature prediction will require detailed drift diffusion simulations to obtain the Joule heating distribution. Figure 4 shows the simulated transient thermal response, which can be used to evaluate temperature rise during pulsed operation - severe thermally induced current slump can be avoided by using a short duty cycle and pulse lengths less than a few μs. The results highlights need for thermal management for reliable β-Ga$_2$O$_3$ RF operation. The simulated local lateral heat flux through the gate metal is larger than through the β-Ga$_2$O$_3$ itself, suggesting that top-side heat extraction could be an effective thermal management strategy. Replacing the SiO$_2$ with a 200 W/m.K diamond thin film (similar to in Ref. [6]) reduces the thermal resistance of the investigated device by 30%. Combining thin film heat spreaders with flip chip mounting onto a high thermal conductivity carrier could result in a significant reduction in thermal resistance.

REFERENCES:
[1] M. Higashiwaki et al., APL 2012
[4] A. Green et al., IEEE ELD 2017

9:00 AM TT02

Thermal Strains in Wafer Bonding and Heteroepitaxial Structures of Monocrystalline β-Ga$_2$O$_3$ and Other IV and III-V Semiconductor Substrates

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Wafer bonding of monocrystalline β-Ga$_2$O$_3$ to other IV and III-V semiconductor substrates with higher thermal conductivity (typically by 3-20 times) and lower cost and heteroepitaxial structures with β-Ga$_2$O$_3$ as either substrates or epitaxial layers are important for the applications of β-Ga$_2$O$_3$ in high-power devices and GaN-based LEDs. It is necessary to understand thermal strains in bonded β-Ga$_2$O$_3$ and epitaxial structures due to thermal mismatch in order to select proper materials for bonding and epitaxial growth and assess the structural and electrical properties in the bonded and epitaxial structures. In this study, thermal strains along six evenly distributed in-plane directions were determined in wafer bonding structures of (0 0 1) β-Ga$_2$O$_3$ bonded to InP, Si, InP, 3C-SiC, and 6H-SiC substrates, and epitaxial structures of MOVCD (0 0 1) β-Ga$_2$O$_3$ with an in-plane orientation relation of (1 1 0) β-Ga$_2$O$_3$ and MOVCD (0 0 1) β-Ga$_2$O$_3$/0 0 1 sapphire with an in-plane orientation relation of (0 0 1) β-Ga$_2$O$_3$/0 0 1 sapphire. The thermal expansion coefficients of β-Ga$_2$O$_3$ single crystal wafers were measured over a range of room temperature to up to 1000°C using X-ray diffraction and a high temperature cell. Measurements that involve single crystals overcome problems associated with previous measurements using powders milled from single crystals, such as strains induced by milling and surface reactions of individual grains. The temperatures used here cover a wider range than had been used earlier in those powder measurements making these measurements more suitable for addressing strains in wafer bonding and high temperature epitaxy. We determined that the ‘b’ and ‘c’ axes expand linearly at about twice the rate of the ‘a’ axis with increasing temperature with expansion coefficients of ~7 × 10$^{-5}$K$^{-1}$ (compared to about 5 × 10$^{-5}$K$^{-1}$ for ‘a’). The angle between the ‘a’ and ‘c’ axes increases slightly (~0.1°) with increasing temperature to 1000°C. Using the measured lattice parameters of β-Ga$_2$O$_3$ single crystal wafers, it is predicted that with a bonding temperature of 600°C each of the (0 0 1), (0 1 0), and (0 0 1) oriented single crystal β-Ga$_2$O$_3$ bonded to InP, 3C-SiC and 6H-SiC have similar tensile thermal strains (except for that along ~1/6-1/2 in-plane directions for (0 0 1) β-Ga$_2$O$_3$ bonded structures having compressive in-plane thermal strains) within a range from ~4.0 × 10$^{-5}$ to ~2.0 × 10$^{-5}$, ~1.5-15 times smaller than that of β-Ga$_2$O$_3$ bonded to Si. Additionally, (0 1 0) oriented β-Ga$_2$O$_3$ bonded to other substrates has more uniform thermal strains along different in-plane directions (~5 times difference between the maximum and minimum values) than (0 0 1) and (0 1 0) oriented β-Ga$_2$O$_3$. The thermal strains of the (0 0 1) β-Ga$_2$O$_3$ single crystal bonded to InP, 3C-SiC and 6H-SiC range from ~2.0 × 10$^{-5}$ to ~1.0 × 10$^{-5}$, smaller than ~6.5 × 10$^{-5}$ of GaAs bonded to InP with the same bonding temperature along ~1/3 in-plane directions. On the other hand, as for the MOVCD (0 0 1) GaN(0 0 1) β-Ga$_2$O$_3$ grown at 1000°C, tensile thermal strains were determined along 5/6 in-plane directions while compressive strains along the other in-plane directions. The thermal strains range from 2.5 × 10$^{-5}$ to 2.2 × 10$^{-5}$ which are smaller than that in GaN grown on sapphire (~2.5 × 10$^{-5}$) while partially (along ~1/2 in-plane directions) smaller than GaN on SiC (~7.2 × 10$^{-5}$). In addition, compressive in-plane thermal strains in β-Ga$_2$O$_3$ were determined for the MOVCD (2 0 1) β-Ga$_2$O$_3$ deposited on (0 0 1) sapphire substrate at 650°C with a range from 1.9 × 10$^{-5}$ to 2.0 × 10$^{-5}$.

9:20 AM TT03

Characterization of Electrical Resistance at Heterointerface of Single-Crystal Ga$_2$O$_3$/Polycrystalline SiC Bonded Substrates
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Kazumichi Yagi1 and Masataka Ito1
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2SICOX Co. Ltd., Tokyo, Japan
Toshiba Corporation, Tokyo, Japan
1Tamura Co. Ltd., Sayama, Japan.

β-Ga$_2$O$_3$ offers great potential for high-power devices with low energy loss owing to its material properties derived from an extremely large bandgap of 4.5 eV. The availability of commercial Ga$_2$O$_3$ substrates with high crystal quality and yet lower cost than GaN and SiC also facilitates the development of vertical power devices. However, the low thermal
conductivity of Ga$_2$O$_3$ (11–24 W/mK) hampers high-power device operation. As for this issue, we consider that heat dissipation from Ga$_2$O$_3$ devices can be improved by directly bonding them to a thermally and electrically conductive substrate. We pursued this idea in a previous work with polycrystalline SiC since these substrates are not only highly conductive but also electrically but also affordable, and successfully demonstrated the formation of a void-free high-quality Ga$_2$O$_3$/SiC interface by using the surface-activated-bonding (SAB) method [1].

The interface presented a negligibly small thermal resistance and a large bonding strength comparable to the Ga$_2$O$_3$ bulk strength. In this work, we characterized the electrical resistance at the Ga$_2$O$_3$/SiC bonded heterointerface. Two-terminal electrical test structures were fabricated on (i) a single-crystal β-Ga$_2$O$_3$ (001) substrate ($n$=3–10$^5$ cm$^{-3}$), (ii) a polycrystalline SiC substrate ($n$=1–10$^6$ cm$^{-3}$), and (iii) a single-crystal Ga$_2$O$_3$/polycrystalline SiC bonded substrate, where (i) and (ii) were used to extract series bulk resistances. Ti/Au ohmic electrodes were blanket evaporated onto the back sides of all the substrates, and circular ohmic emissions from the total series resistance of 0.66 Ω, was 0.06 Ω (a heterointerface was an ohmic junction. The electrical resistance at the bonding strength comparable to the Ga$_2$O$_3$ bonded substrate presented a linear behavior, indicating that the heterointerface was an ohmic junction. The electrical resistance at the bonded substrate presented a linear behavior, indicating that the heterointerface was an ohmic junction.

Field-Effect Transistor based on MBE grown m-Fe$_2$O$_3$—Spectral Dependences on Incident Wavelength and Polarization

Yunshan Wang, Hyunik Park, Satish Kumar; Georgia Institute of Technology, Atlanta, Georgia, United States. ;

MSE, University of Utah, Salt Lake City, Utah, United States; Washington State University, Pullman, Washington, United States; ;

We report polarization dependent photoluminescence studies on unintentionally-, MBE-, and MOCVD grown m-Fe$_2$O$_3$ by the Czochralski method. In particular, we observe wavelength shifts of the highest energy UV emission dependent on the incident polarization. For 240 nm (5.17 eV) excitation, almost no shift of the UV emission is observed between E//b and E//c, while shift of the UV emission centroid is clearly observed for 266 nm (4.66 eV) excitation. These observations are consistent with the UV emission originating from transitions between conduction band electrons and two differentially-populated self-trapped hole (STH) states. This observation implies that the STHs form primarily at the oxygen involved in the original photon absorption event, thus providing the connection between incident polarization and emission wavelength. The data imposes a lower bound on the energy separation between the self-trapped hole states of 10–30 meV.

Breakdown Voltage Improvement of β-Ga$_2$O$_3$ Field-Effect Transistor with a Boron Nitride-Graphene Source-Field Plate

Jinho Bae 1, Hyoung Woo Kim 1, Zhequan Yan and Satish Kumar 1, 2; Georgia Institute of Technology, Atlanta, Georgia, United States.

Because of the large bandgap and the resultant large electrical breakdown strength, β-Ga$_2$O$_3$ emerged as a promising semiconductor which can sustain large voltages, making it attractive for high-power devices. However, high power dissipation in these devices can cause critical challenges, e.g., it can significantly affect the performance and reliability of these devices. It’s necessary to understand the thermal transport in β-Ga$_2$O$_3$ to control the hot spot temperature in its active devices and also for the design of packaging and thermal solutions. A few studies have focused on the prediction and the measurements of the thermal conductivity of β-Ga$_2$O$_3$. However, the computational results don’t have a consistent agreement with the experimental results and the thermal conductivity of the phonon transport in β-Ga$_2$O$_3$ is not well understood yet. In addition, due to the imperfection in growth processes, the crystal lattice of the β-Ga$_2$O$_3$ contains unintentional localized defects such as vacancies. They could also significantly influence the thermal properties of β-Ga$_2$O$_3$ which is not well understood yet. To better understand the influence of defects on the phonon transport mechanism, we used first-principles density functional theory (DFT) along with the Boltzmann Transport Equations (BTE) to predict the phonon transport properties of pristine and defective β-Ga$_2$O$_3$.

The thermal conductivities of β-Ga$_2$O$_3$ crystals along three different crystal directions are calculated based on the iterative solution of the BTE. Our results have a better agreement with the experimental results compared to the previous studies. The largest thermal conductivity of β-Ga$_2$O$_3$ is observed in the direction of [010]. In addition, the oxygen vacancies indicate a significant influence on the thermal transport of β-Ga$_2$O$_3$, which results from the phonon scatterings caused by the mass missing of oxygen atoms. Results indicate that at room temperature, 1% and 2% oxygen vacancies decrease the thermal conductivity by 8.5% and 14.3% in [100] direction, 14.9% and 2% in [010] and 7.5% and 17.4% in [001] direction, respectively. We also find that the optical phonon modes in β-Ga$_2$O$_3$ make a significant contribution to the thermal conductivity compared to the acoustic modes, which is different with most other semiconductors. Furthermore, the oxygen vacancies have more influence on the optical modes than that on acoustic modes, which suppress the contribution of optical modes to the thermal conductivity. In other words, under the influence of defects, the acoustic modes’ contribution to the thermal conductivity increases. The results from this work will help us understand the mechanism of phonon transport considering the influence of defects and provide insights for the future design of β-Ga$_2$O$_3$-based electronic devices.

Photoluminescence from β-Ga$_2$O$_3$ Bulk Crystals—Spectral Dependences on Incident Wavelength and Polarization

Yunshan Wang, Peter Dickens, Xiaojian Ni, Emmanuel Lotubal, Samuel Sprawls, Feng Liu, Srikanth Koduru, Kevin Lymi, Michael Scarpulla, Emmanuel Lotubai; The Ohio State University, Columbus, Ohio, United States; Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States.

We report polarization dependent photoluminescence studies on unintentionally-, MBE-, and MOCVD grown m-Fe$_2$O$_3$ by the Czochralski method. In particular, we observe wavelength shifts of the highest energy UV emission dependent on the incident polarization. For 240 nm (5.17 eV) excitation, almost no shift of the UV emission is observed between E//b and E//c, while shift of the UV emission centroid is clearly observed for 266 nm (4.66 eV) excitation. These observations are consistent with the UV emission originating from transitions between conduction band electrons and two differentially-populated self-trapped hole (STH) states. This observation implies that the STHs form primarily at the oxygen involved in the original photon absorption event, thus providing the connection between incident polarization and emission wavelength. The data imposes a lower bound on the energy separation between the self-trapped hole states of 10–30 meV.

Breakdown Voltage Improvement of β-Ga$_2$O$_3$ Field-Effect Transistor with a Boron Nitride-Graphene Source-Field Plate

Jinho Bae 1, Hyoung Woo Kim 1, Zhequan Yan and Satish Kumar 1, 2; Georgia Institute of Technology, Atlanta, Georgia, United States.

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techniques to enhance the breakdown voltage of the devices are widely employed owing to the simplicity and efficiency. Preventing breakdown by applying gate and source field-plate structure lead the full potential of β-Ga2O3 as a power device. In this work quasi-2D β-Ga2O3 source field-plate metal-semiconductor field effect transistor (MESFET) were fabricated by field-oxidation of β-Ga2O3 film by dry 

dry transfer of graphene as a source field material as a source field-plate structure. By applying h-BN as a dielectric material between β-Ga2O3 channel and graphene field-plate, which has ultrahigh breakdown field of 8~12 MV/cm and atomically flat surface, nanoscale MESFET device by stacking 2D materials was fabricated. Electrical and optical properties, and three-terminal off-state breakdown were analyzed by using semiconductor analysis connected with probe station. Silvaco device simulation framework was employed to study the difference of electric field distributions between field-plated and non-field-plated devices. The details of our work will be discussed.

12:40 AM TT08
Optical Properties of Mg- and Fe-Doped β-Ga2O3, Daniel Hashemi1,2, David Look1,2 and Stefan C. Badescu;1 Air Force Research Laboratory, Wright-Patterson AFB, Ohio, United States; 2Semiconductor Research Center, Wright State University, Dayton, Ohio, United States.

Wide-bandgap semiconductors, such as beta gallium oxide (β-Ga2O3), exhibit a number of interesting physical properties. For instance, β-Ga2O3 has a large breakdown field, high transmittance in the UV-vis region, as well as good thermal and chemical stability. This oxide has attracted a lot of attention not only due to its promising potential in power electronics, but also in transparent electronics. In the former application, deep-center dopants, especially Fe and Mg, are used to increase resistivity, while in the latter, shallow centers, usually Si or Sn, are used to decrease resistivity. These centers can be usefully characterized by UV/VIS/NIR reflectance and transmittance measurements which can yield absorption a and reflection R coefficients. We have developed new methodology for accurately determining both high (above band-gap) and small (below band-gap) values of a. In bulk materials, several mid-gap levels typically appear in the a spectrum. To understand these mid-gap features, structural, electronic, and optical properties of β-Ga2O3 with Mg and Fe impurities are studied by employing first-principles calculations based on density functional theory calculations combined with many-body perturbation theory including quasiparticle and excitonic effects. A detailed comparison done between the computed optical absorptions spectra of the systems within and without the Bethe–Salpeter framework, suggests the electron–hole interaction significantly modifies the spectra. Also, we look at the role of deep defect levels in the gap found in the modeling in the interpretation of features from experiment.

SESSION UU: Transparent Conductors and Contacts
Session Chairs: David Janes and Kin Man Yu
Friday Morning, June 29, 2018
Location: Multicultural Center, MCC Lounge

8:40 AM UU01
(Student) Atomic Structure and Electronic Properties of the InO(111) Cleavage Surface Investigated by STM/STS (Celina Schulze; Robert Zielinski1, Zbigniew Galazka2, Wjatscheslaw Martyanov2, Hendrik Janssen1, Andrea Lenz1 and Holger Eische1; 1Institute of Solid State Physics, Technische Universität Berlin, Berlin, Germany; 2Leibniz-Institute for Crystal Growth (IKZ), Berlin, Germany.

The high electrical conductivity in combination with optical transparency makes InO a very interesting material for optoelectronic and high-power electronic devices including LEDs and LDs, ultraviolet Schottky barrier photodetectors, heterostructure field-effect transistors, and metal-semiconductor-metal photodetector. As for p-InO containing a high density of defects, researchers have developed efficient Schottky contacts with low leakage current and high barrier height. In particular, for the fabrication of transparent electronic devices, Schottky contacts need to be transparent on top of reliable Schottky barrier heights (SBHs). In this study, thus, we investigated the electrical and optical properties of high barrier-height and transparent Ti/ITO Schottky contacts on p-InO for optoelectronic and transparent electronic devices. The SBHs and ideality factors were estimated using current-voltage-temperature (I-V-T), capacitance-voltage (C-V), and barrier inhomogeneity model as a function of annealing temperature. The SBHs and ideality factors estimated using I-V characteristics were estimated to be in the range of 0.36–0.39 eV and 1.74–2.07, respectively, depending on the annealing temperature. On the other hand, the barrier inhomogeneity and C-V methods yielded much larger SBHs of 0.82–1.18 eV, the Ti/ITO/InO/ITO capacitor showed 62.07–94.45%. The XPS Ga 2p core levels originated from the interface regions of the ITO/Ti/InO samples shifted toward higher or lower energies, depending on the annealing temperature. The normalized N/Ga atomic ratio showed that N and Ga vacancies were formed at the p-GaN surface region at 300 and 500 °C, respectively. The XPS Ti 2p, N 1s, and O 1s core level results showed the formation of interfacial TiN and TiO2 phases at 300 and 500 °C, respectively. STEM element mapping results excluded the outdiffusion of Ga atoms in the sample annealed at 500 °C. On the basis of the XPS and STEM results, the dependence of the SBHs on the annealing temperature is described and discussed.

9:20 AM UU03
(Student) The Role of Hydrogen in Binary and Ternary Transparent Conducting Oxides Sebastian Husein1, Michael Stuckelberger2, Bradley West3, Fabien Dauzou4, Monica Morales-Masis1, Martial Duchamp5 and Mariana I. Bertoni1, 1School of Engineering for Matter, Transport, and Energy, Arizona State University, Tempe, Arizona, United States; 2X-Ray Nanoscience and X-Ray Optics, Deutsches Elektronen–Synchrotron (DESY), Hamburg, Germany; 3STI IMT PV-LAB, École Polytechnique Fédérale de Lausanne (EPFL), Neuchâtel, Switzerland; 4Énergie, Matériaux et Télécommunication, Institut National de la Recherche Scientifique (INRS), Québec, Quebec, Canada; 5Electrical, Computer, and Energy Engineering, Arizona State University, Tempe, Arizona, United States; 6Most Resiko Centre for Microscopy and Spectroscopy, Peter Grünberg Institut, Forschungszentrum Jülich PGIS, Jülich, Germany; 7School of Materials Science and Engineering, Nanyang Technological University, Nanyang, Singapore.
For photovoltaic (PV) devices, the transparent conductive oxide (TCO) properties of interest are electrical conductivity and optical transparency. However, finer control of additional TCO properties has become vital due to the advent of complex PV device architectures, such as silicon heterojunction and tandem devices, where optimal charge extraction is crucial for higher charge carrier mobility, as well as a control over band gap (E_g), Fermi level (E_F), and work function (WF). The current commercial TCO of choice is tin doped indium oxide (ITO), which has a typical conductivity of 1-5 x 10⁹ S/cm and a transparency of 85% in thin-film form. While ITO meets present device requirements, research efforts are focused on providing inexpensive and environmentally benign TCO alternatives. Record mobilities 3-4 times greater than that of industry-standard ITO have been demonstrated in hydrogenated indium oxide (IO:H), making it an effective ITO-alternative for incorporation into a wide range of PV devices [2-4].


9:40 AM UU04 (Student) Visible and Ultraviolet Transparency of the Correlated Metal SrNbO₃ Joseph Roth, Yoongsang Park, Alexej Pogrebnyakov and Robert Engel-Hoeger; Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania, United States.

Transparent conductors in the visible spectrum are key enablers of countless display and energy technologies. While many transparent conductors have been developed to be transparent in the visible region, few examples exist in the ultraviolet region. A material that is transparent both in the in the visible and ultraviolet range in particular, 200 – 300 nm, would be universally applicable for display, energy, and UV-specific applications, especially disinfection of water and air. We show that the correlated metal strontium niobate (SrNbO₃) is suitable for applications in both spectral ranges. Correlated metals offer an alternative design strategy compared to traditional paradigms, like doping for higher charge carrier mobilities in semiconductors. Instead of starting with transparent semiconductors and doping them improve conductivity, we start with a conducting material and open a transparency window though tuning the electron effective mass via electron correlation and tuning interband transitions. Adjusting these two parameters allows for a transparency window to extend over a variety of optical spectral ranges. This principle was applied in the correlated metals CaVO₃ and SrVO₃, which were shown to have a similar transparency and resistivity to indium tin oxide (ITO) 1. Here, we report on films of the correlated metal, SrNbO₃, grown by pulsed laser deposition² and magnetron sputtering. Transmission for this material is in excess of 80% throughout the visible range and near ultraviolet (270 – 600nm) while maintaining a resistivity lower than 2×10⁻⁴Ω·cm. Of the extended abstract. The fact that this material lends itself to sputtering allows for easy integration into devices. Ongoing research aims to further optimize the absorption edge to improve transparency further into the ultraviolet region through alloying doping, using lanthanum and titanium to suppress interband transitions.1. Zhang, L. et al. Correlated metals as transparent conductors. Nat. Mater. 15, 204–210 (2016).2. Oka, D., Hihoe, Y., Nakao, S., Fukumura, T. & Hasegawa, T. Intrinsic high electrical conductivity of stoichiometric SnNbO₃ epitaxial thin films. Phys. Rev. B 92, (2015).

10:00 AM BREAK

10:20 AM UU06 Flexible Transparent Conductors Based on Random Networks of Metallic Nanowires—Synthesis, Characterization and Integration into Devices Caroline Cellé, Djadjili Toutouy, Arnaud Cornelis, Thomas Sannicolo, Bruno Laguitton and Jean-Pierre Simonato; CEA LITEN, Grenoble, France.

Transparent conductors are widely used as fundamental part of many day life devices such as solar cells, OLEDs, display technologies and touch panels. More and more, development of the Internet of Things implies that markets push emerging technologies and lead consumer needs to be geared towards flexible or non-planar devices. So new generation of transparent electrodes exhibiting both a really high transparency, a high electrical conductivity and mechanical flexibility should have to be developed. Up to now, the fabrication of transparent conductive films is currently made up of thin films of transparent conductive oxides such as indium tin oxide (ITO). However the as-made ITO electrodes suffer from limitations like costly fabrication process and brittleness. The use of solution-processable nanomaterials, and especially based on metallic nanowires, appears as a promising alternative since it affords a large area, low-cost deposition method. Among metals, silver as the most conductive metal has been widely reported in the literature for easy nanowires synthesis. The very high aspect ratios of metallic nanowires are required to allow fabrication of percolating random networks with the best trade-off between transparency and electrical conductivity. We will herein present first the synthesis of silver nanowires AgNWs based on poloy process to independently control nanowire lengths and diameters. Thanks to compatible large scale printing process, elaboration of homogeneous random networks exhibiting excellent performances with sheet resistance less than 20 Ω/sq at 90 % of transmittance will be detailed. Nanowire dimension tuning will strongly modify optoelectrical properties of transparent thin films in terms of sheet resistance, transparency and haze properties. Understanding of percolation properties of this 2D random network of AgNWs in modern Solar Cells will be discussed. From electrical and thermal distributions will be discussed. Prior to integration into devices, electrode stability will be addressed for emphasising good stability over more than 3 years (storage in air and in the dark) but also for evaluating failure limits under several environmental stresses. To enhance the interest of macroscopic properties of nanoscale materials, we will finally show results dealing with the use of such electrode as transparent film heaters (THF) at large scale with very good performances.

10:40 AM UU07 (Student) Comparative Studies of Thermal Transient Responses of Hotspots in Graphene-Silver Nanowire and Silver Nanowire Transparent Conducting Electrodes Sajia Sadouq1, Yu G. Gong1,2, Amir K. Ziabari1,2, Kerry Maize1,2, Amir M.S. Mohammed1, Ali Shakouri1,2 and David B. Janes3; 1School of Electrical and Computer Engineering, Purdue University, West Lafayette, Indiana, United States; 2Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana, United States.

Nanostructured random networks have attracted wide attention as transparent conducting electrodes (TCEs), providing optical and electrical properties comparable to conventional transparent conductive oxides along with mechanical flexibility [1,2]. Nanowire (NW)/nanotube networks exhibit percolating conduction, with NW-NW junction resistance as the transport bottleneck. Hybrid networks consisting of a 2D layer stacked on a NW network (e.g. monolayer graphene/silver NW network) can provide low resistance at high transparency, via co-percolation through both sub-networks. While the macroscopic characteristics of NW and hybrid networks have been studied extensively, studies of the local conduction pathways and relative differences between the networks at the microscopic scale have been limited. Thermoreflectance (TR) imaging techniques offer the potential to study microscopic self-heating induced by current flow over large areas of the device simultaneously [3-6]. In this study, we use TR imaging technique to compare the thermal transient of hotspots (comprising several NW-NW junctions) in silver NW and hybrid networks (figure 1). Within a time-regime dominated by local self-heating (0-10 µs), we find that hotspots in both networks show similar thermal time constants of less than 1 µs (figure 2), during the heating and the cooling cycle. Compared to the NW network, the hybrid network exhibits ~ 4x fewer hotspots (figure 3a)) and a one-third reduction in average hotspot temperature (figure 3(b)), but ~ 3x more power dissipation per hotspot. These observations can be semi-
quantitatively explained in terms of interconnected resistor network models and estimations of local heat spreading from the NW-NW junctions to the substrate via NWs and graphene. We also analyze the temporal evolution of spatial distribution of the hotspots and find that hotspots in hybrid network are more clustered compared to silver NW network. Since hotspots occur at the most resistive links within otherwise conductive pathways, the hotspot distribution provides at least qualitatively information on current pathways. This comparative study captures the essence of percolating/co-percolating transport and illustrates the important role graphene plays in minimizing electrical and thermal resistance of NW-NW junctions making 1D-2D hybrid network an attractive transparent electrode material for flexible applications.

References


11:00 AM UU08
Facile Engineering of Bandgap, Optical Properties and Morphology of Conjugated Polymers Sunghwan Lee, Grant DREWLOW, Austin S. REED and Barah AHN; Mechanical Engineering, Baylor University, Waco, Texas, United States.

Conjugated polymers with electrical conductivity are garnering much attention for applications in organic electronic and optoelectronic devices including such as field effect transistors, organic solar cells and sensors. Polymers based on poly(3,4-ethylenedioxythiophene) (PEDOT) are particularly promising candidates with a semi-metallic range of conductivity, uniform surface planarity and excellent ductility. In this work, homopolymer PEDOT films deposited using oxidative chemical vapor deposition (oCVD) show the maximum conductivity as high as ~3500 S cm⁻² at a deposition rate <0.5 nm/min. However, their utility is limited due to the relatively low transmittance and abrupt decrease near the red edge in the visible regime. Here, we demonstrate facile oCVD copolymerization strategies that exhibit a powerful ability to tune the band gap of PEDOT-based copolymers. The oCVD technique provides a single-step process for the synthesis and deposition of functional copolymer films. The cross-linking monomers of biphenyl or anthracene are simultaneously evaporated with EDOT monomer and an oxidant of FeCl₃ during the deposition. Due to the engineered band gap, the optical properties of copolymers are significantly enhanced compared to homopolymer PEDOT. Poly(biphenyl-co-EDOT) [p(BPH-co-EDOT)] shows the superior transmittance of ~93% to homopolymer PEDOT (~80%) and poly(biphenyl-co-EDOT) [p(BPH-co-EDOT)] (~88%) at the wavelength of 550 nm. In addition, copolymer films show no significant transmission decay in the red edge regime of the light unlike homopolymer PEDOT that presents an abrupt transmission falloff. An improvement in optical transmittance is in agreement with an increase in band gap of materials (pANTH-co-EDOT), ~2.3 eV vs. PEDOT, ~1.8 eV). Further, the surface morphology of oCVD copolymers is dramatically changed compared to homopolymer PEDOT. These copolymers show much bigger inter-molecular morphological features in atomic force microscopy images, which is expected to be favorable to the carrier transport. To conclude, oCVD-processed band gap tunable PEDOT copolymers with enhanced transmittance and abilities to alter morphology may, therefore, have of great relevance in many organic electronic and optoelectronic devices that require the high optical transparency and better morphologies.