PCSI
Room Keahou I - Session PCSI1-MoM1

Characterization of Interfaces and Devices (Transport, Optical, & Electronic)

Moderator: Roman Engel-Herbert, Paul-Drude Institute for Solid State Electronics, Germany

8:30am **PCSI1-MoM1-1 Atomic Scale Insights into Layered 2D Materials Epitaxy, Dopants and Defects**, ***Jamie Warner***, The University of Texas at Austin **INVITED**

Layered 2D Materials in the monolayer limit are primarily surfaces and interface with other materials through van der Waals interactions. However, the presence of defects creates dangling bonds that act as binding sites and disrupt the periodic van der Waals bonding. Understanding the interfacial coupling between different 2D monolayers and with other atoms, molecules and materials at the atomic scale is essential for building accurate models, and transmission electron microscopy is a leading approach for studying atomic scale behavior. Here, aberration corrected scanning transmission electron microscopy, combined with electron energy loss spectroscopy is used to extract accurate insights into atoms and their local bonding in 2D materials and how epitaxy arises at the interfaces. This will include graphene, hBN and transition metal dichalcogenides of mixed form, including MoS2, WS2, SnS2, PtSe2, PdSe2 and more. Insights into the epitaxy in twisted Moire systems of 2D will be shown, and how 4D-STEM, figure 1, can be used to see structural insights beyond conventional imaging such as electric field mapping around single dislocations [1], figure 2. The atomic structure of several dopant atoms at the interface and the role of surface carbon adsorbates on the adatom adsorption and migration will be presented. These results will provide detailed information about how individual atoms behave on 2D surfaces that are suspended and under in-situ heating up to 1000^{o}C.

9:10am **PCSI1-MoM1-9 Beyond Chemical Composition: How Surface Science Can Measure Electronic Properties**, *James Johns,* ***Sarah Zaccarine***, *Jennifer Mann, Kateryna Artyushkova,* Physical Electronics

X-ray photoelectron spectroscopy (XPS) is a widely used technique to analyze surface composition and chemistry. Often, scientists and engineers aiming to optimize material performance in a device require complementary information about the material's optical and electronic properties. This combined information is necessary in fields such as semiconductors, photovoltaics, (opto)electronics, batteries, and other chemical redox applications.

Fortunately, modern XPS spectrometers offer additional techniques to study the behavior of electrons in a system in addition to the chemical makeup of atoms and molecules in the surface. Reflection electron energy loss spectroscopy (REELS) can be used for optical band gap measurements as well as hydrogen content and carbon hybridization, additional chemical information beyond XPS. Ultraviolet photoelectron spectroscopy (UPS) is a similar method to XPS but with lower-energy UV photons instead of X-rays and higher spectral resolution, illuminating finer details of the valence band structure including work function and ionization potential. Inverse photoemission spectroscopy (IPES), as the name implies, uses the opposite process of XPS and UPS to probe the conduction band of metals and other conductive materials for insight into unoccupied band structure and measuring the electron affinity. Low-energy IPES (LEIPS) is uniquely suited to studying electronic structure of e-beam-sensitive organics that can be damaged by the traditional IPES method [1]. Combined, UPS and IPES/LEIPS can be used to calculate the electronic band gap for conductive materials, an invaluable property for studying charge transfer across an electrochemical interface.

This presentation will discuss the unique information that each of these techniques yields on electronic states in a surface. Guidance will also be shared on choosing an appropriate technique for a given analytical question, how to prepare and mount samples appropriately for the various analyses, and common pitfalls to avoid in data acquisition and interpretation.

[1] Yoshida, H. Chem. Phys. Lett. **539–540**, 180-185 (2012).

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9:15am **PCSI1-MoM1-10 Enhancing Interface and Retention Characteristics in NAND Flash Memory by Increasing Poly-Si Thickness to Prevent Pin-Hole Formation**, ***Chansung PARK***, *ByoungDeog Choi,* Sungkyunkwan University, Korea

In the fabrication of NAND Flash memory cells, the quality of the tunneling oxide (DTOX) layer is crucial for ensuring reliable operation and data retention. This study focuses on the impact of increasing the thickness of the polysilicon (Poly-Si) layer deposited on DTOX following channel hole etching. After tunneling oxide deposition, subsequent processing steps can introduce plasma damage and hydrofluoric acid (HF) damage, leading to the formation of pin-holes at the DTOX interface. These pin-holes adversely affect interface characteristics and compromise data retention. By optimizing the Poly-Si thickness, we aim to mitigate pin-hole formation, thereby enhancing the interface integrity. Our experimental results demonstrate that a thicker Poly-Si layer effectively protects the DTOX from plasma and HF damage, resulting in significant improvements in both the interface properties and data retention performance. This approach not only provides insights into the processing challenges faced in NAND Flash fabrication but also highlights the importance of interface engineering in advancing memory device reliability.

9:20am **PCSI1-MoM1-11 Relation Ship between Defect Density and Photoreflectance Spectroscopy for $InAs_xP_{1-x}$ Metamorphic Buffer Layer**, *Jong Su Kim,* ***Gyoung Du Park***, *Geun Hyeong Kim, Taein Kang,* Yeungnam University, Republic of Korea*; Sang Jun Lee, Dong Wan Kim,* Korea Research Instutue of Standards and Science (KRISS), Republic of Korea

In recent decades, $InAs_xP_{1-x}$ metamorphic buffer layer have applicated in advancing infrared photodetectors, chemical gas sensors, and optical communication devices. To improve the devices performance utilizing metamorphic buffer layer, it is crucial to reduce defect density by growing with graded composition ratios. Therefore, we prepared three samples with different $InAs_xP_{1-x}$ (x=0.7, 0.55, 0.5) compositions to examine the differences in defect density based on composition. Afterward, we investigated how these density differences impacted the PR results, exploring the potential of using photoreflectance (PR) measurements to infer defect densities. First, to determine the dislocation density of each sample, X-ray diffraction (XRD) measurements were conducted, resulting in values of 1.32 x10^7, 5.37 x10^6, and 1.12 x10^7 for the x=0.7, 0.55, and 0.5 samples, respectively, confirming that the x=0.55 sample had the lowest defect density. Following that, the internal electric field (*F*) was calculated from the Franz-Keldysh oscillation (FKO) signals obtained through the PR signal. The calculated *F* at the main peaks were 162, 84, and 160 *kV/cm* for the x=0.7, 0.55, and 0.5 samples, respectively. For the x=0.55 sample, the *F* was approximately 80 *kV/cm* lower. While this result could be attributed to differences in the built-in potential caused by composition variations, the dramatic difference is not observed in the x=0.7 and x=0.5 samples. Therefore, the 80 *kV/cm* difference cannot be fully explained by composition-related built-in potential alone. In General, lower defect density in a semiconductor reduces the number of photo-generated carriers trapped by defect states, enhancing the field screening effect and resulting in a lower calculated *F*, as indicated by the FKO signal. Additionally, we performed PR measurement as a function of modulation frequency to determine the time constant to verify the process of photogenerated carriers being trapped at defect states. The results showed that the x=0.7, 0.55, and 0.5 samples exhibited time constants of 54.4, 43.9, and 51.5 *us*, respectively, with the x=0.55 sample having the lowest time constant. These results are due to the lower defect density in the x=0.55 sample, which reducing the probability of photo-generated carriers being trapped at defect states during transport. In conclusion, we proposed that PR spectroscopy, shows potential as a new method for investigating defect-related properties in metamorphic buffer layer structures.

9:25am **PCSI1-MoM1-12 UPGRADED: Imaging Light-Matter Interactions using Low Kinetic Energy Photoelectrons**, *Andrew Kim, Alex Boehm, Morgann Berg,* ***Taisuke Ohta***, *Chloe Doiron,* Sandia National Laboratories*; Fernando Vega,* Purdue University*; Jaeyeon Yu, Joseph Klesko, Sylvain Gennaro,* Sandia National Laboratories*; Fangze Liu,* los Alamos National Laboratory*; Sean Smith, Guild Copeland,* Sandia National Laboratories*; Calvin Chan,* University of Colorado at Boulder*; Aditya Mohite,* Rice University*; Alexander Cerjan,* Sandia National Laboratories*; Thomas Beechem,* Purdue University*; Michael Sinclair, Igal Brener, Raktim Sarma,* Sandia National Laboratories

In the photoemission process, the electromagnetic fields propagating within the material excite electrons above the vacuum level, with higher field intensity resulting in a greater number of photoemitted electrons.

Photoelectron emission microscope (PEEM) directs the emitted photoelectrons onto an electron detector via electron optics that preserve their spatial origin. By extension, the spatial distribution of the electromagnetic field in engineered nanostructures, such as metasurfaces and photonic crystals, can be decoded from the photoelectron images.

In this talk, we will present results from three optical systems investigated using PEEM across a wide optical spectrum range. Using ultraviolet excitation, we examined Fabry-Perot resonances in thin film cavities of HfO_2 and SiO_2. The ultraviolet light is confined in oxides due to their higher refractive indices than that of the Si substrate. We use the cavity resonances to visualize the nanometer-scale inclusions embedded in the oxides using PEEM [1]. In the visible range, we examined dielectric metasurfaces of TiO_2 rods (i.e., meta-atoms) arranged in a square lattice. By comparing photoelectron images to finite-difference time-domain simulations, we determined the inelastic mean free path (IMFP) of the very low-energy (<1 eV) electrons to be ~35 nm. Because this IMFP is comparable to the height of the meta-atoms, the result highlights the sensitivity of photoelectron imaging to optical resonances supported within the meta-atom volume [2]. Extending to the near-infrared wavelength, we showed the polarization-dependent variation of the spectra of broken symmetry resonator metasurfaces. This work took advantage of potassium deposition on the surface to reduce work function, which enabled two-photon photoemission using near-infrared light [3]. In all three systems, we show exemplars where the real-space near-field variations are intertwined with their spectroscopic signatures. These results demonstrate the applicability of photoelectron imaging with sub-optical wavelength resolution to examine light-matter interactions in volume-type photonic resonances supported by dielectric nanophotonic structures.

[1] M. Berg, F. Liu, S. Smith, R. G. Copeland, C. K. Chan, A. D. Mohite, T. E. Beechem, T. Ohta, Phys. Rev. Applied, **12**, 064064 (2019).

[2] A. R. Kim, C. F. Doiron, F. J. Vega, J. Yu, A. M. Boehm, J. P. Klesko, I. Brener, R. Sarma, A. Cerjan, T. Ohta, in preparation (2024).

[3] A. M. Boehm, S. D. Gennaro, C. F. Doiron, M. B. Sinclair, T. E. Beechem, R. Sarma, T. Ohta, Near-field Imaging of Optical Resonances in Silicon Metasurfaces Using Photoelectron Microscopy, APL Photonics, **9**, 066103 (2024).

9:45am **PCSI1-MoM1-16 Examining Radiation Effects on the Electronic Structure and Defect Density of 1L WS2 through in-situ Photoemission Spectroscopy**, ***Christopher Smyth***, *Alex Boehm,* Sandia National Laboratories*; Kory Burns,* University of Virginia*; Andrew Kim, Taisuke Ohta,* Sandia National Laboratories

Two-dimensional (2D) transition metal dichalcogenides (TMDs) exhibit a unique combination of high radiation tolerance and promising computing performance in an atomically thin profile. However, the relationship between ion irradiation, defect density, and electronic structure in TMDs has not been identified, and must be understood to characterize radiation resilience. Heavy ion fluences of $<10^{12}$ cm^{-2} degrade TMD device performance, but are currently untraceable by conventional TMD characterization techniques. Hence, the relationship between radiation-induced defect density and carrier concentration in monolayer (1L) transition metal sulfides (TMS) remains unresolved. Some reports indicate ion irradiation induces hole doping in TMS, whereas theory predicts electron doping by sulfur vacancies, which are the most abundant defect formed in TMS under ion irradiation.

In this talk, we irradiate suspended 1L WS_2 films with 5 MeV Fe^{2+} ions at fluences of 10^{11}-10^{13} cm^{-2} to controllably introduce defects, and examine the valence band density of states (DOS) using photoemission spectroscopy. Photoemission spectra (PES) show the highest occupied valence band DOS at the Γ-point in the Brillouin zone shift towards the vacuum level and Γ-point peak width increases up to an ion fluence of 10^{13} cm^{-2}. These spectral modifications substantiate a reduced band gap and excited photo-hole lifetime by enhanced screening with increased defect density. By calculating the defect density as a function of ion fluence using the Shockley-Read-Hall recombination model, we demonstrate that the PES exhibits an unprecedented sensitivity to defect concentrations on the order of 10^{12} cm^{-2} generated at an ion fluence of 10^{11} cm^{-2}. We further verify ion beam-induced defect densities using scanning transmission electron microscopy. Additional ion irradiations up to 10^{13} ions cm^{-2} cause electron doping as predicted by theory, but we detect hole doping after ion irradiation beyond the 10^{13} cm^{-2} fluence. This study highlights the high sensitivity of the Γ-point valence band PES to radiation-induced changes in defect density, band gap, and excited photo-hole state behavior in 1L WS_2 down to ion fluences of 10^{11} cm^{-2}.

This work was supported by a LDRD program at SNL. A.R.K. acknowledges support from the U.S. DOE SC, Division of MSE. SNL is a multimission laboratory managed and operated by NTESS, LLC, a subsidiary of Honeywell International, Inc., for the NNSA under contract DE-NA-0003525. The views expressed in the correspondence do not necessarily represent the views of the U.S. DOE or the U.S. Government. This work was performed, in part, at CINT, a User Facility operated for the U.S. DOE SC.

9:50am **PCSI1-MoM1-17 Scalable Synthesis of One-Dimensional Quantum Matter**, ***Ruhin Chowdhury***, *Emma Renteria,* The University of New Mexico*; Sadhvikas Addamane,* Sandia National Laboratories, USA*; Darryl Shima, Divya Prakash, Jordan Neely,* University of New Mexico*; Francesca Cavallo,* The University of New Mexico

We present our recent efforts in the area of controlled synthesis of screw dislocations. Dislocations in semiconductors and other materials are generally considered detrimental in that they create scattering centers that lower carrier mobility, act as non-radiative carrier recombination centers, and induce growth instability of coherent thin films. Therefore, past research efforts have focused on hindering the formation of these line defects or annihilating them. Recent theoretical studies have demonstrated the prospect of repurposing screw dislocations as one-dimensional quantum matter [1,2], with potential applications in quantum computation and spintronics. These findings motivated our research on synthesis protocols of screw dislocations to achieve predictive control of their spacing, arrangement, and width. Specifically, we investigated and established approaches to fabricate SDs in single-crystalline and widely used semiconductors, such as Si, GaAs, and SiC. The semiconductors are in nanomembrane (NM) form or sheets with nanoscale thickness and a lateral size-to-thickness ratio of at least 10^2. Our approach to controlled synthesis of SDs relies on overlaying two arrays of pixelated NMs of the same material at a non-zero twist angle or twisted bicrystals (TBiCs). Through this process, we create an array of disregistries at the interface that will serve as seeds for the growth of SDs. Pixelated NMs are obtained by top-down processing multilayered structures such as epitaxially grown GaAs thin films on AlGaAs sacrificial layers-coated GaAs substrates or SiC on insulator wafers. NMs provide more uniform interfacial bonding than their bulk counterpart and expand the palette of SDs hosts to include epitaxially grown ternary and quaternary alloys. High-temperature furnace annealing of TBiCs fosters the propagation of SDs from the interfacial seeds across the thickness of the NMs. We characterize the spatial distribution of SDs in NMs by plan-view transmission electron microscopy under a weak-beam condition. The spacing between SDs is correlated to theoretically calculated values using the measured twist angle between the NMs. The twist angle is obtained by selected area electron diffraction (SAED) patterns acquired from the TBiC.

[1]L. Hu, H. Huang, Z. Wang, W. Jiang, X. Ni, Y. Zhou, V. Zielasek, M. G. Lagally, B. Huang and F. Liu, “Ubiquitous Spin-Orbit Coupling in a Screw Dislocation with High Spin Coherency”, Phys. Rev. Lett, 121, 066401 (2018).

[2]Y. Ran, Y. Zhang, and A. Vishwanath, “One-Dimensional Topologically Protected Modes in Topological Insulators with Lattice Dislocations”, Nat. Phys. 5, 298 (2009).

9:55am **PCSI1-MoM1-18 Current Characteristics Depending on the Doping Concentration of the Barrier in the GaSb Based Unipolar Detector**, *Jong Su Kim,* ***Jong Hun Lee****, Geun Hyeong Kim, Tae In Kang,* Yeungnam University, Republic of Korea*; Sang Jun Lee, Dong Wan Kim,* Korea Research Instutue of Standards and Science (KRISS), Republic of Korea

The nBn detector consists of an n-type contact layer, a unipolar barrier that prevents electron transport, and an n-type absorber. Compared to the p-i-n structure, the nBn detector offers advantages such as low dark current and high-temperature operation. Due to these characteristic, nBn detector has been actively researched over the past years,particularly regarding the barrier doping concentration.

In the nBn detector, the dark current is known to decrease as the increase of the barrier donor doping concentration [1]. However, Zhuhas reported that Te doping in AlGaSb occur deep trap in 1988 [2]. These deep traps occur the leakage current such as trap assist tunneling (TAT) in the nBn detector. In addition, because the effect of barrier doping concentration on photocurrent has not been further investigated yet, to investigate the current characteristics of GaSb-based nBn detector depending on barrier doping concentration I-V measurements were performed. Dark current density at 80 K, 0.2 V were measured 0.009 A/cm^2 (undoped), 0.013 A/cm^2 ($2x10^{15}cm^{-3}$), 0.108 A/cm^2 ($2x10^{16}cm^{-3}$). Due to the negligible generation-recombination (G-R) current at low temperature,these results indicate the increase of TAT current due to rise of Te-related deep trap concentration.

The exponent proportion of photocurrent to excitation light power at 300 K, 1 V were0.43 (undoped), 0.63 ($2x10^{15}cm^{-3}$), and 1.21 ($2x10^{16}cm^{-3}$).The exponent of lower than unity indicate that the carrier loss due to the recombination[3]. The reduce of carrier loss as the increase doping concentration was attributed that carrier injection due to the TAT and more efficiently carrier extraction due to higher carrier velocity. In conclusion, this study shows the importance of appropriate barrier doping concentration when the design of nBn detector through the rise of dark current and reduce of photocurrent loss as the increase of barrier doping concentration.

10:00am **PCSI1-MoM1-19 MBE-Grown Germanium Quantum Well Planar Josephson Junction***, **Joshua Thompson**, Chomani Gaspe, Riis Card, Jason Dong, Kasra Sardashti,* Laboratory for Physical Sciences*; Shiva Davari, Hugh Churchill,* University of Arkansas*; Kyle Serniak, Thomas Hazard,* MIT Lincoln Laboratory*; Christopher Richardson,* Laboratory for Physical Sciences

At the heart of a transmon qubit is the Josephson junction (JJ) which is engineered to create the anharmonic energy spacing needed to individually populate the two lowest energy levels in the system. Transmon qubits can incorporate two such JJs in a SQUID arrangement to achieve flux tunning of the qubit but require on-chip, current carrying flux lines. This presentation will discuss the characterization of undoped germanium quantum wells (Ge-QW) in a SiGe heterostructure and the fabrication of planar JJs for future integration into voltage tunable transmon qubits.

Strained Ge-QWs host heavy holes with high mobility and low effective mass. When combined with highly transparent superconducting contacts, they create a promising platform for combining voltage-controlled semiconductor materials with high fidelity superconductor qubit circuitry. The Ge-QW with SiGe spacer material is grown using Molecular Beam Epitaxy (MBE) and has a carrier mobility greater than 60,000 cm^2/Vs with a hole density less than $1x10^{12}$ cm^{-2}. Using a series of lithography and etching techniques, 100-nm to 500-nm long JJs are formed on a 2.5 µm tall SiGe mesa that is necessary to isolate the lossy SiGe from the rest of the superconducting circuit. Device design, fabrication challenges, and preliminary junction performance will be shown

10:05am **PCSI1-MoM1-20 Neutron Reflectometry Studies of Interfacial Phenomena in Actinide and Actinide Related Thin Films***, Izabela Kruk, Peng Wang,* Los Alamos National Laboratory*; David D. Allred,* Brigham You*; Kirk D. Rector,* Los Alamos National Laboratory*; **Jaroslaw Majewski**,* Los Alamos National Laboratory, National Science Foundation

Studies of interfacial chemistry of actinides attract much attention due to interest in the power generation. In the power generation field, current research aims to reduce Pu and minor actinides in the spent light water reactor's fuel stockpiles. Therefore, considerable research efforts are underway to evaluate the suitability of Th as a nuclear fuel. Herein, in situ neutron reflectivity technology measures changes in the scattering length density (SLD) and thickness of a thorium, uranium, and cerium metal films in controlled environmental conditions: time-dependent exposition to oxygen and water vapors in various temperature regimes. Among other phenomena, our research uncovered non-stoichiometric thorium oxides, ThOx, preferentially generated between the metal and its thermodynamically favored dioxide layers. The near perfect stoichiometric lattice and relative low O solubility of ThO2 film limits the availability as well as diffusivity of O species interacting with ThO, and hence prevents or slows the successive further oxidation. These observations suggest that ThO has many advantages over ThO2 as a potential nuclear fuel such as good breeding performance, high thermal conductivity and density with good chemical and temperature stability. Our studies of interaction the Cerium thin films with water vapors revealed homogenous penetration of physisorbed water into the layers of various oxygen stoichiometry and its complete removal upon decreasing of the relative humidity.

Key Words: Actinides, Chemistry of Thin Metal Layers, Neutron Reflectometry, Nuclear Fuel.

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