Program Overview

Room /Time	Jefferson 2-3
MoM	AC-MoM: Characterization & Modeling I

Advanced Characterization Techniques
Room Jefferson 2-3 - Session AC-MoM
Characterization & Modeling I

Moderator: Kornelius Tetzner, Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik (FBH), Germany

9:30am **AC-MoM-5 Characterization of Deep Acceptors in β-Ga_2O_3 by Deep Level Optical Spectroscopy**, *H. Ghadi, J. McGlone, E. Cornuelle,* The Ohio State University*; A. Senckowski,* University of Massachusetts Lowell*; S. Sharma, U. Singisetti,* University of Buffalo*; M. Wong,* University of Massachusetts Lowell*; A. Arehart,* ***Steven A Ringel,*** The Ohio State University **INVITED**

Beta phase gallium oxide (β-Ga_2O_3) is a strong contender for next-generation high voltage and RF device applications. A key component of such devices is a semi-insulating, highly resistive buffer layer or substrate. To date, iron (Fe) has been the preferred acceptor impurity to achieve semi-insulating β-Ga_2O_3. Iron produces an energy level at E_C-0.8 eV, which has been substantiated by theoretical and experimental studies and enables highly resistive material. However, it has also been shown that residual Fe impurities can result in device switching instabilities since the Fermi level can modulate the occupancy of the Fe trap state during standard biasing conditions. While progress to mitigate the impact of residual Fe impurities has occurred, there is also interest in exploring acceptors with much deeper energy levels to avoid device instabilities. Magnesium (Mg) and nitrogen (N) have emerged as candidates based on their predicted energy levels of E_C-3.3 eV and E_C-2.8 eV, respectively (H. Peelaers, et al., APL Mater. 7, 022519, 2019). This presentation will compare each acceptor, with a primary focus on N, using deep level optical spectroscopy (DLOS) and thermally based deep level transient spectroscopy (DLTS). Here, N acceptors were introduced into HVPE-grown β-Ga_2O_3 by ion implantation. A uniform N-implantation profile was used targeting multiple doses in different samples, followed by an activation anneal. DLTS and DLOS measurements were applied before and after annealing. After implantation, multiple trap states appeared, most of which were removed by annealing, leaving a single, new state at E_C-2.9 eV, with Frank-Condon energy of 1.4 eV. The concentration of this state is monotonically tracked with nitrogen concentration from SIMS. This energy level closely matches predicted values for an acceptor-like defect due to nitrogen atoms occupying the oxygen III sites, determined by density functional theory (DFT) calculations (Y.K. Frodason, et al. J. Appl. Phys. 127, 075701, 2020), The much deeper energy compared with Fe could imply a significantly lower operational instability than the shallower Fe acceptor at E_C-0.8 eV. However, we found that the below midgap position of the $N_{O(III)}$ level, coupled with its small optical cross-section, complicates the trap concentration analysis by DLOS, which is important for understanding how to characterize very deep states in β-Ga_2O_3. Simultaneous hole emission to the valence band and electron emission to the conduction band was seen. The impact of this behavior on DLOS analysis is discussed, and a method to resolve this complication will be presented.

10:00am **AC-MoM-7 Determination of Cation Vacancy and Al Diffusion Constants in B-$(Al,Ga)_2O_3$ / Ga_2O_3 Superlattices**, *H. Yang, A. Levin, B. Eisner, A. Bhattacharyya, P. Ranga, S. Krishnamoorthy,* ***Michael Scarpulla,*** University of Utah

Cation vacancies have been implicated as the dominant compensating native defect in $(Al,Ga)_2O_3$, and will also mediate the diffusion of many impurities.The hidden influence of native defects on tracer diffusion e.g. of Si, Sn etc is critical to understand, especially in situations such as ion implantation where both tracer atoms and vacancies are introduced far above equilibrium concentrations and with spatial gradients.Additionally, cation vacancies and their accumulation at interfaces have been shown to determine the failure modes of high-power (Al,Ga)N devices.For these reasons, it is imperative to understand the diffusion of cation vacancies in $(Al,Ga)_2O_3$ and their mediation of substitutional diffusion of impurities and matrix atoms.This is clearly a difficult task compared, for example, to measuring tracer diffusion from surface sources.The formation energetics of cation vacancies, which is especially lowered by n-type doping in the $^{3-}$ and $^{2-}$ charge states, and their unusual structure have been computed and observed and much computational progress towards migration barriers has been made.

In this work we utilize $(Al,Ga)_2O_3/Ga_2O_3$ superlattices grown by OMVPE, annealing, SIMS profiling, and a novel finite differences simulation method to reveal and characterize the otherwise-invisible influence of cation vacancies. The diffusion of cations may have both interstitial and substitutional components; we present evidence showing that Al diffusion is probably dominated by the substitutional channel.The use of superlattices allows the differential measurement of Al diffusion at different depths, which in turn reveals gradients in the cation vacancy concentration and its evolution with annealing.For different samples, the initial concentration gradients of cation vacancies differ and diffusion occurs in a transient regime.Coupling these experiments with a model of coupled diffusion allows the extraction of the bare diffusion constant for the vacancies themselves (the hopping barrier alone, without formation enthalpy contributions), as well as determination of the Al diffusion constant including its dependence on vacancy concentration.Besides the fundamental interest in determining these parameters in single crystals (as opposed to prior polycrystalline work), these results will be critical for understanding crystal growth, ion implantation, and the time evolution of device structures subjected to extreme fields and temperatures.

10:15am **AC-MoM-8 Defect Characterization in Gallium Oxide and Related Materials Using Terahertz Electron Paramagnetic Resonance Ellipsometry: Fe in Ga_2O_3**, ***Mathias Schubert,*** University of Nebraska, Lincoln*; S. Richter,* Lund University, Sweden*; S. Knight, P. Kuehne,* Linkoping University, Sweden*; M. Stokey, R. Korlacki,* University of Nebraska-Lincoln*; V. Stanishev,* Linkoping University, Sweden*; Z. Galazka, K. Irmscher,* Leibniz-Institut fuer Kristallzuechtung, Germany*; S. Mu, C. Van de Walle,* University of California at Santa Barbara*; V. Ivády,* MPI Physics of Complex Systems, Germany*; O. Bulancea-Lindvall, I. Abrikosov,* Linkoping University, Sweden*; V. Darakchieva,* Lund University, Sweden

The control over electrical conductivity is critical key to enabling gallium oxide and related materials for high power electronic devices. Understanding the influence of dopants and defects onto the electrical and electronic properties is therefore of paramount importance [1]. Identifying defects and their local electronic properties remains a challenge. Here, we introduce frequency-domain Terahertz Electron Paramagnetic Resonance (EPR) ellipsometry as a new tool to study defects in gallium oxide and related materials at very high magnetic fields and very high frequencies. Traditional EPR methods exist in multiple variants and establish perhaps one of the most ubiquitous measurement techniques in science [2]. In our new concept, we determine the full polarization response of intricate defect spins as a continuous function of both field and frequency. For first investigations, we use our previously developed optical Hall effect setup [3]. We recently demonstrated this new approach analyzing the polarized spin response for the nitrogen defect in SiC [4]. Here, we investigate Fe-doped gallium oxide single crystals, and detect a large range of spin signatures which strongly vary with crystal orientation, frequency, and field. Iron is commonly used to obtain semi-insulating material where Fe2+ acts as compensating acceptor. The neutral defect Fe3+ is a high-spin system with s=5/2 and large zero-field splitting. Iron can incorporate at either Ga site but appears preferentially in octahedral configuration. Different claims exist about the nature of the spin Hamiltonian and approximate values for simplified orthorhombic models have been reported. We obtain the anisotropic g-factor as well as the zero-field Hamiltonian up to fourth order which allows to discuss the relevance of the monoclinic character of the local site symmetry. We compare our results with present knowledge from theory computation approaches. We further discuss the influence of phonons, strain, and local crystal symmetry, and we predict THz EPR ellipsometry as a new tool with potential for characterization of defects in heteroepitaxial systems.

[1] A. J. Greene et al., APL Materials 10, 029201 (2022).
[2] C. Poole, Electron Spin Resonance: A Comprehensive Treatise on Experimental Techniques (Wiley, New York, 1983).
[3] P. Kühne et al., IEEE Trans. Terahertz Sci. Technol. 8(3), 257 (2018).
[4] M. Schubert et al., Appl. Phys Lett. 120, 102101 (2022).

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