

## Advanced Characterization Techniques

Room Davis Hall 101 - Session AC+TM-MoM

### Characterization/Modeling I

Moderators: Michael Scarpulla, University of Utah, Uttam Singiseti, University of Buffalo, SUNY

9:15am AC+TM-MoM-4 Electric Field Induced Defect Redistribution at Ni-Ga<sub>2</sub>O<sub>3</sub> Interfaces, *Daram Ramdin, H. Huang, S. Dhara, S. Rajan, J. Hwang, L. Brillson*, The Ohio State University

$\beta$ -Ga<sub>2</sub>O<sub>3</sub> is a prime semiconductor for high power electronics due to its high intrinsic critical field of  $\sim 8$  MV/cm. However, premature dielectric breakdown that occurs at lower field gradients remains a challenge that is relatively unexplored at the atomic and nanoscale. Here we use UHV depth-resolved cathodoluminescence (DRCLS) correlated with scanning transmission electron microscopy (STEM) to describe how high electric fields in a Ni/Au Schottky diode on HVPE (001) Ga<sub>2</sub>O<sub>3</sub> cause atomic lattice arrangements, depth-dependent phase changes, Ni diffusion and native defect rearrangements all on a nanometer scale and a function of increasing electric field gradient up to and past dielectric breakdown.

Before electrical fields are applied, DRCLS near the Ni/  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> interfacial region exhibits new, above  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> band gap 5.29 eV and 5.82 eV CL emissions corresponding to a  $\gamma$ -Ga<sub>2</sub>O<sub>3</sub> phase. Also present are a set of characteristic intrinsic  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> defect emissions including a  $\sim 2.4$  eV feature which increases under the contact. STEM confirms a defective misaligned  $\gamma$  phase that is of average thickness  $\sim 5$  nm.

With increasing reverse bias at 143 nm below the M-S interface, in-situ DRCLS shows increasing above-bandgap emissions relative to the intrinsic 3.2 eV and 3.6 eV emissions. Prior to breakdown, these  $\sim 5.2$  eV and  $\sim 5.8$  eV emissions remain without applied fields, indicating Ni diffusion and accompanying local phase inhomogeneities. After breakdown, these emissions are reduced, indicating reduced Ni and  $\gamma$ -Ga<sub>2</sub>O<sub>3</sub> phase present at this depth. However, at the intimate interface, STEM imaging confirms that the defective layer thickness triples, with little Ni diffusion observed outside of the defective layer after breakdown.<sup>1</sup> These observations are consistent with Ni diffusion into  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> with metallization and subsequent reverse bias, then diffusion back towards the defective layer during the breakdown process, similar to the effect of annealing on this defective layer (unpublished). Breakdown experiments performed in air show that  $V_{br}$  is 2.7x higher, indicating that thermal effects play a more pronounced role in the breakdown process in UHV. These results provide evidence that dielectric breakdown at the widely used Ni/  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> contact involves an interplay of nanoscale phase change, Ni diffusion, and defect rearrangement.

Support acknowledged from AFOSR Grant No. FA9550-18-1-0066 (DNR & LJB) and AFOSR (GAME MURI) Grant No. FA9550-18-1-0479 (HLH, JH).

1. J. Shi et al., Appl. Mater. Int. 2021, 13, 29083-29092.

9:30am AC+TM-MoM-5 Charge State Transition Levels of Ni in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> Crystals from Experiment and Theory: Eminently Suitable Candidate for Compensation, *Palvan Seyidov*, Leibniz-Institut für Kristallzüchtung, Germany; *J. Basile Varley*, Lawrence Livermore National Laboratory; *Z. Galazka, T. Chou, A. Popp, K. Irmischer, A. Fiedler*, Leibniz-Institut für Kristallzüchtung, Germany

$\beta$ -Ga<sub>2</sub>O<sub>3</sub> has emerged as a next-generation high-power application due to its large bandgap of 4.85eV and a high theoretical breakdown field of  $\sim 8$  MV/cm, which already resulted in established power rectifiers and MOSFETs with excellent characteristics.<sup>1</sup> Bulk single crystals for substrates can be grown with EFG<sup>2</sup> and Czochralski<sup>3</sup> methods. One of the critical criteria for achieving excellent characteristic in lateral devices is the choice of high-resistive free-standing substrates. In this respect, deep acceptor dopants are necessary to counter the unintentional donor impurities. Recently, Mg, Fe, and Co dopants have been proposed as potential deep acceptors for producing semi-insulating  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> crystals. However, if the acceptor level positions above the mid-band gap, it can lead to electron conduction and loss of the semi-insulating state at high fields or high temperatures, as is the case for Fe and Co dopants. On the other hand, the holes are not mobile (in VB) in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> crystals resulting in a high semi-insulating state if the acceptor level positions below the mid-band gap, as is the case in the Mg acceptor dopant. However, the acceptor level of Mg positions only  $\sim 1.2$  eV above the VBM, where thermal ionization is to be expected at higher temperatures leading to loss of the semi-insulating state of substrates. Thus, an acceptor dopant is needed that has its acceptor level

below and very close to the mid-band gap, which is the key factor for producing reliable semi-insulating  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> crystals.

We measured the photoconductivity, optical absorption, and temperature-dependent resistivity (up to 1100K) of Ni-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> crystal grown by the Czochralski method<sup>3</sup>. Fitting results of photoconductivity measurement allow us to identify the energy of the  $E_{ZPL}$ ,  $D_{FC}$ , and  $hw$  of Ni-related deep levels. The first-principal calculations based on DFT support our identifications. Spectral regions observed in optical absorption mainly arise due to the charge transfer from Ni-related deep levels and CB or VB. High-temperature resistivity shows a thermal activation energy of  $\sim 2.0$  eV. Conclusively, from the experiment and theory, a consistent energy scheme: an acceptor level of  $\sim 1.9$  eV (above the VBM), and a donor level of  $\sim 3.8$  eV (below the CBM) were identified. Due to the position of the acceptor level (below and close to the mid-band gap), Ni seems to be a promising acceptor dopant for producing semi-insulating  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates for lateral power devices.

<sup>1</sup> A. J. Green et al., APL Mater **10**(2), 029201 (2022). <sup>2</sup> A. Kuramata et al., Jpn. J. Appl. Phys. **55**(100), 1202A2 (2016). <sup>3</sup> Z. Galazka; J. Appl. Phys. **131** (2022) 031103.

9:45am AC+TM-MoM-6 Comparative Study of Temperature-Dependent Bandgap Transitions in Ga<sub>2</sub>O<sub>3</sub> Polymorphs, *Benjamin M. Janzen, N. Hajizadeh, M. Meißner, M. Marggraf, C. Hartung*, Technical University of Berlin, Germany; *Z. Galazka*, Leibniz-Institut für Kristallzüchtung, Berlin, Germany; *P. Mazzolini, A. Sacchi, R. Fornari*, Department of Mathematical, Physical and Computer Sciences, University of Parma, Italy; *C. Petersen, H. von Wenckstern, M. Grundmann*, Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany; *E. Kluth, M. Feneberg, R. Goldhahn*, Otto-von-Guericke-University Magdeburg, Germany; *T. Oshima*, Department of Electrical and Electronic Engineering, Saga University, Japan; *T. Kato, H. Nishinaka*, Faculty of Electrical Engineering and Electronics, Kyoto Institute of Technology, Japan; *J. Varley*, Lawrence Livermore National Laboratory; *M. Wagner*, Paul-Drude-Institut für Festkörperelektronik, Germany

The temperature dependence of the optical bandgap has rarely been investigated experimentally for the different polymorphs of Ga<sub>2</sub>O<sub>3</sub>. A direct comparison of the temperature dependence as well as the electron-phonon coupling strengths is made considerably more difficult by the different experimental methods (e.g., reflection spectroscopy, absorption spectroscopy or ellipsometry) used to study the various polymorphs. In particular, there is no study in the literature that provides a self-consistent comparison between the band gap values and the electron-phonon coupling strengths of the different polymorphs using the same experimental technique.

We provide a combined experimental-theoretical study to investigate the electronic bandgap transitions in monoclinic [1]  $\beta$ -, orthorhombic rotational-domain [2] as well as single-domain [3]  $\kappa$ -, rhombohedral [4]  $\alpha$ -, defective spinel [5]  $\gamma$ - and cubic bixbyite [6]  $\delta$ -Ga<sub>2</sub>O<sub>3</sub> as a function of the sample temperature. Temperature-dependent UV photoluminescence excitation (PLE) spectroscopy is employed in the temperature range between 5 K and 300 K and the obtained bandgap energies are compared with room temperature measurements of the dielectric function as determined by spectroscopic ellipsometry. The temperature dependencies are discussed in conjunction with DFT calculations regarding the effects of electron-phonon coupling and the averaged phonon energies.

At 5K, we find that  $\gamma$  and  $\alpha$  possess the largest bandgap energy values around 5.36 eV, with the monoclinic  $\beta$ -polymorph's observed polarization-dependent direct band-to-band transitions exhibiting the smallest bandgap energies between 4.72 eV and 4.99 eV. Regarding the strength of the electron-phonon coupling, we observe the strongest coupling for  $\gamma$  or weakest coupling for  $\kappa$  and  $\delta$ , whereas the interaction appears similarly intense for  $\alpha$  with respect to  $\beta$ . In contrast to the rotational domain structured  $\kappa$ -Ga<sub>2</sub>O<sub>3</sub> thin film, the single-domain film reveals a directional dependence of the energy bandgap when polarizing the incident light along the crystallographic a- or b-directions, respectively.

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[2]: P. Mazzolini, B. M. Janzen et al., Adv. Funct. Mater., **33**(2), 2207821 (2023).

[3]: H. Nishinaka et al., Jpn. J. Appl. Phys., **61**(1), 018002 (2022).

[4]: S. Vogt et al., Phys. Status Solidi A, **220**(3), 2200721 (2023).

[5]: L. E. Ratcliff, B. M. Janzen et al., Adv. Mater., **34**(37), 2204217 (2022).

[6]: T. Kato et al., ACS Appl. Electron. Mater., **5**(3), 1715 (2023).

# Monday Morning, August 14, 2023

10:00am **AC+TM-MoM-7 Strain and Composition Dependencies in  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  Alloys**, Rafal Korlacki, J. Knudtson, M. Stokey, M. Hilfiker, University of Nebraska-Lincoln; V. Darakchieva, Lund University, Sweden; M. Schubert, University of Nebraska-Lincoln

Strain caused by the lattice mismatch in heteroepitaxial thin-films can be used to optimize the optical performance, as it has been demonstrated for the ternary system of  $(\text{Al},\text{Ga})\text{N}$ . [1-2] In order to apply the same principle to  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  alloys, the details of the strain relationships for various electronic and optical properties as a function of composition are needed. We use symmetry-based analysis on how the energy eigenvalues and other properties depend on the components of stress and strain tensors. [3] Then, we perform density functional theory (DFT) calculations for a representative set of structures realizing different model deformation scenarios for both,  $\text{Ga}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$ , in monoclinic and rhombohedral phases. We obtain the linear deformation potentials for energy eigenvalues [3,4] and other material properties that can be extracted from first principles calculations, such as band-to-band transitions, effective mid-band energies, refractive indices, components of the dielectric tensors, and effective mass parameters. Then, Vegard's rule allows us to construct a simple universal model of strain and composition dependencies of these properties in heterostructures under specific strain patterns, [5,6] and thus allowing rational strain engineering to aid design of new  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ -based electronic and photonic devices.

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[2] J.-M. Wagner and F. Bechstedt, *Phys. Rev.* **B66**, 115202 (2002)

[3] R. Korlacki, M. Stokey, A. Mock, S. Knight, A. Papamichail, V. Darakchieva, and M. Schubert, *Phys. Rev.* **B102**, 180101(R) (2020)

[4] R. Korlacki, J. Knudtson, M. Stokey, M. Hilfiker, V. Darakchieva, and M. Schubert, *Appl. Phys. Lett.* **120**, 042103 (2022)

[5] R. Korlacki, M. Hilfiker, J. Knudtson, M. Stokey, U. Kilic, A. Mauze, Y. Zhang, J. Speck, V. Darakchieva, and M. Schubert, *Phys. Rev. Appl.* **18**, 064019 (2022)

[6] M. Stokey, R. Korlacki, J. Knudtson, A. Mock, M. Hilfiker, A. Mauze, Y. Zhang, J. Speck, A. Papamichail, S. Knight, V. Darakchieva, and M. Schubert, "Phonon modes and strain effects in  $\beta$ - $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ ," in preparation

10:15am **AC+TM-MoM-8 10 kV  $\text{Ga}_2\text{O}_3$  Schottky Rectifier Operational at 200 °C**, Yuan Qin, M. Xiao, M. Potter, Y. Ma, Center of Power Electronics Systems, Virginia Polytechnic Institute and State University; J. Spencer, Naval Research Laboratory; Z. Du, Ming Hsieh Department of Electrical Engineering, University of Southern California; A. Jacobs, Naval Research Laboratory; K. Sasaki, Novel Crystal Technology Inc., Japan; H. Wang, Ming Hsieh Department of Electrical Engineering, University of Southern California; M. Tadjer, Naval Research Laboratory; Y. Zhang, Center of Power Electronics Systems, Virginia Polytechnic Institute and State University

This work demonstrates a novel lateral  $\text{Ga}_2\text{O}_3$  Schottky barrier diode (SBD) with a  $BV$  over 10kV and a thermally-stable 10kV blocking at high temperatures up to 200°C. The device design to enable such performance is a NiO-based reduced-surface-field (RESURF) structure that achieves a charge balance with the  $\text{Ga}_2\text{O}_3$  channel at high reverse bias.

Fig. 1(a) and (b) show the schematic and top-view scanning electron microscopy (SEM) image of the RESURF  $\text{Ga}_2\text{O}_3$  SBD, respectively. A gap between the p-NiO layer and cathode ( $L_{pc}$ ) is designed to prevent the possible leakage current and punch-through in NiO.

Fig. 1(c) shows the depth profile of the net donor concentration in the  $\text{Ga}_2\text{O}_3$  epi layer. A total charge density ( $\sigma_n$ ) of  $3.8 \times 10^{12} \text{cm}^{-2}$  is estimated in n- $\text{Ga}_2\text{O}_3$ . A NiO/n- $\text{Ga}_2\text{O}_3$  p-n diode is fabricated to extract the acceptor concentration in NiO, which is revealed to be  $8 \times 10^{17} \text{cm}^{-3}$  at 25°C and shows little change at 200°C (Fig. 1(d)). If a charge imbalance margin below 15% is kept for practical device fabrication, the NiO thickness ( $t_{\text{NiO}}$ ) range is estimated to be 61-82 and 58-78nm for the anode-to-cathode length ( $L_{AC}$ ) of 30 and 50 $\mu\text{m}$ .

Fig. 2(a)-(c) show the simulated electric field (E-field) contours of RESURF SBDs with different  $t_{\text{NiO}}$ . In charge balance condition ( $t_{\text{NiO}}=75\text{nm}$ ), the E-field are more evenly distributed in  $\text{Ga}_2\text{O}_3$  channel. Fig. 2(d) manifests that the NiO RESURF region could increase the device on-resistance ( $R_{\text{on}}$ ) due to the vertical depletion effect.

Fig. 3(a) and (b) show the reverse I-V characteristics of the  $\text{Ga}_2\text{O}_3$  RESURF SBDs with various  $t_{\text{NiO}}$  for  $L_{AC}$  of 30 and 50 $\mu\text{m}$ . The breakdown voltage ( $BV$ ) increases with the increasing  $t_{\text{NiO}}$ , reaching >10kV (the measurement limit of our test setup) at  $t_{\text{NiO}}=75\text{nm}$ , and starts to decrease at larger  $t_{\text{NiO}}$ . The two

sets of devices can be swept repeatedly up to 10kV at 200°C (Fig. 3(c)). Fig. 3(d) suggests the determining impact of charge balance on the  $BV$ .

Fig. 4(a) shows the forward I-V characteristics of the non-RESURF and 75-nm-RESURF SBDs, both with  $L_{AC}=30$  and 50 $\mu\text{m}$ . The larger  $R_{\text{on}}$  of RESURF SBDs can be explained by the simulation results in Fig. 2(d). The specific  $R_{\text{on}}$  of the RESURF SBDs with  $L_{AC}=30\mu\text{m}$  is calculated to be  $0.27\Omega\text{-cm}^2$ . Fig. 4(b) shows the temperature-dependent forward I-V characteristics of this RESURF SBD.

Fig. 5 benchmarks the  $R_{\text{on,sp}}$  versus  $BV$  as well as the  $BV$  versus maximum operational temperature for our devices and the state-of-the-art  $\text{Ga}_2\text{O}_3$  devices. Our device shows the highest  $BV$  and the operational temperature in multi-kilovolt  $\text{Ga}_2\text{O}_3$  devices.

# Monday Afternoon, August 14, 2023

## Advanced Characterization Techniques

Room Davis Hall 101 - Session AC+DI+HM+TM-MoA

### Characterization/Modeling II

Moderator: Mike Thompson, Cornell University

3:45pm **AC+DI+HM+TM-MoA-9 The Physics of Low Symmetry Semiconductors: Gallium Oxide for the Future of Green Energy as Example**, *Mathias Schubert*, R. Korlacki, M. Stokey, M. Hilfiker, University of Nebraska-Lincoln, USA; S. Knight, Linköping University, Sweden; S. Richter, Lund University, Sweden; A. Ruder, University of Nebraska-Lincoln, USA; A. Papamichael, V. Stanishev, Linköping University, Sweden; J. Speck, University of California Santa Barbara; V. Darakchieva, Lund University, Sweden

**INVITED**

The physics of GaAs (zincblende structure) and Gallium nitride (wurtzite structure) led to disruptive technologies driven by extreme properties such as small effective mass, large direct bandgap, and piezoelectric polarization. Gallium reappears in a monoclinic-structure oxide with enormous prospects for applications in power electronics for the future of green energy. Numerous new phenomena hitherto unknown for traditional semiconductors occur in monoclinic symmetry semiconductors such as non-parallel phonon-plasmon scattering, hyperbolic shear polaritons, splitting of associated transverse and longitudinal phonon modes, non-degenerate highly anisotropic fundamental excitonic band-to-band transitions, direction-dependent band alignments, and complex defect spin interactions within the highly anisotropic host lattice. The influences of composition, strain, doping, and defects are discussed for Ga<sub>2</sub>O<sub>3</sub> and related alloys, and special emphasis is paid to new semiconductor phenomena, and consequences for thin film growth and device designs are pointed out. Methods such as generalized ellipsometry, the optical Hall effect, Terahertz electron paramagnetic resonance ellipsometry, and density functional theory computations are employed for characterization and analysis.

4:15pm **AC+DI+HM+TM-MoA-11 Investigation of Split Vacancy and Interstitial Defects and Ionic Diffusion Mechanisms in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>: A Direct Approach via Master Diffusion Equations**, *Channyung Lee*, E. Ertekin, University of Illinois Urbana-Champaign

The low symmetry of the monoclinic structure of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> has led to interesting discoveries of a variety of complex configurations of intrinsic defects, such as Ga vacancies split into two or three different Ga sites. These complex defects contribute to the fast, yet highly anisotropic, diffusion of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, making it challenging to understand the dominant diffusion mechanisms of Ga cations. While previous computational studies have analyzed some migration pathways between these complex split defects, a comprehensive understanding of the overall diffusion mechanism, and predictions of the components of the full diffusivity tensor accounting for the full spectrum of intrinsic defects is not yet achieved. In this work, we aim to calculate from the first principles the 3D diffusion tensors for Ga interstitial and vacancy self-diffusion via the direct approach of solving the master diffusion equations. To achieve this, we first explore the maximum extent of "N"-split defects with large configurational complexity, including their formation energies. With the dominant low-energy defects identified, we then construct the complete diffusion network taking into account all stable split defects and all possible hops connecting them (including the interstitialcy mechanism). The nudged elastic band method is next used to accurately determine the hopping barriers, and the barriers and diffusion pathways are used to construct the complete master diffusion equations for Ga cations. Finally, the solution to these equations yields the Onsager transport coefficients, resulting in the 3D diffusion tensors and identification of the most active diffusion paths along three different crystallographic directions. Our analysis includes the identification of over 50 unique interstitial and interstitialcy hops between 20 different configurations of Ga interstitials and more than 30 unique vacancy hops between 15 different configurations of Ga vacancies. Extended N-split Ga defects are remarkably more stable than simple point defects, and play a critical role in creating low-energy pathways for both interstitial and vacancy diffusion. Furthermore, we found that selecting the appropriate supercell size is crucial for accurately describing the formation energies of N-split defects and calculating their associated migration energy barriers. Our study provides a clear understanding of the migration mechanisms of native Ga species in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and the origin of its anisotropic diffusion, which can contribute to further developments in the design and optimization of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>-based electronics.

4:30pm **AC+DI+HM+TM-MoA-12 Hybrid Metal/low-k/BaTiO<sub>3</sub>/ $\beta$ -Ga<sub>2</sub>O<sub>3</sub> Metal-Insulator-Semiconductor Junctions Enable Electric Field of 6.8 MV/cm**, *Ashok Dheenan*, S. Dhara, Ohio State University; A. Islam, A. Green, Air Force Research Laboratory; S. Rajan, Ohio State University

$\beta$ -Ga<sub>2</sub>O<sub>3</sub> is an ultrawide bandgap semiconductor that has attracted interest for use in high-power electronics due to its theoretical breakdown field of 8 MV/cm and availability of native bulk substrates. Integration of high-quality insulator layers is critical to realizing the material breakdown fields of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> devices. Recent work has demonstrated the advantages in using hybrid extreme-k/low-k insulator stacks to enable high average electric fields in the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> [N.K. Kalarickal et al. *IEEE EDL* (2021)]. In this work, we study such hybrid insulator stacks. Four different insulator stacks were used to fabricate metal-oxide-semiconductor capacitors (MOSCAPs) on top of (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> Sn-doped substrates. The first set of samples consisted of a 20 nm Al<sub>2</sub>O<sub>3</sub> low-k layer and BaTiO<sub>3</sub> (BTO) layers of 20 and 35 nm, respectively. The second two samples used 24 nm of SiO<sub>2</sub> with BTO layers of 35 nm and 50 nm, respectively. Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub> were deposited by plasma-assisted atomic layer deposition after a Piranha/HF clean [A.E. Islam et al. *IEEE TED* (2022)]. BTO layers were deposited by RF sputtering. All thicknesses were confirmed by ellipsometry of co-labeled Si. The backside and top contacts were deposited by e-beam evaporation to complete fabrication. The samples were analyzed in terms of breakdown strength, C-V characteristics and supported reverse field in the Ga<sub>2</sub>O<sub>3</sub>. The sample with 50 nm of BTO on 24 nm SiO<sub>2</sub> resulted in a larger oxide capacitance, likely due to the increased permittivity of the BTO due to higher thermal budget. For breakdown measurements, a leakage current of 1 mA/cm<sup>2</sup> was defined as the breakdown limit for all devices. The field in the Ga<sub>2</sub>O<sub>3</sub> was calculated by extracting the effective donor density from C-V and under the assumption of no charge in the dielectric layers. The sample with 20 nm Al<sub>2</sub>O<sub>3</sub> and 20 nm BTO showed the best performance, with a forward breakdown electric field of 5.7 MV/cm in the Al<sub>2</sub>O<sub>3</sub> and reverse breakdown field of 6.8 MV/cm in the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. This is one of the highest reverse breakdown fields reported to date for Gallium Oxide in such a junction and shows the potential of hybrid low-k/high-k stacks to enable extreme fields in ultra-wide bandgap semiconductors. In summary, we have studied the properties of hybrid low-k/high-k insulator stacks on  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and shown that such stacks can enable excellent reverse breakdown fields in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> power devices. We acknowledge funding from Department of Energy / National Nuclear Security Administration under Award Number(s) DE-NA0003921, and AFOSR GAME MURI (Award No. FA9550-18-1-0479, project manager Dr. Ali Sayir).

4:45pm **AC+DI+HM+TM-MoA-13 Towards Controlled Transfer of (001)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> to (0001) 4H-SiC Substrates**, *Michael Liao*, National Research Council Postdoctoral Fellow at the U.S. Naval Research Laboratory; K. Huynh, University of California Los Angeles; J. Lundh, National Research Council Postdoctoral Fellow at the U.S. Naval Research Laboratory; M. Tadjer, K. Hobart, U.S. Naval Research Laboratory; M. Goorsky, University of California Los Angeles

We demonstrate successful blistering of He-implanted (001)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, bonding to (0001) 4H-SiC, and initial results towards large-area transfer of (001)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> to SiC. Compatible with large-scale processing, exfoliation is an important step in controlled-thickness transfer of films for heterogeneous integration. Furthermore, integration of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> to high thermal conductivity materials will be crucial for thermal management of high-power devices. Two-inch (001)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> wafers were implanted with He<sup>+</sup> at an energy of 160 keV and a dose of 5×10<sup>16</sup> cm<sup>-2</sup>, mimicking our previous parameters used to successfully exfoliate (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>.<sup>1</sup> Strain fringes were observed after the implant which corresponded to a maximum strain of ~1.7%, which is higher than the ~1% strain when implanting (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> likely due to the larger Poisson's ratio of (001)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>.<sup>2</sup> The implanted substrates were then bonded to (0001) SiC at room temperature using a ~5 nm Ti interlayer to assist with the bond. Both unbonded implanted substrates and the bonded structures were first annealed at 200 °C for 10 hours to simultaneously initiate He bubble nucleation at the projected range (~0.68  $\mu$ m) and strengthen the bond. Then, even after annealing at 500 °C for 10 hours to initiate bubble growth, the (001)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> did not transfer to the (0001) 4H-SiC. Unlike what was observed for (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>,<sup>1</sup> blistering did not even occur at this temperature. Annealing at 800 °C for up to 12 hours resulted in ~10  $\mu$ m blisters for the unbonded substrates, which is typically an indication that large wafer-area transfer can be achieved if bonding was done prior to annealing.<sup>3</sup> However, the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrate did not wafer split from the bonded structure, and instead only small area transfers up to ~200  $\mu$ m were achieved. Only ~7% of the total bonded area transferred while the entire structure remained bonded.

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Strategies to improve transfer will be presented, including initiating a cold split prior to exfoliation and refined annealing strategies to improve He bubble nucleation and larger bubble growth at the projected range. These are promising results towards achieving large wafer-scale (001)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> composite wafers, and when combined with subsurface damage-free chemical mechanical polishing,<sup>4</sup> these composite wafers would be suitable for subsequent devices and/or epitaxial growth.

## References

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2. K.Adachi, et al., J.Appl.Phys., 124 085102 (2018)
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## Advanced Characterization Techniques

### Room Bansal Atrium - Session AC-MoP

#### Advanced Characterization Techniques Poster Session I

##### AC-MoP-1 Photoluminescence Mapping of Gallium Oxide, *Matthew McCluskey*, Washington State University

Photoluminescence (PL) spectroscopy is an important method to characterize dopants and defects in gallium oxide. Common features in the PL spectrum include the intrinsic UV band, blue and green bands that involve donor-acceptor pairs, and red emission due to  $\text{Cr}^{3+}$  impurities. PL mapping with excitation wavelengths ranging from 266 to 532 nm reveals the spatial distribution of these features with micron resolution. Damage due to high-intensity laser pulses results in significant changes in the intensity and energy of the UV band. In Czochralski-grown  $\beta\text{-Ga}_2\text{O}_3\text{:Fe}$ , the  $\text{Cr}^{3+}$  emission intensity shows striations that are attributed due to inhomogeneities during growth. In addition to defects in the bulk, PL microscopy has revealed several specific defects on the surface. Some of these localized centers are very bright UV emitters. Raman scans of these bright emitters revealed hydrocarbon peaks, which may point toward the origin of the light emission.

##### AC-MoP-2 Linearly Polarized UV, Blue, and IR Photoluminescence from $\beta\text{-Ga}_2\text{O}_3$ , *J. Cooke, M. Lou, Michael Scarpulla*, University of Utah; *A. Bhattacharyya*, University of California, Santa Barbara; *X. Cheng, Y. Wang*, University of Utah; *S. Krishnamoorthy*, University of California, Santa Barbara; *B. Sensale-Rodriguez*, University of Utah

An ultra-wide bandgap of 4.8 eV makes  $\beta\text{-Ga}_2\text{O}_3$  a promising material for power devices and ultra-violet (UV) optoelectronics such as UV-transparent electrodes and solar-blind photodetectors. It is well-known that the optical absorption of  $\beta\text{-Ga}_2\text{O}_3$  is anisotropic, having different threshold energies for different incident linear polarizations. Due to its low symmetry, the polarization of the emitted photoluminescence (PL) of  $\beta\text{-Ga}_2\text{O}_3$  should also be polarized; but this phenomenon which could allow distinguishing between point defects based on their structure has received much less attention. Polarized emission has been predicted and measured to be strongly related to self-trapped holes (STHs) involving O displacements, impurities, and doping. The reported typical  $\beta\text{-Ga}_2\text{O}_3$  PL is composed of UV, blue, green, and red main emission bands. Previously-reported PL has discussed excitation polarization-dependent PL, but there has been no discussion of polarized PL emission which we have found also to be polarization dependent.

Herein we report the emission polarization dependence of various high-crystalline-quality melt-grown bulk  $\beta\text{-Ga}_2\text{O}_3$  samples. It was found that (

We also observed polarized emission for Fe-doped bulk  $\beta\text{-Ga}_2\text{O}_3$  samples. Both the b-orientation and [102]-orientation showed red PL with different intensities. Whereas UV, blue, and green PL in UID and Sn-doped samples come from band transition recombination, red PL in Fe-doped samples comes from  $\text{Cr}^{3+}$ . Therefore, the causes of this emission polarization dependence are different, potentially caused by orbitals within the  $\text{Cr}^{3+}$ .

##### AC-MoP-3 Non-Uniformity and Hysteresis of Capacitance-Voltage Doping Profiling in $\beta\text{-Ga}_2\text{O}_3$ , *Jian Li, A. Charnas, B. Noesges, A. Neal, T. Asel, Y. Kim, S. Mou*, Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

Doping and defects – the important aspects of  $\beta\text{-Ga}_2\text{O}_3$  technology development – are entangled in both their underlying physics and their electrical characterization. Doping uniformity is expected to be key to the feasibility and yield of larger-scale manufacturing of  $\beta\text{-Ga}_2\text{O}_3$ -based electronics. This work is concerned with vertical doping uniformity, which is closely tied to present-day challenges such as out diffusion of compensating impurities (e.g., Fe and Mg) and interfacial accumulation of doping impurities (e.g., Si). The capacitance-voltage (CV) measured doping profiles of  $\beta\text{-Ga}_2\text{O}_3$  materials by this work and others often show a non-uniformity varying from 15% to 140% over the depth of 100s of nm. The ubiquity of this observation and its indifference of the growth and doping methods are inexplicable from sheer growth point of view therefore warrant a close scrutiny.

The apparent doping profile non-uniformity in a Schottky junction may be accompanied by the observation of CV hysteresis, which shares a common electrostatic basis underlying the threshold voltage instability in field-effect transistors. Irmscher et al. in 2013 reported CV hysteresis in a  $\beta\text{-Ga}_2\text{O}_3$  Schottky diode without accompanying analysis but the subject of that report was on deep levels therefore hinting their implicit role in CV

hysteresis. Indeed, works in earlier decades have proven deep states as the origin of CV hysteresis, which manifests the difference of equilibrium and non-equilibrium CV scans. To date, defects in  $\beta\text{-Ga}_2\text{O}_3$  have been detected and characterized by Hall, DLTS, and its variants such as DLOS and admittance spectroscopy. This work explores the case of using illumination-less steady-state room-temperature CV technique for dual-purpose investigation of doping and defect in  $\beta\text{-Ga}_2\text{O}_3$ .

We investigate the relationship between doping non-uniformity and carrier dynamics in deep levels in  $\beta\text{-Ga}_2\text{O}_3$ . We speculate that the carrier density non-uniformity is in part contributed by an artifact due to carrier emission from deep levels and seek experimental evidences from analytical electrostatic modeling of hysteresis observed in cyclic CV measurements. We aim to separate the contributions of doping and deep levels to more accurately quantify their respective parameters, i.e., doping density and spatial distribution for the former, and energy, density, and capture cross-section for the latter. The materials under investigation include bulk substrates and MBE and MOCVD grown epitaxial layers. We will discuss the implication of our findings on MOSFET operation for power electronic applications.

##### AC-MoP-4 Scanning Transmission Electron Microscopy (S/TEM) Investigation of $\gamma\text{-Ga}_2\text{O}_3$ Defective Layers In Aluminum and Scandium Alloyed $\beta\text{-Ga}_2\text{O}_3$ , *Andrew Balog*, The Pennsylvania State University; *A. Chmielewski*, CEMES-CNRS, France; *R. Lavelle, L. Miao*, The Pennsylvania State University; *J. Jesenovec, B. Dutton*, Washington State University; *C. Lee, E. Ertekin*, University of Illinois at Urbana Champaign; *J. McCloy*, Washington State University; *N. Alem*, The Pennsylvania State University

Beta gallium oxide ( $\beta\text{-Ga}_2\text{O}_3$ ) has gained interest recently as an attractive candidate for high power electronics and extreme environment applications. Possessing a monoclinic structure (space group  $C2/m$ ), the anisotropic unit cell creates a unique combination of properties. Most important among these is a band gap around 4.8 eV, 1.4 eV greater than the most widely studied UWBG semiconductor, GaN. This results from the presence of tetrahedral and octahedral gallium sites, as well as three inequivalently coordinated oxygen sites.  $\beta\text{-Ga}_2\text{O}_3$  suffers from a low thermal conductivity an order of magnitude below common UWBG and power semiconductor materials, as well as a lack of achievable p-type doping. However, the material's most fundamental constraint is insufficient knowledge about defect formation, behavior, and their impact on properties. Recent attempts at alloying  $\beta\text{-Ga}_2\text{O}_3$  with scandium and aluminum shows promise mainly in increasing  $\beta\text{-Ga}_2\text{O}_3$ 's band gap, as the monoclinic phases of  $\text{Sc}_2\text{O}_3$  and  $\text{Al}_2\text{O}_3$  demonstrate increases up to 5.48 eV and 7.24 eV, respectively. Increasing the band gap via alloying is vital for producing devices in higher critical field applications. However, the role these elements play in defect formation is still not well understood.

Using Scanning/Transmission Electron Microscopy (S/TEM) imaging and spectroscopy, we study how the addition of scandium and aluminum can change the atomic and electronic structure of  $\beta\text{-Ga}_2\text{O}_3$ . In addition, we identify a nanometer-scale layer of  $\gamma\text{-Ga}_2\text{O}_3$  at the surface of a Czochralski-grown single-crystal of  $\beta\text{-Ga}_2\text{O}_3$ . S/TEM and the suite of tools it provides such as electron energy loss spectroscopy (EELS) and energy dispersive spectroscopy (EDS), also allows for probing local electronic states around defects and general compositional mapping. This provides further information on the environment around defects and their impact on local structure. Using S/TEM imaging we investigate how the  $\gamma$  polymorph of  $\text{Ga}_2\text{O}_3$  forms as a thin film on the surface of  $\beta\text{-Ga}_2\text{O}_3$ , while the local bonding environment is uncovered by studying variations in the oxygen EELS K edge. Understanding the formation and structure of this defect phase is vital for improvement of processing and growth techniques, while also allowing for the study of the role alloys play in the defect formation process.

# Tuesday Morning, August 15, 2023

## Advanced Characterization Techniques

Room Davis Hall 101 - Session AC+MD-TuM

### Characterization/Modeling IV

Moderator: Baishakhi Mazumder, University of Buffalo, SUNY

10:45am **AC+MD-TuM-10 Defects in Ga<sub>2</sub>O<sub>3</sub>: An Ultra-high Resolution Electron Microscopy Study**, *Nasim Alem*, The Pennsylvania State University; *A. Chmielewski*, CEMES-CNRS, France

INVITED

Interest in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> has dramatically increased in recent years due to the material's potential promise for use in power electronics and extreme environments. Its combination of a monoclinic structure (C2/m space group), two inequivalent tetrahedral and octahedral gallium sites and three inequivalent oxygen sites, and a bandgap of 4.8 eV, 1.4 eV above that of gallium nitride, creates a semiconductor material with a unique set of properties. This is further aided by  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>'s uncommon capability among the ultra-wide bandgap oxides to be grown into high quality single crystal substrates using both melt-based bulk and thin film growth and deposition methods. Defects and their stability and dynamics under static and extreme environments can limit the incorporation of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> into new applications. Therefore, a direct visualization and in-depth understanding of the defects and their interplay with the environment is vital for understanding the materials properties and the device breakdown under extreme conditions. In this presentation we will discuss the atomic, electronic, and chemical structure of the defects in doped and UID  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> using scanning transmission electron microscopy (S/TEM) imaging and electron energy loss spectroscopy (EELS). In addition, we will discuss the electronic structure and the local properties in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> under extreme conditions using STEM-EELS. This fundamental understanding is important to uncover the breakdown behavior in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and the impact of defects on its device performance.

11:15am **AC+MD-TuM-12 Sub-oxide Ga to Enhance Growth Rate of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> by Plasma-assisted Molecular Beam Epitaxy**, *Zhuoqun Wen*, *K. Khan*, *E. Ahmadi*, University of Michigan, Ann Arbor

In recent years, there has been significant interest in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> as a potential candidate for the next generation of power electronics, solar-blind ultraviolet (UV) detectors, and as a substrate for UV light emitting diodes (LEDs). This interest stems from its ultra-wide bandgap of 4.8eV. Thin film growth and n-type doping (Si, Sn, Ge) of Ga<sub>2</sub>O<sub>3</sub> have been achieved through various methods such as metal-organic chemical vapor deposition (MOCVD), pulsed laser deposition (PLD), and molecular beam epitaxy (MBE). However, MBE has limitations in terms of the growth rate of Ga<sub>2</sub>O<sub>3</sub> due to the desorption of volatile Ga<sub>2</sub>O, which is formed from the reaction between Ga and Ga<sub>2</sub>O<sub>3</sub>. Using gallium sub-oxide (Ga<sub>2</sub>O) instead of elemental gallium has been previously employed [1] as a technique to enhance the growth rate of Ga<sub>2</sub>O<sub>3</sub> by Ozone-MBE. However, this technique has not yet been investigated in plasma-assisted MBE. In my talk, I will present the results of our recent studies on using Ga<sub>2</sub>O as Ga source in PAMBE. Using the same plasma conditions, we show that using Ga<sub>2</sub>O instead of Ga can at least double the growth rate of Ga<sub>2</sub>O<sub>3</sub>.

Previously, we have demonstrated uniform and controllable silicon doping of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> by utilizing disilane (Si<sub>2</sub>H<sub>6</sub>) as the Si source. [2] In my talk, I will show that this technique is also compatible with utilizing Ga<sub>2</sub>O as Ga source. The silicon doping can be tuned from  $3 \times 10^{16} \text{ cm}^{-3}$  to  $1 \times 10^{19} \text{ cm}^{-3}$  using the diluted disilane source.

References:

1. Vogt, P., Hensling, F. V., Azizie, K., Chang, C. S., Turner, D., Park, J., ... & Schlom, D. G. (2021). Adsorption-controlled growth of Ga<sub>2</sub>O<sub>3</sub> by suboxide molecular-beam epitaxy. *Apl Materials*, 9(3), 031101.
2. Wen, Z., Khan, K., Zhai, X., & Ahmadi, E. (2023). Si doping of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> by disilane via hybrid plasma-assisted molecular beam epitaxy. *Applied Physics Letters*, 122(8)

11:30am **AC+MD-TuM-13 Microscopic-Scale Defect Analysis on Ga<sub>2</sub>O<sub>3</sub> through Microscopy**, *M. Kim*, NIST-Gaithersburg, Republic of Korea; *A. Winchester*, *O. Maimon*, NIST-Gaithersburg; *S. Koo*, KwangWoon University, Korea; *Q. Li*, George Mason University; *Sujitra Pookpanratana*, NIST-Gaithersburg

Crystalline defects of technologically mature materials have been identified and classified by the semiconductor industry [1,2], since it is economically beneficial to isolate failure mechanisms at the source rather than relying on

backend testing. This has significantly improved device reliability. The various defects could be categorized into killer or non-killer defects, where killer defects can hinder the operation of high-performance devices by trapping charge carriers or causing increased leakage current. Although  $\beta$ -gallium oxide ( $\beta$ -Ga<sub>2</sub>O<sub>3</sub>) is expected to surpass silicon carbide (SiC), defects in Ga<sub>2</sub>O<sub>3</sub> are prevalent and largely unclassified. Therefore, screening out defects that cause electrical device degradation must be solved for widespread adoption of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>.

In this work, photoemission electron microscopy (PEEM) is used to visualize micrometer-scale defects and determine their electronic impact. PEEM is based on the photoelectric effect and is a non-destructive analysis method where light is used to excite and eject electrons from the sample surface and these electrons are analyzed. We investigated the defects on commercially-available epitaxially-grown  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> on (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates. The epitaxy was formed by hydride vapor phase epitaxy (HVPE) with a target doping of  $1 \times 10^{18} \text{ cm}^{-3}$  on the (010) semi-insulating  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> wafer. We identified elongated structures on the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> epi-layer as shown in Figure 1a, and they appear in multiple instances of the sample surface and in a parallel configuration. These features resemble the "carrot" defect observed in SiC epitaxy [3]. From the imaging spectroscopy mode of the PEEM (Figure 1b), the base and tip of the carrot were found to have similar valence band maxima but dissimilar work functions. The spectra from the tip of the carrot resembles that of the surrounding  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> epi-layer. We are performing ongoing work to identify this feature as a microscopic defect. For understanding the electrical influence of these elongated features on HVPE epi-layer, we will perform tunneling atomic force microscopy (TUNA) to measure the electrical properties on and off the defect surface. Together, we will present a discussion on the nature of these distinct features and their implication on device performance.

11:45am **AC+MD-TuM-14 Characterization and Processing Improvements for Fabricating and Polishing  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> Substrates**, *Robert Lavelle*, *D. Snyder*, *W. Everson*, *D. Erdely*, *L. Lyle*, *N. Alem*, *A. Balog*, Penn State University; *N. Mahadik*, *M. Liao*, Naval Research Laboratory

As progress continues to be made in fabricating and polishing uniform, high-quality  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates, it is increasingly important to link commercial suppliers and research groups with expertise in crystal growth, substrate processing, epi growth/synthesis, characterization, and devices. This creates a vertically integrated feedback loop that drives answering fundamental research questions and increasing the manufacturability of the substrates. We will review our latest results in optimizing the chemical-mechanical polishing (CMP) methods and related processing steps for  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates and materials characterization. This includes quantifying and minimizing subsurface damage related to processing, investigating the propagation of defects such as nanopipes, fabricating off-cut/off-axis substrates, and extending the fabrication/polishing methods to different alloy compositions.

Previous results showed that an excellent surface finish (Ra < 2 Å over a >0.175 mm<sup>2</sup> area) could be achieved for Czochralski (Cz) grown  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates using a two-step CMP process with a nearly 10X reduction in polishing cycle time. After continuing to develop this process, we observed that a similar surface finish could be achieved by optimizing the pH of the colloidal silica slurry while realizing a further 3-4X reduction in cycle time. This establishes a path toward a milestone 1-day polishing process for  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates. While the surface finish is similar, further reduction in the FWHM of the x-ray rocking curves (XRRCs) was also obtained by reducing the force and optimizing the other polishing parameters during the final CMP step. These processing changes suggest improvement in polishing related subsurface damage, which we assessed using high-resolution x-ray diffraction (HRXRD) by varying the x-ray penetration depth and advanced microscopy techniques.

Uniformity continues to be an important consideration as commercial 2"+ substrates become increasingly available. We continue to map and collect characterization data from across substrates grown by Cz and edge-defined film-fed growth (EFG) and will share our observations. This includes site-specific XRRC measurements as well as etch pit density (EPD) mapping and defect analysis for full substrates. In this discussion, we will also integrate feedback from epi growers for different types of substrates. Finally, we will discuss our methodology for processing off-cut/off-axis as well as alloyed substrates and latest characterization results.

## Material and Device Processing and Fabrication Techniques Room Davis Hall 101 - Session MD+AC+EP-TuA

### Process/Devices II

Moderator: Yuhao Zhang, Virginia Tech

3:45pm **MD+AC+EP-TuA-9 Large Area Trench  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> Schottky Barrier Diode with Extreme-K Dielectric Resurf**, *Saurav Roy, A. Bhattacharyya*, University of California Santa Barbara; *J. Cooke*, University of Utah; *C. Peterson*, University of California Santa Barbara; *B. Rodriguez*, University of Utah; *S. Krishnamoorthy*, University of California Santa Barbara

We report the first combination of high-k dielectric RESURF with trench geometry to realize low reverse leakage large area (1mm<sup>2</sup> and 4mm<sup>2</sup>)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> Schottky Barrier Diodes with high current values (15A pulsed, 9A DC). 1.2  $\mu$ m deep trenches are etched on HVPE-grown 11  $\mu$ m epilayer with 8 $\times$ 10<sup>15</sup> cm<sup>-3</sup> apparent charge density concentration using dry etching and 300 nm BaTiO<sub>3</sub> (BTO) is then sputter deposited which is followed by annealing at 700°C to enhance the dielectric constant. The fins are then opened using dry etching. Pt/Au Schottky contacts are deposited using e-beam evaporation with planetary rotation for conformal deposition. To further improve the breakdown voltage field plates are used with Si<sub>3</sub>N<sub>4</sub> as the field plate oxide. A planar SBD, a BTO field-plated SBD, and a trench SBD with high-k RESURF are fabricated for comparison. The on resistance ( $R_{on,sp}$  normalized to the device footprint) of the planar and field plated SBDs are extracted to be 7.9 and 8.2 m $\Omega$ -cm<sup>2</sup>, respectively, and an increased on resistance of 10.8 m $\Omega$ -cm<sup>2</sup> is measured for small area (200 $\times$ 200  $\mu$ m<sup>2</sup>) trench SBD with high-k RESURF, indicating dry etching induced damage. The breakdown voltage of the BTO field-plated SBD increases to 2.1 kV from 816 V (planar SBD) whereas the breakdown voltage increases to 2.8-3kV for the trench SBD with high-k RESURF. A very low leakage current density of 2 $\times$ 10<sup>-4</sup> A/cm<sup>2</sup> is measured for the trench SBD at 2.8 kV. The 1 mm<sup>2</sup> trench SBD exhibits a current of 3.7A(Pulsed)/2.9A(DC) and the 4mm<sup>2</sup> trench SBD exhibits a current of 15A(Pulsed)/9A(DC) at 5V. The breakdown (catastrophic) voltage of the 1mm<sup>2</sup> and 4mm<sup>2</sup> trench SBDs are measured to be 1.4 and 1.8kV. The leakage currents at breakdown are significantly lower compared to other high current SBDs reported in the literature despite the large area of the device, due to the much-reduced parallel field at the metal/semiconductor interface. Temperature dependence of on resistance shows lower temperature co-efficient ( $\alpha = 0.87$ ) which is lower than SiC SBDs. The large area high-k RESURF trench SBDs also has lowest  $V_{on,leakage}$  product for any  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> SBDs with more than 1kV breakdown voltage and 1A current, which is important to reduce both the on and off-state power dissipation. The 4mm<sup>2</sup> high-k RESURF trench SBD has the highest current (5A(DC)/9A(Pulsed)) at  $V_F = V_{on}+2V$  with breakdown voltage more than 1.3kV and exhibits lowest leakage current for similar rated device from literature.

This material is based upon work supported by the II-VI Block Gift Program and the Air Force Office of Scientific Research MURI award FA9550-21-0078.

4:00pm **MD+AC+EP-TuA-10 Fabrication and Characteristics of Ga<sub>2</sub>O<sub>3</sub> MOSFET using p-NiO for Normally-off Operation**, *Daehwan Chun, Y. Jung, J. Park, J. Hong, N. Joo, T. Kim*, Hyundai Motor Company, Republic of Korea

In order to increase sales of electric vehicles, it is essential to have market competitiveness by reducing price and improving performance, as well as improving mileage. To increase the mileage of an electric vehicle, it is important to efficiently use the limited power of the battery. The inverter/converter/OBC plays a role in converting electrical energy into a form suitable for electrical components, and the power semiconductor performs switching and rectification operations in the components responsible for such power conversion. Therefore, the performance of power semiconductors is directly related to the mileage of electric vehicles.

Existing power semiconductors mainly used Silicon(Si) materials, but recently, Silicon Carbide(SiC) power semiconductors with improved performance have been mass-produced and started to be installed in vehicles. Gallium Oxide(Ga<sub>2</sub>O<sub>3</sub>), which has a wider energy bandgap(4.7~4.9eV) than SiC, has a high critical electric field, excellent electron transport ability, and high-quality large-area substrate growth, so it has the advantage of not only performance compared to existing GaN or SiC semiconductor but also easy manufacturing process. In particular, the unit price of Ga<sub>2</sub>O<sub>3</sub> epitaxial wafer is expected to be reduced to 1/3 of that of SiC. Therefore, the manufacturing cost is also expected to be lower than that of SiC power semiconductors.

In this paper, we present the fabrication results of Ga<sub>2</sub>O<sub>3</sub>-based lateral MOSFETs for inverter/converter/OBC applications of electric vehicles. Normally-off operation was secured through the application of NiO, which does not require an ion implantation process, and a breakdown voltage of 600V was achieved. In addition, Al<sub>2</sub>O<sub>3</sub> was used as a gate insulating film to suppress gate leakage current, and high-concentration ITO was applied to form an ohmic junction.

Applying NiO to form the depletion layer in the channel region when the MOSFET is off-state ensures normally-off operation of the Ga<sub>2</sub>O<sub>3</sub> MOSFET. However, there is a limit to gate voltage application due to leakage current because of the existence of a pn heterojunction diode in the gate region. To solve this problem, an insulating film(Al<sub>2</sub>O<sub>3</sub>) was formed between NiO and the gate metal. The threshold voltage of the MOSFET with this structure formed a high value of 30V or more, so the threshold voltage was lowered by modifying the concentration of the Ga<sub>2</sub>O<sub>3</sub> epitaxial layer. As a result, some drain-source leakage current occurred, but an IV characteristic graph that clearly distinguishes the On/Off state of the MOSFET was obtained.

4:15pm **MD+AC+EP-TuA-11 On the Mg-Diffused Current Blocking Layer for Ga<sub>2</sub>O<sub>3</sub> Vertical Diffused Barrier Field-Effect-Transistor (VDBFET)**, *Ke Zeng, Z. Bian, S. Chowdhury*, Stanford University

To truly realize the potential of the Ga<sub>2</sub>O<sub>3</sub> in a transistor, it is imperative to design a buried gate barrier junction to circumvent the pre-mature breakdown near the gate often seen in lateral structures. Owing to the high diffusivity of dopants and defects in Ga<sub>2</sub>O<sub>3</sub>, in contrast to that of, for example, SiC at a moderate temperature, we propose the use of diffusion doping as a rapid and non-invasive platform to explore the possibility of an effective current blocking layer (CBL) in vertical Ga<sub>2</sub>O<sub>3</sub> transistors. In this work, we will discuss the development and characteristics of the Mg diffused CBL that was recently utilized to demonstrate an efficient Ga<sub>2</sub>O<sub>3</sub> VDBFET with remarkable pinch-off characteristics.

The process (Fig. 1) starts with a commercially available Ga<sub>2</sub>O<sub>3</sub> HVPE epitaxial wafer. The wafer was first coated with a highly Mg-doped spin-on-glass (SOG) layer which was subsequently cured and then patterned by HF to form the selective Mg dopant source. A thick PECVD layer was deposited onto the sample to isolate and stabilize the diffusion doping process. The Mg was then diffused into the wafer under a 950 °C furnace annealing for ~1 hr to form the CBL. The dopant oxide stack was stripped clean by an HF dip afterward. A Ni/Au anode was then deposited on top of the CBL region for the 2-terminal CV and IV studies shown in Fig. 2. Furthermore, for the 3-terminal VDBFET, a high dose titled Si triple ion implantation was done to form the source contact region inside the CBL area, followed by an activation annealing. The Ti/Au and Ni/Au composite source electrode was deposited on top of the source and CBL region respectively. A Ti/Au drain contact was then deposited on the back of the wafer. A 25nm ALD Al<sub>2</sub>O<sub>3</sub> was used as the gate oxide, and a Ti/Ni/Au stack was deposited as the gate contact on top of the wafer.

From a simple CV analysis on the metal-isolation-semiconductor (MIS) structure, it's confirmed that the conductivity of the Ga<sub>2</sub>O<sub>3</sub> epitaxial layer was successfully modulated by the Mg diffusion process for a depth of ~ 1.6  $\mu$ m. The same MIS structure measured a reverse breakdown voltage of 466 V. However, when the surface is further doped with implanted Si<sup>++</sup> layer, the formed NiN diode only blocks ~72V, the same as the final device blocking voltage. The VDBFET showed amazing transistor characteristics with decent saturation, on-current without any optimization, as well as a current on/off ratio > 10<sup>9</sup>. Due to the compensation of electrons by Mg in the gate region, the transistor exhibited enhancement mode operation with a turn-on voltage of ~7V. The breakdown voltage, however, was only measured to be 72 V under a gate bias of 0 V.

4:30pm **MD+AC+EP-TuA-12 Electrical Properties of p-NiO/ $\beta$ -Ga<sub>2</sub>O<sub>3</sub> Vertical PN Heterojunction Diode for Power Device Applications**, *Youngkyun Jung, D. Chun*, Hyundai Motor Company, Republic of Korea

In this paper, the p-type NiO/ $\beta$ -Ga<sub>2</sub>O<sub>3</sub> vertical pn heterojunction diode for power device application was fabricated, and the electrical characteristics of the device was evaluated. The  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> has a wide energy bandgap of about 4.8eV, and that is expected to be a material for next-generation power semiconductors with high breakdown voltage and low power loss. Compared to SiC (Silicon carbide) and GaN (Gallium Nitride), which are used as common materials for power semiconductors, it has a breakdown field (8MV/cm) that is about 3 times higher, and Baliga's FOM (3,400), which represents the semiconductor figure of merit, it has a value 4 to 10 times higher than that of GaN and SiC materials. Recently,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> has been fabricated in the form of an epitaxial layer on a wafer and applied to power devices such as MOSFETs, MESFETs, Schottky barrier diodes, and pn

junction diodes. The p-NiO has a wide band gap of 3.6 eV or more, p-type characteristics of NiO generally is induced by nickel vacancies or oxygen interstitials, that are defects provide the hole carriers. The carrier concentrations of p-NiO can be controlled in the range of  $10^{16}$  to  $10^{19}\text{cm}^{-3}$  with the amount of oxygen gas during the sputtering deposition process. The depletion region width of p-NiO/ $\beta\text{-Ga}_2\text{O}_3$  can be changed according to the change in the carrier concentration of p-NiO. To fabricate the pn vertical heterojunction diode, p-NiO was deposited on the  $\beta\text{-Ga}_2\text{O}_3$  epitaxial layer with a thickness of 250nm by using RF magnetron sputtering, and 100 nm of Ni metal for ohmic contact was deposited on the deposited p-NiO by using DC magnetron sputtering. The I-V characteristics of the fabricated pn heterojunction diode were measured by Keithley 2410, and the C-V characteristics were measured by Keysight 4284A. As a result of measuring electrical characteristics, the pn heterojunction diode has a lower leakage current value than the previously reported Schottky Barrier Diode, and on/off ratio is about  $10^9$ . When the carrier concentration of deposited p-NiO was  $10^{19}\text{cm}^{-3}$ , the turn-on voltage, current density,  $R_{on}$  value and breakdown voltage values of pn heterojunction diode were shown 2.2V,  $242\text{A}/\text{cm}^2@4\text{V}$ ,  $17\text{m}\Omega.\text{cm}^2@4\text{V}$ , and  $-465\text{V}$  respectively.

4:45pm **MD+AC+EP-TuA-13 Effects of Oxygen Reactive Ion Etching and Nitrogen Radical Irradiation on Electrical Properties of  $\text{Ga}_2\text{O}_3$  Schottky Barrier Diodes**, *Shota Sato*, *K. Eguchi*, Department of Physics and Electronics, Osaka Metropolitan University, Japan; *Z. Wang*, National Institute of Information and Communications Technology, Japan; *T. Kitada*, *M. Higashiwaki*, Department of Physics and Electronics, Osaka Metropolitan University, Japan

$\beta\text{-Ga}_2\text{O}_3$  has attracted great attention as a new wide bandgap semiconductor mainly for power devices. Oxygen reactive ion etching ( $\text{O}_2$  RIE) is often used to remove a resist and/or an organic contamination in  $\text{Ga}_2\text{O}_3$  device processing. However, this process usually causes damage to a  $\text{Ga}_2\text{O}_3$  surface degrading device characteristics. On the other hand, we found that nitrogen (N) radical irradiation can significantly restore the  $\text{Ga}_2\text{O}_3$  surface damage. In this study, we investigated effects of the  $\text{O}_2$  RIE and N radical irradiation on electrical properties of Schottky barrier diodes (SBDs) fabricated on  $\beta\text{-Ga}_2\text{O}_3$  (100) and (010) substrates.

$\text{Ga}_2\text{O}_3$  SBD structures were fabricated using unintentionally doped  $\beta\text{-Ga}_2\text{O}_3$  (100) and (010) bulk substrates with an effective donor concentration of less than  $2 \times 10^{17}\text{cm}^{-3}$ . We evaluated electrical properties of the  $\text{Ga}_2\text{O}_3$  SBDs fabricated on the substrates treated by four different processes: (a) no surface treatment, (b)  $\text{O}_2$  RIE, (c) N radical irradiation, (d)  $\text{O}_2$  RIE followed by N radical irradiation. The  $\text{O}_2$  RIE was performed at an RF power of 50 W for 90 seconds. The N radical irradiation was conducted using an RF plasma cell in a molecular beam epitaxy growth chamber at a substrate temperature of  $700^\circ\text{C}$  and an RF power of 500 W for 2 hours.

We first studied current density–voltage ( $J$ – $V$ ) characteristics of the  $\text{Ga}_2\text{O}_3$  (100) SBDs processed by the four different methods. In case of the devices with no treatment, a large variation of the turn-on  $V$  in a wide range of 0.5–1.1 V was observed. The  $\text{O}_2$  RIE process further spread the variation to 0.2–1.0 V, indicating that the  $\text{Ga}_2\text{O}_3$  (100) surface was more damaged. Furthermore, some devices showed kinks in their  $J$ – $V$  curves. The curves with the kinks look like an overlap of  $J$ – $V$  characteristics for a few area with different Schottky barrier heights under the anode electrode. In contrast, with and without the  $\text{O}_2$  RIE,  $J$ – $V$  characteristics of both SBDs treated by the N radical irradiation showed an almost constant turn-on  $V$  of 0.3 V and no kink. These results indicate that the N radical irradiation has effects to significantly restore the  $\text{Ga}_2\text{O}_3$  surface damage and equalize the surface condition. Qualitatively the same effects of nitridation were confirmed for the  $\text{Ga}_2\text{O}_3$  (010) SBDs.

In conclusion, we found that N radical irradiation is effective for restoring  $\text{Ga}_2\text{O}_3$  surface damage, which leads to improvements in electrical properties of the Schottky interface.

This work was supported in part by the Development Program, “Next-Generation Energy-Saving Devices” of the Ministry of Internal Affairs and Communications, Japan (JPMI00316).



## Advanced Characterization Techniques

### Room Bansal Atrium - Session AC-TuP

#### Advanced Characterization Techniques Poster Session II

**AC-TuP-1 Photoluminescence Spectroscopy of Cr<sup>3+</sup> in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and (Al<sub>0.1</sub>Ga<sub>0.9</sub>)<sub>2</sub>O<sub>3</sub>**, *Cassandra Remple*, Materials Science & Engineering Program, Washington State University; *L. Barmore*, Dept. of Physics and Astronomy, Washington State University; *J. Jesenovc*, *J. McCloy*, Institute of Materials Research, Materials Science & Engineering Program, Washington State University; *M. McCluskey*, Dept. of Physics and Astronomy, Washington State University

Alloying  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> with Al<sub>2</sub>O<sub>3</sub> to create (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> enables ultra-wide bandgap material suitable for applications deep into the ultraviolet. In this work, photoluminescence (PL) spectra of Cr<sup>3+</sup> were investigated in monoclinic single crystal  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>:Cr, and 10 mol.% Al<sub>2</sub>O<sub>3</sub> alloyed with  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, denoted  $\beta$ -(Al<sub>0.1</sub>Ga<sub>0.9</sub>)<sub>2</sub>O<sub>3</sub> or AGO. Temperature-dependent PL properties were studied for Cr<sup>3+</sup> in AGO and  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> from 295 K to 16 K. For both materials at room temperature, the red-line emission doublet  $R_1$  and  $R_2$  occurs at 696 nm (1.78 eV) and 690 nm (1.80 eV), respectively, along with a broad emission band at 709 nm (1.75 eV). The linewidths for AGO are larger for all temperatures due to alloy broadening. For both materials, the  $R$ -lines blue-shift with decreasing temperature. The (lowest energy)  $R_1$  line is dominant at low temperatures due to the thermal population of the levels. For temperatures above ~50 K, however, the ratio of  $R_2$  to  $R_1$  peak areas is dominated by nonradiative combination. Additionally, Hall data was taken at low and elevated temperatures which demonstrated n-type behavior.

**AC-TuP-2 Determining the Effects of Traps on the Effective Mobility of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> MOSFETs using the Split C-V Method in Dark and Illumination Conditions and Pulsed I-V**, *Ory Maimon*, George Mason University; *N. Moser*, Air Force Research Lab; *D. Chamria*, Colgate University; *K. Liddy*, *A. Green*, *K. Chabak*, Air Force Research Lab; *S. Pookpanratana*, *P. Shrestha*, National Institute of Standards and Technology (NIST); *Q. Li*, George Mason University

Beta-gallium oxide ( $\beta$ -Ga<sub>2</sub>O<sub>3</sub>) high power and RF device performance is rapidly increasing due to the improved growth and fabrication methods developed in the last few years. Investigation of traps at and near the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and gate dielectric interface is critical for improving reliability and performance of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> MOSFETs. Trap state energies can vary in the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> bandgap, and their occupation can change with device bias. The trap states can also act as scattering sites, reducing the mobility. Here, we report on a study of effective mobility degradation due to traps at the Al<sub>2</sub>O<sub>3</sub>/ $\beta$ -Ga<sub>2</sub>O<sub>3</sub> interface in lateral depletion-mode  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> MOSFETs using the split C-V method in dark and illumination conditions with wavelengths from 730 nm (1.7 eV) to 265 nm (4.7 eV) and pulsed I-V is used to further characterize the traps

The MOSFETs are fabricated on a (010) semi-insulating  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrate. A 50 nm Si-doped epi layer is grown as the channel with a target doping concentration of  $2.4 \times 10^{18} \text{ cm}^{-3}$ . The ohmic contacts are formed using a Ti/Al/Ni/Au metal stack and annealed at 470 °C for 1 min in nitrogen. A 20 nm Al<sub>2</sub>O<sub>3</sub> gate dielectric is deposited using plasma-assisted atomic layer deposition (PE-ALD). The transistors are fabricated with a constant  $L_G$  and  $L_{GS}$  of 2  $\mu\text{m}$  and 0.5  $\mu\text{m}$ , respectively, while  $L_{GD}$  varies between 0.5  $\mu\text{m}$ , 5.5  $\mu\text{m}$ , and 10.5  $\mu\text{m}$ . Most FETs have a threshold voltage of -4 V, good linearity, and  $I_{ON}/I_{OFF}$  ratios between  $10^7 - 10^9$ .

A  $D_{it}$  of  $3 \times 10^{11} \text{ eV}^{-1} \text{ cm}^{-2}$  up to 0.44 eV below the conduction band is determined using the conductance method. Using illumination gives deep trap concentrations 1.7 eV below the conduction band. We observe little change for wavelengths above 455nm (2.7 eV) but see increasingly larger flatband voltage shifts as wavelength decreases, indicating a larger  $D_{it}$ . 2.7 eV below the conduction band. We observe an approximate 1.8x increase in the effective mobility under 265nm (4.7 eV), indicating that it is considerably lowered due to filled traps throughout the bandgap. We will present the analysis of the split C-V method in dark and illumination conditions, with a focus on the impact of traps on the mobility, and use pulsed I-V to analyze traps in comparison to the split C-V measurement.

**AC-TuP-3 Advanced Characterization Methods for Scale-up and Improvement of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> Substrates**, *Robert Lavelle*, *D. Snyder*, *W. Everson*, *D. Erdely*, *L. Lyle*, *A. Balog*, *N. Alem*, Penn State University

Advanced characterization methods are required to scale-up and improve the quality and uniformity of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates. In addition to developing these methods, one of the key challenges is implementing characterization

techniques at each stage of processing and combining these data to understand the interdependency of these steps and, ultimately, the impacts on device performance. PSU/ARL is uniquely positioned to help establish this vertically integrated feedback loop based on its  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrate processing experience and relationships with crystal and epi growers. PSU/ARL has characterized  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> crystals grown by multiple methods, including edge-defined film-fed growth (EFG) and Czochralski (Cz), and mapped full 2" substrates following chemi-mechanical polishing (CMP). In this poster, we will share these results focused on understanding the quality and uniformity of the substrates as well as advanced characterization methods, such as high-resolution x-ray diffraction (HRXRD) and transmission electron microscopy (TEM), for understanding the impacts of processing on defects and the fundamental material properties of the substrates. In this poster, we will highlight our recent progress on etch pit density (EPD) and defect mapping of full  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates. This includes investigating the propagation of defects such as nanopipes and impacts on epi growth. As part of this work, we have utilized a variety of characterization methods from optical mapping of full 2" substrates to performing TEM of individual defects. We will also discuss how we implemented characterization methods, including HRXRD, white light interferometry (WLI), and atomic force microscopy (AFM), for improving the surface finish and minimizing subsurface damage during CMP of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates. These advanced characterization methods have been essential in producing high-quality, uniform substrates during the scale-up process. Finally, we will share our recent work on characterizing off-cut/off-axis substrates and different alloy compositions in collaboration with groups focused on researching crystal and epi growth methods.

**AC-TuP-4 Vacancies in Electron Irradiated  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> Probed with Positrons**, *Marc Weber*, *C. Halverson*, Washington State University; *B. Dutton*, *C. Remple*, Washington State University, United States Minor Outlying Islands (the); *M. McCluskey*, Washington State University, US, United States Minor Outlying Islands (the); *M. Scarpulla*, University of Utah; *J. McCloy*, Washington State University, United States Minor Outlying Islands (the)

Positron annihilation spectroscopy is a powerful tool to evaluate vacancies and vacancy-related defects. To extract absolute defect concentrations data on reference samples or from other techniques must be available. We have examined bulk grown and epi-layer  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> material before and after high dose electron irradiation. Pre-existing and generated defects are probed by depth resolved positron Doppler Broadening and FTIR. Compared to other semiconducting materials, the anisotropic electron momentum distribution of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> poses challenges. Data from samples oriented in the [100], [010], and [001] direction are examined and compared to earlier experiments on oxygen annealed  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>[1] and recent theoretical work.[2] Subsequent annealing studies will further assist in the identification of the created defects. This work generously supported by the Air Force Office of Scientific Research under award number FA9550-18-1-0507 monitored by Dr. Ali Sayir.

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**AC-TuP-5 Artificial Intelligence Assisted Vacancy Detection via 3D Microscopy in Doped and Undoped Ga<sub>2</sub>O<sub>3</sub>**, *Prachi Garg*, *J. Sarker*, Department of Materials Design and Innovation, University at Buffalo; *A. Uddin Bhuiyan*, *L. Meng*, Department of Electrical and Computer Engineering, The Ohio State University; *H. Zhao*, Department of Electrical and Computer Engineering & Department of Materials Science and Engineering, The Ohio State University; *K. Reyes*, *B. Mazumder*, Department of Materials Design and Innovation, University at Buffalo

Recently, gallium oxide (Ga<sub>2</sub>O<sub>3</sub>) has attracted attention in high-power electronics and Schottky barrier diodes, due to their wide bandgap of ~4.8eV and critical breakdown strength of ~8 MV/cm. However, the low electron mobility of Ga<sub>2</sub>O<sub>3</sub> makes it crucial to dope with group IV elements (Si, Sn or Ge) in order to achieve desired electrical conductivity. This dopant incorporation in Ga<sub>2</sub>O<sub>3</sub> contributes to the formation of Ga vacancies. While

the inherent O vacancies in Ga<sub>2</sub>O<sub>3</sub> does not contribute to the electrical conductivity, the formation of Ga vacancies upon doping tends to trap the dopant atoms resulting in charge compensation effect in the material. To further improve semiconductor properties, defects like vacancies are introduced in a controlled manner, which have significant effect on its optical/charge transfer properties. Therefore, identifying and detecting these cationic vacancies are impactful for transport properties, however it is very challenging to detect vacancies from an atomic perspective using nano-analytical tools. Atom probe tomography (APT) is the only characterization tool that is capable of providing atomic resolution in 3D space. However, the latent features remain hidden in the tool complexities and large dimensional data, making it difficult to detect vacancies and distinguish them from missing atoms using APT alone. In this work, we developed a unique approach by integrating artificial intelligence with microscopic data to map the vacancy position in real atom probe data. Here, we applied a deep learning model named U-net for vacancy extraction on the 3D microscopic APT data. U-net is the image segmentation model which works in an end-to-end setting. A raw image is fed to the model, that goes within carefully tuned architecture and results in a segmented image i.e. feature map in this case. This model is trained on the synthetically generated Ga<sub>2</sub>O<sub>3</sub> structure using MD simulation software named LAMMPS (Large scale Atomic/Molecular Massively Parallel Simulator). Large structure is generated and sliced into voxels, fed into U-net model to train it on vacancy identification in each slice. Once the U-net model is trained, we use the APT data, slice it and feed into the model to detect the vacancies in real dataset. The trained U-net model will automatically analyze the APT data to learn and predict the local structure including vacancies to understand the vacancy distribution in doped and undoped Ga<sub>2</sub>O<sub>3</sub> structure. This work will provide an advancement in understanding the effect of Ga vacancies in Ga<sub>2</sub>O<sub>3</sub>. This work can also be expanded to study similar materials systems for developing future high-power transistors and optical devices.

**AC-TuP-6 Silicon Ion Implantation in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>: Effect of Temperature on Atomic Damage and Recovery, Naomi Pieczulewski, K. Gann, Cornell University; T. Asef, B. Noesges, Air Force Research Laboratory; K. Heinselmann, National Renewable Energy Laboratory; M. Thompson, D. Muller, Cornell University**

Si implantation is a promising strategy to reduce contact resistance and improve Ga<sub>2</sub>O<sub>3</sub> device performance.<sup>1</sup> Recent reports have shown a variety of phase transformations into Ga<sub>2</sub>O<sub>3</sub> polymorphs from the  $\beta$  phase upon ion implantation.<sup>2,3</sup> Previously our group has found that by using high angle annular dark field (HAADF) and annular bright field (ABF) scanning transmission electron microscopy (STEM) imaging, we can accurately identify  $\gamma$ -phase of Ga<sub>2</sub>O<sub>3</sub>.<sup>4</sup> Here, we present a systematic study of high Si implant doses over a range of implant temperatures from liquid nitrogen temperature to 600°C to investigate the limits of damage recovery. We found that the kinetically favored defect structure is  $\gamma$ -Ga<sub>2</sub>O<sub>3</sub> under the investigated implant conditions and the implanted films retain  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> resulting in fast and clean recovery.

MBE grown UID  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> [010] film was implanted with Si over a 100nm profile targeting a total carrier concentration of  $5 \times 10^{19}$  to  $1 \times 10^{20} \text{cm}^{-3}$ . The implanted films were characterized by STEM to probe defects at the atomic scale, supplemented by X-ray diffraction (XRD) and Rutherford Back Scattering (RBS). We observe implantations performed at both room temperature and low temperature cause a phase transformation into  $\gamma$ -Ga<sub>2</sub>O<sub>3</sub> as well as interstitial Ga defects in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, but also retain significant  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. Crystallinity in the low temperature implant indicate significant dynamic annealing either during implantation or during warming back to room temperature. Implantation performed at a high temperature shows significantly less lattice damage and retains complete  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. Thermal activation by post-annealing heat treatment is required on all samples to electrically activate carriers.

Finally, lattice recovery and Si activation was investigated after annealing the Si implanted films at 950°C for 20 minutes under high purity nitrogen. Carrier activation was observed in the control implant starting only after a couple minutes, indicating the retained  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> enables fast recrystallization into recovered film. All films showed good recovery and significant dopant activation, indicating the limits of damage recovery can be still pushed.

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**AC-TuP-8 Kinetics of Compensation in Sn-doped Ga<sub>2</sub>O<sub>3</sub> During O<sub>2</sub> Annealing Revealed by FTIR and Modelling, J. High, H. Yang, N. Rock, Mike Scarpulla, University of Utah**

It is well known that annealing n-type doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> in air or O<sub>2</sub> produces insulating surface layers on the micron scale; however the microscopic mechanisms remain a mystery. Besides the identity of the defects involved, the locations of generation and transport are unknown.

At this time, V<sub>Ga</sub>, V<sub>O</sub> and their complexes are believed to be the dominant stable native defects but the mechanisms of their formation are unknown. Do V<sub>Ga</sub> form at structural defects and interfaces then diffuse to permeate the material, or do Frenkel pairs nucleate homogeneously and the Ga<sub>i</sub> diffuse away to sinks? How is the information about oxygen richness imposed transmitted from the surfaces inwards to the bulk; do O<sub>i</sub> play any transient role in mediating these processes? Such details still have not been addressed, and can not be distinguished by their effects on net charge alone; some orthogonal data such as formation or migration barriers must also constrain hypotheses in order to determine the most likely.

We have been utilizing FTIR transmission through wafers approximately 500  $\mu\text{m}$  thick to reveal the kinetics of the conducting-to-insulating transition during annealing. In thick samples, a mechanism with diffusion constant many orders of magnitude faster than that found near the surface (up to  $\sim 1 \mu\text{m}$ ) using electrical methods would be required. Put more concretely, if only the previously-determined mechanism is present, the insulating transition would take centuries in wafers while only days to weeks are required near 1000 °C in pure O<sub>2</sub>.

We developed a coupled defect diffusion, carrier density, dielectric function, multilayer optics model of the samples with which we can test hypotheses for the kinetics of compensating defect formation and transport. Our model spans from the bandgap near 5 eV to the limiting 2-phonon absorption at  $1500 \text{cm}^{-1}$  and, after inclusion of POP phonon-limited momentum scattering lifetime in the Drude component, reproduces the data extremely well. With this level of modelling, we show with high confidence that at least two diffusion-mediated processes are required to reproduce the data. We review possible mechanisms and provide evidence on the kinetic barriers for what is presumably a native defect driven process. Fortunately, the fidelity and predictiveness of computations of defect energetics and migration barriers now allow differentiation between possible mechanisms; we hope that these experiments will motivate detailed studies to uncover the detailed mechanisms of defect processes in Ga<sub>2</sub>O<sub>3</sub> and beyond.

**AC-TuP-9 Cation Vacancy and Dopant Diffusion in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, Nathan David Rock, A. Levin, University of Utah; A. Bhattacharyya, University of California Santa Barbara; H. Yang, B. Eisner, University of Utah; S. Krishnamoorthy, University of California Santa Barbara; M. Scarpulla, University of Utah**

Mechanistic understanding of native and impurity defect diffusion and reaction processes in Ga<sub>2</sub>O<sub>3</sub> is necessary for advanced fabrication of devices and for the long-term reliable operation of those devices. The diffusion of native and impurity atoms and their incorporation into various point defects and complexes is mediated by native defects. Thus, understanding the diffusion of native defects is fundamental to understanding all diffusion processes. Unlike impurities, vacancies are difficult to study because of the difficulty of measuring their concentration. Additionally, the mechanisms of formation of native defects are unknown; for example, cation vacancies may be introduced at surfaces and diffuse inwards, or interstitial-vacancy pairs may form in the bulk with interstitials diffusing outwards.

We introduced superlattices (SLs) of alternating (Al,Ga)<sub>2</sub>O<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub> grown by OMVPE in order to make visible the flux of cation vacancies using Al as a tracer. We demonstrate that in the case of SLs grown on Sn-doped substrates, the diffusion of Al is mediated by the transient diffusion of a large concentration of mediating defects (presumed to be V<sub>Ga</sub> or complexes thereof) from the substrate into the epilayers. This results in faster diffusion near the Sn-doped substrate and slower near the free surface indicating that the introduction of V<sub>Ga</sub> from the free surface is insignificant at the at% level compared to the supply in the substrate. In the case of SLs grown on Fe-doped substrates, the diffusion of Al is much slower and spatially-uniform indicating a uniform density of mediating defects vs depth. Additionally, we document the co-diffusion of Sn and Fe out of the substrates and through the SLs – this implies that V<sub>Ga</sub> is not diffusing alone

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but rather as complexes or with high-correlation with Fe or Sn. This implies that the rates measured are not those of the VGa itself but rather a slowed rate from the mutual effects of solute drag. The role of oxygen is also investigated – annealing in O<sub>2</sub> is generally needed for dopants to diffuse, however the role of O in the diffusion of pre-existing VGa in the substrate is not clear. In addition to the model of vacancy-mediated diffusion introduced last year, we also report on coupled drift-diffusion-reaction-Poisson models for simultaneous diffusion of V<sub>Ga</sub>, Sn, and Fe. We also have documented the presence and diffusion of various other impurities which has implications for device stability. We estimate the contributions of chemical and electrical potential gradients (e.g. surface fields and dopant concentration steps) in the mass transport.

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 Eguchi, K.: MD+AC+EP-TuA-13, 8  
 Eisner, B.: AC-TuP-9, 10  
 Erdely, D.: AC+MD-TuM-14, **6**; AC-TuP-3, 9  
 Ertekin, E.: AC+DI+HM+TM-MoA-11, 3; AC-MoP-4, 5  
 Everson, W.: AC+MD-TuM-14, **6**; AC-TuP-3, 9  
 — F —  
 Feneberg, M.: AC+TM-MoM-6, 1  
 Fiedler, A.: AC+TM-MoM-5, 1  
 Fornari, R.: AC+TM-MoM-6, 1  
 — G —  
 Galazka, Z.: AC+TM-MoM-5, 1; AC+TM-MoM-6, 1  
 Gann, K.: AC-TuP-6, 10  
 Garg, P.: AC-TuP-5, 9  
 Goldhahn, R.: AC+TM-MoM-6, 1  
 Goorsky, M.: AC+DI+HM+TM-MoA-13, 3  
 Green, A.: AC+DI+HM+TM-MoA-12, 3; AC-TuP-2, 9  
 Grundmann, M.: AC+TM-MoM-6, 1  
 — H —  
 Hajizadeh, N.: AC+TM-MoM-6, 1  
 Halverson, C.: AC-TuP-4, 9  
 Hartung, C.: AC+TM-MoM-6, 1  
 Heinselmann, K.: AC-TuP-6, 10  
 Higashiwaki, M.: MD+AC+EP-TuA-13, 8  
 High, J.: AC-TuP-8, 10  
 Hilfiker, M.: AC+DI+HM+TM-MoA-9, 3; AC+TM-MoM-7, 2  
 Hobart, K.: AC+DI+HM+TM-MoA-13, 3  
 Hong, J.: MD+AC+EP-TuA-10, 7  
 Huang, H.: AC+TM-MoM-4, 1  
 Huynh, K.: AC+DI+HM+TM-MoA-13, 3  
 Hwang, J.: AC+TM-MoM-4, 1  
 — I —  
 Irmischer, K.: AC+TM-MoM-5, 1  
 Islam, A.: AC+DI+HM+TM-MoA-12, 3  
 — J —  
 Jacobs, A.: AC+TM-MoM-8, 2  
 Janzen, B.: AC+TM-MoM-6, 1  
 Jesenovec, J.: AC-MoP-4, 5; AC-TuP-1, 9  
 Joo, N.: MD+AC+EP-TuA-10, 7  
 Jung, Y.: MD+AC+EP-TuA-10, 7; MD+AC+EP-TuA-12, 7  
 — K —  
 Kato, T.: AC+TM-MoM-6, 1  
 Khan, K.: AC+MD-TuM-12, 6  
 Kim, M.: AC+MD-TuM-13, 6  
 Kim, T.: MD+AC+EP-TuA-10, 7  
 Kim, Y.: AC-MoP-3, 5  
 Kitada, T.: MD+AC+EP-TuA-13, 8  
 Kluth, E.: AC+TM-MoM-6, 1  
 Knight, S.: AC+DI+HM+TM-MoA-9, 3  
 Knudtson, J.: AC+TM-MoM-7, 2  
 Koo, S.: AC+MD-TuM-13, 6  
 Korlacki, R.: AC+DI+HM+TM-MoA-9, 3; AC+TM-MoM-7, 2  
 Krishnamoorthy, S.: AC-MoP-2, 5; AC-TuP-9, 10; MD+AC+EP-TuA-9, 7  
 — L —  
 Lavelle, R.: AC+MD-TuM-14, **6**; AC-MoP-4, 5; AC-TuP-3, 9  
 Lee, C.: AC+DI+HM+TM-MoA-11, **3**; AC-MoP-4, 5  
 Levin, A.: AC-TuP-9, 10  
 Li, J.: AC-MoP-3, 5  
 Li, Q.: AC+MD-TuM-13, **6**; AC-TuP-2, 9  
 Liao, M.: AC+DI+HM+TM-MoA-13, **3**; AC+MD-TuM-14, 6  
 Liddy, K.: AC-TuP-2, 9  
 Lou, M.: AC-MoP-2, 5  
 Lundh, J.: AC+DI+HM+TM-MoA-13, 3  
 Lyle, L.: AC+MD-TuM-14, **6**; AC-TuP-3, 9  
 — M —  
 Ma, Y.: AC+TM-MoM-8, 2  
 Mahadik, N.: AC+MD-TuM-14, 6  
 Maimon, O.: AC+MD-TuM-13, **6**; AC-TuP-2, 9  
 Marggraf, M.: AC+TM-MoM-6, 1  
 Mazumder, B.: AC-TuP-5, 9  
 Mazzolini, P.: AC+TM-MoM-6, 1  
 McCloy, J.: AC-MoP-4, 5; AC-TuP-1, 9; AC-TuP-4, 9  
 McCluskey, M.: AC-MoP-1, 5; AC-TuP-1, 9; AC-TuP-4, 9  
 Meißner, M.: AC+TM-MoM-6, 1  
 Meng, L.: AC-TuP-5, 9  
 Miao, L.: AC-MoP-4, 5  
 Moser, N.: AC-TuP-2, 9  
 Mou, S.: AC-MoP-3, 5  
 Muller, D.: AC-TuP-6, 10  
 — N —  
 Neal, A.: AC-MoP-3, 5  
 Nishinaka, H.: AC+TM-MoM-6, 1  
 Noesges, B.: AC-MoP-3, 5; AC-TuP-6, 10  
 — O —  
 Oshima, T.: AC+TM-MoM-6, 1  
 — P —  
 Papamichael, A.: AC+DI+HM+TM-MoA-9, 3  
 Park, J.: MD+AC+EP-TuA-10, 7  
 Petersen, C.: AC+TM-MoM-6, 1  
 Peterson, C.: MD+AC+EP-TuA-9, 7  
 Pieczulewski, N.: AC-TuP-6, **10**  
 Pookpanratana, S.: AC+MD-TuM-13, **6**; AC-TuP-2, 9  
 Popp, A.: AC+TM-MoM-5, 1  
 Potter, M.: AC+TM-MoM-8, 2  
 — Q —  
 Qin, Y.: AC+TM-MoM-8, 2  
 — R —  
 Rajan, S.: AC+DI+HM+TM-MoA-12, 3; AC+TM-MoM-4, 1  
 Ramdin, D.: AC+TM-MoM-4, 1  
 Remple, C.: AC-TuP-1, **9**; AC-TuP-4, 9  
 Reyes, K.: AC-TuP-5, 9  
 Richter, S.: AC+DI+HM+TM-MoA-9, 3  
 Rock, N.: AC-TuP-8, 10; AC-TuP-9, **10**  
 Rodriguez, B.: MD+AC+EP-TuA-9, 7  
 Roy, S.: MD+AC+EP-TuA-9, 7  
 Ruder, A.: AC+DI+HM+TM-MoA-9, 3  
 — S —  
 Sacchi, A.: AC+TM-MoM-6, 1  
 Sarker, J.: AC-TuP-5, 9  
 Sasaki, K.: AC+TM-MoM-8, 2  
 Sato, S.: MD+AC+EP-TuA-13, **8**  
 Scarpulla, M.: AC-MoP-2, **5**; AC-TuP-4, 9; AC-TuP-8, **10**; AC-TuP-9, 10  
 Schubert, M.: AC+DI+HM+TM-MoA-9, 3; AC+TM-MoM-7, 2  
 Sensale-Rodriguez, B.: AC-MoP-2, 5  
 Seyidov, P.: AC+TM-MoM-5, 1  
 Shrestha, P.: AC-TuP-2, 9  
 Snyder, D.: AC+MD-TuM-14, **6**; AC-TuP-3, 9  
 Speck, J.: AC+DI+HM+TM-MoA-9, 3  
 Spencer, J.: AC+TM-MoM-8, 2  
 Stanishev, V.: AC+DI+HM+TM-MoA-9, 3  
 Stokay, M.: AC+DI+HM+TM-MoA-9, 3; AC+TM-MoM-7, 2  
 — T —  
 Tadjer, M.: AC+DI+HM+TM-MoA-13, 3; AC+TM-MoM-8, 2  
 Thompson, M.: AC-TuP-6, 10  
 — U —  
 Uddin Bhuiyan, A.: AC-TuP-5, 9  
 — V —  
 Varley, J.: AC+TM-MoM-6, 1  
 von Wenckstern, H.: AC+TM-MoM-6, 1  
 — W —  
 Wagner, M.: AC+TM-MoM-6, 1  
 Wang, H.: AC+TM-MoM-8, 2  
 Wang, Y.: AC-MoP-2, 5  
 Wang, Z.: MD+AC+EP-TuA-13, 8  
 Weber, M.: AC-TuP-4, **9**  
 Wen, Z.: AC+MD-TuM-12, **6**  
 Winchester, A.: AC+MD-TuM-13, 6  
 — X —  
 Xiao, M.: AC+TM-MoM-8, 2  
 — Y —  
 Yang, H.: AC-TuP-8, 10; AC-TuP-9, 10  
 — Z —  
 Zeng, K.: MD+AC+EP-TuA-11, **7**  
 Zhang, Y.: AC+TM-MoM-8, 2  
 Zhao, H.: AC-TuP-5, 9