## **Program Overview**

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## Monday Morning, August 8, 2022

#### 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  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> 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 ( $\beta$ -Ga<sub>2</sub>O<sub>3</sub>) is a strong contender for nextgeneration 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  $\beta\text{-}Ga_2O_3\!.$  Iron produces an energy level at  $E_C\text{-}0.8$  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 Ec-3.3 eV and Ec-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  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> 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 Ec-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  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. 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)<sub>2</sub>O<sub>3</sub> / Ga<sub>2</sub>O<sub>3</sub> 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)<sub>2</sub>O<sub>3</sub>, 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)<sub>2</sub>O<sub>3</sub> 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 <sup>3</sup> 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)<sub>2</sub>O<sub>3</sub>/Ga<sub>2</sub>O<sub>3</sub> 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<sub>2</sub>O<sub>3</sub>, *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 Fedoped 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.

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

## Monday Evening, August 8, 2022

#### Advanced Characterization Techniques Room Jefferson 1 & Atrium - Session AC-MoP

#### **Advanced Characterization Techniques Poster Session**

AC-MOP-1 Advanced Defect Characterization in b-Ga<sub>2</sub>O<sub>3</sub> Without the Arrhenius Plot, J. Li, NCKU, Taiwan; Adam Neal, S. Mou, Air Force Research Laboratory, Materials and Manufacturing Directorate, USA; M. Wong, University of Massachusetts Lowell

Defect is one of the issues that limit the present performance of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> devices. For example, several defects have been observed at 0.6, 0.8. and 1.1 eV below the conduction band edge of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, which are considered to affect doping compensation, leakage current, and threshold stability in transistors. Conventional detection of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> defects (in various forms such as Hall, conductivity, admittance spectroscopy, and deep-level transient spectroscopy (DLTS)) is accomplished by inspecting the electrical charge response, which is based on the Arrhenius behavior of the carrier emission rate from a defect determined by the activation energy  $E_a$  and the attempt-to-escape frequency vo. All thermally activated electrical charge response measurements are conventionally analyzed by the Arrhenius plot procedure, where one fits the Arrhenius plot of ln(v) versus  $T^{-1}$  to a line and extract  $E_a$  from the slope and  $v_0$  from the intercept. Improvement of the measurement expediency for extracting  $E_a$  and  $v_0$  is desirable to understanding their physiochemical origins and devising mitigation strategies in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> material and device engineering.

We investigate a ~0.8 eV defect in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> using a technique that offers substantial improvement over the conventional DLTS technique, specifically in the analytical processing of electrical signal and the extraction of  $E_o$  and  $v_o$ . The technique bypasses both the rate-window treatment and the Arrhenius plot. First, only the raw capacitance transients in the time domain are needed, which can be readily acquired by generalpurpose instruments such as impedance analyzers and lock-in amplifiers. Next, the capacitance transients are projected between the temperature and time domains, as well as to the  $E_o$  and  $v_o$  domains. Extraction of  $E_o$  and  $v_o$  is accomplished by matching the projected and experimental capacitance transients to each other. The efficient utilization of information from the 2D temperature-time domain allows operation in a smaller temperature/voltage range and extraction of the temperature and electricfield dependence of  $E_o$  and  $v_o$ .

#### AC-MOP-2 Infrared-Active Phonon Modes and Static Dielectric Constants of Orthorhombic LiGaO<sub>2</sub>, *Teresa Gramer*, *M. Stokey*, *R. Korlacki*, *M. Schubert*, University of Nebraska - Lincoln

 $Li_2O-Ga_2O_3$  is an oxide system of broader interest.  $LiGaO_2$  (LGO) and multiple phases of Ga<sub>2</sub>O<sub>3</sub> (GO) are ultra-wide bandgap metal oxides for future electronic and optoelectronic applications [1], and both LGO, which is orthorhombic, and the orthorhombic phase of GO are expected to be piezoelectric due to the lack of inversion symmetry [1]. While both GO and LGO have recently been identified to most likely trap holes which makes the achievement of sufficient p-type conductivity difficult [2], LGO is particularly promising as a substrate for heteroepitaxial growth of GaN due to very small lattice mismatch (<1%), and a composite LGO/ $\beta$ -GO substrate has also been demonstrated [3]. Here, we provide a thorough study of the fundamental optical and phonon mode properties of high-quality singlecrystals of LGO using generalized spectroscopic ellipsometry in combination with hybrid-level density functional theory calculations to investigate the optical properties in the mid- to far-infrared spectral range. From this, all 33 infrared-active pairs of transverse and longitudinal optical phonon modes are observed. We derive the anisotropic midband gap indices of refraction and static dielectric constants.

[1] A review of band structure and material properties of transparent conducting and semiconducting oxides: Ga<sub>2</sub>O<sub>3</sub>, Al<sub>2</sub>O<sub>3</sub>, In<sub>2</sub>O<sub>3</sub>, ZnO, SnO<sub>2</sub>, CdO, NiO, CuO, and Sc<sub>2</sub>O<sub>3</sub>, Joseph A. Spencer, Alyssa L. Mock, Alan G. Jacobs, Mathias Schubert, Yuhao Zhang, and Marko J. Tadjer , Applied Physics Reviews 9, 011315 (2022)

[2] Self-trapped holes and polaronic acceptors in ultrawide-bandgap oxides, John L. Lyons, Journal of Applied Physics 131, 025701 (2022)

[3] Composite substrate LiGaO<sub>2</sub> (0 0 1)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> (1 0 0) fabricated by vapor transport equilibration, Jungang Zhang, Changtai Xia, Shuzhi Li, Xiaodong Xu, Feng Wu, Guangqing Pei, Jun Xu, Shengming Zhou, Qun Deng, Wusheng Xu, Hongsheng Shi, Mater. Lett. 60. 3073-3075. (2006)

AC-MOP-3 Spectroscopic Ellipsometry Optical Analysis of Zinc Gallate at Elevated Temperatures, Emma Williams, University of Nebraska-Lincoln, USA; M. Hilfiker, U. Kilic, Y. Traouli, N. Koeppe, J. Rivera, A. Abakar, M. Stokey, R. Korlacki, University of Nebraska - Lincoln; Z. Galazka, Leibniz-Institut für Kristallzüchtung, Germany; M. Schubert, University of Nebraska - Lincoln

Zinc gallate (ZnGa<sub>2</sub>O<sub>4</sub>) is shown to be a promising alternative to gallium oxide. This is due to the material's larger bandgap of 5.27(3) eV, compared to that of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> (5.04 eV), which is linked to a higher Baliga's figure of merit. [1,2] ZnGa<sub>2</sub>O<sub>4</sub> also contains an isotropic structure, which is advantageous compared to both the monoclinic  $\beta$ -phase and uniaxial  $\alpha$ -phase of Ga<sub>2</sub>O<sub>3</sub> in simplifying device design. [2,5] Additionally, ZnGa<sub>2</sub>O<sub>4</sub> growth has rapidly developed to where bulk single crystals can be melt-grown with controllable n-type conductivity. [4]

In this work, the optical properties of  $ZnGa_2O_4$  are modeled using a spectroscopic ellipsometry approach at temperatures between 22°C and 600°C, where material properties drastically change in elevated temperatures. At each 50°C interval a Cauchy dispersion equation is applied to the transparent region of the data where the refractive index and high-frequency refractive index is derived. Furthermore, a critical point model is implemented across the spectral range of 1 eV to 6.5 eV. This allows for the determination of the bandgap, which is found to red-shift linearly with temperature with a slope of -0.72(4) meV K<sup>-1</sup>, resulting from the thermal expansion of the lattice. [3] The linear decrease in the bandgap energy when exposed to increasing elevated temperatures is in congruence with behavior shown by common wide bandgap metal oxides. In particular, the reduction of bandgap width as a function of temperature is comparable to that of the ultrawide bandgap material  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, further justifying ZnGa<sub>2</sub>O<sub>4</sub> as a suitable high-power device material. [2,3] References:

- [1] M. Hilfiker et al. Appl. Phys. Lett. 118, 132102 (2021).
- [2] A. Mock et al. Appl. Phys. Lett. 112, 041905 (2018).
- [3] M. Hilfiker et al. Appl. Phys. Lett. 120, 132105 (2022).
- [4] Z. Galazka et al. APL Materials 7, 022512 (2019).
- [5] S. J. Pearton et al. Appl. Phys. Lett. 5, 011301 (2018).

AC-MoP-4 The Electron Spin Hamiltonian for Fe<sup>3+</sup> in Monoclinic β-Ga<sub>2</sub>O<sub>3</sub>, S. Richter, Lund University, Sweden; S. Knight, P. Kühne, Linköping University, Sweden; **Mathias Schubert**, University of Nebraska - Lincoln; V. Darakchieva, Lund University, Sweden

Large interest in Ga<sub>2</sub>O<sub>3</sub> originates from the possibility to build devices with high breakdown voltage. Understanding electronic defects is essential to utilize the material. As  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is monoclinic, the effect of the low symmetry needs to be studied. Electron (paramagnetic) spin resonance (EPR) spectroscopy gives access to local site symmetry of spin-carrying defects. Deploying THz ellipsometry [1], we can measure high-field EPR at arbitrary variable frequency by reflection a free beam [2]. This allows true distinction of anisotropic g-factor and zero-field spin splitting, and hence examining the local site symmetry of electronic defects.

Iron incorporated on gallium sites can act as compensating acceptor and facilitate semi-insulating material. Here, we investigate the spin Hamiltonian of the neutral Fe<sup>3+</sup> state with spin s=5/2. It is characterized by large zero-field splitting that differs for Fe on octahedral Ga<sub>ii</sub> site (preferential) and Fe on tetrahedral Ga<sub>i</sub> site. Different, partially incorrect, reports exist about the nature of the spin Hamiltonian [3,4]. In contrast to standard EPR measurements at X or Q band with limited access to allowed spin transitions, we obtain EPR scans in the frequency range 110-170GHz at magnetic field between 3 and 7T that capture all five resonances for each Fe site at the same time. Modeling the spin Hamiltonian reveals a slight anisotropy of the g-factor and shows that zero-field splitting up to fourth order is relevant. We will discuss how the monoclinic s=5/2 spin Hamiltonian differs from orthorhombic and/or s=3/2 approximations.

P. Kühne *et al.*, IEEE Trans. Terahertz Sci. Technol. **8**(3), 257 (2018).
S. Schubert *et al.*, Appl. Phys Lett. **120**, 102101 (2022).
R. Büscher *et al.*, Z. Naturforsch. **42a**, 67 (1987).
M. L. Meil'man, Sov. Phys. Sol. State **11**(6), 1403 (1969).

The supplemental material features exemplary experimental data and the form of the spin Hamiltonian.

## Monday Evening, August 8, 2022

AC-MoP-5 Characterization of (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> to Support Fabrication, Wafer Size Scaleup, and Epi Development, David Snyder, Penn State Applied Research Laboratory

Efficient wafer size scaleup of quality (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates and epi development require extensive materials characterization. Over the past two years, the Applied Research Laboratory (ARL) Electronic Materials and Devices Department (EMDD) has partnered with Northrop Grumman's SYNOPTICS division in support of the Air Force Research Laboratory (AFRL)'s initiative to produce 2-inch epi-ready (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates via the Czochralski (Cz) method. As part of this effort, ARL has developed a multitude of techniques specifically for characterizing  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates at various stages of processing. In this poster, we highlight these techniques and describe the rapid feedback loop that ARL enables between those working on crystal growth, substrate fabrication, epi growth, and device processing within the expanding  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> community.

This poster covers defect mapping and identification, surface metrology, and x-ray characterization. Each of these areas provide essential information about the quality of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrates for subsequent epi growth and ultimately device fabrication. We show how etch pit analysis is used to automatically map defects in up to 2-inch wafers in conjunction with the focused ion beam (FIB) approach to prepare cross-sections for imaging the defect structures, including nanopipes. White light interferometry/profilometry and atomic force microscopy (AFM) provide three-dimensional topography information about the wafers, i.e., after polishing, thermal annealing, or free etching. This poster also describes our method for in-situ high-resolution x-ray characterization during fabrication in which a decrease in full-width at half-maximum (FWHM) was correlated with removal amount to optimize  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> polishing. Finally, we discuss how x-ray characterization provides information about curvature and substrate/epi layer quality with grazing incidence x-ray diffraction (GIXRD) being utilized to provide extremely surface-sensitive monitoring.

## AC-MOP-6 Photoluminescence Spectroscopy of $Cr^{3+}$ in $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and (Al<sub>0.1</sub>Ga<sub>0.9</sub>)<sub>2</sub>O<sub>3</sub>, *Cassandra Remple*, *J. Jesenovec*, *B. Dutton*, *J. McCloy*, *M. McCluskey*, Washington State University

Alloying  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> with Al<sub>2</sub>O<sub>3</sub> to create (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> enables ultra-wide band gap material deep into the UV. Here, photoluminescence (PL) spectra of  $Cr^{3+}$  dopant is compared between monoclinic single crystals  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, and 10 mol.% Al<sub>2</sub>O<sub>3</sub> alloyed with  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, denoted  $\beta$ -(Al<sub>0.1</sub>Ga<sub>0.9</sub>)<sub>2</sub>O<sub>3</sub> or AGO. Temperature dependent PL properties were studied for  $Cr^{3+}$  in AGO and  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> from 285 to 16 K. For  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>at room temperature, the red-line emission doublet R1 and R2 occurs at 696 nm (1.78 eV) and 690 nm (1.80 eV) respectively along with a broad emission band at 709 nm (1.75 eV). For both AGO and  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> the R<sub>1</sub> line increases in intensity with decreasing temperature. This can be explained by the thermal depopulation effect of the  $R_1$  state, which occurs with increasing temperature. The  $R_1$  and  $R_2$  lines of both materials were observed to blue-shift with decreasing temperature. Additional emission lines emerge at lower temperatures, with  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> showing more peaks than AGO. R<sub>1</sub> and R<sub>2</sub> peak parameters such as energy, intensity, width, and splitting were studied as a function of temperature, with significant differences between the two materials.

#### AC-MoP-7 Surface Relaxation and Rumpling of Sn Doped B-ga2o3(010),

Nick Barrett, CEA Saclay, France; A. Pancotti, Universidade Federal de Jataí, Brazil; T. Back, AFRL; W. Hamouda, M. Laccheb, C. Lubin, A. Boucly, CEA Saclay, France; P. Soukiassian, Université Paris-Saclay, France; J. Boeckl, D. Dorsey, S. Mou, T. Asel, AFRL; G. Geneste, CEA, France

We have used X-ray Photoelectron Diffraction (XPD), low-energy electron diffraction (LEED), atomic force microscopy (AFM) and X-ray photoelectron spectroscopy (XPS) to determine the surface structure, chemistry and interplanar relaxation and rumpling in single crystal, Sn-doped b-Ga<sub>2</sub>O<sub>3</sub> (010). XPD is a powerful technique, which combines information on local chemistry and atomic structure. By measuring the angular anisotropy of core level intensity one can, by comparison with simulations, deduce the local atomic and chemical environment around each type of emitting atom. The XPS measurements show typical spectra for stoichiometric  $Ga_2O_3(010)$ . Annealing at 823 K yielded a well-ordered surface with sharp (1x1) lowenergy electron diffraction (LEED) pattern. AFM shows unique surface termination with root mean square roughness of 0.1-0.15 nm. The XPD measurements were performed using a laboratory based setup with a monochromatic Al Ka (1486.7 eV) source and a high precision angular manipulator capable of scanning both polar (q) and azimuthal (f) angles. The XPD patterns collected for the Ga  $2p_{3/2}$  and O 1s emission. Surface interlayer relaxation up to 8% of the bulk interplanar distance and 0.11-0.14 Å rumpling are observed at the  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>(010) surface. At the surface,

the oxygen atoms shift toward the vacuum with respect to the gallium atoms. The rumpling decreases to zero and and the interplanar distance reaches the bulk value of 1.52 Å by the sixth atomic layer. The surface structure agrees with that predicted by first-principles density functional theory calculations which, in addition, suggest a significant band gap narrowing of  $\approx 1$  eV in the surface layer, due to surface states spatially localized on surface oxygen atoms of O<sub>II</sub> type.

A. Pancotti et al. Phys. Rev. B102, 245306 (2020)

AC-MoP-8 Probing Vacancies and Hydrogen Related Defects in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> with Positrons and FTIR, Corey Halverson, M. Weber, J. Jesenovec, B. Dutton, C. Remple, M. McCluskey, J. McCloy, Washington State University  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is a promising material for power electronics. Ubiquitous hydrogen and vacancies strongly influence the electronic properties of these materials. Methods to detect and characterize them are desirable. Fourier Transform Infrared Spectroscopy (FTIR) and Positron Annihilation Spectroscopies (PAS) both have been use with success. Here, they are applied to investigate the hydrogen content in gallium vacancies particularly in the top 6 micrometers below the surface. A Czochralski grown bulk single crystal is explored before and after repeated annealing in vacuum with the main goal to remove hydrogen from the sample. The hydrogen reduction method was first applied with success on single crystal ZnO samples.  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is sealed in an evacuated hydrogen-depleted quartz tube together with thin foils of titanium. Before sealing the ampoule, the quartz and the titanium are heated repeatedly to drive out trapped hydrogen. Then  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is annealed at 850C to 900C for up to 8 days while maintaining the Ti-foil at the other end of the ampoule at room temperature. Depth resolved PAS Doppler broadening data reveal significant reduction in the effective positron diffusion length and small changes in the vacancy sensitive width of the annihilation line (Sparameter). These changes reversed by subsequent annealing in hydrogen. The positron data will be presented and correlated with bulk FTIR measurements on the same sample. This work generously supported by the Air Force Office of Scientific Research under award number FA9550-18-1-0507 monitored by Dr. Ali Sayir.

AC-MOP-9 Evolution of Anisotropy and Order of Band-to-Band Transitions, Excitons, Phonons, Static and High Frequency Dielectric Constants Including Strain Dependencies in Alpha and Beta Phase (Al<sub>x</sub>Ga<sub>1</sub>. x)<sub>2</sub>O<sub>3</sub>, *Megan Stokey*, University of Nebraska-Lincoln; *R. Korlacki, M. Hilfiker, T. Gramer*, University of Nebraska - Lincoln; *J. Knudtson*, University of Nebraska-Lincoln; *S. Richter*, Lund University, Sweden; *S. Knight*, Linköping University, Sweden; *A. Mock*, Weber State University; *A. Mauze*, *Y. Zhang, J. Speck*, University of California Santa Barbara; *R. Jinno, Y. Cho, H. Xing, D. Jena*, Cornell University; *Y. Oshima*, National Institute for Materials Science, Japan; *E. Ahmadi*, University of Michigan; *V. Darakchieva*, Lund University, Sweden; *M. Schubert*, University of Nebraska - Lincoln

The rhombohedral alpha and monoclinic beta phases of gallium oxide both make promising candidates for ultra-wide bandgap semiconductor technology. Of particular interest are alloyed films and the evolution of anisotropic optical properties with respect to both alloy composition and strain induced effects. Here, we study alpha and beta phase (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> via a combined density functional theory and generalized spectroscopic ellipsometry approach across a range of alloying. Infrared-active phonon properties, static dielectric constants and midband gap indices of refraction are quantified.[1,2,3] Strain and alloying effects are shown and compared to previous theoretical works.[4] Band-to-band transitions, excitons, and high-frequency dielectric constants are also investigated in the visible to vacuum-ultra-violet (VUV) spectral range.[5,6,7,8] We identify a switch in band order where the lowest band-to-band transition occurs with polarization along the ordinary plane in  $\alpha$ -Ga--<sub>2</sub>O-<sub>3</sub> whereas for  $\alpha$ -Al-<sub>2</sub>O<sub>3</sub> the lowest transition occurs with polarization in the extraordinary direction. With this, we present the most comprehensive picture of optical properties' evolution along composition and strain currently available.

[1] M. Stokey, et al., Phys. Rev. Materials 6, 014601 (2022)

[2] M. Stokey, et al., Appl. Phys. Lett. 120, 112202 (2022)

[3] The influence of strain and composition on the infrared active phonons in epitaxial  $\beta$ -(AlxGa1-x)2O3 deposited onto (010)  $\beta$ -Ga2O3; M. Stokey, *et al.*, *In Preparation* 

[4] R. Korlacki, et al., Rev. B 102, 180101(R) (2020)

[5] M. Hilfiker, et al., Appl. Phys. Lett. 118, 062103 (2021)

[6]Anisotropic dielectric function, direction dependent bandgap energy, band order, and indirect to direct gap cross over in  $\alpha$ -(AlxGa1-x)2O3 (0≤x≤1); M. Hilfiker, *et al.*, Appl. Phys. Lett. XX, XX (2022)

## Monday Evening, August 8, 2022

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AC-MOP-10 Photoluminescence Mapping of Gallium Oxide and Aluminum Gallium Oxide Epitaxial Films, Jacqueline Cooke, P. Ranga, University of Utah; J. Jesenovec, J. McCloy, Washington State University; S. Krishnamoorthy, University of California at Santa Barbara; M. Scarpulla, B. Sensale-Rodriguez, University of Utah

The mechanisms generating photoluminescence (PL) emissions from gallium oxide (Ga<sub>2</sub>O<sub>3</sub>) and aluminum gallium oxide (AGO) have been under intense scrutiny. In general, spectrally-resolved PL is used to characterize the defects leading to radiative recombination processes within a specific material. In this regard, the PL spectra for  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> has generally been deconvoluted in three emission bands: UV, blue, and green. So far, the intense debate in defining the defects and phenomenological explanations of electronic processes that cause Ga<sub>2</sub>O<sub>3</sub> and AGO emissions have only explored point defects as the potential source for the PL emission leaving out whether extended defects could affect PL. Because of the strong electron phonon coupling, emission peak shapes from any defect are expected to be very broad and not have a simple functional peak shape; these attributes make it challenging to fit spectra uniquely. Because of this, there is little chance of directly assigning PL spectral features unambiguously to specific  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> point defects from PL alone.

Here, a systematic PL study on multiple series of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and AGO epitaxial thin films and bulk single crystals is performed. Spectrally-resolved PL, PL intensity mapping, scanning electron microscopy (SEM), atomic force microscopy (AFM), and transmission electron microscopy (TEM) were used along with literature to show that extended structural defects largely determine the PL emission from many samples of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and AGO. Homogeneous films with no extended defects or stacking faults and bulk crystals yield PL emission with a dominant UV peak, while samples of lesser crystalline quality exhibiting stacking faults, rotation domain boundaries, and other such extended defects do not exhibit a UV emission but rather exhibit blue.

Si-doped homoepitaxial (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> samples yield homogeneous crystalline films with a low density of extended defects and an unshifting dominant UV emission in PL. A bulk (-201)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> sample shows a dominant UV emission while heteroepitaxial and homoepitaxial (-201)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> films show dominant blue PL emission (due to the films' poor quality as seen in PL mapping, AFM and SEM). An AGO series shows consistent blue centered PL for AGO grown on both sapphire and  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> (also due to the films' poor quality as seen in TEM, PL mapping, AFM and SEM). Lastly, an improved (reduced number of extended defects) 10% AGO film grown on (010) bulk  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> show a shift in the PL spectrum with a now UV dominant emission. PL mapping shows that areas of extended defects emit blue PL while the crystal film emits UV PL within the sample.

#### AC-MoP-12 Non-Destructive Characterization of Annealed Si-Implanted Thin Film $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, *Aine Connolly*, *K. Gann*, Cornell University; *S. Tetlak*, Air Force Research Laboratory; *V. Protasenko*, Cornell University; *M. Slocum*, *S. Mou*, Air Force Research Laboratory; *M. Thompson*, Cornell University

Selective doping by ion implantation is critical for small-scale device fabrication in wide-bandgap materials such as  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, requiring understanding of both lattice damage due to implantation and subsequent lattice recovery during thermal annealing. Carrier activation, mobility, and diffusion are known to be critically coupled to annealing temperature, time and ambient as well as intrinsic and extrinsic film properties. Electrical measurements provide one measure of annealing behavior, but are limited due to the need for direct metal contacts, the intrinsic spatial averaging, and the inability to directly measure lattice recovery or observe associated defects. To address these limitations, we present Raman spectroscopy and photoluminescence (PL) measurements of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> implanted and annealed samples, evaluating their ability to local carrier activation and lattice recovery non-destructively.

Recent studies of bulk doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> [1] have identified additional Raman peaks in samples with carrier concentrations above the Mott criterion. To determine if these peaks are directly linked to carrier activation, we examined a wide range of Si-implanted (5x10<sup>19</sup> cm<sup>-3</sup>) and annealed samples using a laterally localized Raman probe. A peak at 285 cm<sup>-1</sup> was observed above the noise floor in several samples, with the intensity increasingly linearly with sheet carrier density (N<sub>5</sub>). The effect of the lattice quality (recovery) on the relative intensities of other Raman peaks was also analyzed.

Previous  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> studies suggest that an increase in activated dopants decreases the total PL, due to the higher defect density and the resultant probability of electrons reaching non-radiative recombination centers [2]. PL behavior of the Si-implanted samples was thus measured as a function of lattice recovery with (N<sub>2</sub> ambient) and without (O<sub>2</sub> ambient) carrier activation. The PI signal decreased dramatically after implantation, with partial recovery after thermal anneals and lattice damage recovery. Negative correlation was observed between the PL intensity and carrier activation. Correlations between PL and cathodoluminescence were also measured.

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[2] Shimamura, K., Villora, E.G., Ujiie, T., and K. Aoki. Excitation and photoluminescence of pure and Si-doped B-Ga2O3 single crystals. *Appl. Phys. Lett.* 92, 201914 (2008).

## Tuesday Morning, August 9, 2022

#### Advanced Characterization Techniques Room Jefferson 2-3 - Session AC-TuM

#### Advanced Characterization & Microscopy

Moderator: Ginger Wheeler, Naval Research Laboratory

10:45am AC-TuM-10 Defects in Gallium Oxide - How We "See" and Understand Them, Jinwoo Hwang, The Ohio State University INVITED Due to the low crystal symmetry, gallium oxide can display formation of unique defects ranging from point defects to phase transition that are important to understand, as such defects directly correlate to the properties of the material and performance of gallium oxide-based devices. This presentation will overview the recent progress in the atomic scale characterization of various defects in gallium oxide and aluminum gallium oxide using scanning transmission electron microscopy. We make a direct connection between the atomic structure of these defects and important properties of gallium oxide materials and devices, including growth characteristics of the films as well as their electric and thermal properties. The topics will include: (i) formation of point defects and complexes, (ii) alloy incorporation and phase stability in aluminum gallium oxide, (iii) formation of 2D defects, such as stacking faults and twins, (iv) phase transformation induced by incorporation (or diffusion) of impurity atoms, (v) defects at interfaces with metal contacts and their influence on thermal interface resistance, and (vi) defects created by ion implantation of gallium oxides. The new information that we summarize in this presentation is expected to help achieve atomic scale control of defects in gallium oxide materials and devices for the next generation power electronics applications.

# 11:15am AC-TuM-12 Atomic-Scale Investigation of Point and Extended Defects in Ion Implanted $\beta$ -Ga<sub>2</sub>O<sub>3</sub>, *Hsien-Lien Huang*, *C. Chae*, The Ohio State University; *A. Senckowski*, *M. Wong*, Penn State University; *J. Hwang*, The Ohio State University

Atomic scale scanning transmission electron microscopy (STEM) was used to study the formation of point and extended defects, as well as phase transformations in Si-implanted  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. Quantitative analysis of the atomic column intensities in STEM images acquired with an absolute scale, when combined with precise electron scattering simulations, can directly visualize the detailed structure of atomic and nanoscale defects in materials. For example, our previous studies have revealed the formation of different types of point and extended defects, including the interstitialdivacancy complexes in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> and planar defects and phase transition in (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> that directly correlate with Al incorporation into the lattice. In the present study, we performed a correlative study on the structural change and defect formation in Si implanted β-Ga<sub>2</sub>O<sub>3</sub> (edge-defined, filmfed (EFG)-grown (001)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> substrate) as a function of Si dose, using a combination of STEM and secondary ion mass spectrometry (SIMS). Peak Si concentrations of 10<sup>18</sup>-10<sup>21</sup> cm<sup>-3</sup> were investigated. Different types of point defects and their complexes were observed in lower Si concentrations (< ~ 10<sup>19</sup> cm<sup>-3</sup>), which include cation interstitials and substitutional atoms into the oxygen positions. The types and concentrations of those defects change as a function of the depth of the implantation. The implication of the observed defects to electronic properties will be discussed. High concentration of point defects at a local region also led to the formation of a unique type of extended defect, which apparently involves a large strain field that extends up to a few tens of nanometers. At higher Si concentrations (>  $10^{20}$  cm<sup>-3</sup>), the structure tends to transform into different  $Ga_2O_3$  phases, including  $\gamma\text{-}Ga_2O_3$  which, according to our previous investigation, has a close relationship to the extended defects in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. In situ annealing of the samples was performed to understand the structural evolution and diffusion dynamics of the implanted materials. The precise atomic scale information on defect formation and their evolution provides an important guidance to understand and control the ion implantation of Ga<sub>2</sub>O<sub>3</sub> materials and devices which is crucial to advance them to next generation ultrawide-bandgap applications.

11:30am AC-TuM-13 Microscopic and Spectroscopic Analysis of (100), (-201) and (010) (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> Films Using Atom Probe Tomography, J. Sarker, University at Buffalo-SUNY; A. Bhuiyan, Z. Feng, L. Meng, H. Zhao, The Ohio State University; Baishakhi Mazumder, University at Buffalo-SUNY

(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> is an emerging ultra-wide bandgap semiconductor with a bandgap tunability of 4.8 - 8.7 eV and highly promising for high power electronics [1]. The Al inclusion limit in (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> varies with growth orientation. While (010)–(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> is single β–phase stable till 27% Al, (-201) and (100)–(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> exhibit β–phase for >50% Al [2]. The Al

incorporation in  $(Al_xGa_{1-x})_2O_3$  for different orientations are limited by phase segregations, chemical heterogeneity and domain rotations due to difference in surface free energy. The higher the surface free energy, the lower the Al incorporation at the growth surface. Also, as the surface free energy varies for different growth orientation, the binding energies would be different which play a significant role in Al inclusion range in (100), (-201) and (010)–(Al\_xGa\_{1-x})\_2O\_3 films. Therefore, a comprehensive understanding of the film's structural-chemical morphology and properties (surface energy, binding energy and bond lengths) of (100), (-201) and (010)–(Al\_xGa\_{1-x})\_2O\_3 is needed to achieve films with high Al% for high power transistors.

Here, we employed atom probe tomography (APT), a nanoanalytical tool combining microscopy to provide chemical imaging and spectroscopy to reveal qualitative binding energy/bond length information of material. The nanoscale structure-chemistry of (100), (-201) and (010)–(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> varying Al composition was probed. From the in-plane lateral Al/O distribution, (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> layers with 20% Al are found to be homogeneous in (100), (-201) and (010) orientation while (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> layers with 50% Al are relatively less homogeneous in each case. This is attributed to the higher surface migration length of Al atoms compared to that of Ga atoms. The APT spectroscopy was used to determine the relative bond length information of Ga–O and Al–O for (100), (-201) and (010)–(Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> films varying Al content. The observed APT spectroscopy result reveals that the bond length of Ga–O and Al–O changes as the (Al<sub>x</sub>Ga<sub>1-x</sub>)<sub>2</sub>O<sub>3</sub> growth orientation varies.

This work will provide critical understanding and insights on the structural chemistry and bond lengths of  $(Al_xGa_{1-x})_2O_3$  films with different growth orientations and will aid in optimizing the growth towards developing  $(Al_xGa_{1-x})_2O_3$  films with high Al%.

Acknowledgment: NSF (Grant No. 2114595; 1810041 and 2019753) and AFOSR (FA9550-18-1-0479)

Reference: 1. Bhuiyan et al. APL Materials, 8, 031104 (2020); 2. Bhuiyan et al. Appl. Phys. Lett. 117, 142107 (2020)

11:45am **AC-TuM-14** Phase and Microstructure Evolution of  $\kappa$ -Ga<sub>2</sub>O<sub>3</sub> Thin Films Grown by MOCVD, *Jingyu Tang*, *K. Jiang*, Carnegie Mellon University, China; *M. Cabral*, *A. Park*, Carnegie Mellon University; *L. Gu*, Carnegie Mellon University, China; *R. Davis*, *L. Porter*, Carnegie Mellon University Ga-Oais an ultra-wide bandran semiconductor that has larger values of

 $\mathsf{Ga}_2\mathsf{O}_3$  is an ultra-wide bandgap semiconductor that has larger values of bandgap, Baliga's figure of merit, and breakdown electric field than SiC and GaN. There are four commonly accepted polymorphs of Ga<sub>2</sub>O<sub>3</sub>, namely trigonal  $\alpha$  (corundum structure), monoclinic  $\beta$ , orthorhombic  $\kappa$ , and cubic  $\gamma$ (cation deficient spinel structure) phases. Of those four polymorphs, β-Ga<sub>2</sub>O<sub>3</sub> has been the most investigated, as this phase is the thermodynamically stable phase from room temperature to the melting point at atmospheric pressure<sup>1-2</sup>. However, the lower symmetry of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> results in anisotropic optical and electronic properties. Compared with β-Ga<sub>2</sub>O<sub>3</sub>, κ-Ga<sub>2</sub>O<sub>3</sub> has higher symmetry and some unique properties. κ-Ga<sub>2</sub>O<sub>3</sub> shows spontaneous polarization (Psp) parallel to the c-axis and thus a highdensity two-dimensional electron gas can be formed at the interface without doping. The reported values of Psp are 0.23 C/m<sup>23</sup> and 0.242 C/m<sup>2</sup> <sup>4</sup>, respectively, which are about an order of magnitude higher than those of GaN and AlN. In this study, nominally phase pure  $\kappa\text{-}\text{Ga}_2\text{O}_3$  films were successfully grown on vicinal c-plane sapphire (0.15° offcut toward mplane) by low-pressure metal-organic chemical vapor deposition<sup>5</sup>. Phase and microstructural characterizations were conducted using a complementary suite of tools. High-angle annular dark-field scanning transmission electron microscopy of a κ-Ga<sub>2</sub>O<sub>3</sub> film grown under optimum conditions revealed the pseudomorphic growth of 3-4 monolayers of  $\alpha$ -Ga<sub>2</sub>O<sub>3</sub> at the interface, followed by a 20-60 nm transition layer containing a mixture of  $\beta\text{-}$  and  $\gamma\text{-}\text{Ga}_2\text{O}_3$  which was covered by an ~700 nm-thick layer of phase-pure  $\kappa$ -Ga<sub>2</sub>O<sub>3</sub>. The occurrence of these phases and their sequence of formation will be presented. X-ray diffraction (XRD) and scanning electron microscopy investigations showed that the top layer varied between  ${\sim}100\%~\kappa\text{-}Ga_2O_3$  and  ${\sim}100\%~\beta\text{-}Ga_2O_3\text{,}$  depending on the growth temperature and the growth rate. XRD  $\phi$  scans showed in-plane epitaxial relationships and the presence of the three rotational domains in the ĸ-Ga<sub>2</sub>O<sub>3</sub>. Atomic force microscopy investigations revealed a smooth surface morphology with a root-mean-square roughness of ~3.5nm for optimum growth conditions. In summary, growth conditions have been established that yield 700 nm-thick films, above a thin transition layer, comprising phase-pure  $\kappa\text{-}Ga_2O_3;$  whereas the  $\beta\text{-}phase$  is favored at higher growth temperatures and lower growth rates.

## **Tuesday Morning, August 9, 2022**

12:00pm AC-TuM-15 Investigation of Extended Defects in Ga2O3 Substrates and Epitaxial Layers using X-ray Topography, Nadeemullah A. Mahadik, M. Tadjer, T. Anderson, K. Hobart, Naval Research Laboratory, USA; K. Sasaki, A. Kuramata, Novel Crystal Technology, Japan

Recently, beta-gallium oxide ( $\beta$ -Ga<sub>2</sub>O<sub>3</sub>) has attracted attention for high power devices due to its high bandgap of 4.9eV and possibility of manufacturing large diameter wafers using quasi-equilibrium melt-based techniques, which can have low defects. Extended defects such as dislocations, stacking faults, inclusions, dislocation slip bands etc have proven to have detrimental effects on power and RF device performance and reliability. Defect identification and their mitigation is necessary to fabricate devices that can reach the predicted breakdown and on-state resistance performance for Ga<sub>2</sub>O<sub>3</sub> devices. Investigation of extended defects over large diameter Ga<sub>2</sub>O<sub>3</sub> wafers, including defect delineation and micro-structural properties can be obtained using high resolution x-ray topography (XRT). In this study, various extended defects were investigated in 100 mm diameter Ga<sub>2</sub>O<sub>3</sub> wafers with 10 $\mu$ m thick epitaxial layers using multiple reflection XRT characterization to identify defect types and distinguish defects in both substrates and epitaxial layer.

For this study, a 100 mm diameter, edge-defined, film-fed (EFG) growth  $Ga_2O_3$  wafer with 10 mm epitaxial layer grown via halide vapor phase epitaxy (HVPE) was obtained from Novel Crystal Technology. XRT imaging was performed on a Rigaku XRTMicron system equipped with a 1.2kW Cu/Mo dual rotating anode, high precision X, Y, f goniometer and 5.4mm/2.2mm pixel dual X-ray cameras. Imaging was performed using Mo ka<sub>1</sub> in transmission geometry with g=(020) and in reflection geometry with g=(-809), (607), and (-44,10). Imaging using Cu ka1 was also performed in reflection geometry with g=(224) and (514). Using these various imaging conditions the penetration depth of the X-rays was controlled in the sample. Hence, identification and delineation of a variety of extended defects from both the epitaxial layers as well as the substrates was performed.

A distribution of basal plane dislocations (BPD) was observed across the wafer with a density  $^{3}x10^{3}$  cm<sup>-2</sup>. These BPDs are primarily within the substrate. Few of the BPDs were observed to propagate into the epitaxial layers. Slip bands were observed emanating from the edge of the wafer in several regions and are within the epitaxial layers only. These are likely due to residual damage in the wafer edge processing. Additionally pits were identified within the epitaxial layer, which could be due to pitting occurring by Ga droplets during the HVPE process. Other defects such as inclusions, surface dislocations, and scratches were also observed. Detailed microstructure and dislocation analysis will be presented on the extended defects observed in the multiple XRT images.

## Wednesday Morning, August 10, 2022

Electronic and Photonic Devices, Circuits and Applications Room Jefferson 2-3 - Session EP1-WeM

Process & Devices III

Moderator: Uttam Singisetti, University of Buffalo, SUNY

9:15am EP1-WeM-4 Remarkable Improvement of Conductivity in B-Ga<sub>2</sub>O<sub>3</sub> by High-Temperature Si Ion Implantation, *Arka Sardar*, *T. Isaacs-Smith, S. Dhar,* Auburn University; *J. Lawson, N. Merrett,* Air Force Research Laboratory, USA

Monoclinic Beta Gallium Oxide ( $\beta$ -Ga<sub>2</sub>O<sub>3</sub>) is emerging as a promising wide bandgap semiconductor for high voltage electronics. Ion implantation is a key process for device fabrication as it provides a unique way to carry out selective area doping with excellent control. It has been demonstrated that Si implantation into (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> at room temperature followed by annealing at ~1000°C, results in an activation efficiency (n)of 63% for Si concentrations up to ~5e19 cm<sup>-3</sup>. However, for higher concentrations, a severe drop of the  $\eta$  to 6% occurs [1]. In this work, we demonstrate that high-temperature implantation can be used to significantly improve this for heavily implanted  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. In the case of SiC, implantation at > 500°C results in superior conductivity due to lower defect densities and better recrystallization after annealing [2]. Based on this, we performed room temperature (RT, 25°C) and high temperature (HT, 600°C) Si implants into MBE grown 300 nm (010)  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> films with energies of 275 keV and 425 keV through ~110 nm Mo and ~30 nm  $Al_2O_3$  layers; with a total of fluence of 2.4e15 cm<sup>-2</sup> or 4.8e15 cm<sup>-2</sup>. This was followed by annealing in flowing nitrogen at 970°C for 30 minutes to activate the dopants. SIMS shows the Si profile is ~400 nm deep with an average concentration of ~6.0e19 cm  $^{-3}$  for the lower fluence samples, and expected to be ~1.2e20cm<sup>-3</sup> for the higher fluence (SIMS ongoing). No significant difference in surface roughnesses were detected by AFM throughout the process. HRXRD shows structural defects after the implantation and partial crystallization recovery upon annealing, where the advantage was in favor of HT implantation. The ratio of the free electron concentration from Hall measurements and the total amount of Si in  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> was used to determine the activation efficiencies. For the lower fluence, the HT sample shows only a ~6% improvement of  $\eta$ over the RT sample. Remarkably, for the higher fluence, while the RT sample was too resistive for measurement, the HT sample had n close to 70%, with a high sheet electron concentration of 3.3e15 cm<sup>-2</sup> and excellent mobility of 92.8 cm<sup>2</sup>/V·s at room temperature. These results are highly encouraging for achieving ultra-low resistance heavily doped β-Ga<sub>2</sub>O<sub>3</sub> layers using ion implantation, which will be discussed further in this presentation.

#### References:

[1]K. Sasaki et.al,, Appl. Phys. Express 6, 086502 (2013).

[2]F. Roccaforte, et. al, , Micro 2, 23 (2022).

#### Acknowledgments:

We acknowledge the support of the Department of Physics, Auburn University.

9:30am EP1-WeM-5 Towards Lateral and Vertical Ga2O3 Transistors for High Voltage Power Switching, Kornelius Tetzner, J. Würfl, E. Bahat-Hilt. Treidel. О. Ferdinand-Braun-Institut. Leibniz-Institut für Höchstfrequenztechnik (FBH), Germany; Z. Galazka, S. Bin Anooz, A. Popp, Leibniz-Institut für Kristallzüchtung (IKZ), Germany INVITED Gallium Oxide (Ga<sub>2</sub>O<sub>3</sub>) power switching devices are expected to boost efficiency of power converters predominately operating at comparatively high bias voltage levels in the kV range. Thanks to the extraordinarily high energy band gap of 4.9 eV a high device breakdown strength of about 8 MV/cm is expected. Thus it is possible to efficiently utilize these properties for very compact power devices with aggressively minimized gate to drain separation. This enables low resistive on-state and low leakage off-state properties. Most Ga<sub>2</sub>O<sub>3</sub> devices introduced so far rely on volume electron transport properties; only a few 2DEG devices have been demonstrated. In any case the values of electron mobility and saturation velocity in Ga<sub>2</sub>O<sub>3</sub> crystals may depend on crystal orientation and did not yet reach properties being comparable to more developed wide band gap semiconductor families such as GaN and SiC. - Nevertheless the benefit of Ga<sub>2</sub>O<sub>3</sub> devices

relates to the combination of high breakdown field and electron transport properties and the resulting compact device design strategies are already getting competitive to existing power switching technologies.

The presentation will give an overview on the current status of lateral and vertical  $Ga_2O_3$  devices with a special emphasis on results obtained at FBH and IKZ [1]. For both cases concepts for epitaxial layer structures and device designs suitable for reaching the targeted performance will be discussed especially in terms of breakdown voltage and channel current density. Critical points for device optimization such as type of gate recess in lateral transistors and concepts of critical electric field reduction in vertical transistors will be addressed.

[1] K. Tetzner, IEEE Electron Device letters, vol. 40, No. 9, (2019), pp. 1503 - 1506.

10:00am EP1-WeM-7 Comparison of β-Ga2O3 Mosfets With TiW and NiAu Metal Gates for High-Temperature Operation, Nicholas Sepelak, KBR, Wright State University; D. Dryden, KBR; R. Kahler, University of Texas at Dallas; J. William, Air Force Research Lab, Sensors Directorate; T. Asel, Air Force Research Laboratory, Materials and Manufacturing Directorate; H. Lee, University of Illinois at Urbana-Champaign; K. Gann, Cornell University; A. Popp, Leibniz-Institut für Kristallzüchtung, Germany; K. Liddy, Air Force Research Lab, Sensors Directorate; K. Leedy, Air Force Research Laboratory, Sensors Directorate; W. Wang, Wright State University; W. Zhu, University of Illinois at Urbana-Champaign; M. Thompson, Cornell University; S. Mou, Air Force Research Laboratory, Materials and Manufacturing Directorate, USA; K. Chabak, A. Green, Air Force Research Laboratory, Sensors Directorate; A. Islam, Air Force Research Laboratory, Sensors Directory  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> offers a robust platform for operation of electronic devices at a high temperature because of its large band gap and low intrinsic carrier concentration. We have recently characterized the high temperature performance  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> field effect transistors using different gate metals in vacuum and air ambient at temperatures up to 500 °C.

The devices fabricated using TiW refractory metal gate and Al<sub>2</sub>O<sub>3</sub> gate dielectric exhibited stable operation up to 500 °C in vacuum and up to 450 °C in air [1]. Transfer (I<sub>DS</sub>-V<sub>GS</sub>) characteristics of a device were measured at various temperatures in vacuum and air. Extracted I<sub>MAX</sub>/I<sub>MIN</sub> for the vacuum test reduced from ~10<sup>4</sup> to 10<sup>2</sup> as temperature was increased up to 500 °C. During the vacuum characterization, the contact resistance remained unchanged at all temperatures and, therefore, device characteristics showed no degradation once devices were brought back to RT even after several hours of device operation at 500 °C in vacuum.

The devices, fabricated with Ni/Au gate metal and Al<sub>2</sub>O<sub>3</sub> gate dielectric, exhibited stable operation up to 500 °C in air [2]. The measured I<sub>D</sub>-V<sub>D</sub> characteristics showed no current degradation up to 450 °C. At 500 °C, the device exhibited a drop in I<sub>D</sub>; however, device characteristics recovered once the device is brought back to RT, even after 20 hours of device operation at 500 °C.

For tests in air ambient, both Ni/Au and Ti/W devicesobserved an increase in current with temperature due to activation carriers from dopants/traps in the device, however, both exhibited I<sub>MAX</sub>/I<sub>MIN</sub> < 10<sup>2</sup> at 450 °C because of contact degradation. The barrier height of  $\phi_B \sim 1.0$  eV and 0.77 eV was calculated for the TiW/Al<sub>2</sub>O<sub>3</sub> and the NiAu/Al<sub>2</sub>O<sub>3</sub> interfaces, respectively using thermionic emission theory. Thought the values of  $\phi_B$  for the Ti/W contacts was consistent with that expected from the work-function difference between TiW and Al<sub>2</sub>O<sub>3</sub>, the devices with Ni/Au yielded lower  $\phi_B$  presumably due to the diffusion of Ni and the partial crystallization of the Al<sub>2</sub>O<sub>3</sub> dielectric [3]. Our results suggest that with appropriate choice of metals and gate dielectrics, the stable 500 °C operation using  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> is achievable.

[1] Sepelak *et al.*, "High-temperature operation of  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> MOSFET with TiW refractory metal gate," *DRC, 2022*.

[2] Sepelak et al., "First Demonstration of 500 °C Operation of  $\beta\text{-}Ga_2O_3$  MOSFET in Air," CSW, 2022

[3] Islam et al., "Thermal stability of ALD-grown SiO2 and Al2O3 on (010)  $\beta$ -Ga2O3 substrates," DRC, 2022.

10:15am EP1-WeM-8 High Electron Mobility Si-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> MESFETs, Arkka Bhattacharyya, University of Utah; S. Roy, University of California at Santa Barbara; P. Ranga, University of Utah; S. Krishnamoorthy, University of California at Santa Barbara

A hybrid low temperature - high temperature (LT-HT) buffer/channel stack growth is demonstrated using MOVPE with superior carrier mobility values. An LT-grown ( $600^{\circ}$ C) undoped Ga<sub>2</sub>O<sub>3</sub> buffer (250-330 nm thick) is grown

## Wednesday Morning, August 10, 2022

followed by transition layers to a HT (810°C) Si-doped Ga<sub>2</sub>O<sub>3</sub> channel layers (~220 nm) without growth interruption. The (010) Fe-doped Ga<sub>2</sub>O<sub>3</sub> substrates were cleaned in HF for 30 mins prior to channel growth. From Hall measurements, this stack design is shown to have an effective RT Hall mobility values in the range  $162 - 184 \text{ cm}^2/\text{Vs}$  for doped channel electron densities of 1.5- $3.5 \times 10^{17} \text{ cm}^3$  measured on multiple samples/substrates. These mobility values are higher than the state-of-the-art values in Ga<sub>2</sub>O<sub>3</sub> literature. Two types of (010) Fe-doped Ga<sub>2</sub>O<sub>3</sub> bulk substrates were used in this study:  $5 \times 5 \text{ mm}^2$  diced pieces from  $10 \times 15 \text{ mm}^2$  EFG-grown substrates from NCT, Japan and 2-inch CZ-grown bulk substrates from NG Synoptics, USA.

The charge and transport properties were also verified using CV, TLM, fieldeffect mobility ( $\mu_{FE}$ ) measurements and FET current characteristics. Few samples were processed for regrown ohmic contacts to minimize contact resistance. R<sub>C</sub> values of 1-2  $\Omega$ .mm were achieved. 3D electron densities were verified by CV measurements. Channel charge profile (from CV) showed the absence of any active parasitic charge below the buffer layer. R<sub>sh</sub> values from TLM measurements matched closely with Hall measurements. RT  $\mu_{FE}$  measured on FatFET structures (L<sub>G</sub> ~110um, L<sub>GS</sub>/L<sub>GD</sub> ~ 1um) showed peak values of 158 and 168 cm<sup>2</sup>/Vs in the doped region for electron densities of  $3.5 \times 10^{17}$  cm<sup>-3</sup> and  $2.1 \times 10^{17}$  cm<sup>-3</sup> respectively, which are also the highest values to be ever reported. MOSFETs and MESFETs with device dimensions L<sub>GS</sub>/L<sub>GD</sub> = 1/2.5/5 um show max ON currents of ~200 mA/mm and ~130 mA/mm respectively. MESFETs show very high I<sub>ON</sub>/I<sub>OFF</sub> ~  $10^{10}$  and ultra-low reverse leakage. OFF-state voltage blocking capabilities of these devices will be reported.

These buffer-engineered doped high-mobility  $Ga_2O_3$  channel layers with superior transport properties show great promise for  $Ga_2O_3$  power devices with enhanced performance.

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#### **Author Index**

-A -

Abakar, A.: AC-MoP-3, 3 Abrikosov, I.: AC-MoM-8, 2 Ahmadi, E.: AC-MoP-9, 4 Anderson, T.: AC-TuM-15, 7 Arehart, A.: AC-MoM-5, 2 Asel, T.: AC-MoP-7, 4; EP1-WeM-7, 8

— B —

Back, T.: AC-MOP-7, 4 Bahat-Treidel, E.: EP1-WeM-5, 8 Barrett, N.: AC-MOP-7, **4** Bhattacharyya, A.: AC-MoM-7, 2; EP1-WeM-8, **8** Bhuiyan, A.: AC-TuM-13, 6 Bin Anooz, S.: EP1-WeM-5, 8 Boeckl, J.: AC-MoP-7, 4 Boucly, A.: AC-MoP-7, 4 Bulancea-Lindvall, O.: AC-MoM-8, 2

**— C —** Cabral, M.: AC-TuM-14, 6

Chabak, K.: EP1-WeM-7, 8 Chae, C.: AC-TuM-12, 6 Cho, Y.: AC-MoP-9, 4 Connolly, A.: AC-MoP-12, **5** Cooke, J.: AC-MoP-10, **5** Cornuelle, E.: AC-MoM-5, 2

— D —

Darakchieva, V.: AC-MoM-8, 2; AC-MoP-4, 3; AC-MoP-9, 4 Davis , R.: AC-TuM-14, 6 Dhar, S.: EP1-WeM-4, 8 Dorsey, D.: AC-MoP-7, 4 Dryden, D.: EP1-WeM-7, 8 Dutton, B.: AC-MoP-6, 4; AC-MoP-8, 4

— E -

Eisner, B.: AC-MoM-7, 2

— F -

— G —

Feng, Z.: AC-TuM-13, 6

Galazka, Z.: AC-MoM-8, 2; AC-MoP-3, 3; EP1-WeM-5, 8 Gann, K.: AC-MoP-12, 5; EP1-WeM-7, 8 Geneste, G.: AC-MoP-7, 4 Ghadi, H.: AC-MoM-5, 2 Gramer, T.: AC-MoP-2, **3**; AC-MoP-9, 4 Green, A.: EP1-WeM-7, 8 Gu, L.: AC-TuM-14, 6

— H —

Halverson, C.: AC-MoP-8, **4** Hamouda, W.: AC-MoP-7, 4 Hilfiker, M.: AC-MoP-3, 3; AC-MoP-9, 4 Hilt, O.: EP1-WeM-5, 8 Hobart, K.: AC-TuM-15, 7 Huang, H.: AC-TuM-12, **6** Hwang, J.: AC-TuM-10, **6**; AC-TuM-12, 6 Bold page numbers indicate presenter

## — I —

Irmscher, K.: AC-MoM-8, 2 Isaacs-Smith, T.: EP1-WeM-4, 8 Islam, A.: EP1-WeM-7, 8 Ivády, V.: AC-MoM-8, 2

## — J —

Jena, D.: AC-MoP-9, 4 Jesenovec, J.: AC-MoP-10, 5; AC-MoP-6, 4; AC-MoP-8, 4 Jiang, K.: AC-TuM-14, 6 Jinno, R.: AC-MoP-9, 4

## -K-

Kahler, R.: EP1-WeM-7, 8 Kilic, U.: AC-MoP-3, 3 Knight, S.: AC-MoP-8, 2; AC-MoP-4, 3; AC-MoP-9, 4 Knudtson, J.: AC-MoP-9, 4 Koeppe, N.: AC-MoP-3, 3 Korlacki, R.: AC-MoM-8, 2; AC-MoP-2, 3; AC-MoP-3, 3; AC-MoP-9, 4 Krishnamoorthy, S.: AC-MoM-7, 2; AC-MoP-10, 5; EP1-WeM-8, 8 Kuehne, P.: AC-MoM-8, 2 Kühne, P.: AC-MoP-4, 3 Kuramata, A.: AC-TuM-15, 7

Laccheb, M.: AC-MOP-7, 4 Lawson, J.: EP1-WeM-4, 8 Lee, H.: EP1-WeM-7, 8 Leedy, K.: EP1-WeM-7, 8 Levin, A.: AC-MoM-7, 2 Li, J.: AC-MoP-1, 3 Liddy, K.: EP1-WeM-7, 8 Lubin, C.: AC-MoP-7, 4

Mahadik, N.: AC-TuM-15, **7** Mauze, A.: AC-MoP-9, 4 Mazumder, B.: AC-TuM-13, **6** McCloy, J.: AC-MoP-10, 5; AC-MoP-6, 4; AC-MoP-8, 4 McCluskey, M.: AC-MOP-6, 4; AC-MoP-8, 4 McGlone, J.: AC-MOM-5, 2 Meng, L.: AC-TuM-13, 6 Merrett, N.: EP1-WeM-5, 2 Mock, A.: AC-MoP-9, 4 Mou, S.: AC-MoP-9, 4 Mou, S.: AC-MoP-1, 3; AC-MoP-12, 5; AC-MOP-7, 4; EP1-WeM-7, 8 Mu, S.: AC-MoM-8, 2

— M -

Oshima, Y.: AC-MoP-9, 4

Pancotti, A.: AC-MoP-7, 4 Park, A.: AC-TuM-14, 6 Popp, A.: EP1-WeM-5, 8; EP1-WeM-7, 8

— P

Porter, L.: AC-TuM-14, 6 Protasenko, V.: AC-MoP-12, 5

## — R —

Ranga, P.: AC-MoM-7, 2; AC-MoP-10, 5; EP1-WeM-8, 8 Remple, C.: AC-MoP-6, **4**; AC-MoP-8, 4 Richter, S.: AC-MoM-8, 2; AC-MoP-4, 3; AC-MoP-9, 4 Ringel, S.: AC-MoM-5, **2** Rivera, J.: AC-MoP-3, 3 Roy, S.: EP1-WeM-8, 8

## — S —

Sardar, A.: EP1-WeM-4, 8 Sarker, J.: AC-TuM-13, 6 Sasaki, K.: AC-TuM-15, 7 Scarpulla, M.: AC-MoM-7, 2; AC-MoP-10, 5 Schubert, M.: AC-MoM-8, 2; AC-MoP-2, 3; AC-MoP-3, 3; AC-MoP-4, 3; AC-MoP-9, 4 Senckowski, A.: AC-MoM-5, 2; AC-TuM-12, 6 Sensale-Rodriguez, B.: AC-MoP-10, 5 Sepelak, N.: EP1-WeM-7, 8 Sharma, S.: AC-MoM-5, 2 Singisetti, U.: AC-MoM-5, 2 Slocum, M.: AC-MoP-12, 5 Snyder, D.: AC-MoP-5, 4 Soukiassian, P.: AC-MoP-7, 4 Speck, J.: AC-MoP-9, 4 Stanishev, V.: AC-MoM-8, 2 Stokey, M.: AC-MoM-8, 2; AC-MoP-2, 3; AC-MoP-3, 3; AC-MoP-9, 4

**— T —** Tadjer, M.: AC-TuM-15, 7 Tang, J.: AC-TuM-14, **6** Tetlak, S.: AC-MoP-12, 5 Tetzner, K.: EP1-WeM-5, **8** 

Thompson, M.: AC-MoP-12, 5; EP1-WeM-7, 8 Traouli, Y.: AC-MoP-3, 3

— V —

Van de Walle, C.: AC-MoM-8, 2

Wang, W.: EP1-WeM-7, 8 Weber, M.: AC-MOP-8, 4 William, J.: EP1-WeM-7, 8 Williams, E.: AC-MoP-3, **3** Wong, M.: AC-MoM-5, 2; AC-MoP-1, 3; AC-TuM-12, 6 Würfl, J.: EP1-WeM-5, 8

— X —

Xing, H.: AC-MoP-9, 4

— Y —

Yang, H.: AC-MoM-7, 2

Zhang, Y.: AC-MoP-9, 4 Zhao, H.: AC-TuM-13, 6 Zhu, W.: EP1-WeM-7, 8