Program Overview

Room /Time	Jefferson 1 & Atrium	Jefferson 2-3
MoA		TM-MoA: Characterization & Modelling II
TuM		TM-TuM: Characterization & Modelling III
TuP	Poster Sessions	

Theory, Modeling and Simulation
Room Jefferson 2-3 - Session TM-MoA

Characterization & Modelling II
Moderator: Mike Thompson, Cornell University

3:45pm **TM-MoA-9 Transport, Doping, and Defects in β-Ga_2O_3**, ***Adam Neal,*** Air Force Research Laboratory, Materials and Manufacturing Directorate, USA **INVITED**

The first reports of Ga_2O_3 MESFETs and MOSFETs by the group of Higashiwaki demonstrated the potential of β-Ga_2O_3 for high breakdown voltage, low on-resistance power electronics due to its ultra-wide bandgap and large breakdown electric field. Realizing that potential requires development of high-quality β-Ga_2O_3 material, best guided by an understanding of the electronic transport properties which directly correlate to device performance. In this talk, through a combination of temperature dependent Hall effect and admittance spectroscopy measurements, I will begin by presenting our work characterizing electrically active defects which may ultimately limit the maximally achievable breakdown voltages in Ga_2O_3 devices. Following that, I will present analysis of transport in plasma-MBE grown β-Ga_2O_3 produced at Air Force Research Laboratory, towards understanding the contributions of various scattering mechanisms limiting the electron mobility in our films. Informed by transport studies such as these, material growers and device engineers can continue to push β-Ga_2O_3 to the limits of its performance.

4:15pm **TM-MoA-11 Structural Changes to Beta Gallium Oxide from Ion Irradiation Damage: Model and Relation to in-Situ Experiments**, ***Alexander Petkov,*** *D. Cherns, D. Liu,* University of Bristol, UK*; W. Chen, M. Li,* Argonne National Laboratory, USA*; J. Blevins,* Air Force Research Laboratory, USA*; V. Gambin,* Northrop Grumman*; M. Kuball,* University of Bristol, UK

A good radiation hardness of Ga_2O_3 has been suggested, though its susceptibility to radiation damage is higher than in GaN. To better assess gallium oxide device reliability for nuclear and space applications, more understanding of the structural changes in the material as a result of irradiation is needed. We propose a model for the structural deformation of beta gallium oxide under ion irradiation. Assuming displacements confined primarily to the Ga-atom sublattice, we explain the main features of TEM diffraction patterns from in-situ irradiated gallium oxide using 400 eV Ar ions of fluence 4 x 10^{15} cm^{-1} (equivalent to 2 displacements per atom) (Fig. 1). We propose that displacements of gallium atoms are confined between close-packed O-atom layers (which in beta gallium oxide exist parallel to the (101), (-201), (-3-10), (-310) planes) with a preference for octahedral interstitial positions and recombination. We thus demonstrate the anisotropic evolution of the octahedral-to-tetrahedral Ga-site ratio in the irradiated gallium oxide as a function of displacements per atom, finding it to increase the most along the [-3-10] direction and the least along the [-201] (Fig. 2). The similarity of the structure post irradiation with that of kappa and alpha gallium oxide is examined. We conclude that while the structure post irradiation shares some features similar to kappa gallium oxide (specifically the octahedral-to-tetrahedral site ratio), ion irradiation does not cause a phase transition of beta gallium oxide into kappa as previously thought (Fig. 3).

The authors gratefully acknowledge the NSUF funding (#1393) for beamtime at Argonne IVEM-Tandem User Facility. The authors also thank Mr Peter Baldo (ANL, USA) for dedication on the operation of the ion accelerator during the experiment.

4:30pm **TM-MoA-12 Band Structure Across κ-$(In_xGa_{1-x})_2O_3$/κ-$(Al_yGa_{1-y})_2O_3$ Thin Film Interfaces**, ***Ingvild Julie Thue Jensen,*** *A. Thøgersen, E. Fertitta, B. Belle,* SINTEF Materials Physics, Norway*; A. Langørgen, S. Cooil, Y. Hommedal, Ø. Prytz, J. Wells, L. Vines,* University of Oslo, Norway*; H. von Wenckstern,* University of Leipzig, Germany

Ga_2O_3 is a candidate for development of power electronics components that are faster, smaller and more energy efficient than Si-based technology, permitting devices capable of operating at higher voltages, frequencies and temperatures.[1] The κ-phase of Ga_2O_3 (sometimes labeled ε-phase) is a meta-stable orthorhombic phase where large spontaneous polarization has been predicted by density functional theory.[2] By partial substitution of Ga by In or Al, the original bandgap (~4.9 eV) can be decreased or increased, in principle within the range spanned by the bandgaps of In_2O_3 (2.9 eV) and Al_2O_3 (8.8 eV).This provides a wide parameter space for device development through tailoring of properties such as bandgaps and band offsets. It is believed that interface-localized two-dimensional electron gas (2DEG) may be achieved within this materials system, which opens for potential applications in *so-called* high-electron-mobility transistors (HEMTs).

In the present work the band structure of thin film κ-$(In_xGa_{1-x})_2O_3$/κ-$(Al_yGa_{1-y})_2O_3$ heterostructures are investigated experimentally to evaluate if formation of 2DEG can be within reach. Samples with a selection of *x* and *y* compositions were fabricated by Pulsed Laser Deposition (PLD) on sapphire substrates. Both synchrotron and in-house X-ray Photoelectron Spectroscopy (XPS) were used to investigate the position of the valence band edges relative to the Fermi level in the heterostructure layers and corresponding reference samples. Extraction of valence band maxima from XPS was aided by Density functional theory (DFT) calculations. Local bandgap information was provided by Scanning Transmission Electron Microscope Electron Energy Loss Spectroscopy (STEM EELS), which can determine wide bandgaps with a spatial resolution < 10 nm. Valence band offsets across the heterojunctions were obtained by XPS and combined with bandgap information to find the corresponding conduction band offsets and provide a comprehensive overview of band discontinuities across κ-$(In_xGa_{1-x})_2O_3$/κ-$(Al_yGa_{1-y})_2O_3$ interfaces.

[1] F. Iacopi, M. Van Hove, M. Charles and K. Endo. MRS Bulletin 40 (2015) 390

[2] M.B. Maccioni and V. Fiorentini, Appl. Phys. Express 9 **(2016)** 041102, S.B. Cho and R. Mishra, Appl. Phys. Lett. 112 **(2018)** 162101, J. Kim, D. Tahara, Y. Miura and B.G. Kim Appl. Phys. Express 11 **(2018)** 061101

4:45pm **TM-MoA-13 Aluminum Incorporation Striations in (-201) β-$(Al_xGa_{1-x})_2O_3$ Films Grown on C-Plane and Miscut Sapphire Substrates**, ***Kenny Huynh,*** *Y. Wang, M. Liao,* University of California Los Angeles*; P. Ranga,* University of Utah*; S. Krishnamoorthy,* University of California at Santa Barbara*; M. Goorsky,* University of California, Los Angeles

High aluminum content striations were observed in (-201) $(Al_xGa_{1-x})_2O_3$ thin films (~500 nm) grown on (0001) and 6° miscut (0001) sapphire substrates. A modulated Al composition structure was observed whose orientation depended on the substrate miscut. High resolution x-ray diffraction (XRD) and transmission electron microscopy (TEM) were used to investigate the structural and chemical properties of the $(Al_xGa_{1-x})_2O_3$ films (with $0<x<0.3$) and the in-plane relationship with the underlying sapphire substrate. (-201) $(Al_xGa_{1-x})_2O_3$ films were grown by metalorganic vapor phase epitaxy and the Al composition was controlled by tuning the ratio of trimethylaluminum to triethylgallium flow. The growth was carried out at a substrate temperature of 810 °C and a reduced growth pressure of 15 Torr to minimize Al precursor prereactions.

Scanning transmission electron microscopy measurements (sensitive to Z-contrast) reveal alternating layers of high and low contrasting features throughout the $(Al_xGa_{1-x})_2O_3$ film. In conjunction with energy dispersive spectroscopy, the striations are identified as regions of high Al content. In the films that were grown on c-plane sapphire, the high Al content striations run parallel to the (-201) surface. However, in the case of the 6° miscut sapphire substrates, the high Al content striations are oriented about 8-10° from the surface. In addition, the average period of the striations is smaller with higher Al content ranging from 25 to 7 nm periods for x = 0.04 and x = 0.3 respectively.

XRD (-401) pole figures were measured for $(Al_xGa_{1-x})_2O_3$ films (with $0<x<0.3$) and a commercially available (-201) β-Ga_2O_3 substrate as a reference. XRD (-401) pole figure for the (-201) β-Ga_2O_3 reference substrate shows both (-401) at χ = ~23° and (-400), at χ = ~50° (the 2θ angle difference is less than 0.5°) with no symmetry. However, the pole figures from the $(Al_xGa_{1-x})_2O_3$ thin films grown on sapphire ($0<x<0.3$) all show six-fold symmetry for both (-401) and (-400). We believe the six-fold symmetry is a result of three sets of twins (120° away from each other), plus the existence of anti-parallel domains (0° and 180° pairs). On the other hand, additional 12 spots at χ = ~58° were observed in the $(Al_xGa_{1-x})_2O_3$ films on sapphire. These do not

correspond to any planes with (-201) surface orientation, suggesting grains with different orientation exist. We speculate that the anisotropy of the monoclinic structures, the surface energy differences associated with the miscut substrate, and step edge features impact the formation of the composition striations.

5:00pm **TM-MoA-14 Plasmon-phonon Coupling in Electrostatically Gated *β*-Ga_2O_3 Films with Mobility Exceeding 200 $cm^2V^{-1}s^{-1}$**, *A. Rajapitamahuni, A. Manjeshwar,* University of Minnesota, USA*; A. Kumar, A. Datta,* University at Buffalo*; P. Ranga,* University of California Santa Barbara*; L. Thoutam,* SR University, Warangal, India*; S. Krishnamoorthy,* University of California Santa Barbara*; **Uttam Singisetti,*** University at Buffalo*; B. Jalan,* University of Minnesota, USA

Monoclinic β-Ga_2O_3, an ultrawide-bandgap semiconductor, has seen enormous activity in recent years. However, the fundamental study of the plasmon-phonon coupling that dictates electron transport properties has not been possible due to the difficulty in achieving higher carrier density (without introducing chemical disorder). In this talk, we present a highly reversible, electrostatic doping of β-Ga_2O_3 films with tunable carrier densities using ion-gel-gated electrical double layer transistor configuration. Combining temperature dependent Hall effect measurements, transport modeling and comprehensive mobility calculations using ab-initio based electron-phonon scattering rates, we demonstrate an increase in the room-temperature mobility to 201 $cm^2V^{-1}s^{-1}$ followed by a surprising decrease with an increasing carrier density is due to the plasmon-phonon coupling. The modeling and experimental data further reveal an important “anti-screening” (of electron-phonon interaction) effect arising from dynamic screening from the hybrid plasmon-phonon modes. Our calculations show that a significantly higher room-temperature mobilities of 300 $cm^2V^{-1}s^{-1}$ is possible if high electron densities (> 10^{20} cm-3) with plasmon energies surpassing highest energy LO mode can be realized. As Ga_2O_3 and other polar semiconductors play an important role in several device applications, the fundamental understanding of the plasmon-phonon coupling can pave the way to enhance the mobility by harnessing the dynamic screening of the electron-phonon interactions.

Theory, Modeling and Simulation
Room Jefferson 2-3 - Session TM-TuM

Characterization & Modelling III

Moderator: Michael Scarpulla, University of Utah

9:15am **TM-TuM-4 First-Principles Modeling of Ga_2O_3**, ***Hartwin Peelaers,*** University of Kansas **INVITED**

β-Ga_2O_3 is a wide-band-gap semiconductor with promising applications in high-power electronics and photodetectors that are transparent to visible light. In this talk, I will show how first-principles calculations, based on density functional theory with hybrid functionals, can be used to predict and explain the properties of Ga_2O_3.

We first focus on modifying Ga_2O_3's properties for electronic applications through doping. While n-type doping is straightforward, p-type doping is elusive, with only deep acceptors available. We explore the properties of possible acceptors, and discuss the viability of obtaining semi-insulating material [1]. All dopants we considered lead to deep acceptor levels that are more than 1.3 eV above the valence-band maximum. N and Mg were identified as the most promising deep acceptors. We evaluated incorporation in different configurations, and considered the effect of native defects as well as complexes. We also predict diffusion activation energies, finding that Mg is significantly more mobile.

Alloying allows to modify the lattice constants, band gaps, and conduction-band offsets. We will provide quantitative results for alloys with In_2O_3 and Al_2O_3 [2,3].

When Ga_2O_3 is used as a transparent conducting oxides (TCO), two conflicting properties have to be balanced: transparency and conductivity. The requirement of transparency is typically tied to the band gap of the material being sufficiently large to prevent absorption of visible photons. This is a necessary but not sufficient condition: indeed, the high concentration of free carriers, required for conductivity, can also lead to optical absorption. This absorption can occur through direct absorption to higher-lying conduction band states, or by an indirect process, for example mediated by phonons or charged impurities. We will elucidate the fundamental limitations of optical absorption in Ga_2O_3 and shed light on experimental observations [4,5].

Work in collaboration with J.L. Lyons, S. Seacat, C.G. Van de Walle, and J.B. Varley.

[1] H. Peelaers, J. L. Lyons, J. B. Varley, and C. G. Van de Walle, APL Mater. **7**, 022519 (2019).

[2] H. Peelaers, D. Steiauf, J. B. Varley, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **92**, 085206 (2015).

[3] H. Peelaers, J. B. Varley, J. S. Speck, and C. G. Van de Walle, Appl. Phys. Lett. **112**, 242101 (2018).

[4] H. Peelaers and C.G. Van de Walle, Appl. Phys. Lett. **111**, 182104 (2017).

[5] H. Peelaers and C.G. Van de Walle, Phys. Rev. B **100**, 081202(R)(2019).

9:45am **TM-TuM-6 Theory of Acceptor-Donor Complexes in Ga_2O_3**, *I. Chatratin, F. Sabino,* University of Delaware*; P. Reunchan,* Kasetsart University, Thailand*;* ***Anderson Janotti,*** University of Delaware

Ga_2O_3 has attracted great attention as a promising material for high-power electronic devices due to a very large band gap and high breakdown voltage. It can be easily doped *n*-type, with Si, Ge, or Sn as shallow donors, but difficult to dope *p*-type. All tested candidate acceptor impurities lead to deep acceptor levels, lying at ~1 eV above the valence band. These deep acceptors are quite useful for making semi-insulating Ga_2O_3 layers, which are important components in many device designs. The interactions between acceptors, such as nitrogen or zinc, and donor impurities may play important role in the performance of the Ga_2O_3 semi-insulating layers. Using electronic structure calculations based on hybrid density functional theory, we investigate the interactions between acceptor and donor impurities in different possible configurations of acceptor-donor complexes considering all the inequivalent cation and anion sites of the *β*-Ga_2O_3 crystal structure. We calculate binding energies of the complexes and discuss changes in transition levels compared to those of the isolated species. These results aim at facilitating the experimental characterization of acceptor impurities to further the development of Ga_2O_3-based electronic devices.

10:00am **TM-TuM-7 Donor Doping of Monoclinic and Corundum $(Al_xGa_{1-x})_2O_3$**, ***Darshana Wickramaratne,*** US Naval Research Laboratory*; J. Varley,* Lawrence Livermore National Laboratory*; J. Lyons,* US Naval Research Laboratory

Designs of electronic devices using $(Al_xGa_{1-x})_2O_3$ (ALGO) as the barrier layer and gallium oxide (Ga_2O_3) as the active layer are being considered. The success of these devices is predicated in part on the ability to achieve controlled doping of the ALGO barrier layer. This requires shallow centers across the alloy composition range to be identified. The fact that Ga_2O_3 is most stable in the monoclinic structure, which is different from the ground-state corundum structure of Al_2O_3 also needs to be accounted for.

Using first-principles calculations based on a hybrid functional we investigate the prospects for *n*-type doping monoclinic and corundum ALGO alloys across the entire alloy composition range. We explore the properties of group-IV (C, Si, Ge, and Sn) and transition metal (Hf, Zr, and Ta) substitutional dopants. In Ga_2O_3, all of these dopants are shallow donors. However, in Al_2O_3 they are all deep defects, characterized by the emergence of deep levels within the band gap. Combining our calculations of dopant charge-state transition levels together with information about the ALGO alloy band offsets for both polymorphs, we estimate the critical Al composition at which each dopant transitions from being a shallow to a deep donor. We identify Si to be the most efficient dopant to achieve *n*-type conductivity in high Al-content corundum and monoclinic ALGO [1].

This work was supported by the ONR/NRL 6.1 Basic Research Program.

[1] J. B. Varley, A. Perron, V. Lordi, D. Wickramaratne, and J. L. Lyons, *Appl. Phys. Lett.* **116**, 172104 (2020).

10:15am **TM-TuM-8 The Co-Design, Fabrication, and Characterization of a Ga2O3-on-SiC MOSFET**, ***Yiwen Song,*** Pennsylvania State University*; A. Bhattacharyya,* University of Utah*; A. Karim, D. Shoemaker,* Pennsylvania State University*; H. Huang,* Ohio State University*; C. McGray,* Modern Microsystems, Inc.*; J. Leach,* Kyma Technologies, Inc.*; J. Hwang,* Ohio State University*; S. Krishnamoorthy,* University of California at Santa Barbara*; S. Choi,* Pennsylvania State University

β-phase gallium oxide (Ga_2O_3) is an emerging ultrawide bandgap semiconductor (E_G ~ 4.8 eV) that offers potential for significant improvement in the performance and manufacturing cost of today's commercial wide bandgap semiconductor devices. However, due to the poor thermal conductivity of the Ga_2O_3 (10.9-27 W/mK), overheating has become a major bottleneck to the commercialization of Ga_2O_3 devices.

In response to this critical problem, a Ga_2O_3/4H-SiC composite wafer was fabricated. Thermo-physical properties of the composite wafer were characterized using a combination of laser-based pump-probe methods. Scanning transmission electron microscopy and modeling suggest that the interfacial thermal boundary resistance (TBR) is mainly limited by the low thermal conductivity of the interlayer used for the fusion bonding process. A n-type Ga_2O_3 channel layer was successfully grown on the composite wafer using low-temperature metalorganic vapor phase epitaxy (MOVPE). Metal-oxide-semiconductor field effect transistors (MOSFETs) were subsequently fabricated on the composite substrate. In situ nanoparticle-assisted Raman thermometry was used to compare the self-heating behavior of MOSFETs fabricated on a Ga_2O_3 substrate and the Ga_2O_3/4H-SiC composite wafer. Under steady-state operation, a 56% reduction in channel temperature was achieved in the devices fabricated on the composite wafer as compared to the homoepitaxial devices on the Ga_2O_3 native substrate. However, the improvement in the device thermal resistance is limited under high frequency switching operation due to the low thermal diffusivity of the Ga_2O_3 layer, highlighting the importance of minimizing the Ga_2O_3 layer thickness. Transient electro-thermal device modeling was performed to assess the cooling effectiveness of optimized composite substrates for the case of both single- and multi-finger devices. Simulation results suggest that additional top-side cooling using a high thermal conductivity passivation overlayer such as polycrystalline diamond allows to achieve high heat transfer performance under high frequency operating conditions.

This comprehensive study on both material- and device-levels provides key insight into the effective thermal management of $Ga_{-2}O_3$ device technologies.

Theory, Modeling and Simulation
Room Jefferson 1 & Atrium - Session TM-TuP
Theory, Modeling and Simulation Poster Session

TM-TuP-1 Simulation Study of Single Event Effects in Ga_2O_3 Schottky Diodes, ***Animesh Datta**, U. Singisetti,* University at Buffalo

β-Ga_2O_3 has attracted high interest in the last decade and emerged as a promising material for next-generation power, GHz power switching, and RF applications. The large bandgap opens its possibilities for potential space applications, as the electron-hole pair generation in radiation (LET) is inversely proportional to the bandgap. Under radiation conditions in space, single event effects (SEE) are a potential reliability issue for devices in space-based RF and power systems. Previous reports have explored SEE burnout in SiC MOSFETs and thus SEE could also be an issue in Ga_2O_3 based devices. To date, there have been no reports of study of SEE in Ga_2O_3 based devices. In this work, we present the SEE effect in Ga_2O_3 Schottky diodes by simulation. 2-D simulations were performed using Silvaco TCAD to investigate the effects of ionizing radiation (measured in LET) under various bias conditions to understand the failure mechanism in the device. Breakdown simulations (V_{br}= 1400 V) show that the anode edge has the highest electric field; thus, it is chosen as the ion strike location in simulations. Under the radiation conditions, the time-dependent simulations show that the current recovers even at 1000 V and 40 MeV/mg/cm^2 LETs; even though the instantaneous peak field exceeds 8 MV/cm. It is noted that higher LETs take a longer time to recover. The heat generated due to ion strikes can also lead to the failure of devices due to thermal effects. The ion strike results in an instantaneous high current density within the device and leads to excessive Joule heating. The thermal effects were studied in Ga_2O_3 diodes with a diamond coating. Below radiation conditions of V=500V and LET=5 MeV/mg/cm^2 the device does not show any signatures of single event burnout (SEB) including thermal effects. At higher voltage bias and high LETs, there are signatures of possible thermal runaway where the temperature rises to a high value but only for a short amount of time and then recovers. The total energy dissipated under the ion strike condition is also calculated by integrating the power density spatially across the ion track. Our results indicate that under similar radiation conditions the power dissipated in b-Ga_2O_3 Schottky diodes is lower compared to the experimental data of SiC Schottky diodes. Future work includes investigating the threshold condition of SEB in b-Ga_2O_3 Schottky diodes for potential applications in harsh radiation conditions.

TM-TuP-2 Anisotropic Photoresponsivity and Deviation from Beer-Lambert Law in Beta Gallium Oxide, ***Md Mohsinur Rahman Adnan**, D. Verma, S. Dhara,* The Ohio State University*; C. Sturm,* Universitat Leipzig, Germany*; S. Rajan, R. Myers,* The Ohio State University

Polarization-dependent photoresponsivity measurements on (001) β-Ga_2O_3 are modeled by calculating the anisotropic absorption process via the dielectric tensor[1]. Quasiparticle band structure calculations show that three different transitions from topmost group of O^{2-} 2p valance bands to the lowest Ga^{3+} 4s conduction band can occur that contribute significantly to the excitonic spectra[2]. A linear polarizer is utilized in the excitation path to generate photocurrent in (001) β-Ga_2O_3 Schottky diode. Three excitonic transitions corresponding to P_x, mixed P_x/P_z and P_y valance band sates are observed as peaks in the measured photoresponsivity spectra at 4.9eV, 5.2eV and 5.5eV[2]. The intensity of the peaks depends on the linear polarization of the excitation.

This strongly anisotropic absorption process in β-Ga_2O_3 cannot be modeled using a generic absorption coefficient; the Beer-Lambert law is not strictly accurate in an anisotropic dielectric. To model anisotropic absorption, we solve the electromagnetic wave equation using the Berreman[3] matrix and the measured dielectric tensor of β-Ga_2O_3[1]. The Poynting vector versus the linear polarization of the excitation with respect to the a- and b- axes and absorption depth is calculated and used to determine the generation rate and the photoresponsivity spectrum of β-Ga_2O_3. The modeled photoresponsivity matches the experimentally measured 3-peak spectrum and its variation with polarization angle. The simulations confirm that the photon flux in β-Ga_2O_3 over the energy range of interest (4-6eV) does not decay exponentially with depth over the photocarrier collection region, in violation with the Beer-Lambert law.

The exciton Franz Keldysh effect is observed in the photoresponsivity spectra, where exciton absorption peaks red shift with reverse bias[4]. The magnitudes of red shift for the three photoresponsivity peaks are inversely related to the corresponding interband transition energies i.e. the smallest energy transition peak shows the highest amount of red shift. We will discuss the polarization anisotropy of the field-dependent red-shift in terms of the exciton wave function anisotropy and its impact on the Stark shift.

[1]C. Sturm et al., APL Mater. 3, 106106 (2015).
[2]J. Furthmüller et al., Phys. Rev. B 93, 115204 (2016).
[3]D. W. Berreman, J. Opt. Soc. Am. 62, 4, pp. 502-510 (1972).
[4]M. M. R. Adnan et al., Phys. Rev. Appl. 16, 034011 (2021).

TM-TuP-4 Self-Trapped Holes and Polaronic Acceptors in Ultrawide Bandgap Oxides, ***John Lyons**,* US Naval Research Laboratory

Although Ga_2O_3 is widely believed to be the most promising ultrawide-bandgap semiconductors, its inability to be *p*-type doped hampers its future applications. Recently, other oxide materials have emerged as potential competitors to Ga_2O_3, but their propensity for hole conductivity is less well known. Here the stability of hole polarons in a set of ultrawide-bandgap oxides (Ga_2O_3, Al_2O_3, $ZnGa_2O_4$, $MgGa_2O_4$, $LiGaO_2$ and GeO_2) is examined and compared, both in pristine material and in the presence of acceptor impurities. Holes spontaneously self-trap in all oxides investigated here, with varying stability. Acceptor impurities further stabilize these trapped holes, leading to large acceptor ionization energies. Hole trapping also leads to characteristic distortions and distinct optical transitions, which may explain some experimentally-observed signals. These results indicate that achieving *p*-type conductivity in any of these oxides is unlikely.

This work was supported by the ONR/NRL 6.1 Basic Research Program.

TM-TuP-5 Modeling for a High-Temperature Ultra-Wide Bandgap Gallium Oxide Power Module, ***Benjamin Albano**,* Virginia Tech Center for Power Electronics Systems*; B. Wang, C. DiMarino, Y. Zhang,* Virginia Tech Center for Power Electronics

The ultra-wide bandgap (UWBG) of Ga_2O_3 allows it to achieve over 10-times lower intrinsic carrier concentration than Si permitting Ga_2O_3 devices to operate at much higher temperatures. However, its low thermal conductivity and the associated self-heating could cause the device to exceed its safe operating temperature as prescribed by gate dielectric and packaging material limitations. The objective of this study is to develop a physics-based simulation and computation framework for the co-design of Ga_2O_3 devices and packaging.

Table I outlines the benefits and limitations of different models that are conventionally used for device and packaging design. In the design of the package and the micro-/nano-scale device structures, it is critical to observe the interactions between the two [1] [2]. The traditional package-level FEA simulation usually assumes a uniform power density and junction temperature in the devices, while neglecting the temperature variations in the sub-micron device structures; this variation can be up to tens of kelvin under high-power device operations. Conversely, the typical physics-based TCAD simulation accurately models the electrothermal behaviors within the device but the high computational power required (due to the large difference in length scales between the electrically active regions and the thermal diffusion regions) limits their use when package components need to be considered. These models instead simplify the packaging into nominal boundary thermal resistances, neglecting larger packaging elements in the heat flow path that are critical to overall thermal management and reliability [3].

The simple bottom-side cooled diode shown in Fig. 1. was modeled in ANSYS Workbench, Silvaco 2D TCAD, and Silvaco 3D TCAD. As can be seen in Fig. 2., there were stark differences in the heat distribution between the models. These hot spots are severe reliability liabilities and would need to be accounted for in the package design.

In order to build a platform that accounts for the additional electro-thermal effects while still being practical and efficient, a series of models were built to integrate the physics-based material/device-level simulation with a package-level FEA simulation. These models were then evaluated against more traditional methods of device-package simulation, seen in Table II, to understand the potential benefits of such a method. In end effect, this method would guide both device and package design with the hope of identifying and optimizing the thermal and electric field management needs.

[1] IEEE EDL, vol. 90, no. 6, p. 1065-1076, 2002.

[2] IEEE WiPDA, 2018 p. 287-294.

[3] APL, vol. 115, no. 173508, 2019.

TM-TuP-6 Atomic Surface Structure of Sn doped β-Ga_2O_3(010) Studied by Low-energy Electron Diffraction*, **Alexandre Pancotti,*** Universidade Federal de Jataí, Brazil*; J. T. Sadowski,* Center for Functional Nanomaterials, Brookhaven National Laboratory*; A. Sandre Kilian,* Universidade Federal de Jataí, Brazil*; D. Duarte dos Reis,* Universidade Federal do Mato Grosso do Sul, Brazil*; C. Lubin,* SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay , France*; A. Boucly,* SPEC, CEA, CNRS, Université Paris-Saclay, France*; P. Soukiassian,* SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, France*; J. Boeckl, D. Dorsey ,* Air Force Research Laboratory*; M. Shin, T. ASEL,* Air Force Research Lab*; J. Brown, N. Barrett ,* SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay , France*; T. Back,* SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay

The surface crystallographic and electronic structure of bulk single crystals of transparent, wide gap semiconductor gallium oxide β-Ga_2O_3(010) has been studied using Spot Profile Analysis Low-Energy Electron Diffraction (SPA-LEED) and X-ray Photoelectron Spectroscopy (XPS). The XPS measurements show typical spectra for Ga_2O_3(010). The surface structure of Sn doped single crystal β-Ga_2O_3 Using quantitative LEED I-V. The surface shows a (1 x 1) LEED pattern without reconstruction. The comparison between experimental I-V curves and theoretical LEED simulations using Green's function formalism indicates the formation of a single surface termination layer. There are significant displacements in the first topmost slab surface, moreover, experiment and theory suggest important atomic rumpling between gallium and oxygen atoms in the topmost surface layers. The surface structure agrees with that predicted by first-principles density functional theory calculations and X-ray photoelectron diffraction.

Author Index

Bold page numbers indicate presenter

— A —

Adnan, M.: TM-TuP-2, **5**
Albano, B.: TM-TuP-5, **5**
ASEL, T.: TM-TuP-6, 6

— B —

Back, T.: TM-TuP-6, 6
Barrett , N.: TM-TuP-6, 6
Belle, B.: TM-MoA-12, 2
Bhattacharyya, A.: TM-TuM-8, 4
Blevins, J.: TM-MoA-11, 2
Boeckl, J.: TM-TuP-6, 6
Boucly, A.: TM-TuP-6, 6
Brown, J.: TM-TuP-6, 6

— C —

Chatratin, I.: TM-TuM-6, 4
Chen, W.: TM-MoA-11, 2
Cherns, D.: TM-MoA-11, 2
Choi, S.: TM-TuM-8, 4
Cooil, S.: TM-MoA-12, 2

— D —

Datta, A.: TM-MoA-14, 3; TM-TuP-1, **5**
Dhara, S.: TM-TuP-2, 5
DiMarino, C.: TM-TuP-5, 5
Dorsey , D.: TM-TuP-6, 6
Duarte dos Reis, D.: TM-TuP-6, 6

— F —

Fertitta, E.: TM-MoA-12, 2

— G —

Gambin, V.: TM-MoA-11, 2
Goorsky, M.: TM-MoA-13, 2

— H —

Hommedal, Y.: TM-MoA-12, 2
Huang, H.: TM-TuM-8, 4
Huynh, K.: TM-MoA-13, **2**
Hwang, J.: TM-TuM-8, 4

— J —

Jalan, B.: TM-MoA-14, 3
Janotti, A.: TM-TuM-6, **4**
Jensen, I.: TM-MoA-12, **2**

— K —

Karim, A.: TM-TuM-8, 4
Krishnamoorthy, S.: TM-MoA-13, 2; TM-MoA-14, 3; TM-TuM-8, 4
Kuball, M.: TM-MoA-11, 2
Kumar, A.: TM-MoA-14, 3

— L —

Langørgen, A.: TM-MoA-12, 2
Leach, J.: TM-TuM-8, 4
Li, M.: TM-MoA-11, 2
Liao, M.: TM-MoA-13, 2
Liu, D.: TM-MoA-11, 2
Lubin, C.: TM-TuP-6, 6
Lyons, J.: TM-TuM-7, 4; TM-TuP-4, **5**

— M —

Manjeshwar, A.: TM-MoA-14, 3
McGray, C.: TM-TuM-8, 4
Myers, R.: TM-TuP-2, 5

— N —

Neal, A.: TM-MoA-9, **2**

— P —

Pancotti, A.: TM-TuP-6, **6**
Peelaers, H.: TM-TuM-4, **4**
Petkov, A.: TM-MoA-11, **2**
Prytz, Ø.: TM-MoA-12, 2

— R —

Rajan, S.: TM-TuP-2, 5
Rajapitamahuni, A.: TM-MoA-14, 3
Ranga, P.: TM-MoA-13, 2; TM-MoA-14, 3
Reunchan, P.: TM-TuM-6, 4

— S —

Sabino, F.: TM-TuM-6, 4
Sandre Kilian, A.: TM-TuP-6, 6
Shin, M.: TM-TuP-6, 6
Shoemaker, D.: TM-TuM-8, 4
Singisetti, U.: TM-MoA-14, **3**; TM-TuP-1, 5
Song, Y.: TM-TuM-8, **4**
Soukiassian, P.: TM-TuP-6, 6
Sturm, C.: TM-TuP-2, 5

— T —

T. Sadowski, J.: TM-TuP-6, 6
Thøgersen, A.: TM-MoA-12, 2
Thoutam, L.: TM-MoA-14, 3

— V —

Varley, J.: TM-TuM-7, 4
Verma, D.: TM-TuP-2, 5
Vines, L.: TM-MoA-12, 2
von Wenckstern, H.: TM-MoA-12, 2

— W —

Wang, B.: TM-TuP-5, 5
Wang, Y.: TM-MoA-13, 2
Wells, J.: TM-MoA-12, 2
Wickramaratne, D.: TM-TuM-7, **4**

— Z —

Zhang, Y.: TM-TuP-5, 5