higher reverse leakage currents compared to continuously-grown p-n junctions. A common phenomenon is the presence of a high concentration of Si ("Si spike") incorporated at the regrown interface. We report experiments to identify the source(s) of the Si spike and to characterize its effect on the electrical properties of GaN p-n diodes. Secondary ion mass spectroscopy (SIMS) was used to measure Si concentrations at a metal-organic chemical vapor deposition (MOCVD)-regrown interface using various regrowth strategies. SIMS consistently shows a Si spike (Si ~ 2-5E17 cm^-3) when the wafer is taken from the growth system and chemically cleaned before reintroduction to the growth chamber for regrowth. Alternatively, samples grown with an in-situ growth interrupt, (sample cooled to room temperature, warmed back up to the growth temperature for regrowth without being removed from the reactor) show a significant reduction in the Si spike (Si < detection limit), indicating the growth chamber and regrowth process are not significant sources of Si for this hardware configuration. Current-voltage performance was measured for four structures to determine the Si spike effect on diode performance. The structures included: a) a continuously grown junction, b) a planar, regrown junction (with Si spike), and two continuously grown junctions with intentional Si spike doping at the p-n junction (Si = 5E17 cm^-3 and Si = 6E16 cm^-3). The structures used HVPE GaN substrates and consisted of a 10 μm, n-type (~ 3-5E16 cm^-3) drift layer and a 0.4 μm, p-type GaN layer. For the structures with intentional Si doping, a 5-nm-thick Si spike GaN layer was grown prior to growing the p-type layer. The SiH4 flow for the intentional Si spikes was chosen to mimic the Si spike observed in regrown diodes. Diodes with no field management structures to increase reverse bias breakdown were fabricated and the forward and reverse-bias currents were measured as a function of voltage. Forward-bias behaviors were nearly identical for all structures with ~ 3 V turn on voltages and forward leakage currents ~ 1E-11 A up to ~ 1.6 V. Similarly, reverse-bias performances were nearly identical for all structures with reverse breakdown voltages of 550-750 V, defined by a reverse leakage current of ~ 10 μA. Differences in the reverse breakdown voltages are likely due to drift layer doping differences amongst the wafers. These results reveal: 1) the primary source of Si originates from ex-situ contamination during wafer handling prior to loading for regrowth, and 2) the presence of Si at the p-n junction, at these concentrations, did not impact the forward or reverse-bias performance of these regrown diodes compared to a continuously-grown diode with no Si at the junction. Additional work is underway to investigate selective area p-n diodes to enable advanced, vertical device structures. The information, data, or work herein was funded in part by the Advanced Research Projects Agency – Energy (ARPA-E), U.S. Department of Energy under the PNDIODES program directed by Dr. Isik Kizilyalli. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

*Plenary Speaker
8:20 AM Awards Ceremony
8:30 AM *A01
Electronics Anywhere or Will We Ever Have Flexible Electronics?
Thomas N. Jackson; The Pennsylvania State University, State College, Pennsylvania, United States.

A Google search for “flexible electronics” or “printed electronics” brings ~4x10^5 and ~5x10^5 hits, respectively. Yet commercial applications of active flexible electronics are hard to find. In fact, large scale commercial applications of active thin film electronics on any substrate, rigid or flexible, are few. They include the outstanding success of active matrix displays (~$100 billion and ~200 million m^2/year), and limited, but significant, product areas in x-ray detectors and thin film photovoltaics. The list of active devices used in commercial applications is similarly limited, perhaps starting and ending with transistors used mainly as simple switches, and diodes. Both the current applications and the current scope of devices and circuits appear disconnected from the level of research and business interest. What are the key enablers for ubiquitous thin film electronics and especially flexible electronics? What application areas make the best use of developing thin film technology? Thin film transistors (TFTs) on flexible substrates have been demonstrated using a-Si:H, polysilicon, organic semiconductor, oxide semiconductors, and other materials. Among these, a-Si:H has relatively poor performance (NMOS only FETs and typical field effect mobility <1 cm^2/Vs), yet is the backbone for most of the ~$100 billion active matrix display industry. Organic semiconductors have similar (poor) performance in FETs and have thus far failed commercially in transistor applications, yet have had significant and growing success in organic light emitting diode (OLED) displays. Low-temperature polysilicon has found significant application (for example, in OLED displays) and high performance devices (field effect mobility >100 cm^2/Vs) have been demonstrated on polymeric substrates, but commercial applications have not followed. Using organic and oxide thin film transistors as examples, this talk will consider approaches to flexible electronics, what characteristics are most important and what approaches may fail. 9:20 AM BREAK

SESSION B: GaN Power Electronic Materials
Session Chairs: Andrew Allerman and Jennifer Hite
Wednesday Morning, June 27, 2018
Location: Music Building, Lotte Lehmann

10:00 AM B01
Regrown GaN P-N Diodes with Low Reverse Leakage Currents—Investigating the Si Spike
Gregory W. Pickrell, Andrew M. Armstrong, Andrew Allerman, Mary Crawford, Karen C. Cross, Caleb E. Glaser and Vincent M. Abate; Sandia National Laboratories, Albuquerque, New Mexico, United States.

Vertical GaN-based power electronics promise higher-performance than Si- and SiC-based devices for applications including consumer electronics, electric vehicles, and the power grid. Poor selective-area p-type doping is the critical remaining materials challenge that has precluded devices such as junction field effect transistors (JFETs) and merged p-n Schottky (MPS) diodes in GaN. Ion implantation and epitaxial regrowth have been used, with limited success. GaN p-n diodes, where the p-GaN layer was formed by regrowth, have so far yielded lower breakdown voltages and/or GaN-based high electron mobility transistors (HEMTs) are of significant interest for next-generation RF power amplifiers. However, for power switching devices there are still significant challenges preventing mass production and widespread adoption. In particular, lateral HEMT devices lack avalanche capability for rugged power switching, vertical device technology is not mature, and the manufacturing cost associated with small diameter substrates is relatively high. As a scalable substrate solution, Qromis, Inc. has developed commercial engineered substrates designated QST?. As the substrates are engineered to be thermally matched to GaN, thick epitaxial layers capable of >1kV devices can be grown on 200 mm diameter wafers suitable for fabrication in a CMOS fabrication facility. Taking advantage of this platform, we present a GaN-based lateral junction (JFET) device gate field effect transistor (JFET) device technology for robust power switching. The p-GaN gate functions to collect secondary electron avalanche breakdown, a critical capability for power switching that has not been demonstrated in lateral GaN JFETs to date. In this work we present process development to realize such lateral JFET devices, focusing on foundry-compatible processes to facilitate cost-effective manufacturing. The layer structure consisted of a semi-insulating GaN buffer layer for...
blocking, a n-GaN channel layer, and a p-GaN cap for gate control and electric field spreading. The critical process steps are reliable, low-damage dry etching to recess the source and drain regions, N+ source and drain contact regions by Si ion implantation, and multi-zone N implant to compensate p-GaN in the access region for appropriate electric field management. Optimization of each of these steps and their impact on device performance will be discussed in detail. Implanted activation is achieved by applying a protective capping layer and using a modified RTA-based technique to accumulate long cycle time in the 1150-1250 °C range without damaging the GaN layers. Following fabrication, JFET devices and test structures were characterized. CTCM characterization indicated that the addition of n-GaN ohmic, but p-GaN ohmic contact resistance was poor. The first devices exhibited modulating transistor behavior with a large negative threshold voltage. Simulations indicate that such normally-on behavior is expected. Off-state leakage current was relatively high, indicating that the semi-insulating buffer layer was not optimized. Capacitance-voltage measurements were implemented to characterize the active epilayer layers and understand the differences between the initial prototype structures, and vertical breakdown measurements were used to characterize the blocking capability. A dynamic ON-resistance evaluation is in-progress. The n-GaN ohmic process was improved utilizing a N+ contact region formed by Si ion implantation and activation annealing, and the p-GaN ohmic process was improved by using a sub-bandgap light illumination. The results of the initial testing have been used as feedback to new epitaxial structures, which will be evaluated and discussed in detail. This is a promising proof-of-concept and further work is in-progress to improve problems in the epitaxial layer structure and optimize doping in the material stack, especially in the channel and gate layer, is in-progress and will be shown at this conference. In conclusion, it is expected that with overall gallium nitride breakdown avalanche breakdown and have the capability to block >1kV.

10:40 AM B03

(Student) Franz-Keldysh Effect in GaN Schottky Barrier Diodes and p-n Junction Diodes Under High Reverse Bias Voltage Takuya Inoue 1, Masaya Okada 1, Masaki Ueno 1, Yoshiyuki Yamamoto 1, Tetsuo Narita 1, Masakazu Kanenchika 1, Tsutomu Uesugi 2, Tetsu Kachi 3, Tsunenobu Kimoto 4, Masahiro Horita 4, and Jun Suda 4, 1: Kyoto University, Kyoto, Japan; 2: Sumitomo Electric Industries, Ltd., Hyogo, Japan; 3: Toyona Central R&D Labs., Aichi, Japan; 4: Nagoya University, Nagoya, Japan.

Under a high electric field, a direct-bandgap semiconductor exhibits sub-bandgap light absorption, which is known as the Franz-Keldysh (FK) effect. GaN is a direct-bandgap semiconductor and has a high critical electric field. Thus, the FK effect can be observed significantly in GaN power devices under a high reverse voltage. In this study, we investigated the photocurrent in undoped and p-sub-bandgap light illumination GaN Schottky barrier diodes (SBDs) and p-n junction diodes (PNDs) under a high reverse voltage. The voltage and wavelength dependences of the photocurrent can be explained by the light absorption due to the FK effect. In addition, the temperature dependence of the photocurrent due to the FK effect was investigated and can be explained by red shift of its absorption edge. To characterize the FK effect on a Schottky barrier diode, devices used in this study were fabricated on GaN homoepitaxial layers to suppress a leakage current due to threading dislocations. The net donor concentration of the n-epilayer of the GaN SBDs was 5.5×10^{19} cm^{-3}. In the GaN SBDs under a low reverse voltage, the photocurrent induced by the internal photoemission (IPE) was observed, which did not depend on a voltage. Under a high reverse voltage, the photocurrent significantly increased with the voltage. The increase in the photocurrent was striking as the wavelength got closer to the absorption edge of GaN. These additional photocurrents were considered to originate from the sub-bandgap optical absorption due to the FK effect. We calculated the photocurrent considering the light absorption due to the FK effect in the depletion layer and the absorption in the volume. The volume mass is critical to determine the electric field dependence of the absorption coefficient, and we used the value (0.16md) obtained from the electron and hole effective masses in GaN reported in the past. The calculated curves considering the IPE and the FK effect showed good agreement with the experimental curves in terms of the voltage and wavelength dependences. In the GaN SBDs under a reverse voltage of 200 V and the photocurrent induced by the FK effect was clearly observed in the range from 390 nm to 400 nm. Under a higher voltage, the leakage current due to the thermionic field emission becomes larger and cannot be neglected. To investigate the FK effect in a higher electric-field range, we fabricated the GaN PNDs with a relatively high doping concentration. The Si concentration of the n-epilayer and the Mg concentration of the p-epilayer were 6.3×10^{19} cm^{-3} and 5.0×10^{19} cm^{-3}, respectively. The photocurrent was observed under a high reverse voltage and significantly increased with a reverse voltage. In the GaN PNDs, the maximum electric field was 1.8 MV/cm under a reverse voltage of 200 V and the photocurrent due to the FK effect was clearly observed in the range from 390 nm to 420 nm. Since the electric field in the GaN PND was higher than that in the GaN SBD under the same reverse voltage, the photocurrent in the GaN PND was larger than that in the GaN SBD for the same wavelength. The calculated photocurrent in the GaN PND also showed good agreement with the experimental results as well as the case of the GaN SBD. In addition, we investigated the photocurrents induced by the FK effects in the GaN PND at 223, 298, and 373 K. The photocurrent for the same wavelength increased with a temperature. The increases were successfully explained by the temperature dependence of the bandgap of GaN.

11:00 AM B04

(PStudent) Polarization-Induced Doping in Buried P-Type GaN—Unique Advantage in Reverse Blocking Wenshen Li 1, Mingda Zhu 1, Kazuki Nomoto 2, Zongyuan Hu 3, Xiang Gao 3, Manyam Pilla 4, Debdeep Jena 4, Huili Grace Xing 4, Electrical and Computer Engineering, Cornell University, Ithaca, New York, United States; 3: Qorvo Inc., Richardson, Texas, United States; 4: Material Science and Engineering, Cornell University, Ithaca, New York, United States.

Polarization-induced (PI) doping is a unique doping scheme in GaN material system, offering advantages such as fully activated dopants independent of temperature [1] and increased breakdown field with the introduction of Al. Buried p-type structures are prevalent in GaN vertical power devices, offering capabilities including reverse blocking, avalanche and reduced surface field (RESURF). However, it is well-known that p-GaN gets passivated by hydrogen in metal-organic chemical vapor deposition (MOCVD) grown material. The activation of the Mg dopants is much more difficult in buried p-GaN structure in comparison with structures with exposed p-GaN surface. Since PI-doping does not rely on impurity dopants in principle, the incorporation of PI-doping in buried p-type structures is a promising proof-of-concept and further work is in-progress to identify the unique advantage of utilizing PI-doping in GaN vertical power devices.

11:10 AM B04


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The growth and fabrication of GaN homojunction tunnel diodes demonstrating negative differential resistance (NDR) at $-1.25 \text{ V}$ and high reverse bias current densities above $1.2 \text{ kA/cm}^2$ necessary for tandem series connected devices and tunnel contacts is reported. Tunnel junctions for the III-nitrides are being heavily investigated to increase design freedom in order to realize tandem series connected devices, simplify fabrication with less metallization and lithography, and enable substantially better contact resistances to n-type material. Unfortunately, metal-organic chemical vapor deposition (MOCVD) grown films lack the doping abruptness necessary to form small depletion width low loss tunnel junctions. Additionally, MOCVD grown beam-epitaxy (MBE) grown films are limited in hole concentrations. The metal modulated epitaxy (MME) growth technique performed in an MBE system enables high hole concentrations above $7 \times 10^{19} \text{ cm}^{-3}$, as well as electron concentrations above $4 \times 10^{19} \text{ cm}^{-3}$ and the abrupt interfaces required to form low specific resistance tunnel junctions without the need for polarization engineered interlayers. GaN $p++/n$ tunnel diodes and $n++/p$ tunnel contacted diodes with varied silicon doped n-type layers exhibiting electron concentrations of $1 \times 10^{20} \text{ cm}^{-3}$, $6 \times 10^{19} \text{ cm}^{-3}$ and $4 \times 10^{20} \text{ cm}^{-3}$ and magnesium doped p-type layers with hole concentrations above $5 \times 10^{18} \text{ cm}^{-3}$ are presented. The highest silicon doped $p++/n++$ tunnel diode is the only device that demonstrates NDR in forward bias around $1.25 \text{ V}$, and the lowest reverse bias to reach a current density of $1.2 \text{ kA/cm}^2$. Additionally the reverse breakdown voltage is $-1 \text{ V}$. The intermediate silicon doped $p++/n+$ diode showed reverse break down at $-2 \text{ V}$, while the lowest silicon doped $p++/n+$ diode showed the highest reverse breakdown voltage greater than $-3 \text{ V}$ and forward voltage turn on at $-2.8 \text{ V}$. The highest silicon doped $n++/p++/n$ tunnel contact diode demonstrates a low $-0.1 \text{ V}$ increase in turn-on voltage when compared to a $p/n$ control diode demonstrating a turn-on voltage of $-2.9 \text{ V}$. The medium and lowest silicon doping $n++/p++/i/n$ diodes increasing turn on voltages of $3.2 \text{ V}$ and $4.5 \text{ V}$ respectively and increasing series resistance compared to the $p/n$ control diode. These results are promising for improving performance of a wide array of III-nitride devices including light emitting diodes (LEDs), lasers, and solar cells.

Heterogeneous combinations of two-dimensional (2D) layered materials provides us with an ability to tune several electronic and optical properties tailored for specific applications. Transition metal dichalcogenides (TMDs) are attractive 2D materials in the “beyond graphene” realm of materials. To utilize their unique electronic properties, it is important to develop low resistance contacts to these materials. Graphene is a promising candidate and has been shown to produce low-resistance contacts to a few TMDs. But this has been done by manual stacking via exfoliation or polymer-assisted transfer, which is not a scalable method. One avenue that is still in its infancy, yet could provide significant potential for scalability and be enroute “all-2D” electronics is the utilization of as-grown graphene contacts to 2D materials beyond graphene. Here, we discuss electronic properties resulting from the interface of the as-grown lateral heterostructures between epitaxial graphene and TMDs. Using powder vaporization to grow the TMDs on patterned epitaxial graphene, directly yields 2D lateral heterostructure between graphene and TMDs like MoS$_2$, without the need for transfer of any 2D layers. Investigation of this synthetic lateral heterostructure via several advanced characterization techniques leads to an understanding of the structure of this interface. Cross-sectional transmission electron microscopy shows that the interface between graphene and MoS$_2$ is in fact, a pristine overlap of the MoS$_2$ onto the graphene for a few hundred nanometers. This unique combination allows for improved electronic coupling and reduced contact resistance to these TMDs using graphene as the contacting material instead of conventional metals like Ti/Au. The flexibility of being able to tune the doping of the epitaxial graphene allows us to explore the option of matching the Fermi level of the graphene to the Fermi level of the TMD, thus for the elimination of the doping of the TMD, thus reducing the barrier for electrons and making contacts much superior to conventional metals.
analogous to graphene. Among them, transition metal dichalcogenides (TMDCs) own a special place for many extraordinary properties and applications that have been reported in the recent years. 

While graphene based field effect transistors (FETs) perform poorly in terms of switching because of its zero band gap; MoS₂, a TMDC, has been reported to deliver far superior field from the second constituent. Additionally, few atomic layer thick MoS₂ layers on SiO₂/Si. The process oxidizes patterned metallic Mo to form a mixture of volatile Mo-oxides at <400 °C and then proceeds with sulfidation at <500 °C for about 50 min to produce 3-5 monolayer (ML) thick MoS₂ thin film, as confirmed by Raman spectroscopy and atomic force microscopy. High quality mono or bi-layer graphene was grown on Cu foil using chemical vapor deposition technique on a variety of substrates.

In our earlier work, we reported a 2D heterojunction between graphene and MoS₂, which offered a Schottky barrier that could be tuned by over 0.6 eV using a back-gate voltage, turning it into an excellent barristor (variable barrier transistor). A key property of this barristor is that each constituent of the heterojunction is so thin that it cannot completely screen an electric field from the second constituent. As a result, voltage-induced interfacial tunability is achievable. For the same reason, any donor or acceptor molecule adsorbed at the top surface of the device can effectively influence the barrier height at the interface, by interacting with both materials simultaneously. In our current work, we focus on such gas sensing applications. We start with a top-down growth technique for synthesizing large area, few atomic layer thin MoS₂ layers on SiO₂/Si. The process oxidizes patterned metallic Mo to form a mixture of volatile Mo-oxides at <400 °C and then proceeds with sulfidation at <500 °C for about 50 min to produce 3-5 monolayer (ML) thick MoS₂ thin film, as confirmed by Raman spectroscopy and atomic force microscopy. High quality mono or bi-layer graphene was grown on Cu foil using chemical vapor deposition technique on a variety of substrates.

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stability and portability of silicone devices. Due to air-sensitive nature of silicone, it is unfeasible to make silicone through widely used transfer and fabrication process. A unique growth-transfer-fabrication integrated process has been employed with key features including: i) in-situ AlOx/silicone/Ag sandwiched encapsulation, ii) native Ag film to stabilize silicone and serve as source with drain electrodes, iii) direct forming back gate dielectrics and electrodes (an ex-situ atomic layer deposition of 15 nm AlOx followed by 200-300 nm Ag or Au deposition seen in Fig. 1) on top of in-situ AlOx/silicone/Ag/mica stack. Consequently, back gate silicone device structures is built-in ready to be delaminated from mica substrate for device study. Besides interface engineering, it is crucial to employ thermal release tape in the delamination transfer step for better transfer quality. Under optimized temperature and surface conditions, this approach can transfer silicone device stack over a 1 x 1/2 in2 area with decent coverage and uniformity (Fig. 1b), leading to potentially high yield of device fabrication. This newly developed process not only provides a more reliable outcome in seamless transfer and fabrication of silicone devices, but it also preserves intact silicone (Fig. 2), by forming functional layers of silicone devices beforehand. In addition, we also discovered that material attribution, such as the number of layers, also played a role in stabilizing silicone devices. Electrostatic measurements on fabricated silicone transistors revealed ambipolar charge transport characteristics in drain current (I) response to gate voltage (Vg) for both monolayer and multilayer silicone devices (Fig. 3) proving certain theoretical calculations3. Monolayer silicone could yield field-effect mobility ~100 cm2/V·s at residual carrier density of ~5 x 1012 cm-2 with gate modulation around 10%, whereas multilayer silicone showed an enhanced mobility up to 200 cm2/V·s at residual carrier density ~8 x 1011 cm-2 with slightly reduced gate modulation. There are two interesting features in multilayer silicone device performance: one is a broader I-V response curve especially close to Dirac point, and the other is a notably longer lifetime up to 48 hrs (2 mins for monolayer). The results indicate that number of layers is a key knob to tune the stability of silicone devices. This work suggests a promising route to minimizing the risk of degradation during transfer and device fabrication, providing a new type of layered 2D materials such as phosphorene and germanane. Importantly, the allotropic affinity of silicone with crystalline bulk silicon suggests a more direct path for silicene integration with ubiquitous semiconductor technology. Reference: 1. S. Cahangirov, et al., Phys. Rev. Lett. 102 (23), 2009.2. C.-C. Liu, et al., Phys. Rev. Lett. 107 (7), 2011.3. Y. D. Nelson, et al., J. Phys. Cond. Matter 22 (57), 2010.4. Q.-X. Pei, et al., J. Appl. Phys. 114 (3), 2013.5. L. Tao, et al., Nature Nanotech. 10 (10), 2015.6. P. Vogt, et al., Phys. Rev. Lett. 108 (15), 2012.2. Supported by NSF (#51602051), Fundamental Research Funds for the Central Universities (#22424017R30008)

SESSION D: Organic and Hybrid Optoelectronics

Session Chairs: Tse Nga Ng and Adrienne Stiff-Roberts

Wednesday Morning, June 27, 2018
Location: University Center, Flying A Studios

10:00 AM D01

300% Enhancement of Carrier Mobility in Uniaxial-Oriented Perovskite Films Formed by Topolectric-Oriented Attachment

Donghoo Kim, Zhen Li, Mengjin Yang, Joseph J. Berry and Kai Zhu; Chemistry and Nanoscience Center, National Renewable Energy Laboratory, Golden, Colorado, United States.

Organic-inorganic perovskites with intriguing optical and electrical properties, such as excellent absorption coefficient, long carrier diffusion length, and unique defect physics, have attracted significant research interests due to their excellent performance in optoelectronic devices. Recent efforts on preparing uniform and large-grain (micrometer-sized) polycrystalline perovskite film have led to enhanced carrier lifetime up to several μs. However, the mobility (~5-10 cm2/V·s) and trap density (1015–1017 cm–3) of polycrystalline perovskite films which are closely related to device characteristics are significantly less than the values (~105–106 cm2/V·s and 1010–1015 cm–3, respectively) of their single-crystal counterparts. We recently showed for perovskite films with a grain size beyond 400 nm there is little if any correlation with grain size and carrier mobility. This suggests that the details of materials processing could limit the transport properties within the bulk rather than at the boundaries. This motivates the development of strategies for reducing trap density in the bulk to further enhance the electrical properties of polycrystalline perovskite films for various optoelectronic applications. In addition, controlling crystalline orientation in polycrystalline films can also enhance charge transport over their randomly oriented counterparts by reducing structural disorder. Oriented attachment involving spontaneous self-organization along a common crystallographic orientation between neighboring particles is one of the most well-known mechanisms for synthesizing oriented nanocrystals with improved crystallinity and reduced defect density, but it has never been adopted, so far, for perovskite growth. Here, we demonstrate a facile topolectric transformation with oriented attachment (we called this process as a topolectric-oriented attachment, TOA) to grow highly oriented perovskite films, featuring strong uniaxial-crystallographic texture, micron-grain morphology, high crystallinity, and low trap density (~4×1010 cm–3). These uniaxial-oriented TOA-perovskite films exhibit unprecedented 9-GHz charge-carrier mobility of 71 cm2/V·s which approaches the reported mobilities for CH3NH3PbI3 single crystals (115±15 cm2/V·s). TOA-perovskite based n-p planar solar cells show minimal discrepancies between stabilized efficiency (19.0%) and reverse-scan efficiency (19.7%). The reverse-scan efficiencies exhibit no dependence on the scan delay time.

10:20 AM D02

(Student) In-Plane Transport Pathways Promote Out-of-Plane Charge Percolation in Bulk Heterojunctions

Jeremy S. Mehta and Jeffrey M. Mativetsky; Physics, Binghamton University, Binghamton, New York, United States.

Solution processed organic photovoltaics is a promising low-cost, green, and mechanically-flexible energy conversion technology. The bulk heterojunction (BHJ) architecture, with its nanoscale interpenetrating donor-acceptor structure, allows for ample light absorption while satisfying the need for a high density of donor-acceptor interfaces required for efficient charge photogeneration. Nevertheless, the BHJ’s locally varying composition and crystallinity lead to a complex landscape for charge transport. Despite the importance of nanoscale structuring, optoelectronic characterization has been predominantly limited to large-area device measurements. In this presentation, we discuss the key structural features that impact out-of-plane charge transport in high-performance small-molecule/fullerene BHJ active layers comprising p-FTSiPcBM. A series of 15 BHJ films with varying compositions and degrees of phase separation were characterized electrically by conductive atomic force microscopy (C-AFM) and structurally by grazing incidence x-ray diffraction (GIXD). Hole mobility was quantified and mapped at the nanoscale by performing a series of C-AFM current-voltage measurements at thousands of sample positions. GIXD provided the donor crystallite size and population along n-π and alkyl stacking directions. We find that, contrary to conventional wisdom, lateral aromatic stacks play a critical role in facilitating out-of-plane charge transport in BHJ active layers. We identify the in-plane n-π crystallinity as the strongest predictor of out-of-plane hole mobility across all studied film morphologies. This result is further supported by nanoscale hole mobility maps that show a halo of moderate hole mobility regions concentrated around high hole mobility hot spots. As the in-plane n-π stacking population increases, the width of the halo surrounding conductive hot spots also increases, indicating increased lateral access of charge from the surrounding regions to the hot spots. Additional insight into the dependence of hole mobility on active layer composition and phase separation is provided by percolation theory. Both the spatial mobility maps and the percolation model point towards three-dimensional charge percolation across the active layer. This analysis indicates the importance of three-dimensional connectivity with lateral access to vertical pathways.

10:40 AM D03

Extended PDI Small Molecules and their Optoelectronic and Film Forming Properties

Julia A. Schneider1, Kyle Clark2, Yonghao Zheng1, Hengbin Wang1, Hidenori Nakayama1, Fred Wudl1, Michael Chabinyc1, Javier Read de Alaniz1, 1 Mitsubishi Chemical Center for Advanced Materials, Santa Barbara, California, United States; 2 University of California, Santa Barbara, Santa Barbara, California, United States; 3 School of Optical-Electronic Information, University of Electronic Science and Technology of China, Chengdu, Sichuan, China.

Perylene diimides (PDIs) exhibit excellent redox properties, environmental stability, and high charge mobilities, making them popular non-fullerene acceptors and electron transport layers in photovoltaics. While several studies have examined PDIs to achieve a variety of characteristics, there has been less focus on tailoring the electronic and optical properties of PDI itself. In this work we discuss how modifications to the PDI core can lead to advantageous electronic and film forming properties. We will present the synthesis of expanded PDI structures and
compare their performance in a variety of devices, including bulk-heterojunctions and perovskite solar cells.

11:00 AM D04
(Studnet) The Effect of Donor-Acceptor Ratio on Novel Organic Short-Wave Infrared Photodetectors

Zhelin Yao1, Zhengui Wu1, Jason Azoulay2 and Tse Nga N1; 1Electrical and Computer Engineering, University of California, San Diego, La Jolla, California, United States; 2School of Polymers and High Performance Materials, University of Southern Mississippi, Hattiesburg, Mississippi, United States.

With the key applications in environmental monitoring, biomedical diagnosis and spectroscopic instrumentation, the state-of-the-art short-wave infrared (SWIR) photodetectors comprised of conventional inorganic semiconductors are expensive, and thus not economically viable for large scale sensing. As an alternative class of materials, semiconducting polymers can substantially lower the production cost with the ease of low-temperature processing. To achieve the SWIR absorption, a low energy bandgap is required. However, low bandgap polymers with optoelectronic functionality are scarce due to synthetic difficulty; In addition, reducing bandgap inevitably increases the dark current noise resulted from the lowered barrier to thermally generated carriers. Here we report a SWIR polymer that exhibits a spectral redshift of 100 nm in the bulk heterojunction photodiode with properties deriving the absorption profile of its pristine film. We investigated the optimal donor-acceptor (D-A) ratio to achieve the balance of spectral broadening and device performance. The performance of photodiodes was monitored by current-voltage characteristics, external quantum efficiency, electrochemical impedance spectroscopy and noise measurement. An improved photocurrent-voltage fitting model was implemented to identify the collection and dissociation loss for the respective D-A ratio, and the results were supported by the transient photocurrent measurement. Capacitance measurements were also carried out to correlate the trap density induced by different D-A ratio to the extracted collection loss. The study provides an in-depth understanding of how D-A ratio affects the spectral shift and device performance with the SWIR polymer.

11:20 AM D05
Small molecule C60 Organic Light-Emitting Diodes with Reduced Turn-On Voltage, the Role of Charge Transfer States and Triplet-Triplet Annihilation in Organic Light Emitting Diodes

Weichuan Yao1, Zhengui Wu1, Jason Azoulay2, Eugene G. Bittle1, Lee Richter1 and David Gundlach1; 1National Institute of Standards and Technology, Gaithersburg, Maryland, United States; 2Theis Research, La Jolla, California, United States.

Low-power solid state lighting and large area displays for consumer electronics have been drivers for the development of more and more efficient organic light emitting diodes. Since the drive voltages for most OLEDs are comparably higher than for their inorganic counterparts, research recently focused on more efficient device geometries and device physics enabling a lower device turn-on. Common for the organic semiconductor community is the belief that in most OLED device configurations the turn-on voltage must be larger than the emitter bandgap for efficient light emission. However, there have been devices reported with electroluminescence (EL) turn-on at about half of the bandgap voltage for a series of heterojunctions. These devices commonly share a small molecule emitter (and hole transport layer) like rubrene and an electron transport layer such as C60. The mechanism which leads to the reduced turn-on voltage was attributed to either an Auger-assisted energy up-conversion process at the heterojunction interface; or and Dexter transfer of triplet charge transfer (CT) states into triplet excitons, followed by triplet-triplet annihilation (TTA). For rubrene based devices, TTA was assigned to be the origin of the observed low-voltage turn-on and the formation of an intermediate CT-state and recombination rate. We find that suppressing the CT-state formation by a 3nm thick BCP interlayer yield in device luminance compared to the rubrene/C60 device, while maintaining the same low turn-on voltage. The increased luminance of devices with BCP interlayer suggest a reduction in parasitic effects of the CT-state. Examining the current density-voltage-characteristics, J(V), of the OLEDs more closely, we observe diode ideality factors of about 1.5 in the heterojunction devices, whereas this value is 2 in a rubrene-only devices not exhibiting the low turn-on voltage. The effective value of 1.5 rules out a coherent triplet formation process and auger-recombination in the C60 based heterojunctions. The overserved luminescence-current density-characteristics, L(J), show a linear dependence in the small current limit, whereas a quadratic dependence is expected for coherent as well as incoherent triplet-triplet annihilation processes. Our electrical analysis suggests that the origin of the observed low-voltage turn-on is not due to an Auger or triplet-triplet annihilation process. Rather, it suggests that classical radiative band-to-band recombination is the most favourable recombination process.

11:40 AM D06
Halide Perovskite/Polymer Composites for Fully Printed LEDs

Zhixin Yu; Industrial and Manufacturing Engineering, Florida State University, Tallahassee, Florida, United States.

Recently, remarkable optoelectronic properties have been discovered in a group of materials called halide perovskites. Their potential to invigorate the current solar cell and light-emitting diode (LED) industries has been demonstrated by achieving very high device efficiencies in relatively short periods. In this conference meeting, we hope to present our recent work of developing perovskite/polymer composites towards the realization of fully printable LEDs. The perovskite/polymer composites possess all the remarkable optoelectronic characteristics of pure perovskites. For instance, we have demonstrated their use for blue, green and red LEDs. In addition the device efficiencies exceeded those of pure perovskite LEDs. The perovskite/polymer composites have shown advantages in improving the processability and quality of the perovskite thin films; and enhancing the structural stability of the perovskites especially at high humid fabrication and service environments. By embedding the perovskite crystals inside a polymer matrix, the perovskites can be less toxic and more environmentally benign compared to pure perovskite.

SESSION E: Materials for Memory Applications

Session Chairs: W. Alan Doolittle and Taakee Lee

Wednesday Morning, June 27, 2018
Location: University Center, State Street

10:00 AM E01
(Studnet) Understanding Intercalation Enabling Device Structures Resulting in Non-Volatile Behavior of Lithium Niobite Memristors

Marshall B. Teliekamp, Bill Zivasatien, Alex S. Weidenbach and W. Alan Doolittle; Georgia Institute of Technology, Atlanta, Georgia, United States.

Neuromorphic computing has grown in interest as the performance limits of Von Neumann based devices are approached. The brain performs certain computational tasks significantly more efficiently than the current CMOS Von Neumann architecture, which has led to the desire to realize a solid-state equivalent of the biological neural network. The memristor has been accepted as a potential element of neuromorphic computing, but the field is currently dominated by filamentary devices that provide a binary memory response for a constant period stimulus, disallowing adaptive learning without active control of the stimuli. Lithium niobite (LiNbO3), a lithium intercalated sub-oxide of the maturely studied lithium niobate (LiNbO3), exhibits an analog memristive response with a continuum of resistive states, which enables replication of biological processes such as short-term (STP), long-term (LTP), and spike-timing dependent plasticity (STDP) and through drift and diffusion of non-filamentary Li, accurately replicates many aspects of mammalian neurobiology. Lithium niobate contains mobile lithium ions acting as dopants that move within the potentiated material to cause resistive changes. Without the presence of an electrical bias, these ions are shown to diffusively equilibrate to a uniform concentration, and the film exhibits its as-grown resistance, an effect that is useful for realizing STP and STDP. Although inherently a volatile material, LiNbO3 has been experimentally confirmed to exhibit non-volatile behavior by means of using electrode materials that are known to reversibly capture/release lithium, facilitating intercalation and de-intercalation of LiNbO3. These electrodes known to alloy with lithium, such as aluminum, dissolve, capture and/or alloy with lithium, effectively changing the LiNbO3 acceptor concentration and possibly forming resistive interface layers between the metal and the LiNbO3. However, the mechanism by which this non-volatile behavior arises is not well understood. Specifically, whether the segregation of Li from the LiNbO3 is driven by thermionic emission over an energy barrier or by electrochemical means has important consequences on the future scaling of these promising neuromorphic devices. To understand the effect governing the transition from the volatile behavior of LiNbO3 towards non-volatility, both non-volatile and volatile device contacts were
(Nb2O5-x) is investigated as an insulating layer in metal-insulator-metal rectification and hysteresis properties required to imitate a biological Niobium Oxide (NbO2) memristors created by electroforming a channel Binghamton, New York, United States.

Matthew Wahila

Memdiode Electrical Response

Reports 6, Article number: 27506 (2016)

silicon nanowires, K Saranti, S Alotaibi and S Paul, Nature's Scientific for two terminal electronic memory devices - Storing information on


Organic resistive memory is one of the promising next-generation data storage technologies due to several advantages such as versatility of organic materials, low-cost device fabrication, and application on printable and flexible devices. However, the mechanism of the resistive switching phenomenon in organic resistive memory devices has not been clearly understood [1]. In this study, we investigated the time-dependent current behavior of unipolar-type organic memory devices under a constant voltage stress. In this measurement, the current abruptly increased several times and reached ON state even when the applied voltage was below the threshold voltage. The distribution of the time required to reach ON state (defined as turn-on time) could be described with Weibull distribution, which has often been used for studying time-dependent gate dielectric breakdown in semiconductor transistors [2]. Through a statistical analysis of the turn-on time values, we found that the probability of the current increase over time depended on both the magnitude of the applied voltage and temperature, but not on the current level itself (i.e. resistance state). We explain these observations by the formation of percolation networks of conducting paths during the turn-on process.

Organic memristors are fabricated using electroforming a channel inside an insulating layer of bulk Nb2O5 have been shown to replicate the rectification and hysteresis properties required to imitate a biological neuron. However, Nb2O5 memristors have no reported capacitance and therefore require a bulky separate parallel capacitor which limits scalability of the memristive device, particularly when used in a neuromorphic circuit. Conversely, oxygen deficient niobium pentoxide (Nb2O5-x) is investigated as an insulating layer in metal-insulator-metal (MIM) memdodis, rectifying devices with state memory, for the use in memristive applications. A sputtered film of Nb2O5-x fabricated into a memdiode is shown to have similar rectifying and hysteresis properties as the NbO2 memristor as well as an added intrinsic capacitance useful in large scale integration. The removal of electroforming along with the addition of an intrinsic capacitance allows a sputtered Nb2O5 memdiode to replace the NbO2 memristor and increase the device density of neuromorphic circuits. The current-voltage characteristics are found to be tunable in proportion to the number of oxygen-vacancies created in the sputtering process. Nb2O5 memdiodes have been deposited in a DC sputtering tool using a pure Nb target sputtered at powers of 30W, 40W, and 50W in an oxygen environment. The sputter chamber is held at a pressure of 10 mTorr with a constant oxygen flow of 15 sccm. The sputtering of an amorphous Nb2O5 film under oxygen deficient conditions introduces the necessary oxygen vacancies to achieve a sufficient conductivity through defect mediated Poole-Frenkel conduction in the active layer of the memdiodes. Rectification is achieved from a transition from tunneling to Poole-Frenkel conduction. The oxygen vacancy concentration of Nb2O5-x can be controlled through the sputtering power. By holding the oxygen flow constant during deposition and adjusting the power applied to the Nb target, different oxygen vacancy concentrations were achieved. By increasing the Nb:O ratio above the stoichiometric ideal value of 0.4, tunable current rectification and hysteresis is realized without the need for electroforming. The oxygen to niobium ratio was measured at various sputter powers using x-ray photoelectron spectroscopy (XPS) and hard x-ray photoelectron spectroscopy (HAXPES). The compositional analysis of 3 differing Nb target power levels (30W, 40W, and 50W) showed a positive trend in the Nb:O ratios. The averaged Nb:O ratio (omitting surface oxygen contaminants) of the 3 Nb target power levels were determined to be 0.481±0.023, 0.486±0.016, and 0.497±0.018 compared to the ideal stoichiometric value of 0.400 for the 30W, 40W, and 50W films, respectively. To corroborate the role of oxygen vacancies in the Nb2O5-x memdiodes, XPS was performed using harder x-rays (HAXPES) to study the electronic structure of the bulk. As the Nb:O ratio increased (i.e. with increasing Nb power) in-gap defect states near the conduction band minimum were filled. The recorded current indicates an activation energy of 0.22 eV confirming the current is dominated by the oxygen vacancy defect. This activation energy is consistent with the energetic location of the in-gap states observed by HAXPES and suggests the filling of these oxygen vacancy states. Increased oxygen vacancy content results in higher current and smaller turn-off voltage of the memdiodes. The hysteresis in ON-state switching is also enhanced by an increase in the oxygen vacancy content. In conclusion, sputtered Nb2O5 enables scalable fabrication of memdiodes without electroforming using an easy process for tuning the current-voltage and hysteresis response, rectification, and capacitance crucial via oxygen vacancy engineering for high density neuromorphic circuitry.
filters, data recording, signal transduction in sensing systems, as optoelectronic switches, or as a molecular electronic element such as a Read-Only memory. Despite the variety of uses of these systems, many photochromic molecules have proven to be difficult to switch when placed on a metal surface, limiting their utility for integration with electronic systems. This work demonstrates that such switching can be achieved from the metastable norbornadiene (NB)-state to the quadricyclane (QC)-state, which is normally controlled optically, can also be electrically induced on metal surfaces. We utilize the Single-Molecule Break Junction (SMBJ) technique to make contact to and investigate the switching properties of these molecules. Because the switching action breaks the conjugation pathway within the molecule, it causes a large conductance change of a factor of ~10. Interestingly, at room temperature under high vacuum, the transition between the NB- and QC-states occurs at low biases, at a bias of 50 mV, the high conductance NB-state is detected, but at 200 mV, the low conductance QC-state is observed. Alternatively, when the single-molecule conductance measurements are performed in a mesitylene solvent environment, this transition does not occur below a bias voltage of ~1.2 V. This change in the switching voltage suggests that the solvent serves as a cold bath and that a local heating effect is responsible for the observed switching behavior. By systematically controlling the ambient temperatures over a range from 78K to 300K shows a clear correlation between the switching bias and the ambient temperatures. The bias/temperature dependence can be explained by a local heating mechanism which yields a local effective temperature of 325K within the molecular junction when switching occurs. By modeling the behavior with an Arrhenius-type relation we are able to examine the effects of surface binding on the switching energy barrier and determine the kinetics for the switching behavior. This understanding of an electrically controlled thermal switching behavior also indicates that the back reaction is also possible and controllable. Since similar thermal excitation has not been realized in the solvent phase, this work also signifies potential tuning approaches of molecular behavior by engineering the surface adsorption and molecular properties. By electrically controlling the switching behavior in both direction, this molecule represents a new opportunity to develop electrically-controlled single-molecule resistive memory devices.

SESSION F: Epitaxial Materials and Devices I
Session Chairs: Minjoo Lee and Christine Wang
Wednesday Morning, June 27, 2018
Location: University Center, Santa Barbara Harbor

10:00 AM F01
Kinetic Compositional Instability and Phase Separation in MBE-Grown InGaAs
Mark E. Twigg, Nadeemullah Mahaidik, Nicole A. Koutlas, Stephanie Tommaso and Michael K. Yates; Naval Research Laboratory, Washington, District of Columbia, United States.

Phase separation in III-V semiconductor alloys remains a problem that limits the performance of electronic materials. As the first stage in a comprehensive program addressing this issue, we have begun investigating an alloy system in which only the group III elements differ: InGaAs. Lattice-matched InGaAs alloy films were deposited at three temperatures (400, 450, and 500°C) by molecular beam epitaxy on a (001) InP substrate. Using transmission electron microscopy (TEM), we have found phase separation in all three growths to varying degrees. According to the kinetic compositional instability (KCI) model developed by Glas [1], the critical exponent for kinetic spinodal phase separation in InGaAs is 814°C, a temperature well above the growth temperatures used in this study. Dark-field (DF) cross-sectional TEM (XTEM) measurements, using the composition sensitive g=202 reflection, find that the amplitude of composition modulations averaged over the thickness of the XTEM sample are 0.7, 0.5, and 0.4 atomic percent for the growth temperatures 400, 450, and 500°C, respectively. X-ray reflectivity and 2-dimensional small angle x-ray measurements also indicate that the 400°C growth shows significantly greater phase separation than the 450 and 500°C growths. Atom probe tomography indicates that the amplitude of composition modulation for the 400°C growth is approximately 1 atomic percent, a value that compares favorably with the 0.7 atomic percent measured by DF XTEM. The KCl model examines the different roles played by thermodynamics and kinetics in the deposition of III-V alloy thin films. The thermodynamic model that serves as the starting point for KCI, that of Ipatova et al. [2], arrives at a critical temperature of spinodal decomposition of 160°C for InGaAs, a value at variance with the appearance of phase separation at 400-500°C, and therefore clearly too low. The kinetic contribution of KCl theory, however, raises the critical temperature to a value of 814°C that is consistent with our observations. The KCl model explicitly addresses the kinetics of the volatile near-surface region of the film, where surface undulations driven by surface diffusion introduce the kinetic component that undermines compositional stability beyond the point dictated by thermodynamics alone. KCl theory considers the surface-undulation related depth profile of the composition undulation of this near surface region, which assumes the form of exponential growth with the thickness of the kinetically active near-surface layer. The coefficient of exponential growth in the KCl model is a function of the difference between the critical and growth temperatures, such that the exponential growth coefficient is larger for growth temperatures farther below the critical temperature. In order to understand the composition modulation in these films as a function of growth temperature, we have used KCI theory to evaluate the average amplitude of composition modulation for a given growth temperature by integrating the KCI vertical composition profile over thickness. We then determine which value of thickness yields an average composition for each growth temperature which is consistent with the trend observed by DF XTEM. This analysis finds that the kinetically unstable layer terminating the surface during InGaAs deposition is approximately 2 nm thick when the lateral composition modulation wavelength is 3 nm. The thickness of this kinetically unstable layer corresponds to features marking both lateral and vertical composition modulation observed in DF XTEM for cross-sections that are cut along the [100] direction. The thickness of composition modulations in III-V semiconductor alloys generally run in the elasticity-soft [100] direction, its is found that [100]-oriented XTEM samples best reveal composition modulation.[1] F. Glas, Phys. Rev.B, 62, 7393 (2000).[2] I. P. Ipatova, V. G. Malyshevkin, and V. A. Shchukin, J. Appl. Phys. 7198 (1993).

10:20 AM F02
Calculating the Peach-Koehler Force on a Threading Dislocation Arm in a Semiconductor Film with a Blocking Layer and Free Surface
Mark E. Twigg and Glenn G. Jernigan; Naval Research Laboratory, Washington, District of Columbia, United States.

A familiar strategy for decreasing the density of threading dislocations penetrating the surface of a heteroepitaxial semiconductor film is one that employs an artificial superlattice. The differences in the mechanical stiffness of the superlattice layers play a role in blocking or redirecting threading dislocations that is ultimately traceable to the Peach-Koehler force acting on the leading edge of threading dislocation segments. The calculation of Peach-Koehler forces influenced by the presence of a heteroepitaxial layer, with mechanical stiffness differing from that of the buffer layer, is addressed by the formalism developed by Choi and Earmre for treating dislocation image forces generated by two heteroepitaxial interfaces [1,2]. This method relies on analytical continuation arguments applied to the dislocation strain field for a non-anisotropic material. The formalism for treating two epitaxial interfaces is derived from the Schwarz-Neumann reflection principle that satisfies alternating interfacial boundary conditions for the two interfaces in question, an approach that generates a convergent series. Each term of this series is proportional to the difference V in the mechanical stiffness of the two materials bounding a given interface, taken to a specific power (e.g. V⁰, V¹, V²). This approach can be extended to three interfaces, which is the strategy utilized in this study. A case of particular interest is that where two of the interfaces define a dislocation-blocking heteroepitaxial layer, and the third interface defines the free surface that terminates the film. The ability to include the effects of the film surface, as well as the interfaces defining the blocking layer, is especially important because the semiconductor/vacuum interface generates a much larger image force than the blocking layer interfaces. In addition, it is the image force generated by the free surface that plays the dominant role in drawing threading dislocation loops to the film surface. We consider a specific materials system, one designed to block threading dislocation arms in a Ge film deposited by molecular beam epitaxy on a (001) Si substrate, where the Ge film is intended to support the growth of a GeSn alloy. In this system, the Ge film constitutes the buffer layer, the blocking layer is composed of SiGe alloy, which is followed by a Ge capping layer terminated by the Ge/ vacuum interface that corresponds to the film surface. Because Si has a greater mechanical stiffness than Ge, the SiGe layer has the ability to repel dislocations originating in the GeSn layer. By adding the ability to include the influence of the film surface in the calculation, we now have a model capable of determining the appropriate composition and thickness for a SiGe dislocation-blocking layer. We have applied this formalism to a film with SiGe blocking layers having critical thicknesses below the threshold for dislocation generation when grown on a Ge buffer: 100 nm 90 atomic % Ge, 50 nm 80 atomic % Ge, and 10 nm 70 atomic % Ge. Preliminary results indicate that the most important factor in the SiGe blocking layer is the degree to which it stiffer than the Ge buffer, while the thickness of the SiGe blocking layer is found to be of secondary
importance. For the range of composition and thickness for the SiGe blocking layers described here, it has also been determined that only first order terms associated with the Si/SiGe interface (i.e. those proportional to the difference in stiffness Si/Ge:V) need to be retained to assure accurate calculation of the Peach-Koehler force. The efficacy of this first order theory indicates that this computational procedure can be extended to more complex layered thin film structures. [1] S. T. Choi and Y. Y. Earmme, Int. J. Solids Struct. 39, 943 (2002).[2] M. B. Katz, M. E. Twigg, N. A. Mahakik, C. L. Canedy, and C. A. Affouda, J. Electronic Mater. 45, 2102 (2016).

10:40 AM F03
(Student) Thin-film Engineering of Nanomembranes with Amorphous Silicon by Employing a Highly Integrated Coherently with Silicon. The limits of boron miscibility in III-V materials approach to strain-free, direct-bandgap, luminescent layers that can be >14% tensile strain with conventional III-V substrates, making epitaxial investigation. The small lattice constants of the B-V compounds result in systems, with many fundamental properties still awaiting experimental investigation. The boron pnictides (B-V) remain one of the least explored III-V materials for the incorporation of mixed boron alloys with silicon via commercially available GaP-on-Si substrates. Here we present the first epitaxial growth of BGaAs layers on GaP to probe both the fundamental properties of BGaAs alloys and the limits of boron miscibility in III-V alloys. BGaAs films with thicknesses ranging from 50 to 200 nm were grown on (100) oriented GaP substrates by solid-source molecular beam epitaxy. X-ray diffraction (XRD) measurements indicate that unity substitutional boron incorporation was maintained in relaxed BGaAs films for boron concentrations <12%. In-situ high-energy reflection electron diffraction results indicate that the films remained smooth and ordered during crystal growth despite strain relaxation, further indicating that unity substitutional boron incorporation was maintained in the BGaAs/GaP heterostructures. As the boron concentration was increased >12%, evidence of potential phase segregation was observed in XRD omega-2theta scans through the emergence of a GaAs diffraction peak, which we attribute to preferential solid-phase segregation of GaAs (SPE) over GaP. This is consistent with boron-induced growth of amorphous Ge on the SPE-GaAs growth. Work is underway to mitigate this extrinsic effect, as well as to characterize the fundamental optical properties of BGaAs; details will be presented at the conference. This work was supported by the Northrop-Grumman Corporation and an AFOSR STTR award (FA6517-17-2-0070).[1] K. Toko et al., J. Crystal Growth 436 (2016).[2] B. Tsang et al., J. Crystal Growth 351 (2004).[3] N. A. Mahakik et al., J. Alloys Compd. 506 (2010).[4] McNicholas et al. J. Alloys Compd. 497 (2010).[5] McNicholas et al. J. Alloys Compd. 506 (2010).

11:00 AM F04
(Student) Epitaxial Growth of a Light Absorbing Ge Layer on an Al-Induced Crystallized Ge Seed Layer. Layer engineering of a Ge layer on an Al-induced crystallized Ge seed layer is presented. This work was supported by the Semiconductor Research Corporation (SRC) and the National Science Foundation (NSF). This work was supported by the National Science Foundation (NSF).

11:20 AM F05
(Student) Epitaxial Growth of a Light Absorbing Ge Layer on an Al-Induced Crystallized Ge Seed Layer. The Ge layer was grown on the Ge seed layer by molecular beam epitaxy (MBE) and lifted off in HF. The Ge layer was then annealed at 300 °C, 350 °C, and 450 °C for 50 h in a N₂ ambient.

References
Alkaline-earth silicides have been widely investigated because of their useful functions for many technological applications such as solar cells, thermoelectrics, and optoelectronics. However, the study of germanides has not been active compared to that of silicides even though some studies have predicted interesting electrical and optical properties for germanides. SrGe, one of the alkaline-earth germanides, is a ternary compound material (~0.9 eV) and has a high optical absorption coefficient (~10^4 cm⁻¹ at 1.5 eV). These properties are suitable for the long wavelength absorption layer of a multijunction solar cell. Here we have studied to fabricate SrGe thin films by using our knowledge of epitaxial growth technology of alkaline-earth silicides and firstly revealed the electrical properties of SrGe. We fabricated high quality BaSi thin films on Si substrates using a two-step way: BaSi, template layer is formed by reactive deposition epitaxy (RDE), which is Ba deposition on a heated Si substrate, followed by molecular beam epitaxy (MBE) [2]. This method will be applicable for SrGe, (Fig. 1). In RDE, Sr was deposited on Ge (100), (110), and (111) substrates at substrate temperatures in the range between 300 and 700 °C. The deposition rates of Sr were, respectively, 0.7 nm/min and 120 nm for Ge (001), 1.4 nm/min and 30 min for Ge (011), and 1.3 nm/min and 60 min for Ge (111). MBE growth of SrGe thin film (~100 nm) was attempted using RDE-SrGe, on Ge (110) as a seed crystal because of its good crystallinity. During the MBE, the deposition rates of Sr and Ge were set at 1.4 and 0.84 nm/min, respectively, at Ge substrates temperatures between 150 and 500 °C. The θ-2θ X-ray diffraction (XRD) patterns and the reflection high-energy electron diffraction (RHEED) pattern of the samples after RDE indicate that SrGe thin films were formed on the Ge substrates (Fig. 2). The optimum substrate temperature for SrGe growth was different, depending on the Ge substrate orientation: 300 °C for Ge (100), 400 °C for Ge (110), and 600 °C for Ge (111). Scanning electron microscopy images show that the surface morphology of the samples, i.e., the shape of the SrGe crystals, reflects the substrate orientation (Fig. 3). Furthermore, it was found from the cross-sectional TEM observation of the samples that the Ge (110) substrate is optimal for the formation of SrGe, having a single composition and single orientation (Fig. 4(a))[3]. MBE growth of SrGe, thin film (~100 nm) was attempted using SrGe, grown by RDE on Ge (110) as a seed crystal. After the MBE, only SrGe, (411) peak was observed in the θ-2θ XRD pattern with RDE. (Fig. 4(b)). The electrical properties of the SrGe, thin film fabricated by MBE at 250 °C showed a high electron density (~10^19 cm⁻³) and high electron mobility (~460 cm²/Vs). This result indicates that SrGe, is applicable not only for solar cells but also for thermoelectric conversion elements. This is the first report to synthesize SrGe, thin films and to evaluate their electrical properties, demonstrating the excellent potential of SrGe, in the presented work, we will also discuss the relationship between growth conditions and electrical characteristics.[1] M. Kumar et al., J. Alloys Comp. 630, 126 (2015)[2] T. Suemasu and N. Usami, J. Phys. D: Appl. Phys. 50, 023001 (2017)[3] T. Imao et al., Nanoscale Res. Lett. 13, 22 (2018).

**SESSION G**: Gallium Oxide Devices

**Session Chairs**: Masataka Higashikawa and Rebecca Peterson

**Wednesday Afternoon, June 27, 2018**

**Location: Music Building, Lotte Lehmann**

1:50 PM G01

**Student** High Electron Mobility in Modulation-Doped β-(Al Ga) \(_2\)O/β-(Al 2O 3) Heterostructures

**Yuewei Zhang**

**Adnan T. Neaf**

**Zhanbo Xiu**

**Chandan Joshi**

**Yuanhua Zheng**

**Sanyam Bajaj**

**Mark Brenner**

**Shin Mou**

**Donald Dorsey**

**Kelson Chabak**

**Greg Jessen**

**Jinwoo Hwang**

**Joseph Heremans**

**Siddharth Rajan**

**Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States**

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**Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States**

**Air Force Research Laboratory, Materials and Manufacturing Directorate, Dayton, Ohio, United States; **

**Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States**

**Air Force Research Laboratory, Sensors Directorate, Dayton, Ohio, United States; **

**Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States**

**We report on high mobility two dimensional electron gas (2DEG) channels formed through modulation doping in β-(Al Ga) \(_2\)O/β-(Al 2O 3) heterostructures. A degenerate 2DEG was confirmed through temperature dependent Hall measurements, with a peak mobility of 2790 cm²/Vs. Shubnikov-de Haas oscillation was also observed for the first time in Ga 2O 3. Beta-phase Ga 2O 3 has emerged as a promising candidate for a wide range of device applications, including power electronic devices, radio-frequency devices and solar-blind photodetectors. The wide bandgap energy and the predicted high electric field breakdown field of β-(Al Ga) \(_2\)O suggest the potential for high performance devices.**

2:10 PM G03

**Strain Engineering and Two-Dimensional Electron Gas in ε-Ga 2O 3**

**Sung Beom Cho**

**Rohan Mishra**

**Mechanical Engineering and Materials Science, Washington University in St. Louis, St Louis, Missouri, United States**

**Institute of Materials Science and Engineering, Washington University in St. Louis, St Louis, Missouri, United States**

As a wide gap semiconductor, Ga 2O 3 is rapidly emerging as a promising candidate for power electronics applications. While most of the studies have focused on its stable β-phase, there are a handful of reports on its metastable ε-phase that has a spontaneous polarization. Numerous experimental groups have recently attempted to stabilize ε-Ga 2O 3, using epitaxial strain using substrates such as Al 2O 3(0001) [1], GaN(0001) [1], AlN(0001) [1], MgO(111) [2] and Si(001) [3]; however, due to the lack of an understanding of the stability of various Ga 2O 3 phases under epitaxial strain, these trials and-error based attempts have been limited in success. All the films are observed to be of inherently poor quality. There are also diverging reports on the structure and properties of the deposited thin films. A recent experimental report of ε-Ga 2O 3 grown on Al 2O 3(0001) substrate has even suggested the film to be ferroelectric, where the direction of the spontaneous polarization could be switched with an external electric field [4]. It implies that the stabilization of ε-Ga 2O 3 will open new avenue of polarization engineering in Ga 2O 3 power electronics. We have used first-principles density-functional theory (DFT) calculations in combination with coincidence-site lattice models to develop a phase diagram of Ga 2O 3, under epitaxial strain. We show that all the previously used substrates impose an epitaxial strain over 3% on ε-Ga 2O 3, which explains the poor structural quality of the deposited thin films. In this presentation, we will discuss promising commercially available substrates that can stabilize ε-Ga 2O 3 with epitaxial strain < 1%. We will discuss the electronic structure of ε-Ga 2O 3 under epitaxial strain using phase diagrams such as the band gap, polarization constants and its ferroelectric nature. We will demonstrate a way to achieve two-dimensional electron gas (2DEG) at the heterointerface of ε-Ga 2O 3 with an epitaxially-matched

**References:**


**Applied Physics Letters**

2:30 PM G04 (Student) DC and RF Characteristics of Submicron Delta-Doped $\beta$-Ga$_2$O$_3$ Field Effect Transistors Zhanbo Xia*, Chandan Joshi**, Sriman Krishnamoorthy*, Sanjay Bagai*, Yuewei Zhang*, Mark Brener*, Saurabh Lodha* and Siddharth Rajan*; 1 Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, United States; 2Department of Electrical & Computer Engineering, The University of Utah, Salt Lake City, Utah, United States; 3Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio, United States; 4Department of Engineering, Indian Institute of Technology Bombay, Mumbai, India.

We report delta-doped Gallium Oxide ($\beta$-Ga$_2$O$_3$) field effect transistors with MBE regrown contact for RF applications, with $I_{\text{off}}$ = 310 mA/mm and current gain cut-off frequency of 4 GHz at $\beta$-Ga$_2$O$_3$ is the largest bandgap (4.5 eV) semiconductor that can be grown directly on the GaN, forming a part of the semiconductor that can form the GaN in a single crystal form. The predicted breakdown electric field (6-8 MV/cm) is higher than that of GaN or SiC (~3 MV/cm), which when combined with electron mobility (predicted ~250-350 cm$^2$/Vs) and electron velocity (predicted ~2 x 10^7 cm/s) amongst the highest figures of merit for power electronic and high frequency devices. As a result, $\beta$-Ga$_2$O$_3$ possesses transformational potential for future electronic and optical applications. High frequency devices require scaling of the gate to channel distance and high channel charge density/velocity. Delta doped channel is one of the structure which can enable high charge density with gate to channel distance and high channel charge density/velocity. Delta doped channel is one of the structure which can enable high charge density as well as high channel charge density with high mobility [4]. In this work, we report Ga$_2$O$_3$ delta doped MOSFET with MBE regrown ohmic contact for RF performance. The device structure used in this work was grown on Fe-doped semi-insulating (010) oriented $\beta$-Ga$_2$O$_3$ substrates. Oxygen plasma power of 300W with a chamber pressure of 1.5 x 10^-2 Torr, and Ga flux of 8x10^-4 Torr, resulted in a Ga-limited growth rate of 3.3 nm/hour. One silicon delta doped layer with concentration of 1.5 x 10^{22} cm^-3 capped with 33-nm thick of Ga$_2$O$_3$ layer was grown on top of the 100nm undoped buffer layer. Source and drain regions were patterned and etched for heavily doped n-type Ga$_2$O$_3$ regrowth. Contact regrowth was carried out under close condition with the precious growth. Ti/Au/Ni metal stack was patterned after BCl$_3$ treatment for the Ohmic contact formation. Device isolation was performed using ICP-RIE etch with a BCl$_3$-based chemistry. Ohmic contacts were annealed at 470°C for 1 minute. Gate metal stack of Ni/Au/ Ni was deposited to form a schottky barrier contact. Contact resistance of 0.1 Ω mm and sheet resistance of 6.7 kΩ/ square were measured from transfer length method. Hall measurement indicates there is a 1.4x10^17 cm$^{-2}$ channel charge density with electron mobility of 65 cm^2/Vs. Capacitance-voltage measurement suggested a flat-C-V curve. A 2-D electron gas (2DEG) with density of 1.2 x 10^{12} cm^-2 was extracted. Frequency dispersion of C-V curve was observed near pinch-off voltage. Electrical characteristics of delta-doped FET with gate length of 0.8 μm shows a maximum DC drain current $I_{\text{D(max)}}$ of 310 mA/mm measured at $V_{\text{DS}}$ = 1 V and $V_{\text{GS}}$ = 10 V, and a maximum transconductance $g_{m}$ of 45 mS/mm measured at gate bias of -3 V. The channel was pinched off at $V_{\text{DS}}$ = -8 V, and on/off ratio of 1 x 10^5 was obtained. Using a drain current of 0.1 mA/mm for breakdown, a breakdown voltage ($V_{\text{BR}}$) of 70 V was estimated in a 0.5 μm gate-drain spacing device. Small signal characteristics were measured on the same device. Peak $g_{m}$ of 46 mmhos was obtained at $V_{\text{DS}}$ = -3 V and $V_{\text{GS}}$ = 10 V. $f_{\text{MAX}}$ reached 9 GHz at gate bias of -4 V. The small signal performance is mainly limited by channel electron mobility. The results reported in this work indicate the promise of delta-doping based devices for high current density/mobility and could open a new device architecture for high performance $\beta$-Ga$_2$O$_3$-based high frequency devices. The project was funded by the Department of the Defense, Defense Threat Reduction Agency (Grant HDTRA11710034), ONR EXEDE MURI program, and the OSU Institute for Materials Research Seed Program. Redman test [1] H. Higashiwaki, M. Higashiwaki, et al., IEEE Electron Device Lett. 37, no. 2, pp. 212-215, Feb. 2016. [2] Nan Ma, et. al., Appl. Phys. Lett. 109, 212101 (2016). [3] Krishnendu Ghosh, et. al., Journal of Applied Physics 122, 035702 (2017); [4] E. F. Schubert, et. al., IEEE Transactions on Electron Devices, vol. 33, no. 5, pp. 625-632, May 1986.
conduction of AlN and AlGaN. The underlying challenges include the very large p-type dopant (Mg) activation energy (up to 600 meV) in Al-rich AlGaN, the formation of compensating defects including nitrogen vacancies, and the unintentional impurity incorporation (carbon and oxygen). Previous studies have been largely focused on metal organic chemical vapor deposition (MOCVD). Here we report on the epitaxy and characterization of Mg-doped Al-rich AlGaN by molecular beam epitaxy (MBE). In this context, we have studied the epitaxy and charge carrier transport properties of Mg-doped Al0.6Ga0.4N using plasma-assisted MBE. Under optimized growth conditions, we have measured free hole concentrations -8.7×10^{17} cm^{-3} at room-temperature. Moreover, hole Hall mobilities up to 10^{10} cm^{2}/V●s at 170 K can be reliably achieved at room-temperature. Significantly, a minimum resistivity of 0.7 Ω cm was measured, which is five to ten times smaller than the values previously reported for Mg-doped Al-rich AlGaN grown by MOCVD. In this work, Mg-doped AlGaN epilayers were grown on AlN templates on sapphire substrate using a Veeco Gen 930 MBE system equipped with a radio frequency plasma-assisted nitrogen source. The samples were grown under nearly metal-rich conditions by carefully controlling the nitrogen flow rate. The sample thicknesses are ~0.4 μm.

AlGaN epilayers with different Mg doping concentrations were investigated and studied. The Mg doping concentrations were derived based on secondary-ion mass spectroscopy (SIMS) measurements. In these studies, we have shown that Mg has a negligible influence on the mobility of Mg-doped AlGaN under uniform Al composition, i.e., ~60%. We have studied the charge carrier transport properties of Mg-doped AlGaN epilayers by performing Hall effect measurements. A maximum free hole concentration ~8.7×10^{17} cm^{-3} was measured at room-temperature, which is higher than the previously reported values for Mg-doped AlGaN epilayers with similar Al composition. The hole mobility values in the range of 10-17 cm^{2}/V●s can be reliably measured for Mg-doped AlGaN epilayers with hole concentrations of 2.8×10^{17} cm^{-3}. Variations of the overall resistivity vs. Mg concentration are also studied. A minimum resistivity ~0.7 Ω cm was measured, which is nearly five to ten times smaller compared to previously reported values for Mg-doped AlGaN with similar Al compositions. To elucidate the p-type conduction mechanism of Mg-doped AlGaN epilayers, we have further performed temperature-dependent Hall measurements. The hole concentrations showed a very weak dependence on temperature in the range of 300 to 550 K, suggesting that the temperature-dependent band conduction. The hole concentration exhibited a drastic increase above 550 K, which is due to hole activation to the valence band. The activation energy is in the range of 300 to 350 meV, which is close to previously reported Mg activation energy values for AlGaN with similar Al compositions. We have further fabricated and characterized AlGaN multiple quantum well LEDs grown by metalorganic chemical vapor deposition (MOCVD), and we have been able to obtain excellent results. The LED exhibited strong emission at ~280 nm at room-temperature, with a turn-on voltage of ~5 V. The realization of high efficiency AlGaN quantum well UV-C LEDs is currently in progress and will be reported.

3:50 PM G07
Terrestrial Alloy Rare Earth Scandate as Dielectric for β-Ga2O3 MOS Structures
Hannah N. Masten, Jamie Phillips and Rebecca L. Peterson; Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan, United States.

Here we demonstrate a ternary alloy rare earth scandate, (Y,Sc)2O3, as a dielectric insulator for β-Ga2O3 MOS devices. The wide bandgap semiconductor β-Ga2O3 has generated great interest for power devices due to its large expected breakdown field. For enhanced performance of Ga2O3 MOSFETs, the gate dielectric should have a large conduction band offset and low interface state density (Dit) to Ga2O3. In addition, for power devices, we desire dielectrics with a high crystallization temperature. We have previously developed a solution-process to deposit (Y,Sc)2O3 films with low leakage current, a high relative dielectric constant of 9.6, a large breakdown field of 4.0 MV/cm, and a crystallization temperature of ~600°C, higher than that of many binary metal oxide combinations. In the present work, we explore the ALD growth of amorphous (x)H2O/(y)Al2O3 on Al-rich AlGaN with a gate dielectric to constant voltage stress (CVS) with periodic, multi-frequency C-V measurements interspersed through the stress. Prior to executing CVS, representative C-V and I-V data were collected. Results demonstrated that negligible frequency dispersion was observed, indicating no appreciable interface state traps (Dit) which indicates that Al2O3 can form a robust interface with β-Ga2O3. After these pre-stress measurements, the MOSCAPs were subjected to the CVS. Results demonstrate a positive flat band voltage (VFB) shift with increasing stress time at different stress voltages. This positive VFB shift is maintained after 1000s with post-stress hysteresis being slightly larger than the pre-stress hysteresis. This suggests the large shift observed in the CVS data is not due to pre-existing defects.

4:30 PM G09
Combined XPS-UPS Study of Conduction Band Offsets for High-k Dielectric Nanolaminates Grown on Single-Crystal GaN and Ga2O3(010) by Atomic Layer Deposition
David J. Mandia1, Angel Yangus-Gil1, Jian Liu1, Jacob H. Leach2, Keith R. Evans1 and Jeffrey W. Elam1; 1’Energy Systems Division, Argonne National Laboratory, Lemont, Illinois, United States; 2’Kyma Technologies, Inc., Raleigh, North Carolina, United States; 3’Chemistry, Northwestern University, Evanston, Illinois, United States.

The search for adequate binary metal oxide dielectric nanolaminates (NLs) to prevent degradation of power semiconductor devices is ongoing and involves the atomic layer deposition (ALD)-grown of binary metal oxide combinations. In the present work, we explore the ALD growth of amorphous (x)H2O/(y)Al2O3 on Si (with native SiO2 layer) substrates and then on both GaN and Ga2O3 single crystals. A variety of
samples ranging from their homogeneous mixtures to HfO	extsubscript{2} or AlO	extsubscript{2}-rich NLs are assessed before and after a thermal annealing by spectroscopic ellipsometry (SE), XAS techniques such as X-ray photoelectron spectroscopy (XPS) and X-ray absorption fine structure (EXAFS) measurements in order to elucidate the structural evolution of the NL at the GaN (or AlGaN)-Si interface. By quantifying the HfO	extsubscript{2} incorporation throughout the AlO	extsubscript{2} layer and using the programmable nature of ALD to alternate layers of the HfO	extsubscript{2} and AlO	extsubscript{2} in an (AB)\(_2\)-(CD) fashion, the influence of HfO	extsubscript{2} mobility within AlO	extsubscript{2} layer on the NL dielectric constant can be verified unequivocally. EXAFS is a powerful tool for determining the local coordination environment of the Hf at the GaN or AlGaN-O-NL interface and, at low super-cycle numbers (sub-nm scale), the ultimate stability of the NLs can be probed and optimized such that the bulk material properties are retained. Finally, via a modified Kraut's method,\textsuperscript{1}\textsuperscript{1} Ultraviolet photoelectron spectroscopy (UPS) is used to obtain the valence band maximum of the GaN and GaO	extsubscript{2} substrates and combined with the high-resolution XPS data for the Hf and Ga shallow core-level photoelectrons ejected from the thin HfO/AI O	extsubscript{2} overlayer in order to assess the conduction band offset (CBO) at the ilum-substrate heterojunction. Probing the insulator properties imparted by the high-k overlayer on the wide bandgap semiconductor surfaces of GaN and GaO	extsubscript{2} is crucial in order to understand and prevent the degradation problem in GaO	extsubscript{2}-based power semiconductor devices. Moreover, photoluminscence (PL) studies of the coated and pristine samples will corroborate the effect of the bulk defect concentration on the conduction/ valence band properties of the material.\textsuperscript{1}\textsuperscript{1} E.A. Kraut, R.W. Grant, J.R. Waldrop, S.P. Kowalczyk, Phys. Rev. Lett. 44, 1620 (1980).

SESSION II: III-Nitrides—LEDs and Lasers

Wednesday Afternoon, June 27, 2018

Location: University Center, Corwin East

1:30 PM H01
Stimulated Emission at 375 nm from Optically Pumped Vertical-Cavity Surface-Emitting Lasers with Air-Gap/Al\textsubscript{x}Ga\textsubscript{1-x}N Distributed Bragg Reflectors

Youngjae Park\textsuperscript{1}, Theeradetch Detchprohm\textsuperscript{1,2}, Karan Mehta\textsuperscript{1}, Oliver Moreno\textsuperscript{1}, Yuh-Shiu Liu\textsuperscript{1}, Shuo Wang\textsuperscript{1}, Shyh-Chiang Shen\textsuperscript{1}, P. Douglas Yoder\textsuperscript{1}, Fernando Ponce\textsuperscript{1} and Russell Dupuis\textsuperscript{1};\textsuperscript{1} Georgia Institute of Technology, Atlanta, Georgia, United States;\textsuperscript{2} Arizona State University, Tempe, Arizona, United States.

The field of ultraviolet (UV) photonics at wavelengths λ<400 nm is an area of increasing practical interest and coherent light sources and fast, high-power UV detectors are becoming of increasing practical interest and coherent light sources and fast, high-power UV detectors are becoming.

The InGaN/(Al)GaN multiple quantum wells (MQWs) laser is a crucial to the achievement of the IQE=95% (lowest threshold current density of 6 kW/cm\textsuperscript{2}) can achieve high internal quantum efficiencies (IQE=95%). However, significant efforts, no electrically injected laser has been demonstrated. Apart from doping and carrier injection, waveguide and MQW design is of utmost importance as it will directly influence the output characteristics of AlGaN-based lasers. For example, we have reported that the Quantum Confined Stark Effect (QCSE) is significant in c-plane AlGaN MQW devices and the radiative recombination rate can be significantly influenced by Al concentration of AlGaN wells and barriers; thickness of wells and barriers. Because of this, it is necessary to optimize these parameters to achieve the highest possible IQE and efficiency.

AlGaN-based optoelectronic devices have a wide range of applications, including bio-sensing, air and water purification. Recently, it was demonstrated that AlGaN multiple quantum well (MQW) lasers grown on low-pressure metalorganic chemical vapor deposition (LP-MOCVD) with AlQW ranging from 3 to 15. Since each QW pair (well + barrier) has a thickness of approximately 0.1 nm, the MQW thickness ranges between 24 nm and 120 nm. Taking into account a refractive index of 2.5 for bulk AlGaN in the UV, the optical path distance in MQW devices is on the order of 24 nm to 300 nm, which in the latter case is enough to serve as a waveguide for a laser with a wavelength of 280 nm. In order to measure n\textsubscript{eff} in waveguides, we developed a method based on measuring longitudinal modes in short cavities. This is based on mode spacing (λ) and its functionality with emission wavelength λ, cavity length L and n\textsubscript{eff} (Xie et al.).

For the case of 3xAlGaN/AIN MQWs, cavities ranging from 120 μm to 400 μm were fabricated. Using this method, n\textsubscript{eff} was determined to be 3.6 for this structure. Using the same measurement method, n\textsubscript{eff} is expected to have a larger value in 15xAlGaN/AIN MQW laser.

1:50 PM H02
(Student) Waveguide Design for AlGaN-Based Deep-Ultraviolet (DUV) Laser

Youngjae Park\textsuperscript{1}, Ronny Kirste\textsuperscript{2}, Shyun Washiyama\textsuperscript{1}, Seiji Mita\textsuperscript{1}, Will Mecouch\textsuperscript{1}, Pramod Reddy\textsuperscript{1}, Ramón Collazo\textsuperscript{2} and Zlatko Sitar\textsuperscript{1};\textsuperscript{1} Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina, United States;\textsuperscript{2} Adroit Materials, Cary, North Carolina, United States.

AlGaN-based optoelectronic devices have a wide range of applications, including bio-sensing, air and water purification. Recently, it was demonstrated that AlGaN multiple quantum well (MQW) lasers grown on low-pressure metalorganic chemical vapor deposition (LP-MOCVD) with AlQW ranging from 3 to 15. Since each QW pair (well + barrier) has a thickness of approximately 0.1 nm, the MQW thickness ranges between 24 nm and 120 nm. Taking into account a refractive index of 2.5 for bulk AlGaN in the UV, the optical path distance in MQW devices is on the order of 24 nm to 300 nm, which in the latter case is enough to serve as a waveguide for a laser with a wavelength of 280 nm. In order to measure n\textsubscript{eff} in waveguides, we developed a method based on measuring longitudinal modes in short cavities. This is based on mode spacing (λ) and its functionality with emission wavelength λ, cavity length L and n\textsubscript{eff} (Xie et al.).

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injection current density of 4.0 kA/cm². The second LD device with a shorter stimulated emission peak wavelength of 381.9 nm is then fabricated. The threshold current density and the voltage is 2.8 kA/cm² and 5.5 V, respectively. In order to demonstrate the LDs with even shorter stimulated emission wavelength, we grew AlGaInN/GaN MQW with EL peak wavelength of 370 nm.

**2:30 PM H04**

(LATE NEWS) Mg Induced Composition Change in InGaN Alloys

**Jilan Gherasoiu**, Kin Man Yu1,2, Mike Hawkridge1, L.A. Retcher1z and Wladek Walukiewicz3, College of Engineering, State University of New York at Polytechnic PI: Baldo, UTica, New York, United States; 1School of Physics, City University of Hong Kong, Kowloon Tong, Hong Kong; 2PANalytical, Westborough, Massachusetts, United States; 3Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California, United States.

We present the investigation of the effect of Mg doping on the InGaN crystal properties over a large range of Mg fluxes and indium fractions in the range from 30% to 40%, using secondary ion mass spectroscopy (SIMS) and transmission electron microscopy (TEM). InGaN thin films were grown on GaN/sapphire templates and doped with Mg at an effusion cell temperatures between 300 °C and 390 °C. The growth of InGaN takes place under liquid phase epitaxy conditions at a temperature and compositions that place the mixture in the spinodal decomposition region. We have found that the doping efficiency of Mg in GaN is limited due the formation of compensating defects while that in InGaN is limited due the kinetics of magnesium diffusion leading to the depletion of indium at the growth interface. We propose a model explaining this phenomenon that is supported by the experimental observations. A flux-modulation doping method that was used to avoid the in-die depletion is described. The hole concentrations were measured by Hall method and electrochemical capacitance voltage (ECV) and have been found in the range from 5x10¹⁸/cm³ to 6x10¹⁹/cm³. The range of III-group/magnesium flux ratios (PIII/PMg) that allows doping without indium depletion was determined. The SIMS and TEM data is also discussed in the context of recently published information that is in contrast with our findings and we provide an explanation for the differences observed. Finally, the effectiveness of the doping was verified through fabrication of InGaN pn-junctions that have demonstrated electroluminescence with a central wavelength of 585 nm (~2.1 eV).

**2:50 PM H05**

(Student) Carrier Dynamics in High-Speed III-Nitride Light-Emitting Diodes for Visible-Light Communication

**Armam Rashidi**, Morzeta Monavarian, Andrew Aragon, Ashwin Rishinaraman and Daniel Feezell; Center for High Technology Materials (CHTM), University of New Mexico, Albuquerque, New Mexico, United States.

High-speed InGaN/GaN light-emitting diodes (LEDs) are of interest for visible-light communication due to their potential to simultaneously provide efficient lighting and data communication. In the past decade, micro-scale LEDs have achieved large modulation bandwidths ranging from 100s of MHz to 1 GHz, leading to multi-Gb/s data communication rates. Higher modulation bandwidth is usually achieved by reducing the size of the device to minimize the transport and RC effects and by increasing the drive current, which results in a reduction of the recombination lifetime. However, reduction of the recombination lifetime is accompanied by efficiency droop at high current densities. To better optimize micro-LEDs for both speed and efficiency, characterization of carrier lifetime also aids in the understanding of fundamental material properties, low yield, and premature microplasma breakdown in the active region of the detector. In this study, GaN p-i-p-i-n SAM-APD arrays with separate absorption and multiplication (SAM) regions were fabricated by wet chemical methods.

**3:00 PM I01**

(Student) Demonstration of GaN p-i-p-i-n Separate-Absorption and Multiplication Ultraviolet Avalanche Photodiodes Arrays with Large Detection Area

**Mi-Hee Ji**, Jeoomoh Kim2, Hoon Jeong1, Marzieh Bahktiary Noodish, Theeradetch Detchprohm1 and Russell Dupuis2; 1Georgia Institute of Technology, Atlanta, Georgia, United States; 2LG Electronics, Seoul, Korea (the Republic of).

Wide-bandgap III-nitride-based avalanche photodiodes (APDs) are promising candidates for optical detection in the ultraviolet (UV) spectral region because of their potential capabilities of intrinsically visible-blind operation, high optical gain, and high detection sensitivity as well as chemical and thermal stability. Recently, UV-APD arrays with large detection area have been demonstrated for improving the conversion efficiency and sensitivity for weak signals. Moreover, separate absorption and multiplication (SAM) APD structures have been widely studied in order to reduce multiplication noise and increase optical gain. However, the realization of high-performance SAM-APDs with large detection areas has been hampered by high threading dislocation densities resulting from heteroepitaxial growth and it eventually leads to non-uniform electrical properties, low yield, and premature microplasma breakdown in the active region of the detector. In this study, a p-AlGaInN/Mg:Si layer was introduced as window layer instead of a p-GaN/Mg window layer to reduce UV absorption loss in the p-type contact layer. The epitaxial layer structure consisted of a 1-μm thick n-GaN/Si layer (n~5.0×10¹⁸ cm⁻³), a 0.21-μm thick i-GaN:Si layer as multiplication layer (n~1.5×10¹⁸ cm⁻³), a 90-nm thick p-GaN/Mg with linearly graded [Mg] up to ~1.5×10¹⁹ cm⁻³ as a charge layer, 0.24-μm thick i-GaN as absorption layer ([Mg]=2.5×10¹⁹ cm⁻³), a 30-nm thick p-Al:+GaInN:Mg window layer ([Mg]=1.0×10¹⁹ cm⁻³) and a 20-nm thick heavily doped p-AlGaInN:Mg:Mg metal contact layer ([Mg]=1.0×10²⁰ cm⁻³). The growth and doping conditions for epitaxial layers were carefully optimized to achieve improved crystalline quality and doping properties. The SAM-APD arrays were defined into square mesas with the size of 100×100 μm² by standard photolithography and inductively coupled plasma (ICP) etching. After mesa definition, Ti/Au was deposited on the wafers, followed by dry etching for accessing via holes. Finally, Ti/Au metal stacks were evaporated for metal interconnects and wire-bonding pads. In order to verify the uniformity of a 4×4 SAM-APD array, the dark current and photocurrent of the 16 individual SAM-APDs in the array were measured. The dark current densities of the 100×100 μm² devices in the SAM-APD array were below (5.1±0.8)×10⁻⁸ A/cm² at a reverse bias (Vᵢ) of 46 V except for two of the devices. Also, the average on-set point of the breakdown voltage (V₉₀) of the 16 devices in the SAM-APD array was 73±1.20 V and no microplasma was visually observed. These results indicate that the devices in the SAM-APD array show a uniform and reliable distribution of onset point of V₉₀ and low leakage current density.
In addition, multiple reverse-bias I-V scans were performed for selected devices in the SAM-APD array to verify the reliability and stability. The selected SAM-APDs in the array exhibited superior reliability and stability compared to our previous APD arrays that did not employ a window and SAM structure. The detailed growth, device fabrication processing and device characterization including spectral response will be further discussed.

3:50 PM 102

(Student) Billion-Fold Reduction in Screw Dislocation Related Dark Current in Al0.50Ga0.50N Solar-Blind Metal-Semiconductor-Metal Photodetectors

Shashwat Rathkanthiwar, Digbijoy N. Nath and Srinivasan Raghavan

High Efficiency, Monolithically Integrated (In)GaN/Si Photocathode for Stable Generation of Solar Fuels

Shashwat Rathkanthiwar, Digbijoy N. Nath and Srinivasan Raghavan

Utilizing the nitrogen polarity of III-Nitride materials has led to recent developments in the improvement of 2DEG confinement in GaN/AlGaN HEMTs and enhancement of InGaN quantum well LEDs. We have recently reported on the simulation and realization of increased efficiency of N-polar Cs-free GaN photocathodes. While the N-polarity allows for favorably harnessing the spontaneous polarization charge at interfaces, its differing surface structure compared to the well-studied Ga-polar surface poses a challenge. An increased dangling bond density at N-polar surfaces leads to a higher density of trap states and a thicker surface oxide. Due to the stability of Ga-polar GaN structures, growth interruption and subsequent exposure to ambient condition is possible without significantly impacting device performance. In the Ga-polar orientation, carrier transport simulations of devices match closely with experimental measurements for samples with growth/layer interruption. In the nitrogen polarity however, experimental results fail to match simulated transport efficiency across interfaces. To better understand the impact of interface properties on carrier transport across N-polar interfaces, multilayer N-polar III-Nitride photocathode structures with and without interruption between growth layers were simulated and reported here. GaN/AlGaN photocathode structures have been grown on-on-axis sapphire substrate in a MOCVD growth system. A systematic study has been conducted to study the impact of growth interruption at interfaces between device layers. Unintentional impurity incorporation studied through secondary ion mass spectroscopy (SIMS) shows an increase in oxygen concentration overall in the epitaxial layers by a factor of two for samples with interruption between layers compared to uninterrupted samples. Additionally, a further oxygen concentration increase is seen by SIMS at interfaces for interrupted layer growth compared to uninterrupted growth. We characterize the impact of this increased impurity concentration at interrupted interfaces on photocathode efficiency using ultraviolet/visible/photoemission from 2.7 % quantum efficiency to 9.1 % quantum efficiency through the use of uninterrupted interfaces. Atomic force microscopy (AFM) and x-ray diffraction (XRD) are used to study the surface morphology and crystal quality, respectively. Through AFM we report similar surface morphologies and RMS roughness values of 0.40 nm for interrupted and 0.56 nm for uninterrupted structures.

4:30 PM I04

(Student) High Efficiency, Monolithically Integrated (In)GaN/Si Photocathode for Stable Generation of Solar Fuels

Shashwat Rathkanthiwar, Digbijoy N. Nath and Srinivasan Raghavan

Artificial photosynthesis on semiconductor photoelectrodes is a clean and efficient route to the generation of solar fuels, including hydrogen and hydrocarbons directly from sunlight, water, and carbon dioxide, which can simultaneously address the challenges associated with energy storage for conventional solar cells. III-nitride semiconductors are promising materials to realize high efficiency photoelectrodes: their energy bandgap can be varied across nearly the entire solar spectrum by changing the alloy composition and they are the only known semiconductors whose energy band edge positions straddle water oxidation and reduction potentials under deep visible and near-IR light irradiation. In this work we report on band-engineered n-GaN/n-IntGaN nanowire arrays grown on planar n+-Si substrates using plasma-assisted molecular beam epitaxy, and have further demonstrated that such semiconductor photocathodes can exhibit N-polar high efficiency half-cell solar hydrogen conversion efficiency (>11%) and long-term stability. The diameter and length of the nanowires are ~50 nm and 250 nm, respectively, and can be well controlled by tuning the growth parameters. The flat-band potential (V_f) for this photocathode is measured to be 0.45 V vs NHE. Due to the small offset between the conduction band edges of Si and InGaN (with In composition ~ 10%), photoelectrons of the underlying Si wafer can readily inject into the n-InGaIn nanowire segment. The migrated electrons to the surface of GaN/InGaIn nanowires participate in proton reduction, due to the reduced surface band bending and the highly uniform Pt nanoparticles coverage on the nanowire surfaces. We have demonstrated that such a monolithically integrated n-GaN/n-InGaIn nanowire/Si photocathode can exhibit a saturated photocurrent density of ~42 mA/cm², half-cell solar hydrogen conversion efficiency of 11.3% at 0.32 V vs NHE and very high stability for 46 hours in 0.5 M H₂SO₄ under 1 Sun AM 1.5G illumination. To our knowledge, this is the most stable semiconductor photocathode ever reported at such high efficiency and high current density level. The superior performance is attributed to the unique lateral carrier extraction of 10D nanowires, efficient carrier transport on conductive n-type GaN nanowires, and efficient light absorption of the underlying n+-Si substrate. High stability of these nanowires is attributed to the N-rich surfaces of N-polarity GaN nanowire structures, which protect against photocorrosion and oxidation. Studies are currently in progress to further improve the efficiency with the use of indium rich InGaN nanowires.

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In this work, we report on a zero-bias external quantum efficiency (EQE) of 67% for back-illuminated AlGaN p-i-n UV photodetector. This is the highest zero-bias EQE reported for solar blind UV detectors realized on template-free and mask-free III-nitrides grown using Metal Organic Chemical Vapor Deposition (MOCVD) on a sapphire substrate. Devices with a peak detection at 290 nm exhibited a UV-to-Visible rejection ratio $>5 \times 10^4$ which is one of the highest reported for wide band gap photodetectors. Direct, wide and tunable energy gap of AlGaN can be utilized for realization of photodetectors operating in the solar blind regime (230-290 nm) of the electromagnetic spectrum. Despite complexities in growth and device fabrication, development of high efficiency p-i-n photodetectors has been gaining attention due to the self-powered nature of this detector geometry and for their potential application in realisation of arrays. In this work, we utilised a simple growth technique involving a 7 nm nominally thick low temperature AlN nucleation layer (LT-AlN NL) grown at 800°C followed by 500 nm high temperature AlN grown at 1100°C. This was used as the buffer for the growth of the detector epilayer. The introduction of the LT-AlN NL helped attain a 3-times reduction in both the screw and edge dislocation density in the active detector epilayer ($A_{\text{LT-AlN NL}}$). This ultimately led to the development of large-area detectors (0.1 mm$^2$) exhibiting a high zero-bias spectral responsivity (SR) of 156 mA/W (corresponding to 67% EQE) under back-illumination which is the highest reported value for AlGaN epistacks grown using a relatively simple, cost-effective and scalable growth technique. The only higher value of zero-bias EQE (80%) for AlGaN p-i-n detector reported has been achieved using more complicated growth technique such as pulsed atomic layer epitaxy (PALE). The devices had a high forward current density of 120 A/cm$^2$ and a turn-on voltage of 4.8 V (estimated at 20 mA forward current). From the forward $V$-characteristics, an ideality factor of 2.8, a series resistance of 34 ohms and shunt resistance of 1.2 x 10$^6$ ohm were estimated. Furthermore, EQE exceeds 95% at 2V and was found to increase exponentially with applied bias, indicative of an internal gain mechanism operating in these devices. A signature of this was also observed in the variation of photocurrent ($I_{\text{ph}}$) with the optical power density ($P_{\text{opt}}$). For voltages $>2$V, the photocurrent increased linearly for low optical powers ($<7$ mW/cm$^2$); the dependence becoming sub-linear at higher optical densities ($>7$ mW/cm$^2$). This could be attributed to the presence of hole-traps in the semiconductor bulk which become saturated at higher illumination densities, leading to the observed sub-linearity. Though growth optimization helped improve both the dark and photo characteristics of the detectors fabricated in this study, the dark current for the lowest leakage sample was comparatively higher (1.4 $\mu$A at 5 V) than the values commonly reported in literature. To investigate the cause of the relatively high dark current, temperature-dependent current-voltage (I-V-T) characterization was performed in the 25-400 K temperature range. Analytical modelling of the obtained I-V-T characteristics revealed hopping conduction through localized defect states within the semiconductor band-gap as the dominant carrier transport mechanism operating in the 6-20 V bias regime. The calculated activation energy for hopping was found to be 80 meV and 144 meV for the high and low-leakage current samples respectively. Further growth and device optimization to reduce the dark current are underway and will be presented. In summary, we report on the demonstration of high EQE UV p-i-n detectors using relatively simple III-nitride growth techniques. This is the also first report on the observation and analysis of gain in AlGaN p-i-n detectors leading to a SR as high as 156 mA/W at an applied bias of 10 V.

### 1:30 PM J01

**Operation of High-Frequency Vertical Organic Transistors**

Hans Kleemann, Markus P. Klinger, Axel Fischer, Bahman Kheradmand-Boroujeni, Frank Ellinger and Karl Leo

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Due to their inherent flexibility organic electronic devices such as organic thin-film transistors (OTFT) are prime candidates for large-area flexible circuits. However, despite continuous improvements on important semiconductor properties such as charge carrier mobility, organic transistors still fall short of performance when comparing to their inorganic counterparts. In particular, with regard to cut-off frequency and intrinsic gain, the current performance of organic transistors does not meet the requirements for applications such as wireless communication or active-matrix display backplanes. Moreover, for planar organic thin-film transistors, typical device improvements strategies such as down-scaling of the length are not easily applicable because of either contact-resistance restrictions or cost considerations. Vertical organic transistors represent an interesting alternative because they obey different scaling laws due to their ultra-short channel length and hence open a new perspective for high power and high frequency applications.

In this contribution, we discuss device improvement strategies for vertical organic transistors. In a case study, we focus on the organic permeable-base transistor (OPBT) and elucidate the device physics of these vertical transistors having a physical channel length $L$ of $< 300$ nm [1]. Deriving dependencies connecting material properties such as charge carrier mobility, device dimensions such as channel length, and device performance parameters such as transconductance and capacitance, we systematically improve the OPBTs [2]. In this way, we demonstrate that an outstanding performance can be achieved with cutoff frequencies $f_c > 30$ MHz at low voltages ($< 10$ V) marking a new record for organic transistors [3]. Moreover, due to the high carrier densities during operation at high frequency, we discuss the effect of self-heating leading to a positive thermal feedback which ultimately affects the dynamic device properties. Because of this heating, transistor parameters such as $f_c$ cannot be accurately determined from static measurements of e.g. the transconductance and capacitance. The parameters rather dependent on the driving condition and become time-dependent quantities. Based on a model describing the thermal feedback [4], we conclude on the device temperature during operation, which can be used to derive optimized driving schemes enabling a significantly improved dynamic transistor response [1].

planar zigzag structure within the amorphous polymer. While standard spin coating techniques can easily deposit the α phase, β-phase deposition is more challenging. β-PFO exhibits greater charge-carrier mobility and color purity [1], allowing superior device performance; however, β-PFO shows increased defect concentration when formed by solvent annealing [2]. Poor coherence in the morphology of such a thin film can reduce its performance and provide new parameters with which to optimize film deposition. [4]In previous work depositing PFO with RIR-MAPLE prepared for MRS Fall, it was shown that the emulsion-based approach is an effective method to increase β-phase concentration in thin films without increasing surface roughness. Due to the low vapor pressure of trichlorobenzene, it allows β-phase formation. The emulsion when used in conjunction with RIR-MAPLE effectively transfers the polymer to a substrate while maintaining the crystalline character. The current work investigates the film quality and relative concentration of β-phase in PFO films deposited using emulsion-based RIR-MAPLE as a function of emulsion preparation parameters, namely, emulsion mixing time and secondary solvent concentration. The secondary, unreactive, isopropyl alcohol, is added to the emulsion in order to lower the vapor pressure of the emulsion, allowing greater stability under vacuum. Phenol is also unable to effectively dissolve PFO, therefore, increasing PFO self-interactions during preparation increases β-phase concentration. Thus, the optimal mixing time and secondary solvent concentration will be determined for maximum β-phase concentration. Films deposited by RIR-MAPLE from the different emulsion targets are characterized by photoluminescence and UV-Vis absorbance spectroscopy, as well as atomic force microscopy. Films containing β-phase exhibit a characteristic shoulder in UV-Vis spectra at 430nm. Normalizing these spectra with respect to the 390nm α-PFO characteristic peak provides a method for calculating β-phase concentration. Reference [1], [2], [3], [4], [5], [6]

2:10 PM J03
Thermoelectric Response of Conducting Polymers Doped by Solid-State Diffusion and Their Electronic Applications

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Katharina Broch
Guillaume Schweicher
Youngrok Kim
Cameron Jelett
Christian B. Nielsen
Iain McCulloch
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Doping has been a key topic in organic electronics since the demonstration of a metallic conductivity in doped pi-conjugated polymers by various doping methods. However, most of conducting polymers still suffer from dopant-induced structural and energetic disorder. We have recently demonstrated an efficient solid-state doping method to achieve a coherent charge transport in poly(2,5-bis(3-hexadecyloxyphen-2-yl)thiophene-3,4-diyl) (P3HT) doped with 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) with one of the highest Hall mobilities for conducting polymer [1]. The observed coherent charge transport in the doped P3HT film could be attributed to a preserved 2D microstructural order upon doping. The doping method was also found to be effective for other thiophene-based and donor-acceptor polymers which potentially can be extended to a wide range of organic systems. In addition, a controllable de-doping recipe was employed to systematically study the thermoelectric effect in these highly conducting polymers over a wide temperature range [2]. Their charge transport and the underpinning strong energy dependence which can be correlated to their thermoelectric power factors. Furthermore, the doping by solid-state diffusion can achieve a superior thermoelectric power factor than a conventional solution-doping which is favorable for developing thermoelectric power generation technology. Lastly, we demonstrate that the doping method can also be employed to enhance the device characteristics in organic field-effect transistors. References [1, 2, 3]

2:30 PM J04
A Programmatic Molecular-Scale Rectifier Driven by the Interface-Engineered Molecular Junction Consisting of the 2D Semiconducting Layer and the Self-Assembled Monolayers

Jaeho Shin
Seunghoong Yang
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Since Aviram and Ratner initially proposed the possibility of a molecular-scale rectifier in 1974, diverse type of molecular diodes driven by a specific molecular itself or the asymmetric interfacial property has been studied. Recent studies suggested that the rectification substrate without the vacuum deposit is essential. In this study, we propose a new class of molecular-scale rectifier based on a hybrid molecular junction system that is composed with stacked of the Au (or graphene)/the 2D material (MoS2, or WSe2) the standard self-assembled monolayer (SAM) (alkyl- or conjugated molecules)/Au probe tip. The 2D material and the SAM are sandwiched between the Au probe tip and conducting electrode (graphene or Au) using conducting atomic force microscopy (CAFM) technique. In case of the molecular junction without 2D semiconducting material, the typical tunneling behavior through molecular barrier has been observed when the tip-loading force was 1 nN. When the tip-loading force was increased from 1 to 100 nN, however, the intriguing transition of the Fowler–Nordheim tunneling regime was observed, which can be interpreted by the correlation effects of the molecular-tilt configuration and the vdW interactions on the tunneling barriers [5]. In case of the molecular junction with the 2D MoS2 material, the diode feature with rectification ratio > -10 was observed [6]. Furthermore, this ratio can be programmed according to the number of MoS2 layers, molecular length, and energy-alignment between 2D layers. Another interesting point is that the rectifying polarity can be changed depending on the type of 2D materials, i.e., MoS2, and WSe2. Our suggested rectifier architecture can provide potential benefit to simply implement the molecular-scale diode function and propose the idea to improve the diode performance [1].

2:50 PM J05
High Piezoelectric Coefficient PVDF-TrFE Films for Flexible Electronics - Deepak1,2, Karishma Jain1,2 and Anshu Gaur1,2; 1Materials Science and Engineering, Indian Institute of Technology Kanpur, Kanpur, India; 2National Centre for Flexible Electronics, Indian Institute of Technology Kanpur, Kanpur, India.

The phenomenon of piezoelectricity in poly(vinylidenefluoride) was first described by Kawai in 1969 and its copolymer poly(vinylidenefluoride-trifluoroethylene) (PVDF-TrFE) is among the widely used organic material for pressure sensing applications. Also PVDF-TrFE has high mechanical flexibility and low processing temperature, thus making it the best material for flexible electronic applications. Still its commercialization for fabrication of pressure sensors is elusive due to low piezoelectric coefficient (d33) than inorganic piezoelectric materials such as PZT. Another major factor influencing the commercialization is the fabrication route for polymer which can match the industry standards and provide greater yield. Earlier we had reported record piezoelectric coefficient (d33) than inorganic piezoelectric materials such as PZT. Another major factor influencing the commercialization is the fabrication route for polymer which can match the industry standards and provide greater yield. Earlier we had reported record piezoelectric coefficient (d33) than inorganic piezoelectric materials such as PZT. Another major factor influencing the commercialization is the fabrication route for polymer which can match the industry standards and provide greater yield. Earlier we had reported record piezoelectric coefficient (d33) than inorganic piezoelectric materials such as PZT. Another major factor influencing the commercialization is the fabrication route for polymer which can match the industry standards and provide greater yield.
the knife coated, annealed and ice-quenched films show higher value of $d_0$, the dry only films, that is, without annealing and quenching still show similar values as reported for solution casted and annealed/quenched films. In short, we are able to make PVDF-TrFE films with higher $d_0$ values without annealing/quenching and/or UV treatment which simplifies the overall process and makes it compatible with high yield roll to roll manufacturing method. The reason of enhancement of piezoelectric properties in all these processing methods is alignment of polymer chains which increase crystallinity as determined by XRD and AFM. In knife-coating method, the same alignment in polymer chains is observed during the coating process and therefore no further processing steps are necessary. 3:10 PM BREAK

SESSION K: Materials Integration Session Chairs: Daniel Ewing and Patrick Shea Wednesday Afternoon, June 27, 2018 Location: University Center, Flying A Studios

3:30 PM K01 (Student) Characterization of Wafer-Bonded Silicon with Surfaces Treated with an Ion-Bombardment Procedure to Form Oxide-Free Interfaces Michael E. Liao1, Chao Li1, Christoph Floetgens2 and Mark Goorsky1; 1: Materials Science & Engineering, University of California, Los Angeles, Los Angeles, California, United States; 2: EV Group, Sankt Florian am Inn, Austria.

Direct wafer-bonding has not only provided a method of device fabrication, but also a way of characterizing and understanding the properties of interfaces across bonded materials. Ion bombardment in the range of a few eV to several thousand eV are often used to modify the pre-bonded surfaces. In this work, native oxides on (001) p-type silicon wafers are removed via an ion bombardment process with varying ion energies in an ion-bombardment® high vacuum wafer-bonding system [1]. Argon ions are used in this study with ion energies varying by an order of magnitude around a baseline energy, Eo. The removal of oxide layers between two bonded materials can lead to electrically conductive interfaces of the bonded structure. However, while ion bombardment can remove oxides from the silicon surface, this process also induces surface and sub-surface damage of the wafer, which limits the bonded interface’s electrical conductivity. X-ray reflectivity (XRR) and spectroscopic ellipsometry (SE) were used to characterize thicknesses and densities of the damaged layers. XRR and SE also both revealed a transition layer at the interface between the bulk (crystalline) silicon and the damaged silicon region. XRR results show that upon increasing the ion energy from 0.2Eo to 0.4Eo, the damaged layer thickness remains constant or even decreases slightly (from 2.2 ± 0.3 nm to 1.8 ± 0.3 nm while the transition layer thickness maintains ~ 1.0 nm in both samples. However, increasing the ion energy from 0.4Eo to 2Eo results in an increase in the damage layer thicknesses from 1.8 ± 0.3 nm to 3.5 ± 0.3 nm as well as a thickness increase of transition layers from ~ 1.0 ± 0.2 nm to 3.0 ± 0.2 nm. Interestingly, the damaged silicon layer density is approximately the same across all ion energies used. The resulting damaged silicon region has a density of 1.85 g/cm$^3$, which is 20% less than that of crystalline Si (2.33 g/cm$^3$) and deposited amorphous silicon (= 2.2 g/cm$^3$). Cross-sectional transmission electron microscopy (X-TEM) images of the 0.4Eo and 2Eo samples show that the damage region between the bonded wafers spans 3.68 nm and 7.49 nm (IonBond®) respectively, in agreement with the XRR and SE results for single wafer thicknesses. Bonded pairs with thicker damaged regions exhibit lower electrical conductivity across the interface. Current-voltage (IV) measurements show that the 0.4Eo and 2Eo samples exhibited interfacial resistances of about 0.8 kΩ and 39 kΩ, respectively. X-TEM images show that annealing at 450 °C reduces the damage region width; and after 12 hours of annealing, nearly all of the damaged region is removed. The removal of the damaged region after annealing is consistent with subsequent IV measurements that show negligible interfacial resistance in the 0.4Eo to 2Eo samples. In other words, the electrical conductivity across the bonded interface is comparable to the conductivity within the individual wafers, which suggests the energy barrier across the interface due to the damaged region is mitigated after annealing. References 1. C. Flötgen, N. Razeck, V. Dragoi, and M. Wimpfen, ECS Transactions 64, pp. 103-110, (2014).

3:50 PM K02 The Effect of In-Plane Rotational Misalignment on Electrical Conductivity of Wafer-Bonded n-InP/n-InP Structures Michael E. Liao, Victor Tran, Matthew Yue and Mark Goorsky; Materials Science & Engineering, University of California, Los Angeles, Los Angeles, California, United States.

Wafer-bonding of III-V semiconductors has led to the fabrication of high-efficiency multijunction solar cells.1 Without the restrictions of lattice parameter mismatch, wafer-bonding opens up a myriad of possibilities of various materials combinations for many electronic devices. Understanding the surfaces of materials is crucial in wafer-bonding since the bonded interface controls the electrical performance of wafer-bonded systems. We previously studied the effect of miscut (relative tilt) in GaAs and InP bonded homojunctions and heterojunctions.3 By determining the barrier height across the bonded interfaces, relative tilt across the interface leads to larger barrier heights. Additionally, systems with at least one side InP (i.e. InP homojunctions or InP/GaAs heterojunction) corresponded to lower barrier heights than the GaAs homojunction system. We concluded that the key factors that affect interfacial barrier height are surface passivation, materials choice, and relative misorientation of the bonded materials. Thus, in this work, we investigated the effect of in-plane rotational misalignment between wafer-bonded (001) n-InP wafers for rotations of 0°, 15°, 30°, 45°, 60°, and 90°. First, 50-mm diameter InP wafers were cleaved into quartets and submerged in an NH$_3$OH solution to remove the native surface oxide and then submerged in a 20% aqueous (NH$_4$)$_2$SO$_4$ solution for 5 minutes. After drying the wafers with N$_2$, the wafers were brought face-to-face and very low pressure (kPa) was applied manually at room temperature and in ambient air pressure. The relative rotational misalignment was induced by rotating the top wafer prior to applying pressure. The wafers were then annealed at 400 °C for 2 hours to strengthen the bonded interface. Ohmic contacts were fabricated on the InP bonded samples using AuGe/Ni/Au via electron beam evaporation. The deposited metals were then alloyed by annealing at 400 °C for 2 minutes in N$_2$ atmosphere. The samples were then rapidly thermal annealed for 2 minutes at 600 °C. All samples were then diced into ~ 2 x 2 mm squares and current-voltage measurements were performed at room temperature ranging from -0.1 V to 0.1 V. Over 20 samples were made for each angle group; the average of the top 5 lowest resistance for each group is reported. There is a discrepancy in literature on the effect of rotational misalignment. Kiss et al.4 claimed rotational misalignment (001) III-V wafers by 20° and 90° result in the same decrease in electrical conductivity across the bonded interface compared to their 0° bonded wafers. However, Okuno et al.5, 6 found that 0° and 90° bonded samples result in nearly equal electrical performance. We measured the interface resistance across our range of samples and find that 0° and 90° result in nearly equal, and highest, electrical conductivity (lowest interfacial resistance) while a rotation of 45° results in the lowest electrical conductivity. The interfacial resistance increases from 0° to 45° and decreases from 45° to 90°. The interfacial resistance across the 0°, 15°, 30°, 45°, 60°, and 75°, and 90° samples are (6.0 ± 0.2)×10$^3$ Ω·cm, (7.0 ± 0.4)×10$^3$ Ω·cm, (7.2 ± 0.1)×10$^3$ Ω·cm, (7.8 ± 0.2)×10$^3$ Ω·cm, (7.0 ± 0.2)×10$^3$ Ω·cm, and (6.2 ± 0.4)×10$^3$ Ω·cm, respectively. We conclude that the effect of rotational misalignment on the electrical conduction across bonded interfaces follows a sinusoidal pattern and its periodic effect on interfacial conductivity depends on the lattice symmetry of the wafer’s surface orientation, which has implications for bonding wafers with different surface symmetry. References 1. F. Dimroth, et al., Prog. in Photovolt.: Res. and App. 22, 277, 2014.; 2. P. T. Chiu, et al., IEEE J. of Photovolt. 4, 493, 2014.; 3. M. Sale, et al., IEEE 42nd Photovolt. Spec. Conf., 1, 2015.; 4. F. Kish, et al., Appl. Phys. Lett. 67, 2060, 1995.; 5. Y. Okuno, et al., Appl. Phys. Lett. 66, 451, 1995.; 6. Y. Okuno, et al., IEEE J. of Quan. Elec. 33, 959, 1997.

4:10 PM K03 (Student) Wafer-Scale Lift-Off of Epitaxial GaN Transistors from Silicon to Glass Substrate and Their JDEC Reliability Tests Pavani Vamsi Krishna Nittala, Nayana Remesh, Nagabooapathy K. Mohan, Rangarajan Muralidharan, Srinivasan Raghavan, Digbijoy N. Nath and Prosenjit Sen; Centre for Nano Science and Engineering, Indian Institute of Science, Bangalore, India.

We report on the wafer-scale epitaxial lift-off of GaN-based high electron mobility transistors (HEMTs) from silicon to glass substrate, and their JDEC reliability tests which revealed negligible performance degradation during the transfer process. This technology is expected to pave ways for the transfer of GaN-based devices with high performance to dissimilar platforms which can enable heterogeneous integration of III-nitride technology for a range of futuristic applications. GaN-based HEMT stacks for the fast-expanding power electronics market, are typically grown on silicon for cost and
scalability reasons. However, apart from threading dislocations which adversely affect device performance, the interface between III-nitride and silicon is a probable source of leakage. To realize novel technologies such as flexible/conformal/transparent III-nitride electronics, epitaxial lift-off technique [1] has enabled the transfer of as-grown AlGaN/GaN HEMTs from silicon (111) to a foreign substrate. In our earlier reports [2,3], we presented a simpler technique for the transfer of AlGaN/GaN HEMT’s from as-grown silicon substrates to glass wafer using epoxy-mediated transfer technology. Using this technique, a two order of magnitude reduction in the mesa and 3-terminal leakage currents was achieved in the HEMTs. And, to ensure the reliability of the transfer process, the devices were subjected to the industry standard Joint Electron Device Engineering Council (JEDEC) standard electrical reliability tests JESD22-A120A and JESD22-A104E. The first test (JESD22-A120A) is a test method for the measurement of moisture diffusivity and water solubility of organic materials used in electronic devices while the second test JESD22-A104E is a temperature cycling test to determine the device capability in withstanding extreme thermal and mechanical stresses. JESD22-A120A involves exposure to 85°C for 24 hours and JESD22-A104E-G involves sudden alternating low (−40°C) and high (+125°C) temperatures for 10 cycles each for a period of 30 minutes at each temperature. The devices in this study were found to exhibit a negligible change in performance after JDEC reliability tests, indicating the robustness of the wafer-scale transfer process. Although glass is used as an example of a substrate here, the process outlined here can be replicated on other substrates to facilitate better heat extraction from the devices and/or enable conformal/transparent electronics. References: [1] Jingshang Wang et al., APL, 110, 173503 (2017) [2] N.P.Vamsi Krishna et al., IEEE ECTC 2017; [3] N.P.Vamsi Krishna et al., IWPSD 2017;

4:30 PM K04 A New Relaxation Mechanism Enabling High-Quality, Laterally Grown Ge Films on Si Nato Quittoruing: McGill University, Montreal, Quebec, Canada.

We have recently grown Ge thin films on Si using a metal-catalyzed, lateral growth technique at 380°C. There are two surprising results from this work; first, the films are fully relaxed, despite the low growth temperature and, second, the cross-sectional transmission electron micrographs suggest high-quality (low threading dislocation density) films. Standard predictions of the growth of Ge on Si do not include the nucleation and glide of dislocations to relax the 4% lattice mismatch between the two materials; the nucleation of dislocations implies highly defective films, which is why the high-quality state of the lateral films is surprising. Dislocation glide is a thermally activated process and so, at these low temperatures, it would be greatly impeded and should result in a strain-free film, which is why the fully relaxed state of our laterally grown Ge on Si is surprising. Given these surprising results we propose a new relaxation mechanism which enables the high-quality growth of large lattice-mismatched materials. We hypothesize that the strain induced by the lattice mismatch can be relaxed by extending the preexisting misfit dislocations and that lateral growth can “build in” dislocations as it grows. This technique could be applied to other materials systems like GaN on Si or InP on Si, providing a pathway to fabricate high-performance device on low-cost, lattice-mismatched substrate.

4:50 PM K05 (Student) Formation of Si/Ge Nanowires and Quantum Dots via Ge Diffusion During Oxidation of Si/Ge Heterostructures Emily Turner, William Brewer1, Yan Xin1, Christopher Hatem1, Van Truong1, Kevin Jones1, Keshab R. Sapkota2 and George T. Wang2; 1University of Florida, Gainesville, Florida, United States; 2Sandia National Laboratories, Albuquerque, New Mexico, United States; 3National High Magnetic Field Laboratory, Tallahassee, Florida, United States; 4Applied Materials, Gloucester, Massachusetts, United States.

Si and SiGe Quantum Dots (QDs) have exciting potential as on-chip optical sources and in microelectronics and quantum computing. These QDs could enable single electron devices, spin qubits, and on-chip light sources for integrated SiGe based photonics and electronics. However, scalable methods for creating size-controlled and on-chip position-controlled Si/Ge QDs at dimensions less than 5nm do not currently exist. To address this challenge, we explore the use of a unique Ge diffusion process during the oxidation of Si/Ge heterostructures to create Si/Ge QDs. Initial oxidation work using patterned Si/Ge superlattice fins resulted in the formation of vertically stacked, horizontal Si nanowires. After oxidation, these Si nanowires were encapsulated in defect-free epitaxial strained SiGe. High angle annular dark field scanning transmission electron microscopy (HAADF-STEM) analysis revealed that Ge rapidly diffused along the Si/SiO2 interface during oxidation, effectively encapsulating the Si layers in SiGe as the oxidation continued. Further, the formation of these Si nanowires was significantly influenced by the oxidation temperature. At 900°C, rounded Si nanowires with diameter down to 2nm were fabricated. Lower temperature oxidations did not result in encapsulation of the Si layers as the diffusion of Ge along the Si/SiO2 interface continued at the rate of the SiGe oxidation. At higher oxidation temperatures the diffusivity of Ge into Si was sufficient to dilute the Si nanowire with Ge. We extend this study to the oxidation of vertical Si/Ge nanowires, defined via electron beam lithography and reactive ion etching, in order to create Si/Ge QDs. Si/Ge nanowires are oxidized at both high (900°C) and low (650°C) temperatures to control the diffusion of Ge along the sidewalls of the nanowires. Results on the formation of Si and SiGe QDs within the nanowires will be presented. These findings could lead to the way to scalable manufacturing of Si/Ge QDs for single electron devices as well as on-chip light emission and sensing.

SESSION L: 2-D Materials Synthesis
Session Chairs: Jason Hagmann and Shruti Subramanian
Wednesday Afternoon, June 27, 2018
Location: University Center, State Street

1:50 PM L01 (Student) Diffusion-Controlled Epitaxy of Large Area Coalesced WSe2, Monolayers on Sapphire Xiaotian Zhang1, Tanushree H. Choudhury2, Mikhail Chubarov3, Yu Xiang4,5, Bhakti Jariwala1, Fu Zhang6, Nasim Alemi2, Gwo Ching Wang7, Joshua A. Robinson8 and Joan M. Redwing1; 1Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, United States; 22D Crystal Consortium, Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania, United States; 3Department of Physics, Applied Physics & Astronomy, Rensselaer Polytechnic Institute, Troy, New York, United States; 4Center for Materials, Devices and Integrated Systems, Rensselaer Polytechnic Institute, Troy, New York, United States.

Monolayer WSe2 is a direct-gap 2D semiconductor with a large exciton binding energy and thus is of interest for optoelectronics and heterostructure devices. Prior studies demonstrated that gas source chemical vapor deposition (CVD) is a promising approach to prepare WSe2 crystal domains and films, but control of the film growth rate at the monolayer and few-layer level remains a challenge. The realization of large area single crystal WSe2 monolayer films requires the ability to control the density and orientation of nuclei on the substrate surface and the lateral growth rate of the domains to achieve fully-coalesced 2D growth. In this study, a multi-step process also provides a way to study fundamental mechanisms associated with surface diffusion of W adatoms or migration of W-rich clusters. Based on 2D Smoluchowski ripening, the tungsten-species diffusion-mediated process was developed for the epitaxial growth of coalesced monolayer WSe2 films on c-plane sapphire. The studies were carried out in a cold-wall CVD reactor using W(CO)6 and H2 as source gases in a H2 carrier gas. The multi-step process consists of an initial nucleation step which used a high W(CO)6 flow rate along with H2 at 800°C and 700 Torr to promote nucleation. The W(CO)6 was then switched out of the reactor and the sample was annealed in H2Se to promote surface diffusion of tungsten-containing species to form oriented WSe2 islands with uniform size and controlled density. The W(CO)6 was then switched back into the reactor at a lower flow rate to suppress further nucleation and grow the WSe2 islands laterally to form a fully coalesced monolayer film in less than one hour. Reflection high energy electron diffraction (RHEED) and in-plane X-ray diffraction measurements further confirm that the coalesced WSe2 monolayer film is epitaxially oriented on sapphire as [10-10] WSe2 || [10-10] α-Al2O3. High resolution annular dark field scanning transmission electron microscopy (ADF-STEM) and selected area diffraction analysis of WSe2 removed from the sapphire also indicate that the films are predominately single crystal with anti-phase boundaries that result from merging of 0° and 60° oriented domains. The multi-step process also provides a way to study fundamental mechanisms of WSe2 monolayer growth. By varying the W(CO)6 flow rate and time during the nucleation step, it was possible to control the size and spacing of initial WSe2 domains. The evolution of domain size and cluster density was measured in situ using a 2D imaging process, which is associated with surface diffusion of W adatoms or migration of W-rich WSe2 clusters. Based on 2D Smoluchowski ripening, the tungsten-species surface diffusivity was estimated as 1.2×10-14 cm2/s at 800°C, comparable to the diffusivities of ~5 nm Pt particles on alumina (1.5×10-14 cm2/s at 600°C) and ~6 nm Au particles on sapphire (2.0×10-14 cm2/s at 500°C). As the surface coverage increased above ~50% (15 min), the lateral growth
rate of the monolayer decreases due to precursor adsorption occurring more frequently on existing WS\textsubscript{2} monolayers rather than on the sapphire surface. The adatoms must diffuse a longer distance to reach the domain edges due to the increasing domain size; therefore, it becomes more likely that they will contribute to bilayer growth rather than fill in the initial monolayer. The lateral growth rates of domains was found to be relatively independent of the substrate temperature over the range of 700-900°C suggesting that the growth is limited by gas phase mass transport. However, the domain shape became more truncated at higher temperature due to local variations in the Se:W adatom ratio. The high vapor pressure of selenium results in a significant decrease in the sticking coefficient of Se on sapphire at elevated temperature, which consequently reduces the local Se:W ratio on the surface. The results provide an important step toward atomic level control and understanding of the epitaxial growth of WSe\textsubscript{2} monolayers in a scalable process that is suitable for the fabrication of large area devices.

2:10 PM L02

(Student) Wafer-Scale Synthesis of Monolayer WSe\textsubscript{2}—A Multi-Functional Photocatalyst for Efficient Overall Pure Water Splitting

Yongjie Wang, Yuanpeng Wu and Zetian Mi; EECS, University of Michigan, Ann Arbor, Michigan, United States.

High efficiency artificial photosynthesis, that can convert solar energy directly into chemical fuels, is one of the key sustainable technologies to enable a carbon-free, storable and renewable source of energy. A multifunctional photocatalyst combining the catalytic functions of water oxidation and proton reduction together with light harvesting capacity is highly desired, but do not yet exist for achieving stable solar fuel production. Monolayer WSe\textsubscript{2}, with a direct energy gap of \(1.65\) eV is a nearly ideal light absorber to convert sunlight to hydrogen fuels through solar water splitting. To date, however, the controlled synthesis of monolayer WSe\textsubscript{2} on a wafer scale and the realization of overall water splitting on WSe\textsubscript{2} has remained elusive. Here, we report the van de Waals epitaxy of crystalline monolayer WSe\textsubscript{2} on large area amorphous SiO\textsubscript{2} substrates. We have demonstrated, for the first time, the multi-functionality of monolayer WSe\textsubscript{2}, in solar water splitting, including extraordinary capacities for efficient light harvesting, water oxidation, and proton reduction. In this study, 2D WSe\textsubscript{2} layers were grown on amorphous SiO\textsubscript{2} substrates using a Veeco GENxplor MBE system. Streaky RHEED feature due to quantum confined WSe\textsubscript{2} layers was observed, implying an unambiguous evidence for the achievement of crystalline WSe\textsubscript{2} directly on amorphous substrates with smooth surface. Similar streaky RHEED feature was reported for WSe\textsubscript{2} epitaxy previously, but the growth took place on crystalline GaAs and graphite substrates. The high quality of single and few layer WSe\textsubscript{2} was further confirmed by detailed photoluminescence, micro-Raman and high resolution transmission electron microscopy studies. Significantly, we observed, for the first time, that monolayer WSe\textsubscript{2} can drive solar water splitting under visible light without using other cocatalyst. The absorbed photon conversion efficiency exceeds 12% for a single monolayer WSe\textsubscript{2}, and the turnover number exceeds 80,000 for 2h unassisted solar water splitting. Moreover, when normalized by the mass of WSe\textsubscript{2}, photocatalyst material, the \(H\)\textsubscript{2} production rate is 1,972 \text{L H\textsubscript{2}} g\textsuperscript{-1} (under 100 mW cm\textsuperscript{-2}) for CoO\textsubscript{2} nanoparticles. The continuous evolution of \(H\)\textsubscript{2} and \(O\)\textsubscript{2} confirms that the conduction and valence band edges of monolayer WSe\textsubscript{2} meet the thermodynamic and kinetic requirements for solar water splitting. This work provides a viable strategy for wafer-scale synthesis of multi-functional photocatalysts for the development of efficient, low cost, and scalable solar fuel devices and systems.

2:30 PM L04

Wafer Scale Epitaxial Growth of Monolayer and Few-Layer WS\textsubscript{2}, by Gas Source Chemical Vapor Deposition

Michael Chaban, Tanushree H. Choudhury and Joan M. Redwing; 1Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania, United States; 2Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, United States.

Two dimensional (2D) materials have great potential for future applications in a wide range of fields. Efforts are underway to develop scalable synthesis routes for the preparation of large area 2D monolayer and few-layer films. There are various reports on the large area growth of different 2D materials on amorphous substrates (e.g. SiO\textsubscript{2}). Thus, resulting films, having large domains before coalescence will also have high angle grain boundaries which can act as scattering and recombination centers for charge carriers. The way to avoid formation of high angle grain boundaries is the use of crystalline substrate and epitaxial growth. In the present work, we use c-plane substrate as the substrate for WS\textsubscript{2} growth. To achieve layer-by-layer growth mode, we implemented a multi-step growth process, previously developed for WSe\textsubscript{2}, which consists of nucleation, ripening and lateral growth of islands. In this work, we employ a cold wall horizontal low pressure gas source chemical vapor deposition reactor for the growth of WS\textsubscript{2} on 2 inch c-plane sapphire substrate. Monolayer to bi-layer growth is achieved in a scalable process that is suitable for the fabrication of large area devices.

2:50 PM L05

(Student) Two-Dimensional Tantalum Disulide—Controlling Structure and Properties via Synthesis

Rui Zhao1, Benjamin Grisafe2, Ram Krishna Ghosh1, Suman Datta1 and Joshua A. Robinson1; 1Materials Science and Engineering, Pennsylvania State University, University Park, Pennsylvania, United States; 2Department of Electrical Engineering, University of Notre Dame, Notre Dame, Indiana, United States.

Tantalum disulfide (TaS\textsubscript{2}) is a member of transition metal dichalcogenides (TMD). It is a charge density wave (CDW) material that undergoes periodic structural and electronic changes. There are many polymorphs in the TMD family (1T, 2H, 3R, 6H, etc.) and one must begin with the proper phase to apply their unique characteristics. For instance, 1T-TaS\textsubscript{2} is special for its metal-insulator transition (MIT) which is of interest for the next generation electronic applications. In this work, we demonstrate one way to directly synthesize TaS\textsubscript{2} flakes via powder vapor deposition. The growth has been successfully achieved on different kinds of substrates (sapphire, SiO\textsubscript{2}/Si, and epitaxial graphene). This process leads to single crystalline flakes (both 1T-TaS\textsubscript{2} and 2H-TaS\textsubscript{2}) with lateral size of 10-20\textmu m and vertical size of 20-100\textmu m. A series of characterization tools (AFM, SEM, Raman spectroscopy, XPS, TEM) are conducted to evaluate their physical and chemical properties. The phase of the synthesized flakes (1T, 2H-TaS\textsubscript{2} or TaS\textsubscript{2} nanowires) can be controlled by either temperature, intercalate agent or additional dopants. Via electric means, we have firstly demonstrated MIT in pure 1T-TaS\textsubscript{2} flakes from PV synthesis method. With this synthesis route, we are able to manipulate their phases by intercalation or doping, which opens up possibilities of directly integrating this phase material into novel devices for beyond-CMOS applications.

3:10 PM BREAK
The realization of epitaxial graphene has enabled new perspectives and interest in many research areas, serving not only as an atomically-smooth substrate for material growth or versatile contact material for device technology, but also as a means of artificially confining materials to low dimensions. Specifically, the epitaxial graphene/silicon carbide (EG/SiC) system has led to studies of intercalation of elements such as nitrogen, hydrogen, and fluorine through graphene layers to the EG/SiC interface. We show that intercalation of elemental gallium and indium readily occurs in systems of epitaxial graphene, where atomic layers of gallium or indium reside between the first two layers of graphene rather than between individual graphene layers. Such studies reveal that the EG/SiC interface plays a key role promoting elemental intercalation and in stabilizing atomically thin layers of materials. We show that two to three atomic layers of the group-III elements gallium and indium can be achieved through a simple process in which metallic sources are heated beneath substrates of EG/SiC. To promote intercalation, graphene layers are first exposed to a plasma treatment, resulting in an increased defect density in the graphene. Following this treatment, graphene is placed face-down over metallic gallium or indium, and heated in an argon atmosphere in a tube furnace from 600-800°C. Scanning transmission electron microscopy of resulting samples shows predominant formation of trilayer gallium and bilayer indium located between SiC and the first EG layer. Auger electron spectroscopy indicates intercalation on the lateral scale of 10s of microns. Additionally, increased gallium and indium signals are observed in x-ray photoelectron spectroscopy following intercalation in plasma-treated graphene samples, supporting the hypothesis that intercalation occurs at the EG/SiC interface rather than in graphene layers. To further investigate the nature of bonding in the SiC/intercalant/EG stack, preliminary density functional theory calculations are performed. Results indicate covalency between the first and second layers of intercalated gallium in SiC/Ga/EG structures and decreased covalency between the second and third gallium layers, further supporting the notion that the SiC surface layer is a key role in the formation of these two-dimensional metals. Ongoing work aims to investigate the superconducting behavior of the atomic gallium in SiC/Ga/EG samples through combined density function theory and low-temperature experimental efforts. Further work aims to realize additional two-dimensional metals with this EG/SiC system, in an effort to understand repercussions of the intercalant and the role of the SiC substrate, the unique properties of metallic elements confined to ultra-thin dimensions. 1. Wang, Z. et al. Simultaneous N-intercalation and N-doping of epitaxial graphene on 6H-SiC (001) through thermal reactions with ammonia. Nano Res. 6, 399–408 (2013).2. Riedl, C., Coletti, C., Iwasaki, T., Zakharov, A. A. & Siegel, M.; Sofer, Z. Adv. Mater. 2017, 1605299.; 2] E. Aktürk et al., Phys. Rev. B, 2016, 94, 1–9.; [3] Y. Yamaguchi et al., J. Phys. Soc. Japan 2008, 77, 14701.; [4] H. Hirahara et al., Phys. Rev. B, 2010, 81, 165425.; [5] T. G. C. Tan et al., Phys. Status Solidi RRL, 2017, 1700511.; [6] T. Nagao et al., Phys. Rev. Lett., 2004, 93, 105501.

3:50 PM L07

(Studenst) Epitaxial Growth and Characterization of 2-D Bil-Xsbx Alloys on Si(111) Sarah F. Muschinske, Emily S. Walker, Christopher J. Brennan,Yunying Alice You, Tzu-Yu D. March, Andrew F. Briggs, Erica M. Krivoy, Deji Akinwande, Minjoo L. Lee, Edward T. Yu and Seth Bank. 1Department of Electrical and Computer Engineering, The University of Texas at Austin, Austin, Texas, United States; 2Department of Electrical and Computer Engineering, The University of Illinois at Urbana-Champaign, Urbana, Illinois, United States. Two dimensional (2-D) allotropes of Group V materials including phosphorus (P), arsenene (As), antimonene (Sb), and bismuthene (Bi) have attracted great interest due to their unique electronic, optical, and structural characteristics compared to the corresponding bulk structures. The puckered-layer 2-D allotrope of bismuthene is of particular interest due to its large spin-orbit coupling, high bulk mobility, and the predicted direct band gap in single monolayers, which may enable the isolation of its spin-split surface states and zero-band gap behavior. Experimental studies of this 2-D structure have not been reported. Ongoing studies using exfoliation and the epitaxial Bi suggests that, while puckered-layer bismuthene is less metallic than bulk Bi, an overall metallic band structure is maintained in most films. Additionally, the propensity of few-layered puckered-layer Bi to exhibit island mode growth up until the point at which it transitions to its bulk (001) oriented structure further complicates characterization of this 2-D structure’s unique properties. Allowing Bi films to be established to open a small direct band gap and induce topologically insulating (TI) behavior in the composition range of 7-22% Sb, and the electronic properties of few-layer Bi_{1-x}Sb_{x} may potentially be similarly tunable through the Sb composition. While first-principles calculations predict the stability of puckered-layer Bi_{1-x}Sb_{x}, and in situ reflective high energy electron diffraction (RHEED) studies indicate that Bi_{1-x}Sb films may exhibit a similar growth mode to Bi on Si(111), structural and electrical characterization of Bi_{1-x}Sb on Si(111) is so far very limited. In this work, we explore the epitaxial growth of Bi_{1-x}Sb alloy films on Si(111) through molecular beam epitaxy (MBE). We demonstrate, using X-ray diffraction (XRD), that ultrathin Bi_{1-x}Sb films form an (012)-oriented crystal structure analogous to the expected (012) orientation of the puckered-layer Bi allotrope. Using XRD, atomic force microscopy (AFM), and temperature-dependent sheet conductance measurements, we examine the influence of the film thickness and Sb concentration on the structure, morphology, and electronic properties of Bi_{1-x}Sb films between 2-50 nm (6-150 ML) and 0-15%. We observe that the transport behavior of both Bi and Bi_{1-x}Sb films becomes more metallic as the film thickness decreases – suggesting the presence of the predicted metallic surface states in both compositions. We additionally demonstrate, through high-resolution AFM, that alloying with Sb improves the continuity of Bi_{1-x}Sb films between 3-12 ML by accelerating island coalescence, which facilitates ex situ measurements of thinner films than are possible to measure in Bi. We have found that Bi_{1-x}Sb films exhibit extremely similar crystal structure and temperature dependent conductance to pure Bi. This indicates that the incorporation of Sb in low concentrations may be used to facilitate continuous growth without significantly modifying the properties of the films, and will potentially allow for the further characterization of the puckered-layer allotrope through defect-free Bi_{1-x}Sb films. Pandey, M.; Sofer, Z. Adv. Mater. 2017, 1605299.; [2] E. Aktürk et al., Phys. Rev. B, 2016, 94, 1–9.; [3] Y. Yamaguchi et al., J. Phys. Soc. Japan 2008, 77, 14701.; [4] H. Hirahara et al., Phys. Rev. B, 2010, 81, 165425.; [5] T. G. C. Tan et al., Phys. Status Solidi RRL, 2017, 1700511.; [6] T. Nagao et al., Phys. Rev. Lett., 2004, 93, 105501. 4:10 PM L08

Chemical Vapor Deposition of Black Phosphorus Michael Smure, Gene Siegel, Shivashankar Vangala, Timothy A. Prusnisk, Daniel Hashemi and Stefan C. Badescu; Air Force Research Lab, Wright Patterson AFIA, Ohio, United States. Black phosphorus (BP) has attracted significant attention as a two dimensional (2D) semiconductor due to its high p-type mobility, thickness tunable direct band gap, and anisotropic properties. These properties make BP a unique 2D material well suited for numerous novel device applications. Unfortunately, thin film synthesis remains to be a major challenge to further advance BP beyond the laboratory. As such, almost all work (characterization, device, etc.) has been performed using exfoliated bulk material. The few exceptions include BP films synthesized by high pressure and temperature conversion from red phosphorus and pulsed laser deposition of amorphous-BP films. However, use of more traditional thin film methods, like chemical vapor deposition (CVD) or molecular beam epitaxy (MBE), have not been successful in producing large area films with excellent quality, uniformity, and thickness control (mono- to many-layer) and development of similar methods for BP would have a major impact. In this paper we describe efforts to develop CVD methods for growth of black phosphorus thin films. The high vapor pressure, multiple phases (white, red, blue, violet, green, and black), complex chemical, and high reactivity of phosphorus present major challenges. In this work we have investigated numerous metal, utilizing, and semiconducting substrates and phosphorus precursors (tertiarybutylphosphine (TBP), phosphine and elemental phosphorus). We find that on mostly inert substrates, like sapphire, there is competition between the high vapor pressure of phosphorus and the high temperature required to form crystals on BP. This was found to result in no growth at high temperatures and deposition of only red phosphorus at low temperature. In other 2D materials, metals have shown to enable growth, stabilizing nucleation and serving as a
catalyst. Phosphorus is quite reactive and is known to form phosphides with numerous metals restricting their use. We have found that Cu, Ni, Pt, Ag and other common metals will readily form a stable phosphide at temperatures below 500 °C. On Au we find the formation of small black phosphorus islands on the order of a few microns. Investigation of the growth mechanisms shows evolution of an intermediate phase (Au-P) at low temperatures to black phosphorus at higher temperatures. Characterization of these films shows this evolution with increasing growth temperature and supported by first-principles calculations. The work presented here describes the challenges to CVD growth of BP thin films and initial results to overcome some of these issues, which could lead to methods for growth of large area, high quality BP films from mono- to many-layers thick.

4:30 PM L09

(Students) Properties of MBE-Grown GaN on MoS2, Heterojunctions Choon Hee Lee1, Yuewei Zhang1, Jared Johnson1, Rachel Kolton1, Vincent Gambini1, Jinwoo Hwang1 and Siddharth Rajan1; 1Ohio State University, Columbus, Ohio, United States; 2Northrop Grumman Aerospace Systems, Redondo Beach, California, United States.

We report on molecular beam epitaxy (MBE) growth of GaN on a CVD-grown Nb-doped p-MoS2 for three-dimensional two-dimensional (3D/2D) heterojunction diodes. A distinct feature of 2D materials is the van der Waals bonding, indicating chemical reaction between Ga atoms and MoS2 during growth without lattice matching constraints. Integration of narrow gap 2D materials with wide bandgap semiconductors, such as ZnO or III-Nitrides, enables new combinations of heterostructures. 3D/2D heterojunction diodes achieved through direct growth or layer transfer of various 2D materials on to GaN substrates have been developed with excellent electrical properties. Here we report on GaN layers grown on MoS2 heterostructured materials, especially MoS2, is challenging, because the chemical reaction between MoS2 and Ga atoms at elevated growth temperatures could lead to the decomposition of MoS2. Here, we report the growth of GaN on p-type MoS2 at various growth conditions using plasma-assisted molecular beam epitaxy (PAMBE). The GaN growths on CVD-grown MoS2 were carried out using a Veeco Gen 930 PAMBE system equipped with standard effusion cells for Ga and Si. To explore the GaN growth condition on MoS2, 50 nm of GaN films were grown on MoS2, with different substrate temperatures and Ga:N flux ratios. The growth was monitored in situ using reflection high-energy electron diffraction (RHEED). Raman spectroscopy (≈785 nm) and XRD were used to characterize the films after growths. The effect of either Ga or N flux exposure to MoS2 films was first investigated by monitoring the RHEED patterns of MoS2. Prior to the growth, sixfold symmetry of the MoS2 films was confirmed with streaky RHEED patterns. No change was observed under N2 plasma irradiation, whereas the RHEED pattern transitioned to a ring shape immediately after Ga flux exposure, indicating chemical reaction between Ga atoms and MoS2 during growth. This was further confirmed by a standard Ga-rich growth condition, indicating growth was obtained at Tsub < 500°C. X-ray diffraction (XRD) scans revealed c-axis oriented crystal structure for GaN grown at 550 °C with (002) family diffraction peaks for MoS2. No MoS2 decomposition was detected from Raman as well. 50 nm undoped GaN showed a relatively rough surface morphology (RMS roughness = 3.69 nm) due to N-rich growth condition. From cross-sectional scanning transmission electron microscopy (STEM), mixed hexagonal (ABAB stacking) and zincblende structure (ABCABC stacking) were both observed for the sample grown at the optimized condition. This is consistent with the observed transitions in RHEED patterns, which changed from a streaky MoS2/RHEED pattern to a spotty and eventually a ring pattern as GaN grew up to 500 nm thick. Unlike MBE-grown 2D material on GaN, no clear van der Waals gap between GaN and MoS2 was observed from the TEM images, which might be due to the strong interaction between Ga and MoS2. GaN/GaM (30 nm, Nsub = 1019 cm-3) UD-GaN (45 nm) films were then grown at the optimized condition to demonstrate heterojunction diodes using a selective area growth method. Current-voltage measurements of the diodes exhibit rectifying behavior; however, further analysis and process optimization will be carried out to study the detailed electrical characteristics and energy band lineup for the MBE-grown GaN on MoS2. The characterization of this junction illustrates the feasibility of exploring 3D/2D heterojunctions to elucidate their utility for demonstrating novel applications such as heterojunction bipolar transistor.

4:50 PM L10

(LATE NEWS) Plasma-Enhanced Atomic Layer Deposition of MoS2, Suzanne Mohney1, Asad Mughal1, Timothy Walter1 and Kayla Cooley1; 1Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania, United States; 2Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania, United States.

Due to their promising physical properties, semiconductor two-dimensional transition metal dichalcogenides (TMDs) are a materials class receiving intense research attention. Molybdenum disulfide is one of the most widely studied materials in this class and has potential for applications ranging from electronics to catalysis. However, achieving large-area uniform growth of MoS2 has proved challenging and is typically accomplished at elevated temperatures using chemical vapor transport, chemical vapor deposition, or related techniques. Plasma-enhanced atomic layer deposition (PEALD) is a promising method for achieving control of film thickness and atomic scale within the temperature range low enough for integration into traditional semiconductor device fabrication processes. In this work, we use PEALD to grow thin layers of MoS2. Using the co-reactants (N2/2Me2H2Mo and H2:Ar plasma, depositions were carried out in a hot-walled PEALD system from 250–540 °C. Films were characterized by spectroscopic ellipsometry, XPS, TEM, AFM, and Raman spectroscopy to determine growth rate, morphology, film purity, and crystalline quality. Interesting differences were observed among films prepared on thermally oxidized silicon, c-plane sapphire, and c-plane GaN/sapphire substrates. We discovered that PEALD MoS2 films can be controllably grown down to single layers by adjusting the number of growth cycles. Very thin films were polycrystalline with the (0001) plane parallel to the substrate, although substrate-dependent out-of-plane growth was observed for thicker films. Higher growth temperatures as well as post-deposition annealing under sulfur vapor were shown to increase the crystallinity of the films. We anticipate that this PEALD growth technique will be suitable for a wide array 2D TMDs thin films and devices.

SESSION M: Computational Electronic Materials

Location: University Center, Lobero

1:30 PM M01

(Students) Refractive Indices of BAIN and BGN Alloys from First-Principal Calculations Feraz S. Ahnaf1; Kuang-Hui Li1, Kaikai Liu2 and Xiaohang Li2; 1King Abdullah University of Science and Technology, Thuwal, Saudi Arabia; 2Huazhong University of Science and Technology, Wuhan, China.

Classical wurtzite III-nitride (AIN, GaN, and InN) materials are widely accepted as compatible with applications in high frequency optoelectronics and high power devices. Optoelectronics made with III-nitride materials can operate over a large spectrum of wavelengths; from infrared (IR) to ultraviolet (UV). They owe this property to their highly tunable bandgaps from around 2 to around 6 eV. Highly reflective distributed Bragg reflectors (DBRs), have also been investigated as possible applications of III-nitride alloys. The search for materials with larger bandgaps, motivated by the rising interest in optical devices in the UV range, has inspired multiple studies of BN-based nitrides and their alloys with traditional III-nitrides. Additionally, alloying III-nitrides with boron can reduce the lattice parameters allowing for lattice matching with a variety of substrates. Knowing the refractive index of B III-nitride alloys allows for design and simulation of optoelectronic devices. It has been experimentally shown that a small incorporation of boron in GaN and AlN can cause a significant change in the refractive index of the material. However, no experimental study has investigated the effect on the refractive index for an unstrained single crystal of B III-nitride as far as we know. Additionally, the predicted large miscibility gap in wurtzite B III-nitride as has been shown in zinc-blende structures, prevents further studies on the experimental front. The effect of alloying on the refractive index has also been theoretically investigated over a large range of compositions for BGAN alloys. It seems clear that boron incorporation has the potential for allowing high tunability of the refractive indices of BAIN and BGN alloys. In this work we further investigate this theoretically using hybrid density functional theory (DFT). Additionally, we confirm our model by calculating the refractive indices of the well-known AlGaN alloys and comparing them to experimental values as well.

We found that...
our values are well within an acceptable range with a slight understimation when compared with experimental data. When looking at the results of the boron alloys we find a very interesting behavior. The static refractive index (at 9 eV) of both BAIN and BGAN seems to bow rather than change linearly as the composition is varied. Additionally we find that the refractive index curves at different boron compositions cross with each other at certain photon energies. Our hypothesis to explain this odd behavior comes from the classical model of light propagation inside materials. This model tells us that the refractive index of a material depends on electron resonances at different energies. These energies occur when electrons transition between bands. It has been found in previous studies that different bands (or their associated bandgaps) bow at different rates as boron content is increased. We believe that the refractive index bowing phenomenon is the result of these different bowing rates. To confirm this hypothesis, an extensive study of how the refractive index relates to different band transitions is needed. Such a model is called Interband Transition Contributions model (ITC); ITC has been developed in previous studies for other III-V materials to predict their refractive index.

1:50 PM M02
Band Structures and Direct-to-Indirect Bandgap Transition in BGAN Alloys Che-Hao Liao, Advanced Semiconductor Laboratory, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia.

Wide bandgap III-nitride materials have attracted great attention due to their excellent properties for device applications. As an emerging member of the III-nitride family, alloys based on BGN ternary have the potential to be lattice matched to AlN and SiC substrates, at boron compositions of ~12% and ~17% respectively [1], and also offer the possibility of using BALGaN quantum materials leading more degrees of freedom in designing much sophisticated and reliable high frequency, high-power microelectronic and optoelectronic devices such as high electron mobility transistors and ultraviolet emitters. However, BGN as an emerging material, its basic electronic and structural properties are still not well known [2]. In particular for high electron mobility transistors, BGN layer could be used as semi-insulating buffer layer [3] or back-barrier layer [4] to provide a polarization-induced band discontinuity and a resistive barrier originating from its excellent insulation properties. The electrical resistivity increases strongly by raising the boron content in BGN and the n-type carrier concentration decreases while the mobility increases. This boron-controlled resistivity is very promising for using the BGN based materials in microelectronic and optoelectronic devices. The growth of BGN is still challenging due to a large difference in atom radius between boron and gallium, which is expected to result in a wide miscibility gap and phase separation at several percents of boron. Growing BGN layers by using different substrates have been demonstrated, and BGN layers with the boron content up to 5.5% and 4.3% have been reported in BGN deposited on SiC substrate and AlN/sapphire templates, respectively [5]. The highest reported boron content of 7% in BGN film was obtained using ion implantation into GaN film grown on sapphire [6]. There is still room for crystal growth improvement and innovation in this field by exploring boron nitride-based alloys. In this work, the band structures of B Ga N are systematically studied through first-principles calculation based on density functional theory (DFT) using hybrid functional of Heyd, Scuseria, and Emzerhof (HSE) in the MedeA-VASP code [7]. The band structures of B Ga N with varying B compositions were calculated and plotted. The direct and indirect bandgap energies are extracted and plotted as a function of B composition, and a direct-indirect bandgap crossover is observed. Furthermore, the variation of direct and indirect bandgap energies is further broken down for the comparison at different high symmetry points, the Γ−A indirect bandgap became the dominate indirect bandgap at B composition larger than 0.44 has been demonstrate. The direct-indirect bandgap transition of B Ga N alloys at B concentration around 44% has been identified through our first-principles calculation.[1] B. P. Gunning et al., J. Cryst. Growth 460, 190 (2017).[2] A. Said et al., Optik 127, 9212 (2016).[3] T. Baghdadi et al., Phys. Status Solidi C 6, 1029 (2009).[4] V. Ravindran et al., Appl. Phys. Lett. 100, 243503 (2012).[5] J. Jurkevičius et al., Physica B 492, 23 (2016).[6] A.Y. Polyakov et al., J. Electron. Mater. 26, 237 (1997).[7] M. Zhang et al., Phys. Status Solidi B 254, 1600749 (2017).

2:10 PM M03
Wurtzite B Al N and B Ga N Heterointerface for Optical and Power Electronics Haiding Sun, Kaikai Liu, Muwei Zhang, Feras S. Alqtairi and Xiaohang Li; King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia.

Wurtzite (WZ) B Al Ga N alloys with tunable direct bandgap which can cover 200 to 360 nm wavelength. WZ B Al N alloys are expected to possess similar wide bandgap for UV devices. A few groups have grown B Al N epitaxially and showed effective refractive index modification by minor boron (B) incorporation. High reflectivity distributed Bragg reflectors have been demonstrated by employing B Al Ga N/AlN structures. Also, theoretical studies indicated the benefits of introducing B in the active region for optoelectronics, where UV emission could be enhanced by four times using BALGaN/AlN quantum wells. Though these studies show the potentials of B Al N alloys, many issues have yet to be solved. For example, due to the phase separation, short diffusion length of B, and strong parabolic reaction in the gas phase, the compositional in the B Al N alloys remains low. Recently, a high B incorporation of 14.4% in a single-phase 100 nm thick WZ BAIN was achieved. Numerically, first-principle calculations of zinc-blend (ZB) B Al N have been done, where a small bowing parameter of lattice constants was observed and a first transition from indirect bandgap to direct bandgap occurred at a low B composition of 0.12. Furthermore, it is found that the direct bandgap occurs at a relatively low B composition (x<0.12) is observed, above which the bandgap of B Al N maintained indirect, thus desirable for low-absorption optical devices. Furthermore, previously, researchers have estimated spontaneous polarization (SP) and piezoelectric (PZ) constants of WZ B Al N and B Ga N (0≤x≤1) ternary alloys by linear interpolation of the compositions binary BN, GaN, and AlN. However, the estimation may not be accurate since the constants may be nonlinear versus the composition. Here, we also calculated the SP constants of B Al N and B Ga N with the hexagonal structure as reference. The PZ constants are also obtained. The SP constants show moderate nonlinearity, due to the volume deformation and the dipole moment difference between the hexagonal and wurtzite structures. The PZ constants exhibit considerable bowing because of the large lattice difference between the binary alloys. Furthermore, the PZ constants of B Al N and B Ga N become zero at boron compositions of ~87% and ~74%, respectively, indicating non-piezoelectricity. The large range of SP and PZ constants of B Al N and B Ga N can be beneficial for the design of mini- and micro-sized optical and electronic devices. For instance, zero heterointerface polarization can be formed for BAIN- and BGAN-based heterojunctions with proper B compositions, potentially eliminating quantum-confined Stark effect for optical devices.

2:30 PM M04
(Students) Towards Automating High-Throughput Calculations of Intrinsic Point Defect Properties with Semi-Local DFT Daniel Broberg and Mark Asta; Materials Science and Engineering, University of California, Berkeley, San Francisco, California, United States.

Density-functional-theory (DFT) based methods for the calculation of charged point-defect properties in semiconductors and insulators have been extensively developed over the past three decades. Defect calculations performed with semi-local DFT are often severely hampered by the underestimation of the bandgap and by supercell-size effects, such as the weakly decaying coulomb interaction between periodic neighbors in a supercell. To address these inaccuracies, several \textit{a-posteriori} corrections have been developed to correct the self-energy. The most utilized empirical approaches involve the use of charge corrections, band edge re-assignment, band filling corrections, and shallow level corrections. While these corrections have been applied extensively within the framework of semi-local DFT calculations, and shown to yield results consistent with experiment, a major outstanding issue is the lack of standardization with which many of these corrections are applied: namely, which types of corrections are applied and the use of several system-specific choices in their practical implementations. In this presentation, we summarize our efforts to standardize the process of computing point defect properties within semi-
local DFT using an automated workflow tool that enables high-throughput calculations. To do this, we make use of a growing test set (>30) of GGA-PBE computed point defects and bench mark against results from relaxed HSE calculations. Several approaches to implementing automated point-defect calculations are tested to determine an optimal route for automation of these techniques. In this study we place an emphasis on assessing the practical quantities which can be recovered from semi-local approaches. The lessons learned from this study provide a basis for increasing the scale of calculations done to a fully automated framework within the Materials Project infrastructure. This work was intellectually led by the Materials Project Center, supported by the Office of Basic Energy Sciences (BES) of the U.S. Department of Energy.

2:50 PM M05
**Ab Initio Design of Two-Dimensional Electron Gas at Perovskite Oxide Interface**

Kesong Yang; Department of NanoEngineering, University of California San Diego, La Jolla, California, United States.

Perovskite-based oxide heterointerfaces between two wide-band-gap insulators are attracting increasing interests because of their novel electronic properties such as the two-dimensional electron gas (2DEG) at the interface that have potential applications in the next-generation nanoelectronic devices. In this talk, I will present our recent work on the computational design of perovskite-based 2DEG systems using ab-initio calculations. Specifically, I will talk the high-throughput design of the perovskite-based nonpolar/polar 2DEG systems based on polar catastrophe mechanism and polarization discontinuity mechanism. Three types of interfacial configurations including polar/nonpolar, nonpolar/nonpolar, and polar/polar interfaces will be summarized from their fundamental electronic and geometrical properties. These research findings may provide some avenues to achieve 2DEG in the perovskite-oxide-based interface materials.

3:30 PM M06
**Stability, Novel Materials and Physics of Perovskite Semiconductors for Solar Cells**

Chao Zheng and Oleq Rubel; Materials Science and Engineering, McMaster University, Hamilton, Ontario, Canada.

Degradation of hybrid halide perovskites under the influence of environmental factors impairs future prospects of using these materials as absorbers in solar cells. First principle calculations can be used as a guideline in search for new materials, provided we can rely on their predictive capabilities. We show that the instability of perovskites can be captured using ab initio total energy calculations for reactants and products augumented by interfacial conductive DFT data to determine formation energies for finite temperature effects[1]. Our results suggest that the instability of CH$_3$NH$_3$Pbl$_3$ in moist environment is linked to the aqueous solubility of the CH$_3$NH$_3$I salt, thus making other perovskite materials with soluble decomposition products and weak dissociation enthalpy prone to degradation.Simple criteria for predicting the intrinsic stability of halide perovskites, such as the Rashba’s spin-orbit coupling strength and geometrical factors, do not fully capture formability of hybrid halide perovskites. We extend the Born-Haber cycle to partition the decomposition enthalpy of various perovskite structures into lattice, ionization, and molecularization energy components. The analysis of various contributions to the decomposition enthalpy points to an ionization energy of an organic molecule and an inorganic complex ion as an additional criterion for predicting chemical trends in stability of perovskites[2].Using a low ionization energy and a suitable size of an A site molecule as a predictor for the thermodynamic stability of AIPb$_3$ hybrid halide perovskites, we identified an aziridinum lead iodide (CH$_3$)$_2$NH$_3$PbI$_3$ as a new, stable, low bandgap hybrid halide perovskite for photovoltaics[3]. Ab initio calculations were used to evaluate a polymorphism of the crystal structure of the proposed halide hybrid perovskite, its stability and electronic properties in comparison to the mainstream perovskites. Our results highlight the importance of van der Waals interactions for predicting a correct polymorphism of the perovskite vs a hexagonal crystal structure. In perovskites that lack spatial inversion symmetry, the bulk spin-orbit coupling becomes odd in the electron’s momentum, which gives rise to a splitting of the spin sub-bands in energy. Application of this effect to solar cells can lead to the development of new high-efficiency materials. Such materials are expected to combine benefits of direct and indirect band gap semiconductors, namely a very long lifetime of optical excitations and the strong optical absorption. It is believed that a very long time of optical excitations combined with optical absorption. It is believed that a very long time of optical excitations is crucial for solid-state photovoltaics in hybrid halide perovskites is associated with the presence of a Dresselhaus-Rashba splitting at the band edges[4, 5]. In this presentation, we will analyze the structural origin and chemical trends of the Dresselhaus-Rashba effect in perovskites, robustness of the splitting with respect to a dynamic disorder, as well as consequences of the spin texture for the radiative recombination of optical excitations.[1] E. Tenuta, C. Zheng, and O. Rubel, “Thermodynamic origin of instability in hybrid halide perovskites,” Sci. Rep., vol. 6, no. 1, p. 37654, Dec. 2016.[2] C. Zheng and O. Rubel, “Optical Excitation as a Stability Criterion for Halide Perovskites,” J. Phys. Chem. C, vol. 121, no. 22, pp. 11977–11984, Jun. 2017.[3] C. Zheng and O. Rubel, “Aziridinium lead iodide: a stable, low bandgap hybrid halide perovskite for photovoltaics,” arXiv:1711.05380 [cond-mat.matr-sci], Nov. 2017.[4] O. Rubel and A. Bokhanchuk, “Robust Bloch character at the band edges of hybrid halide perovskites,” arXiv:1508.03612 [cond-mat.matr-sci], Aug. 2015.[5] D. Niesen et al., “Giant Rashba Splitting in CH3NH3PbBr3 Organic-Inorganic Perovskite,” Phys. Rev. Lett., vol. 117, no. 12, pp. 1–6, 2016.

3:30 PM M07
**Identification of Intrinsic Defects in BiI$_3$ for Photovoltaic Applications**

Sung Beom Cho; Jaume Gazquez; Yoon Myung; Parag Banerjee; and Rohan Mishra; Mechanical Engineering and Materials Science, Washington University in St. Louis, St. Louis, Missouri, United States; 2Sejong University, Seoul, Korea (the Republic of); 3Institut de Ciència de Materials de Barcelona, Bellaterra, Spain.

BiI$_3$, a layered-structure semiconductor with a moderate bandgap of 1.7 eV and has high electron-hole pair generation efficiency [1]. Historically, it has been intensively investigated for X-ray and gamma-ray detector [2]. More recently, it has gained attention as a promising photovoltaic material. Based on its antibonding band edge characteristics, BiI$_3$, despite the presence of defects, is predicted to retain the electronic structure and properties of its pristine form [3]. However, all the above applications require an atomic-scale understanding of the defect landscape and their effect on the electronic properties, which has been lacking. We have used a combination of density-functional theory (DFT) calculations and aberration-corrected scanning transmission electron microscopy (STEM) to identify stable point defects and stacking faults in BiI$_3$ films and their effect on its functionalities. Based on DFT calculations, we predict intrinsic defects, such as both Bi antisites and I vacancies, have sufficiently low formation energy to be present under ambient conditions. We confirm these prediction through direct STEM observation of the defects in synthesized samples. While these dominant intrinsic point defects show deep thermodynamic transition levels, they do not lead to mid-gap states that can act as optical recombination centers. As a result, we find intrinsic defects in BiI$_3$, act as centers to trap thermally excited carriers. We have also calculated the effect of intrinsic doping using the calculated formation energies. Though the deep-level defects do not affect the optical properties of BiI$_3$, they act as compensating defects that pin the Fermi-level. From STEM Z-contrast imaging, we also observe plenty of intergrowths in the BiI$_3$ thin films. We have identified the atomic configuration of these intergrowths using a combination of STEM images and the total energy of promising models calculated using DFT. We find the intergrowths are triggered by Bi bulk-like line defects that can be formed by the alignment of Bi interstitials and Bi antisites. These line defects have a formation energy of 1.8 eV/nm and are observed to span a length between 3-8 nm. This Bi bulk-like line defect separates one I layer, then triggers formation of intergrowths. Also, interestingly, this line defect shows metallic character according to DFT calculations. We will discuss the implications of these defects on the optical properties including the excitonic states. Our combined study of intrinsic defects in BiI$_3$, provides guidance to control the defect structure for improved photodetector and photovoltaic applications by modulating the growth condition.[1] N. J. Podraza, W. Qiu, B.B. Hinojosa, M.A. Motyka, S.R. Philpott, J.E. Baciak, S. Troller-Mckinstry, and J.C. Nino: Journal of Applied Physics 114, 033110 (2013).[2] A. Beer, R.K. Willardson, and E. Weber, Semiconductors for Room Temperature Nuclear Detector Applications, Academic Press (1995).[3] R. E. Brandt, V. Stevanović, D. S. Ginley, and T. Buonassisi, *MRS Commun.* 5, 265 (2015).

4:10 PM M08
**Phase Transitions and Self-Assembled Nanostructure in Chalcopyrite Semiconductors and Similar Compounds**

Paul Quayle; Kyma Technologies, Inc., Raleigh, North Carolina, United States.

The II-V-V, and I-III-VI$_2$ compounds form a large materials set that has applications in thermoelectrics and nonlinear optics, and is being explored for (opto)electronics. Lattice disorder phenomena has long been observed in these materials and many ternaries undergo order-disorder phase transitions. Understanding the nature of this disorder is not complete though. The properties of these phase transitions are characterized by a randomization of the cation sublattice at high temperatures so that the structure adopts the higher symmetry of the binary parent phases, i.e. the III-Vs or II-VIs. However, recent experimental and theoretical observations
conflict with this picture. Here, the terrains are discussed within the framework of Landau theory, and it is shown that they fall neatly within the class of materials that exhibit lattice disorder via domain formation, characterized by a kagome-like (or k-type) group-subgroup relation between competing phases. Based on this, it is proposed that this set of materials undergoes a first-order, reorientational transition between a lower symmetry, low temperature phase and a higher symmetry, high temperature phase, with a transient mixed phase regime that occurs around the Curie temperature, which accounts for the observed disorder.

4:30 PM M09
First-Principal Predictions of Integer Anomalous Quantum Hall Effect in 2D Chern Insulator and Transition to Weyl Semimetal in Bulk—Bi,MnX (X= Se, Te) Sugata Chowdhury1, Kevin Garrity2, Joseph A. Hagmann1, Curt Richter3, Careylin Campbell4 and Francesca Tavazzia5; 1PML, National Institute of Standards and Technology, Gaithersburg, Maryland, United States; 2MML, National Institute of Standards and Technology, Gaithersburg, Maryland, United States.

The quantum anomalous Hall effect (QAHE), which arises from topologically protected states in materials with strong spin−orbit coupling (SOC) and broken time reversal symmetry (TRS), has been the subject of an enormous interest in the last few years. In the presence of broken TRS, 2D insulators can be characterized by the Chern number (C), a topological invariant that takes on integer values, and these materials display quantized Hall conductance when C is non-zero, $$\sigma_y = C (e^2/h)$$ where e is carried by spin-polarized edge states even in the absence of an external magnetic field. Experimentally, Chern insulators have thus far been limited to magnetically doped Z2 topological insulators at very low temperatures (~1 K), but there is no fundamental reason for this limit, and significant work has gone into finding materials that display the QAHE at higher temperatures. Recently, we have reported the growth of a thin film of magnetic topological insulator (TI) with stoichiometric composition Bi,MnSe (BMS) by molecular beam epitaxy (MBE). In this work, we have investigated the electronic structure of BMS and the related materials (Bi,MX (M=Pb, Mn; X=Se,Te)) using density functional theory (DFT), and we predict a series of topologically non-trivial phases. We calculate the formation energies, charge states, band structures, and magnetic properties of these materials, as well as the evaluating their topological invariants. Our calculations reveal that Bi,MnX (X=Se, Te) are a strong (Z2) TIs when their spins are aligned antiferromagnetically, and become Weyl semimetals when their spins are aligned ferromagnetically. In thin film form, Bi,MnX (BMX) has a non-zero C value when the system thickness is around 1.2 nm and it is three or four layers, due to band inversion at the Γ point. As we increase the thickness of the system, it approaches a magnetic Weyl semimetal, with the Fermi level located in the Weyl point, which is characterized by the Chern number (C). This semimetallic state also displays interesting behavior, including a pair of half Fermi arcs on opposite surfaces. We have investigated the concentration of magnetic atoms in TI materials needed for insulator-to-metal transition. Relatedly, we find that Bi,PbX (X=Se, Te) are strong (Z2) TIs. With these results, we provide an avenue to achieve a magnetic Weyl semimetal and a higher temperature QAHE.J. A. Hagmann et al., New J. Phys. 19, 085002 (2017)

SESSION N: Nanoscale Characterization
Session Chairs: Heayoung Yoon and Edward Yu
Wednesday Afternoon, June 27, 2018
Location: University Center, Santa Barbara Harbor

1:50 PM N01
Structural- and Chemical Characterization and Bandgap Measurements at the Nanoscale of (ZnO), (GaN) Thin Films Using (S)TEM Methods Calliope Biazioti, Cecille Granered, Vegard S. Olsen, Lasse Viness, Beng G. Svensson and Oystein Prytz; Department of Physics, Center for Materials and Nanotechnology, University of Oslo, Oslo, Norway.

Bandgap engineering plays an important role in designing novel semiconductor materials, offering tunable optical and electronic properties. In recent years, ZnO and GaN, two wide-bandgap semiconductors with similar bandgaps and wurtzite structure, have been at the focus of scientific research due to their versatile applications. Interestingly, recent studies revealed that alloying GaN with the two with each other leads to wide-bandgap due to a strong band bowing effect. The fact that the bandgap can be reduced by only changing the concentration (x) between the two materials gives the opportunity to tailor the optical properties of the alloys towards optoelectronic devices. In our present work, we studied RF magnetron sputtered (ZnO), (GaN) thin films deposited on c-sapphire substrates. Due to the different plasma conditions, ZnO versus GaN, chemically and structurally induced phenomena, may severely affect the functional properties. Hence tailoring material properties by controlling nanometer scale structure and composition is of increasing importance. In this respect, structural and chemical characterization was performed, applying TEM/STEM methods and employing dispersive x-ray spectroscopy (EDX), X-ray diffraction, and Raman microscopy and down to the atomic scale. Bandgap measurements were acquired by performing electron energy loss spectroscopy (EELS) providing an excellent tool for investigations of local band gap gradients on the scale of semiconductor. This has spurred interest in synthesis other 2D materials with wurtzite structure, such as BN [1] and more recently 2D GaN [2], which have a tunable direct bandgap as a function of its thickness, as theoretically expected [3]. In this focus, 2D Indium Nitride (InN) is interesting because its bulk bandgap changed from the infrared range (0.65 eV) at 300 K to the violet light range (3.4 eV) at 2 K over a change in dimension of 2D material [4]. Therefore, controlling the thickness of a 2D InN layer will contribute new light emitting devices. The synthesis of 2D Nitrides was first reported in 2016 by applying Confined Heteroepitaxy (CHet) process to form a 2D Gallium Nitride (GaN) layer with 1-2 atom thickness [5]. In this technique, Silicon Carbide (SiC) substrate is graphitized and then directly damaged using oxygen plasma to provide an intercalation path. Then, Ga flakes located below the SiC substrate are evaporated in a tube furnace at 700 °C. The Ga atoms intercalated the defected graphene and deposited between the graphene and the SiC substrate. To complete the half reaction, nitrogen is introduced by Ammonia annealing at 700 °C. In this study, we extend this growth method from GaN to InN. We employed a coordinated approach in order to understand the chemistry and synthesis path link through microscopy using a variety of electron microscopy techniques, including Auger Electron Spectroscopy (AES), Scanning Electron Microscopy (SEM), and transmission electron microscopy (TEM). Firstly, the sample was imaged by SEM to investigate different gray-levels on the surface. Then, AES mapping was employed to explore the areas that intercalated successfully using the In encapsulated within the tears of graphene. After that, the samples were coated with SiO2 to protect the interface for transport. We used focused ion beam milling for site-specific characterization. TEM techniques such as Bright-field, Dark-field, aberration-corrected STEM-HAADF imaging, electron energy loss spectroscopy (EELS) and Energy Dispersive X-ray Spectroscopy (EDS) mapping were all applied to characterize the SiC/In-containing/graphite/SiO2 interface. The results of this study had three observations. Firstly, HAADF images corresponding to “dark” gray levels in SEM imaging confirm the existence of 1-2 atom thickness of In encapsulated within the graphene. Secondly, we investigated the role of graphene thickness/folding on the oxidation stability, and the result is that folded (multi-layer) graphene provides better oxidation resistance to the In-containing layer comparing to mono-layer graphene. Finally, both EDS and EELS maps show an In-peak encapsulated between the SiC substrate and a carbon layer. Mapping of Nitrogen “N−K” was challenging because of the overlapping between In-M edge (443 eV), N-K edge (401 eV) and a large c-Si background (217 eV). Through EDS mapping, STEM-EDS analysis, and post-processing steps, we demonstrate that nitrogen is co-located with Indium. This is model dependent, and, to date, unambiguous data on nitrogen incorporation has not been achieved. Further characterization is proceeding to investigate better signal of the Nitrogen by using a direct electron EELS detector (K2 from Gatan). We will continue to explore the properties of these materials with the aim of improving the QY efficiency. The discovery of graphene in 2004 [1] has there been a flurry of activity in investigating Two Dimensional (2D) materials, because of their superlative properties: spin−orbit coupling, massless Dirac fermions, flexiblity, thermal and chemical stability [2]. Remarkably, the in-plane hexagonal symmetry of graphene is largely responsible for its behavior. However, the zero-band gap of graphene presents hurdles to use it as a...
a few nanometers. Quantitative high resolution TEM (qHRTEM), comprising nanoscale strain measurements was performed by geometric phase analysis (GPA). The primary aim of this work was to obtain a significant bandgap reduction and at the same time ensure good crystal quality of the films. In this respect, a series of samples were studied by X-ray diffraction (XRD) and the GaN content. A range of x ≤ 0.2 was achieved in the composition and film thickness. Furthermore, comparative studies between as-deposited and post-deposition annealed samples were performed in order to study the effect of annealing in the film properties. Results revealed that for high x, single-domain films of high crystalline quality were grown, having a good heteroepitaxial relationship with the substrate "GaAs-like" (0001) (out-of-plane) and "GaP-like" (11-20) (in-plane) (the so-called ‘aligned’ domains). Reduction of x resulted in films that exhibited a columnar structure, with cone-shaped grains, highly oriented along the c-axis. Except for the ‘aligned’ domains that were the dominant type, also ‘30°-twisted’ domains were observed that are metastable due to the higher mismatch with the substrate. GPA revealed that the films were almost fully relaxed due to the generation of a dense array of misfit dislocations (MDs) along the interface. Threading dislocations (TDs) were a dominant defect and their density was slightly reduced after annealing while the overall morphology of the films was almost the same. EDX maps verified that the (ZnO), (GaNx) alloy was random without clusters or GaN agglomerations. The interface between the GaN alloy and the GaAs substrate was free of any chemical gradient was taking place close to the interface and cubic nano-sized areas were detected. EELS measurements revealed a bandgap reduction of the alloys with respect to pure ZnO.

2:30 PM N04

Glide in GaAs/Si Thin Films Using Electron Channeling Contrast Imaging

Brian B. Haidel, Patrick Callahan, Gareth Seward, Dachwan Jung, John Bowers and Kunal Mukherjee; Materials, University of California Santa Barbara, Santa Barbara, California, United States; Earth Sciences, University of California Santa Barbara, Santa Barbara, California, United States; Institute for Energy Efficiency, University of California Santa Barbara, Santa Barbara, California, United States; Electrical and Computer Engineering, University of California, Santa Barbara, Santa Barbara, California, United States.

We demonstrate the remarkable ability to induce and observe dislocation motion in heteroepitaxial GaAs/Si films at room temperature in a scanning electron microscope with no sample preparation. These samples are technologically relevant as templates for directly-integrated quantum dot laser growth, and the dislocations present in them are key to important device degradation mechanisms. Electron Channeling Contrast Imaging (ECCI) is a technique that leverages electron diffraction effects to image dislocations and small defects to allow for the imaging of strain fields caused by lattice imperfections such as dislocations and stacking faults near the surface of a sample. Additionally, when an electron beam is impinging upon a strained semiconductor sample, the energy deposited by the beam via non-radiative recombination at dislocations can allow them to overcome the Peierls barrier and glide, a process known as Recombination Enhanced Dislocation Glide (REDG). We have combined these two phenomena to capture movies of dislocation evolution in GaAs films grown heteroepitaxially on silicon substrates. As these observations take place at room temperature and not growth temperature, there is significant residual strain arising from thermal expansion mismatch between these materials. We have made extensive use of ECCI to characterize dislocation motion in strained thin films towards developing an understanding of REDG. Threading dislocations have been observed gliding, gliding by cross-slip, annihilating, and even interacting with other dislocations to inhibit further motion. A key process identified is the formation of stacking faults in the material by glide of misfit dislocations towards the surface which have decomposed into partials. We have also explored the kinetics of REDG with temperature-dependent measurements, and the thermal strain driving force with sample thickness-dependent measurements. Additionally, we will present preliminary data on the immediate vicinity of the interface. Nonetheless, corroborating STEM/EDX also reveals Si incorporation into the HZO layer near the Si interface and therefore the L-APT finding is substantiated. Such (intentional or unintentional) Si present in the HZO layer may be consequential since Si-doped (5%) HfO2 is known to be ferroelectric. Moreover, ambiguous peak assignments involving TiN and SiO2 in the HZO layer are similarly ruled-out by the STEM/EDX analysis, which thus dispensed with a premise L-APT conclusion that a thin Ti layer is present at the HZO/Si interface. L-APT also revealed a concentration of ZrN near the TiN/HZO interface. This finding is consistent with the views that crystallization should initiate on the TiN interface and that HfO2 should experience partial phase separation. In this regard, as would assist in the formation of small grains near the interface. L-APT analysis includes the use of a new, automated peak finding engine, developed in-house, which helps to reduce the uncertainty in making mass-spectral assignments.1. N. A. Sanford, et al., Micron 94, 53 (2017).2. M. H. Lee et al., IEDM 22.5.1 (2015); samples used in this study were graciously provided by M. H. Lee

2:50 PM N05

Laser-Assisted probe tomography and STEM/EDX

Norman Sanford, Paul Blanchard, Alexana Roskho, Andrew Kummel, Michael Katz and Albert Davydov; National Institute of Standards and Technology, Boulder, Colorado, United States; University of California, San Diego, San Diego, California, United States.

HfO2 and ZrO2 are high-k dielectrics that are commonly used in logic and memory. Furthermore, the HfZr1-xO2 (HZO) ferroelectric alloy is a good candidate for integration with Si, SiGe, or Ge since there is a large process window for Hf/Zr composition. Ferroelectric-dielectric hybrid structures enable functionality for applications in non-volatile memories and negative capacitance FETs. Laser-assisted atom probe tomography (L-APT) is an attractive method to study these materials since it will, in principle, provide 3D, sub-nm resolution and identification of chemical constituents. L-APT was therefore performed on TiN/HZO/Si structures to help determine the film composition, the nature of the interfaces, and possible phase separation in HZO films near their interfaces with TiN; this interface is critical since HZO almost always requires a crystalline capping layer to induce formation of the orthorhombic ferroelectric phase. Such phase separation could promote nanocrystal formation which is thought to be critical to formation of the metastable ferroelectric phase. However, L-APT analysis of these and related materials can be complicated by the dependencies of both elemental and molecular species that appear in various charge states [1]. Such artifacts may render mass-spectral assignments ambiguous and thus introduce significant uncertainties in L-APT-derived 3D chemical composition. In general, it is advisable to underpin L-APT with complementary metrology methods, such as STEM/EDX used herein, to thus attach more confidence to the results. As described elsewhere, TiN/ HZO/Si structures were grown by HZO ALD, capped with sputtered TiN, and annealed at 600C [2]. L-APT specimens and TEM lamellae for this study were prepared and examined in a manner similar to previous work on TiN [1]. The thicknesses of the HZO and TiN layers as revealed by STEM were used to scale the 3D reconstruction of L-APT data. Possible Pt contamination arising from FIB processing during specimen preparation is of concern because it may introduce mass spectral peaks that overlap with HfO2+, HfO2+ and TiO2+ assignments. However, STEM/EDX analysis of the HZO layer ruled-out Pt contamination. L-APT of the HZO/Si interface finds Si incorporation in the HZO layer as decomposed from SiO2 molecular species in the mass spectra. However, this conclusion is weakened by the separate 28-Da ambiguity between SiO2+ and O2+ that is within the immediate vicinity of the interface. Nonetheless, corroborating STEM/EDX also reveals Si incorporation into the HZO layer near the Si interface and therefore the L-APT finding is substantiated. Such (intentional or unintentional) Si present in the HZO layer may be consequential since Si-doped (5%) HfO2 is known to be ferroelectric. Moreover, ambiguous peak assignments involving TiN and SiO2 in the HZO layer are similarly ruled-out by the STEM/EDX analysis, which thus dispensed with a premise L-APT conclusion that a thin Ti layer is present at the HZO/Si interface. L-APT also revealed a concentration of ZrN near the TiN/HZO interface. This finding is consistent with the views that crystallization should initiate on the TiN interface and that HfO2 should experience partial phase separation. In this regard, as would assist in the formation of small grains near the interface. L-APT analysis includes the use of a new, automated peak finding engine, developed in-house, which helps to reduce the uncertainty in making mass-spectral assignments.1. N. A. Sanford, et al., Micron 94, 53 (2017).2. M. H. Lee et al., IEDM 22.5.1 (2015); samples used in this study were graciously provided by M. H. Lee

3:10 PM BREAK

3:30 PM N06

Laser-Assisted Atom Probe Studies of AIoO Tunnel Junctions on Silicon

Norman Sanford, Paul Blanchard, Russell Lake, Xian Wu and Davood Nafissipour; National Institute of Standards and Technology, Boulder, Colorado, United States.

AIoO tunnel junctions in an overlap geometry have yielded high-coherence superconducting qubits [1]. The fabrication scheme used to realize these structures involves multiple lithographies that require breaking vacuum between different metal deposition steps; in the course of the process, a bottom Al electrode is formed. The sample is then exposed to atmosphere during lithographic patterning of the top electrode. A short Ar plasma surface treatment is used to remove the native AlOx before controlled in situ oxidation of the tunnel barrier and deposition of the top electrode. Since the degree of Al oxidation is critical to device performance, it is compelling to compare the oxygen content of tunnel junctions fabricated in situ to those that were exposed to ambient air between processing steps. Laser-assisted atom probe tomography (L-APT) is attractive for such assessments since it will, in principle, provide sub-nm-scale resolution of
elemental constituents. Notably, L-APT studies of aluminum oxide tunnel barriers in magnetic tunnel junctions have been described previously [2]. Since Ga readily alloys with Al, we found it impossible to employ standard Ga-beam FIB techniques to prepare L-APT specimens from planar samples [3]. Alternatively, we fabricated test structures by depositing the Al/AIOx/Al films on pre-sharpened, degenerately-doped, Si microspot coupon arrays [4]. However, this approach has complications since the surfaces of the specimen tips are decorated with Al grains measuring roughly 2–10 nm. With such caveats in mind, we fabricated and analyzed two sets of specimens as follows. Set 1: 20 nm Al, followed by in situ oxidation at 150 mTorr in O2, for 20 minutes, capping with 20 nm of Al. Set 2: 20 nm of Al specimen removed to ambient air for 24 h, returned to vacuum system and Ar plasma cleaned for 1 minute, in situ oxidation in O2 at 150 mTorr for 2 minutes, and capped with 20 nm Al. L-APT returned complex mass spectra displaying various elemental and molecular species, likely ambiguous assignments, interfacial C contamination, and evidence for surface contaminant species. However, by confining our attention to Si, O, and Al we can nonetheless draw useful conclusions. We have generated reconstructions of specimen tips that illustrate the underlying Si tip encased in AlOx and Al. The composition of the AlOx was evaluated using cuboid (20×12×20 nm³) ROI sampling volumes scattered about the Si/AIOx interface regions. The O2 concentration averaged over these ROIs is roughly 10 ionic-% for specimens from set 1. Performance analysis of the reconstruction from set 2 returns an O2 concentration of roughly 20 ionic-%. Note, it is not the aim of our reconstruction analysis to accurately reproduce the true layer thicknesses; we are only interested in the relative O2 concentration between the two sample types where identical reconstruction parameters are used. More discussion of mass-spectral ambiguities, contaminants revealed, details of the reconstruction analysis, etc., will be presented at the meeting. Separate electrical transport measurements suggest that the thermal oxidation rate of aluminum is faster on the surface exposed to Ar plasma than on the as-deposited polycrystalline aluminum. Device behavior is also consistent with L-APT assessment of O2 concentrations for the two types of specimens.1. Wu, et al., Appl. Phys. Lett. 111, 033502 (2017).2. Perford-Long, J. Appl. Phys. 98, 124904 (2005).3. Thompson, et al., Ultramicroscopy 107, 131 (2007).4. Larson, et al., Local Electrode Atom Probe Tomography (Springer, New York, 2013).

3:50 PM N08
Optimization and Limitations of Scanning Spreading Resistance Microscopy
Jay Mody and Jochonia Nxumalo; GLOBALFOUNDRIES, Malta, New York, United States.

In this paper, we present SSRM measurements in various ambient conditions for optimization of SSRM. We also evaluate the optimization based on repeatability, reproducibility and the signal-to-noise ratio (SNR). In air, high-resolution SSRM, performed with full diamond tips (FDT) instead of the coated diamond tips (CDT) has emerged as the solution towards sub-nanometer spatial resolution (Figure 1). This resolution is achieved with the CDT because they provide a stable contact with much lower indentation forces in comparison to the CDT. Nevertheless, with both tips the force has to be controlled accurately to minimize the plastic deformation (determined by the spatial resolution) and to minimize sample and tip wearing. Although optimum resolution would require minimum force, the requirements in terms of contact stability and reproducibility may necessitate a higher force for long term stable operation. Parameters considered to be responsible for the observed variations include surface contamination as well as the growth of native oxide on the cleaved Si cross-section at room temperatures. Thus, when changing the ambient conditions (e.g., N2 & vacuum) reduction in the contaminants at the surface of the sample and preventing the growth of a native oxide induced by the natural humidity of air can be expected. This will influence the quality of the SSRM electrical contact, the repeatability/ reproducibility and SNR of the technique. Thus, we have carried out a detailed investigation on the influence of ambient conditions (e.g., N2 & vacuum) on SSRM measurements. The sample used in this study is a one-dimensional (1D) diode structure fabricated on a low doped p-type substrate (p/p+/n++) covered with a 200 nm SiO2 protective layer as seen in Figure 2. For the SSRM measurements in N2 environment the samples are cleaved in-situ. Hence, the layer of contaminants, water layer and growth of native oxide on the cross-sectional cleaved surface is suppressed. Similarly, for the SSRM measurements in vacuum the samples are cleaved and instantaneously placed in the vacuum chamber where the pressure is reduced to (1e-5 torr). This reduces the layer of absorbed contaminants, of water layer and growth of native oxide. After analyzing the samples in various conditions, repeatability and reproducibility can be substantially improved in N2 and high-vacuum environment when compared to air as shown from Figure 3 to Figure 6.

4:10 PM N10

Since the inception of scanning tunneling microscopy [1], electrochemists have sought to take advantage of scanned probe microscopy techniques to manipulate the spatial position of a probe with high resolution to facilitate simultaneous high resolution topographical, conductometric, and amperometric/voltammetric imaging of surface and interfaces. Lately, scanning ion conductance microscopy (SICM) [2], has emerged as a versatile non-contact imaging tool and been employed for a variety of applications. SICM has been used to investigate the surface topography of both synthetic and biological membranes, ion transport through porous materials, dynamic properties of living cells, and suspended artificial black lipid membranes. In addition, integration of complementary techniques with SICM has led to many exciting new applications including scanning near-field optical microscopy and patch-clamping [3]. Powerful as it is, SICM remains insensitive to electrochemical properties, or, in other words, SICM is inherently chemically-blind and has no chemical specificity. To obtain spatially-resolved electrochemical information, scanning electrochemical microscopy (SECM), also known as the chemical microscope, has been adapted. SECM analysis on specie, transport, and electroanalysis has been widely employed to examine localized electrochemical properties and reactivity of various materials/interfaces, such as electrode surfaces and interfaces, membranes [4], and biological systems. Despite its many applications, SECM, however, lacks reliable probe-sample distance control, and the probe is usually kept at a constant height during conventional SECM scanning. As a result, any variation in surface topography will result in changes in probe-sample distance, and thus lead to convolution to the measured faradaic current, which will complicate the subsequent data interpretation [4]. To address the above-mentioned issues for SICM and SECM, hybrid SICM-SECM techniques have been developed, in which the SICM compartment provides the accurate probe-sample distance control, while the SECM compartment measures the faradaic current for electrochemical information collection. In this work, we demonstrate the use of an AFM (Park NX10) in combination with an ammeter for concurrent topography imaging and electrochemical mapping. The SICM-SECM probe utilized here consisted of a Au crescent electrode (AuE) on the tip of a nanopipette. High-resolution probe-substrate distance control was obtained by the ion current feedback from SICM, while the simultaneous electrochemical signal collection was achieved via the AuE from SECM. As a proof-of-concept experiment, a Au/Pyrex pattern standard sample was imaged with the SICM-SECM technique. The Au bar and the Pyrex substrate were clearly resolved from the SICM topography image, with the bar height and pitch width closely matching the actual values. In terms of the electrochemical property mapping, the higher Faradaic current was seen when the probe was scanned over Au bar as a result of redox cycling, while lower Faradaic current was observed when the probe was over Pyrex substrate due to hindered diffusion. The capability of the SICM-SECM technique described here holds the promise of many exciting applications in the field of electrochemistry, material science, and battery research [1] Binnig, G., Rohrer, H., Gerber, C. and Weibel, E., Tunneling through a controllable vacuum gap. Appl. Phys. Lett., 1982, 40, 178-180. [2] Hansma, P. K., Drake, B., Marti, O., Gould, S. A. C. and Prater, C. B. The scanning ion-conductance microscope. Science, 1989, 243, 641. [3] Shi, W., Zeng, Y., Zhou, L., Xiao, Y., Cummins, T.R. and Baker, L.A., Membrane patches as ion channel probes for scanning ion conductance microscopy. Faraday Discussions, 2016, 193, 81-97. [4] Shi, W. and Baker, L.A., Imaging heterogeneity and transport of degraded Nafion membranes. RSC Adv., 2015, 5, 99284-99290.
 SESSION O: Materials for Energy Storage and Catalysis  
Session Chairs: Zachary Lebens-Higgins and Shuji Ogata  
Wednesday Afternoon, June 27, 2018  
Location: Multicultural Center, MCC Theater

1:30 PM O01  
Li$_2$Ti$_4$O$_7$/Li Hybrid Solid-State/Ionic Liquid Electrolyte Batteries  
Isaiah O. Oladeji$^1$ and Robert E. Peale$^1$; $^1$Physics, University of Central Florida, Orlando, Florida, United States; $^2$Sisom Thin Films LLC, Orlando, Florida, United States.

Low cost, extremely safe, long-cycle life, and high specific energy lithium metal or ion batteries are desired for widespread adoption of lithium batteries worldwide. We propose to use our proprietary engineered particles to make the cathode, and modify Li anode surface, and combine these with hybrid Li,La,Zr,O$_x$ solid-state/ionic liquid electrolyte that is nonflammable, is electrochemically stable, and has high ionic conductivity over wide temperature range to fabricate extremely safe hybrid solid-state/ionic liquid electrolyte based lithium metal batteries with high rate capability. Preliminary results are reported for a cell with the proposed architecture. Li$_2$Ti$_4$O$_7$ (LTO) is used as cathode and the protected Li as anode. The cell is infiltrated with ionic liquid. The cell shows excellent LTO charge/discharge voltage profile and charge/discharge capacities over the first 100 cycles, where Coulombic efficiency remained at 100% throughout. The results confirm the validity of our design. Nail test generated no fire nor temperature rise.

1:50 PM O02  
Large-Scale First-Principles Molecular Dynamics Simulation of Organic Molecules@SWCNT for Novel Cathode Material of Li-Ion Battery  
Shujie Ou, Takahiro Tsuzuki and Masahiro Uraganagase; Nagoya Institute of Technology, Nagoya, Japan.

Recently the system of quinone molecules encapsulated in the SWCNT, which is free from rare metals, has been proposed as a next-generation cathode electrode material [1]. In the experiment [1], the phenanthrenequinone (PhQ) was used. The PhQ molecule is composed of 14 C, 8 H, and 2 O atoms and has 3 benzene rings. Single PhQ can capture as much as 2 Li atoms around the two O atoms. Dissolution of the PhQ toward the electrolyte, which occurs for the simple aggregate, was suprisingly significantly in the encapsulated system [1]. Despite the success of the encapsulated system as the electrode material, little is known about the configuration of the PhQs in the SWCNT and about the dynamics of Li-atoms in their insertion and extraction processes. In the present study, we will address those issues through large-scale, first-principles molecular-dynamics simulation. We will consider the SWCNT with its diameter 1.5nm corresponding to the experimental value. We have analyzed the PhQ-encapsulated SWCNT system with or without the Li atoms by performing the first-principles molecular dynamics simulation using our original DFT code. We adopt our divide-and-conquer-type real-space grid implementation code of the density-functional theory (DC-RGDFT) [2] with the norm-conserving pseudopotential and the PBE-GGA xc-functional. The eigenfunctions are described on the real-space grid and therefore are free from the basis set. We here add the DFT-D2 [3] to the DC-RGDFT to incorporate the Van der Waals forces in an empirical manner. The system temperature is controlled with the Langevin thermostat method. We perform the following four cases of the simulation: Case 1. Relaxation of the PhQs encapsulated in the SWCNT. Case 2. Relaxation of the PhQs with Li atoms encapsulated in the SWCNT. Case 3. Dynamics of Li insertion in the encapsulated system. Case 4. Dynamics of Li extraction from the encapsulated system. Cases 1 and 2 are considered to find the relaxed configurations of the PhQs in the encapsulated systems in two extreme settings: no Li atom exists in case 1, while 16 Li atoms exist in case 2. We thereby find that the shape of the SWCNT changes significantly in the relaxed state depending on the extent of Li atoms inserted. The SWCNT shows a circular cylinder shape when no Li exists. With sufficient Li atoms inserted, the SWCNT is flattened. Substantial electron transfer from the PhQs to SWCNT is found. Cases 3 and 4 are considered to investigate the Li dynamics, particularly the paths of Li atoms within the insertion and extraction processes. When the center of mass of the Li atoms is shifted gradually to the outside of the SWCNT, the Li atoms transfer either along the inner wall of the SWCNT or hopping on the PhQs. In addition, the SWCNT changes its shape to a round shape when the Li atoms go outside the SWCNT.


2:10 PM O03  
Investigating the Electrochemical Performance of One Pot Synthesized MnO$_2$, Nanorods  
Neha Kanaujia$^1$, Nagesh Kumar$^2$, Yogesh Sharma$^1$ and Ghanshyam D. Varma$^{1,2}$; $^1$Physics, I.I.T. Roorkee, Roorkee, India; $^2$Centre of Nanotechnology, I.I.T. Roorkee, Roorkee, India.

Global warming, increasingly worsened environmental pollution and the compulsion for energy security have stimulated the impulse to develop such energy storage devices that can store energy produced from renewable sources like solar, wind turbines, hydropower, and supply the same whenever required. In this regard, electrochemical supercapacitors are the preferable alternative due to their very short charging-discharging times (few seconds), excellent power density (>10 kW kg$^{-1}$) and higher cycle stability (>10$^5$ cycles). In this work, we are reporting the synthesis of one dimensional and high aspect ratio MnO$_2$, nanorods through facile one-pot hydrothermal route. The synthesized sample has been further characterized by X-ray diffraction (XRD), Transmission Electron Microscopy (TEM), Field Emission Scanning Electron Microscopy (FESEM) and Fourier Transform Infrared Spectroscopy (FTIR) techniques. The electrochemical Cyclic Voltammetry (CV), Galvanostatic Charging-Discharging (GCD) and Electrochemical Impedance Spectroscopy (EIS) have been performed in 2M KOH aqueous electrolyte solution. Maximum specific capacitances of 174 Fg$^{-1}$ at current density of 1 Ag$^{-1}$ and 135 Fg$^{-1}$ at scan rate 5 mVs$^{-1}$ have been recorded by CV and GCD, respectively. The structural and morphological characterizations are further correlated in detail with electrochemical behavior of the as prepared sample in this paper.

2:30 PM O04  
(Small, LATE NEWS) Resonant Tunneling Transport as a Sensitive Measurement Probe of the Internal Polarization Fields in III-Nitride Tunneling Heterostructures  
Jimy Encencadero$^1$, S.M. Islam$^1$, Vladimir Protasenko$^1$, Patrick Fay$^1$, Debdeep Jena$^1$ and Huili Grace Xing$^{1,2}$; $^1$School of Electrical and Computer Engineering, Cornell University, Ithaca, New York, United States; $^2$Department of Materials Science and Engineering, Cornell University, Ithaca, New York, United States; $^3$Department of Electrical Engineering, University of Notre Dame, South Bend, Indiana, United States.

The internal pyroelectric and piezoelectric polarization fields present in III-Nitride semiconductors play a crucial role in the design and performance of various electronic and photonic devices. Their effects are usually measured for samples with a complex structure and are difficult to study. However, resonant tunneling diodes (RTDs) offer a unique way to directly probe the strength of these internal fields by identifying a critical turn-on voltage in the tunneling current characteristics of polar resonant tunneling diodes (RTDs). In this scheme, the exponentially sensitive tunneling current is employed to determine the magnitude of the polarization fields at a level of unprecedented accuracy. Recently, room temperature resonant tunneling transport has been successfully engineered in GaN/AIN double barrier RTDs. The robust and repeatable nature of this quantum transport regime allowed us to uncover the intimate connection between the strong polarization fields and the unique tunneling features present in the RTD’s current-voltage characteristics. A general electrostatic model was developed for polar RTDs considering the effects of the internal polarization fields. Using this model, analytical expressions are derived for the peak voltage and peak tunneling current in forward bias, which show a clear dependence on the magnitude of the polarization fields. However, it is in reverse bias where the strong polarization fields exhibit a more dramatic effect by inducing a characteristic turn-on threshold voltage which depends only on two variables: 1) the strength of polarization fields and 2) the thickness of the tunneling barriers.In the present study, the characteristic threshold voltage has been measured at cryogenic temperatures in a set of GaN/AIN RTDs which exhibit variable barrier thickness. Molecular beam epitaxy (MBE), was employed to grow the different device structures which feature tunneling barriers between 1.5 and 2.4 nm. From these measurements, the magnitude of the polarization field (Fn) generated at the GaN/AIN heterojunction was extracted, obtaining a value of Fn=11±0.25 MVcm$^{-1}$. This value is comparable with previous reports in which the polarization fields were also experimentally measured. These results show that this method can be employed to accurately determine the magnitude of the internal
polarization fields in any polar heterostructure by relying on the strong effects that the polarization fields exert on the resonant tunneling current.

2:50 PM O05 MOVED TO H04

3:10 PM BREAK

3:30 PM O06

Engineering Monolayer MoS\textsubscript{2} Films to Be Better Hydrogen Evolution Catalyst than Pt (Guoning Li and Linyou Cao; North Carolina State University, Raleigh, North Carolina, United States).

Developing catalysts better than Pt for the hydrogen evolution reaction (HER) consists of one holy grail in the field of clean energy. We demonstrate that monolayer MoS\textsubscript{2} films may be engineered to show better HER catalysis than Pt. This is realized by optimizing the density of sulfur vacancies in the film and leveraging proper interactions of the film with substrates. Pt substrate is used as an example to highlight the proper interaction. The substrate does not participate the catalytic reaction, but may boost the activity of the film by forming a lower interface tunneling barrier and affecting the electronic structure of the film, such as through charge transfer. A minimal amount of Pt like 1 nm thick is enough to enable the superior performance at the film, and the performance of the film is very stable with no degradation for more than two months. This result indicates that MoS\textsubscript{2} may be engineered to be better than Pt in HER catalysis, although more studies would be necessary to find out non-noble materials as the proper substrate.

3:50 PM O07

(LATE NEWS, Student) Revealing Transition Metal and Oxygen Charge-Compensation in the Delithiation of Conventional Layered Oxide Cathodes (Zachary Lebens-Higgins\textsuperscript{1}, Nicholas V. Faenza\textsuperscript{2}, Maxwell Radin\textsuperscript{3}, Liao Liu\textsuperscript{4}, Shawn Salliss\textsuperscript{5}, Jatinikumar Rana\textsuperscript{6}, Mateusz Zuba\textsuperscript{7}, Julina Vicenckievicu\textsuperscript{8}, Nathalie Pereira\textsuperscript{9}, Karena W. Chapman\textsuperscript{10}, Tien-Lin Lee\textsuperscript{11}, Anton Van der Van\textsuperscript{12}, Glenn G. Amatucci\textsuperscript{13}, Wanli Yang\textsuperscript{14} and Louis Piper\textsuperscript{15}; 1Department of Physics, Binghamton University, Binghamton, New York, United States; 2Energy Storage Research Group, Department of Materials Science and Engineering, Rutgers, The State University of New Jersey, North Brunswick, New Jersey, United States; 3Materials Department, University of California, Santa Barbara, Santa Barbara, California, United States; 4Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois, United States; 5Harwell Science and Innovation Campus, Diamond Light Source Ltd., Didcot, United Kingdom; 6Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, United States.

Li-rich systems have gained increased attention due to their utilization of oxygen redox to access higher capacities beyond the transition metal (TM) redox couples. While higher energy densities are desirable for practical applications, these systems are currently unsuitable due to sluggish kinetics and poor cyclability. Despite lower theoretical capacities, conventional layered oxides, LiMO\textsubscript{2}, currently offer superior performance, though there remains a gap between the theoretical and practical capacities. In conventional layered oxides, the extractable lithium is accounted for solely by the transition metals. Oxygen redox has long been debated in LiMO\textsubscript{2} systems yet any oxygen participation in charge-compensation is considered to relate to the TM-O covalency. This type of oxygen participation does not provide excess capacity and is considered distinct from the oxygen redox process in Li-rich systems involving lone pair states at the VBM. Overcoming the capacity gap of conventional layered oxides requires identifying the charge-compensation mechanisms and their influence in the LiMO\textsubscript{2} system. Here, we focus on the state of the art Li\textsubscript{Ni0.8Co0.15Al0.05}O\textsubscript{2} system to elucidate the charge-compensation mechanisms up to high degrees of delithiation. Utilizing a combination of x-ray absorption spectroscopy and extended x-ray absorption fine structure, we find limited TM evolution at high degrees of delithiation. By mapping the resonant inelastic x-ray scattering of the O K-edge, we directly probe the oxygen environment to evaluate the nature of oxygen participation at high degrees of delithiation. Our work provides new insights into oxygen participation in LiMO\textsubscript{2} systems. Moreover, we link our results to the oxygen redox process for Li-rich systems to provide a better understanding for the oxygen redox mechanism.
on-chip nanoelectronic signaling approaches as new tools for the fundamental study of important chemical and biological catalytic systems. In specific, we have developed an on-chip electrical transport spectroscopy (ETS) approach for directly probing the electrochemical surfaces of metallic nanocatalysts under in operando conditions, using ultrathin PtNWs as model electrocatalysts. Our results not only show a high degree of consistency with generally accepted conclusions in platinum electrochemistry, but also provide important insights into various technically important electrocatalytic reactions. This study defines a novel nanoelectronic on-chip characterization strategy, as an alternative to the traditional spectroscopic characterization techniques, for in situ electrochemical surface studies with high surface sensitivity and surface specificity. The on-chip nanoelectronic investigations have further been applied to investigate the charge transport mechanism and the electrochemical behavior in electrogenic microbes (including *Shewanella* and *Geobacter*), which has been a subject of ongoing debate. Our results elucidate the complex basis of electrical conductivity of both individual microbial cells and biofilms, and have led to a new model revealing the electrochemical origin of microbial conductivities.

**4:50 PM O10**

(Graduate, LATE NEWS) Formation of Low Defect Density BaSi, Light Absorbers for Solar Cell Applications

**Yudai Yamashita,** Takuma Sato, Kaoru Toko and Takashi Suemasu; University of Tsukuba, Tsukuba-shi, Japan.

Barium disilicide (BaSi2) shows great promise as a new material for thin-film solar cells. It has a suitable bandgap of 1.3 eV, large optical absorption coefficients exceeding those of CIGS, and a large minority-carrier diffusion length of about 10 μm. We achieved a conversion efficiency of 9.9% in p-BaSi2/n-Si heterojunction solar cells. We next target BaSi2 pn homojunction solar cells. To this end, high-quality BaSi2 light absorbers with low defect density (N_d) are inevitable. In this work, we investigated defect levels and their values of N_d around the BaSi2/Si interface and in the BaSi2 layers by DLTS, and succeeded in forming BaSi2 films with N_d ~10^{13} cm^{-2}. In the first experiment, we investigated the Si pretreatment method for removing RCA-prepared oxides on n-Si(111) (ρ = 1–4 Ωcm). For sample A, we etched the surface oxide layers using 5% HF solution, followed by thermal cleaning (TC) under UHV at 800°C. For sample B, the Si substrate underwent TC at 800°C under UHV in addition to the simultaneous deposition of a 1-nm-thick Si layer. After that, 100-nm-thick p-BaSi2 layers (ρ = 2 × 10^{16} cm^{-2}) were grown at 600°C by MBE for both samples. The open-circuit voltage and the short-circuit current density under AM1.5 illumination changed significantly for sample A depending on the position of front ITO electrodes in a 2×2 cm² area. In contrast, any variations were very small for sample B, and the reproducibility was high. In DLTS, the forward filling bias voltage V_0 was set at 0.5 V, the pulse width t_p was 50 ms and the reverse bias voltage V_{rev} was set at −0.01 V. The DLTS profiles show that there were significantly higher defect levels with N_d ~10^{14} cm^{-2} in the vicinity of the interface in sample A. On the other hand, the N_d decreased markedly by approximately 100-fold or more in sample B. Thus, we decided to take this Si pretreatment method hereafter. In the second experiment, we investigated the defect levels in undoped BaSi2 absorber layers by DLTS. After the Si pretreatment mentioned above, we grew a 500-nm-thick undoped BaSi2 layer by MBE using an optimized Ba/Si ratio on n-Si (111) (ρ = 1–4 Ωcm) to form a heterojunction diode. The electron concentration (n) of the BaSi2 is below 10^{15} cm^{-3}. The n of the Si substrate was 2 × 10^{18} cm^{-3} at RT. Hence, the depletion region stretches in both sides. However, the defects on the Si substrate decrease to a value below the detection limit as described in the first experiment. For this reason, the detected peaks indicate defects in BaSi2. An upward facing peak caused by minority-carrier (hole) trap level (H1) was observed at approximately 126 k. The hole trap level was calculated to be approximately 0.27 eV from the valence band maximum, and N_d was 1×10^{17} cm^{-3}. This value is approximately 100 times smaller than that reported. As the DLTS signal near 125 K decreased as |V_{rev}| decreased and hence it approached the BaSi2/Si interface. This result shows that the defects in BaSi2 and their density are still high around the interface. When we changed the number of injected carriers by changing the pulse width t_p, the DLTS signal increased sharply as the t_p increased from 0.1 to 10 ms, indicating the presence of point defects. First-principles calculation has revealed that V_{rev} is most likely to occur. One of the calculated defect levels due to V_{rev} is in good agreement with H1. Based on the SRH recombination model, N_d ~10^{13} cm^{-2} does not cause detrimental influence on the minority-carrier properties of BaSi2.

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