International Workshop on Gallium Oxide and Related Materials (IWGO-6)
Room ESJ 0202 - Session IWGO-MoA1

Defects Science I

Moderators: John Lyons, Naval Research Laboratory, **Matthew McCluskey**, Washington State University

2:00pm **IWGO-MoA1-1 Toward Quantitative Modeling of Temperature-Dependent Defect Physics in β-Ga_2O_3***, Elif Ertekin,* University of Illinois*; Michael Scarpulla,* University of Utah*; Joel Varley,* Lawrence Livermore National Lab*; Nasim Alem,* Penn State University*; Channyung Lee, Grace McKnight,* University of Illinois*; Aaditta Arnab,* University of Utah **INVITED**

β-Ga_2O_3 is a promising semiconductor for next-generation power electronics due to its ultrawide band gap and high critical breakdown field. While first-principles methods have provided substantial insight into its ground-state properties, many of the key processes governing synthesis and device operation occur at elevated temperatures, where defect thermodynamics, diffusion, and electron–phonon interactions become central. In this presentation, I will discuss efforts to develop a quantitatively predictive description of these temperature-dependent effects, with the goal of achieving direct and reliable agreement with experiment.

Temperature plays a dual role in β-Ga_2O_3, simultaneously influencing defect populations and enabling mass transport. The low-symmetry monoclinic structure gives rise to complex, anisotropic diffusion pathways for both native defects and impurities, with migration governed by a competition between interstitial, interstitialcy, and trap-limited mechanisms. When coupled with the strong temperature dependence of defect formation energies, including contributions from chemical potentials, band gap renormalization, and vibrational entropy, this leads to significant changes in predicted dopability and compensation behavior under realistic growth and annealing conditions.

These same thermodynamic and kinetic effects extend beyond point defects. Under conditions of elevated temperature and nonstoichiometry, polymorphic transformations become accessible, and the formation of γ-Ga_2O_3 within β-Ga_2O_3 can be understood in terms of vacancy-mediated pathways and configurational entropy contributions to phase stability. Such mechanisms are consistent with experimental observations of nanoscale γ-phase inclusions and interfacial layers.

Temperature also directly modifies the electronic structure through lattice expansion and electron–phonon coupling, producing substantial band-edge shifts across device-relevant temperature ranges. Taken together, these effects highlight the interconnected roles of temperature, defects, and lattice dynamics in determining the behavior of β-Ga_2O_3, and underscore the importance of incorporating finite-temperature physics into predictive modeling of ultrawide-band-gap semiconductors.

2:25pm **IWGO-MoA1-6 Characterization of β-Ga_2O_3 Deep Acceptor/n$^-$ Junction Diodes Grown by Molecular Beam Epitaxy***, **Steve Rebollo,** Wolfgang Buchmaier, Sriram Krishnamoorthy, James Speck,* UC Santa Barbara

β-Ga_2O_3 lacks p-type conductivity in part due to the lack of shallow acceptors. Despite this, deep acceptor doping is of interest because deep acceptor doped layers can be used to create potential energy barriers in devices. Unlike shallow dopants, which are always fully ionized at room temperature, the ionization of deep dopants may change with operating conditions which may impact device performance. Here, we investigate the electrical properties of β-Ga_2O_3 deep acceptor/n$^-$ junction diodes.

An epitaxial stack consisting of a 320 nm thick, 3×10^{17} cm^{-3} Si-doped n$^-$ layer followed by a 20 nm thick, 8×10^{19} cm^{-3} Mg-doped layer was grown by plasma-assisted molecular beam epitaxy (PAMBE) on a Sn-doped, n$^+$(001) β-Ga_2O_3 substrate. Metal-oxide-catalyzed epitaxy (MOCATAXY) was used to enable high quality growth. A wet-etch only process with hot-H_3PO_4 was used to co-fabricate both mesa deep-acceptor/n$^-$ junction diodes and planar Schottky barrier diodes (SBDs). Ni/Au was used to contact the Mg-doped and n$^-$ layers while Ti/Au was used as a backside ohmic contact. The band diagram for virgin devices is similar to that of a pn diode.

The deep acceptor/n$^-$ diodes exhibit rectifying behavior. Compared to a SBD, which has a minimum ideality factor of 1.1, a specific on-resistance of 6.0 mΩcm^2, and a turn-on voltage of 0.8 V, the deep acceptor/n$^-$ diode has a minimum ideality factor of 1.9, an $R_{on,sp}$ of 24.9 mΩcm^2, and a turn-on voltage of 2.4 V. The virgin deep acceptor/n$^-$ diode exhibits a built-in voltage of 3.1 V as determined from capacitance-voltage measurements. The V_{bi} increased to 3.6 V when the measurement was repeated following the initial IV measurements. The IV and CV characteristics remain unchanged over the span of 5 weeks. The V_{bi} further increases to 4.5 V following a proper burn-in (5 V for 60 s). The CV characteristics are unaffected by AC frequency or by large pre-soak voltages.

The observed behavior is attributed to deep acceptor states trapping electrons when the diode is turned on. This increases the depletion region width and built-in voltage when compared to virgin devices. Detrapping appears to be a slow process. It is hypothesized that the diode is a majority carrier device with overflow electrons that reach the Ni/Au contact contributing to current flow. The quadratic turn-on behavior implies space-charge limited transport, but additional experiments are required to confirm this. Of note, the V_{bi} demonstrated here is significantly larger than what has been demonstrated in β-Ga_2O_3 SBDs and heterojunction devices. The large V_{bi} and the stable device characteristics suggest that Mg may be a promising deep acceptor candidate for β-Ga_2O_3 devices.

2:40pm **IWGO-MoA1-9 Identification and Suppression of Carbon-Related Trap States and Carrier Compensation in MOCVD-Grown β-Ga_2O_3***, **Miranda Carver**, Hemant Ghadi, Lingyu Meng, Dong Su Yu, Hongping Zhao, Aaron Arehart, Steven Ringel,* Ohio State University

Beta-phase gallium oxide (β–Ga_2O_3) is a promising ultra–wide–bandgap semiconductor for next–generation power and high–frequency devices due to its large bandgap (~4.8 eV), high theoretical breakdown field (>8 MV/cm), and availability of melt-grown native substrates. Epitaxial growth by metal-organic chemical vapor deposition (MOCVD) produces high–quality β–Ga_2O_3 layers with low background impurity concentrations [1]. The conventional precursor, triethylgallium (TEGa), yields material with excellent mobility but is limited to growth rates below 3 µm/hr, which constrain vertical device architectures that require thick drift layers [1,2]. Trimethylgallium (TMGa) enables faster growth rates (up to ~10 µm/hr); however, faster growth with TMGa is often accompanied by unintentional compensation from extrinsic impurities (e.g. carbon). Previous work shows that increasing O_2 flow during growth can mitigate this compensation while maintaining high growth rates [3]. In this study, we investigate the effects of oxygen in MOCVD TMGa–based growth of β–Ga_2O_3 to identify compensating defects in the bandgap using quantitative defect spectroscopy.

Si-doped β-Ga_2O_3 epilayers were grown on Sn-doped (010) EFG substrates via MOCVD using TMGa at a growth rate of 6.1 µm/hr while varying the O_2 flow from 800 to 3000 sccm. Growths were performed at 950 °C and 60 Torr with constant TMGa and SiH_4 flow rates. Schottky barrier diodes with 8 nm Ni were fabricated for defect characterization. All devices exhibited rectifying behavior and a quality factor ($Q=\omega C/G$) >10, indicating good diode characteristics for defect measurements. The net ionized carrier concentration extracted from C-V measurements varied from 3×10^{17} cm^{-3} to 4×10^{18} cm^{-3} with increasing O_2 flow despite a constant SiH_4 flow, suggesting increased compensation at lower oxygen flow rates. Deep level transient spectroscopy (DLTS) measurements revealed two traps with a dominant state near E_C–0.6 eV, with the concentration decreasing monotonically with increasing O_2 flow. Deep level optical spectroscopy (DLOS) measurements revealed states at E_C–1.6 eV, E_C–2.2 eV, and E_C–4.4 eV, with the E_C-1.6 eV trap exhibiting the strongest dependence on O_2 flow, decreasing in concentration as the O_2 flow increased. The correlated reduction of the E_C–0.6 eV and E_C –1.6 eV traps with increasing O_2 flow suggests that both are associated with carrier compensation that is suppressed under oxygen-rich growth conditions. Further details will be presented at the conference.

[1] Z. Feng, Appl. Phys. Lett. 114(25), 250601 (2019).

[2] S. Bin Anooz, Appl. Phys. Lett. 116(18), 182106 (2020).

[3] L. Meng, Crystal Growth & Design 22(6), 3896–3904 (2022).

2:55pm **IWGO-MoA1-12 Deep Trap States in Mg/N Co-Implanted β-Ga_2O_3 Current Blocking Layers Revealed by Thermally Stimulated Current Spectroscopy***, **Hitoshi Takane**, Yusuke Yamashita,* Toyota Central R&D Labs., Inc., Japan*; Fenfen Fenda Florena, Hironobu Miyamoto, Kohei Sasaki,* Novel Crystal Technology, Inc., Japan*; Daigo Kikuta,* Toyota Central R&D Labs., Inc., Japan

Deep acceptor doping to form a quasi-*p*-type current blocking layer (CBL) in *β*-Ga_2O_3 via ion implantation is crucial for achieving both high-voltage blocking and enhancement-mode operation [1]. Mg/N co-implantation has been proposed, achieving a significant improvement in current blocking capability compared with Mg- or N-implantation alone [2]. Since deep traps that compensate free carriers strongly affect CBL performance, their properties need to be clarified to optimize the fabrication process and ensure device reliability. In this study, we performed thermally stimulated current (TSC) spectroscopy to examine deep traps in Mg/N co-implanted CBLs. The TSC study revealed four trap levels in the Mg/N co-implanted CBLs.

To form CBLs in β-Ga_2O_3, N-implantation ([N]: 1.2×10^{19} cm^{-3}, 650-nm box profile) and Mg/N co-implantation ([Mg]: 6.0×10^{18} cm^{-3}, 300-nm box profile, [N]: 6.0×10^{18} cm^{-3}, 650-nm box profile) were carried out, followed by thermal annealing at 900 or 1000°C under an O_2 atmosphere for 30 min. Reverse *I*–*V* measurements (up to –200 V) at room temperature showed that the Mg/N co-implanted samples exhibited superior current blocking capability compared with the N-implanted samples.

We performed the TSC measurements for both samples. The Mg/N co-implanted CBLs showed clear TSC spectra, whereas such spectra could not be obtained for the N-implanted samples due to high dark leakage current. For the Mg/N co-implanted CBLs, we extracted trap energy levels by two methods. One is to fit the spectra based on Eq. (1) [3], where E_T is the energy level of deep traps.

$I = I_0 \{-E_T/kT - kD_T/\beta\ T^4\ e^{-E_T/kT} \times [1 - 4kT/E_T + 20(kT/E_T)^2]\}$ **(1)**

The other method is direct extraction from the peak temperature (T_m) with Eq. (2) [4].

$E_T = kT_m \ln(T_m{}^4/\beta)$ **(2)**

Four trap levels near the conduction band minimum (E_C) were identified at E_C–E_T ~0.72, 0.83, 0.93, and 1.02 eV. The values obtained by the two methods were in good agreement, supporting the reliability of the extracted energy levels. The trap levels at E_C–E_T ~0.72 and 1.02 eV may correspond to the previously reported E2* and E3 traps, respectively, which are likely associated with implantation-induced damage [3].

This paper is based on results obtained from a project, JPNP22007, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

[1] K. Zeng, *J. Phys. Mater.* **8** 031002 (2025). [2] F.F. Florena *et al.,* will be presented at *IWGO-6* (2026). [3] M. Pavlovic *et al., JAP* **84**2018 (1998). [4] B. Wang *et al., JAP* **125**, 105103 (2019). [5] A.Y. Polyakov *et al., JVST A* **40**, 020804 (2022).

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3:10pm **IWGO-MoA1-15 Effects of 230 MeV Ca Swift Heavy Ion Irradiation on β-Ga_2O_3 Schottky Diodes**

Yanzhen Zhao, Ohio State University*; Cale Overstreet,* University of Tennessee, Knoxville*; Hemant Ghadi, Quentin Shuai,* Ohio State University*; Kay-Obbe Voss,* GSI Helmholtz Centre For Heavy Ion Research*; Maik Lang,* University of Tennessee, Knoxville*; Steven Ringel, Aaron Arehart,* Ohio State University

Radiation exposure can degrade semiconductor device performance and lead to failure. β-Ga_2O_3 is a promising material for aerospace applications due to its ultra-wide bandgap (~4.8 eV) and strong atomic bonding [1]. While previous studies have examined the radiation response of β-Ga_2O_3 devices, heavy-ion-induced damage remains relatively underexplored [1]. Heavy ions can introduce displacement damage and generate defects degrading device performance. Therefore, investigating radiation-induced trap formation is important.

A systematic investigation of displacement damage in halide vapor phase epitaxy (HVPE)-grown β-Ga_2O_3 Schottky diodes was conducted under 230 MeV Ca irradiation up to relatively high fluence. The net carrier concentration decreases with irradiation fluence with a carrier removal rate (CRR) of 2.5×10^6 cm^{-1}. To identify the radiation-induced defects, deep-level transient and optical spectroscopies (DLTS/DLOS) were performed.Lighted C-V (LCV) measurements were used to improve trap concentration accuracy for the DLOS levels. Based on the combination of measurements, the E_C - 0.70 eV and E_C - 0.80 eV traps showed negligible trap concentration changes, whereas three DLOS-identified levels (E_C - 2.0 eV, E_C - 3.0 eV, and E_C - 4.4 eV) increased with radiation fluence. The trap concentrations-fluence dependence yields introduction rates of 8.4×10^4 and 6.1×10^5 for E_C - 2.0 and E_C - 3.0, and 1.4×10^6 cm^{-1} for DLOS optical feature E_C - 4.4 eV, respectively. The results establish a defect spectrum for radiation damage in β-Ga_2O_3, are consistent with the CRR, overall require high fluences for obvious changes, and provide insight for radiation-tolerant devices design.

[1] J. Kim, S. J. Pearton, C. Fares, J. Yang, F. Ren, S. Kim, and A. Y. Polyakov, Journal of Materials Chemistry C **7**, 10 (2019).

3:25pm **IWGO-MoA1-18 Machine Learning Quantification of Dislocation Defects in Ga_2O_3 Using X-Ray Topography**

James Gallagher, NRL*; Christian Reimann,* Rigaku, Germany*; Caroline Reilly, Jacob Leach, Heather Splawn,* Kyma Technologies*; Nadeemullah Mahadik, Marko Tadjer, Karl Hobart, Michael Mastro,* NRL

Ga_2O_3 is a promising ultra-wide bandgap semiconductor, as it is one of the least expensive to manufacture while maintaining a high breakdown voltage, resistance to radiation, and the ability to operate at high temperatures. In many maturing semiconductors, defects are present in concentrations exceeding 10^3 cm^{-2}. These defects often reduce the reliability of devices and lead to unpredictable performance. To both learn the effect of defects on performance and optimize the manufacturing of Ga_2O_3 wafers, quick, non-destructive methods for defect mapping are needed. Multiple techniques exist and are well known; however, the defect quantity can easily exceed 10^4 cm^{-2}. To rapidly quantify the defects, computational algorithms are needed. However, since defects vary in size, shape, and intensity, pattern-matching algorithms are unreliable. This work discusses using machine learning techniques to evaluate the concentration of defects in Ga_2O_3, with a focus on evaluating defects using X-Ray topography (XRT) images.

Figure 1a shows an XRT image of a (001) Ga_2O_3 wafer using the g=[-204] reflection. Defects are clearly oriented with a dislocation line direction of £= [010]. These are likely edge dislocations, as the imaging vector g is perpendicular to the dislocation line £ [1]. Applying a U-Net model yields the image in Figure 1b, where white pixels indicate a high probability of belonging to a defect. Figure 1c shows a contour plot circling the predicted locations on the original image. This model can evaluate high-resolution (<4 µm/pixel) wafer-scale images in minutes on a standard desktop computer. Figures 1d-1f demonstrate the model's application at a wafer scale. At such scales, the model maps defects with high accuracy, and most disagreements between the model's output and manual labeling arise from the subjective nature of defining defect boundaries.

[1] Y. Yao, Y. Tsusaka, K. Sasaki, A. Kuramata, Y. Sugawara, and Y. Ishikawa, “Large-area total-thickness imaging and Burgers vector analysis of dislocations in ***β*** -Ga2O3 using bright-field x-ray topography based on anomalous transmission,” *Applied Physics Letters*, vol. 121, no. 1, p. 012105, Jul. 2022, doi: 10.1063/5.0098942.

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