International Workshop on Gallium Oxide and Related Materials (IWGO-6)
Room ESJ 0202 - Session IWGO-MoA2

Defects Science II

Moderators: Emmanouil Kioupakis, University of Michigan, **Hartwin Peelaers**, University of Kansas

4:10pm **IWGO-MoA2-27 Advancing Understanding in Conductivity Control in Ga2O3 Polymorphs and Alloys Through Atomistic Simulations*, Joel Varley,*** Lawrence Livermore National Laboratory **INVITED**

Exploiting chemical and structural control of gallium oxide (Ga_2O_3) through doping, alloying, and epitaxy is an attractive way of further expanding the properties of this promising ultra-wide bandgap platform for next-generation power electronics. For example, Ga_2O_3 exhibits a number of (metastable) polymorphs with superior properties to the thermodynamically favored β-phase, and alloying with other elements like In and Al alloys can lead to tunability of the band gap to potentially access higher power device figures of merit, analogous to the III-nitride system but spanning a much larger rage of bandgaps exceeding 8 eV eV.[1,2] Here we survey the current understanding of dopability, common trap levels, and other types of in Ga_2O_3 and related alloys, focusing on their potential optical and electrical consequences from insights gained through first-principles-based calculations employing hybrid functionals. Specifically, we discuss what is known about the influence of crystal structure and composition on the prospects of donor doping and electrical compensation, as well the role(s) of native defects and impurities incorporated through growth and processing steps. We summarize the behaviour predicted for a number of conventional dopants and lesser-explored dopants and impurities that can impact the performance of Ga_2O_3-related materials and devices.[3-8] These results provide guidance for understanding the roles of different defect populations in the family of Ga_2O_3 polymorphs and related alloys.

This work was performed under the auspices of the U.S. DOE by Lawrence Livermore National Laboratory (LLNL) under contract DE-AC52-07NA27344.

4:35pm **IWGO-MoA2-32 High-Throughput, High-Resolution, Three-DimensionalObservationof Threading Dislocations in β-Ga2O3 Using Phase-Contrast Microscopy*, Yukari Ishikawa,*** *Daiki Katsube,* Japan Fine Ceramics Center, Japan*; Yongzaho Yao,* Mie Univ., Japan Fine Ceramics Center, Japan*; Koji Sato,* Japan Fine Ceramices Center, Japan*; Kohei Sasaki,* Novel Crystal Technology, Japan

Wafer-scale, depth-resolved inspection of threading dislocations remains a critical challenge in the development of β-Ga_2O_3 ultrawide-bandgap semiconductors. We report a laboratory-implementable, nondestructive approach for high-throughput, high-resolution, three-dimensional visualization of threading dislocations using phase-contrast microscopy (PCM). PCM can be implemented in a conventional laboratory environment under ambient conditions and achieves millisecond-scale acquisition of each field of view, providing a practical and scalable platform for rapid wafer-level inspection. The detection capability of PCM is quantitatively validated through direct comparison with synchrotron radiation X-ray topography (SR-XRT), demonstrating excellent correspondence exceeding 96% in identical regions. PCM further offers superior lateral spatial resolution, enabling the separation of closely spaced dislocations. By systematically shifting the focal plane, depth-resolved imaging of dislocation propagation through the crystal thickness is achieved, allowing three-dimensional reconstruction of dislocation networks. Projection analysis of sequential PCM images reveals dislocation trajectories and their crystallographic characteristics. These results establish PCM as an accessible and growth-relevant platform for wafer-scale, three-dimensional dislocation evaluation in β-Ga_2O_3, opening a pathway toward process feedback and reliability-oriented materials engineering.

4:50pm **IWGO-MoA2-35 Origin of Donor Compensation in $(Al_xGa_{(1-x)})_2O_3$ Alloys*, Sierra Seacat,*** *Hartwin Peelaers,* University of Kansas

Many Ga_2O_3 devices require the formation of heterostructures to confine charge carriers. Typically, monoclinic AlGaO alloys are used for this purpose, as the larger bandgap of Al_2O_3 results in an alloy with a conduction-band offset relative to Ga_2O_3 enabling charge carrier confinement. However, intentional *n*-type doping can be difficult to achieve in these alloys, with donor compensation observed in alloys with 25% Al content or higher when doped with Si. The source of this compensation cannot be ascribed to Si alone, as density functional theory (DFT) calculations predict that Si should remain shallow up to 70% Al content. This implies that another defect is acting as a compensating acceptor.

Here, we propose cation vacancies as the source of donor compensation in monoclinic AlGaO alloys. Using DFT with the HSE06 hybrid functional, we calculate the formation energies of cation vacancies in monoclinic Al_2O_3 and $AlGaO_3$ as compared to the Si donor. We find that the split vacancy ic configuration is also the lowest energy vacancy in Al_2O_3 and $AlGaO_3$. By determining the point where this vacancy becomes lower in energy than Si at the CBM as a function of alloy composition, we predict that vacancies will compensate donor doping for 16% Al content or greater under O-poor conditions and are therefore the likely source of donor compensation in monoclinic AlGaO [1].

[1] S. Seacat and H. Peelaers, https://doi.org/10.48550/arXiv.2602.02879 (2026).

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