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 $R_{on,sp}$.

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