PCSI
Room Ballroom South - Session PCSI-WeA2
Oxides III

Moderator: Alessandro Mazza, Los Alamos National Laboratory

4:30pm **PCSI-WeA2-31 Epitaxial Engineering of Emergent Phenomena in Tantalate Perovskites**, ***Kaveh Ahadi,*** Ohio State University **INVITED**

Epitaxial tuning knobs, including epitaxial strain, could serve as a powerful parameter that significantly alter the lattice symmetries, affect phase stability, and reshape the energy landscape. In this presentation I will discuss the epitaxial tuning of tantalate perovskites ($KTaO_3$ and $EuTa_2O_6$) grown using a sub-oxide molecular beam epitaxy method, which we recently developed for tantalates [1]. Next, I will talk about the effect of epitaxial tuning knobs, such as epitaxial strain, on the lattice and electronic structures. Here, I will discuss that$KTaO_3$, a cubic perovskite, can be epitaxially strained into a highly tunable ferroelectric. $KTaO_3$ films, grown commensurate to $SrTiO_3$ (001), experience an in-planecompressive strain of -2.1 % that transforms the otherwise cubic structure into atetragonal polar phase with a transition temperature of 475 K, consistent with ourphase-field calculations. The Curie temperature and the spontaneouselectric polarization are systematically controlled with epitaxial strain. Scanning transmission electron microscopy reveals cooperative polar displacements of thepotassium columns with respect to neighboring tantalum columns at room temperature. Optical second harmonic anisotropic rotation results are described by a tetragonal polar point group (*4mm*), indicating emergence of a global polar ground state.

Finally, I discuss our recent results on epitaxial control of ordering in fractionally occupied double perovskite, $EuTa_2O_6$ [2]. The intrinsic crystal anisotropy of $EuTa_2O_6$ plays a pivotal role, underscoring how targeted structural modifications can facilitate the emergence of novel quantum states. The crystal and electronic structures of $EuTa_2O_6$ are investigated. X-ray diffraction and electron microscopy reveal the layered *A*-site ordering. Angle-resolved photoemission spectroscopy, along with density functional theory calculations, provide direct insight into the electronic structure, unveiling the potential for engineered confined states within bulk materials. These findings highlight $EuTa_2O_6$ as a platform for studying 2D-like electronic phenomena in a 3D context, paving the way for novel device architectures.

[1] T. Schwaigert, S. Salmani-Rezaie, M. R Barone, H. Paik, E. Ray, M. D Williams, D. A Muller, D. G Schlom, K. Ahadi,Journal of Vacuum Science & Technology A **2**, 41(2023).

[2] T. Schwaigert, A. Barooni, B. Gregory, P. Malinowski, A. Tenneti, S. Hasko, B. Palazzolo, J. W Hodgson, B. Faeth, P. M Woodward, K. M Shen, A. Singer, M. Ghazisaeidi, S. Salmani-Rezaie, D. G Schlom, K. Ahadi, Advanced Functional Materials e13656 (2025)

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5:10pm **PCSI-WeA2-39 Pockels Effect in Single-Domain a-Oriented BaTiO3 on Vicinal Si (001)**, ***Jason Tischler,*** University of Texas at Austin*; Agham Posadas,* La Luce Cristallina*; David Smith,* Arizona State University*; Kamyar Barakati, Kalinin Sergei,* University of Tennessee Knoxville*; Alexander Demkov,* University of Texas at Austin

Silicon (Si) integrated photonics is an emerging technology developed for the communications industry with emerging applications in quantum and neuromorphic computing [2, 3]. These devices provide advantages in data transmission rates by modulating optical signals in Si waveguides. However, Si by itself is a poor modulator of light as it has no intrinsic electro-optic effect. Barium titanate (BTO) demonstrates a large electro-optic response known as the Pockels effect due to it being a non-centrosymmetric medium. The Pockels effect is the change in refractive index of the material due to an external electric field. This response is described by a tensor and the largest component for BTO is r_{42}, which is reported to be 1,300 pm/V in bulk [4], and 923 pm/V in thin films [5,6]. To access this large value in a waveguide phase-shifter, one uses thin BTO films with the so-called a-axis orientation [7]. When BTO is epitaxially grown on Si (001) in the a-axis orientation, meaning the long c-axis is in-plane, two orthogonal in-plane crystallographic domains form. This creates problems in the form of Rayleigh scattering at the domain boundaries and not being able to fully utilize the high r_{42} coefficient.

In this talk we demonstrate the use of a 4° miscut vicinal Si (001) substrate to stabilize a single in-plane orientation growth of a-axis BTO on strontium titanate (STO) buffered Si by molecular beam epitaxy (MBE). In this study, utilizing x-ray diffraction (XRD) techniques and scanning transmission electron microscopy (STEM), we detail the crystalline microstructure confirming a single in-plane BTO orientation; The ferroelectric domain structure is characterized using piezo-force microscopy (PFM) and the electro-optic response is probed via transmission geometry Pockels measurements.

5:15pm **PCSI-WeA2-40 Epitaxial Single Crystal MgO Buffers on Si (100)**, ***Pablo Espinosa Argaiz****, Alexander Demkov,* University of Texas at Austin

The integration of functional metal oxides with silicon has been a persistent challenge due to the thermodynamic instability of their resulting interfaces [1]. Crystalline oxide buffer layers have been used as a solution by providing a thermodynamically stable transition layer. Magnesium oxide (MgO) buffers have been shown to work as effective pseudo-substrates for metal oxide epitaxy [2, 3], and its deposition on silicon has been shown to be stable [4].

In this talk we report an extensive study of high-quality MgO buffer layers using molecular beam epitaxy (MBE) on Si(100) substrates. The buffers were grown through electron-beam evaporation of single crystal MgO, which was deposited at 300°C under an oxygen partial pressure of $3.7x10^{-5}$ Torr. The reflection high-energy electron diffraction (RHEED) pattern (Figure 1.a) reveals a modulated pattern along the MgO[100] direction, indicating the beginning of small island formation and surface faceting. The thickness dependence on the films' crystallinity was studied through the FWHM of the (200) MgO Bragg peak rocking curve as seen in Figure 1.b. The trend suggests an improvement in the crystallinity as the layers become thicker. Figure 1.c shows the scanning transmission electron microscopy (STEM) image of a cross section of the MgO/Si interface, revealing an in-plane epitaxial relationship of MgO <100> || Si <100> with a 4:3 coincident site arrangement between the MgO and Si conventional unit cells. The figure also reveals the presence of tilted MgO grains and small-angle grain boundaries. The interface layer observed in Figure 1.c was investigated using x-ray photoelectron spectroscopy (XPS), suggesting the formation of Mg-O-Si bonds at the interface. Additionally, the measured band alignment at the MgO/Si interface and its relation to first principles calculations of various interface models will be discussed.

[1] K. J. Hubbard, D. G. Schlom, J. Mater. Res. 11, 2757 (1996).[2] K. Nashimoto, D. Fork, T. H. Geballe, Appl. Phys. Lett. 60, 1199 (1992).[3] D. K Fork, F. A. Ponce, J. C. Tramontana, T. H. Geballe, Appl. Phys. Lett. 58, 2294 (1991).[4] T. Abukawa, S. Sato, Y. Matsuoka, Surface Science 604, 1624 (2010).

5:20pm **PCSI-WeA2-41 Plasma-Induced Surface Modification of Indium for Improved Bonding**, ***Kristen Steffens****, Sujitra Pookpanratana, Junyeob Song, Marcelo Davanco, Tammy Lucas, John Biesecker, Daniel Schmidt,* National Institute of Standards and Technology (NIST)

Bonding plays an important role in advanced microelectronics integration and packaging by bringing together components and devices produced separately.Surface-pretreatments on bonding materials have been consistently found to be crucial to achieving a high-quality bond, despite incomplete understanding of why certain treatments have greater success than others.Our project aims to improve understanding of some of these bonding pre-treatment effects to provide information to enable more efficient development of bonding protocols.

Indium is a critical material for conductive contacts in the fabrication of cryogenic low-temperature electronics and optical detectors for infrared and microwave applications, because In is a superconducting material which retains its ductility and adhesion properties during thermal cycling.Certain pre-bond plasma treatments increase the success of In-In bond adhesion.We have observed that plasma chemistries such as H_2/He, which do not include N_2 as a plasma gas, promote more successful In-In bonding.To understand why, we investigate the effects of atmospheric plasma exposure on In surfaces for several plasma chemistries including He/H_2/N_2, He/H_2 and He/N_2.X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) are used to characterize In surfaces prior to and after ambient pressure plasma treatment.All plasma treatments decreased the amount of carbon and increased the amount of In-oxide present when compared to an untreated film.N-$_2$-containing plasmas resulted in the appearance of an additional high binding energy peak in the N 1s XPS spectrum.We postulate that this may be due to nitrate species formed on the In native oxide surface. Additional experiments are planned to assess the plausibility of this explanation.In foil was measured prior to and after Ar sputter cleaning for comparison to treated samples.

UPS measurements showed that all plasma chemistry treatments lowered the work function compared to the non-treated control.Greater spatial variation in work function was observed for chemistries with high N_2 versus those with little to no N_2.This finding possibly correlates with poorer bonding for N_2 containing plasmas.

5:25pm **PCSI-WeA2-42 High-Temperature Resilient Neuromorphic Device based on Optically Configured Monolayer MoS2 for Cognitive Computing**, ***Pukhraj Prajapat***, *Govind Gupta,* National Physical Laboratory, India

High-temperature neuromorphic devices are becoming more and more essential as technology progresses to support space exploration and survive extreme conditions such as those found in factories. To overcome this need, the researchers are devising technologies that imitate human brain structure and operation. In this work, we present a scalable neuromorphic device based on a monolayer of MoS_2, that demonstrates operation at 100°C. The device portrays excellent electrical performances mostly due to the great thermal stability of monolayer MoS_2 and its mechanical flexibility. Among these performances are low power consumption, fast switching, high resistance ratio, low switching voltage, and long stable endurance (~10^3 cycles). Besides, the device mimics neuromorphic behavior by embedding the synaptic plasticity that is the major functional property of biological neural networks, thus allowing advanced cognitive computing in extreme environments. This is the first step toward a combination of materials science and neuromorphic computing, and it clears the way for smart resilient electronics that could survive in a variety of harsh conditions. This research is targeting a major change in the area of high-temperature electronics, and this progress is paving the way for obtaining future high-performance electronics that can meet the needs of modern technology.

5:30pm **PCSI-WeA2-43 Understanding Dielectric Breakdown Using EDMR and NZFMR**, ***Colin McKay***, Sandia National Laboratories; *George Bodenschatz, Kaila Burges, Elijah Allridge, Michael Elko, Patrick Lenahan,* Penn State University; *David Hughart, Gaddi Haase,* Sandia National Laboratories

Time dependent dielectric breakdown (TDDB) is a fundamental problem in solid state electronics which is still not fully understood. Different models in the literature provide very different expected lifetimes. A deeper understanding of the physical mechanisms of TDDB can be gained from using electrically detected magnetic resonance (EDMR) and near zero field magnetoresistance (NZFMR). This abstract shows data from such a study. We report a fundamental advance in our understanding of TDDB in SiO_2 and the first direct observation of the generation of a specific point defect, the E' center, due high field gate stress using EDMR, NZFMR, and other techniques at room temperature. EDMR and NZFMR are spectroscopic techniques sensitive only to electrically active defects.

In this study, gate oxides in large arrays of silicon on insulator (SOI) n-MOSFETs were subjected to high electric field stress at 7.5V. Damage caused by the stress was characterized using the Fitzgerald-Grove gated diode method, capacitance vs voltage (CV), EDMR, and NZFMR measurements. The gate oxides were 7 nm thick and the gate areas of the transistor arrays were between 5,000 μm^2 and 50,000 μm^2.The early increase in peak DCIV current indicates that the first stage of damage is characterized by interface state generation, specifically Pb centers, with no appreciable increase in bulk oxide defects. The generation of interface states is accompanied by the redistribution of hydrogen away from recombination centers shown by the NZFMR results. The interface state density eventually starts to saturate, followed by an increase in bulk oxide defects, specifically E' centers, represented by a shift in the voltage of the DCIV peak current. The Pb and E' centers were identified via their EDMR signals. The E' spectrum only appears after long stress durations. This new understanding of the different stages of damage provides a fundamental insight into the physics of damage mechanisms during the leadup to TDDB.

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5:35pm **PCSI-WeA2-44 Interfacial Polarization in Polymer-Based Dielectric Composites with 2d Nanomaterials**, *So-Yeon Jun,* ***SeGi Yu***, Hankuk University of Foreign Studies, Republic of Korea

The dielectric behavior of polymer-based composite films was systematically investigated with a particular focus on the interfacial polarization phenomena arising from the incorporation of conducting two-dimensional (2D) nanoplatelets. Ferroelectric $BaTiO_3$ (BTO) nanoparticles were employed as a primary filler; while MXene, graphene oxide (GO), and reduced GO (rGO) served as co-fillers to modulate the interfacial effects. Cyanoethyl pullulan (CEP) was used as a polymer matrix due to its high dielectric behavior among polymers. A reference sample, containing BTO nanoparticle fillers only in a CEP matrix, was also prepared to isolate the contribution of the 2D nanomaterials, which resulted in four dielectric composite samples. MXene platelets were delaminated in dimethyl sulfoxide (DMSO) via ultrasonication for 2 hours, and rGO was chemically reduced from GO using hydrazine over 8 hours—both conditions optimized in prior studies [1,2] to enhance dielectric performance. All components were dispersed in dimethylformamide (DMF) and spin-coated onto ITO substrates to form uniform dielectric films.

The incorporation of conducting 2D nanoplatelets significantly enhanced the dielectric constant of the composites. The highest value was achieved with the MXene-incorporated film (~200 at 1 kHz), followed by GO films (~130) and rGO films (~120), all substantially higher than the reference film containing BTO only (~90). However, this enhancement was accompanied by an undesirable increase in the dielectric loss (tan δ) due to percolative linkage of fillers. The loss increased, from 0.048 for the reference sample, to 0.053 for GO, 0.10 for MXene, and 0.22 for rGO, respectively.The observed dielectric enhancement is attributed to pronounced interfacial polarization at the filler-matrix boundaries, facilitated by the high aspect ratio and conductivity of the 2D nanoplatelets. Among them, MXene demonstrated superior interfacial coupling due to its metallic conductivity, leading to more effective charge accumulation at interfaces. In addition, MXene can successfully suppress the increase in the dielectric loss which is difficult to control for nanomaterial incorporation within a polymer matrix. Raman spectroscopy and X-ray photoemission spectroscopy (XPS) analyses corroborated the structural and electronic characteristics responsible for these effects. These findings demonstrate the critical role of interfacial polarization in tailoring the dielectric properties of polymer-based composites and suggest that MXene-based systems hold promise for next-generation electronic and energy storage applications, where high permittivity and controlled loss are essential.

5:40pm **PCSI-WeA2-45 Switchable Electron-Phonon Scattering Strength in Monolayer Hexagonal Boron Nitride**, *Alv Johan Skarpeid,* University of Oslo, Norway; *Noah Joseph Hourighan,* Graz University of Technology, Austria; *Richard Justin Schenk,* University of Oslo, Norway; ***Håkon Ivarssønn Røst***, University of Bergen, Norway; *Giovanni Di Santo, Luca Petaccia,* Elettra-Sincrotrone Trieste, Italy; *Bodil Holst,* University of Bergen, Norway; *Anton Tamtögl,* Graz University of Technology, Austria; *Justin William Wells,* University of Oslo, Norway

In the past decade, the layered compound hexagonal boron nitride (hBN) has drawn considerable attention due to its compatibility with various low-dimensional van der Waals (vdW) materials [1]. While hBN resembles graphene in lateral size, crystalline structure, and Debye frequency, its two distinct sub-lattices give rise to a significant energy band gap between the valence and conduction bands [2]. Recently, it was predicted that hBN should host strong electron-phonon coupling (EPC) in its electronic π- and σ-bands [3], reminiscent of the reported (and debated) interactions in the graphene σ-bands [4]. Since then, we have confirmed this EPC from observable energy renormalizations in the hBN band structure [5].

We will showcase the electron-phonon coupling (EPC) in hBN, highlighting how changing the substrate interaction, e.g., by adatom intercalation, can influence coupling strength (see Fig. 1). By combining angle-resolved photoemission and neutral helium atom scattering, we will demonstrate how these techniques together help demystify the scattering modes involved in electron-hole recombination. We will also mention the broader implications of EPC in materials with finite electronic band gaps.

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[2] J. Robertson, *Phys. Rev. B* **29**, p. 2131 (1984).

[3] E. Thingstad et al., *Phys. Rev. B* **101**, p. 214513 (2020).

[4] F. Mazzola et al., *Phys. Rev. B* **95**, p. 075430 (2017).

[5] H. I. Røst et al., *Nano Lett*. **23**, pp. 7539-7545 (2023).

5:45pm **PCSI-WeA2-46 Epitaxial Growth of Superconducting $CoSi_2$ for Advancements in Quantum Information Sciences**, ***Julian Choi***, *Teun van Schijndel, Yu Wu, Christopher Palmstrom,* University of California Santa Barbara

Josephson junctions (JJs) are superconductor/insulator/superconductor structures crucial in superconducting quantum circuits due to their non-linear inductance creating an anharmonic oscillator that can be used as a qubit. They are often created using amorphous materials. The amorphous

oxide and its interfaces with the superconductor are believed to result in two-level energy loss systems that limit performance. One way to progress in this field is to carefully select materials that best minimize this loss. In this context, $CoSi_2$ is particularly interesting for these systems because it has the potential to be fully epitaxial with silicon, thus eliminating any amorphous materials. This is due to the capability of growing a single crystalline Si barrier on $CoSi_2$, which is possible because of their similar crystal structures and small lattice mismatch of approximately 1.2% [1].In this talk, we demonstrate the Si substrate preparation and epitaxial growth of superconducting $CoSi_2$ by molecular beam epitaxy (MBE). We systematically investigate the crystalline structure, topography, and superconducting properties of the resulting films. The reflection high-energy electron diffraction (RHEED) patterns after the cleaning process exhibited Laue arcs, indicating an oxide-free and smooth surface. During the growth, Co is deposited and $CoSi_2$ is formed through reaction with the Si substrate heated to at least 200 C. 2 x 2 diffraction patterns are visible in RHEED, which indicate epitaxial growth, later confirmed by high resolution X-ray diffraction (XRD). Atomic force microscopy (AFM) shows grain formation on the surface and measurements using an adiabatic demagnetization refrigerator show the superconducting transition temperature (T_c) of the $CoSi_2$ film as 0.58 K, which is lower than the bulk value of 1.4 K [2]. This T_c reduction suggests that the film is too thin or may not be completely single crystalline. We then investigate the growth of $CoSi_2$ films at different temperatures, evaluate the impact of post-growth anneals, and determine how these factors influence their superconducting properties.

[1] J.C.Hensel, A.F.J Levi, R.T. Tung, et al, Appl. Phys. Lett. 47, 151 (1985); https://doi.org/10.1063/1.96245

[2] Matthias, B. T., and J. K. Hulm. "Superconducting properties of cobalt disilicide." Physical Review 89.2(1953): 439.

5:50pm **PCSI-WeA2-47 Interfacial Oxidation in Niobium Films Probed by HAXPES**, ***Ananya Chattaraj,*** Brookhaven National Laboratory

Niobium (Nb) thin films are widely used in superconducting quantum circuits owing to their relatively high superconducting transition temperature (T_c) and compatibility with microfabrication processes [1,2]. Device performance, however, is often limited by dielectric losses originating from interfacial oxides in which two-level systems introduce parasitic energy dissipation [2,3]. A deeper understanding of the structural and chemical evolution of Nb oxides, as well as their depth distribution, is therefore critical for improving thin-film quality and coherence in superconducting devices. In this presentation we demonstrate the deposition of Nb thin films using DC magnetron sputtering. The oxidation behavior and interfacial chemistry of the films were investigated using laboratory-based X-ray photoelectron spectroscopy (XPS) together with variable-photon-energy Hard X-ray Photoelectron Spectroscopy (HAXPES) performed at the NSLS-II synchrotron. HAXPES measurements spanning photon energies from 2000–5500 eV enabled non-destructive, depth-resolved analysis from the surface oxide to the metallic Nb bulk. Quantitative fitting of the Nb 3d and O 1s core-level spectra revealed multiple suboxide species (Nb_2O_5, NbO_2, and NbO_x) and their gradual evolution across the Nb/NbO_x interface [2,4]. The variable-energy approach provided nanometer-scale insight into oxidation gradients and interfacial structure that are inaccessible to conventional XPS, highlighting the power of synchrotron-based depth profiling for complex superconducting thin films. Electrical transport measurements confirmed a T_c of approximately 9 K, demonstrating that high-quality superconducting properties can be achieved using sputtered Nb growth. The integrated structural, spectroscopic, and transport characterization establishes a framework for understanding interfacial oxidation mechanisms in Nb thin films and provides guidance for mitigating oxide-related losses in superconducting and quantum device technologies.

[1] Joshi et al Physical Review Applied. 2023 Aug 1;20(2):024031.

[2] Murthy et al. ACS nano. 2022 Sep 26;16(10):17257-62.

[3] Verjauw et al. Physical Review Applied. 2021 Jul 1;16(1):014018.

[4] Burnett et al. arXiv preprint arXiv:1512.02553.

5:55pm **PCSI-WeA2-48 Room Temperature Electrically Detected Magnetic Resonance of Performance Limiting Defects in GaN Pn Junction Diodes**, *Dustin T. Hassenmayer,* ***Patrick M. Lenahan,*** *M.J. Elko,* Penn State University*; David A. Fehr, Michael E. Flatte,* University of Iowa*; B.R. Tuttle,* Penn State University*; R. Chu, Yuxin Du,* University of Illinois at Urbana-Champaign

In order to utilize any semiconductor material, it is important to understand the physical and chemical nature of its most important electrically active defects. Multiple studies have been reported on defects in GaN but direct experiment evidence linking specific defect structures to their properties is very limited. Electrically detected magnetic resonance (EDMR) along with conventional electron paramagnetic resonance (EPR) has unrivaled analytical power for identifying point defects. However, EDMR has many orders of magnitude greater sensitivity than conventional EPR [1-2]. In this work, we report on the EDMR detection of an important defect in GaN devices with detailed observation of hyperfine structure. These observations involve room temperature EDMR measurements of GaN pn diodes. The measurements involved device active region of <10-7 cm3. There have been longstanding sensitivity barriers which have limited the application of magnetic resonance techniques on III-V materials. This work may have cleared a path to identifying point defects in a variety of III-V devices. The first and second derivative EDMR signal shown in figure 1 was obtained on a GaN pn junction diode at room temperature with 3.05 V forward bias (B $\perp$ c). The EDMR signal has a g $\approx$ 2.005, and a rich, partially resolved hyperfine structure consisting of 10 lines. These are the first reported room temperature EDMR or EPR results reported on GaN devices. In figure 1, we show a model calculation involving an unpaired electron shared with three equivalent Ga nuclei with 60% 69Ga and 40% 71Ga and a hyperfine coupling constant of 32.1 G and 44.4 G, respectively. The hyperfine structure is similar to the previously observed L1 center in undoped GaN irradiated by 2.5 MeV electrons reported by Watkins et al. [3].

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