PCSI
Room Redondo - Session PCSI-SuA
Novel Device Characterization

Moderator: Holger Eisele, Otto-von-Guericke-Universität

4:00pm **PCSI-SuA-1 Welcome and Opening Remarks*,***

4:05pm **PCSI-SuA-2 Electroemission Spectroscopy of GaN-Based Diodes – Revealing the Inner Working of LEDs and More!*, Jim Speck,*** University of California Santa Barbara **INVITED**

In this talk, we introduce the technique of electroemission spectroscopy (EES) and its application to GaN-based LEDs.The technique is based on electron emission from p-GaN surfaces that have been cessiated to realize negative electron affinity (NEA).For LEDs the p-GaN surface is exposed through open apertures in a grid metal contact.We have developed this technique to measure electron emission into vacuum that are the result of (i) three-body Auger nonradiative recombination (n2p process (assuming n ≈p, scaling as n3)), trap-assisted Auger recombination (TAAR, n2 process); and electron overflow.

In this talk we review the evolution of the EES technique as applied to LEDs and reference p-n and p-i-n diodes.We review four different techniques that have identified the first conduction band upper valley (UV1) at 0.9 eV above the CBM.We show evidence for the next upper valley (UV2) at 1.7 eV above the CBM.Additionally, we review systematic measurements to assure that the emitted electrons from the p-GaN surface are indeed a result of processes occurring at the internal diode junction.

Recently we have performed EES measurement on electrically driven InGaN/GaN commercial blue c-plane (peak wavelengths λ = 465 nm) light emitting diode (LED) with 60 nm of p-GaN on top of the active region (this is relatively thin p-GaN).The signal-to-noise ratio of semiconductor peaks is improved on the thin p-GaN LED due to reduced loss of electrons en route to emission into vacuum during transit through the thin p-GaN.This further proves that hot electrons are generated in the bulk region and not by light or other hot electron generation mechanisms at the surface.Using square root of the light output power as a proxy for the active region carrier density, n, the hot electron integrated peak intensity is shown to be proportional to n3 and, thus, is directly attributed to a 3-body Auger process.Since there are significant Auger recombination currents even at low injection current densities, it is expected that Auger recombination current will dominate over radiation recombination and Shockley–Read–Hall (SRH) currents at higher current densities.

4:45pm **PCSI-SuA-10 Characterization of Semiconductor Nanostructures using Ultra-high Resolution STEM-CL*, Gordon Schmidt,*** *J. Christen, F. Bertram,* Otto-von-Guericke-University Magdeburg, Germany **INVITED**

For a comprehensive understanding of complex semiconductor heterostructures and the physics of devices based on them, a systematic determination and correlation of the structural, chemical, electronic, and optical properties on a nanometer scale is essential. Luminescence techniques belong to the most sensitive, non-destructive methods of semiconductor research. The combination of luminescence spectroscopy – in particular at liquid He temperatures – with the high spatial resolution of a scanning transmission electron microscope (STEM) as realized by the technique of low temperature cathodoluminescence microscopy in a STEM (STEM-CL), provides a unique, extremely powerful tool for the optical nano-characterization of quantum structures.

Typical results, which will be presented, include the nm-scale analysis of group III-V semiconductor nanostructures visualizing the enormous capability of STEM-CL characterization.

The direct identification of the emission of a two-dimensional electron gas (2DEG) in a lateral GaN/AlN/AlGaN heterostructure field-effect transistor (HFET) will be shown.The characteristic emission of the 2DEG channel is observed on the low-energy side of the dominating donor-bound exciton luminescence. Beside this spectral fingerprint, the exact local origin of the 2DEG CL is verified to be close to the GaN/AlN interface. Due to the superposition of several possible recombination channels in the near-band-edge spectral region, this local verification is essential for the unambiguous identification of the 2DEG luminescence. The transport of the generated excess minority carriers (i.e. holes) into the 2DEG region leads to an intensity onset of the 2DEG emission already 60 nm below the GaN/AlN interface (already in the GaN drift region).

Single dot spectroscopy by means of low temperature STEM-CL provides a detailed insight into the energy structure of individual quantum dots (QDs) and directly correlates those properties with the real structure on a nanoscale. We characterize the vertical and lateral transfer of carriers within a 7-fold layer stack with high-density InP quantum dots grown via Stranski-Krastanov mode. We observe a characteristic change of the excitonic emission lines during scanning across an individual InP QD in a lateral CL linescan. This reveals the change of the numbers of excess carriers reaching the dot - i.e. altering the quantum dot population. The shift of emission energies visualize the renormalization of the ground-state energy of the single dot and the intensity ratio of the excitonic recombinations verifies this change in occupation.

5:25pm **PCSI-SuA-18 Optimizing Tof-SIMS Depth Profiles of Semiconducting Heterostructures*, Jan Tröger,*** University of Münster, Germany*; R. Kersting, B. Hagenhoff,* Tascon GmbH, Germany*; D. Bougeard,* University of Regensburg, Germany*; H. Riemann, N. Abrosimov,* Institute for Crystal Growth Berlin, Germany*; J. Klos, L. Schreiber,* RWTH Aachen University, Germany*; H. Bracht,* University of Münster, Germany

In order to meet the demand for increased performance with progressive miniaturization, microelectronic components are being developed into multilayer structures with increasing complexity. Since the material composition, the layer thickness and the diffusion behavior between the individual layers have a sensitive effect on both the performance and the service life of the components, such a development is only possible through analytical monitoring of the materials properties on an atomistic scale.

A suitable analytical method to investigate semiconductor multilayer structures is Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS). The particular strength of the method is the possibility to determine all elements including their isotopes. In addition, the information depth of only about 0.5 nm (< 3 monolayers) makes SIMS a very surface-sensitive tool. By sputtering it becomes possible to obtain the composition of materials in deeper layers.

In this presentation we focus on optimizing ToF-SIMS depth profiling of semiconductor heterostructures. As model system, we investigate while varying sputter parameters a state-of-the-art Molecular Beam Epitaxy (MBE) grown multilayer structure consisting of ultra-thin layers with 2 nm in thickness. We measure atomic concentration profiles and use an error function based description model to quantify layer thicknesses as well as interface sharpness. Using this approach the multilayer structure is well resolved. The optimized instrumental setting for high depth resolution in ToF-SIMS profiling is applied to analyze a MBE grown SiGe/^{28}Si/SiGe heterostructure. The strained and isotopically purified 28Si layer of this structure represents a Quantum Well that has been proven to be an excellent host for an electrostatically defined electron spin qubit [1].

[1] Struck, T.; Hollmann, A.; Schauer, F.; Fedorets, O.; Schmidbauer, A.; Sawano, K.; Riemann, H.; Abrosimov, N. V.; Cywiński, ; Bougeard, D.; Schreiber, L. R. Low-frequency spin qubit energy splitting noise in highly purified 28Si/SiGe. npj Quantum Information 2020, 6, 2056–6387.

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PCSI
Room Redondo - Session PCSI-SuE
Characterization Methods

Moderator: Chip Eddy, Jr., ONR Global

7:30pm **PCSI-SuE-1 Atomic Scale Structural Characterization of Material Surfaces and Interfaces via Atomic Electron Tomography*, Yongsoo Yang,*** Korea Advanced Institute of Science and Technology, Republic of Korea **INVITED**

A high degree of anisotropy and even completely new phenomena can be often found at the materials surface/interface systems, and their properties are governed by the 3D arrangement of individual atoms at the surface/interface. To achieve a proper understanding of structure-property relations at the interface, a precise determination of the 3D interface atomic structures and their dynamics is a definite prerequisite, which has been limited to lower-dimensional measurements or simulations. Traditional crystallography, which is reliant on periodicity, cannot determine their real structures because the periodic symmetry breaks down at the surface/interface. Without any prior assumption of underlying structure, atomic electron tomography (AET) is now able to locate the 3D coordinates of individual atoms and their dynamics with picometer precision and with elemental specificity. A variety of complex internal atomic structures can be measured with 3D atomic-level details; including grain boundaries, chemical order/disorder and phase boundaries [1]. Recently, combined with deep-learning based neural network, it now became possible to precisely measure the 3D surface/interface structure of nanomaterials with high precision, revealing surface-substrate boundary effect, coalescence dynamics, core-shell strain relation and surface catalytic activity at the atomic scale [2-4]. Understanding the atomic resolution structural properties and their dynamics at the nanomaterial interfaces together with the relationship between atomic structure and material properties will allow the rational design of novel materials with desired surface/interface properties at the atomic scale.

[1] Y. Yang et al., Nature 542, 75 (2017).

[2] J. Lee, C. Jeong and Y. Yang, Nat. Commun, 12, 1962 (2021).

[3] J. Lee, C. Jeong, G. Lee, S. Ryu and Y. Yang, Nano Lett. 22, 665 (2022).

[4] H. Jo et al., arXiv:2207.06677 (2022).

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8:10pm **PCSI-SuE-9 Understanding Interface Effects in Van der Waals Heterostructures with Neutron Reflectometry*, Alex Grutter,*** National Institute for Science and Technology (NIST) **INVITED**

Layered Van der Waals (VdW) systems are among the most exciting playgrounds in condensed matter physics and include topological insulators, Weyl and Dirac semimetals, and 2D magnetic systems. In particular, heterostructures incorporating different classes of topological or magnetic orders are promising platforms for next generation quantum and spintronic devices. However, these systems represent a difficult materials engineering challenge in which reactive, often easily oxidized, materials must coexist and interact across sharp interfaces while preserving the target properties. It is in this context that simultaneous magnetic and structural depth profiling with polarized neutron reflectometry (PNR) has drawn considerable interest. With sub-Ångstrom resolution, sensitivity to magnetic signals originating within a single atomic monolayer, and the ability to detect chemical changes with precision, PNR is a powerful and non-destructive tool for probing low-dimensional nanostructures.

In this talk, we will introduce the basic concept of neutron reflectometry and use a series of recent examples to explore the unique insights PNR provides into the chemical and magnetic properties of VdW interfaces. Specifically will show how PNR identifies changes in surface chemistry, low-dimensional magnetism, magnetic proximity effects, and other forms of magnetic interface coupling in systems such as perovskite membranes, $(Bi,Sb)_2Te_3$, $MnBi_2Te_4$, $CrTe_2$, and Cd_3As_2.[1-7] Special emphasis will be placed on multimodal characterization approaches combining PNR with X-ray scattering, spectroscopy, muon spin relaxation spectroscopy, and electron microscopy for an even more comprehensive picture of the interface. By decomposing the magnetic and electronic properties on a layer-by-layer and element-resolved basis, new quantum material systems may be robustly understood and designed. We will conclude with a discussion on the future of ultra-sensitive magnetic interface probes and the potential impact from highly multiplexing neutron instrumentation such as a CANDOR reflectometer currently being commissioned at NIST.

References:

1. C.-Y. Yang et al., Science Advances 6, eaaaz8463 (2020)
2. W. Yanez et al., Physical Review Applied 16, 054031 (2021)
3. N. Bhattacharjee et al., Adv. Materials 34, 2108790 (2022)
4. L. J. Riddiford et al., Phys. Rev. Lett. 128, 126802 (2022)
5. P. Deng et al., Nano Letters 22, 5735 (2022)
6. Q. Lu et al., ACS Nano 16, 7580 (2022)
7. P. Chen et al., Nat. Electronics *In Press* (2022)

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Room Redondo - Session PCSI-MoM1

2D and VdW Materials

Moderator: Anthony Rice, National Renewable Energy Laboratory

8:30am **PCSI-MoM1-1 Step-Edge Nucleation and Domain Orientation Control in Epitaxy of Transition Metal Dichalcogenides on Sapphire***, H. Zhu,* The Pennsylvania State University*; T. Choudhury,* The Pennsylvania State University, India*; N. Nayir,* The Pennsylvania State University, Turkey*; T. Mc Knight, N. Trainor, A. van Duin,* ***Joan Redwing,*** The Pennsylvania State University **INVITED**

Wafer-scale synthesis of semiconducting transition metal dichalcogenide (TMDs) monolayers is of significant interest for device applications to circumvent size limitations associated with the use of exfoliated flakes. Promising results have been demonstrated for epitaxial films deposited by vapor phase techniques such as CVD and MOCVD. However, the three-fold symmetry of TMDs such as MoS_2 and WSe_2, results in two energetically equivalent domain alignments, often referred to as 0°and 60° domains, when grown on flat high symmetry substrates such as c-plane sapphire. The oppositely oriented domains give rise to inversion domain boundaries (IDBs) upon coalescence which exhibit a metallic character and are generally undesirable. In this study, we demonstrate the epitaxial growth of unidirectional TMD monolayers on 2” diameter c-plane sapphire substrates with a significantly reduced density of inversion domains. Steps on the sapphire surface are shown to play a key role in TMD nucleation and impart a preferred orientation to the domains depending on the step edge structure and chemistry.

Metalorganic chemical vapor deposition (MOCVD) was used for the epitaxial growth of WSe_2 monolayers on c-plane sapphire, miscut ~0.2^{o} toward the m-axis, in a cold-wall horizontal quartz-tube reactor. A three-step nucleation-ripening-lateral growth process, carried out at temperatures ranging from 850^{o}C to 1000^{o}C, was used to achieve epitaxial films using $W(CO)_6$ and H_2Se as precursors in a H_2 carrier gas. Density functional theory calculations demonstrate that the extent of Se passivation of the sapphire surface and the presence of oxygen remnants near the step edge are critical factors in determining the location of TMD nucleation on the step edge and the subsequent domain orientation relative to the underlying sapphire. By changing the reactor pressure, which modifies the sapphire surface via changes in the chemical potential of H and Se, the site of WSe_2 nucleation can be modified which switches the preferred orientation of the domains. Fully coalesced TMD monolayers are obtained with a reduced density of inversion domain boundaries (<15% areal coverage).The results demonstrate the important role of step structure and chemistry in nucleation and epitaxial growth of TMD monolayers.

9:10am **PCSI-MoM1-9 Effects of Strain and Local Topography on Electromechanical Coupling in Monolayer Transition Metal Dichalcogenides***,* ***Claire Ganski****, A. De Palma, E. Yu,* The University of Texas at Austin

Two-dimensional transition metal dichalcogenides (2D TMDs) have been extensively studied in recent years due to their remarkable electronic, optical, and mechanical properties. Their ability to withstand high levels of strain without fracture makes 2D TMDs attractive candidate materials for devices such as quantum emitters and energy harvesters. However, the high sensitivity of 2D material properties to nanoscale morphology and strain can just as easily interfere with as aid in optimal device performance if not fully understood and accounted for. In this work, we use piezoresponse force microscopy (PFM) to demonstrate that nanobubbles present in exfoliated MoS_2 monolayers significantly alter the electromechanical behavior of these samples and exhibit strong out-of-plane PFM responses due to flexoelectricity. Small bubbles with diameters under 100 nm consistently exhibit enhanced piezoresponse compared to flat regions. Without filtering images for these ubiquitous features, effective piezoelectric coefficients based on PFM of exfoliated monolayer MoS_2 will be systematically overestimated. Large bubbles with diameters on the order of hundreds of nanometers present an even more remarkable pattern. Rather than increasing monotonically from perimeter to apex, the piezoresponse amplitude of large bubbles reaches its peak at the perimeter and subsequently decreases toward a local minimum at the bubble apex. This profile can be correlated with the curvature of the bubble topography, which is related to the local strain gradient. These correlations suggest a link between local electromechanical properties and strain gradients present in these regions. We argue that the large strain gradients at the bubble edges induce a local reduction in spatial symmetry, which produces out-of-plane polarizations via the flexoelectric effect. On subsequent characterization using PFM, these regions effectively behave not as a 2H MoS_2 monolayer, but as a low-symmetry material exhibiting out-of-plane piezoelectricity.

9:15am **PCSI-MoM1-10 Probing Edge State Conductance in Ultra-Thin Topological Insulator Films***, A. Leis,* ***Jonathan Karl Hofmann****, M. Schleenvoigt, K. Moors, H. Soltner, V. Cherepanov, P. Schüffelgen, G. Mussler, D. Grützmacher, B. Voigtländer, F. Lüpke, F. Tautz,* Forschungszentrum Juelich GmbH, Germany

Quantum spin Hall (QSH) insulators have unique electronic properties, comprising a band gap in their 2D interior and 1D spin-polarized edge states in which current flows ballistically. In scanning tunneling microscopy (STM), the edge states manifest themselves as an enhanced local density of states (LDOS). However, there is a significant research gap between the observation of edge states in nanoscale spectroscopy, and the detection of ballistic transport in edge channels which typically relies on transport experiments with microscale lithographic contacts. Here, few-layer films of the 3D topological insulator (BixSb1−x)2Te3 are studied [1], for which a topological transition to a 2D topological QSH insulator phase has been proposed. The samples were grown on silicon-on-insulator substrates by MBE [1]. After the growth, a vacuum transfer into the room temperature 4-tip STM was carried out. Indeed, an edge state in the LDOS is observed within the band gap. Yet, in nanoscale transport experiments with a four-tip STM, two-quintuple-layer (QL) films do not exhibit a ballistic conductance in the edge channels, as the measured 4-point resistance is fully in accord with finite element calculations using the measured terrace conductivities [2]. Thus, no QSH edge states are present at the 2 QL films. This demonstrates, that the detection of edge states in spectroscopy can be misleading with regard to the identification of a QSH phase. In contrast, nanoscale multi-tip transport experiments are a robust method for effectively pinpointing ballistic edge channels, as opposed to trivial edge states, in quantum materials.

[1] A. Leis et al., Adv. Quantum Technol. 4, 2100083 (2021)
[2] A. Leis et al., Adv. Quantum Technol. 5, 2200043 (2022)

9:20am **PCSI-MoM1-11 MBE Growth of Transition-Metal Dichalcogenides***,* ***Wojciech Pacuski,*** University of Warsaw, Poland **INVITED**

Monolayer transition-metal dichalcogenides (TMDs) are two-dimensional materials with exceptional optical properties such as high oscillator strength, valley-related excitonic physics, efficient photoluminescence, and several narrow excitonic resonances. Long time the above effects have been explored for structures produced by techniques involving mechanical exfoliation or post-growth transfer, and more recently, also encapsulation in hBN, inevitably inducing considerable large-scale inhomogeneity. On the other hand, techniques which are essentially free from this disadvantage, such as molecular beam epitaxy (MBE), have yielded only structures characterized by considerable spectral broadening, which hinders most of the interesting optical effects. In this talk, I will present the MBE-grown TMD ($MoSe_2$) exhibiting narrow and fully resolved spectral lines of neutral and charged exciton [1]. Moreover, our monolayers exhibit unprecedented high spatial homogeneity of optical properties, with variation of the exciton energy as small as 0.16 meV over a distance of tens of micrometers. Importantly, good optical properties are achieved for as-grown samples, without any post-growth exfoliation and encapsulation in hBN. Our best recipe for MBE growth includes an extremely slow growth rate, the annealing at very high temperatures, and the use of atomically flat hBN substrate in the form of flakes exfoliated from bulk. Moreover, comparable results we also obtained using an hBN buffer that we grow by MOCVD on 2” Al_2O_3 wafers [2]. Our optical characterization includes Raman scattering, second-harmonic generation, and low-temperature photoluminescencere. Thanks to sharp and intense exciton lines, we were able to perform also magneto-spectroscopy and time resolved spectroscopy [3], which reveal subtle differences between 2D epilayers and mechanically exfoliated materials. We compare structural and optical properties of $MoSe_2$ grown on hBN to properties of various TMDs ($MoTe_2$ [4,5], $NiTe_2$ [6], WSe_2, VSe_2) grown on various substrates (2D, 3D, polycrystalline). This reveals particularly high diffusion parameters of transition metals on hBN [5], the role of distribution of orientation of TMD grain domains, the tendency to merge grains, form bilayers and 1D or 3D structures.

[1] W. Pacuski et al., Nano Letters 20, 3058 (2020).

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PCSI
Room Redondo - Session PCSI-MoM2
Semiconductor Heterostructures/Nanostructures/Interfaces/Surfaces

Moderator: Norbert Esser, TU Berlin and Leibniz-Institut für Analytische Wissenschaten-ISAS-e.V.

10:40am **PCSI-MoM2-27 UPGRADED: Hydrogen Cleaning Induced Surface Modifications of GaAs(110)*, Dorothee Sophie Rosenzweig,*** Technische Universität Berlin, Germany*; M. Hansemann,* Paul Drude Institut Paul Drude Institut für Festkörperelektronik, Germany*; P. Ebert, M. Schnedler,* Peter Gruenberg Institut Forschungszentrum Juelich, Germany*; M. Daehne,* Technische Universität Berlin, Germany*; H. Eisele,* Otto-von-Guericke-Universität, Germany

Zincblende III/V nanowires typically exhibit non-polar (110) surfaces as side facets [1]. Since characterization is mostly performed in a different (UHV)-chamber than growth, such nanowires are commonly exposed to the atmosphere. For the nanoscopic analysis of such III/V nanowire (110) growth surfaces, hydrogen cleaning is a commonly used procedure to remove residual adsorbates, such as e.g., oxygen. While hydrogen cleaning is reported to be destruction free [2] and to achieve clean, atomically flat surfaces with well-defined electronic properties—as they are expected directly after growth—the actual processes and dynamics during cleaning are rarely examined. However, a detailed understanding of these issues is crucial for the interpretation of electronic surface properties, of the growth of nanowires, as well as the incorporationand distribution of dopant atoms.

Here, we investigate the modifications of *n*-type GaAs(110) surfaces as a model system upon controlled atomic hydrogen exposure at room temperature and under commonly used cleaning conditions at the atomic level. For depiction and measurement at the atomic scale, we used scanning tunneling microscopy and spectroscopy under UHV conditions. Using these methods, we study the geometric arrangement of the adsorbed atoms, the newly introduced defects, as well as additional electronic (defect) states and Fermi level pinning. First, we confirm the debuckling and roughening of the (110) surfaces by hydrogen adsorption at the atomic level. This was predicted by Ref. [3] from methods showing integral information without atomic resolution. We see both effects in images with atomic resolution: Hydrogen adsorption debuckles the surface while the roughening is in fact related to the formation of very specific defects derived from arsenic vacancies. Further, we link the structural changes to changes in electronic properties and confirm our STS results by tunnel current simulations. Second, the effects of hydrogen cleaning itself are shown in images with atomic resolution. Two effects are observed: The formation of native defects as well as the (re)creation of atomically flat surfaces. Again, electronic properties are evaluated from tunneling spectra and confirmed by tunnel current simulations. These findings lead to a comprehensive picture of the processes involved in the hydrogen cleaning procedure of III/V semiconductor surfaces.

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[1] Motohisa et al., Phys. E 23, 298 (2004)

[2] Webb et al., Nano Lett. 15, 4865-4875 (2015)

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11:00am **PCSI-MoM2-31 Surface Work Function Engineering of Diamond-like Carbon Through Spatial Selective Gallium Implantation*, Jiayun Liang,*** *Z. Al Balushi,* University of California at Berkeley

Bottom-up synthesis of materials with high spatial selectivity has long been a goal of nanotechnology. However, to obtain spatially selective nucleation and exact control over the size and shape of the domain during the synthesis, spatial modification of the surface work function landscape of substrate must be realized at the growth temperature. Herein, a spatially controllable surface work function landscape of diamond-like carbon (DLC) thin layer was achieved through spatially selective implantation of gallium into DLC using focused ion beam (FIB). Under various FIB conditions, two typical features with a size of 5 µm and 5 µm were obtained: “valley” with a step height of 3.5 nm, and “hill” with a step height of 4 nm. Gallium precipitated after one-hour-long in-situ annealing process at 500°C or 300°C in a high-vacuum environment (10^{-9}torr). At 500°C, the surface work function of valley feature was 51 meV higher than that of the unimplanted region, while the surface work function of hill feature was 16.8 meV lower than that of the unimplanted region. However, as the annealing temperature dropped to 300°C, the surface work functions for hill and valley featuressurface were 51.8 meV and 88 meV lower than those of the unimplanted region, respectively. Both gallium precipitation and change of DLC properties contributed to the shift in surface work function. Therefore, a spatially controllable surface work function landscape can be realized by carefully tuning the annealing conditions and spatial arrangement of hill and valley features, facilitating the selective area growth of materials in various nanofabrication processes.

11:05am **PCSI-MoM2-32 Nanotrench Formation along Step Edges of Vicinal Si(111) Surfaces by Wet-chemical Treatments*, Kenta Arima,*** *Z. Ma, T. Takeuchi, R. Hashimoto, R. Sun, K. Yamamura,* Osaka University, Japan

We aim at forming atomic-thick Si ribbons from a silicon-on-insulator (SOI) layer possessing a vicinal (111) surface by combining multiple wet-chemical treatments. Among the treatments, the most important one is to cut neighboring Si terraces along atomic step edges by metal-assisted chemical etching (MacEtch). To test this MacEtch performance, we have started experiments using a Si(111) bulk wafer. The Si surface has the miscut angle of 0.2°.

After a cut sample was wet cleaned, it was immersed in water in which the concentration of dissolved O_2 molecules was very low, or a ppb level. This process is referred to as the first LOW (Low dissolved-O_2 Water) treatment. We find that a Si(111) surface composed of flat terraces and biatomic steps was formed by this first LOW treatment. Then it was immersed in LOW containing Ag^+ ions at a concentration of 5 ppm, which is referred to as the second LOW treatment. It was demonstrated that Ag atoms were selectively reduced at the edges of atomic steps on Si(111) to form Ag nanowires, as reported by another group. Finally, the Si sample with Ag nanowires was immersed into a mixture of HF and H_2O_2. The resultant AFM image indicates that the self-assembled Ag nanowires after the second LOW treatment were replaced by almost continuous nanotrenches. This is probably because the Ag nanowires acted as a catalyst to enhance chemical etching of the Si surface underneath [1]. By applying this sequence for a thin SOI layer, we expect to form Si ribbons of which both a width and a thickness are controlled in a self-assembled manner.

[1] Z. Ma, S Masumoto, K. Kawai, K. Yamamura, and K. Arima, *Langmuir*, **38**, 3748 (2022).

11:10am **PCSI-MoM2-33 III-V Materials Grown Directly on V-groove Si for Solar Cells*, Theresa Saenz,*** *J. Mangum, J. Boyer, A. Neumann, R. France, W. McMahon,* National Renewable Energy Laboratory*; J. Zimmerman,* Colorado School of Mines*; E. Warren,* National Renewable Energy Laboratory

III-V solar cells offer superior performance to other technologies, reaching light conversion efficiencies above 40% [1]. However, their high cost has limited their use to space applications, with the GaAs or Ge substrate contributing a large portion of the overall cost [2]. The direct growth of III-Vs on Si is a compelling strategy to combine the high performance of III-V solar cells with the low cost of Si substrates. Nanopatterned V-groove Si offers both additional cost savings through its compatibility with low-cost wafer polishing and an ideal crystallographic surface for preventing the formation of antiphase domains that typically plague III-V on Si growth. In this work, we demonstrate the growth of low-dislocation-density GaAs on GaP grown via metalorganic vapor phase epitaxy (MOVPE) on V-groove Si substrates.

Fig. 1: a) SEM cross-sectional image of coalesced GaP on V-groove Si. b) AFM of the coalesced GaP with a R_q of 0.2 nm. c) ECCI image of GaAs on GaP on V-groove Si after TCA and DFLs showing a TDD of $3´10^{6}$ cm^{-2}.

We studied a number of MOVPE nucleation conditions for GaP on V-groove Si and found that a high V/III ratio and growth temperature produces uniform nucleation at the bottom of the grooves that later coalescences into a thin film as shown by cross-sectional scanning electron microscopy (SEM, Fig. 3a) [3], with the exact geometry of the nanopatterns also playing an important role in coalescence. The coalesced GaP was very smooth, with a RMS roughness (R_q) of 0.2 nm measured by atomic force microscopy (AFM, Fig. 3b). However, with a threading dislocation density (TDD) of 5´10^{7} cm^{-2} as measured by electron channeling contrast imaging (ECCI, Fig. 3c), the defects in this GaP on Si template would be limiting for solar cells applications. To decrease the TDD, we grew GaAs on the GaP/Si templates and employed thermal cycle annealing combined with a dislocation filter like the one described in Ref. 4. This resulted in relaxed GaAs with a TDD of 3´10^{6} cm^{-2} as measured by ECCI, achieving a low TDD in a material with a bandgap suitable for solar cells. We will present solar cell results and discuss the materials science consideration involved in achieving smooth and high-quality III-V growth on V-groove Si.

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[2] J. S. Ward et al., Prog. Photovolt. **24**, 1284-1292 (2016).

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11:15am **PCSI-MoM2-34 Improved Passivation Performance of Atomic-layer-deposited (ALD)-MoO$_X$ Film by Introducing an Al$_2$O$_3$ Interlayer***, **Hyo Sik Chang,*** Chungnam National University, Republic of Korea

The carrier-selective contact solar cell structure allows transition metal oxides to bend the band gap to stabilize energy, and adjusts the energy band to induce barrier tunneling such that holes and electrons can move efficiently to both electrodes, thereby reducing recombination loss and increasing efficiency. Conventional hole selection candidates, such as WO$_X$, VO$_X$, and MoO$_X$, have been investigated as hole-selective contacts (HSC) [1]. In this study, we introduce a low-temperature ALD-Al$_2$O$_3$ interlayer for continuous processing with the ALD-MoOx film. Therefore, based on the HSC structure using ALD-MoOx, we conducted a study on the change in passivation performance by controlling the ALD-MoO$_X$ interface state by introducing ultra-thin ALD-Al$_2$O$_3$ grown at a low temperature of 170 °C, which is the same as the deposition temperature of ALD MoOx.The deposition rate of the ALD-MoO$_X$ thin film using 250 g/Nm^3 ozone was approximately 0.036 nm/cycle. MoO$_X$ deposition was performed at 150, 250, and 350 cycles for proper thickness selection of the carrier selective contact. The best passivation performance of the MoO$_x$ thin film at 250-ALD cycle exhibits a carrier lifetime of 22 *us* and an implied *iVoc* of 568 *mV*, as shown in Fig. 1. Although the best values of the MoOx thin film are shown in the 250-ALD cycle, the passivation characteristics are relatively low. This phenomenon can be explained by the fact that thin SiO$_X$ generated between MoO$_X$ and Si substrates causes defects. the Al$_2$O$_3$ interlayer helps to reduce interface defects because Al$_2$O$_3$ layers reduce Si^{1+} and Si^{3+} sub-oxide states and changes to Si^{4+} to form network components that mimic SiO$_2$. This induces stabilization of the interface and the work function of the MoOx was found to ~7.0 eV. The composition of the MoO$_3$ thin film close to that of Mo^{6+} was confirmed.

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11:20am **PCSI-MoM2-35 UPGRADED: Determining the Arrangement of sub-Surface Dopants in a Silicon Quantum Device Platform***, **Håkon Røst,*** Norwegian University of Science and Technology (NTNU), Norway*; E. Tosi,* Instituto de Ciencia de Materiales de Madrid, Spain*; F. Strand, A. Åsland,* Norwegian University of Science and Technology (NTNU), Norway*; P. Lacovig, S. Lizzit,* Elettra-Sincrotrone Trieste, Italy*; J. Wells,* University of Oslo, Norway

Recently, efforts to realize a silicon-based, CMOS-compatible quantum computer have been intensifying. Central to its development are so-called Si:P δ-layers: i.e., ultra-sharp layers of phosphorus atoms placed beneath the silicon surface [1]. Until recently, one key property has remained elusive: the arrangement of the P dopants within the δ-layer. The answer to this question is of crucial importance, as the dopant arrangement will directly impact the energy separation (i.e., valley-splitting) of the supported quantum well states [2].

In this talk, we will demonstrate how the local neighborhood around encapsulated dopants in a bulk semiconductor can be directly probed using X-ray photoelectron diffraction (XPD). By utilizing subtle core level energy shifts that are concomitant with the coordination of a dopant, chemically specific diffractive images can be formed [3]. Through comparison with XPD simulations that are derived from models of the local atomic environment around the dopants, the true dopant atom placement can be ascertained. Typically, XPD is only used as a probe of surface structure [4]. We demonstrate here that – under the right conditions, it also can be used to determine the local arrangement of sub-surface atoms. Therefore, XPD is well suited for solving the long-standing mystery of the Si:P δ-layer structure.

References:

[1] F. A. Zwanenburg *et al*., Rev. Mod. Phys. **85**, 961 (2013).

[2] D. J. Carter *et al*., Nanotechnology **22**, 065701 (2011).

[3] D. Woodruff, Surf. Sci. Rep. **62**, 1 (2007).

[4] A. J. U. Holt *et al*., 2D Mater. **8**, 035050 (2021).

11:40am **PCSI-MoM2-39 Cross-sectional Scanning Tunneling Microscopy Study of 6.1 Å Family Semiconductors for ULTRARAM™ Memory***, **Aurelia Trevisan,*** Eindhoven University of Technology, The Netherlands*; P. Hodgson,* Lancaster University , UK*; D. Lane,* University of Adelaide, Australia*; M. Hayne,* Lancaster University, UK*; P. Koenraad,* Eindhoven University of Technology, The Netherlands

The peculiar band alignments of the 6.1 Å semiconductor family (InAs, GaSb and AlSb) have been exploited for the development of a new non-volatile memory technology, ULTRA**RAM**™[1]. The basis of the nonvolatility of ULTRA**RAM**™ is the large InAs/AlSb conduction band offset (2.1 eV). Multiple ultrathin InAs/AlSb heterojunctions form a triple-barrier resonant tunnelling (TBRT) structure between the channel and the floating gate (FG) [2]. Electrons are allowed to move across the TBRT layers when a low voltage is applied (~ 2.5 V), while when no bias is applied, electrons cannot be transferred in or out the FG [1]. ULTRA**RAM**™is presently grown by molecular beam epitaxy. However, for commercial production, the growth would be ideally transferred to MOCVD as it is more scalable. We performed room temperature and low temperature cross-sectional scanning tunneling microscopy (X-STM) measurements on a ULTRA**RAM**™sample grown on a GaAs n-doped wafer. With X-STM, the various layers of ULTRA**RAM**™ were investigated at the atomic scale. The main goal of the experiment was to probe the quality of the layers and their interfaces, in terms of thickness uniformity and sharpness, in particular the TBRT. In the investigated sample, the TBRT is positioned between an InGaAs layer (readout channel) and an InAs layer (FG). We studied the morphology of the TBRT, the quality of the InAs/AlSb layers and the uniformity in their composition. We observed the formation of slip planes starting from the interface between the InGaAs layer and the GaSb layer below it, most probably due to the lattice mismatch of the grown layers. The slip planes either end at the top most layer of the sample (FG) or at the interface between the InGaAs channel layer and the AlSb barrier B1. The latter typically give rise to small, down-triangle-shaped AlSb accumulation regions below B1 of the TBRT (Quantum Pits, QPs). However, we also observed the formation of AlSb QPs in the absence of an identified slip plane. Due to presence of the QPs the InGaAs/AlSb interface is not sharp and the thickness of B1 is uneven. Interestingly, the subsequent InAs and AlSb layers in the TBRT are typically characterized by sharper interfaces and more uniform thickness. We investigated possible mechanisms for the formation of the QPs and a possible relation with the presence of the slip planes.

[1] P. D. Hodgson, D. Lane, P. J. Carrington, E. Delli, R. Beanland, and M. Hayne, Adv. Electron. Mater., 2101103 (2022)

[2] D. Lane, M. Hayne, J. Phys. D: Appl. Phys. **54**, 355104 (2021)

11:45am **PCSI-MoM2-40 Surface Reaction and Plasma Induced Damage by Atomic Layer Etching Process***, **Sung Gyu Pyo,*** Chung-Ang University, Republic of Korea

As the semiconductor integrated process enters the region below 10 nm, the removal of contaminants on the silicon wafer surface is crucial for high-integration device products and has a great influence on the yield, quality, and reliability of these products. Therefore, a cleaning method with high efficiency and high selectivity is required.

Correspondingly, the NOR (native oxide removal) dry cleaning method, which removes the native oxide films by using indirect plasma with hot H$_2$ or H$_2$/NF$_3$ gases, has attracted attention as a next-generation cleaning process because it can etch various thin-films with profile control. According to Toshio Hayashi et al. the mechanism for the dry cleaning process using hot H$_2$ gas and down flow NF$_5$ gas, which are not decomposed at the plasma source, is that fluorine, which has high electronegativity, is adsorbed well on the surface of the silicon wafer and reacts with hydrogen gas; it then generates NH$_4$-F-NH$_4$ because of Coulomb interaction. Therefore, (NH$_4$)$_2$SiF$_6$ is formed on the silicon substrate and vaporized at above 100 °C.

Dry cleaning can control selectivity of the contaminants and roughness of the wafer surface, depending on gas flow, temperature, pressure, plasma power, and pressure distribution. However, controlling various process parameters is very difficult; It is necessary to understand the mechanism of gas reactions based on the plasma used for controlling etch rate and selective thin-film uniformity.

In this study, we investigated the method of surface planarization as well as removal of contaminants during dry cleaning using down flow H_2 and NH_3 gas. According to the gas flow, dry cleaning of oxide, nitride, and p-doped wafers was performed. On analyzing the quality of each film, we propose an analysis method for controlling etch rate to selective thin-films and contaminants in a trench region below 10 nm.

In this experiment, the characteristics of each thin-film were analyzed by Raman spectroscopy, which can quantify and provide qualitative analysis of selective parts through beam focusing. When the characteristics of p-doped thin-films are analyzed by selective removal of oxide and nitride films, which are deposited on p-doped silicon in trenches with a width of 10 nm or less, we can use Raman spectroscopy to determine the appropriate etch rate and time.

PCSI
Room Redondo - Session PCSI-MoA1
Semiconductor Discovery/Interface/Surface Characterization

Moderator: Dorothee Sophie Rosenzweig, Technische Universität Berlin

2:00pm **PCSI-MoA1-1 (Al,Gd)N as a Novel Material for Neutron Detection: Materials Discovery and Interface Design**, ***Nancy Haegel,*** National Renewable Energy Laboratory **INVITED**

Ultra-wide bandgap nitrides, with their exceptional optoelectronic and charge transport properties, have already delivered transformative impact for light emitting diodes ((Al,Ga)N) and cell phone resonators ((Al,Sc)N), with potential for future impact for power electronics, sensors, and other optoelectronic/magnetic applications. This class of pseudo-binary alloys and ternary nitrides is rapidly expanding due to advances in high-throughput computational discovery and non-equilibrium synthesis [1]. In this work, Al1-xGdxN alloys have been synthesized and characterized [2]. These new materials offer exciting integration opportunities for thin film devices leveraging significant concentration of the ferromagnetic and strongly neutron absorbing 157Gd constituent in an AlN wide bandgap host.

Metastable Al1-xGdxN alloys have been synthesized using non-equilibrium combinatorial thin film deposition via radio frequency co-sputtering. First-principles calculations show that the limiting critical composition for a wurtzite to rocksalt phase transition is xc = 0.82. However, theory also suggests that at temperatures below 1000 K there is a large miscibility gap limiting Gd incorporation in AlN to only a few percent. By higher effective temperature through non-equilibrium growth we have achieved the highest Gd3+ incorporation into the wurtzite phase reported to date. Single-phase compositions up to x ≈ 0.25 are confirmed by high resolution synchrotron grazing incidence wide angle X-ray scattering and transmission electron microscopy.

Integration of these materials into devices will require electrical contact functionality and interface control. We will discuss needs and opportunities for detailed understanding and synthesis control strategies at incommensurate interfaces between rocksalt and wurtzite structures for device integration.

[1] S.R. Bauers et. al., “Ternary nitride semiconductors in the rocksalt crystal structure,” Proc. of the National Academy of Sciences, 116, 14829-14834, 2019.

[2] R.W. Smaha, K. Yazawa et al., ”Prediction and Synthesis of Gd-rich Al1−xGdxN Alloys,” DOI:10.26434/chemrxiv-2022-k32j0

2:40pm **PCSI-MoA1-9 Surface Calibrated Electron Holography: Anomalous Strain Relaxation and Minimization of Polarization Changes at III-Nitride Hetero-Interfaces**, ***Michael Schnedler****, Y. Wang, Q. Lan, F. Zheng, L. Freter, Y. Lu, U. Breuer,* Forschungszentrum Jülich GmbH, Germany*; H. Eisele,* Otto-von-Guericke-Universität Magdeburg, Germany*; J. Carlin, R. Butté, N. Grandjean,* EPFL, Switzerland*; R. Dunin-Borkowski, P. Ebert,* Forschungszentrum Jülich GmbH, Germany

Polarization and electron affinity changes at $Al_{0.06}Ga_{0.94}N$/GaN and $In_{0.05}Ga_{0.95}N$/ $Al_{0.06}Ga_{0.94}N$ interfaces are quantified by off-axis electron holography (EH) in transmission electron microscopy (TEM), in conjunction with scanning tunneling microscopy and spectroscopy, as well as self-consistent simulations of the electrostatic potential and electron phase maps. The central problem of quantitative EH is that at the surfaces of the thin TEM lamellae a defect-induced pinning occurs, which alters the phase contrast. Therefore, we calibrated the electron optical phase maps using a d-doped layer at the GaN buffer/substrate interface by determining the energy of the pinning level at the surface to 0.69 eV above the VBM (consistent with pinning by nitrogen vacancies). The such calibrated EH provides quantification of the key interface properties: The biaxially relaxed $In_{0.05}Ga_{0.95}N$/ $Al_{0.06}Ga_{0.94}N$ interface exhibits polarization and electron affinity changes as theoretically expected. However, at the $Al_{0.06}Ga_{0.94}N$/GaN interface anomalous lattice relaxations and vanishing polarization and electron affinity changes occur, whose underlying physical origin is anticipated to be total energy minimization by the minimization of Coulomb interactions between the polarization-induced interface charges. [1]

[1] Y. Wang *et al.*, Phys. Rev. B **102**, 245304 (2020)

2:45pm **PCSI-MoA1-10 Surface Carrier Density in 2D and 3D Indium Nitride Structures**, ***Fernando Maia de Oliveira****, A. V. Kuchuk,* Institute for Nanoscience and Engineering, University of Arkansas*; C. Romanitan,* National Institute for Research and Development in Microtechnologies, Romania*; H. V. Stanchu,* Institute for Nanoscience and Engineering, University of Arkansas*; M. E. Ware,* Department of Electrical Engineering, University of Arkansas*; Y. Mazur, G. J. Salamo,* Institute for Nanoscience and Engineering, University of Arkansas

Narrow-bandgap materials have gained increased attention due to their great applicability in infrared systems. [1] In particular, indium nitride (InN) offers extraordinary advantages to the industry of ultra-fast high-power electronics due to its high mobility, low effective electron mass, and widely tunable plasmonic activity. But, the challenging fabrication of InN-based devices makes it difficult to explore its benefits. The accumulation of electrons at the surface of indium nitride structures has been previously reported for 2D and 3D materials. However, the control of such charge accumulation using growth parameters is yet to be explored. [2] In this study, we investigate the morphology, structure, and optical features of a series of 2D and 3D InN structures grown using different In/N flux ratios. By evaluating the longitudinal optical phonon-plasmon coupled modes of InN using Raman spectroscopy, we measure the surface carrier concentration increasing from approximately 10^{17} to 10^{18} cm^{-3} as the surface-to-volume ratio decreases. By simulating the InN structures using the k.p method we show that the morphological evolution from 3D to 2D structures modifies the electron occupation near the surface, as shown in Figure 1. Our key finding shows that the charge profile along the InN structure is influenced by its structural features, such as porosity, surface-to-volume ratio, in-plane strain, and roughness of the material by modifying the bending of the conduction and valence bands along the InN material.

2:50pm **PCSI-MoA1-11 Structure and Chemistry of $ZnGeN_2$ Quantum Wells in GaN for use in Green LEDs**, *M. Tellekamp,* National Renewable Energy Laboratory*;* ***Moira Miller****,* Colorado School of Mines*; A. Rice,* National Renewable Energy Laboratory*; D. Diercks,* Colorado School of Mines*; A. Tamboli,* National renewable Energy Laboratory

Hybrid II-IV-N_2/III-N heterostructures, based on current commercialized (In,Ga)N light-emitting diodes (LEDs), are predicted to significantly advance the design space of highly efficient optoelectronics in the visible spectrum, specifically in the green to amber regions where LED efficiencies are orders of magnitude lower than other colors. Yet, there are few epitaxial studies of II-IV-N_2 materials. $ZnGeN_2$, a ternary analogue of GaN, is explored as a potential green-to- amber emitter which can be integrated into existing GaN LED heterostructures due to structural similarity. $ZnGeN_2$ is wurtzite when disordered, and is structurally and electronically similar to GaN, possessing a lattice mismatch of ~0.8%. Previous work by this group has demonstrated epitaxial growth of $ZnGeN_2$ on GaN and AlN via molecular beam epitaxy (MBE) [1-2]. Here we present the growth of abrupt quantum wells (QW) of $ZnGeN_2$ within GaN by nitrogen plasma-assisted MBE, including successful five-layer multiple quantum well (MQW) structures.

Detailed structural and elemental analysis of the heterostructures was performed, including X-ray diffraction (XRD), scanning transmission electron microscopy (STEM), energy dispersive X-ray spectroscopy (STEM-EDS), and atom probe tomography (APT). These methods demonstrate high-quality and abrupt interfaces in the heterostructures after multiple repeating heterointerfaces and some compositional nonidealities in each layer. Through changes in growth methodology, we demonstrated methods to improve unintentional impurities including associated improvements in structural quality. We also investigated conduction band offset using X-ray photoelectron spectroscopy (XPS) in the GaN/$ZnGeN_2$ heterostructures, important for LED design. Together, these data demonstrate both the promise of heteroepitaxially integrated hybrid ternary/binary nitride systems along with the challenges associated with growing such systems, including an outlook on methods to improve the materials and eventual devices.

[1] M. B. Tellekamp et al 2020, Crys. Growth Des. 20, 3, 1868–1875.

[2] M. B. Tellekamp et al 2022, Crys. Growth Des. 22, 2, 1270–1275.

PCSI

Room Redondo - Session PCSI-MoA2

Organics, Semiconductors, and Molecules

Moderator: Nancy Haegel, National Renewable Energy Laboratory

3:40pm **PCSI-MoA2-21 Single-Molecular Tunnel Junctions: The BN/CC Isosterism Effectiveness in PAH Models*, Sandra Rodriguez Gonzalez,*** Universidad Autónoma de Madrid, Spain

Boron-Nitrogen (BN)/Carbon-Carbon (CC) isosterism constitutes one of the most versatile and efficient doping techniques to improve the Polycyclic Aromatic Hydrocarbons (PAHs) properties in organic optoelectronic devices.[1] The diatomic polar BN unit modifies the electronic structure, and hence the aromaticity, simply by swapping its orientation; but maintains the good co-planarity and rigidity of the backbone. Motivated by the scarcely employ of this type of isoelectronic substitution to modulate the electronic transport properties in single-molecule devices, we report the BN/CC isosterism effect on the aromaticity and single molecule conductance in a series of 1,4 azaborine acene derivatives, as PAHs models.

Studied molecules were strategically designed and synthesized, to reveal a first, the unequivocal and utmost effect of BN doping on the conductance. Scanning tunneling microscope break-junction (STM-BJ) measurements, in combination with the nonequilibrium Green´s function (NEGF) formalism coupled to self-energy corrected Density Functional Theory (DFT+Σ) method,[2] within the Landauer framework, were employed.[3] A comprehensive study was possible considering different molecular polarization orientations in the [Au-molecule-Au] theoretical model junctions, and conformational changes related to the BN-substitution.

[1]. (a) C. Chen, C-Z. Du, X-Y, Wang, Adv. Sci., 2022, 2200707; (b) X-Y. Wang, et. al., Angew. Chem. Int. Ed., 2013, 52, 3117; (c) J. S. A. Ishibashi, et. al., Dalton Trans., 2019, 48, 2807; (d) J. Huang, Yl Li, Frontiers in Chemistry, 2018, 341,1. [2]. (a) J. G. Fallaque, S. Rodríguez-González, F. Martín, C. Diaz, J. Phys.:Condens.Matter., 2022, 34, 435901; (b)J. G. Fallaque, S. Rodríguez-González, C. Diaz, F. Martín, Nanoscale, 2022, 14, 464. [3]. L. Palomino Ruiz, S. Rodríguez González, I. R. Márquez, A. G. Campaña, J. M. Cuerva, F. Martín, C. Díaz, A. Millán, M. T. González, Angew. Chem. Int. Ed. 2021, 60, 6609.

3:45pm **PCSI-MoA2-22 Surface Resonant Raman Scattering: Analysis of Vibrations at Clean Surfaces and Monolayer Films*, Norbert Esser,*** TU Berlin and Leibniz-Institut für Analytische Wissenschaten-ISAS-e.V., Germany **INVITED**

Raman spectroscopy is a standard analytical method to study organic and inorganic material structures. For analysing ultrathin films, plasmonic surface enhancement (SERS) or tip enhancement (TERS) is common nowadays. However, even without such plasmonic field enhancement, Raman spectroscopy can be sensitive enough to record surface phonons, surface resonances or adsorbate vibrations. This is strongly favoured by surface resonant Raman scattering, i.e. resonance enhancement involving surface electronic transitions. By choosing an appropriate energy of the exciting laser line, a surface specific resonance enhancement may be achieved.

On clean surfaces, confined phonons and phonon resonances have been detected using surface resonant excitation on Si, Ge, III-Vs and Cu. The termination of surfaces by adsorbates has been analysed with sub-monolayer precision, e.g. for Sb on III-V(110) substrates, Pb and Au on Si(111), H on Si(111) and O on Cu(110).

In collaboration with theory groups, DFT-based calculations of the structure and electronic bands have revealed the mechanism of surface resonant Raman Scattering. Moreover, comparison of theory and experiment allows one to conclude on particular surface/adsorbate structures. In particular, I will discuss the interplay between atomic and electronic structure, metal-semiconductor transition and the effect of strong electron-phonon-coupling in quasi 1D-nanowires (In and Au on Si(111) and Si(553)).

On conductive samples, Raman scattering by the charge transfer mechanism may play an important role, in addition to deformation potential scattering. Please note that charge transfer is an important part of SERS and TERS, called chemical enhancement effect. The free carrier concentration in the scattering volume may lead to a notable difference for Raman spectroscopy on surfaces as well, e.g. for conductive nanowire structures and for metals.

4:25pm **PCSI-MoA2-30 Ordered Monolayer Growth of N-Heterocyclic Carbenes on Silicon Surfaces***, M. Franz,* Technische Universität Berlin, Germany*; S. Chandola,* Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany*; M. Koy,* Westfälische Wilhelms-Universität Münster, Germany*; **Robert Zielinski,*** Technische Universität Berlin, Germany*; H. Aldahhak,* Universität Paderborn, Germany*; M. Das, M. Freitag,* Westfälische Wilhelms-Universität Münster, Germany*; U. Gerstmann,* Universität Paderborn, Germany*; D. Liebig, A. Hoffmann, C. Kosbab, M. Rosin,* Technische Universität Berlin, Germany*; W. Schmidt,* Universität Paderborn, Germany*; C. Hogan,* Università di Roma 'Tor Vergata', Italy*; F. Glorius,* Westfälische Wilhelms-Universität Münster, Germany*; N. Esser,* Leibniz-Institut für Analytische Wissenschaften – ISAS e.V., Germany*; M. Dähne,* Technische Universität Berlin, Germany

N-Heterocyclic carbenes (NHCs) have been shown to be excellent modifiers and anchors for the functionalization of surfaces, but the investigation has been limited to metals. Thus a controlled functionalization of silicon surfaces by ordered NHC layers is particularly interesting. Here, we present an extensive scanning tunneling microscopy (STM), density functional theory, and X-ray photoemission spectroscopy study of the growth of NHCs on Si(111) and demonstrate a binding to the surface via a single Si–C bond. We varied the molecule–substrate interaction by using different model NHCs on a Si(111)√3×√3R30°-B surface. This substrate is deactivated by the subsurface incorporation of B atoms and thus particularly suited for the ordered growth of organic films. We find that the NHC molecules bind via a single covalent C-Si bond in an upright adsorption geometry and demonstrate the formation of highly ordered monolayers that are thermally stable and show strong work function reductions. The degree of ordering in the monolayers as well as their periodicity depends on the NHC molecule, in particular on the nature of its sidegroups, as well as on the defect density of the substrate.

4:30pm **PCSI-MoA2-31 Arrangement and Electronic Properties of Cobalt Phthalocyanine Molecules on B-Si(111)-√3 × √3 R30°*, Susi Lindner-Franz,*** *M. Kubicki,* Technische Universität Berlin, Germany*; H. Eisele,* Otto-von-Guericke-Universität Magdeburg, Germany*; M. Dähne, M. Franz,* Technische Universität Berlin, Germany

In this contribution, we investigate the molecular arrangement and electronic properties of cobalt phthalocyanine CoPc on the passivated B-Si(111)-√3 × √3 R30° (Si:B) surface in detail by means of scanning tunneling microscopy (STM) as well as tunneling (STS) and photoemission spectroscopy (PES). The STM images clearly show that submonolayers of CoPc lie flat on the surface, with either a four-leaf cloverlike or a circular appearance, depending on the presence of neighboring molecules or surface defects, which affect the molecular rotation, and that a selective orbital hybridization occurs. Furthermore, PES data explain that the spectral changes are mostly related to the chemical interactions, while the previously discussed changes of the band bending only play a minor role. For high CoPc coverages, in contrast, the molecules are tilted with respect to the Si:B surface, establishing exceedingly ordered molecular arrangements. The STS data in show that several monolayer thick films of CoPc exhibit identical electronic properties as compared with pure CoPc.

4:35pm **PCSI-MoA2-32 Bio-Resorbable Memristorwith Alginate as an Active Layer for Transient Electronics*, Hojung Jeon,*** *Y. Rim,* Department of Intelligent Mechatronics Engineering, and Convergence Engineering for Intelligent Drone, Sejong University, Republic of Korea

Bio-resorbable and transient electronics that imply chemically or physically dissolution after a certain period operation have drawn considerable attention due to the demand of biocompatibility for eco-friendly applications [1]. This work presents alginate-based resistive random-access memory (RRAM) to establish bio-resorbable memristive system. Alginate is assumed as the switching layer by using solution process and prove its bipolar switching behavior, which refers we can apply set/reset operations in small ranges(-2V~3V) of voltage to enhance power consumption efficiency. High stability was also verified by endurance and retention time due to tolerance and long-term maintenance. Bio-resorbable properties of RRAMs, which were fabricated with water-soluble Mg electrodes was investigated by fully dissolving in DI water and dissolving time controllability was also demonstrated by modulating the thickness of Al_2O_3 capping layer, which was deposited using atomic layer deposition(ALD). With this approach, it is expected that biocompatible RRAMs can apply to a neuromorphic system by fitting two terminal devices which have closely characterized structures with artificial synapses [2]. Controlling the dissolving time, we can also consider of the hardware-security. Furthermore, the devices have implantable characteristics in human-body so it can be used in the area of medical surgery or health-care problems.

Fig. Set and reset of bio-resorbable alginate memristor devices

Acknowledgments

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[2] Aristide Gumyusenge, Armantas Melianas,Scott T. Keene, Alberto Salleo, Annu. Rev. Mater. Res. 2021. 51:47–71

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PCSI
Room Redondo - Session PCSI-MoE
Novel Materials

Moderator: Christopher Palmstrøm, University of California, Santa Barbara

7:30pm **PCSI-MoE-1 Machine Learning in the Quantum Regime Through Physical-Principle-Informed Representations***, **Qimin Yan**,* Department of Physics, Northeastern University **INVITED**

Materials design in the quantum regime call for the integration of multi-tier materials information that goes beyond atomic structures. Especially, many quantum behaviors are greatly controlled by local bonding environments and physical constraints related to symmetry. In this talk, I will give several examples of how domain knowledge and physical principles for quantum material systems can be incorporated into machine learning frameworks through representation learning to greatly improve the performance of machine learning models for property predictions. Motivated by Pauling's rules, I will show that local bonding environments (structure motifs) can be incorporated into a graph-based machine-learning architecture to make reliable property predictions for solid-state quantum materials including complex metal oxides. The proposed atom-motif dual network model demonstrates the feasibility to incorporate beyond-atom materials information in a graph network framework and achieves state-of-the-art performance in predicting the electronic structure properties of complex metal oxides. Through unsupervised learning, abstracted material information such as chemical formulas and motif connections can be combined with national language processing technologies to effectively represent fundamental elements in materials and use them in downstream learning tasks. I will demonstrate how contrastive representation learning can be used to incorporate physical constraints that control the collective behavior of electron densities into neural-network-based density functional design. At the end of the talk, I will discuss the continued development of machine learning models for quantum materials that embrace local/global symmetries and symmetry-based interactions.

8:10pm **PCSI-MoE-9 UPGRADED: Ultra-Thin Freestanding Membranes Enables New Discovery of Interfacial Properties***, **Xiao Zhao**, Y. Lu, M. Salmeron,* LBNL

Many surface-sensitive techniques have been improved recently to narrow the gap between measuring environmental conditions from vacuum to practical gas and liquid environments. To extend the pressure range and to enable measurements of the liquid phase, thin film membranes acting as windows in environmental cells have been fabricated. Herein, we present a new generation of ultrathin free-standing membranes made with graphene, oxide films (2-10nm Al_2O_3, TiO_2, etc.) or metal (3-10nm Pt)[1]. The films are mechanically robust and transparent to electrons and photons. Their applicability for various environmental spectroscopies, such as X-ray Photoelectron Spectroscopy (XPS, 1bar for gas or for liquid), Infrared Nanospectroscopy (nano-FTIR, solid-liquid interface), Kelvin Probe Force Microscopy (KPFM) and Sum Frequency Generation (SFG) is demonstrated[1,2]. With this platform we investigated the structure and profile of electrical double layer, self-assembly of protein and electrocatalyst evolution. The remarkable properties of such ultra-thin membranes open up broad opportunities for atomic/molecular level studies of interfacial phenomena (corrosion, catalysis, electrochemical reactions, energy storage, geochemistry, and biology) in a broad range of environmental conditions.

8:30pm **PCSI-MoE-13 UPGRADED: Extreme Spatiotemporal Imaging and Control of Nanophotonic Components and Their Neuromorphic Applications***, L. Wittenbecher, D. Winge, A. L'Huillier,* Lund University, Sweden*; J. Vogelsang,* Oldenburg University, Germany*; D. Zigmantas,* Lund University, Sweden*; **A Mikkelsen**,* NanoLund and Department of Physics, Lund University, Sweden

During the past decade we achieved unprecedented abilities to probe and exploit light-matter interaction down to the nanometer and sub-femtosecond spatiotemporal scales. This opens for new fundamental physical insights as well as to rationally design of a variety of novel functional materials and devices with applications for energy harvesting and alternative computing. The presentation has two parts:

First, we combine the femtosecond and attosecond time resolution of advanced laser systems with the nanoscale spatial resolution of PhotoEmission Electron Microscopy (PEEM). We use this to unravel the hot electron dynamics in InAs nanowires [1] and observe the dynamics of near-field enhancement in hybrid metal-semiconductor nanostructures [2,3]. We will include new works using very high fields on Ag nanowires and attosecond pulse excitation on ZnO.

Second, we propose an artificial neural network concept [4] in which the weighted connectivity between nodes is achieved by overlapping light signals inside a shared quasi 2D waveguide – a broadcasting concept. This decreases the circuit footprint by two orders of magnitude compared to existing optical solutions. The evaluation of optical signals is performed by neuron-like nodes constructed from efficient III–V nanowire optoelectronics. This minimizes power consumption of the network. Detailed simulations of the central network parts, demonstrate feasibility [4] and new experimental data on wire-to-wire on chip communication circuits will be shown.

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PCSI

Room Redondo - Session PCSI-TuM1

Electronic and Structural Properties of Films and Surfaces

Moderator: Jia Li, Brown University

8:30am **PCSI-TuM1-1 UPGRADED: Strain Soliton Formation in Epitaxial Bismuth Thin Films***, **Jason Dong**, H. Inbar, C. Dempsey, A. Engel, C. Palmstrøm,* University of California Santa Barbara

Strain solitons are topological defects which have been observed in van der Waals materials [1]. Strain solitons are generated as a result of thin film strain and form as ripples in the films, separating commensurate and incommensurate regions. The solitons are analogous to misfit dislocations and cause local relaxation of the crystal. Solitons have been of interest due to their potential for generating novel spatially confined states within two-dimensional materials [2].

In this talk, we report the formation of strain solitons in epitaxial (111) bismuth thin films grown by molecular beam epitaxy on InSb(111)B substrates. The 0.9% lattice mismatch between bulk bismuth and the InSb(111)B substrates results in strain relaxation via strain soliton formation and in-plane edge dislocation formation. Edge dislocations are observed to induce large angle bending of the solitons. The solitons appear to form at the interface and propagate throughout the film. The strain state of the bismuth thin films is characterized by *in-situ* low temperature scanning tunneling microscopy and ex-situ X-ray diffraction. The effect of the solitons on local strain and lattice rotation is mapped from the STM images using the Lawler-Fujita algorithm [3]. Partial relaxation of bismuth is observed to begin at 2 bilayers, and the thin films become fully relaxed by 30 bilayer thick. The evolution of the soliton network and their strain fields as a function of thickness is characterized. Our results indicate that bismuth primarily relaxes by strain soliton formation and enables future investigation of novel states hosted in the bismuth solitons.

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8:50am **PCSI-TuM1-5 Epitaxial Growth and Surface Studies of Bi/ Hexagonal ζ- Phase Mn_2N/MgO (001) using Molecular Beam Epitaxy and Scanning Tunneling Microscopy***, **Ashok Shrestha**, A. Abbas, A. Smith,* Ohio University

The growth and structure of the cubic manganese nitrides, namely θ- MnN, η- Mn_3N_2, and ε- Mn_4N, has already been investigated intensively on MgO (001) substrates [1,2]. However, the hexagonal ζ- Mn_2N has remained unexplored. Thin films of hexagonal ζ- Mn_2N were grown successfully on MgO (001) using molecular beam epitaxy (MBE) and used as a substrate to grow a very thin layer of bismuth.

In this presentation, the epitaxial growth of ζ- Mn_2N and multilayer of bismuth will be discussed. The sample growth process was monitored by *in-situ* reflection high energy electron diffraction. RHEED shows a streaky pattern indicating the smooth sample surface throughout the sample growth. During the Mn_2N growth, 1/4th order fractional streaks are observed along $[100]_{MgO}$ + R30° direction. These fractional streaks indicate the 4× reconstruction on the Mn_2N surface. The presence of a 4× reconstructed surface is also verified by room temperature scanning tunneling microscopy. Moreover, the RT-STM images show the atomically flat terraces, steps, and the atomic resolution of the hexagonal array of the Mn_2N surface. Various *in-situ* and *ex-situ* measurements are performed to calculate the *in-plane* and *out-of-plane* lattice constants. The calculated lattice parameters are in good agreement with the theoretically reported values of ζ- Mn_2N (a=b= 2.83 Å, c= 4.54 Å) [3]. Furthermore, the surface chemistry of the samples was determined by *in-situ* Auger electron spectroscopy at different locations on the sample surface. The stoichiometric ratio of Mn: N on the film is nearly 2:1 which is consistent with ζ- Mn_2N. After successfully growing ζ- Mn_2N, a very thin film of Bi is deposited, and the surface is studied by RT-STM. Interestingly, the measurements show multiple steps with a height of ~1.6 Å which is not matching the step height of bulk Bi (111) (3.94 Å) [4], but it is consistent with the step height of bismuthene grown on Ag (111) as reported by Sun *et al.* (2022) [5]. Although the step heights suggest multilayer bismuthene, atomic resolution images show a rectangular lattice.

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8:55am **PCSI-TuM1-6 One-Dimensional Spin-Polarized Surface States on Bi(112) Compared to States on Other Vicinal Surfaces of Bi***, **Anna Cecilie Åsland**, J. Bakkelund,* Norwegian University of Science and Technology (NTNU), Norway*; E. Thingstad,* University of Basel, Switzerland*; H. Røst,* Norwegian University of Science and Technology (NTNU), Norway*; S. Cooil,* University of Oslo, Norway*; J. Hu,* Norwegian University of Science and Technology (NTNU), Norway*; I. Vobornik, J. Fujii,* Instituto Officina dei Materiali (IOM)-CNR, Italy*; A. Sudbø,* Norwegian University of Science and Technology (NTNU), Norway*; J. Wells,* University of Oslo, Norway*; F. Mazzola,* Instituto Officina dei Materiali (IOM)-CNR, Italy

Vicinal surfaces of bismuth have been found to be great test-beds for investigating one-dimensional (1D) spin-polarized surface states that can be used in spintronic devices [1,2]. We used angle-resolved photoemission spectroscopy (ARPES) and spin-resolved ARPES together with tight-binding (TB) and density functional theory (DFT) calculations to investigate two such surface states on Bi(112). The surface states resemble elongated Dirac cones: 1D and close to dispersionless in the k_y direction, but dispersing in energy along the k_x-direction, forming elongated, X-like features (see Figure). The spin-polarization is pointing mainly in-plane and along the 1D lines, but there are signs of an out-of-plane component for one of the two states. In this talk, we will compare the energy vs. momentum (E vs. k) dispersion and spin-polarization of the measured surface states of Bi(112) to those calculated from the tight-binding model, and the surface states on two other vicinal surfaces of bismuth [1,2]. Similar surface states were found on all three surfaces, suggesting that their existence and general properties are robust properties of bismuth vicinal surfaces. In addition, differences in the details of the states, especially regarding spin-polarization, indicate that their properties may be tuned simply by cutting and polishing the crystal precisely along different high-symmetry directions.

9:00am **PCSI-TuM1-7 Epitaxial Growth and Electronic States of Ultrathin Bi (0001) Films on InSb (111)B***, H. Inbar, J. Dong, A. Engel,* UC Santa Barbara*; M. Zubair,* University of Delaware*; C. Dempsey, Y. Chang,* UC Santa Barbara*; A. Fedorov,* ALS-LBNL*; A. Janotti,* University of Delaware*; **Chris J. Palmstrøm**,* UC Santa Barbara

Synthesizing high-quality single-domain bismuth films with controlled strain, interface chemistries, and thin thickness remains a fundamental materials science challenge with significant consequences such as obtaining high spin-polarization in spintronic devices [1] and 1D-edge transport in the quantum spin Hall phase [2]. Tensile strain in quantum-confined (0001) bismuth films is predicted to lead to a band gap opening [3], allowing surface states to contribute mainly to transport signatures. Yet, only small-area planar Bismuthene wetting layers [4] or thick (>6 bilayers, BL) compressively strained films were studied on semiconducting substrates [5].

In this work, ultrathin large-area Bi (0001) layers were grown on InSb (111)B substrates by molecular beam epitaxy (MBE) and in vacuo transferred for synchrotron-based angle-resolved photoemission spectroscopy (ARPES). In vacuo scanning tunneling microscopy (STM) and ex situ x-ray diffraction (XRD) confirm the successful synthesis of single-crystal Bi epitaxial films. Through a core-level photoemission study, we show that large-area single-domain ultrathin Bi films can be stabilized through strong film-substrate interactions. With decreasing film thickness from 200 BL to 1 BL, we quantify the confinement-induced shifts in the bulk band structure and trace the quantum well energy levels with a phase accumulation model. Significant film-substrate bonds breaking inversion symmetry affect the surface state dispersion leading to a surface state degeneracy which allows us to assign the topological order in Bi (0001) thin films. The findings of this study offer a new route for epitaxial growth and integration of band-engineered Bi films with III-V substrates.

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9:05am **PCSI-TuM1-8 Thermal Stability and Sn Segregation in GeSn Structures***, **Hryhorii Stanchu,*** Institute for Nanoscience and Engineering, Department of Electrical Engineering, University of Arkansas*; O. Olorunsola, A. Kuchuk, A. Said, F. de Oliveira, Y. Mazur, M. Benamara, S. Yu, G. Salamo,* University of Arkansas

Group IV GeSn alloys are extensively studied for efficient Si-based photonics. The interest is elevated recently due to the demonstration of direct bandgap emission in Ge [1]. Specifically, a combination of strain and *n*-type doping reduces the small separation (~140 meV) between the indirect (L) and direct (Γ) valleys in Ge [2] and raises the Fermi level for sufficient electron population in the Γ valley. Nonetheless, the high level of strain (2%) and doping (10^{19} cm^{-3}) only allows a tunable Ge bandgap between 1.3 and 1.6 µm. Alternatively, alloying Ge with the negative bandgap α-Sn results in a fundamental direct bandgap GeSn material with better tunability.The theoretical and experimental estimations indicate an indirect to direct bandgap transition for Sn compositions above 6%.

Achieving Sn-rich GeSn alloys is difficult. This relates to (i) the low equilibrium solid solubility of Sn in Ge (<1%) and (ii) the large lattice mismatch between Ge and α-Sn (15%). However, Sn-rich GeSn alloys have been demonstrated by non-equilibrium growth techniques. The thermal stability of such structures is an issue. We study the structural and optical properties of CVD grown GeSn films in detail. The strain relaxation and Sn segregation is reported for thermal treatment at 300 °C. We discuss on the mechanism of Sn segregation trough the interaction with dislocation.

9:10am **PCSI-TuM1-9 Growth of Ge$_{1-x}$Sn$_{X}$ Heteroepitaxial Layers with High Sn Content on InAs (001) Substrate***, **Nirosh M Eldose,*** Nanoscale Material Science Engineering, University Of Arkansas*; H. Stanchu,* Department of Electrical Engineering, University Of Arkansas*; C. Gunder, C. Li, F. Maia de Oliveira, Y. Mazur, M. Benamara,* Nanoscale Material Science Engineering, University Of Arkansas*; S. Yu,* Department of Electrical Engineering*; G. J. Salamo,* Nanoscale Material Science Engineering, University Of Arkansas

Group IV alloys of Ge and Sn (Ge$_{1-x}$Sn$_x$) are extensively studied for various electronic and optoelectronic applications on a Si platform. Alloying GeSn with α-Sn concentrations as low as 6% [1] allows for an indirect to direct optical transition compared to Ge. Higher Sn content makes possible mid and even long-range infrared optical emission and detection [2,3]. At the same time, due to the low solid solubility of Sn in Ge (~1%) as well as the large lattice mismatch of α-Sn with Ge (~14%), the realization of Sn-rich Ge$_{1-x}$Sn$_x$ structures is challenging.

We will discuss the growth and investigation of crystalline Ge$_{1-x}$Sn$_x$ heteroepitaxial layers with Sn percentage higher than 14% on InAs (001) substrates. Utilizing the small lattice mismatch between Ge$_{1-x}$Sn$_x$ layers and the InAs (001) substrate, we achieved epitaxial growth of Ge$_{1-x}$Sn$_x$ with a high Sn percentage (>30%) by applying a high Sn gradient during growth. The strain induced in the GeSn layers was investigated and the effect of gradually increasing the Sn content of the GeSn lattice significantly affected the composition and morphology of the GeSn layers. Supporting data (Figs 1-3) on the structural properties of Ge$_{1-x}$Sn$_x$alloys using X-ray diffraction, SIMS analysis, XTEM and Raman spectra will be discussed and are shown below.

9:15am **PCSI-TuM1-10 Black Phosphorus/GaAs Heterojunctions for Infrared Detection***, **Emma Renteria,*** University of New Mexico*; S. Addamane,* Center for Integrated Nanotechnologies, Sandia National Laboratories*; T. Rotter, G. Balakrishnan, F. Cavallo,* University of New Mexico

We report our recent results on the development of ultra-thin black Phosphorus (bP)/GaAs junction photodiodes for infrared (IR) detection. The devices comprise an epitaxially grown n-type GaAs nanomembrane and a p-type bP flake exfoliated from commercially available bulk crystals. bP is a promising material for the realization of visible-to-mid-IR detectors as its direct bandgap can be tuned from 0.3 eV to 2 eV by varying its thickness at the nanoscale [1]. The GaAs nanomembrane is multifunctional in that it serves as the n-side of the IR junction photodiode, and it is expected to shield the device from radio-frequency (RF) waves as it has been heavily doped. The fabricated devices have a strong potential to implement RF-waves hardened electronic sensing of IR radiation, a capability of tremendous interest for military and commercial applications. An additional value of the GaAs/bP ultra-thin photodiodes is that they can conform to non-planar surfaces such as aircraft windows and domes of IR cameras, and they can be readily integrated into soldiers' uniforms.

We have established a process to integrate large-area bP flakes onto 220 nm-thick GaAs nanomembranes and used conventional top-down photolithography to fabricate bP-GaAs p-n diodes with areas up to 1.27 x 10^{-4} cm^2. Measured dark-current-voltage characteristics showed a turn-on voltage of 1.4 V with a maximum forward current density of ~ 90 A/cm^2 at 2 V and a dark current density of ~ 2 A/cm^2 at -2 V. We correlate the materials and devices parameters extracted from the current-voltage characteristics with electronic band-structure diagrams and the structure of surfaces and interfaces probed by electron microscopy and x-ray photoelectron spectroscopy. In this talk, we will show the geometry of the bP/GaAs photodiode and the physical-chemical structure of surfaces and interfaces at the nanoscale determine the dominant transport mechanisms and the performance parameters of the device.

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9:20am **PCSI-TuM1-11 UPGRADED: Sub-Nanoscale Chemical Analysis with Nano-Confined Localized Surface Plasmons***, **Nan Jiang,*** University of Illinois - Chicago

It is of significant importance but a challenging task to probe how local chemical environments affect single-molecule behaviors with angstrom scale resolution. Tip-Enhanced Raman Spectroscopy (TERS) affords the spatial resolution of traditional Scanning Tunneling Microscopy (STM) while collecting the chemical information provided by Raman spectroscopy. By using a plasmonically-active probe tip, the Raman signal at the tip-sample junction is incredibly enhanced, allowing for single-molecule probing. This method, further aided by the benefits of ultrahigh vacuum, is uniquely capable of controlling localized plasmons via an atomistic approach. We are able to obtain (1) single-molecule chemical identification;[1] (2) adsorbate-substrate interactions of individual molecules on the surface;[2] (3) local strain effects in 2D heterostructures;[3] (4) atomic-level insights into surface oxidation reactions.[4] By investigating substrate structures, molecular superstructures, 2D material lattices, and adsorption geometries obtained from vibrational modes, we extract novel surface-chemistry information at an unprecedented spatial (< 1 nm) and energy (< 10 wavenumber) resolution. Another important application of localized surface plasmons is to achieve site-selective chemical reactions at sub-molecular scale. Recently, we selectively and precisely activated multiple chemically equivalent reactive sites one by one by scanning probe microscopy tip-controlled plasmonic resonance.[5] Our method can interrogate the mechanisms of forming and breaking chemical bonds at the angstrom scale in various chemical environments, which is critical in designing new atom- and energy-efficient materials and molecular assemblies with tailored chemical properties.

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Author for correspondence: njiang@uic.edu

9:40am **PCSI-TuM1-15 Light Induced Surface Tension Gradients for Hierarchical Assembly of Particles from Liquid Metals***, **Jiayun Liang**, Z. Al Balushi,* University of California at Berkeley

Achieving control over the motion of dissolved particles in liquid metals is of importance for the meticulous realization of hierarchical particle assemblies in a variety of nanofabrication processes. Brownian forces can impede the motion of such particles, impacting the degree of perfection that can be realized in assembled structures. Here we show that light induced Marangoni flow in liquid metals (i.e., liquid-gallium) with Laguerre-gaussian (LG_{pl}) lasers as heating sources, is an effective approach to overcome Brownian forces on particles, giving rise to predictable assemblies with high degree of order. We show that by carefully engineering surface tension gradients in liquid-gallium using non-gaussian LG_{pl} lasers, the Marangoni and convective flow that develops in the fluid drives the trajectory of randomly dispersed particles to assemble into 100-µm wide ring-shaped particle assemblies. Careful control over the parameters of the LG_{pl}laser (i.e., laser mode, spot size, and intensity of the electric field) can tune the temperature and fluid dynamics of the liquid-gallium as well as the balance of forces on the particle. This in turn can tune the structure of the ring-shaped particle assembly with a high degree of fidelity. The use of light to control the motion of particles in liquid metals represents a tunable and rapidly reconfigurable approach to spatially design surface tension gradients in fluids for more complex assembly of particles and small-scale solutes. This work can be extended to a variety of liquid-metals, complementary to what has been realized in particle assembly out of ferrofluids using magnetic fields.

9:45am **PCSI-TuM1-16 Charge Transport in $SrTiO_3$:Rh and $BiVO_4$ Nanoparticle Photocatalysts for Z-scheme Water Splitting***, **Brian Zutter**,* Sandia National Laboratories*; Z. Chen,* University of California Irvine*; L. Barrera,* University of Michigan, Ann Arbor*; A. Lapp, A. Bhandarkar,* Sandia National Laboratories*; K. Watanabe, A. Kudo,* Tokyo University of Science, Japan*; D. Esposito,* Columbia University*; R. Chandran,* University of Michigan, Ann Arbor*; S. Ardo,* University of California Irvine*; A. Talin,* Sandia National Laboratories

Solar-powered water splitting using nanoparticle photocatalyst suspensions is a promising route to economical, clean hydrogen production. In the Z-scheme approach, hydrogen and oxygen-evolving photocatalysts, such as $SrTiO_3$:Rh and $BiVO_4$, are coupled with a redox mediator to improve light absorption compared to single-photocatalyst systems. A key step in the water-splitting process is the separation and transport of photo-excited electrons and holes to the photocatalyst surface. Here we characterize charge transport in individual $SrTiO_3$:Rh and $BiVO_4$ nanoparticles using a nanoprobe within a scanning electron microscope, and directly map internal electric fields with electron-beam induced current. Charge transport in $SrTiO_3$:Rh particles is limited by bulk defect states within the nanoparticle, in contrast to nearly Ohmic conduction in $BiVO_4$ nanoparticles. $SrTiO_3$:Rh particles contain insignificant built-in E fields, while $BiVO_4$ nanoparticles contain built-in E field between different facets of the nanoparticle which can efficiently separate e-h pairs. Inefficient charge transport and lack of built-in electric field explain why the H_2-evolving $SrTiO_3$:Rh nanoparticles are the limiting component within this Z-scheme system.

9:50am **PCSI-TuM1-17 Improvement of Thermal Stability of Ultrathin NiAl Films***, **Kyeong Youn Song**,* Sungkyunkwan University, Republic of Korea

The current copper interconnect technology beyond the 7nm node is facing a crucial challenge of rapidly increasing metal line resistance as the downscaling of device dimensions [1]. In a narrow metal linewidth, the electrical resistivity of Cu increases rapidly due to its relatively high electron mean free path increasing the surface electron scattering. Recent studies have disclosed that binary intermetallic compounds such as NiAl have a high potential to replace Cu due to their low resistivity and high reliability at small dimensions [2]. The critical drawback of NiAl, however, is its rapid increase of resistance upon post-annealing due to the formation of surface oxide and subsequent composition shift of the compound [3].

In this talk, we propose the employment of an aluminum oxide capping layerwith thickness varied from 1-5 nm to improve the thermal stability of ultrathin NiAl films. We found that employing a capping layer effectively prevented the Al out-diffusion from NiAl to aluminum oxide thus the compositional change was no occurred during thermal annealing. Thickness-dependent resistivity of NiAl films was measured, and the NiAl film with 1-nm-thick capping layer shows remarkably low resistivity (49.7mW·cm) for 3.2 nm NiAl film after annealing at 450°C.

9:55am **PCSI-TuM1-18 Frequency-Dependent Conductivity of Granular Metals***, **Laura Biedermann**, M. McGarry, S. Gilbert, W. Bachman, J. Flicker,* Sandia National Laboratories*; P. Kotula,* Sandia*; M. Siegal,* Sandia National Laboratories

We explore the frequency-dependent conductivity, σ, of granular metals (GMs). Granular metal comprise nanoscale metal islands embedded in a dielectric matrix. We target the metal volume fraction, ϕ, so that the few-nm diameter metal islands are separated by a ~1 nm dielectric barrier. These metal/insulator composites can be modelled as a complex resistor-capacitor network with complementary tunneling and capacitive conduction paths [1]. At low frequencies, ideal GMs are highly insulating with thermally-assisted tunneling between islands occurring at high E-fields. At high frequencies, capacitive transport dominates; conductivity increases orders of magnitude.

We compare M-SiN_x and M-YSZ (M = Mo or Co; YSZ = yttria-stabilized-zirconia) GM thin films grown via rf co-sputtering on sapphire. Frequency-dependent conductivity is evaluated using impedance spectroscopy at ambient and cryogenic temperatures. Temperature and field-dependent DC conductivity provide insight into tunneling mechanisms. Granular metal structure (Fig. 1a, b) and composition are determined by scanning transmission electron microscopy (STEM) and x-ray photoemission spectroscopy (XPS).

Through careful selection of the metal-insulator system and synthesis optimization, we prepared GM films having $\sigma_{MHz}/\sigma_{DC} >10^5$ (Fig. 1c). This σ_{MHz}/σ_{DC} ratio was achieved for Mo-SiN_x using deposition conditions that significantly reduced the vacancies present in the sputtered insulator. Analysis of metal/insulator interfaces via XPS showed metal-oxide formation in M-YSZ and metal-silicide formation in M-SiN_x [2]. Control of deposition conditions can minimize these defects, allowing σ_{MHz}/σ_{DC} optimization for high-pass filters.

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PCSI

Room Redondo - Session PCSI-TuM2

Materials for High Power Electronics

Moderator: Gordon Schmidt, Otto-von-Guericke-University Magdeburg, Germany

10:40am **PCSI-TuM2-27 Challenges in SiO_2/Si Interface Engineering for SiC Power MOSFETs***, **Takuji Hosoi**,* Kwansei Gakuin University, Japan*; T. Shimura, H. Watanabe,* Osaka University, Japan **INVITED**

High on-resistance due to low channel mobility and threshold voltage instability due to charge trapping are major concerns of SiC-based power MOSFET, and both issues are deeply correlated with poor SiO_2/SiC interface property grown by thermal oxidation. One of the main causes of this severe interface degradation is residual carbon impurity remained near SiO_2/SiC interface. Although the most common technique to improve SiO_2/SiC interface quality is N incorporation into SiO_2/SiC interface by post-oxidation annealing in NO (NO-POA), the effect on mobility improvement is limited [1] and enhanced hole trapping is pointed out [2]. In this talk, we review the scheme of thermal oxidation and control of N atom profile to improve performance and reliability of SiC MOSFETs based on our recent results.

We demonstrated ultrahigh-temperature oxidation at low oxygen partial pressure to enhance C ejection from SiO_2/SiC interface during thermal oxidation [3]. Passive/active oxidation boundary for 4H-SiC(0001) surface was found to be at around 1600°C under 0.3% O_2/Ar ambient. In SiC MOS capacitors, nearly ideal C-V curve can be obtained by ultrahigh-temperature oxidation, while large hysteresis and positive flatband voltage shift were observed for conventional oxidation. The field-effect mobility of nMOSFET increased from 3 to about 10 cm^2/Vs by performing ultrahigh-temperature oxidation. The reduction in C-related defects was confirmed by electron-spin-resonance (ESR) spectroscopy [4]. We also found that SiC can be oxidized to form SiO_2 under CO_2 ambient at ultrahigh temperatures [5]. Furthermore, a combination of NO-POA and subsequent CO_2 annealing at moderate temperature is effective in obtaining high-channel mobility and stable threshold voltage thanks to the selective removal of N atoms on SiO_2 side at SiO_2/SiC interface and compensation of oxygen vacancies [6].

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11:20am **PCSI-TuM2-35 Epitaxial Growth of Ga_2O_3 Films with Different Ligand Structures by Mist Chemical Vapor Deposition***, **Jang Hyeok Park**, Y. Rim,* Sejong University, Republic of Korea

Recently, gallium oxide (Ga_2O_3) has been receiving attentions for the next generation power semiconductors such as electric vehicles, solar inverters, and energy storage devices because of having a wide band gap of 5.3eV. In particular, beta phase gallium oxide is thermally stable and is formed as a large and single crystal wafer. In order to form epitaxial β-Ga_2O_3 films, hydride vapor phase epitaxy, metal organic chemical vapor deposition, pulsed laser deposition, molecular beam epitaxy, and mist chemical vapor deposition (mist-CVD) have been proposed. Among them, mist-CVD can easily control the chemical compositions and phases as well as do low cost deposition due to simple equipment without vacuum systems.

Here, we studied the effect of precursor ligand types ($Ga(acac)_3$, $GaBr_3$, GaI_3) and growth temperatures (400℃ - 700℃) on heteroepitaxial Ga_2O_3 films on the (0001) sapphire substrates using mist-CVD method.

We confirmed that crystallinity and phases strongly depended on precursor ligands and temperatures. Through the x-ray diffraction, we analyzed the crystal structures of Ga_2O_3 films. At 400℃ and 500℃ temperatures, the (0006) α-phase was observed in Ga_2O_3 films and the optimal phase of α-Ga_2O_3 films was grown by $Ga(acac)_3$. At 600℃ temperature, the (0004) ε-phase was observed in Ga_2O_3 films and the optimal phase of ε-Ga_2O_3 was grown by GaI_3. At 700℃ temperature, the (-402) β-phase was observed in Ga_2O_3 films and the optimal phase of β-Ga_2O_3 was grown by GaI_3. The images of electron backscattering diffraction showed that the crystallinity of Ga_2O_3 grown by precursor ligand types is the single crystal epitaxial growth.

As a result, we confirmed that a carbon free xxx precursor was a good candidate to form high quality β-Ga_2O_3 epitaxial films and it would be useful to understand the epitaxial growth of metal oxide semiconductors using a mist-CVD method.

11:25am **PCSI-TuM2-36 Investigating SiC/Graphene/SiC(0001) Remote Epitaxy Using Hot-wall CVD***, **Daniel Pennachio,*** US Naval Research Laboratory*; J. Hajzus,* ASEE Research Associate at the US Naval Research Laboratory*; A. Lang,* US Naval Research Laboratory*; R. Stroud,* Former: US Naval Research Laboratory, Current: SESE, Arizona State University*; R. Myers-Ward,* US Naval Research Laboratory

Remote epitaxy (RE) is a promising new technique for epitaxial film removal and substrate reuse that utilizes monolayer graphene as a release layer [1]. Graphene grown directly on SiC(0001) substrates through Si sublimation or through propane chemical vapor deposition (CVD) is an ideal platform for remote epitaxy of wide bandgap (WBG) semiconductors as there is no need for a graphene transfer step, reducing the risk of introducing contamination or defects that can complicate the study of the remote epitaxy process. In addition, this materials system is compatible with commercially-viable WBG semiconductor growth and processing. However, SiC CVD growth is typically conducted using high-temperature hydrogen-based chemistries that could damage or remove graphene. This study investigates the effect of alternate CVD growth conditions on SiC/graphene/SiC(0001) remote epitaxy and optimizes CVD parameters to produce high-quality SiC epilayers while reducing damage to the graphene barrier. In addition, since the effect of epitaxial graphene features such as SiC macrostep morphology and associated layer inhomogeneity on the RE process is currently unknown, graphene preparation and associated morphology are varied to explore its effect on SiC epilayer formation.

Semi-insulating nominally on-axis 6H-SiC(0001) and n-type 4° off-axis 4H-SiC(0001) substrates were used to produce different SiC surface morphologies and graphene layer numbers. $Ar:H_2$ process gas flow ratio, growth precursor C/Si ratio, and growth temperature were optimized during hot-wall CVD RE to promote smooth film morphology. Nomarski optical microscopy, scanning electron microscopy, and atomic force microscopy found CVD deposition at 1620°C with Ar/H_2 ratios <20/5 slm, and C/Si ratios <1.55 to have the smoothest surface morphology and fewest polytype inclusions. Substrates with offcuts <0.1° from SiC(0001) exhibited lower epilayer macrostep density, but showed evidence of polytype impurities and 3D growth at C/Si ratios > 1.0. Point defect density in RE SiC epilayers using a graphene interface was shown to be lower than SiC homoepitaxy using similar conditions without graphene. Cross-sectional transmission electron microscopy was utilized to assess the growth interface and graphene layer integrity after CVD growth. Through this study, optimal RE growth processes are suggested for a balance of graphene survivability and SiC film morphology.

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11:30am **PCSI-TuM2-37 Investigating the Structurally and Chemically Heterogeneous Interface of AlGaN on (111) TaC***, D. Roberts,* National Renewable Energy Laboratory*; M. Miller,* Colorado School of Mines, USA*; A. Rice, **M. Brooks Tellekamp**,* National Renewable Energy Laboratory

The lack of lattice matched substrates for AlGaN is the primary limitation to achieving high-performance power electronics, high-frequency electronics, and deep UV (DUV) LEDs. This substrate limitation affects both material quality, through the formation of misfit-induced threading dislocations and strain-induced phase separation, and limitations to device geometry due to resistive or insulating electrical behavior. Dislocations and phase separation prevent AlGaN from reaching its full materials potential, and in the case of semiconducting substrates the primary loss mechanism in a vertically conductive device is resistive loss in the substrate itself. Thus, AlGaN alloys coulddrive disruptive technology iflong-standing substrate issues can be solved [1]. For $Al_xGa_{1-x}N$ there are competing effects of increasing alloy scattering, increased bandgap with increasing Al fraction, and decreasing dopant activation such that ideal compositions for power devices fall in the range 0.3 < x < 0.85 [2]. For these compositions pseudomorphic growth on GaN and AlN is very difficult or impossible.

Recently we have reported the design of virtual substrates for $Al_xGa_{1-x}N$epitaxy consisting of (111) TaC_x grown on sapphire substrates via RF sputtering [3]. The crystallinity is subsequently improved by face-to-face annealing. These substrates offer several opportunities to improve power electronic devices through lattice and thermal conductivity matching, high electrical conductivity, high stability, and epitaxial liftoff.

In this talk we will discuss the nucleation of AlGaN on TaC templates as performed by molecular beam epitaxy (MBE). Annealed TaC substrates show streaky-smooth reflection high-energy electron diffraction (RHEED) patterns and 6-fold rotational symmetry. The epilayers consist of $Al_xGa_{1-x}N$ in the range 0.7 < x < 1. Using RHEED, X-ray diffraction, atomic force microscopy, and transmission electron microscopy we investigate the impact of nucleating conditions on the structure of the film and interface. During metal-rich growth we observe incommensurate RHEED features associated with laterally contracted bilayers of metal which are not observed in nitrogen-rich growth. For $Al_{0.7}Ga_{0.3}N$ we observe relaxed growth on TaC and strained growth on co-loaded AlN templates, and corresponding to this relaxed growth only the film on TaC exhibits a step-terrace structure in AFM observed as spiral hillocks.

11:35am **PCSI-TuM2-38 Tailoring Growth Interfaces of Virtual Substrates for Power Electronics***, **Dennice Roberts**, M. Miller, A. Norman, B. Tellekamp,* National Renewable Energy Laboratory

Power electronics materials are poised to play a critical role in fulfilling next generation energy needs, with up to 90% of future energy demand predicted to flow through power electronics at some point.[1] Among a number of candidate materials, AlxGa1-xN is the strongest, having bipolar dopability, thermal and chemical stability, an ultra-wide bandgap, and demonstrated experimental feasibility. However, AlGaN growth is limited by a lack of lattice-matched substrates, ultimately stunting material quality at higher thicknesses needed for power electronics applications. Further, high power applications increasingly call for fully vertical device structures, necessitating a conductive substrate. [1] Recently our group identified the (111) plane of TaC as a conductive surface lattice-matched to $Al_{0.55}Ga_{0.45}N$, taking inspiration from prior work of AlN and GaN binaries on carbide and boride substrates. [2,3,4]

In this talk we demonstrate the growth of (111)-oriented TaC by RF sputtering. We investigate the interface of TaC with sapphire and SiC substrates and identify means to suppress competing Ta_2C nucleation in order to stabilize (111)-oriented TaC. Potential stacking sequences are identified with respect to crystal structure and observed twinning in the TaC films. We next assess structural changes and film recrystallization that results from face-to-face annealing of TaC thin films at high temperatures above 1500 ºC. Changes to grain structure and domain size are assessed by x-ray diffraction and surface morphology is explored using atomic force microscopy. **Fig 1** shows significant improvements to in- and out-of-plane strain following annealing along with the formation of terraced step edges at the film surface. Strain as a function of material composition and thickness is considered, as this may play a major role in future nucleation of AlGaN layers.

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11:40am **PCSI-TuM2-39 Titanium Dioxide Gate Dielectrics for ScAlN Barrier HEMT Structures*, Neeraj Nepal*,** *V. Wheeler, B. Downey, M. Hardy, D. Meyer,* U.S. Naval Research Laboratory

There has been increased interest in ScAlN-barrier high electron mobility transistors (HEMTs) as ScAlN has larger spontaneous and piezoelectric polarization fields than those in GaN and AlN, which can lead to larger two dimensional electron gas (2DEG) densities. Also, ScAlN with 18% Sc content is nearly latticed matched with GaN and has bandgap of 5.65 eV. Thus, ScAlN can provide a strain-free barrier for GaN HEMT structures with high carrier concentration. Recently, we have demonstrated ScAlN-barrier GaN HEMT structures with electron mobility of 910 cm^2/V-s and 2DEG density >3x10^{13} cm^{-2} [1]. However, these ScAlN/GaN HEMT devices still suffer from high leakage current [2]. Integrating gate dielectrics into these novel ScAlN-barrier HEMTs is necessary to decrease the leakage current, maintain high electric field breakdown and mitigate dc-RF dispersion in order to realize the full potential of these devices.

In this talk we report growth optimization and electrical properties of atomic layer deposition (ALD) grown TiO_2 gate dielectric on ScAlN-barrier HEMTs using Ultratech Fiji Gen2 ALD reactor. ALD process windows were initially monitored and optimized on Si substrates using *in-situ* ellipsometry. Films were deposited using tetrakis(dimethylamino)titanium (TDMAT) and an Ar/O_2 plasma at 300W. The TDMAT precursor temperature was maintained at 75 ^{o}C, while the pulse duration was varied from 0.25 to 0.35 sec. The plasma gas chemistry was also optimized. Optimal deposition parameters were used as initial condition to further optimize ALD conditions on ScAlN surface. On ScAlN barrier HEMT structures, deposition temperature was varied from 150 to 350 ^{o}C.

Atomic force microscopy was measured before and after ALD deposition showing minimal change in roughness as a result of the TiO_2 deposition.Contactless resistivity measurements performed before and after ALD and were also consistent, indicating that no plasma induced damage was occurring during ALD gate deposition. Vertical current-voltage and capacitance-voltage measurements were made on a Schottky-contacted HEMT structure and compared to devices with TiO_2 gate dielectrics deposited at different temperatures to discern the full electrical impact. As an example, an extracted dielectric constant of TiO_2 layer deposited at 200°C with O_2 flow of 20 sccm was 50 with no significant change in 2DEG density (changed from 2.7x10^{13} cm^{-2} to 2.6x10^{13} cm^{-2}after TiO_2 layer). Finally, we will present the band alignment of an optimum ALD TiO_2 on ScAlN structure using x-ray photoelectron spectroscopy.

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11:45am **PCSI-TuM2-40 Effect of Substrate and Growth Method on Vanadium Dioxide Thin Films by RF Magnetron Sputtering*, Adam Christensen*,** *A. Posadas, A. Demkov,* The University of Texas at Austin*; B. Zutter, P. Finnegan, S. Bhullar, S. Bishop, A. Talin,* Sandia National Laboratories

Interest in vanadium dioxide (VO_2) comes from its ability to undergo a metal-to-insulator transition (MIT) from monoclinic, semiconducting M1 phase to the metallic, rutile R phase. This transition occurs at a temperature of 340 K [2] and is generally characterized by a rapid change in electrical conductivity. This makes VO_2 attractive for many electronic and optical switching applications [1,3-4].Research on VO_2 thin film deposition has run the gamut in terms of the substrates and deposition methods used, but the use of bulk yttria-stabilized zirconia (YSZ) substrates and RF sputtering in combination or CMOS compatible fabrication has not been emphasized.

In this talk, we demonstrate that the growth of VO_2 (M1) thin films and the magnitude of the MIT (on/off ratio) are strongly impacted by choice of substrate and deposition method, and these choices are not trivial. This is achieved by comparing reactive RF sputtering deposition and oxidation of a polycrystalline vanadium metal film sputtered on (100)- and (111)-oriented YSZ substrates. The dioxide stoichiometry of these films is confirmed by x-ray photoelectron spectroscopy (XPS) and Raman spectroscopy. X-ray diffraction (XRD) reveals that direct reactive sputtering on both substrate orientations yields VO_2 (B), a metastable phase epitaxially stabilized by lattice matching. The metal sputtering and subsequent oxidation process (Fig. 1a) on (100)-oriented YSZ results in (010)-oriented VO_2 (M1) exhibiting an MIT on the order of 10^3confirmed by temperature dependent conductance measurements (Fig. 1b) in CMOS compatible devices. With the same metal sputtering and subsequent oxidation process on (111)-oriented YSZ, we achieve slightly overoxidized films with similar magnitude of MIT.

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PCSI
Room Redondo - Session PCSI-TuE
Spin Transport and Spintronics
Moderator: Scott Crooker, Los Alamos National Laboratory

7:30pm **PCSI-TuE-1 Proximitized Materials: From Spintronics to Majorana States*, Igor Zutic,*** University at Buffalo-SUNY **INVITED**

Advances in scaling down heterostructures and atomically-thin two-dimensional (2D) materials suggest a novel approach to systematically design materials as well as to realize exotic states of matter. A given material can be transformed through proximity effects [1] whereby it acquires properties of its neighbors, for example, becoming superconducting, magnetic, topologically nontrivial, or with an enhanced spin-orbit coupling. Such proximity effects not only complement the conventional methods of designing materials by doping or functionalization, but can also overcome their various limitations. In proximitized materials it is possible to realize properties that are not present in any constituent region of the considered heterostructure. Unlike the superconducting proximity, which could exceed mm, other proximity effects extend over only several nm. After some background on proximity effects, we discuss implications of magnetism leaking into initially a non-magnetic region [1-3]. We show that gate-tunable band topology allows helicity reversal of the emitted light [4] and novel paths to spin-lasers [5]. Motivated by the search for elusive spin-triplet topological superconductivity hosting Majorana states, which are considered for fault-tolerant quantum computing, we explain the importance of proximity effects. Instead of epitaxially-defined, topological nanostructures could be designed using magnetic textures and combining magnetic and superconducting proximity effects in 2D systems [6]. Measurements of proximity-induced topological superconductivity in planar Josephson junctions [7] provide novel opportunities for controlling Majorana states [8].

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8:10pm **PCSI-TuE-9 Spin/Valley Pumping and Long-Distance Spin Transport in Monolayer TMD Semiconductors*, Cedric Robert,*** LPCNO, CNRS INSA Toulouse, France **INVITED**

Monolayers of transition metal dichalcogenides (TMD) are ideal semiconductor materials to control both spin and valley degrees of freedom either electrically or optically. Nevertheless, optical excitation mostly generates excitons species with inherently short lifetime and spin/valley relaxation time. In this presentation we will show that we can strongly polarize (up to 75%) the resident electrons in n-doped WSe_2 and WS_2 monolayers by using a circularly polarized continuous wave laser [1]. Then, using a spatially-resolved optical pump-probe experiment (see Figure 1), we measure the lateral transport of spin/valley polarized electrons over very long distances (tens of micrometers) [2]. These results highlight the key role played by the spin-valley locking effect in TMD monolayers on the pumping efficiency and the polarized electron transport.

PCSI

Room Redondo - Session PCSI-WeM1

Topological and Magnetic Materials

Moderator: Joan Redwing, The Pennsylvania State University

8:30am **PCSI-WeM1-1 Development of Thin Film Platforms for Tunable Topological Materials*, Anthony Rice,*** NREL **INVITED**

Cd_3As_2 is a prototypical Dirac semi-metal, a class of materials with gapless topologically protected electronic states. These materials could play a role in a large number of applications, including transistors, spintronics, photodetectors, and thermoelectrics. To be used in these technologies, however, significant progress needs to be made in developing routes to tune their properties as well as combining them with materials that are already technologically relevant. Here, a II-VI/III-V platform is first developed which allows for growth of Cd_3As_2 on GaAs(111) with high electron mobility. This platform is extended for both (110) and (001) film orientations, ultimately allowing for growth of heterostructures relevant for photodetectors. Analogous approaches also allow for integration of Cd_3As_2 with Si(001). Ways to alter the electronic properties of Cd_3As_2 will also be discussed. This work demonstrates routes toward developing quantum materials for a variety of applications and may be extended to a variety of other materials system.

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9:10am **PCSI-WeM1-9 Electrical Transport of Zn-doped Dirac Semimetal Cd_3As_2 Films*, Ian Leahy,*** *J. Nelson, A. Rice, K. Alberi,* National Renewable Energy Laboratory

Topological semimetals (TSMs) are emerging as materials with potential use in low powered electronics and spintronic devices [1-4]. In order to translate the useful properties of TSMs to device applications, studies focusing on reliable epitaxial growth, disorder, and the control of electronic states in TSM films are needed. Here, wefocus on the use of alloying with Zn to modify the electronic structure and electrical transport of $(Cd_{1-x}Zn_x)_3As_2$ with x = 0-0.23.

Zn doping of Cd_3As_2 has been used to lower the carrier concentration and move the Fermi energy closer to the Dirac point. However, the addition of Zn is also expected to modify the band structure, causing a change in the electronic structure from Dirac semimetal to semiconductor [5]. By tuning the growth conditions to suppress native defects in our films [6] we are able to produce $(Cd_{1-x}Zn_x)_3As_2$ films with carrier concentrations a full order of magnitude smaller (as shown in Fig. 1b, $\sim 10^{17}$ cm^{-3}) than other literature reports ($>10^{18}$ cm^{-3}) [7]. Lowering the starting carrier concentration enables us to tune the Fermi energy with smaller amounts of Zn doping.

Figure 1 shows the Zn doping dependence of the low-field mobility and the carrier density for our films. For x < 0.1, we observe a slight reduction in mobility with increasing x paired with an order of magnitude reduction in the carrier density. By x = 0.23, the dominant carrier switches from n-type to p-type accompanied by a 100x reduction of the carrier mobility, consistent with the transition from TSM Cd_3As_2 to semiconducting Zn_3As_2 behavior. We will present a careful analysis of the electrical transport properties to explore the low Zn doping regime where the n-type carrier densities reach their lowest values before the electronic structure is significantly altered.

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9:15am **PCSI-WeM1-10 Epitaxial Growth of Weyl Semimetal TaAs on GaAs(001)*, Jocienne Nelson,*** *A. Rice, I. Leahy,* NREL*; R. Kurleto,* University of Colorado at Boulder*; J. Mangum,* NREL*; A. Shackelford,* University of Colorado at Boulder*; M. van Schlifgaarde,* NREL*; M. Holtz,* Colorado School of Mines*; D. Dessau,* University of Colorado at Boulder*; K. Alberi,* NREL

Three dimensional topological semimetals (TSMs) were experimentally discovered in the past decade and exhibit extraordinary properties such as extremely high mobility [1], conductivity [2] and magnetoresistance [3] stemming from their protected bandstructure. They are now emerging as excellent candidates for a wide variety of applications including photovoltaics [4], spintronics [5], thermoelectrics [6], and catalysts [7]. Weyl semimetals in particular have unique bandstructures with a singly degenerate linear band crossings. While there has been a great deal of success studying novel bulk single crystal TSMs, they are not suitable for device applications. Instead, epitaxial thin films are needed to access unique behaviors such as the Chiral anomaly and also insert them into more conventional device structures. Thus, there is a need to develop thin film TSMs compatible with semiconductor manufacturing to accelerate the adoption of TSMs into device applications.

We report epitaxial growth of the Weyl semimetal TaAs on GaAs(001) substrates using molecular beam epitaxy. TaAs has been widely studied in bulk crystal form but has not previously been synthesized as a single crystal film, likely due to the challenge posed by a lack of lattice matched substrates. In this presentation we discuss growth strategies to realize single crystal films and eliminate secondary phases. Fig. 1 shows x-ray diffraction and reflection high energy electron diffraction (RHEED) measurements demonstrating that the TaAs is single crystal. We will also discuss the impact of epitaxial growth on intrinsic doping and magnetoresistance.

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9:20am **PCSI-WeM1-11 Quasi Van Der Waals Epitaxy of Magnetic Topological Insulator on GaAs (111) Substrate*, Yuxing Ren,*** *L. Tai, S. Chong, G. Qiu, K. Wang,* University of California, Los Angeles

Magnetic topological insulator could achieve quantum anomalous Hall (QAH) effect and spin-orbit torque (SOT) switching in the same structure. This is promising for its future applications in memory or switching applications with its robust surface properties by topological protection. In this work we have grown $Cr{:}(Bi_xSb_{1-x})_2Te_3$ and $MnBi_2Te_4$ on GaAs (111) substrate through modulation doping by MBE (Molecular Beam Epitaxy). The doping level and the thickness of each layer is examined to tune the bandgap and the Fermi level of the whole sample. In this way, we can tune the Fermi level into the bandgap and optimize the total resistivity to achieve quantization.

Considering the van der Waals nature of the epitaxial layers, it has very weak van der Waals bonding with the substrate. This gives rise to a quasi Van der Waals epitaxial growth mode at the interface of GaAs (111) and epitaxial layers. In this growth mode strain relaxes quickly within the 1st epitaxial layer. Growth mechanism and the influence on its transport properties are also discussed.

9:25am **PCSI-WeM1-12 UPGRADED: Asymmetric Magnetic Proximity Interactions in Ferromagnet/Semiconductor van der Waals Heterostructures*, Scott Crooker,*** Los Alamos National Laboratory

Magnetic proximity interactions (MPIs) between atomically-thin semiconductors and two-dimensional magnets provide a means to manipulate spin and valley degrees of freedom in nonmagnetic monolayers, without the use of applied magnetic fields.In such van der Waals (vdW) heterostructures, MPIs originate in the nanometer-scale coupling between the spin-dependent electronic wavefunctions in the two materials, and typically their overall effect is regarded as an effective magnetic field acting on the semiconductor monolayer. Here we demonstrate that this picture, while appealing, is incomplete: The effects of MPIs in vdW heterostructures can be *markedly asymmetric*, in contrast to that from an applied magnetic field [1].Valley-resolved optical reflection spectroscopy of $MoSe_2/CrBr_3$ vdW structures reveals strikingly different energy shifts in the *K* and *K'* valleys of the $MoSe_2$, due to ferromagnetism in the $CrBr_3$ layer. Strong asymmetry is observed at both the A- and B-exciton resonances. Density-functional calculations indicate that valley-asymmetric MPIs depend sensitively on the spin-dependent hybridization of overlapping bands, and as such are likely a general feature of such hybrid vdW structures. These studies suggest routes to selectively control *specific* spin and valley states in monolayer semiconductors.

9:45am **PCSI-WeM1-16 Atomic Layer Epitaxial Growth of Kagome Magnet Fe_3Sn_2 Thin Films***, **Shuyu Cheng**, B. Wang, I. Lyalin, N. Bagués, A. Bishop, D. McComb, R. Kawakami,* Ohio State University

Kagome magnets are attractive family of materials due to complex spin textures and topological band structures [1]. As a typical example of kagome magnet, Fe_3Sn_2 has been shown to exhibit spin frustration [2] and magnetic skyrmions [3] in real space, and massive Dirac fermions [4] in momentum space. However, most of these studies were done on bulk crystals. The development of epitaxially grown Fe_3Sn_2 thin films will be an exciting future direction, as the thin films of kagome magnets enable potential applications in devices as well as the discovery of new phenomena.

In this presentation, we report our progress in atomic layer molecular beam epitaxy (AL-MBE) growth of kagome magnet Fe_3Sn_2 thin films on Pt(111) buffer layer on Al_2O_3(0001) substrates. During the growth, the RHEED intensity shows oscillatory behavior, indicating layer-by-layer growth mode (Fig. 1(a)). AL-MBE allows us to grow Fe_3Sn_2 at much lower temperatures and therefore produces a sharp interface. The high quality of the sample is confirmed by various methods (Fig. 1(b)). The magnetic properties of Fe_3Sn_2 thin films are also presented here (Fig. 1(c)) [5]. We further show that the anomalous Hall effect (AHE) only has intrinsic contribution, suggesting the magnetic Weyl semimetal nature of Fe_3Sn_2 (Fig 1(d)).

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9:50am **PCSI-WeM1-17 Selectively Oriented Crystalline Growth of Mn_3Sn on Al_2O_3(0001) using Molecular Beam Epitaxy***, **Sneha Upadhyay**, T. Erickson , H. Hall, A. Shrestha,* Ohio University*; J. Moreno,* Universidad Autónoma de Puebla, Instituto de Física, Apartado , Mexico*; D. Ingram ,* Ohio University*; K. Sun,* The University of Michigan*; A. Smith ,* Ohio University

Kagome antiferromagnet Mn_3Sn has garnered attention due to the presence of interesting properties such as anomalous Hall effect below 420K[1], Nernst effects and presence of exchange bias[2]. Until now most thin film growths have been conducted by using sputter deposition or by cleaving. Recently, Higo *et al* reported the finding of the 100% perpendicular full switching of the (01$\underline{1}$0) oriented Mn_3Sn which was grown using molecular beam epitaxy on a MgO (110) substrate having a thin W buffer layer [3]. This result indicated that the orientation and possible strain of the film can be key for film transport properties and therefore its of great interest to explore how one can achieve different crystalline film orientation of Mn_3Sn.

In this talk, we demonstrate the synthesis of crystalline Mn_3Sn on Al_2O_3(0001) without a buffer layer using molecular beam epitaxy. The samples were deposited at two different temperatures T_h (500 ± 9 °C) and T_l (416 ± 9 °C) with Mn: Sn flux ratio of 3.2:1 for 90 minutes. Our analysis indicates that for the two temperatures, the resulting orientations of the films are different, with the T_h sample being predominantly *c*-oriented and T_l sample being 43% *a*-oriented but in our recent template growth method at room temperature we achieved 82% *a*-oriented film. In both cases the reflection high energy electron diffraction (RHEED) patterns were streaky indicating a crystalline film and the cross-sectional scanning tunneling electron microscopy (STEM) gave an insight into the morphology of the samples. In both cases the sample are discontiguous with presence of 3D morphology for sample grown at T_h and quasi-2D morphology for the T_l grown sample. Template grown sample are contiguous and show streaky RHEED patterns throughout the growth. Orientation relationships between the Mn_3Sn films and the sapphire substrate are determined from *in-plane* and *out-of-plane* measurements. The composition of the samples, the strain effects as well as the pseudomorphic overlay will be discussed in detail. Furthermore, we are in the process of doing STM measurements of the samples and performing theoretical calculations.

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PCSI

Room Redondo - Session PCSI-WeM2

Oxide Semiconductors nd Memristor Materials

Moderator: Holger Eisele, Otto-von-Guericke-Universität

10:35am **PCSI-WeM2-26 Advancement and Prospects of Ultra-Wide-Bandgap Oxide Semiconductors***, **Shizuo Fujita,*** Kyoto University, Japan*; K. Kaneko,* Ritsumeikan University, Japan*; K. Tanaka,* Kyoto University, Japan **INVITED**

It is a general trend of semiconductors that the wider bandgap materials show the higher characteristic breakdown field E_c, exhibiting high Baliga's figure of merit, which is proportional to E_c^3. The bandgap of gallium oxide (Ga_2O_3), 4.5-5.7 eV dependent on its crystal phase, is wider than those of SiC and GaN, and therefore Ga_2O_3 is attracting high attention as a material for future power devices. In addition, Ga_2O_3 bulk substrates are grown by the conventional solution-based methods, and the device-oriented research is done based on the homoepitaxial growth, similarly to the traditional III-V semiconductor research like GaAs and InP. Since the first demonstration of MESFETs and MOSFETs in 2012 and 2013, respectively by NICT, Japan, rapid progress of the devices, including 1.4 kV SBD, normally-off MOSFETs, 2.66 kV vertical FINFETs, high frequency MOSFETs (f_{max}=27 GHz), high-frequency HFETs (f_{max}=37 GHz), and 4.4 kV MESFETs, are going on.

Ga_2O_3 takes at least five polymorphs, and β-phase is the most stable phase. The Ga_2O_3 substrates are the β-phase, and the most advanced device research shown above is based on the β-phase. Other phases are semi-stable, but interesting characteristics which are not realized by the β-phase are expected. For example, the crystal structure of α-phase (corundum) is the same as that of sapphire, allowing complete bandgap engineering from that of Ga_2O_3 to Al_2O_3. Our group has been contributing to the research on α-Ga_2O_3, which was grown on sapphire substrates by the mist CVD method. FLOSFIA Inc. has developed SBDs of α-Ga_2O_3, and they may be supplied at a low cost because of the use of low-cost sapphire substrates. P-type conductivity of Ga_2O_3 is a difficult problem, but there is a p-type corundum-structured α-$(Ir,Ga)_2O_3$ closely lattice matched to α-Ga_2O_3, allowing the pn junction of ultra-wide-bandgap semiconductors. For α-Ga_2O_3, heteroepitaxial growth on sapphire results in dislocation defects, and how to overcome this problem is now one of the most important subjects of our research. The orthorhombic ε (or named as κ) phase is expected to cause strain-induced in-axis polarization, preferrable to heterojunction FETs like AlGaN/GaN.

At the conference, we plan to show the up-to-date research achievements on ultra-wide-bandgap oxide semiconductors and their devices. The focus is given to Ga_2O_3 semiconductors, but may not be limited to Ga_2O_3. The efforts on developing other promising ultra-wide-bandgap oxide semiconductors will also introduced.

A part of our research works was conducted under the support by JSPS KAKENHI (20H00246) and MIC research and development (JPMI00316).

11:15am **PCSI-WeM2-34 Adsorpion of Gases on β-Ga2O3 Surfaces***, **Jonathan Karl Hofmann**,* Forschungszentrum Juelich GmbH, Germany*; C. Schulze, D. Rosenzweig,* Technical University of Berlin, Germany*; Z. Galazka,* Leibnitz-Institut für Kristallzüchtung, Germany*; M. Dähne,* Technical University of Berlin, Germany*; H. Eisele,* Otto-von-Guericke-Universität, Magdeburg, Germany

β-Ga2O3 is a transparent conductive oxide with a fundamental bad gap of E_G=4.9 eV [1]. Its typical n-type conductivity is controllable via the growth conditions, intentional doping or post-growth heat treatment [2]. Due to its large band gap, β-Ga2O3 is a promising candidate for applications in high power electronics e. g. in field effect transistors with high breakdown voltages [3]. Additionally, since its conductivity is dependent on the ambient conditions, β-Ga2O3 can be used in oxygen sensors [4]. In this contribution, we address the question how its surface properties develop under typical ambient conditions, i. e. under H2O and O exposure, but in a controlled way. Therefore, we used a gas-inlet for H2O vapor and an atomic O source. The β-Ga2O3 single crystals were grown with the Czochralski method [5] and cleaved under UHV-conditions in order to achieve intrinsic surface conditions before gas adsorption. Using Auger electron spectroscopy (AES), low energy electron diffraction (LEED), and scanning tunneling microscopy/spectroscopy (STM/STS), we show how the different adsorbed atoms/molecules change the structure and electronics properties of β-Ga2O3(100) and (001) surfaces in comparison to the freshly cleaved surfaces. On the (100) surface, large clusters of H2O with an undisturbed surface in between were observed. However, STS showed no change in the electronic states. All spectra exhibit a large apparent band gap due to upwards band bending. Negative tunneling voltages gave rise to an accumulation current. Also, an additional exposure to atomic O did not lead to a change in the electronic states, although it lead to a higher surface coverage. On the (001) surface, oxygen covered almost the complete surface. STS showed that O lifts the band bending inherent in clean β-Ga2O3 surfaces.

The project was supported by the Leibnitz association, Leibnitz Science Campus GraFOX, project C2-3.

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[2] Z. Galazka et al., Journal of Crystal Growth 404, 184 (2014)
[3] K. Tetzner et al., IEEE Eletrcon Device Letters 40, 1503-1506 (2019)
[4] M. Bartic, physica status solidi (a) 213, 457-462 (2015)
[5] Z. Galazka, J. Appl. Phys. 131,031103 (2022)

11:20am **PCSI-WeM2-35 Design of Rare-Earth Nickelate Memristors***,* ***Olivia Schneble,*** Colorado School of Mines*; B. Tellekamp,* National Renewable Energy Laboratory*; J. Zimmerman,* Colorado School of Mines

Rare-earth nickelates (*R*NiO$_3$) are distorted perovskite oxides that exhibit a charge-transfer insulator-metal transition (IMT) at temperatures dependent on the rare-earth cation size. LaNiO$_3$ is the exception, remaining metallic at all temperatures. Materials with this thermally driven transition lend themselves memristor applications because they can be switched from high-resistance to low-resistance states via Joule heating. Rare-earth nickelates (RNOs) also span the ideal transition temperature range (400-500 K) and the IMT can be modified by alloying as well as strain state [1]. Previous research in other material systems has found that higher transition temperatures require more energy per operation, but transitions too close to room temperature would require active cooling[2]. This work focuses on the control of RNO material properties for biomimetic neuronal devices.

Our proposed vertical device consists of an LaNiO$_3$ layer that acts as both a bottom electrode and an epitaxial buffer, an epitaxial RNO switching layer, and metallic top contacts. This structure can be translated to dense crossbar arrays and can be grown on numerous crystalline substrates. However, the different bulk structure of LaNiO$_3$ (rhombohedral) from the other RNOs and the relevant substrates (orthorhombic) complicates the heteroepitaxial picture. Factors such as biaxial strain alter the NiO$_6$ octahedral distortions that govern electronic structure, so understanding the substrate/LaNiO$_3$ and LaNiO$_3$/RNO interfaces is critical.We have employed both pulsed laser deposition and RF sputtering to grow epitaxial layers and heterostructures. Preliminary studies focus on NdNiO$_3$, which is more widely studied and easier to stabilize. Both deposition techniques can produce fully-strained, highly-crystalline NdNiO$_3$ on LaNiO$_3$ buffer layers. However, crystallinity does not predict electrical behavior, which we find to be highly dependent on deposition conditions even with nominally constant composition and strain state. These effects are not fully explained by thickness variation, and we will discuss additional mechanisms underlying this variability. We also use measured material properties to model RNO memristors in LT-SPICE, which provides insight into the necessary electrical behavior as we optimize our thin films.

11:25am **PCSI-WeM2-36 Image Recognition Process of IGZO/CsPbBr$_3$ Photo-synaptic Transistors Imitating Human Learning Processes***,* ***Goeun Choi****, Y. Rim,* Department of Intelligent Mechatronics Engineering, and Convergence Engineering for Intelligent Drone, Sejong University, Republic of Korea

Neuromorphic devices are consisted of mimic structures of neurons and synapses in the human brain, which can simultaneously process computation and memory roles for the high- speed computations and high-power efficiencies. Recently, light-applied optical synapses with light applied among neuromorphic semiconductors systems have received attentions due to low crosstalk, wide bandwidth, fast computation, and lower energy consumption [1].

In this study, perovskite CsPbBr3 photo absorber embedded IGZO semiconductor-based photo-synaptic transistors were proposed. Oxide semiconductor (IGZO) is being actively studied because it can realize high mobility and high transparency with low process temperature and low manufacturing cost [2]. However, since the bandgap is wide, there is a limitation in not recognizing light in the visible ray region. CsPbBr3 has a low bandgap (~2.3 eV) and can be formed easily onto the IGZO surface using a solution process. In the optical synaptic arrangement, as the number of pulses increased and the intensity of light increased, the image tended to be clearly recognized [3]. It is consistent with the fact that the more often humans meet, the more facial features they remember [4]. We prove that the image recognition process of the produced photo-synaptic array is similar to that of human learning.

11:30am **PCSI-WeM2-37 IGZO Synaptic Transistors Using Ionic Gel-Based Electric Double Layer Operation for Low Voltage Driving***,* ***Kyongjae Kim****, Y. Rim,* Sejong University, Republic of Korea

Neuromorphic computing, which mimics the behavior of biological neurons and synapses is a method that dramatically solves the problem of the traditional von Neumann structure by performing information processing and data storage simultaneously. Transportation of neurotransmitter from pre-synaptic neurons to post-synaptic neurons induce excited post-synaptic potential, and this process of excitatory post-synaptic potential is the key factor in conducting memory function and data processing simultaneously. Here we propose a coplanar structure having an ionic gated electric double layer transistor (EDLT) with indium gallium zinc oxide (IGZO) for low voltage driving and its synaptic behavior based on modulated channel conductivity induced by an electric double layer (EDL) [1]. The EDL is formed at the interface between IGZO and ionic gel dielectric, and we confirmed that the operation voltage was below 1 V due to the formation of large capacitance (~2μF) [2]. We studied the physical phenomenon at the interface between the IGZO channel and the ionic gel where EDL was formed by the oxygen vacancy of the channel and the ion contents of the ionic gel. This interface is a crucial point for the synaptic behavior owing to the variations of conductance of the interface with the ion movements. The ionic gated EDLT achieves subthreshold swing of 0.1/dec, on/off ratio of 105, and 103 range of excitatory post-synaptic current (EPSC). We successfully demonstrated that the gate bias applied in the form of a pulse and source/drain bias linearly controls the conductance of the channel and shows potentiation, depression, and memory characteristics, revealing its potential to be industrialized in next-generation neuromorphic computing.

11:35am **PCSI-WeM2-38 UPGRADED: Electrostatic *S*haping of Magnetic Transition Regions in La$_{0.7}$Sr$_{0.3}$MnO$_3$***,* *Q. Lan,* Forschungszentrum Jülich GmbH, Germany*; C. Wang,* Tsinghua University, China*; L. Jin, M. Schnedler, L. Freter,* Forschungszentrum Jülich GmbH, Germany*; K. Fischer,* National Institute of Technology, Japan*;* ***Philipp Ebert****, R. Dunin-Borkowski,* Forschungszentrum Jülich GmbH, Germany

We report a magnetic transition region in La$_{0.7}$Sr$_{0.3}$MnO$_3$ with gradually changing magnitude of magnetization, but no rotation, stable at all temperatures below T_C. Spatially-resolved magnetization, composition and Mn valence data reveal that the magnetic transition region is induced by a subtle Mn composition change, leading to a charge transfer at the interface due to carrier diffusion and drift. The electrostatic shaping of the magnetic transition region is mediated by the Mn valence which affects both, magnetization by Mn^{3+}-Mn^{4+} double exchange interaction and free carrier concentration.[1]

[1] Q. Lan *et al.*, Phys. Rev. Lett. **129,** 057201(2022)

PCSI

Room Redondo - Session PCSI-WeA1

Photoemission Spectroscopy and high-k Dielectrics

Moderator: Igor Zutic, University at Buffalo-SUNY

2:00pm **PCSI-WeA1-1 Optical Field-Driven Ultrafast Electron Control Inside of Graphene and at the Surface of Metal Needle Tips*, Peter Hommelhoff,*** Friedrich-Alexander-University Erlangen-Nürnberg (FAU), Germany **INVITED**

With femtosecond laser pulses, electrons can be driven on ultrafast timescales. If these laser pulses are just two optical cycles long (roughly 5 fs pulse duration at 800 nm center wavelength, 1 fs = 10^{-15} sec), it matters how the exact optical field looks like within the laser pulse envelope – but this optical field can be well controlled these days in so-called phase-stable laser pulses.

This talk will give an overview of our work circling around controlling electrons on sub-femtosecond time scales with phase-controlled laser pulses. After a brief introduction to these laser pulses, the first part of the talk will focus on strongly driven electrons inside of graphene. We could show that electrons undergo coherent coupled intraband motion and interband transitions. More specifically, we could demonstrate subsequent coherent Landau-Zener transitions, allowing us to realize Landau-Zener-Stückelberg-Majorana interferometry with electrons inside of graphene. Based on this physics, we could demonstrate a record-fast current switch, with a turn-on time of around 1fs, leading to real charge carrier generation [1].Just recently, we also gained deep insights into how the graphene-gold interface can be used to read out virtual charge carriers. Based on these insight, we could demonstrate a logic gate potentially providing petahertz bandwidths [2].

The focus of the second part of the talk will be on strongfield physics at the surface of metal needle tips. Here we could demonstrate that we can control photo-emitted electrons with the help of phase-controlled laser pulses fully coherently. We observe all hallmarks of strongfield physics, now at the surface of a solid [3]. With more complex two-color laser fields, we could fully reconstruct the attosecond-fast emission dynamics (1 as = 10^{-18} sec). In particular, we find a tunneling time of 710 ± 30 attosec, i.e., we can now trace electron emission dynamics from solids with attosecond time resolution [4].

[1] Higuchi et al., Nature **550**, 224 (2017); Heide et al., PRL **121**, 207401 (2018); Heide et al., Nat. Phot. **14**,

219 (2019); Heide et al. NanoLett. **21**, 9403 (2021); Heide et al., PRA **104**, 023103 (2021)

[2] Boolakee et al., Nature **605**, 251 (2022);

[3] Krüger et al., Nature **475**, 78 (2011); Krüger et al., J. Phys. B **51**, 172001 (2018);

[4] Dienstbier et al., manuscript submitted

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2:40pm **PCSI-WeA1-9 The Diamond (111) Surface Reconstruction and Epitaxial Graphene Interface*, Simon Cooil,*** University of Oslo, Norway

A rejuvenated interest in diamond as a state-of-the-art electronic material has occurred over the last couple of decades as its potential for use in emerging quantum information and sensing technologies becomes apparent.The growing demand for miniaturisation has also led to increased interest in the nanoscale properties of diamond and the production of diamond-graphene (sp3 – sp2) interfaces. However, fundamental studies of the diamond (111) surface electronic structure remain incomplete and controversy surrounding the metallic[1] or semiconducting[2] nature of the (2×1) surface reconstruction remains unresolved. We therefore follow the evolution of the diamond (111) surface electronic and physical structure as it undergoes reconstruction and subsequent graphene formation with angle-resolved photoemission spectroscopy, low energy electron diffraction, and compare to complementary density functional theory calculations.

The studies begin on the hydrogen terminated H:C(111)-(1×1) surface, proceeding to the C(111)-(2×1) surface reconstruction that occurs following detachment of the surface adatoms at 920 °C. We then continue through to the liberation of the reconstructed surface atoms into a free-standing monolayer of epitaxial graphene at temperatures above 1000 °C. Our results show that the C(111)-(2×1) surface is metallic as it has electronic states that intersect the Fermi-level. This is in strong agreement with a symmetrically π-bonded chain model and should contribute to resolving the controversies that exist in the literature surrounding the electronic nature of this surface. The graphene formed at higher temperatures exists above a newly formed C(111)-(2×1) surface and appears to have little substrate interaction as the Dirac-point is observed at the Fermi-level. Finally, we demonstrate that it is possible to hydrogen terminate the underlying diamond surface by means of plasma processing without removing the graphene layer, allowing for tuneable substrate interactions at the graphene-semiconductor interface[3].

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2. Graupner, R., et al., *Dispersions of surface states on diamond (100) and (111).* Physical Review B, 1997. **55**(16): p. 10841.
3. Reed, B.P., et al., *Diamond (111) surface reconstruction and epitaxial graphene interface.* Physical Review B, 2022. **105**(20): p. 205304.

2:45pm **PCSI-WeA1-10 Hard X-Ray Photoelectron Spectroscopy for Material Science Applications***, P. Amann,* Scienta Omicron, Germany*; **Takahiro Hashimoto,*** Scienta Omicron

Investigating buried interfaces, device electronics or batteries by chemically sensitive instrumentation is highly desired in materials science applications. X-ray photoelectron spectroscopy (XPS) is a powerful method to investigate the chemical nature of surfaces. However, investigations of buried interfaces occurring in, e.g., device electronics are difficult as the energies of the created photoelectrons are not high enough and scattering inside the material's bulk limit the detected signal intensity.

During the past decade, increased attention has been shown to hard X-rays in the photoelectron spectroscopy field [1]. This is primarily due to the increased information depth enabled by the higher photon energies.

Using Scienta Omicron's HAXPES Lab, featuring a monochromatic Ga Ka X-ray source in combination with a hemispherical electron analyzer that includes a +/- 30 degree acceptance angle [2], we were able to investigate buried interfaces, in-operando devices and real world samples (Fig.1 A). [3] In this presentation we will give an overview of applications with a focus on bias-applied measurements from device electronics. Si-based materials are widely used in the semiconductor industry and are subject to chemical changes upon voltage application. Investigating a layered structure of 4 nm thick ZrO_2 on 20 nm TiN on p-doped Si, the binding energy shift could be characterized upon applied voltage in-operando without sample destruction. These changes can be assigned to trapped carriers in the defect level at the Ti-N/p-Si interface. (Fig. 1 B, C).

2:50pm **PCSI-WeA1-11 Advanced Semiconductor-Oxide Interfaces of Ferroelectric and RRAM Devices*, Rainer Timm,*** Lund University, Sweden **INVITED**

Ferroelectric field effect transistors (FeFET) with ultrathin (below 5 nm) ferroelectric $Hf_{1-x}Zr_xO_2$ (HZO) layers or resistive random access memory (RRAM) stacks based on oxygen vacancy HfO_2 layers are currently in the focus of research towards steep-slope transistors, neuromorphic networks, and computation-in-memory application. Especially promising is their combination with III-V semiconductor substrates such as InAs, which offers superior charge carrier mobility compared to Si. Our collaborators at the Nanoelectronics group of Lund University are pioneering in developing InAs nanowire-based FeFET gate-all-around [1,2] and RRAM [3,4] devices including 1 transistor 1 resistor structures integrated in a single nanowire [4]. These novel devices have in common that their performance critically relies on the quality and structure of the semiconductor-oxide interface. Here, I will present in-depth studies of such interfaces using *operando* soft- and hard X-ray photoemission spectroscopy (XPS/HAXPES), complemented by other synchrotron-based methods, which are resulting in a paradigm change in the understanding of MOS structures.

For InAs/HfO_2 RRAM devices, we found that the existence of a sufficiently thick As-oxide interface layer, obtained through extended oxygen plasma pulses, below the HfO_2 film is crucial for enabling resistive switching [4]. This is contrary to the case of conventional InAs-based MOSFETs where we previously were aiming for the perfect self-cleaning and observed complete As-oxide removal during HfO_2 deposition [5]. Furthermore, also the structure of the HfO_2/TiN top metal interface of RRAM devices is relevant, where substantial band-bending can result in strong Schottky barriers [3].

From initial *operando* HAXPES studies of FeFET devices, with applied dc bias or upon positive-up-negative-down (PUND) switching pulses, we derived the unexpected result that the applied bias does not drop across the ferroelectric HZO oxide layer, but instead only across a very thin interfacial InAs-oxide layer. Simulations explain this behavior by the defect density in the interfacial oxide. Nevertheless, the FeFETs show high polarization values and good endurance.

The close connection between state-of-the-art device development and detailed characterization of the involved materials science aspects are the key to an improved understanding of the device functionality.

[1] A. E. Persson et al., Appl. Phys. Lett. **116**, 062902 (2020).
[2] R. Atle et al., Adv. Mater. Interfaces **2022**, 2201038 (2022).
[3] Z. Yong et al., Appl. Surf. Sci. **551**, 149386 (2021).
[4] M. S. Ram et al., Nature Electronics **4**, 914 (2021).
[5] R. Timm et al., Nature Communications **9**, 1412 (2018).

3:30pm **PCSI-WeA1-19 Stoichiometric Control and Optical Properties of $BaTiO_3$ Thin Films Grown by Hybrid MBE**, ***Benazir Fazlioglu Yalcin**, A. Suceava, T. Kuznetsova, Z. Wang, I. Dabo, V. Gopalan,* Penn State University*; R. Engel-Herbert,* Paul Drude Institute, Germany

$BaTiO_3$ is a technologically tremendously relevant material in the perovskite oxide class with above room temperature ferroelectricity and a very large electro-optical coefficient, making it highly suitable for emerging electronic and photonic devices. [1,2] An easy, robust, straightforward, and scalable growth method is required to synthesize epitaxial BaTiO3 thin films with reproducible thin film properties allowing sufficient control over the film's stoichiometry. Here, we report on the growth of BaTiO3 thin films by hybrid molecular beam epitaxy. A self-regulated growth window was identified using complementing information (Fig. 1a, b), the evolution of reflection high energy electron diffraction images during film growth, the deviation of the intrinsic lattice parameter, and film surface morphology. Subsequent optical characterization of the BaTiO3 films by spectroscopic ellipsometry revealed refractive index and extinction coefficient values closely resembling stoichiometric bulk BaTiO3 (Fig. 1c, 1d). In addition to the expected degradation of optical properties with increasing deviation from the self-regulated growth window, an optical absorption peak emerged at 700 nm even in the absence of a detectable lattice parameter expansion of BaTiO3 thin films. This feature was identified by first-principles calculation as Ba vacant lattice site. In addition, optical second harmonic generation analysis was performed to determine the polar symmetry of the films which revealed bulk-like SHG coefficients. In this talk, we will discuss how the optical properties of BaTiO3 can be utilized as a much finer probe than intrinsic lattice parameter expansion to determine the stoichiometry level present in BaTiO3 films. This work is supported by the US Department of Energy, Basic Energy Sciences, under Award Number DE-SC0020145 as part of the Computational Materials Sciences.

Figure 1. (a) A RHEED image taken along the [100] direction (b) an AFM micrograph of a BaTiO3 film grown at 58 mTorr (c) Ordinary refractive indices, n_o, and (d) ordinary extinction coefficients, k_o, of $BaTiO_3$ thin films plotted together with bulk $BaTiO_3$

[1] S. Abel et al., Nat. Mater. 18, 42 (2019)

[2] L. Mazet, et al., Sci. Technol. Adv. Mater. 16, 36005 (2015)

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PCSI

Room Redondo - Session PCSI-WeA2

Graphene

Moderator: Cedric Robert, LPCNO, CNRS INSA Toulouse

4:20pm **PCSI-WeA2-29 Diodic Transport in Graphene Moiré Systems***, **Jia Li**,* Brown University **INVITED**

The discovery of magic-angle graphene moiré systems has unlocked a wide variety of intriguing emergent phenomena. Inside the nearly dispersionless band structures, the combination of isospin symmetry breaking and strong correlation gives rise to an intricate landscape of emergent quantum phases, such as superconductivity and orbital ferromagnetism. The subtle interplay between the flat moiré band and strong Coulomb interaction provides an ideal venue for exploring novel electronic orders. For instance, a recent experiment reported a prominent zero-field superconducting diode effect in twisted trilayer graphene, revealing a new type of symmetry breaking order [1]. The nonreciprocal superconducting transport behavior, evidenced by the direction-dependence in the critical current points towards spontaneous breaking of both parity and time-reversal symmetry in the superconducting state, which motivates our search for a parity-breaking electronic order in metallic states of graphene-based moiré systems.

Such an electronic order can be identified based on highly nonreciprocal, diode-like current-voltage characteristics throughout the moiré flatband, which exhibits a one-fold or three-fold symmetric angular dependence as a function of the azimuth direction of current flow (Figure 1). We show that this parity-breaking order can be described as a valley-polarized loop current state, which is highly tunable with magnetic field, current flow, and field-effect doping. Our findings point towards the universal presence of valley-polarized isospin order and rotational symmetry breaking across the moiré flatband, with important implications for understanding intertwined and competing orders, such as ferromagnetism, nematicity, and superconductivity, in graphene-based moiré systems.

[1] Lin, J-X. et al. Zero-field superconducting diode effect in small-twist-angle trilayer graphene. Nature Physics, in press (2022).

5:00pm **PCSI-WeA2-37 UPGRADED: Proximity-Induced Superconductivity in Epitaxial Topological Insulator/Graphene/Gallium Heterostructures***, **Cequn Li**,* Pennsylvania State University

A topological insulator/superconductor heterostructure may support a novel superconductor called a topological superconductor through the proximity effect. In this work [1], we synthesize high-quality, large area $(Bi,Sb)_2Te_3$ (BST)/graphene (Gr)/gallium (Ga) heterostructures with atomically sharp hetero-interfaces combining confinement heteroepitaxy and molecular beam epitaxy (Fig. 1a). Atomically thin Ga film superconducts at T_c~4 K, and the growth of $(Bi,Sb)_2Te_3$ preserves its superconductivity extremely well. A lithography-free, van der Waals tunnel junction is developed to perform transport tunneling spectroscopy. Our results show a robust, proximity-induced superconducting gap formed in the Dirac surface states of 5-10 quintuple-layer BST/Gr/Ga heterostructures (Fig. 1b). This novel synthesis approach opens up new avenues for the understanding of topological superconductivity and the realization of topological quantum computing. This work is supported by the Penn State Materials Research Science and Engineering Center under award NSF-DMR 2011839.

5:20pm **PCSI-WeA2-41 Stabilizing Phosphorus Oxides at Confined Heterointerfaces***, **Jiayun Liang**, Z. Al Balushi,* University of California at Berkeley

A clean interface is crucial to obtain complex heterostructures with pre-determined properties. Intercalation, a polymer-free method to realizing vertical stacks with a clean interface, remained challenging for large intercalants. In this work, we reported the intercalation of P_2O_5 via chemical reactions at the graphene-Ge (110) heterointerface. Strong P and O signals from energy dispersive X-ray spectroscopy (EDS) were detected underneath the graphene layer on the cross-section of the graphene-Ge (110) heterointerface. A two-step mechanism for the intercalation process was that P_2O_5 decomposed into small fragments (i.e., P, O). These small fragments intercalated through graphene, reacted, and formed P_2O_5 at the graphene-Ge (110) interface. The P_2O_5 intercalated not only tunning the electronic structure of graphene on top with charge transfer but also converting metal (e.g., Ga) to its phosphate form. This study offers an important opportunity for advancing the understanding of mechanism for unstable large molecule intercalation at the graphene-substrate heterointerface.

5:25pm **PCSI-WeA2-42 Origin of Rectangular-like Lattice on Nanographene in STM Images Unveiled by First-Principles Calculations***, **Junhuan Li**, K. Inagaki, R. Sun, K. Yamamura, K. Arima,* Osaka University, Japan

We performed atomic-scale scanning tunneling microscopy (STM) of a cleaved highly oriented pyrolytic graphite [1]. Together with a (√3×√3)*R*30° phase (Fig. 1(c)), a unique rectangular-like lattice (Fig. 1(d)) was resolved on a graphene nanosheet at a sample bias (V_s) of -0.05 V. To clarify the origin of this rectangular lattice, we conducted first-principles calculations [2] based on density functional theory and obtained simulated STM images of armchair-edged graphene nanoribbons (AGNRs) with different widths. In terms of the ribbon width (Fig. 2(a)), W is defined as the number of dimer lines across the ribbon width [3]. To avoid inaccuracies in the Fermi level, we used the sum of the electron density of orbitals in [$\varepsilon_{\mathrm{HOMO}}+eV_s$, $\varepsilon_{\mathrm{HOMO}}$] for a negative sample bias, where $\varepsilon_{\mathrm{HOMO}}$ indicates the energy level of the highest occupied molecular orbitals (HOMO). The band structure was magnified in Fig. 2(c). V_1 and V_2 denote different energy levels at k=0. Fig. 2(d) shows simulated STM images at both sample bias of V_1 and V_2. At the lower sample bias (V_1), we find a rectangular superstructure similar to our experimental results [1]. The other image at V_2 indicates the ring-like shapes within the AGNR, which is in good agreement with the hexagonal lattice of graphene.

5:30pm **PCSI-WeA2-43 Valley-Controlled Even-Denominator Fractional Quantum Hall Effect in Bernal-Stacked Bilayer Graphene***, **Ke Huang**, H. Fu,* Department of Physics, The Pennsylvania State University*; D. Reifsnyder Hickey,* Department of Chemistry, The Pennsylvania State University*; N. Alem,* Department of Materials Science and Engineering, The Pennsylvania State University*; X. Lin,* International Center for Quantum Materials, Peking University, China*; K. Watanabe,* Research Center for Functional Materials, National Institute for Materials Science, Japan*; T. Taniguchi,* International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan*; J. Zhu,* Department of Physics, The Pennsylvania State University

The braiding statistics of non-abelian anyons is the foundation for topological quantum computation. The even-denominator fractional quantum Hall (FQH) effect in a two-dimensional electron system is expected to host such quasi-particles. In Bernal-stacked bilayer graphene (BLG), even-denominator FQH states at filling factors ν = -5/2, -1/2, 3/2 and 7/2 have been observed. In this presentation, I'll discuss our observation of a new even-denominator state at filling factor ν = 5/2 in samples of unprecedented quality and by manipulating the valley isospin degrees of freedom in BLG using a perpendicular electric field. We show that the 5/2 state is spontaneously polarized in the limit of zero valley Zeeman splitting. Theory proposes three possible topological orders for the even-denominator states, i.e. the Moore-Read Pfaffian, its particle-hole conjugate the anti-Pfaffian, and a particle-hole symmetry state. Both the Pfaffian and the anti-Pfaffian break the particle-hole symmetry. They are predicted to have different FQH daughter states. We observe the daughter states of the Pfaffian near ν =3/2, 7/2 and of the anti-Pfaffian near ν = 5/2 and -1/2. These results provide new information on the rich physics of the FQH effect.

PCSI

Room Redondo - Session PCSI-ThM1

Spin Dynamics for Quantum Sensing

Moderator: Christopher Palmstrom, University of California, Santa Barbara

8:30am **PCSI-ThM1-1 Theory of Spin Center Sensing of Diffusion*, Denis Candido,*** University of Iowa **INVITED**

Defects in solids with spins (also known as spin centers) have been shown as promising room temperature solid-state qubits with the ability to be optically initialized and interrogated[1]. Additionally, they have also been demonstrate to be great non-evasive quantum sensors due to their high energy levels sensitivity to both magnetic and electric fields. In general, static electromagnetic fields can be inferred from the shift of the emitted spin center photoluminescence, while dynamical fluctuating fields (generating noise) are inferred from the change of the spin center coherence times[2].

Here we study the electric noise in spin defects due to both fluctuation of the surface charged density and the electrostatic potential at the surface of our crystal [3]. Surprisingly, we show in Fig. 1 that the depth dependence of the electric noise spectral density is strongly influenced by the two-point correlation function of both the charged particles' positions, rather than solely by the character of the charge fluctuators, e.g., point-like or dipole. Furthermore, we are able to recognize the fingerprints and signatures of diffusion phenomena of charged particles through the spin defect's T1 and T2. This is seen on both the defect spin decay and dephasing containing a crossover as function of time around the characteristic correlation time of the fluctuators, determined by the diffusion coefficients (Fig. 2). Hence, spin defects can also be used for sensing of diffusion phenomena and extraction of its corresponding correlation time and diffusion constant.

Work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0021314.

[1] D. D. Awschalom, R. Hanson, J. Wrachtrup,and B. B. Zhou, Nature Photonics12, 516 (2018).
[2] R. Schirhagl, K. Chang, M. Loretz, and C. L. Degen, Annual Review of Physical Chemistry 65, 83 (2014).
[3] D. R. Candido and M. E. Flatté, arXiv:2112.15581 (2021).

9:10am **PCSI-ThM1-9 Probing Spin Dynamics on Diamond Surfaces Using a Single Quantum Sensor***, N. de Leon, **Jared Rovny,*** Princeton University **INVITED**

Nitrogen vacancy (NV) centers in diamond are atom-scale defects with long spin coherence times that can be used to sense magnetic fields with high sensitivity and spatial resolution. Typically, the magnetic field projection at a single point is measured by averaging many sequential measurements with a single NV center, or the magnetic field distribution is reconstructed by taking a spatial average over an ensemble of many NV centers. In averaging over many single-NV center experiments, both techniques discard information. Here we propose and implement a new sensing modality, whereby two or more NV centers are measured simultaneously, and we extract temporal and spatial correlations in their signals that would otherwise be inaccessible. We analytically derive the measurable two-point correlator in the presence of environmental noise, quantum projection noise, and readout noise. We show that optimizing the readout noise is critical for measuring correlations, and we experimentally demonstrate measurements of correlated applied noise using spin-to-charge readout of two shallow NV centers. We also implement a spectral reconstruction protocol for disentangling local and nonlocal noise sources, and demonstrate that independent control of two NV centers can be used to measure the temporal structure of correlations. Our covariance magnetometry scheme has numerous applications in studying spatiotemporal structure factors and dynamics, and opens a new frontier in nanoscale sensing.

9:50am **PCSI-ThM1-17 UPGRADED Quantum Decoherence in Superconducting Circuits: Contrasting Loss Mechanisms of Nb and Si Surface Oxides***, **D Frank Ogletree,*** Molecular Foundry, Lawrence Berkeley Lab*; V. Altoé, A. Schwartzberg, C. Song, D. Santiago,* Molecular Foundry, LBL*; I. Siddiqi,* Physics Department, UC Berkeley and Materials Sciences, LBL

The performance of quantum sensors or qubits based on superconducting circuits is limited by "two level system" (TLS) loss associated with amorphous layers at the metal and substrate interfaces [1,2]. Through selective chemical etching of niobium-on-silicon quantum resonators, correlated with millikelvin microwave loss measurements and interfacial materials analysis [3], we found clear differences in contributions of Si and Nb surface oxides. XPS and STEM analysis of resonator cross-sections were used to correlate physical and chemical changes in the surface oxides with reductions in decoherence [4,5]. Surface SiO_x hosted 70% of TLS loss, with only 24% associated with NbO_x. Although TLS loss dominated decoherence, 39% of loss did not show the characteristic TLS power dependence [1]. NbO_x hosted 68% of non-TLS losses, with only 17% associated with SiO_x. We localized 92% of all loss in the surface oxides. TEM diffraction showed an epitaxial relation between the Nb superconducting film and the Si substrate, with no evidence for the commonly-reported metal-substrate amorphous oxide layer. Post-fabrication surface oxide etching improved our median quantum-resonator quality factors from 0.93 to 5.26 million.

PCSI

Room Redondo - Session PCSI-ThM2

Si Qubits and Spin Centers

Moderator: Christopher Palmstrom, University of California, Santa Barbara

10:50am **PCSI-ThM2-29 Interface-Dependent Valley Splitting in Si Quantum Dot Qubits***, **Mark Friesen,*** University of Wisconsin-Madison **INVITED**

Degenerate "valleys" in the silicon conduction band represent a potentially dangerous degree of freedom that can compete with "spin" as the dominant quantum variable in quantum dot qubits. Scaling up to large numbers of qubits therefore requires controlling the valley energy splitting. Unfortunately, this splitting depends strongly on atomistic properties of the interface, including interface sharpness, roughness and various types of disorder, which are unavoidable. In this talk, I will describe our current understanding of the wide variability observed in valley splitting measurements, even in devices fabricated 100 nm apart on the same chip. I will show that typical strategies for mitigating this variability are often only weakly effective, and that ubiquitous alloy disorder in the SiGe quantum well barriers plays a significant role in determining the valley splitting in many cases of interest. I will conclude by suggesting alternative strategies for controlling the valley splitting in future generations of devices.

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11:30am **PCSI-ThM2-37 Experimental Signature of Topologically Protected Surface States in a New-Type Centrosymmetric Superconductor $PdBi_2$***, **Jinbang Hu,*** Norwegian University of Science and Technology (NTNU), Norway*; J. Wells,* University of Oslo (UiO), Norway

Topological superconductors (TSCs) is a novel quantum phase of matter characterized by a fully gapped bulk state and gapless boundary states hosting exotic Majorana fermions. [1] The prospect of harboring vortex confined Majorana zero mode (MZM) for potential applications in quantum computation has attracted considerable experimental research interest. Recently, topologically protected surface states in a centrosymmetric layered superconductor, β-PdBi2 was confirmed by Sakano et al,[2] and the corresponding possible spin triplet superconducting phases were examined and reported by Sun et al. [3]

In this work, we demonstrate how high-quality PdBi2 samples growing layer-by-layer to the bulk phase by molecular beam epitaxy (MBE) and measured the atomic and electronic structures by scanning tunnelling microscopy (STM) and angle-resolved photoemission spectroscopy (ARPES) for comparison with first principles calculations. As compared to the β-PdBi2 bulk single crystal hosting a topologically protected surface Dirac cone band with the binding energy of the Dirac point around 2.4 eV below Fermi level. Our results shift the Dirac point up to ∼1.1 eV is an important step towards realizing MBS in this robust system.

11:35am **PCSI-ThM2-38 PCSI Closing Remarks***,*

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