PCSI
Room Ballroom South - Session PCSI-MoE
Oxides I

Moderator: Alex Demkov, The University of Texas

7:30pm **PCSI-MoE-1 Phonon Decoupling as a Route to Unit-Cell-Scale Ferroelectricity***, Yeongrok Jin, **Jaekwang Lee**,* Pusan National University, Republic of Korea **INVITED**

The ultimate scaling limit in ferroelectric switching has been attracting broad attention in the fields of materials science and nanoelectronics. Despite immense efforts to scale down ferroelectric features, however, only few materials have been shown to exhibit ferroelectricity at the unit-cell level.

Here we report a controllable unit-cell-scale domain in brownmillerite oxides [1] consisting of alternating octahedral/tetrahedral layers. Our machine-learning force-field (MLFF) phonon calculations reveal that the phonon modes related to oxygen octahedra are decoupled from those of the oxygen tetrahedra in brownmillerite oxides, and such localized oxygen tetrahedral phonons stabilize the sub-unit-cell-segmented ferroelectric domain (Fig.1) [2]. The discovery of unit-cell-scale ferroelectricity opens new possibilities for designing ultrahigh-density memory devices through phonon-mode engineering and interlayer decoupling [3].

[1] Y. Xing*, I. Kim*, K. T. Kang* *et al*., Nature Chemistry 17, 66-73 (2025).

[2] J. Jang*, Y. Jin*, Y. Nam* *et al*., Nature Materials 24, 1228 (2025).

[3] J. Hwang*, S. Jeong* *et al*., under review in Physical Review Letters (2025).

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8:10pm **PCSI-MoE-9 Accelerated Dielectric and Ferroelectric Materials Discovery by High-Throughput Thin Film Synthesis***, **Aiping Chen**,* LANL

Dielectric and ferroelectric materials are fundamental to modern electronic and energy storage technologies, enabling applications ranging from high-κ gate dielectrics to capacitors and nonvolatile memories. However, the discovery and optimization of new materials through conventional trial-and-error approaches remain slow and resource-intensive. Establishing a general-purpose platform that integratesmaterials informatics, combinatorial synthesis, and high-throughput characterization can dramatically accelerate the exploration of complex composition-structure-property relationships. Such an approach enables rapid mapping of materials phase space, identification of promising candidates, and iterative feedback between data-driven prediction and experimental realization, ultimately transforming the pace of dielectric and ferroelectric materials innovation.

In this talk, I will discuss our progress on developing high-throughput thin film synthesis for ferroelectric and dielectric thin films. In the first part, I will discuss the design of $(Ba_{0.7}Ca_{0.3})TiO_3$ (BCT) and $Ba(Ti_{0.8}Zr_{0.2})O_3$ (BZT) superlattices via a high-throughput combinatorial approach. In the second part of the talk, I will discuss strategies to further optimize domain structures and suppress the leakage current in BZT-BCT films via a machine learning approach. The large polarization and the delayed polarization saturation led to greatly enhanced energy density of 80 J/cm^3 and transfer efficiency of 85% over a wide temperature range. Such a data-driven design recipe for a slush-like polar state is generally applicable to quickly optimize functionalities of ferroelectric materials. Figure 1 shows the schematics of the combinatorial synthesis approach of growing the BCT-BZT thin films.

8:15pm **PCSI-MoE-10 Fabrication and Characterization of GeO_2/Ge-based MOS Capacitors after Controlled Adsorption of Water Molecules***, **Hiroki Takano**, Shuto Sano, Kouji Inagaki, Kenta Arima,* The University of Osaka, Japan

The GeO_2/Ge interface is known to generate positive fixed charges upon air exposure, posing challenges for device applications. Our research group has focused on the role of water molecules and their interaction with GeO_2/Ge surfaces. Using *in situ* X-ray photoelectron spectroscopy (XPS) with synchrotron radiated light, we systematically studied the relationship between relative humidity and the thickness of the adsorbed water layer. We also revealed substantial positive charging of GeO_2 films at humidity levels above 10^{-4}%, coinciding with the onset of water adsorption. While this effect was attributed to water penetration into the oxide, possible contributions from X-ray interactions complicated the interpretation.

In this talk, we present an investigation of the charging characteristics of GeO_2/Ge structures pre-exposed to controlled humidity conditions, evaluated through capacitance–voltage (*C–V*) measurements of metal-oxide-semiconductor (MOS) capacitors. To enable these experiments, we developed an integrated reaction chamber capable of annealing, controlled water adsorption, electrode formation via vacuum deposition, and electrical measurements on thermally oxidized GeO_2/Ge samples (550 °C) under high vacuum [1]. As part of the performance assessment of this system, MOS structures were fabricated on GeO_2/Ge structures exposed for 3 h to five different humidity levels (10^{-6}%, 0.01%, 0.1%, 0.9%, and 2.0 %) in the reaction chamber, as well as on an as-oxidized reference sample transported in air. The *C–V* curves of samples exposed to 1% RH or higher, as well as that of the as-oxidized sample, showed hysteresis and a significant negative shift. Furthermore, this hysteresis was identified as injection-type behavior. This phenomenon is attributed to the adsorption of water molecules onto the GeO_2/Ge structure at humidity higher than approximately 1% [1].

[1] S. Sano, H. Takano et al., J. Appl. Phys. **137**, 155304 (2025).

8:20pm **PCSI-MoE-11 Optical and Structural Characterization of Group-IV Oxides Produced by Rapid Thermal Annealing***, Haley Woolf, Danissa Ortega, Carlos Armenta,* New Mexico State University*; Matthew Mircovich, John Kouvetakis, Jose Menendez,* Arizona State University*; **Stefan Zollner**,* New Mexico State University

This project investigates the rapid thermal oxidation of Ge(Sn) on Si by examining their optical and structural changes. Group-IV oxides, particularly GeO_2, are promising piezoelectric materials suitable at high-temperature environments. As-received samples, prepared by chemical vapor depositino, underwent ultrasonic cleaning before oxidation. The samples were rapidly thermally oxidized at a pressure of 2.7 atm with an oxygen flow rate of 0.2 L/min. Spectroscopic ellipsometry measurements revealed that oxide thickness increased with both annealing temperature and time. Depolarizationand surface discoloration indicated non-uniformity within the oxide, which was incorporated into their optical modeling. X-ray diffraction confirmed formation of α-GeO_2. Reciprocal space maps were used to determine the strain state of the Ge epilayer and the relaxation/Sn content for the GeSn epilayer. The Deal-Grove model described Ge oxidation on Si, resulting in an activation energy of 4±2 eV for oxygen diffusion in Ge. The oxidation consumption rates for Ge and GeSn epilayers were determined to be 0.56-0.57 and 0.54, respectively.

8:25pm **PCSI-MoE-12 Surface Characterization of Implanted Arsenic on Si(100) Using Scanning Tunneling Microscopy and Spectroscopy***, **Abigail Berg**, Evan Anderson, DeAnna Campbell, Shashank Misra,* Sandia National Lab

Many quantum and classical device technologies require understanding tunneling in semiconductors, which are sensitive to defects in the tunnel barrier. Characterizing these defects is challenging because the devices involve heterogeneous interfaces and tight sub-10 nm dimensions. Meanwhile, it has been difficult to interpret data about the role of specific defects in semiconductors from scanned probe because of both the non-perturbative role of the tip and features of the electronic structure that are specific to surfaces [1][2][3][4]. Here, we present a method of identifying surface and subsurface features by creating local density of states (LDOS) maps using a scanning tunneling microscope at the surface of hydrogen-terminated silicon. We find that most defects that show up in the topography either do not show up in the LDOS maps or come from imperfections in the hydrogen passivation. By contrast, donors and acceptors are generally not visible in the topography, but can be detected as bright regions from the shift they impart in one of the band edges. The figure on the left provides an example of how we have identified different defects based on their LDOS. The grey boxes show dangling bonds which produce a high LDOS centered around zero bias, independent of the parent electronic structure. The blue and yellow boxes outline where there are donor and acceptor defects that produce bright features at the conduction and valence band edges in the LDOS. We also find some unexpected mid-gap defects in white. With this methodology in place, we plan on investigating mechanisms of dopant diffusion and defect formation more generally in devices ranging from tunnel field effect transistors to single-donor qubits.

8:30pm **PCSI-MoE-13 In_2O_3 Thin Films Deposited Using $InCl_3$ by Mist CVD Method***, **Ryo Ishikawa**, Tomohiro Yamaguchi, Takeyoshi Onuma, Tohru Honda,* Kogakuin University, Japan

In_2O_3 is an oxide semiconductor with high transparency and conductivity, widely used in transparent conducting films and channel layers of thin-film transistors (TFTs). For application to high-mobility TFTs, we have been studying the deposition of ~10 nm In_2O_3 films on SiO_2/Si substrates by the mist chemical vapor deposition (Mist CVD) method. Mist CVD is a technique in which the precursor solution is atomized by ultrasonic vibration and thermally decomposed on a heated substrate. The precursor solution is typically prepared by dissolving metal powders in an acidic solvent such as HCl. In our previous studies, it was confirmed that decreasing the HCl concentration in the solution during Mist CVD resulted in thinner In_2O_3 films [1]. On the other hand, when the concentration approaches the solubility limit, undissolved In_2O_3 powder remains, which negatively affects the film quality. To address this issue, we focused on $InCl_3$ as an alternative precursor. Since $InCl_3$ is easily soluble in deionized water, HCl is not required to prepare the solution, and it is expected that thinner In_2O_3 films can be obtained simply by reducing the $InCl_3$ concentration [2]. In this study, In_2O_3 thin films were deposited on SiO_2/Si substrates by Mist CVD using $InCl_3$ solutions with concentrations between 0.0050 and 0.20 mol/L. The solutions were used after visually confirming complete dissolution by visual inspection.

Figure 1 shows the film thickness as a function of $InCl_3$ concentration measured using SE and TEM. The results show that the In_2O_3 films became thinner as the $InCl_3$ concentration decreased.An In_2O_3 film thickness of about 10 nm was achieved at the concentration of 0.0050 mol/L. Figure 2 shows the bird's-eye FE-SEM images of In_2O_3 films grown at the $InCl_3$ concentrations of 0.0050 and 0.20 mol/L. At the concentration of 0.0050 mol/L, the smoother surface was obtained with smaller crystal grain sizes, while at 0.20 mol/L, the three-dimensional surface was obtained with large crystal grain sizes. The flattening of the surface with decreasing $InCl_3$ concentration can be explained by the smaller grain size. In the presentation, we will comprehensively discuss the structure of the grown In_2O_3 thin films, including their electrical properties.

8:35pm **PCSI-MoE-14 UPGRADED: Quantum Interference at the $(La_{0.3}Sr_{0.7})(Al_{0.65}Ta_{0.35})O_3/SrTiO_3$ Interface***, **Km Rubi**,* Los Alamos National Laboratory*; Kun Han, Huang Zhen,* National University of Singapore*; Michel Goiran, Duncan Maude, Walter Escoffier,* Laboratoire National des Champs Magnétiques Intenses, Toulouse, France*; Ariando Ariando,* National University of Singapore

Quantum interference – whether observed in the form of Aharonov-Bohm effect, the Altshuler–Aronov–Spivak effect, or quantum conductance fluctuations – offers valuable insights into electron dynamics within an electromagnetic environment. These phenomena allow direct measurement of the phase coherence length, which is critically important for developing quantum technologies such as quantum sensing, quantum computing, and quantum communication.

We report quantum oscillations in magnetoresistance that are periodic in magnetic field (B), observed at the interface between $(La_{0.3}Sr_{0.7})(Al_{0.65}Ta_{0.35})O_3$ and $SrTiO_3$ [1]. Unlike Shubnikov–de Haas oscillations, which appear at magnetic fields > 7 T and diminish quickly as the temperature rises, these B-periodic oscillations emerge at low fields and persist up to 10 K. Their amplitude decays exponentially with both temperature and field, specifying the dephasing of quantum interference. Increasing the carrier density through electrostatic gating results in a systematic reduction in both the amplitude and frequency of the oscillations, with complete suppression beyond a certain gate voltage. We attribute these oscillations to the Altshuler–Aronov–Spivak effect, likely arising from naturally formed closed-loop paths due to the interconnected quasi-one-dimensional conduction channels along $SrTiO_3$ domain walls. The relatively long phase coherence length (~ 1.8 μm at 0.1 K), estimated from the oscillation amplitude, highlights the potential of complex oxide interfaces as a promising platform for exploring quantum interference effects and advancing device concepts in quantum technologies, such as mesoscopic interferometers and quantum sensors.

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