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,* Linkoping University, Sweden*; S. Richter,* Lund University, Sweden*; A. Ruder,* University of Nebraska-Lincoln, USA*; A. Papamichael, V. Stanishev,* Linkoping 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 Ga2O3 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 β-Ga_2O_3: A Direct Approach via Master Diffusion Equations**, ***Channyung Lee***, *E. Ertekin,* University of Illinois Urbana-Champaign

The low symmetry of the monoclinic structure of β-Ga_2O_3 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 β-Ga_2O_3, 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 β-$Ga_2O_3$and the origin of its anisotropic diffusion, which can contribute to further developments in the design and optimization of β-Ga_2O_3-based electronics.

4:30pm **AC+DI+HM+TM-MoA-12 Hybrid Metal/low-k/$BaTiO_3$/*β*-Ga_2O_3 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

β-Ga_2O_3 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 *β*-Ga_2O_3 devices. Recent work has demonstrated the advantages in using hybrid extreme-k/low-k insulator stacks to enable high average electric fields in the *β*-Ga_2O_3 [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) *β*-Ga_2O_3 Sn-doped substrates. The first set of samples consisted of a 20 nm Al_2O_3 low-k layer and $BaTiO_3$ (BTO) layers of 20 and 35 nm, respectively. The second two samples used 24 nm of SiO_2 with BTO layers of 35 nm and 50 nm, respectively. Al_2O_3 and SiO_2 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 coloaded 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_2O_3. The sample with 50 nm of BTO on 24 nm SiO_2 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^2 was defined as the breakdown limit for all devices. The field in the Ga_2O_3 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_2O_3 and 20 nm BTO showed the best performance, with a forward breakdown electric field of 5.7 MV/cm in the Al_2O_3 and reverse breakdown field of 6.8 MV/cm *in the β-Ga_2O_3*. 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 *β*-Ga_2O_3 and shown that such stacks can enable excellent reverse breakdown fields in *β*-Ga_2O_3 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) β-Ga_2O_3 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) β-Ga_2O_3, bonding to (0001) 4H-SiC, and initial results towards large-area transfer of (001) β-Ga_2O_3 to SiC. Compatible with large-scale processing, exfoliation is an important step in controlled-thickness transfer of films for heterogeneous integration. Furthermore, integration of β-Ga_2O_3 to high thermal conductivity materials will be crucial for thermal management of high-power devices. Two-inch (001) β-Ga_2O_3 wafers were implanted with He^+ at an energy of 160 keV and a dose of 5×10^{16} cm^{-2}, mimicking our previous parameters used to successfully exfoliate (010) β-Ga_2O_3.[1] 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) β-Ga2O3[1] likely due to the larger Poisson's ratio of (001) β-Ga_2O_3.[2] 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 µm) and strengthen the bond. Then, even after annealing at 500 °C for 10 hours to initiate bubble growth, the (001) β-Ga_2O_3 did not transfer to the (0001) 4H-SiC. Unlike what was observed for (010) β-Ga_2O_3,[1] blistering did not even occur at this temperature. Annealing at 800 °C for up to 12 hours resulted in ~10 µm 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.[3] However, the β-Ga_2O_3 substrate did not wafer split from the bonded structure, and instead only small area transfers up to ~200 µm were achieved. Only ~7% of the total bonded area transferred while the entire structure remained bonded.

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) β-Ga_2O_3 composite wafers, and when combined with subsurface damage-free chemical mechanical polishing,[4] these composite wafers would be suitable for subsequent devices and/or epitaxial growth.

References

1. M.E.Liao,et al., ECS J.Sol.State Sci.Technol., 8(11) P673 (2019)

2. K.Adachi,et al., J.Appl.Phys., 124 085102 (2018)

3. M.Bruel,et al., Jpn.J.Appl.Phys., 36 1636 (1997)

4. M.E.Liao,et al., J.Vac.Sci.Technol. A, 41 013205 (2023)

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