International Workshop on Gallium Oxide and Related Materials (IWGO-6)
Room ESJ 0202 - Session IWGO-ThM1

Theory, Modeling, and Simulation

Moderators: Jinwoo Hwang, The Ohio State University, **Joel Varley**, Lawrence Livermore National Laboratory

8:00am **IWGO-ThM1-1 Breakfast**

8:30am **IWGO-ThM1-7 Impact of Defects and Impurities on the Properties of Al2O3*, Chris G. van de Walle,*** UCSB **INVITED**

Aluminum oxide (Al_2O_3) has a broad range of applications. Alloys of Al_2O_3 and Ga_2O_3 of course also serve as barrier layers in heterojunctions for Ga_2O_3-based devices. In metal-oxide-semiconductor (MOS) technologies, it can be used as a high-k gate dielectric, to passivate the surface of Si substrates, or as the tunneling layer of non-volatile flash memory devices. Al_2O_3 is also frequently used in superconducting qubits, as a tunneling barrier in the Josephson junction and/or as a substrate and capacitor dielectric.

Defects in the oxide layer affect the performance, for instance by leading to changes in threshold voltage. In quantum applications, the qubits are sensitive to defects in the substrate or in the tunnel barrier of the Josephson junction. Dielectric loss can also lead to decoherence. Enhanced control over devices thus requires a thorough understanding of the structural, electronic, and optical properties of potential defects and impurities.

We have performed first-principles calculations to elucidate these issues. For point defects, we focused on the dominant species, which are the oxygen and aluminum vacancies, and provided detailed characterization of their optical properties, which can aid experimental observation and identification [1]. For dielectric loss, we focused on mechanisms that could affect coherence at the operating frequencies of superconducting qubits, which are around about 5 GHz. We identified a mechanism by which charged defects or impurities can absorb electromagnetic radiation at GHz frequencies by emission of acoustic phonons [2]. Finally, for donor impurities, we have complemented our study of Si [3] with a comprehensive study of alternative impurities in both the corundum and monoclinic phase of Al_2O_3, identifying candidate dopants that are remarkably shallow in light of the very large band gap of this material.

Work performed in collaboration with J. L. Lyons, S. Mu, Y. Shin, S. Mu, M. Turiansky, J. B. Varley, H. Wang, M. Wang, D. Wickramaratne, and C. Wilhelmer, and supported by DOE, ONR and AFOSR.

[1] C. Wilhelmer, M. E. Turiansky, D. Waldhör, L. Cvitkovich, C. G. Van de Walle, and T. Grasser, Phys. Rev. Mater. **9**, 096202 (2025).

[2] M. E. Turiansky and C. G. Van de Walle, APL Quantum **1**, 026114 (2024).

[3] S. Mu, M. Wang, J. B. Varley, J. L. Lyons, D. Wickramaratne , and C. G. Van de Walle, Phys. Rev. B **105**, 155201 (2022).

8:55am **IWGO-ThM1-12 GeO_2 and $Ge_xS_{n1-x}O_2$ Alloys: Emerging Ultra-Wide-Band-Gap Materials for Power Electronics*, Emmanouil (Manos) Kioupakis,*** University of Michigan, Ann Arbor **INVITED**

In this talk, I will present recent advances by my research group, our collaborators, and the broader community on rutile GeO_2 and its alloys with SnO_2, a new UWBG semiconductor materials platform for power electronics. I will survey our first-principles investigations of the thermodynamic stability, electronic structure, defect physics, carrier transport, and thermal properties of rutile GeO_2 and $Ge_xSn_{1-x}O_2$ alloys. Complementing the theoretical insights, I will highlight recent experimental progress from our collaborators on the synthesis and characterization of GeO2-based materials. These results provide critical validation of theoretical predictions and shed light on the practical challenges associated with materials quality and phase stability. Moreover, I will provide a brief overview of broader efforts by the global research community on rutile GeO_2 and its alloys SnO_2, spanning different growth techniques, doping strategies, and characterization approaches. This perspective will help identify key bottlenecks and opportunities for advancing these materials toward device applications.

9:20am **IWGO-ThM1-17 Rutile $Ge_xSn_{1-x}O_2$ Alloys for Ultra-Wide Bandgap Electronics: Phase Stability and Bandgap Engineering*, Alp Kurbay,*** University of Michigan, Ann Arbor*; Yann Müller,* EPFL, Switzerland*; Xiao Zhang,* University of Michigan, Ann Arbor*; Anirudh Natarajan,* EPFL, Switzerland*; Emmanouil Kioupakis,* University of Michigan, Ann Arbor

$Ge_xSn_{1-x}O_2$ alloys have recently attracted attention as candidate ultra-wide bandgap (UWBG) materials for power electronics due to their predicted ambipolar dopability, high carrier mobilities, and high thermal conductivity. Experiments show that these alloys can be grown as thin films over a wide composition range, have carrier mobilities that are insensitive to alloy disorder at low Ge content, and exhibit breakdown fields as high as 7.0 ± 1.4 MV/cm [1]. In this study, we perform a comprehensive investigation of the thermodynamic stability, structural parameters, and electronic properties of $Ge_xSn_{1-x}O_2$ alloys using first-principles atomistic calculations. The large positive mixing enthalpy produces a miscibility gap with a critical temperature above 2300 K, which agrees with the experimental phase diagram for bulk materials [2]. This indicates that the high solubilities observed in thin-film synthesis cannot be explained by the incoherent phase diagram alone. We demonstrate that coherency strain during epitaxial growth substantially alters phase stability, and calculations of the coherent spinodal show significant suppression of the miscibility gap, reducing the critical temperature to ≈ 900 K. Our calculations show that these alloys exhibit only weak short-range order, with a slight tendency for Ge–Sn nearest-neighbor clustering, and can be approximated as random solid solutions. Our calculated lattice parameters exhibit a nearly linear dependence on composition, consistent with Vegard's law and experimental measurements. Hybrid-functional calculations show a direct band gap at the Γ-point ranging from ~3.6 eV in SnO_2 to ~4.7 eV in GeO_2 with strong compositional bowing and light carrier effective masses. The calculated bandgaps in the Sn-rich region show a ~200 meV difference between thin films and bulk alloys, and we explore possible causes such as compressive strain and interfacial effects from the substrates. Our results reveal the thermodynamic origin of the metastability of $Ge_xSn_{1-x}O_2$ thin films and demonstrate the potential of this system for band-gap engineering in ultra-wide-bandgap oxide semiconductors [3].

[1] U. Mansur et al., Phys. Status Solidi A, 202501029 (2026).

[2] Watanabe, J. Am. Ceram. Soc. 66, c104 (1983).

[3] Müller et al., arXiv:2601.12184 , https://doi.org/10.48550/arXiv.2601.12184.

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9:35am **IWGO-ThM1-20 Single Ga-Layer Reconstruction Mediates Ga_2O_3 Heteroepitaxy: A Multiscale Atomistic Study*, Ilaria Bertoni,*** *Aldo Ugolotti, Anna Marzegalli,* Universita' degli Studi di Milano-Bicocca, Italy*; Flyura Djurabekova,* University of Helsinki, Finland*; Leonida Miglio,* Universita' degli Studi di Milano-Bicocca, Italy

Ga_2O_3 heteroepitaxy on c-plane sapphire displays a rich polymorphic competition, with different phases stabilizing depending on growth conditions [1]. Under high-temperature/ low-rate conditions—approaching quasi-equilibrium growth— largely relaxed β-Ga_2O_3 crystallites grow on sapphire, often mediated by a thin α wetting layer at the interface [2]. The coherent β/substrate interface is characterized by a strongly anisotropic mismatch strain, as large as ~9% along one of the two in-plane directions, thus making the observed stabilization of β without classical misfit dislocations particularly remarkable. The thermodynamic and atomistic mechanism behind this α/β sequence remains poorly understood.

Through a multiscale framework combining density functional theory, classical nucleation theory and continuum elasticity modeling, we show that α wetting of sapphire is thermodynamically driven by surface energetics, justifying the formation of a thin α interlayer of up to ~3 bilayers. Beyond this thickness, a crossover emerges: three-dimensional β islands, relaxing elastically through their free surfaces, become thermodynamically favored above a critical size, providing a purely thermodynamic rationale for the experimentally observed α→β sequence.

Moreover, upon thermal activation, molecular dynamics simulations reveal a collective atomic rearrangement at the β/α interface that goes well beyond elastic relaxation, enabling near-complete strain release. This plastic reconstruction is confined to a single Ga atomic plane: as the β island expands toward its bulk lattice parameter, at the interface the relaxed β oxygen sublattice periodically overlaps with different sites of the underlying strained α sublattice, causing the interfacial Ga layer to respond to the local oxygen-sublattice environment by adopting an α-like or β-like coordination within the same atomic plane. The oxygen framework remains

perfectly crystalline across the interface, with strain accommodated entirely via this cation redistribution — a mechanism fundamentally distinct from dislocation-mediated relaxation.

This interfacial plasticity provides a permanent, size-independent strain-relief pathway that explains how β-Ga_2O_3 can stabilize on a strained α wetting layer even after island coalescence, consistent with experimental observations under quasi-equilibrium growth conditions.

[1] ACS Appl. Mater. Interfaces 17, 62261−62276 (2025)

[2] Applied Physics Express 8, 011101 (2015)

9:50am **IWGO-ThM1-23 Carrier Mobility in $Ge_xSn_{1-x}O_2$ Alloys from First Principles***, **Amanda Wang**, Alp Kurbay, Xiao Zhang, Nick Pant, Emmanouil Kioupakis,* University of Michigan

SnO_2 and GeO_2 are both transparent conducting oxides in the rutile crystal structure, with band gaps of 3.6 eV and 4.7 eV, respectively. Alloying the two enables tunability of the band gap and of the lattice constants, as well as potential for ambipolar doping due to the predicted ambipolar dopability of GeO_2. However, a shortcoming of many semiconductor alloys is that the disordered potential landscape caused by the random arrangement of atoms results in carrier scattering, impeding mobility. Despite this, experiments have found high electron mobilities in $Ge_xSn_{1-x}O_2$ alloys that are insensitive to alloy composition, indicating a lack of alloy scattering [1,2]. In this work, we calculate the electron and hole mobilities in $Ge_xSn_{1-x}O_2$ alloys using first-principles electronic structure methods to predict the theoretical upper limit of mobility and examine the role of alloy scattering across the composition range. The carrier mobility limited by phonon- and ionized-impurity scattering is calculated for the binary end compounds, in good agreement with experimental measurements for SnO_2. To characterize the alloy scattering, we model random alloys using supercells and perform slab calculations to align the band edges across the composition range. The alloy scattering is combined with the phonon- and ionized-impurity scattering to determine the total alloy mobility. We find that the insensitivity of the band edges with respect to composition results in weak alloy scattering and high electron mobilities that are invariant to composition, especially in the range of low Ge composition, reproducing the trend from experiments as seen in Figure 1. This confirms that $Ge_xSn_{1-x}O_2$ alloys are promising wide-band-gap semiconductors with efficient carrier transport.

[1] Y. Nagashima, *et al.*, Chem. Mater. 34(24), 10842–10848 (2022).

[2] H. Takane, *et al.*, Phys. Rev. Mater. 6(8), 084604 (2022).

10:05am **IWGO-ThM1-26 Refractive Indices, Band-to-Band Transitions, and Ultraviolet Dielectric Functions of Unintentionally-Doped (x = 0 . . . 0.3) and Silicon Doped (x = 0 . . . 0.25) Single Crystal (100) β-(AlxGa1−x)$_2$O$_3$***, **Preston Sorensen**,* University of Nebraska - Lincoln*; Alyssa Mock,* Weber State University*; Megan Stokey,* Milwaukee School of Engineering*; Ufuk Kilic,* University of Nebraska - Lincoln*; Rafal Korlacki,* J. A. Woollam Co., Inc.*; Akhil Mauze, Yuewei Zhang, James Speck,* University of California Santa Barbara*; Zbigniew Galazka,* Leibniz Institute for Crystal Growth, Germany*; Vanya Darakchieva,* Lund University, Sweden*; Mathias Schubert,* University of Nebraska - Lincoln

The monoclinic beta phase of gallium oxide is an ultra-wide bandgap semiconductor that has been widely studied for potential use in high power switching applications. Advances in crystal growth techniques enable us to investigate high quality β-$(Al_xGa_{1-x})_2O_3$ films and bulk substrates. For the first time, the properties of unstrained bulk substrates are investigated, permitting for the decoupling of the effects of strain and the native properties of the lattice. Understanding the fundamental properties of the substrates also permits the investigation of compressive and tensile strain of epitaxial β-$(Al_y Ga_{1-y})_2O_3$ or β-Ga_2O_3 on a different solid solution β-$(Al_xGa_{1-x})_2O_3$ crystal substrate, which has not yet been done.

Here, we study β-$(Al_xGa_{1-x})_2O_3$ (x = 0.05, 0.1, 0.15, 0.2, 0.25, and 0.3) and Silicon doped (x = 0.05, 0.1, 0.15, 0.2, and 0.25) both with (100) surface orientation. Bulk β-$(Al_xGa_{1-x})_2O_3$ crystals were grown by the Czochralski method using Ir crucibles and oxidizing atmosphere. We present model dielectric functions in the near ultraviolet to the vacuum ultraviolet. We investigate the changes in the optical bandgap and band-to-band transitions associated with the increasing aluminum concentration. We compare the results to our previous work done on an additional sample set of pseudomorphically strained β-$(Al_xGa_{1-x})_2O_3$ films on (010) β-Ga_2O_3, with aluminum molar content up to 21%. We contrast the data obtained from the doped samples to the unintentionally-doped samples to resolve the effects of doping on free charge carrier concentration, bandgap, and higher photon energy band-to-band transitions.

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