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