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towards the defective layer during the breakdown process, similar to the effect of annealing on this defective layer (unpublished).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 $0.27\Omega\cdot cm^2$. 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.

Theory, Modeling and Simulation
Room Davis Hall 101 - Session TM-TuM

Characterization/Modeling III

Moderators: Uttam Singisetti, University of Buffalo, SUNY, **Joel Varley**, Lawrence Livermore National Laboratory

9:15am **TM-TuM-4 Electron–Phonon Effects and Temperature-Dependence of the Electronic Structure of Monoclinic β-Ga_2O_3 from First Principles**, ***Elif Ertekin***, *C. Lee,* University of Illinois at Urbana-Champaign, USA*; M. Scarpulla, N. Rock, A. Islam,* University of Utah **INVITED**

A primary reason that β-Ga_2O_3 is a promising semiconductor for next-generation high-power electronics is its ultra-wide band gap, resulting in desirable high critical breakdown field. While first-principles approaches have provided key insights into the ground state electronic structure of β-Ga_2O_3, temperature-dependent properties however have remained challenging to model. Yet, they are important: temperature effects underlie key semiconductor properties such as carrier mobility, band edge positions, and optical absorption. To utilize the unique electrical properties of β-Ga_2O_3 for real-world applications, an accurate description of electronic structure under device-operating conditions is required. In this presentation, I will highlight our recent progress in modeling key temperature-dependent aspects of the electronic structure of β-Ga_2O_3 -- namely, how electron-phonon coupling affects the band structure and band gap. Utilizing the quasi-harmonic approximation and the recently developed "one-shot" frozen phonon method, we have been able to predict the temperature-dependent electronic band structure of β-Ga_2O_3 in a wide temperature range from T = 0 to 900 K using first-principles simulations. Band edge shifts from lattice thermal expansion and phonon-induced lattice vibrations known as electron–phonon renormalization together are found to induce a substantial temperature-dependence on the band gap, with the latter giving the dominant contribution. We find that the band gap is reduced by more than 0.5 eV between T = 0 and 900 K. Our prediction of temperature-dependent band gap matches well with previously reported and our new experimental optical measurements, further emphasizing the need for accounting for such effects in first-principles simulations of wide band gap semiconductors. As the temperature dependence and the band gap reduction is quite a bit larger than that observed in other wide band gap materials, key implications for device performance will be discussed. These implications include an increase in carrier concentrations, a reduction in carrier mobilities due to localization of band edge states, and a ~20% reduction in the critical breakdown field at 900 K. Future directions for analysis -- including challenges in modeling thermal-disorder induced Urbach effects and breakdown -- will be discussed as well.

9:45am **TM-TuM-6 Ab-Initio Calculation of Low Field Electron Transport in Disordered Bulk β-$(Al_xGa_{1-x})_2O_3$ Semiconductor Alloy**, ***Ankit Sharma***, *U. Singisetti,* University at Buffalo-SUNY

β-Ga_2O_3 is an emerging UWBG semiconductor with potential applications in power and RF devices due to its large bandgap, high critical electric field and low on-resistance. The availability of bulk substrates with a matured crystal growth methodology makes it a strong contender to SiC and GaN, the two widely used materials for power and RF applications. With all is benefits, overcoming the low bulk electron mobility due to large polar scattering is a major challenge in this material. As such the Ga_2O_3 device research has pivoted to using AlGaO/GaO heterostructures to harness the high electron mobility of the 2DEG formed at the interface as a result of the band offset. Many devices employing this heterostructure have already been successfully demonstrated. In order to improve and optimize performance of the devices, the fundamental understanding of the charge transport mechanism lies at the crux. Extensive theoretical and experimental investigations have been performed for the bulk GaO, but for the AlGaO alloy the results are scarce. This is further complicated by the fact that with aluminum substitution the translational symmetry in the crystal is lost which forms the basis for the theoretical modeling of the charge transport mechanism. In this work, we extend the periodic crystal based formulation of the electron and phonon dispersion to this disordered system through the Brillouin zone unfolding method where the disorder is modeled using supercell special quasirandom structures. The analysis is further extended to calculate the shortrange deformation potential, longrange polar optical, ionized impurity and alloy disorder scattering from first principles. The Boltzmann transport equation (BTE) is subsequently solved under the Rode's iterative framework to obtain electron mobility. The currently available results for AlGaO alloy solve the BTE for periodic structures and then interpolate the result at intermediate alloy fractions using Vegard's law. Our application of the ab-initio approach at intermediate alloy fractions is novel and eliminates the need for interpolation along with providing insight into the mobility limiting scattering mechanisms under low applied electric fields. We also propose a method to calculate the IR spectra of disordered systems such that theoretical and experimental observation could be compared directly. Some of the results obtained as the part of our initial work in the calculation of the electron mobility in the AlGaO disordered system from first principles is presented in the supplementary material.

10:00am **TM-TuM-7 Quantitative Modelling of Defect Concentrations in β-Ga_2O_3 for Equilibrium, Full Quenching, and Generalized Quenching Scenarios**, ***Khandakar Aaditta Arnab***, *I. Maxfield,* University of Utah*; C. Lee, E. Ertekin,* University of Illinois at Urbana Champaign*; J. Varley,* Lawrence Livermore National Laboratory*; Y. Frodason,* University of Oslo, Norway*; M. Scarpulla,* University of Utah

β-gallium oxide (β-Ga_2O_3) is of intense current interest because of its ultra-wide bandgap, high critical field, and availability of melt-grown substrates. Point defects and complexes determine the properties of bulk crystals as well as epitaxial layers, thus, predictive models of defect concentrations under various impurity and processing scenarios are of very high value. First-principle calculations of defect energetics have provided critical insights into the defect system in β-Ga_2O_3, but translating computed enthalpies into defect concentrations corresponding to real-world crystal growth requires additional steps. Material processing in terms of growth or annealing typically controls the sample's thermochemical trajectory in terms of temperatures and partial pressures, while computational papers frequently present results holding chemical potentials constant.

Here we report quantitative modelling of equilibrium defect concentrations in Ga_2O_3, considering especially the temperature dependence of the bandgap and temperature-dependent chemical potentials from the Ga-O binary system's known thermochemistry. Additionally, we compute results for realistic sample types such as Fe- or Sn-doped wafers accounting for the fixed concentrations of these impurities as opposed to their fixed chemical potentials. Results are presented for various background n-type doping and for equilibrium and quenching, corresponding respectively to 0 or infinite cooling rates. We find significant departures from prior simpler predictions, especially in the case of the bandgap temperature dependence which tends to suppress V_{Ga}. We compare our predicted results to experimental cases such as annealing in O_2 or Ga_2O vapors.

Finally, to give semi-quantitative insight into defect concentrations expected in finite-sized samples subjected to finite cooling rates without full-fledged defect reaction-diffusion simulations, we introduce the concept of generalized quenching as a 3rd type of computation. At the heart of generalized quenching is the insight that, because of their different diffusion constants, different types of defects located at different distances from free surfaces will be "frozen-in" at different temperatures. By combining the correct series of equilibrium and quenching calculations, it is possible to predict defect concentrations present in real-world samples e.g. as a function of radius within a boule or for thin films of different thicknesses. We compare these results to the known phenomena from bulk crystal growth, indicating differences in carrier density between the center and periphery of CZ-grown boules.

10:15am **TM-TuM-8 Exploring Gallium Oxide (β-Ga_2O_3) Drift Layer Design: Theoretical Analysis and Trade-offs**, ***Sundar Isukapati***, *S. DeBoer, S. Jang,* SUNY Polytechnic Institute, Albany*; Y. Jung,* Hyundai Motor Company, Republic of Korea*; W. Sung,* SUNY Polytechnic Institute, Albany

Gallium Oxide (Ga_2O_3) has emerged as a highly promising material for power devices due to its wider bandgap and high critical electric field. In this paper, we investigate the drift layer design for Ga_2O_3 power devices through theoretical analysis and trade-offs. The drift layer, similar to other wide-bandgap materials, plays a crucial role in the performance of Ga_2O_3 power semiconductor devices. The two primary drift layer configurations, non-punch through (NPT) and punch-through (PT), are analyzed with a focus on key design parameters such as drift layer thickness (W_D) and doping concentration (N_D), and their impact on specific on-resistance ($R_{on,sp}$) for both NPT and PT structures. Furthermore, we extend the specific on-

resistance to breakdown voltage (BV) trade-off analysis by considering the additional resistance components for both lateral and vertical MOSFETs, providing a practical guide for device researchers to pursue the appropriate architectures based on the voltage rating.

The ionization rate of the electrons in Ga_2O_3 shown in Fig. 1, is utilized for the evaluations. The electric field at the onset of BV (referred to as the critical electric field, E_c) is extracted iteratively by solving the ionization integral with the ionization rates for both non-punch through (NPT) and punch-through (PT) structures. The critical electric field exhibits a strong dependence on the doping concentration for both non-punch through (NPT) and punch-through (PT) structures (with varying widths) as illustrated in Fig. 2. The impact of doping concentration and width on the BV for both NPT and PT structures (with varying widths) is depicted in Fig. 3. The ionization ratio as a function of doping concentration is extracted from the ionization energies of donors is shown in Fig. 4. With reduced doping concentration and width, the optimal $R_{on,sp}$ of the punch-through (PT) structure is about 8% lower than that of the non-punch through (NPT) structure at a particular BV, as depicted in Fig. 5. To further explore the trade-off analysis, a Ga_2O_3 MOSFET with both lateral and vertical architectures was considered. Using reasonable assumptions and practical specifications, the channel, drift, and substrate resistances were evaluated. Fig. 6 depicts the individual and total resistance components associated with lateral devices (channel and drift resistances represented by red curves) and vertical devices (channel, drift, and substrate resistances represented by blue curves). It is evident from Fig. 6 that, at breakdown voltages lower than ~2kV, the lateral device offers the lowest possible $R_{on,sp}$ but beyond ~2kV, the vertical device dominates by offering a lower $R_{on,sp}$.

Theory, Modeling and Simulation
Room Bansal Atrium - Session TM-TuP

Theory, Modeling and Simulation Poster Session

TM-TuP-1 Investigation of Oxygen Interstitial Diffusion Pathways in β-Ga2O3, ***Grace McKnight***, *C. Lee, E. Ertekin,* University of Illinois at Urbana-Champaign

Monoclinic β-Ga_2O_3 is a highly stable wide band gap semiconductor that exhibits a wide spectrum of complex defects. Understanding the diffusion of these defects may enable the precise optimization of the electronic and optical properties through controlled doping, making β-Ga_2O_3 a promising candidate for a diverse range of applications. While recent computational studies have investigated the diffusion of intrinsic defects including Ga interstitials and Ga and O vacancies as well as extrinsic defects like Si and Sn interstitials, the diffusion of O interstitials has received comparatively less attention. This is because, in many oxide semiconductors, O and H interstitials exhibit faster diffusion than other types of cation interstitials or vacancies, owing to their low diffusion barriers and small ionic sizes, thus making them highly mobile within the material. However, high anisotropy of the monoclinic crystal structure of β-Ga_2O_3 implies significant variations in the diffusion coefficients along different crystallographic directions. In this study, we aim to (1) understand the complete diffusion mechanism of oxygen interstitials and (2) predict directionality in diffusivity of oxygen interstitials in β-Ga_2O_3 from first principles calculations based on total energy density functional theory. We first explore all possible configurations of oxygen interstitials and their formation energies including extended structures, such as O interstitials split into two or three O sites. We construct a diffusion network that includes every possible hop between each identified low-energy configuration and obtain the migration barriers by the nudged elastic band method. The migration paths and barriers of the diffusion network are used to construct and then solve the master diffusion equations, resulting in high anisotropy in Onsager transport coefficients, which illuminate the most dominant pathways in each crystallographic direction. Our study provides valuable insights into the migration of O interstitials, which contributes to the further developments and characterizations of β-Ga_2O_3 based applications.

TM-TuP-2 Optoelectronic Properties of $(In,Ga)_2O_3$ using First Principles Calculations, *E. Welch,* Prairie View A&M University*; P. Borges,* Federal University of Vicosa - Rio Paranaiba, Brazil*;* ***Luisa Scolfaro****, M. Talukder, R. Droopad,* Texas State University

Preliminary experimental results for In alloyed Ga_2O_3 ($In_{2x}Ga_{2-2x}O_3$) reveal these materials as to be promising for use as an n-type layer in a pn-junction with lattice matched, p-type materials like NiO [1]. This n-type conductivity is somewhat anomalous as In substitution/alloying alone is not expected to result in shallow defect states. O vacancies have been shown to exist in abundance in these materials but are known to not contribute to the conductivity as the compensating native defect formation in the material passivates these vacancies. Thus, a better understanding of point and complex defects are required to explain this behavior. Here, we studied In-based defects in Ga_2O_3 using hybrid density functional theory to understand potential sources of this n-type conductivity. The defects studied in Ga_2O_3 were single substitutional In (In_{Ga}), single interstitial In (In_i), and a defect complex comprised of a single In substitution and a single In interstitial (In_{Ga} + In_i). Formation energy calculations were used to quantify the stability of each defect where a negative value indicates relative stability. In_i can form during alloying of $(In_xGa_{1-x})_2O_3$ when the In content is low enough that individual In atoms settle into one of two Ga-O cages within the crystal; In interstitials are shown to prefer the larger Ga-O cage with an energy 1 eV lower than in the smaller cage. The In_i defect introduces 3 valence electrons which reside within the electronic band gap. This results in a partially filled band gap state which can be an intermediate transition state between the bulk electronic band edges. As the In content is elevated, In may become a substitutional defect at the cation site where octahedral O coordination is preferred over tetrahedral coordination; In is isoelectronic to Ga and is stable as a substitutional atom. The increase of In leads to substitution at higher content of In which leads to a reduction of the band gap and eventually to a phase transition, which is seen experimentally [2]. The In_{Ga}+ In_i complex defect can also occur, where the two defects can either be near one another (adjoined) or far in the crystal (disjointed). The formation energy for all systems in their neutral charge state except the single In substitution is positive and therefore these neutral defects are unstable. However, the prospect of polaron formation in the charged defect states indicates potentially stable defects with inter band gap states that may help to explain the anomalous n-type conductivity.

[1] Md Abdul Ahad Talukder, PhD Dissertation, 2022, Texas State University.

[2] J. E. N. Swallow, et al., *ACS Appl. Mater. Interfaces* 13, 2807, **2021**.

TM-TuP-3 Modeling of β-$(Al_xGa_{1-x})_2O_3/Ga_2O_3$ High Electron Mobility Transistor (HEMT) and Current Aperture Vertical Electron Transistor (CAVET), ***Dawei Wang****, D. Herath Mudiyanselage, H. Fu,* Arizona State University

Due to its ultra-wide bandgap, high critical electric field, and large Baliga's figure of merit (FOM), beta-phase gallium oxide (β-Ga_2O_3) has attracted significant research attention for high-power, high-voltage, and high-frequency applications.

For the Ga2O3 HEMT simulation, the effects of delta-doping concentrations, width, and positions on the device performance, such as V_{TH}, transconductances, and breakdown voltages, were elucidated. Increasing delta-doping concentrations can reduce V_{TH} and improve transconductances due to larger 2DEG concentrations in the channel. However, it can also induce a parasitic leakage channel in the delta-doped region due to severe band bending of the conduction band and decrease the device breakdown voltages due to high electric fields at the gate edge. Varying the delta-doping concentrations resulted in a linear change in V_{TH}, which can be used as a reliable method to tune device V_{TH}. Closer delta-doping positions led to better channel quality and high transconductance of the devices. However, the delta-doped region should not be too close to the channel since it may extend into the channel, and degrade the electron mobility, impeding the high-frequency operation of the devices.

For the Ga2O3 CAVET, the conventional β-Ga_2O_3 CAVET showed concentrated electric fields under the gate with a low breakdown voltage (BV) of 260 V and a low peak electric field of 1.4 MV/cm, which is caused by insufficient gate control over the channel. For the introducing delta-doped β-$(Al_xGa_{1-x})_2O_3/Ga_2O_3$ heterostructure, it can reduce the R_{ON} due to the high density of 2DEG and suppress the OFF-state leakage due to the confined electron in the unintentionally doped channel layer. The OFF-state leakage from the aperture and CBL region in the β-Ga_2O_3 CAVETs was studied by simulation for the first time. A longer channel length can prevent the OFF-state leakage from the aperture but also increase the R_{ON} of HEMT-CAVETs. For small L_{ap} of <2 µm, the R_{Dep} became dominant in the R_{ON} due to the encroachment of the aperture by the depletion regions from the CBLs, while the R_{ap0} became dominant for large aperture lengths of >2 µm. For the breakdown simulation of the CBL region, the *BV* increased linearly with the thickness of the CBL increased. The peak electric field of β-Ga_2O_3 limit (~8 MV/cm) was obtained when the CBL layer increased to 6 µm. The *BV* of the CBL region increased linearly with the acceptor doping concentration. These results can serve as a critical reference for the future development of kV-class low R_{ON} β-Ga_2O_3 HEMT-CAVETs for high power, high voltage, high efficiency, and high-frequency applications.

TM-TuP-4 Electronic Band Structure and Excitons in $LiGaO_2$ and $LiGa_5O_8$, *N. Dadkhah,* Case Western Reserve University*; K. Dabsamut,* Kasetsart University, Thailand*;* ***Walter R. L. Lambrecht****,* Case Western Reserve University

Lithium gallate β-$LiGaO_2$ is mostly known as an optical insulator, but it may become an active ultra-wide-band-gap semiconductor by doping with Si, Ge [1]. Recently, we carried out studies of the band structure using the quasiparticle self-consistent (QS) *GW* method (*G* Green's function, *W* screened Coulomb interaction) [2,3] . Recent progress in the *GW* method allows us to include ladder-diagrams (electron-hole) interactions in the evaluation of the screening entering *W:* this method is here called QSGWΓ. Second, in the optical dielectric function, excitonic effects need to be included. We showed in [3] that the quasiparticle gap obtained in QSGWΓ is 7.0 eV, but electron-phonon coupling zero-point motion renormalization reduces it to 6.6 eV and excitonic effects are as large as 0.7 eV and lead to an exciton gap close to 6.0 eV, in excellent agreement with recent photoluminescence excitation and ellipsometry measurements [4]. The Bethe-Salpeter-Equation (BSE) calculations of the optical dielectric function reveal a modified Rydberg series of excitons, including dark excitons related to Wannier envelope functions that break the symmetry. The main luminescence bands were proposed in [4] to be donor-acceptor pair type. Using hybrid density functional defect pair calculations we identify the donor as Ga_{Li} and the acceptor as the Li vacancy and Li_{Ga} in the two observed DAP bands. Meanwhile it was found that CVD growth by Hongping Zhao's group (OSU) of Li-Ga-O films can lead to films with a composition of $LiGa_5O_8$. A compound with this composition is known to

have a spinel type structure with Ga in both tetrahedral and octahedral sites. We have calculated its band structure in the QSGWΓ method to be 5.8 eV, while the BSE calculations indicate large exciton binding energy with an estimated lowest exciton or exciton gap at about 5.5 eV. Electron-phonon band gap renormalization is expected to lower these by ~0.3 eV.

[1] K. Dabsamut, A. Boonchun, and W. R. L. Lambrecht, J. Phys. D: Appl. Phys. 53, 274002 (2020).

[2] S. K. Radha, A. Ratnaparkhe, and W. R. L. Lambrecht, Phys. Rev. B 103, 045201 (2021)

[3] N. Dadkhah, W. R. L. Lambrecht, D. Pashov and m. van Scbhilfgaarde, arXiv:2302.03150v2 and Phys. Rev. B, accepted

[4] L. Trinkler, A. Trukhin, B. Berzina, V. Korsaks, P. Šc

TM-TuP-5 Two–Dimensional Analytical Modeling of the Surface Potential of a Double–Gate Vertical Fin–Shaped Ga_2O_3 Power Transistor*, **Twisha Titirsha**, M. Hossain, M. Shuvo, Q. Huang, J. Gahl, S. Islam,* University of Missouri, Columbia

In recent years, the ultra-wide bandgap semiconductors, such as β-Ga_2O_3, have received significant attention owing to their ultra-wide bandgap (>4 eV), high breakdown strength (~8 MV cm^{-1}) and reasonable electron mobility (200-250 cm^2/Vs). The utilization of vertical Ga_2O_3 power devices presents new prospects in high-power applications. However, stable p-type doping in Ga_2O_3 remains challenging. Researchers expect FinFET structures to address this problem since these do not require p-type doping while designing on an n-type substrate. The dual-channel gating in vertical FinFET yields a highly resilient control of gate electrostatics. In addition, handling high voltages through a thick drift layer minimizes the ungated access zone between the gate and the source, reducing the source resistance and resulting in high output currents and breakdown voltages. Vertical power devices can overcome the challenges associated with short-channel effects (SCE) in ultra-high density in integrated circuits and provide efficient carrier movement, and fast operational speed. Although highly relevant, the analytical model of the surface potential of fin-shaped vertical Ga_2O_3 powerFET has not been reported in the literature yet. This work presents a physics-based surface potential model for fin-shaped vertical Ga_2O_3 powerFET. The model reveals that variations in the doping concentration of Ga_2O_3 lead to distinct work functions, producing a channel potential profile resembling a step function-like profile which creates an additional peak in the electric field profile at the two junctions. The average velocity of the electrons in the channel rises due to this electric field peak, increasing the current value and strengthening the resistance to hot carrier leakage. Consequently, the reduction of the hot carrier effect leads to a significant increase in the breakdown voltage. Besides, the study indicates that the surface potential at the drain end exhibits a noteworthy increase compared to conventional lateral devices. In summary, this work highlights the improved carrier transport efficiency and SCE suppression of the fin-shaped vertical Ga_2O_3 powerFET device, demonstrating the potential applications in high-voltage and high temperature electronics.

Author Index

Bold page numbers indicate presenter