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Science and Technology of Materials, Interfaces, and Processing

2017 Spring Meeting Hudson Mohawk AVS Chapter May 15, 2017 4:00 – 8:00 PM

Rensselaer Polytechnic Institute (RPI) Materials Research Center (MRC) Room 136 Troy, NY 12180

Meeting Agenda^{*}:

4:00 PM – 4:05 PM	Welcome
4:05 PM – 6:25 PM	Oral Presentations
6:25 PM – 6:35 PM	Break – Pizza and beverages
6:35 PM – 7:35 PM	Poster presentations and networking
7:35 PM – 7:45 PM	Best presentation and poster announcement
7:45 PM – 8:00 PM	AVS Local Chapter Executive meeting

*Complete presentation schedule is available in the next page.

*Presentation Schedule: (Oral presentations are of 15 minutes with 5 more minutes for Q&A.)

4:00 – 4:05 PM Welcome note by **Dr. Michael Burrell**, Chair 2016, AVS Hudson Mohawk Chapter

Oral Presentations

- 4:05 4:25 PM **PATH TOWARD 23% EFFICIENCY CdTe SOLAR CELLS** <u>Hongying Peng</u>¹, Zhibo Zhao², Gang Xiong², Markus Gloeckler² ¹GE Global Research, Niskayuna, NY, USA ²First Solar Inc, Perrysburg, OH, USA
- 4:25 4:45 PM INVESTIGATION OF DRY ASH DAMAGE FOR SiOxNy FILMS <u>Yibin Zhang</u>¹, Lei Jiang¹, Zhiguo Sun¹, Jeffrey Riendeau¹ GLOBALFOUNDRIES, 400 Stone Break Rd Extension, Malta, NY, USA
- 4:45 5:05 PM IONOLUMINESCENCE MEASUREMENT AND MODELING FOR ORGANIC SCINTILLATORS Subha Chakraborty and Mengbing Huang SUNY Polytechnic Institute, Albany, NY 12203
- 5:05 5:25 PM PULSE WIDTH MODULATION TO ACHIEVE MULTI-LEVEL RESISTANCE WITH TaO_x BASED RRAM USING Hf AS OXYGEN EXCHANGE LAYER Zahiruddin Alamgir, Joshua Holt, Karsten Beckmann, Nathaniel Cady Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, 257 Fuller Road, Albany, New York 12203

5:25 – 5:45 PM HETEROINTERFACIAL TOUGHENING USING A MOLECULAR NANOLAYER DURING STRESS CORROSION AND FATIGUE Matthew Kwan¹, Muriel Braccini^{1,2}, Jackson Wong¹, Michael W. Lane³, and Ganpati Ramanath^{1*} ¹Rensselaer Polytechnic Institute, Materials Science and Engineering Department, Troy, NY, 12180, USA ²CNRS, Laboratoire Science et Ingénierie des Matériaux et Procédés (SIMAP), F-38000 Grenoble, France ³Emory and Henry College, Chemistry Department, Emory, VA 24327, USA

5:45 – 6:05 PM **TUNABLE BAND GAP IN PHOSPHORENE ANTIDOT LATTICES** <u>Andrew Cupo¹, Paul Masih Das², Gopinath Danda^{2,3}, Neerav Kharche¹, Marija Drndić², and Vincent Meunier¹ ¹Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York, 12180, USA ²Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania, 19104, USA ³Department of Electrical and Systems Engineering, University of Pennsylvania, Philadelphia, Pennsylvania, 19104, USA</u>

6:05 – 6:25 PM VALENCE ELECTRON CONCENTRATION AS AN INDICATOR OF MECHANICAL PROPERTIES IN HARD COATINGS Karthik Balasubramanian¹ and Daniel Gall² ¹Department of Mechanical, Nuclear and Aerospace Engineering, Rensselaer Polytechnic Institute, Troy, New York, 12180, USA ²Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, New York, 12180, USA

6:30 – 7:30 PM

Poster Presentations

REVEALING THE GLOBAL CRYSTALLINE INTEGRITY OF WAFER SCALE GRAPHENE ON SiO₂/Si: AN AZIMUTHAL RHEED APPROACH

Zonghuan Lu¹, Xin Sun¹, Yu Xiang², Morris Washington^{1, 2}, Gwo-Ching Wang^{1, 2}, and Toh-Ming Lu^{1, 2}

¹Center for Materials, Devices, and Integrated Systems ²Physics, Applied Physics and Astronomy Department, Rensselaer Polytechnic Institute, Troy, NY 12180

OPTIMIZATION OF ANNEALING PARAMETERS FOR SILICON CARBIDE (SIC) NANOWIRE FABRICATION

<u>Casey Biederman</u>, Lukas Kiehl, Natasha Tabassum, Brian Ford, Vasileios Nikas, Spyros Gallis

Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, 257 Fuller Road, Albany, New York 12203

VAN DER WAALS EPITAXY OF CdTe THIN FILM USING GRAPHENE AS BUFFER LAYER

Dibyajyoti Mohanty^{1,2}, Zonghuan Lu¹, Xin Sun¹, Shengbai Zhang³, Morris Washington³, Gwo-Ching Wang³, Toh-Ming Lu³ and Ishwara B. Bhat² ¹Center for Materials, Devices, and Integrated Systems ²Electrical, Computer and Systems Engineering Department, ³Physics, Applied Physics and Astronomy Department, Rensselaer Polytechnic Institute, Troy, NY 12180

NEAR INFRARED REFLECTORS AS SMART-GLASS FOR SOLAR PANELS AND BUILDINGS

<u>Mark Altwerger</u>¹, Iulian Gherasoiu² and Harry Efstathiadis¹ ¹Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, 257 Fuller Road, Albany, New York 12203 ²College of Engineering, SUNY Polytechnic Institute, 100 Seymour Rd, Utica, NY 13502

INVESTIGATING THE HETEROEPITAXY OF NATURALLY-FORMED ULTRATHIN

V2O5 OXIDE PASSIVATION LAYER ON VO2/SAPPHIRE(001) FILM

<u>A. J. Littlejohn</u>,^{a*} Y. Yang,^a Z. Lu,^a E. Shin,^{bc} K. C. Pan,^b G. Subramanyam,^{bc} V. Vasilyev, ^c K. Leedy,^c T. Quach,^c T.-M. Lu^a and G.-C. Wang^a

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VAN DER WAALS EPITAXY OF SnS FILM ON SINGLE CRYSTAL GRAPHENE BUFFER LAYER ON AMORPHOUS SiO₂/Si

<u>Yu Xiang</u>^{1,2}, Yunbo Yang^{1,2}, Fawen Guo^{1,2}, Xin Sun^{1,2}, Zonghuan Lu^{1,2}, Dibyajyoti Mohanty^{1,3}, Ishwara Bhat^{1,3}, Morris Washington^{1,2}, Toh-Ming Lu^{1,2} and Gwo-Ching Wang^{1,2}

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EFFECT OF DISPLACEMENT DAMAGE ON TANTALUM OXIDE RESISTIVE MEMORY DEVICES

<u>Joshua Holt</u>¹, Karsten Beckmann¹, Zahir Alamgir¹, Jean Yang-Scharlotta², Nathaniel Cady¹

¹Colleges of Nanoscale Science and Engineering, SUNY Polytechnic Institute, Albany, New York 12203

²Jet Propulsion Laboratory, NASA, California Institute of Technology

CHARACTERIZATION OF THE METALLIC PROPERTY OF VANADIUM DISULFIDE (VS₂)

<u>Poomirat Nawarat</u>, Zhaodong Li, David Frey, Gwo-Ching Wang, and Kim M. Lewis

Department of Physics, Applied Physics, and Astronomy Rensselaer Polytechnic Institute, 110 Eighth Street, Troy, NY 12180

CLEANROOM GLOVES CHARACTERIZATION – A STUDY

Kok Hin Teo¹, Steven Molis², Shannon Kauderer ¹, Joshua Moore¹, Jeffrey Riendeau¹

¹GLOBALFOUNDRIES, 400 Stone Break Rd Extension, Malta, NY, USA ²GLOBALFOUNDRIES, 2070 Route 52, Hopewell Junction, NY 12533

VAN DER WAALS HETEROSTRUCTURE OF CdS THIN FILMS ON GRAPHENE

Xin Sun^{1,*}, Zonghuan Lu¹, Weiyu Xie¹, Yiping Wang², Jian Shi², Shengbai Zhang¹, Morris A. Washington¹ and Toh-Ming Lu¹

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TRANSFER MOLDING FOR MESOSCALE REFRACTIVE INDEX CONTROL

<u>Michael Deagen</u>, Linda Schadler, and Chaitanya Ullal Materials Science & Engineering Department, Rensselaer Polytechnic Institute

DEVELOPMENT and TCAD SIMULATIONS of Ge p-i-n INFRARED DETECTORS

<u>Caitlin Philippi1</u>, John Zeller², Harry Efsathiadis¹, Pradeep Haldar¹, Ashok Sood² ¹State University of New York, Polytechnic Institute, Albany, NY ²Magnolia Optical Technologies, Inc., Woburn, MA

PATH TOWARD 23% EFFICIENCY CdTe SOLAR CELLS

Hongying Peng¹, Zhibo Zhao², Gang Xiong², Markus Gloeckler²

¹GE Global Research, Niskayuna, NY, USA ²First Solar Inc, Perrysburg, OH, USA Email: <u>Hongyingpeng.2017@gmail.com</u>

CdTe has proven to be one of the most promising absorbers for producing high-efficiency and low-cost thin-film solar cells. The world-record efficiencies of CdTe solar cells have significantly increased in the last five years, from 17.3% in 2011 to 22.1% in 2016. The remarkable improvement was not only seen in short-circuit current (Jsc), but also fill factor (FF) and open-circuit voltage (Voc). However, the record efficiency is still far below the theoretical prediction of 32%. In the past few years, we have explored various approaches to improve the performance of CdTe-based thin-film solar cells. In this talk, we will review our recent progresses, including (1) the realization of high figure of merit transparent conductive oxide (TCO); (2) achieving high open circuit voltage via alternative dopant of Ag incorporation and better long term stability via more accurate dosage control; (3) enhancing short circuit currents using engineered window layers. Our results indicate that improvements of the open circuit voltage, short circuit current, and fill factor of CdTebased thin-film solar cells through dedicated synthesis and interface engineering. At material level, further progress has been made to-date to bring CdTe material properties on par with GaAs, in particular on the reduction of interface recombination velocities, minority carrier lifetime improvement, as well as the increase of p-type doping in CdTe. At device level, accomplishment on individual IV parameters (Voc, Jsc and FF) has led us to believe that 23% cell efficiency can be achieved in foreseeable future.

INVESTIGATION OF DRY ASH DAMAGE FOR SIOxNy FILMS

Yibin Zhang¹, Lei Jiang¹, Zhiguo Sun¹, Jeffrey Riendeau¹

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As the semiconductor device continues to shrink, new dielectric materials are implemented with lower the dielectric constant to improve device performance. The need to shrink dimensions has required the use of different patterning materials to achieve critical dimensions. Prior to the 20nm technology node the back end of line (BEOL) post-lithography rework process was usually considered as a non-critical process compared to other process steps. When technologies get into sub-20nm node, rework and cleaning process become a challenge for manufacturers, because new dielectric materials do not stand up to the older rework/strip processes. In this work, it was investigated how dry ash treatment causes damage of SiOxNy by using X-ray Photoelectric Spectroscopy and ellipsometry. SiNO2 was found after the treatment. The composition of the top surface of SiOxNy films was changed. This will result in reducing thickness of SiOxNy films, which will cause defects and degrade device performance. Different recipes of the dry ash treatment were evaluated to minimize the damage.

IONOLUMINESCENCE MEASUREMENT AND MODELING FOR ORGANIC SCINTILLATORS

Subha Chakraborty and Mengbing Huang

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Growing need of miniaturization of semiconductor devices have motivated interest in sensing and controlling the impact location of energetic ions over nano-devices during doping and lithography processes. For this purpose, we have investigated the properties of Helium ion induced luminescence from organic scintillator thin film. The scintillators are prepared by spin-coating undoped and eight different types of fluorophore-doped polystyrene (PS) films on silicon wafers. We have developed a model of ionoluminescence yield by combining Birk's model of scintillation yield and excited state rate equations. Our work shows that an increase in fluorescence efficiency by doping, and an energy transfer mechanism between spatially correlated triplet excited states, known as the Triplet-Triplet Annihilation (TTA) mechanism, are responsible for a linearly increasing singlet fluorescence yield of the plastic scintillators when the ion-flux is increased. The ionoluminescence yields (emitted photons/incident ions) of the doped and undoped scintillators are measured and compared with our theoretical model. As examples shown in FIG. 1 and FIG. 2, our theoretical modeling shows a good agreement with our experimental results, suggesting that singlet-upconversion resulting from triplettriplet annihilation processes may be responsible for enhanced singlet emission of the fluorophores at high ion beam flux densities, and energy transfer from the polystyrene matrix to the fluorophore molecules is an effective pathway to increasing the fluorescence efficiency in the doped scintillator films.



FIG. 1: Comparison of measured ionoluminescence yield (emitted photon/incident ion) of undoped and fluorophore-doped PS scintillator thin films as a function of Helium beam current density *J*. Kinetic energy of He ions, E_k = 350 keV. Coumarin 6 and POPOP dopant fluorophores are used in the doped samples having a mass-ratio PS:Dopant = *m*:1. The dashed straight lines are linear fitting results based on our model of TTA induced yield enhancement. Increase in TTA rate and fluorescence efficiency of doped films contribute towards higher singlet yield (Y_{FL}) of the doped films.



FIG. 2: Comparison of measured ionoluminescence yields from nine different scintillators (Pure PS and eight doped). The dashed lines are fitted based on our theoretical model to find best-fit results of TTA rate and fluorescence efficiency. A comparison of the fluorescence efficiency from the best-fit results with the theoretical calculations based on the dopant concentration show very good agreement.

PULSE WIDTH MODULATION TO ACHIEVE MULTI-LEVEL RESISTANCE WITH TaO_x BASED RRAM USING Hf AS OXYGEN EXCHANGE LAYER

Zahiruddin Alamgir, Joshua Holt, Karsten Beckmann, Nathaniel Cady

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Resistive Random Access Memory (RRAM), also commonly referred to as the "memristor", is a very strong candidate to replace existing non-volatile memory (NVM) such as flash. RRAM has drawn considerable attention among researchers as a potential candidate for next-generation NVM due to its simple structure, fast switching speed, endurance, and retention. The basic structure of RRAM is a metal-insulator-metal (MIM) structure where single or several layers of insulators are sandwiched between two metal electrodes. Besides down-scaling of memory cells, another effective way to increase the memory density is to store more information in one device known as multilevel cell (MLC) storage. For RRAM, multilevel resistive switching has been demonstrated in previous reports by setting the current compliance, changing the reset voltage, and modifying the amplitude of the voltage pulse; however, many of these reports have not shown sufficient endurance for these states or exhibited overlapping states that could lead to bit errors in multilevel storage. We have developed a bilayer tantalum oxide based device with hafnium as the oxygen exchange layer (OEL). Multiple discrete uniform resistance levels were achieved by modulating the reset pulse width and height. For a fixed pulse height. off state resistance was found to vary with the square power of pulse width. By changing reset pulse width, we were modulate resistance gradually, yet each resistance level was distinct and discrete without any overlap. The device also demonstrated endurance more than 10⁸ cycles with satisfactory Roff/Ron ratio and good retention. Excellent cycle-tocycle uniformity with very low standard deviation was also observed. Using I-V curve fitting, it was demonstrated that the device undergoes a transition from Schottky emission to trap assisted tunneling during switching from set to reset state.



Fig. 1 Fourteen resistance levels obtained from 10⁵ consecutive switching pulses were achieved by applying fixed set pulses and reset pulses with different width/height. Level one corresponds to ON state.

HETEROINTERFACIAL TOUGHENING USING A MOLECULAR NANOLAYER DURING STRESS CORROSION AND FATIGUE

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Tailoring the chemistry of heterointerfaces is crucial to control the fracture toughness of a variety of composite materials. Our results demonstrate that introducing an organosilane molecular nanolayer at a copper-silica interface can lead to multifold toughening under both static (stress corrosion) and cyclic loads (fatigue). We find during stress corrosion under controled humidities, nanolayer-induced interface strengthening and consequent metal plasticity activation lead to fracture toughening. We will show that interfacial bond strength weakening decreases metal plasticity, which is activated only above a critical metal film thickness. However, once activated, the metal plasticity increases with increasing temperature due to decreasing yield stress. Cyclic stress fatigue fracture tests of a layered polymer-metal-ceramic structure with a molecular nanolayer at the metal-ceramic interface reveal unusual loading-frequency-dependent multifold toughening in the ~75-300 Hz regime. These frequency-dependent peaks increase the fracture toughness from ~1 Jm⁻² to 3 Jm⁻², exceeding the toughness of statically opened interfaces, ~1.5 Jm⁻² by two-fold. Our fracture surface analyses reveal that cyclic stress fatigue fracture toughening is underpinned by polymer plasticity facilitated by load transfer across the nanolayer-strengthened interface. Experiments with and without the nanolayers show that while nanolayer-induced strengthening is a necessary condition for interface toughening, the toughening extent and frequency regime are dependent on the rheological properties of the polymer. In particular, the

fatigue fracture energy peak height, frequency and width, are sensitive to the polymer glass transition temperature. These results suggest that the fatigue fracture toughening is tunable by appropriate choices of nanomolecular layer and polymer(s). Our findings collectively open up a completely new set of possibilities for tailoring the mechanical properties of layered composites and soft-hard heterointerfaces through nanomolecular functionalization for diverse applications, such as, load-bearing structures, flexible electronics and biomedicine.



TUNABLE BAND GAP IN PHOSPHORENE ANTIDOT LATTICES

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We used first-principles density functional theory (DFT) calculations to investigate the properties of phosphorene antidot lattices. It was found that the stability (quantified by the edge energy) decreases when the density of edges increases. This trend can be broken for H-passivated systems, where in some cases incrementing to a larger radius can increase stability. Most importantly, the band gap can be widely tuned through variation of the perforation spacing and radius. Moreover, deviations from the expected quantum confinement trends are due to edge effects in general. Spatial distributions of the band gap are roughly bimodal with larger band gap atoms emanating from the zigzag edge, which can be explained by the presence of stronger quantum confinement effects in phosphorene nanoribbons with zigzag termination as compared to armchair termination. Transport will be favored along the armchair direction, which contains a continuous path of the lowest band gap atoms. A system with an electronic signature for metals has bands near the Fermi level that are localized to a new self-passivating 4x1 reconstruction of the zigzag edge and are flat (large effective mass), which suggest transport is not supported. The ability to tune phosphorene's band gap extends its applicability in optoelectronics.



VALENCE ELECTRON CONCENTRATION AS AN INDICATOR OF MECHANICAL PROPERTIES IN HARD COATINGS

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Transition metal nitrides are widely used as hard coatings in many applications such as diffusion barrier coatings and coatings for cutting tools. Conventionally used transition metal nitrides, in the rocksalt structure, are relatively brittle which has propelled the search for high toughness coatings. First principle calculations are employed to determine the mechanical properties of transition metal nitrides, carbides, carbonitrides and metallic alloy nitrides from group IV B to XII B to predict a unified indicator of mechanical properties - valence electron concentration. The pugh's ratio and poisson's ratio of the transition metal nitrides/carbides show a parabolic trend as a function of valence electron concentration with early transition metal nitrides/carbides showing brittleness and moving into the regime of ductility at a valence electron concentration between 5 and 5.5. The C_{44} of the transition metal nitrides and carbides show a similar trend varying from a positive C_{44} for nitrides and carbides and become mechanically unstable with a negative C_{44} , for a valence electron concentration of 5.5 and remain mechanically unstable until a valence electron concentration of 7.5 beyond which the C_{44} becomes positive again. To obtain the critical valence electron concentration at which the onset of mechanical instability begins, the C₄₄ of carbonitrides and metallic alloy nitrides from group IV B to VI B are calculated, which indicate a general parabolic descent trend steadily decreasing as the valence electron concentration moves from 4 to 5.5 with a critical valence electron concentration of 5.35 \pm 0.05 at which mechanical instability happens for binary and ternary systems. The elastic moduli and hardness of the transition metal carbonitrides and metallic alloy nitrides exhibits a trend similar to C_{44} with a parabolic decrease starting from a valence electron concentration of 4 to a critical valence electron concentration of 5.3 beyond which the elastic moduli and hardness are not determined due to a negative C44. These calculations provide significant insight into the mechanical properties of nitrides, carbides and carbonitrides of transition metals and valence electron concentration can be used as an indicator for alloy design to achieve the desired mechanical properties.

REVEALING THE GLOBAL CRYSTALLINE INTEGRITY OF WAFER SCALE GRAPHENE ON SiO₂/Si: AN AZIMUTHAL RHEED APPROACH

Zonghuan Lu¹, Xin Sun¹, Yu Xiang², Morris Washington^{1, 2}, Gwo-Ching Wang^{1, 2}, and Toh-Ming Lu^{1, 2}

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Single crystalline graphene is always desirable comparing to the polycrystalline graphene for electronic applications because the grain boundaries would undermine the extraordinary properties from a single crystal graphene. To date, chemical vapor deposition (CVD) is the most widely used method to produce high quality graphene at large scale with the aid of metal/non-metal catalysts. Among those catalysts, the Cu(111) surface has been a favorable choice due to its advantages in symmetry matching with graphene, effectiveness of catalyzing, low carbon solubility, and relative ease in preparing single-crystalline form. However, 60° in-plane rotational twinning in these Cu films have frequently encountered which caused graphene growth direction rotation of 30° across the Cu twin boundaries and also served as the carbon segregation and nucleation sites. Methods have been explored to remove the twinning in Cu films since it appears to be a concern for the growth of single-crystalline graphene. On the other hand, the symmetry of graphene is usually determined by low-energy electron diffraction (LEED) method when the graphene is on the conductive substrates. But LEED cannot handle graphene transferred to SiO₂/Si substrates due to the charging effect. While transmission electron microscopy can generate electron diffraction on post-transferred graphene, this method only reveals local information of the graphene film.

Herein, we employed a novel azimuthal reflection high-energy electron diffraction (RHEED) method to construct the reciprocal space mapping and determine the symmetry of wafer size graphene both pre- and post-transfer. In this work, single-crystalline Cu(111) films were prepared on sapphire(0001) and spinel(111) wafers with sputtering. Then, the graphene was epitaxially grown on single-crystalline Cu(111) films with a low pressure chemical vapor deposition. The reciprocal space mapping using azimuthal RHEED confirmed that the graphene grown on Cu(111) films was single-crystalline, in the form of either monolayer or multilayer structure. While the Cu(111) film grown on sapphire(0001) may occasionally consist of 60° in-plane rotational twinning, the reciprocal space mapping revealed that the in-plane orientation of graphene grown atop was not affected in this work. The proposed structural characterization of the post-transferred graphene sheets is an important step in the realization of the graphene as a platform to fabricate electronic and optoelectronic devices. The results will be presented in POSTER at the Chapter meeting.

Acknowledgements: This work is supported by the NYSTAR Focus Center at RPI, C130117 and by NSF Award under DMR 1305293.

OPTIMIZATION OF ANNEALING PARAMETERS FOR SILICON CARBIDE (SiC) NANOWIRE FABRICATION

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Silicon carbide (SiC) has been of great interest in semiconductor research due to its superior mechanical, optical, and electrical properties as well as both hemo- and biocompatibility. One-dimensional (1D) nanostructures (NSs), i.e. nanowires (NWs) and nanotubes (NTs), have been of interest as a result of their unique properties in comparison to their bulk counterparts. With the combination of excellent intrinsic properties and low dimensionality, SiC NWs have great potential in the fields of nanoelectronics and biotechnology, with applications such as biosensors and single photon emitters.

In most cases, a bottom-up approach is used to fabricate nanowires, which usually results in random orientation or size. To this end, the current investigators have been carrying out a study on catalyst-free self-aligned growth strategies for synthesizing ultrathin (<10 nm) polycrystalline SiC NWs that could be deterministically grown onto ordered arrays. This process includes a conformal CVD step to deposit SiC material, which is an amorphous in nature. However, a polycrystalline SiC is desired for application needs. In that regard, a post-deposition annealing is necessary.

To investigate the optimum conditions for annealing (temperature, duration, ambient), a systematic study has been carried out on thin films with 10, 20, 40 and 80nm thickness. Fourier transform infrared (FTIR) spectroscopy and atomic force microscopy (AFM) were used to assess the bonding configuration and surface morphology, which gives the optimum conditions to be 1100°C for 1 hour under forming gas (5% H₂ and 95% Ar) at atmospheric pressure.

VAN DER WAALS EPITAXY OF CdTe THIN FILM USING GRAPHENE AS BUFFER LAYER

<u>Dibyajyoti Mohanty</u>^{1,2}, Zonghuan Lu¹, Xin Sun¹, Shengbai Zhang³, Morris Washington³, Gwo-Ching Wang³, Toh-Ming Lu³ and Ishwara B. Bhat²

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Conventional heteroepitaxy requires well matched crystalline symmetry, lattice constant, and thermal expansion coefficient between the grown film and the substrate to produce a strain and defect free film. In order to overcome these constraints, van der Waals epitaxy (vdWE) technique has garnered significant interest in recent times. Unlike the epitaxy involving covalent bonds, the bonding between the overlayer and substrate is due to weak van der Waals forces instead of strong covalent bonds. As a result, not only the lattice matching requirement is relaxed, but also significantly fewer defects are present in the grown film, due to the dangling bond free interface. Traditionally, layered materials, owing to their existing van der Waals forces between layers, have been successfully used as substrates to grow other layered materials epitaxially, i.e., 2D on 2D. But the growth of 3D materials on layered materials has proved to be very challenging, with very few materials successfully grown. Among II-VI semiconductor materials, CdTe has invoked intense interest in recent years due to its applicability in photovoltaics, aerospace, and radiation detection related applications. Hence, it is highly desirable to produce low cost, epitaxially grown CdTe films on various substrates, which can be fulfilled by vdWE. We have studied 3D CdTe film on graphene buffer layer owing to graphene's inherent advantages such as high thermal stability, high mechanical strength, high decomposition temperature, ease of producing high guality graphene and transferring to any substrate of interest.

Single layer graphene deposited via chemical vapor deposition (CVD) process and then transferred to SiO₂ (285 nm)/Si (100) substrate was used as a buffer layer for the CdTe film growth. CdTe thin film (~3 μ m thick) was grown using metalorganic CVD (MOCVD) system. The XRD θ -2 θ scans indicated that the preferred out-of-plane orientation of the CdTe films is along the [111] direction. A 10-fold increase in the intensity and reduction in the FWHM of rocking curve of [111] peak was observed as compared to the reference sample without graphene buffer layer. It indicated an improvement in crystallinity of the CdTe film. We have conducted further experiments to compare the effect of monolayer and multilayer graphene as substrates for vdWE of CdTe. The results will be presented in details at the Chapter meeting.

Acknowledgements: This project is supported by the National Science Foundation Award # DMR-1305293.

[1] D. Mohanty et al., Applied Physics Letters 109 (14), 143109 (5 pp.) (2016).

NEAR INFRARED REFLECTORS AS SMART-GLASS FOR SOLAR PANELS AND BUILDINGS

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Solar panels are ensembles of solar cells that convert solar light into electricity. During the operation, the temperature of the solar panel can reach as much as 90°C. With each degree centigrade the conversion efficiency of the solar generator decreases by 0.46%. Thus, in a hot summer day, the power generated can decrease by almost 30%. Moreover, the amount of energy that is spent annually for thermal conditioning of the buildings in United States is of more than 400 billion kilowatt-hours, according to the U.S. Energy Information Administration and the windows are the surfaces that enable the wasteful heat exchange.

Therefore the development of a versatile and robust, metamaterial that can reflect near infrared heat radiation (NIR) in the range 0.7-2.5 μ m while transmitting more than 90% of the visible light intensity is highly desirable. Metal oxides can be used to manage the light reflectance over the long wavelength range. However, to obtain high reflectivity starting at shorter wavelengths, the doping concentration of the metal oxide has to be increased above the level of 1×10^{21} /cm³. At these concentrations the dopant incorporates not only substitutionally but large amounts will also be found interstitially. Interstitial dopants have been shown to produce carriers with heavier effective mass, decreased mobility, and deeper donor states that significantly decrease the transmittance. Ultimately substitutional dopants degrade the crystallinity of the host material, generating compensating defects that limit the achievable carrier density.

To circumvent the need for excessive dopant incorporation we propose a structure that alternates insulating and conducting layers of silicon dioxide (SiO₂) and silicon doped zinc oxide film (ZnO:Si). This structure is deposited by magnetron sputtering from Si and ZnO targets at low temperature. The structure uses the electric-field enhancement of carrier density to regulate the bandwidth of the NIR and in turn the amount of heat reflected. This is achieved through the formation of a quasi 2-dimensional electron gas in a thin layer at the dielectric/ZnO:Si interface. Overall the technology could find many applications, from the passive reduction of heating on solar cells, to the reduction of the cooling demands in buildings and cars, as well as in the field of photonics.

INVESTIGATING THE HETEROEPITAXY OF NATURALLY-FORMED ULTRATHIN V2O5 OXIDE PASSIVATION LAYER ON VO2/SAPPHIRE(001) FILM

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Vanadium oxide thin films exhibit properties which adjust in response to external stimuli such as temperature, photons, electric fields, and magnetic fields, making them ideal for applications including electronics, optical devices, and sensors. Vanadium dioxide (VO₂) in particular, undergoes a reversible semiconductor to metallic phase transition at 68 °C, which has attracted attention to its fundamental mechanism and potential uses. The epitaxial growth of heterostructures comprised of multiple single-phase V-oxides is challenging due to the possibility of multiple V valence states and non-stoichiometry in thin films. As with many other materials, the surfaces of lower-valency (0 to 4+) vanadium oxides form oxide passivation layers due to atmospheric exposure. The formation of ultrathin (< 5 nm) V₂O₅ layers on the surfaces of our tens-of-nm thick VO₂ films deposited by pulsed laser deposition on single crystal Al₂O₃(001) substrates is indicated by X-ray photoelectron spectroscopy and Raman spectroscopy. Furthermore, using our unique surface-sensitive reflection high energy electron diffraction (RHEED) pole figure analysis technique, we show the passivation layer forms heteroepitaxially and are able to simultaneously characterize the in-plane crystalline orientations of both the ultrathin V₂O₅ layer as well as the underlying VO₂ film. The observed heterostructure may be useful for a variety of electronic and optoelectronic applications. The RHEED pole figure characterization technique is general, and may be utilized to determine the epitaxial relationships of other ultrathin heterostructures.

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VAN DER WAALS EPITAXY OF SnS FILM ON SINGLE CRYSTAL GRAPHENE BUFFER LAYER ON AMORPHOUS SiO₂/Si

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Conventional hetero-epitaxy films are typically grown on lattice and symmetry matched single crystal substrates. We demonstrated the epitaxial growth of orthorhombic SnS films (~500 nm thick) on hexagonal monolayer graphene (grown in our laboratory) and transferred to the amorphous substrate SiO₂/Si. SnS has sparked interest in photovoltaic community due to its direct energy band gap of 1.3 eV, a high optical absorption coefficient of > 10^4 cm⁻¹ above the photon energy threshold, low cost, and nontoxicity. We used a method developed at Rensselaer to map the 2D reciprocal space structure of transferred graphene on SiO₂/Si using reflection high energy electron diffraction (RHEED) [1]. The mapping shows the transferred graphene is single crystal and has a six-fold symmetry. See the left figure below.

Using X-ray pole figure analysis, we examined the structure, quality and epitaxy relationship of the SnS film grown on the homemade graphene. The results showed that the SnS film has the (010) out-of-plane orientation and the {160} pole figure has 12 poles. See the right figure below. Comparing the structure of SnS film and the graphene substrate, we found that the SnS film follows the symmetry of graphene with two dominant orientation domains that are rotated 30° relative to each other. RHEED was also used to measure the near surface texture of SnS film. It shows the near surface texture is less perfect as compared with that of the entire film. This surface texture of a film will impact the growth and quality of film grown on top of it as well as the interface formed. Our result offers an alternative approach to grow a hetero-epitaxial film on an amorphous substrate through a single crystal graphene buffer layer. We also show that the texture near the surface of a film may differ from that in the entire film.

[1] Y. Xiang, .F-W. Guo, T.-M. Lu and G.-C. Wang, Nanotechnology 27, 485703 (2016).



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EFFECT OF DISPLACEMENT DAMAGE ON TANTALUM OXIDE RESISTIVE MEMORY DEVICES

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Radiation effects are a primary concern for electronic devices in aerospace or nuclear environments. Electronics developed for these applications must be designed for radiation tolerance. However, existing rad-hard design approaches cannot fully protect devices from radiation effects. For aerospace applications, the implementation of damage mitigation strategies is further limited by mass and power limitations. Resistive memory (RRAM) is an emerging memory technology that has strong potential as a radhard memory element, as well as considerable potential as an alternative memory technology. While transistors rely on the tight control of charge within the channel, RRAM depends on the movement of much larger ions through an insulator. Switching occurs based on the formation and partial destruction of a conductive filament of oxygen vacancies within an insulating oxide. Since the filament is composed of oxygen vacancies, a sudden increase in electrons and holes due to radiation is very unlikely to affect the filament. High mass ionic radiation can affect the filament through displacement damage, generating oxygen vacancies and oxygen interstitials within an oxide. Changes in TaO_x-based device behavior due to radiation have been observed at 10¹⁹ radiationgenerated oxygen vacancies per cm³, as calculated by Stopping Range of lons in Matter (SRIM).

We present a study of radiation-induced displacement damage in tantalum oxidebased RRAM. Devices were irradiated with 170 keV Ar⁺ ions, to fluences expected to disrupt the resistance states of the devices. Beam energy was chosen to minimize ionization damage as calculated in SRIM, enabling study of displacement damage effects. Fluences were chosen to deliver 10²⁰ or 10²¹ vacancies per cm³. The lower fluence was expected to have some effect on devices left in the high resistance state (HRS), while the higher fluence was expected to have a large effect. One device irradiated in HRS at the lower fluence switched to low resistance state (LRS). At the higher fluence, more than half of devices in HRS switched to LRS. It was expected that switching the devices would enable many of the generated oxygen vacancies to recombine. Switching of the irradiated devices quickly mitigated most of the resistance shift, indicating that device switching likely does accelerate vacancy recombination.

CHARACTERIZATION OF THE METALLIC PROPERTY OF VANADIUM DISULFIDE (VS $_2$)

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Ultrathin films of layered transition metal dichalcogenides (TMDCs) have proven to be interesting materials due to their similarities to graphene, such as the deviation from its bulk properties when reaching two-dimension. Among TMDCs, vanadium disulfide (VS₂) has shown its unique properties related to applications of super-capacitors, moisture sensors, and electrochemical catalyst [1]. However, the research is still limited due to the challenge in fabricating high-quality ultrathin VS₂ films. Chemical vapor deposition (CVD) appears to be one of the promising methods to produce ultrathin VS₂ flakes of lateral sizes of tens of microns [1]. Temperature dependent resistivity measurements by Yuan's et al. confirmed that a ~40 nm thick VS₂ flake show metallic behavior [1]. In these measurements, the electrical contacts were fabricated on top of a VS₂ flake using electron beam lithography. At Rensselaer the single crystal VS₂ flakes with a lateral size ranging from tens to 100 µm (figure1), and a thickness below 40 nm has been successfully synthesized for ten micron sized flakes by using the CVD technique. In this project, we propose to mechanically position the ultrathin flake on top of prefabricated electrical contacts. This alternative way can avoid the direct exposure of VS₂ to photoresist and solvents during the probes' fabrication process. We have successfully used the ex situ lift out micromanipulator to maneuver a few micron sized VS₂ flakes grown on Mica or SiO₂ substrates to our desired locations with controlled precision (figure 2 inset). The quantitative analysis from energy-dispersive X-ray spectroscopy (EDS) indicates the atomic ratio of vanadium to sulfur is close to 1:2 (figure 2). Our next step is to position a VS₂ flake on top of four electrical contacts, then perform temperature dependent resistivity measurements. By comparing our result to the literature [1], we aim to verify the metallic property of our VS₂ as well as the validity of our method to characterize the electrical transport properties of VS₂.

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[1] Jiangtan Yuan, et al., Facile Synthesis of Single Crystal Vanadium Disulfide Nanosheets by Chemical Vapor Deposition for Efficient Hydrogen Evolution Reaction, Adv. Mater. 27, 5605 (2015).



Figure 1: Optical image of VS₂ flakes grown by CVD at Rensselaer.

Figure 2: Energy-dispersive X-ray spectroscopy spectrum showing the atomic ratio of V to S is close to 1:2. Inset: Scanning electron microscope image of a few micron sized VS_2 flake.

Poster presentation

CLEANROOM GLOVES CHARACTERIZATION – A STUDY

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Gloves are typically use as consumables in a Cleanroom and Laboratory environment. Nitrile has been the preferred choice, due to its comfort and reliable nature, for the past decade. It provides superior barrier protection, minimizes allergic reactions and has good electrostatic discharge properties. This study investigates the cleanliness of the nitrile gloves using multiple techniques. How clean is the nitrile glove when it first arrives from the manufacturer? If there are contaminants on the glove, can they transfer during usage? Can we minimize the contaminants? We did a series of evaluation and testing on two different vendor's nitrile gloves. Particle Characterization was done by SEM/EDX techniques. A method was developed to determine the number of particles before and after rinsing in water using Liquid particle counting. Residues caused by gloved fingerprints on a clean Si wafer surface were tested using TOF-SIMS. Both set of gloves show metallic contaminations which can transfer to other surfaces (e.g. tool components, production parts, cleanroom apparel, etc). Cleaning of unused gloves helps to reduce particles.

VAN DER WAALS HETEROSTRUCTURE OF CdS THIN FILMS ON GRAPHENE

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Van der Waals epitaxy (vdWE) is a concept of locking up substrates and overlayers through the van der Waals force. In contrast to chemical epitaxy where a small latticemismatch is often an important requirement to grow quality overlayers, vdWE exempts this requirement since no chemical bonding forms at the interface in vdWE. The level of interest in vdWE has been growing in the past years owing to the rapid development of two-dimensional (2D) materials which naturally fit the regime of vdWE. vdWE systems involving 2D materials consist of three subgroups, namely, 2D-3D, 2D-2D, and 3D-2D. There have been numerous studies of 2D-3D and 2D-2D vdWE. However, reports on 3D-2D vdWE are fewer. In particular, vdWE of 3D materials on graphene has been shown challenging. Planar films, compared to clusters, are even more challenging to epitaxially grow on graphene, because a typical 3D material would not "wet" the graphene surface.

CdS is a technologically important semiconductor with a host of applications, including photovoltaics, light emitting diode, photodetector, laser, and anti-Stokes cooling. Given its extraordinary electronic properties, optical transparency, and transferability to arbitrary substrates, graphene is considered to be an attractive choice as the electrode material for CdS-based optoelectronic devices such as CdS/CdTe thin film solar cells. Currently, transparent conductive oxide (TCO) is in place for this role, but semiconductors cannot be grown in single-crystalline form on TCO. Thus, it would be highly desirable if CdS thin film epitaxy can be achieved on graphene that buffers TCO.

In this work, we investigate vdWE of CdS thin films on both single-crystalline graphene) graphene/Cu(111)/spinel(111) (pre-transferred and single-crystalline graphene/SiO₂/Si (post-transferred graphene) substrates with thermal evaporation. X-ray and electron backscatter diffraction pole figures reveal that the CdS films are a Wurtzite structure with a weak epitaxy on graphene and accompanied with a fiber texture background. The epitaxial alignment between CdS and graphene is observed to be an unusual non-parallel epitaxial relationship with a 30° rotation between the unit vectors of CdS and graphene. A geometrical model based on the minimization of superlattice area mismatch is employed to calculate possible interface lattice arrangement. It is found that the 30° rotation between CdS and graphene is indeed the most probable interface epitaxial lattice alignment. The vdWE of CdS on graphene, transferrable to arbitrary substrates, may represent a step forward for the growth of guality CdS thin films on arbitrary substrates through a graphene buffer.

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TRANSFER MOLDING FOR MESOSCALE REFRACTIVE INDEX CONTROL

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Residual-layer-free transfer molding offers a low-cost approach to nanofabrication of isolated structures, useful in applications such as printed electronics and photonics. Discontinuous dewetting enables residual-free-filling of micro-channels combined with dewetting of the macroscopic coating meniscus. For a blade meniscus coating process, a regime for discontinuous dewetting is proposed by combining both macro- and micro-scale wetting considerations. Patterns comprised of parallel channels showed vastly different meniscus morphologies based on the azimuthal angle of the stamp, suggesting a mechanism for 1-D discontinuous dewetting that differs from the qualitative picture often presented in the literature. By tuning ink viscosity, stamp surface energy and blade velocity, the critical dewetting velocity of the meniscus was quantified. Residual-layer-free filling and transfer are demonstrated with high resolution (300 nm) across relatively large areas (>1 cm²).

Development and TCAD Simulations of Ge p-i-n Infrared Detectors

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Germanium (Ge) on silicon (Si) offers a low-cost alternative to conventional infrared detector materials such as InGaAs, InSb and HgCdTe in order to develop near-infrared (NIR) photodetector devices that do not require cooling and can operate with a relatively low dark current. As a result of tensile strain incorporated into the Ge film, the bandgap of the Ge is modulated and the photodetector's absorption range can be increased to even longer wavelengths. We have used high throughput, large area complementary metal-oxide-semiconductor (CMOS) processes in order to fabricate Ge based p-i-n NIR photodetector devices on 300 mm Si wafers. P-i-n junctions offer many benefits such as a strong built-in electric field (~several kV/cm) which can overcome recombination losses, and the ability to tune the width of the depletion region. The Ge is deposited in a two-step process to reduce the dislocation density which could form recombination centers and contribute to a higher dark current. Characterization, including TEM and SIMS, has been done to ensure a quality, crystalline film. We have also performed electrical testing of the device. The device exhibited strong diode behavior as well as an exceptionally low dark current of ~1.35 nA. Simulations using Sentaurus TCAD are underway in order to find the parameters for optimal device performance.