

PCSI

Room Ballroom South - Session PCSI-WeA

Semiconductor Growth III/Wide Gap/Oxide Interfaces/Low-D Structures

Moderators: Chang-Beom Eom, University of Wisconsin-Madison, Stefan Fölsch, Paul-Drude-Institut für Festkörperelektronik, Gaudenzio Meneghesso, University of Padova - DEI, Markus Wohlgemant, University of Iowa

2:00pm **PCSI-WeA-1 The Application of Bismuth as a Surfactant During the Growth of Strain-balanced InAs/InAsSb Superlattices, Shane Johnson, P Webster, Arizona State University** **INVITED**

Recent investigations of the optoelectronic properties of MBE grown strain-balanced type-II InAs/InAsSb superlattices indicate that they have the minority carrier lifetimes and absorption properties necessary for high performance infrared photodetectors [1,2]. The optical performance of this material system can be enhanced by optimizing the constituent layer thicknesses and the Sb mole fraction [2], and through the utilization of bismuth as a surfactant during growth. The presence of a Bi surface layer reduces the incorporation of surface Sb into the InAs/InAsSb superlattice structure and enhances the photoluminescence intensity for dilute Bi fluxes (Bi/In ratio ~ 1%) [3]. As a surfactant, Bi can be applied during the growth of the entire superlattice structure or only during the growth of the constituent InAs layers as a means to moderate the unintentional incorporation of Sb into the InAs material. The figure shows photoluminescence from strain-balanced InAs/InAsSb superlattices grown at 430 °C using Bi/In flux ratios ranging from 0 to 3%. The inset provides the integrated photoluminescence intensity versus Bi/In flux ratio (%). The peak efficiency occurs at a Bi/In flux ratio around 1% for 430 °C growth temperatures. These results and the examination of the unintentional incorporation of Sb into the InAs layers will be presented.

2:30pm **PCSI-WeA-7 Atomic Scale Study of Isovalent Bi Atoms in the (110) InP Surface, Christian Krammel, Eindhoven University of Technology, Netherlands; F Davis-Tilley, M Roy, P Maksym, University of Leicester, UK; L Zhang, P Wang, K Wang, Y Li, S Wang, Chinese Academy of Sciences, China; P Koenraad, Eindhoven University of Technology, Netherlands**

Recent advances in semiconductor growth technology have led to the development of highly mismatched III-V semiconductors, such as dilute nitrides and bismides. This novel material class has attracted much attention from both a fundamental and application-oriented point of view [1,2]. Compared to the well-studied dilute nitrides, little is known about dilute bismides at the atomic length scale, which are in many ways complementary to dilute nitrides [3,4]. We address this issue in state of the art Bi:InP by cross-sectional scanning tunneling microscopy (X-STM) [5].

Bi atoms up to the second monolayer below the (110) InP surface are identified with the help of a geometrical hard sphere model [6] and complementary density functional theory (DFT) calculations. It is found that the contrast of Bi atoms in and directly beneath the (110) surfaces is mainly related to local strain effects of the large Bi atoms on the InP matrix. Besides these structural effects, the influence of Bi impurities on the local electronic structure is addressed in dI/dU point spectra. Here, specific Bi related resonances in the valence band of Bi atoms in the first three surface layers are discussed with respect to theoretical expectations. Bi:InP shows compared to other Bi doped III-Vs an unusual sub band gap photoluminescence. In this light, the short-range ordering of Bi atoms is addressed in Bi doped InP quantum wells and films. The X-STM measurements revealed an enhanced tendency for the formation of first nearest neighbor Bi pairs. At higher Bi contents additional Bi clustering is observed. Bi:InP/InP quantum wells show in contrast to dilute nitrides characteristic segregation patterns.

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- [1] D. G. Cooke et al., Appl. Phys. Lett. **89**, 122103(2006)
- [2] A. Janotti et al., Phys. Rev. B **65**, 115203(2002)
- [3] D. L. Sales et al., Appl. Phys. Lett. **98**, 101902(2011)
- [4] G. Ciatto et al., Phys. Rev. B **78**, 035325(2008)
- [5] K. Wang et al., Scientific Reports **4**, 5449(2014)
- [6] F. J. Tilley et al., Phys. Rev. B **93**, 035313(2016)

2:45pm **PCSI-WeA-10 Current State-of-the-Art of Gallium Oxide Power Device Technology, Masataka Higashiwaki, M Wong, K Konishi, National Institute of Information and Communications Technology, Japan; K Sasaki, K Goto, Tamura Corporation, Japan; R Togashi, H Murakami, Y Kumagai, Tokyo University of Agriculture and Technology, Japan; B Monemar, Linköping University, Sweden; A Kuramata, S Yamakoshi, Tamura Corporation, Japan** **INVITED**

Recently, gallium oxide (Ga₂O₃) has emerged as a new competitor to SiC and GaN in the race toward next-generation power devices by virtue of the excellent material properties and the relative ease of mass wafer production. Following a short introduction of material properties and features of Ga₂O₃, this presentation will review our recent development progress in device processing and characterization of Ga₂O₃ metal-oxide-semiconductor field-effect transistors (MOSFETs) and Schottky barrier diodes (SBDs).

Ga₂O₃ MOSFETs were fabricated with unintentionally-doped (UID) Ga₂O₃ epitaxial layers grown on semi-insulating Fe-doped β-Ga₂O₃ (010) substrates by ozone molecular beam epitaxy [1]. Selective-area Si-ion implantation doping of the UID Ga₂O₃ epitaxial layer formed the device channel and ohmic contacts [2], while the high resistivity of UID Ga₂O₃ was utilized for planar device isolation without mesa etching. SiO₂-passivated depletion-mode MOSFETs with a gate-connected field plate (FP) demonstrated a high off-state breakdown voltage (V_{br}) of 755 V, a large drain current on/off ratio of over nine orders of magnitude, DC-RF dispersion-free output characteristics, and stable high temperature operation against thermal stress at 300°C.

We also fabricated and characterized Pt/Ga₂O₃ FP-SBDs on n⁻Ga₂O₃ drift layers grown on n⁺-Ga₂O₃ (001) substrates [3], owing to the success of halide vapor phase epitaxy for high-speed growth of high-quality Ga₂O₃ thin films [4, 5]. The illustrative device with a net donor concentration of 1.8×10¹⁶ cm⁻³ exhibited a specific on-resistance of 5.1 mΩ·cm² and an ideality factor of 1.05 at room temperature. Successful FP engineering resulted in a high V_{br} of 1076 V. Note that this was the first demonstration of V_{br} of over 1 kV in any Ga₂O₃ power devices.

In summary, the FP-MOSFETs and FP-SBDs revealed excellent device characteristics and demonstrated great potential of Ga₂O₃ devices for power electronics applications.

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- [1] M. H. Wong et al., IEEE Electron Device Lett **37**, 212 (2016), [2] K. Sasaki et al., Appl. Phys. Express **6**, 086502 (2013), [3] K. Konishi et al., 74th Device Research Conference IV-A.5, 2016, [4] K. Nomura et al., J. Cryst. Growth **405**, 19 (2014), [5] H. Murakami et al., Appl. Phys. Express **8**, 015503 (2015).

3:15pm **PCSI-WeA-16 CO₂ Reduction with H₂O over Ga₂O₃ Photocatalysts Prepared at Various Calcination Temperatures, Masato Akatsuka, Nagoya University, Japan**

Gallium oxide (Ga₂O₃) photocatalysts can reduce CO₂ with H₂O to produce CO, although the reaction rate of CO production is very low. It has been reported that the loading of Ag on Ga₂O₃ promoted CO production [1], on the other hand, improvement of Ga₂O₃ structure should be also essential. In our previous work [2], Ga₂O₃ loaded Al₂O₃ samples (Ga₂O₃/Al₂O₃) were prepared to change coordination structures around Ga atoms, and we succeeded to enhance CO production rate. Recently, we found that the photocatalytic activity of Ga₂O₃ depended on the calcination temperature for a Ga₂O₃ precursor in the preparation stage. Therefore, in this study, we will discuss the reason why the CO production was enhanced by controlling calcination temperature.

Ga₂O₃ samples were prepared by calcination of Ga(NO₃)₃·8H₂O powder in the air at given temperatures (673 - 1173 K) for 4 h. We carried out photocatalytic CO₂ reduction with H₂O over the Ga₂O₃ samples. Fig.1 shows CO production rate for each Ga₂O₃ sample. Ga₂O₃ prepared by calcination at 823 K (Ga₂O₃(823 K)) showed a specifically high activity for CO production, although the H₂ production rate for this sample was comparable with those for Ga₂O₃ (673, 773, 873 K). It was found that the H₂ production rate increases with the surface area of the sample.

In XRD measurement of Ga₂O₃(823 K), very weak and broad diffraction peaks were observed, suggesting the formation of low crystallinity β-Ga₂O₃. Taking into account that a low crystallinity photocatalyst has many defects

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to promote the recombination of excited electron-hole pairs, high CO production activity for Ga₂O₃(823 K) would be resulted from an improvement of CO₂ adsorption process rather than electrons and holes diffusion process. Therefore We performed FT-IR measurements for chemisorbed species on Ga₂O₃ samples after introduction of CO₂. It was revealed that adsorbed species on Ga₂O₃(823 K) are different from those on other Ga₂O₃ samples. The FT-IR spectrum of Ga₂O₃(823 K) indicated preferential formation of CO₂ species interacting with water adsorbed on Ga₂O₃ surface.

3:20pm **PCSI-WeA-17 ZrO₂ as a High-k Gate Dielectric for Enhancement-mode AlGaIn/GaN MOS HEMTs**, *Charles Eddy, Jr., V Wheeler*, U.S. Naval Research Laboratory; *D Shahin*, University of Maryland; *T Anderson, M Tadjer, A Koehler, K Hobart*, U.S. Naval Research Laboratory; *A Christou*, University of Maryland; *F Kub*, U.S. Naval Research Laboratory

Advanced applications of AlGaIn/GaN high-electron-mobility transistors (HEMTs) in high-power RF and power switching are driving the need for an insulated gate technology. We present here basic and early applied studies of the use of zirconium oxide (ZrO₂) as a high-k, high breakdown gate dielectric for reduced gate leakage and a fully-recessed barrier structure for enhancement-mode operation of AlGaIn/GaN HEMTs. We include the study of GaN surface preparations for dielectric deposition, surface/interface characterization and device operation wherein a world record threshold voltage of +3.99V is achieved.

An optimum GaN surface preparation involving a piranha etch followed by a thermal oxidation of the surface has previously been shown [1] to result in smooth, clean GaN surfaces that exhibit the best electrical performance when ALD high-k dielectrics are deposited thereon. This same preparation is applied to ALD ZrO₂ dielectrics. ZrO₂ films were deposited by atomic layer deposition (ALD) using two different metal precursors [zirconium (IV) tert-butoxide (ZTB) and tetrakis(dimethylamido)zirconium(IV) (TDMAZ)] and water. For the former we also assessed both water and ozone as the oxygen precursor. ZrO₂ films grown by ALD with ZTB were found to be slightly oxygen rich whether ozone or water were used as the oxygen source. However, films grown with ZTB and ozone did have carbon contamination. Films grown with TDMAZ and water were found to be stoichiometric and free of carbon.

Films grown with ZTB and water on optimally prepared surfaces again shown the best electrical performance for the dielectric-semiconductor interface in terms of smoothness, low leakage in forward and reverse bias (< 10⁻⁵ A cm⁻²) and low hysteresis. Unlike in previous studies with ALD deposited Al₂O₃ and HfO₂, where total trapped charge was in the mid-10¹¹ to low 10¹² cm⁻² range, ZrO₂ films show considerably higher trapped charge densities in the high 10¹² to mid-10¹³ cm⁻² range. The nature of this charge is uncertain at this time but believed to be due to excess oxygen in ZTB deposited films and is directly responsible for a 1.5 – 2 V positive shift in threshold voltage.

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[1] C.R. English, et al., J. Vac. Sci. & Technol. B 32,03D106 (1-17) (2014).

3:25pm **PCSI-WeA-18 Defects and Electrical Characteristics of Pt-based Ohmic and Schottky Contacts to ZnO Nanowires**, *Jon Cox, G Foster, A Jarjour*, The Ohio State University; *H Von Wenkster, M Grundmann*, Universität Leipzig Institut für Experimentelle Physik II, Germany; *L Brillson*, The Ohio State University

Zinc oxide has emerged as a promising wide bandgap material (3.35eV at 300K) for use in next-generation nanoelectronics, with important piezoelectric, gas sensing, and optoelectronic (UV) properties. We report the *in-situ* fabrication of both Ohmic and Schottky contacts to single ZnO nanowires prepared by pulsed laser deposition (PLD) and carbothermal vapor phase transport, using only Pt metal and Ga-ion surface modification.

In bulk ZnO, defects have been shown to strongly affect the behavior of metal contacts, by modifying band bending and allowing trap-assisted tunneling transport through the metal-ZnO Schottky barrier [1].

A Ga focused ion beam (FIB) was operated at 30 keV to implant NW surfaces before metallization for creation of Ohmic contacts, and at 5 keV to gently mill the outer annulus and reduce defect concentrations at the surface, promoting formation of Schottky contacts. Electron beam induced deposition (EBID) was used to pattern Pt metal contacts to the wires, and current-voltage characteristics were measured. Depth-resolved

cathodoluminescence spectroscopy (DRCLS) was used to measure native point defects at the nanowire surface, into the bulk, and under 30nm Pt contacts. Depth profiles of DRCL spectra at and under Ga-implanted Ohmic contacts reveals interfacial segregation of copper on zinc site defects (Cu_{Zn}, 2.34eV) and oxygen vacancies (V_O, 2.54eV). Ohmic contact resistivity was also found to decrease with increasing 30 keV Ga-implantation dose. A depth profile of DRCL spectra at the interface of a Ga-milled area and 30nm Pt contact demonstrates that milling of the NW surface decreases concentration of Cu_{Zn} by an order of magnitude, promoting the formation of Schottky contacts. A Schottky contact with 2 orders of magnitude rectification was fabricated to the thin end of a tapered NW, whose diameter increases linearly from 400nm to 1µm at the other end. Investigation of defect dependence on NW diameter also demonstrated a 2x linear increase in Cu_{Zn} from 500nm to 1µm diameter. To cause pinch-off, the depletion width must be comparable to the NW diameter [2]. Thus, thinner wires are easier to pinch-off and have a lower inherent concentration of surface defects, promoting easier formation of Schottky contacts.

The interfacial physics of contacts to NW's is influenced by the diameter of the NW and its defect profile at the interface. Through the control of defects in these NW's by Ga-ion surface modification, Ohmic and Schottky contacts can be fabricated *in-situ* using a single metal. The authors gratefully acknowledge support from National Science Foundation Grant No. DMR-1305193 (Charles Ying and Haiyan Wang).

4:30pm **PCSI-WeA-31 Investigation of Schottky Contacts and Traps in β-Ga₂O₃**, *Aaron Arehart, S Ringel, E Farzana, Z Zhang*, The Ohio State University; *E Ahmadi, Y Oshima, J Speck*, University of California, Santa Barbara

INVITED

Beta-phase gallium oxide (β-Ga₂O₃) is an ultra-wide bandgap (UWBG) semiconductor that is promising for a broad range of applications including power electronics and chemical sensing, but the understanding of this material is still in its infancy. β-Ga₂O₃ is attracting particular interest due to its large, direct bandgap of ~ 4.8 eV, the availability of *n*-type doping, the ability to create heterostructures, and the availability of native substrates to support homoepitaxial growth. Additionally, several groups have reported promising initial results with high breakdown voltage transistors demonstrating the promise of this material [1-3]. However, there has been little research so far to understand the source and concentration of defects or their impact on device behavior so far [4]. Additionally, the properties of Schottky contact metals are not well explored, but is essential for metal semiconductor field effect transistors (MESFET) and similar devices. This presentation will focus on characterization of defects in β-Ga₂O₃ (Fig. 1), exploration of Schottky barrier heights for Ni, Au, Pt, and Pd metals (Fig. 2) using internal photoemission, capacitance-voltage, and current-voltage-temperature (I-V-T) measurements, and the carrier transport in the Schottky contacts using I-V-T.

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[1] M.H. Wong et al., Electron Dev. Lett. **37**, 212 (2016).

[2] M. Higashiwaki et al., Phys. Stat. Sol. A **211**, 21 (2014).

[3] M. Higashiwaki et al., Semicond. Sci. Tech. **31**, 034001 (2016).

[4] Z. Zhang, et al., Appl. Phys. Lett. **108**, 052105 (2016).

5:00pm **PCSI-WeA-37 Defect Distribution and Electronic Properties of the IrO_x/ZnO Interface**, *Geoffrey Foster*, The Ohio State University; *G Mackessy*, Columbus School for Girls; *A Hyland, M Allen*, University of Canterbury, New Zealand; *L Brillson*, The Ohio State University

We used depth-resolved cathodoluminescence spectroscopy (DRCLS) to measure the spatial distribution of native point defects at Zn- and O-polar ZnO interfaces with iridium oxide (IrO_x) and their impact on Schottky barrier formation. Oxidized metal, such as IrO_x and PtO_x, have sparked interest in their high work functions allowing them to be used as both Ohmic and Schottky contacts[1]. These oxidized metal layers produce Schottky contacts with the ZnO. These diodes have rectification of 8.6 and 5.5 orders of magnitude, respectively, with barrier heights of 0.89 eV and 0.67 eV. For the same RF sputter of a 32 nm IrO_x layer, on ZnO, sample on both Zn-polar and O-polar ZnO, incident electron beams with energies E_B = 1 -5 keV generated electron-hole (e-h) pairs that recombined to exhibit DRCLS spectra past the IrO_x layer, with 3.35 eV intrinsic band gap transitions in ZnO, and 2.01 eV and 2.08 eV V_{Zn} transitions in the Zn-polar and O-polar ZnO respectively. V_{Zn} acts as a compensating defect, acting to increase the depletion width at the IrO_x/ZnO interface creating the Schottky diode [2]. DRCLS enabled us to profile the V_{Zn} density across the IrO_x/ZnO interface on a near nm scale as defined by Monte Carlo

simulations of electron-hole (e-h) pair creation rate vs. depth. This defect depth precision revealed interfaces with V_{Zn} profiles in the ZnO that varied with the Zn-Polar and O-polar ZnO orientations. The depth profiles show a clear difference in the density of V_{Zn} in each sample with nearly a 1.5 times increase in V_{Zn} density from the O-polar to the Zn-polar sample.

The variation of the V_{Zn} between each is significant since it explains the higher barrier height in the Zn-polar ZnO. This increased barrier height from growing oxidized metals on semiconductor films could have implications since these high work function metals could be used as Ohmic contacts on p-type semiconductors. The authors gratefully acknowledge support from National Science Foundation Grant No. DMR-1305193 (Charles Ying and Haiyan Wang).

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[1] G. T. Dang, T. Uchida, T. Kawaharamura, M. Furuta, A. R. Hyndman, R. Martinez, S. Fujita, R. J. Reeves, and M. W. Allen, "Silver oxide Schottky contacts and metal semiconductor field-effect transistors on SnO₂ thin films," vol. 041101, 1882.

[2] Y. Dong, F. Tuomisto, B. G. Svensson, A. Y. Kuznetsov, and L. J. Brillson, "Vacancy defect and defect cluster energetics in ion-implanted ZnO," *Phys. Rev. B - Condens. Matter Mater. Phys.*, vol. 81, no. 8, pp. 3–6, 2010

5:05pm **PCSI-WeA-38 Ultrasound Treatment Influence on the Si-SiO₂ Interface Defects Structure**, *Daniel Kropman, T Laas*, Tallinn University, Estonia; *A Medvids*, Riga Technical University

The effect of ultrasonic treatment (UST) on the defect structure of the Si-SiO₂ system by means of electron spin resonance (ESR), metallography, MOS capacitance technique and secondary ions mass-spectroscopy is presented. The non-monotonous dependence of the point defect densities on the US wave intensity has been observed. The US frequency influence on the ESR signal intensity of the defect centres depended on the defects type and may be caused by vibrational energy dissipation which are a function of defect centre's type. The density of point defects and absorbed impurities at the Si-SiO₂ interface can be reduced by appropriate choice of UST.

Before UST a signal with $g=1.9996$ (Pa centers) connected with vacancy complexes is observed. After UST appears another signal with $g=2.0055$ (broken bonds of Si atoms). Investigation of the dependence of the spin density on the US frequency of the UST in Si-SiO₂ samples with [111] and [100] crystallographic orientation was carried out. It has been shown that the influence of the US frequency and the sample orientation on the ESR signal intensity varies for different centres. The frequency and orientation dependence of the ESR signal with $g=1.9996$ and the lack of this dependence for the centres with $g=2.0055$ show that the vibrational energy dissipation depend on the type of defect centres and their orientation. Defect density grows with an increase of the US intensity or changes nonmonotonously depending on the oxides thickness. In the samples with thick oxide there is a maximum in the dependence of the charge carriers life time on the US wave amplitude, while in samples with thin oxide - a minimum. This shows that the structural defects form electrically active centres and their density can be varied by UST.

5:10pm **PCSI-WeA-39 The Effects of B and Ga Co-doped ZnO Electron Transporting Layer on the Properties of n-ZnO/p-GaN UV Photodetector**, *J Huang, Linjun Wang, K Tang, Y Shen, F Gu*, Shanghai University, China

Recently, ZnO has attracted much attention in short wavelength optoelectronic devices and sensors [1-2] due to its direct wide optical bandgap (3.37eV) and high exciton binding energy (60meV). Also ZnO is intrinsically an n-type semiconductor and can easily be a heterojunction with other p-type materials, such as p-Si, p-NiO, p-SiC, p-GaN as well as some p-type organic-polymers. Based on the very good characteristics of ZnO mentioned above, it is very popular to be chosen as electron selective layer in ultraviolet (UV) photodetectors (PDs) [3-4].

B and Ga co-doped ZnO (BGZO), as a transparent conduction oxide electrode, has many good physical properties, such as high electrical conductivity, excellent optical transparency and thermal stability, which would replace the traditional ITO or FTO due to its low cost and easy process [5]. Herein, we prepared BGZO with different thicknesses as an electron transporting layer of the ZnO/GaN heterojunction and the ultraviolet photoresponse characteristics of the devices were investigated. From the results, we find that the PDs with BGZO coating showed higher responsivity.

[1] T.J. Hsueh, C.L. Hsu, S.J. Chang, P.W. Guo, J.H. Hsieh, I.C. Chen, *Scr. Mater.* **57**, 53 (2007).

[2] H. Zhou, G.J. Fang, L.Y. Yuan, C. Wang, X.X. Yang, H.H. Huang, C.H. Zhou, X.Z. Zhao, *Appl.Phys.Lett.* **94**, 013503 (2009).

[3] T.C. Zhang, Y. Guo, Z.X. Mei, C.Z. Gu, X.L. Dua, *Appl.Phys.Lett.* **94**, 113508 (2009).

[4] S. Mridha, D. Basak, *J. Appl.Phys.* **101**, 083102 (2007).

[5] R.G. Gordon, *Mater. Res. Bull.* **25**, 52 (2000).

5:15pm **PCSI-WeA-40 2D Silica and Aluminosilicate Bilayers on Pd(111): From Incommensurate to Commensurate Crystalline**, *Jin-Hao Jhang, C Zhou, G Hutchings, E Altman*, Yale University

Zeolite silicate frameworks are essential in facilitating numerous catalytic reactions. Although zeolites have been used for decades, it is still a long-term challenge to understand how surface properties of zeolites promote catalytic reactions. Recently, two-dimensional (2D) van der Waals silica and aluminosilicate bilayers have been successfully prepared on metal substrates, e.g. Pd(100) [1], Pt(111) [2], and Ru(0001) [3,4]. This achievement creates a new pathway for investigating zeolites using surface science approaches.

Both silica and aluminosilicate bilayers can grow in crystalline and amorphous forms. On Pt(111) only amorphous silica bilayer can be formed likely due to the relatively large lattice mismatch with the crystalline form, whereas on Ru(0001) both crystalline and amorphous bilayers are seen due to a low lattice strain. However, the structural information of the bilayer-growth transition between crystalline and amorphous phases is still lacking. Pd(111) thus becomes a suitable substrate to gain the information because of the degree of the lattice mismatch: Pt(111) = 4.6% > Pd(111) = 3.7% > Ru(0001) = 2%. We report structural studies of silica and aluminosilicate bilayers on Pd(111) via low energy electron diffraction and scanning tunneling microscopy, complemented by density functional theory (DFT) calculations. Our results reveal that silica bilayers grow in an incommensurate crystalline form on Pd(111) which is found neither on Pt(111) nor Ru(0001) and is in contrast to Pd(100) where a commensurate form is observed. It puts the maximum biaxial tensile strain that can be imparted on the bilayer to less than 3.7%. The aluminosilicate bilayer was successfully prepared by replacing 25% of the Si with Al, and importantly, it grows commensurately on Pd(111). The DFT calculations reveal that the longer Al-O bonds reduce the strain energy by decreasing the mismatch to 1.9% as well as by softening it; thereby explaining the transition from incommensurate to commensurate forms. Overall, this work clearly provides an insight into the possibility of manipulating the structure of a 2D material.

[1] E. I. Altman et al., *J. Phys. Chem. C* **117**, 26144-26155 (2013).

[2] X. Yu et al., *Appl. Phys. Lett.* **100**, 151608 (2012).

[3] D. Loeffler et al., *Phys. Rev. Lett.* **105**, 146104 (2010).

[4] J. A. Boscoboinik et al., *Angew. Chem. Int. Ed.* **51**, 6005-6008 (2012).

5:20pm **PCSI-WeA-41 Electron-phonon Coupling Dynamics for Tunable Bandgap of Transition Metal Dichalcogenide Atomic Layers**, *Quinton Rice, T Neupane, D Jayakodige, B Tabibi, F Seo*, Hampton University

The atomic layers of 2-dimensional transition metal dichalcogenides (TMDCs, MX₂; M=Mo or W; X=S, Se, or Te) are of great interest in the areas of optoelectronic and photonic applications due to the bandgap conversion from direct for monolayer and indirect for bilayer or multilayer; unique properties of valley orbital, spin, and optical helicity; and compositional tuning of exciton bandgaps in visible and near-infrared region. In this work, the average acoustic phonon energy involved in the electron-phonon interaction as well the coupling strength between electrons and phonons is analyzed using the O'Donnell and Chen relation for the temperature-dependent bandgap of TMDCs. The analysis shows that as the temperature is increased the exciton band energy is decreased. When the electron-phonon coupling strength is large (small) the tunability of exciton bandgap is wide (narrow) for a constant acoustic phonon energy. Weak electron-phonon coupling ($S=2$) leads to a linear decrease in the bandgap energy for temperature above ~85 K but strong coupling ($S=30$) above ~60 K. The bandgap was changed from 2 eV to 0.5 eV for both weakly and strongly coupled electrons, however, for a constant electron-phonon coupling strength, large (small) acoustic phonon energy results in narrow (wide) tunability of the bandgap. The ability to control the exciton bandgap through the electron-phonon interaction and average acoustic phonon energy at various temperatures leads to tunable optoelectronic and photonic devices based on 2-dimensional TMDCs. Acknowledgement: This work at HU is supported by ARO W911NF-15-1-0535, NSF HRD-1137747, and NASA NNX15AQ03A.

5:25pm **PCSI-WeA-42 Nonlinear Absorption Characteristics of Monolayer and Bilayer/Multilayer of TMDC**, *Tikaram Neupane, Q Rice, D Jayakodige, B Tabibi, F Seo*, Hampton University

The nonlinear absorption properties of TMDC depends on the changes of band gap where monolayer of TMDC has a direct bandgap and the bilayer and multilayer have an indirect band gap. The bandgap of the monolayer is wider than that of bilayer and multilayer. This absorption process is described by Jablonski diagrams which may include two-step absorption with one-photon for each step, two-photon absorption to the real final state through a virtual intermediate state. In the one-photon excitation, the electric dipole transition $|i\rangle$ to $|f\rangle$ is allowed due to other parities between two states. Hence the saturable (negative) absorption (SA) is observed due to the higher ground-state absorption cross-section than the excited-state absorption cross-section, $\sigma_g > \sigma_e$. But in the two-photon excitation, the electric dipole transitions $|i\rangle$ to $|n\rangle$ and $|n\rangle$ to $|f\rangle$ are allowed due to same parities between the initial and final states via intermediate virtual state. Therefore, the reverse saturable (positive) absorption (RSA) is dominant due to the higher value of the excited-state absorption cross-section than the ground-state absorption cross-section. The band gap changes due to the number of layers and temperature switches RSA to SA or vice versa. The atomic layers with SA are utilized for laser Q-switch and mode-locker, while the atomic layers with RSA are utilized for optical power limiter. Acknowledgement: This work at HU is supported by ARO W911NF-15-1-0535, NSF HRD-1137747, and NASA NNX15AQ03A.

5:30pm **PCSI-WeA-43 Graphene Moiré Pattern Ultra-High Resolution Atomic Force Microscopy**, *B Kim, Gerald Pascual, K Lee*, Park Systems Corporation

The ultra-high resolution of AFM was demonstrated in a Graphene/hexagonal Boron Nitride (hBN) sample evaluation conducted by AFM. The sample consisted of hBN substrate overlaid with a Graphene layer and was scanned under ambient air. The purpose of the evaluation was to assess the AFM ability to characterize the topography of the moiré pattern that was created when one layer was set on top of the other and offset by rotation. Using non-contact AFM mode and a standard AFM probe tip, the AFM was able to successfully image the moiré pattern super lattice constant of the sample in scans as large as 500 x 500 nm (Figure (a)). In the higher magnification image of Figure (b) taken at a scan size of 60 x 60 nm provides the clear evidence that not only are the super lattice constants of the moiré pattern about 15 nm [1] in width, but that the spacing between each striation on the moiré pattern is roughly 4-5 nm in length. Observations of such striations in Graphene/hBN systems have been previously reported [2]. This latter distance is in line with the expected tip radius curvature values for the AFM tip used to acquire all four sets of data.

5:35pm **PCSI-WeA-44 Nucleation of Cu₂Te Layer by a Closed Space Sublimation Method Toward the Growth of Te Based Chalcopyrite**, *Youhei Sakurakawa, A Uruno, M Kobayashi*, Waseda University, Japan

The two-step closed space sublimation (CSS) growth of high quality AgGaTe₂ layer was successfully achieved by the formation of the Ag₂Te layer as a first step. This AgGaTe₂ layer was successfully applied to the solar cells. CuGaTe₂ has been focused on because of the lower material cost than AgGaTe₂. Based on the success of AgGaTe₂/Ag₂Te, CuGaTe₂/Cu₂Te was proposed and the growth of Cu₂Te by the CSS method was attempted in this study. It has been confirmed that the surface morphology was widely varied depending on the growth parameter in case of the Ag₂Te layer growth. The realization of the membrane-filter structure for the Ag₂Te layer was the key for the formation of high quality AgGaTe₂ layer. In this study, Cu₂Te layer was formed on various substrate materials and surface orientations using various source materials. Judging from the phase diagram of Cu-Te, Cu-Te compounds would exhibit various structures depending on the temperature and the mole ratio, hence the surface structure of the layer could be drastically controlled. The substrate surface chemistry (dangling bond density, polarity, and so on) would also affect the formation process of Cu-Te compounds.

Cu₂Te layers were grown using 3N Cu₂Te powder or 3N CuTe powder. The substrate temperature during the layer growth was varied from 590 °C to 700 °C. The substrates used were Si(001), Si(111) and Al₂O₃(0001). The surface structure of the obtained layer was characterized using scanning electron microscope (SEM). The crystallographic property of the layer was mainly analyzed by the θ -2 θ profile of the x-ray diffraction.

Figure 1 shows the SEM image of the layer grown on Si (001) at 590 °C. Plateaus and cells surrounding them were observed. This surface structure

was probably associated with the peritectoid reaction of Cu and Te [3]. The size of plateau and their spacing were sub-micrometer scale, and such structures would be useful for fabricating various nano-structures. The size and the shape of the plateau revealed to be affected by the substrate temperature and the surface orientation of the substrate. The nucleation of the CuGaTe₂ layer on this surface structure would be also reported.

5:40pm **PCSI-WeA-45 Gallium Nanoparticles Based Heterostructures for Full Color Thermally Stable Plasmonic and Photonic Platforms**, *Maria Losurdo*, Cnr-Nanotec, Institute of Nanotechnology, Italy; *A Suvorova*, The University of Western Australia; *K Hingerl*, Johannes Kepler University Linz; *J Humlicek*, Masaryk University, CEITEC, Brno.; *A Brown*, Duke University

Gallium, Ga, a group-III metal, is of fundamental interest due to its polymorphism, unusual phase transition behaviors and optical properties. In recent years, substrate-supported Ga nanoparticle ensembles have been shown to be efficacious for plasmonics applications in the full NIR-VIS-UV spectral range [1]. Although bulk Ga is liquid under ambient conditions, new solid phases have been observed when Ga is confined at the nanoscale. Herein, we discuss structural, thermal and optical properties of Ga nanoparticles (Ga NPs) creating heterostructures with silicon, silicon carbide, graphene, and sapphire. We show that at the nanoscale the support plays a fundamental role in determining Ga nanoparticle phases. Specifically, we demonstrate the stable coexistence in sapphire/Ga NPs and SiC/Ga NPs of the Ga solid g-phase core and a liquid shell. The driving forces for the nucleation of the g-phase are a combination of surface energies, the Laplace pressure in the nanoparticles and its epitaxial relationship to the substrate. Amorphous, deformable substrates, like glass and graphene as well as chemically reactive substrates, such as Si, inhibit solid phase nucleation. Sapphire and SiC, which are rigid and non-reactive with Ga, creates a semi-coherent lattice nucleating a g-phase solid core when the nanoparticles are above 50 nm. The solid-liquid phase coexistence is stable from 180K to 800K [2]. We present extensive correlations between structural, using HRTEM and TERS, and optical characterisations using ellipsometry and magneto-spectroscopy, from the infrared to visible and ultraviolet range, to describe phenomena arising from coupling wavelength-resolved light into the various heterostructures. Therefore, impacts of the stable solid-liquid phase coexistence and of superheating and supercooling in core-shell NPs on plasmonics are discussed.

The study is extended also to a variety of Ga-based bimetallic nanoparticles to provide a general framework for understanding how nanoscale confinement, metals interfacial and surface energies, and crystalline relationships to the support (graphene, semiconductor, or insulator) enable and stabilize the coexistence of unexpected phases providing criteria for choosing heterostructure type to control nanoparticle optical behavior and interfacial charge transfer.

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[1] Y. Yang et al. ACS Photonics, 1, 582 (2014)

[2] M. Losurdo et al., Nature Materials. 15, 995 (2016).

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