Program Overview

Room /Time	Jefferson 2-3
TuM	TM-TuM: Characterization & Modelling III

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-$_2O_3$ device technologies.

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