

International Workshop on Gallium Oxide and Related Materials (IWGO-6)

Room ESJ 0202 - Session IWGO-ThM2

Defects Science IV

Moderators: Emma Rocco, Naval Research Laboratory, Chris G. van de Walle, University of California Santa Barbara

10:50am IWGO-ThM2-35 4D-STEM and Machine Learning Investigation of Defects and Polymorphism in Ultra Wide Band Gap Oxides and Nitrides, Jinwoo Hwang, The Ohio State University **INVITED**
Four dimensional scanning transmission electron microscopy (4D-STEM) has expanded the detector space of STEM, enabling efficient acquisition of electron nanodiffraction patterns with site specificity [1-4]. This capability allows detailed study of local defects and polymorphism in ultra wide band gap materials, including Ga₂O₃ and nitride based systems under active investigation. However, the massive data volume generated by 4D-STEM makes analysis inherently a big data problem, which bottlenecks the synthesis-characterization feedback loop that must be iterated multiple times to optimize thin film structure and properties. To address this, we incorporate machine learning analysis of 4D-STEM nanodiffraction data (Fig. 1a) to identify structural heterogeneity, bond anomalies, and phase separation in Ga₂O₃ films and II-IV-N₂ thin films. We demonstrate that this approach effectively identifies nanoscale polymorphs in Ga₂O₃, as well as structural distortion and different domains in MgSiN₂ based thin films. This combined 4D-STEM and machine learning framework enables fast throughput analysis of structure and defects in thin films [5], which is essential for accelerating the discovery and development of next generation materials for microelectronics in harsh environments. This presentation also includes high resolution STEM studies of twin boundaries in bulk Ga₂O₃ substrates, along with heterointerfaces involving emerging p-type materials such as LiGaO (Fig. 1b) [6,7].

[1] G. Calderon et al., Acta Mater. 298, 121402 (2025).

[2] G. Calderon et al., ACS Applied Materials & Interfaces 16, 55852 (2024).

[3] M. Abbasi et al., APL Materials 11, 011102 (2023).

[4] S. Im et al., Ultramicroscopy 195, 189 (2018).

[5] M. Zhu et al., Scientific Reports 14, 4198 (2024).

[6] K. Zhang et al., Phys. Status Solidi RRL 19 (12), 2500192 (2025).

[7] D. Yu et al., APL Electron. Devices 1, 046104 (2025).

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11:15am IWGO-ThM2-40 Bandgap Renormalization in Si-doped β -Ga₂O₃ Films, Takeyoshi Onuma, Kai Yamamoto, Kyohei Tanaka, Kogakuin University, Japan; **Yoshiki Iba,** Tokyo University of Agriculture and Technology, Japan; **Junya Yoshinaga,** TAIYO NIPPON SANSO CORPORATION, Japan; **Yuma Terauchi,** Tokyo University of Agriculture and Technology, Japan; **Tomohiro Yamaguchi,** Kogakuin University, Japan; **Masataka Higashiwaki,** Osaka Metropolitan University/NICT, Japan; **Yuzaburo Ban,** TAIYO NIPPON SANSO ATI CORPORATION, Japan; **Yoshino Kumagai,** Tokyo University of Agriculture and Technology, Japan; **Tohru Honda,** Kogakuin University, Japan

Burstein-Moss (BM) shift in β -Ga₂O₃ has been reported for single-crystal substrates [1], while bandgap renormalization (BGR) has been addressed for Si-doped films [2]. Recently, Yoshinaga et al. reported growth of Si-doped films by low-pressure hot-wall metal organic vapor phase epitaxy (MOVPE) [3]. In this study, optical spectra were measured for the MOVPE-grown Si-doped films to discuss BGR. 2.5-2.6- μ m-thick Si-doped films were grown on semi-insulating Fe-doped (010) substrates by inserting 1- μ m-thick undoped layer [3]. Room temperature carrier densities n were in a range from 1.77×10^{16} to 1.29×10^{19} cm⁻³. Polarized photoluminescence (PL) and PL excitation (PLE) spectra at 300 K are summarized in Fig. 1. All the PL spectra exhibited a peak around 3.35 eV (370 nm) due to donor-acceptor pair (DAP) emission involving Si donor [4]. A peak associated with the exciton transition at the Γ point was observed in the PLE spectra. The PLE peak energies are plotted as a function of n in Fig. 2. The BM and BGR shifts (Δ_{BM} and Δ_{BGR}) were calculated according to the $n^{2/3}$ and $n^{1/3}$ laws, respectively. As shown by the solid lines, the PLE peak energies were well reproduced by the Δ_{BGR} . The result implies the occurrence of BGR due to hybridization between band and Si levels. This work was supported by MIC under a grant entitled "R&D of ICT Priority Technology (JPMI00316): Next-Generation Energy-Efficient Semiconductor Development and Demonstration Project

(1st and 2nd periods) (in collaboration with MOEJ)." [1] N. Ueda et al., APL 71, 933 (1997). [2] J. Zhang et al., PRB 106, 205305 (2022). [3] J. Yoshinaga et al., APEX 18, 055503 (2025). [4] T. Onuma et al., JAP 124, 075103 (2018).

11:30am IWGO-ThM2-43 Formation and Stabilization of Ga Vacancies in β -(Al,Ga)₂O₃: Effects of Al-alloying, Si-doping, and Proton Irradiation, Iuliia Zhelezova, Ilja Makkonen, University of Helsinki, Finland; **Zbigniew Galazka,** Leibniz-Institut für Kristallzüchtung, Germany; **Filip Tuomisto,** University of Helsinki, Finland

While n -type doping is readily achieved in β -Ga₂O₃, its realization in wider bandgap β -(Al,Ga)₂O₃ alloys remains challenging due to compensating defects. Here, we investigate cation vacancy formation in Si-doped β -(Al,Ga)₂O₃ single crystals using positron annihilation spectroscopy. Eight Czochralski-grown compositions with Al contents of 0–25% were studied in undoped and Si-doped forms. Crystals were grown at Leibniz-Institut für Kristallzüchtung [1]. Residual Si concentrations in undoped samples are $2\text{--}3 \times 10^{17}$ cm⁻³, while intentional doping yields $3\text{--}6 \times 10^{18}$ cm⁻³. Hall measurements show n -type conductivity in undoped samples, whereas doping efficiency decreases with increasing Al content and the 25% alloy becomes insulating [1].

Temperature-dependent positron lifetime and 4D Doppler measurements [2] reveal clear differences between undoped and Si-doped materials. Undoped crystals exhibit strong anisotropy characteristic of β -Ga₂O₃, while Si-doped samples show reduced anisotropy independent of Al content. Positron lifetimes are longer in Si-doped samples (190–220 ps) than in undoped ones (170–195 ps), indicating enhanced vacancy trapping. Si-doped alloys with 10–25% Al show nearly identical annihilation characteristics, consistent with dominant unrelaxed Ga vacancies. Undoped samples show signatures of split Ga-vacancy configurations, with unrelaxed vacancies appearing only at elevated temperatures for higher Al contents (20–25%). Below 100 K, negatively charged defects are observed only in Al-containing samples. The similar signatures of Si-doped alloys indicate that the insulating behavior of the 25% Al sample cannot be explained by Ga vacancies alone but likely involves additional acceptor-type defects.

To further probe defect formation, selected samples were subjected to 6 MeV proton irradiation. Undoped samples show increased lifetimes, reduced anisotropy, and decreased W_2 parameters, consistent with formation of unrelaxed Ga vacancies. In contrast, only minor changes occur in Si-doped samples, indicating that such vacancies are already dominant.

Overall, Al-alloying, Si-doping, and proton irradiation stabilize unrelaxed Ga vacancies and promote compensating defects, limiting doping efficiency and contributing to insulating behavior in β -(Al,Ga)₂O₃.

[1] Z. Galazka et al., JAP, 133, 035702 (2023).

[2] I. Zhelezova et al., JAP, 136, 065702 (2024).

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11:45am IWGO-ThM2-46 Nitrogen-Doped (AlGa)₂O₃/n-Ga₂O₃ Junctions Grown by Plasma-Assisted Molecular Beam Epitaxy, Kohki Tsujimoto, Toshiki Nakaoka, Yusuke Teramura, Shoma Takeda, Satoko Honda, Masataka Higashiwaki, Osaka Metropolitan University, Japan

Nitrogen (N)-doped (AlGa)₂O₃ layers are effective in forming a large energy barrier in various Ga₂O₃ device structures. For instance, a N-doped (AlGa)₂O₃ back barrier is expected to significantly suppress leakage current at an interface between an epitaxial layer and a semi-insulating substrate in lateral Ga₂O₃ field-effect transistors (FETs). In this study, we developed plasma-assisted molecular beam epitaxy (PAMBE) growth techniques of N-doped (AlGa)₂O₃ thin films on Ga₂O₃ (010) substrates and investigated their structural and electrical properties.

We first characterized structural properties of N-doped (AlGa)₂O₃ layers with a N density of 4×10^{19} cm⁻³ and Al compositions of 0.06, 0.11, 0.15, and 0.18 by X-ray diffraction ω - 2θ measurement. (AlGa)₂O₃ (020) peaks and clear fringe patterns were observed for all compositions, indicating high crystal quality and smooth epilayer/substrate interfaces.

To evaluate electrical properties, we fabricated vertical Schottky barrier diodes (SBDs) using the PAMBE-grown N-doped (AlGa)₂O₃ layers on n -Ga₂O₃ (010) substrates. The SBDs had Ni/Au Schottky anode electrodes on the N-doped (AlGa)₂O₃ layer and a Ti/Au cathode ohmic electrode on the substrate backside. Note that a highly Si-doped n^+ -Ga₂O₃ region ($Si \sim 3 \times 10^{19}$ cm⁻³) was unintentionally formed at the epilayer/substrate interface due to Si contamination of the substrate surface.

The capacitance–voltage (C – V) characteristics of the N-doped (AlGa)₂O₃ SBDs showed a monotonic decrease in C with decreasing V regardless of the Al composition, indicating that the depletion layer expanded into the

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substrate over the whole V range. This behavior was in contrast with that of a N-doped Ga_2O_3 reference SBD ($N = 4 \times 10^{19} \text{ cm}^{-3}$) in which the C remained nearly constant for $V > -7 \text{ V}$ and began to decrease for $V < -7 \text{ V}$ with decreasing V , indicating that a two-dimensional electron gas (2DEG) was formed at the epilayer/substrate interface due to the highly Si-doped n^+ - Ga_2O_3 region, pinned the Fermi level, and prevented the depletion layer from expanding into the n - Ga_2O_3 substrate for $V < -7 \text{ V}$. This was because N deep acceptors in the N-doped Ga_2O_3 layer compensated for only a small portion of the Si donors at the interface. This comparison demonstrates that the N-doped $(\text{AlGa})_2\text{O}_3$ layer is more effective to compensate for interface Si donors than the N-doped Ga_2O_3 one and thus suggests that a N-doped $(\text{AlGa})_2\text{O}_3$ layer is more promising than a N-doped Ga_2O_3 layer as a back barrier of lateral Ga_2O_3 FETs.

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