Advanced Characterization Techniques
Room Davis Hall 101 - Session AC+TM-MoM

Characterization/Modeling I

Moderators: Michael Scarpulla, University of Utah, **Uttam Singisetti**, University of Buffalo, SUNY

9:15am **AC+TM-MoM-4 Electric Field Induced Defect Redistribution at Ni-Ga_2O_3 Interfaces***, **Daram Ramdin**, H. Huang, S. Dhara, S. Rajan, J. Hwang, L. Brillson,* The Ohio State University

β-Ga_2O_3 is a prime semiconductor for high power electronics due to its high intrinsic critical field of ~ 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_2O_3 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/ β-Ga_2O_3 interfacial region exhibits new, above β-Ga_2O_3 band gap 5.29 eV and 5.82 eV CL emissions corresponding to a γ-Ga_2O_3 phase. Also present are a set of characteristic intrinsic β-Ga_2O_3 defect emissions including a ~2.4 eV feature which increases under the contact. STEM confirms a defective misaligned γ phase that is of average thickness ~ 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 ~5.2 eV and ~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 γ-Ga_2O_3 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.[1] These observations are consistent with Ni diffusion into β-Ga_2O_3 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towards the defective layer during the breakdown process, similar to the effect of annealing on this defective layer (unpublished).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/ β-Ga_2O_3 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 *β*-Ga_2O_3 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. Irmscher, A. Fiedler,* Leibniz-Institut für Kristallzüchtung, Germany

β-Ga_2O_3 has emerged as a next-generation high-power application due to its large bandgap of 4.85eV and a high theoretical breakdown field of ~8MV/cm, which already resulted in established power rectifiers and MOSFETs with excellent characteristics.[1] Bulk single crystals for substrates can be grown with EFG[2] and Czochralski[3] 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 *β*-Ga_2O_3 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 *β*-Ga_2O_3 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 ~1.2eV 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 *β*-Ga_2O_3 crystals.

We measured the photoconductivity, optical absorption, and temperature-dependent resistivity (up to 1100K) of Ni-doped *β*-Ga_2O_3 crystal grown by the Czochralski method[3]. Fitting results of photoconductivity measurement allow us to identify the energy of the E_{ZPL}, D_{FC},and hω 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 ~2.0 eV. Conclusively, from the experiment and theory, a consistent energy scheme: an acceptor level of ~1.9 eV (above the VBM), and a donor level of ~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 *β*-Ga_2O_3 substrates for lateral power devices.

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

9:45am **AC+TM-MoM-6 Comparative Study of Temperature-Dependent Bandgap Transitions in Ga_2O_3 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_2O_3. 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] β-, orthorhombic rotational-domain [2] as well as single-domain[3] κ-, rhombohedral [4] α-, defective spinel [5] γ- and cubic bixbyite [6] δ-Ga_2O_3as 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 γ and α possess the largest bandgap energy values around 5.36 eV, with the monoclinic β-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 γ or weakest coupling for κ and δ, whereas the interaction appears similarly intense for α with respect to β. In contrast to the rotational domain structured κ-Ga_2O_3 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.

[1]: Z. Galazka, Semicond. Sci. Technol., 33(11), 113001 (2018).

[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).

10:00am **AC+TM-MoM-7 Strain and Composition Dependencies in $(Al_xGa_{1-x})_2O_3$ 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 (Al,Ga)N.[1-2] In order to apply the same principle to $(Al_xGa_{1-x})_2O_3$ 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, Ga_2O_3 and Al_2O_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 $(Al_xGa_{1-x})_2O_3$-based electronic and photonic devices.

[1] D. Li, K. Jiang, X. Sun, and C. Guo, *Adv. Opt. Photon.***10**, 43-110 (2018)

[2] J.-M. Wagner and F. Bechstedt, *Phys. Rev. B***66**, 115202 (2002)

[3] R. Korlacki, M. Stokey, A. Mock, S. Knight, A. Papamichail, V. Darakchieva, and M. Schubert, *Phys. Rev. B***102**, 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 β-$(Al_xGa_{1-x})_2O_3$," in preparation

10:15am **AC+TM-MoM-8 10 kV Ga_2O_3 Schottky Rectifier Operational at 200 ℃**, ***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 Ga_2O_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 Ga_2O_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 Ga_2O_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 Ga_2O_3 epi layer. A total charge density (σ_n) of $3.8\times10^{12}cm^{-2}$ is estimated in n-Ga_2O_3. A NiO/n$^+$-Ga_2O_3 p-n diode is fabricated to extract the acceptor concentration in NiO, which is revealed to be $8\times10^{17}cm^{-3}$ at 25°C and shows little changeat 200°C (Fig. 1(d)). If a charge imbalance margin below 15% is kept for practical device fabrication, the NiO thickness (t_{NiO}) range is estimated to be 61-82 and 58-78nm for the anode-to-cathode length (L_{AC}) of 30 and 50µm.

Fig. 2(a)-(c) show the simulated electric field (E-field) contours of RESURF SBDs with different t_{NiO}. In charge balance condition (t_{NiO}=75nm), the E-field are more evenly distributed in Ga_2O_3 channel. Fig. 2(d) manifests that the NiO RESURF region could increase the device on-resistance (R_{on}) due to the vertical depletion effect.

Fig. 3(a) and (b) show the reverse I-V characteristics of the Ga_2O_3 RESURF SBDs with various t_{NiO} for L_{AC} of 30 and 50µm. The breakdown voltage (*BV*) increases with the increasing t_{NiO}, reaching>10kV (the measurement limit of our test setup) at t_{NiO}=75nm, and starts to decrease at larger t_{NiO}. The two sets of devices can be swept repeatedly up to 10kV at 200°C (Fig. 3(c)).Fig. 3(d)suggeststhe 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 50µm. The larger R_{on} of RESURF SBDs can be explained by the simulation results in Fig. 2(d).The specific R_{on} of the RESURF SBDs with L_{AC}=30µm is calculated to be 0.27Ω·cm^2. Fig. 4(b) shows the temperature-dependent forward I-V characteristics of this RESURF SBD.

Fig. 5 benchmarks the $R_{on,sp}$ versus *BV* as well as the *BV* versus maximum operational temperature for our devices and the state-of-the-art Ga_2O_3 devices. Our device shows the highest *BV* and the operational temperature in multi-kilovolt Ga_2O_3 devices.

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