Program Overview

Room /Time	Jefferson 2-3
MoA	TM-MoA: Characterization & Modelling II

Theory, Modeling and Simulation
Room Jefferson 2-3 - Session TM-MoA
Characterization & Modelling II

Moderator: Mike Thompson, Cornell University

3:45pm **TM-MoA-9 Transport, Doping, and Defects in β-Ga_2O_3**, ***Adam Neal,*** Air Force Research Laboratory, Materials and Manufacturing Directorate, USA **INVITED**

The first reports of Ga_2O_3 MESFETs and MOSFETs by the group of Higashiwaki demonstrated the potential of β-Ga_2O_3 for high breakdown voltage, low on-resistance power electronics due to its ultra-wide bandgap and large breakdown electric field. Realizing that potential requires development of high-quality β-Ga_2O_3 material, best guided by an understanding of the electronic transport properties which directly correlate to device performance. In this talk, through a combination of temperature dependent Hall effect and admittance spectroscopy measurements, I will begin by presenting our work characterizing electrically active defects which may ultimately limit the maximally achievable breakdown voltages in Ga_2O_3 devices. Following that, I will present analysis of transport in plasma-MBE grown β-Ga_2O_3 produced at Air Force Research Laboratory, towards understanding the contributions of various scattering mechanisms limiting the electron mobility in our films. Informed by transport studies such as these, material growers and device engineers can continue to push β-Ga_2O_3 to the limits of its performance.

4:15pm **TM-MoA-11 Structural Changes to Beta Gallium Oxide from Ion Irradiation Damage: Model and Relation to in-Situ Experiments**, ***Alexander Petkov,*** *D. Cherns, D. Liu,* University of Bristol, UK*; W. Chen, M. Li,* Argonne National Laboratory, USA*; J. Blevins,* Air Force Research Laboratory, USA*; V. Gambin,* Northrop Grumman*; M. Kuball,* University of Bristol, UK

A good radiation hardness of Ga_2O_3 has been suggested, though its susceptibility to radiation damage is higher than in GaN. To better assess gallium oxide device reliability for nuclear and space applications, more understanding of the structural changes in the material as a result of irradiation is needed. We propose a model for the structural deformation of beta gallium oxide under ion irradiation. Assuming displacements confined primarily to the Ga-atom sublattice, we explain the main features of TEM diffraction patterns from in-situ irradiated gallium oxide using 400 eV Ar ions of fluence 4 x 10^{15} cm^{-1} (equivalent to 2 displacements per atom) (Fig. 1). We propose that displacements of gallium atoms are confined between close-packed O-atom layers (which in beta gallium oxide exist parallel to the (101), (-201), (-3-10), (-310) planes) with a preference for octahedral interstitial positions and recombination. We thus demonstrate the anisotropic evolution of the octahedral-to-tetrahedral Ga-site ratio in the irradiated gallium oxide as a function of displacements per atom, finding it to increase the most along the [-3-10] direction and the least along the [-201] (Fig. 2). The similarity of the structure post irradiation with that of kappa and alpha gallium oxide is examined. We conclude that while the structure post irradiation shares some features similar to kappa gallium oxide (specifically the octahedral-to-tetrahedral site ratio), ion irradiation does not cause a phase transition of beta gallium oxide into kappa as previously thought (Fig. 3).

The authors gratefully acknowledge the NSUF funding (#1393) for beamtime at Argonne IVEM-Tandem User Facility. The authors also thank Mr Peter Baldo (ANL, USA) for dedication on the operation of the ion accelerator during the experiment.

4:30pm **TM-MoA-12 Band Structure Across κ-$(In_xGa_{1-x})_2O_3$/κ-$(Al_yGa_{1-y})_2O_3$ Thin Film Interfaces**, ***Ingvild Julie Thue Jensen,*** *A. Thøgersen, E. Fertitta, B. Belle,* SINTEF Materials Physics, Norway*; A. Langørgen, S. Cooil, Y. Hommedal, Ø. Prytz, J. Wells, L. Vines,* University of Oslo, Norway*; H. von Wenckstern,* University of Leipzig, Germany

Ga_2O_3 is a candidate for development of power electronics components that are faster, smaller and more energy efficient than Si-based technology, permitting devices capable of operating at higher voltages, frequencies and temperatures.[1] The κ-phase of Ga_2O_3 (sometimes labeled ε-phase) is a meta-stable orthorhombic phase where large spontaneous polarization has been predicted by density functional theory.[2] By partial substitution of Ga by In or Al, the original bandgap (~4.9 eV) can be decreased or increased, in principle within the range spanned by the bandgaps of In_2O_3 (2.9 eV) and Al_2O_3 (8.8 eV).This provides a wide parameter space for device development through tailoring of properties such as bandgaps and band offsets. It is believed that interface-localized two-dimensional electron gas (2DEG) may be achieved within this materials system, which opens for potential applications in *so-called* high-electron-mobility transistors (HEMTs).

In the present work the band structure of thin film κ-$(In_xGa_{1-x})_2O_3$/κ-$(Al_yGa_{1-y})_2O_3$ heterostructures are investigated experimentally to evaluate if formation of 2DEG can be within reach. Samples with a selection of *x* and *y* compositions were fabricated by Pulsed Laser Deposition (PLD) on sapphire substrates. Both synchrotron and in-house X-ray Photoelectron Spectroscopy (XPS) were used to investigate the position of the valence band edges relative to the Fermi level in the heterostructure layers and corresponding reference samples. Extraction of valence band maxima from XPS was aided by Density functional theory (DFT) calculations. Local bandgap information was provided by Scanning Transmission Electron Microscope Electron Energy Loss Spectroscopy (STEM EELS), which can determine wide bandgaps with a spatial resolution < 10 nm. Valence band offsets across the heterojunctions were obtained by XPS and combined with bandgap information to find the corresponding conduction band offsets and provide a comprehensive overview of band discontinuities across κ-$(In_xGa_{1-x})_2O_3$/κ-$(Al_yGa_{1-y})_2O_3$ interfaces.

[1] F. Iacopi, M. Van Hove, M. Charles and K. Endo. MRS Bulletin 40 (2015) 390

[2] M.B. Maccioni and V. Fiorentini, Appl. Phys. Express 9 **(2016)** 041102, S.B. Cho and R. Mishra, Appl. Phys. Lett. 112 **(2018)** 162101, J. Kim, D. Tahara, Y. Miura and B.G. Kim Appl. Phys. Express 11 **(2018)** 061101

4:45pm **TM-MoA-13 Aluminum Incorporation Striations in (-201) β-$(Al_xGa_{1-x})_2O_3$ Films Grown on C-Plane and Miscut Sapphire Substrates**, ***Kenny Huynh,*** *Y. Wang, M. Liao,* University of California Los Angeles*; P. Ranga,* University of Utah*; S. Krishnamoorthy,* University of California at Santa Barbara*; M. Goorsky,* University of California, Los Angeles

High aluminum content striations were observed in (-201) $(Al_xGa_{1-x})_2O_3$ thin films (~500 nm) grown on (0001) and 6° miscut (0001) sapphire substrates. A modulated Al composition structure was observed whose orientation depended on the substrate miscut. High resolution x-ray diffraction (XRD) and transmission electron microscopy (TEM) were used to investigate the structural and chemical properties of the $(Al_xGa_{1-x})_2O_3$ films (with 0<x<0.3) and the in-plane relationship with the underlying sapphire substrate. (-201) $(Al_xGa_{1-x})_2O_3$ films were grown by metalorganic vapor phase epitaxy and the Al composition was controlled by tuning the ratio of trimethylaluminum to triethylgallium flow. The growth was carried out at a substrate temperature of 810 °C and a reduced growth pressure of 15 Torr to minimize Al precursor prereactions.

Scanning transmission electron microscopy measurements (sensitive to Z-contrast) reveal alternating layers of high and low contrasting features throughout the $(Al_xGa_{1-x})_2O_3$ film. In conjunction with energy dispersive spectroscopy, the striations are identified as regions of high Al content. In the films that were grown on c-plane sapphire, the high Al content striations run parallel to the (-201) surface. However, in the case of the 6° miscut sapphire substrates, the high Al content striations are oriented about 8-10° from the surface. In addition, the average period of the striations is smaller with higher Al content ranging from 25 to 7 nm periods for x = 0.04 and x = 0.3 respectively.

XRD (-401) pole figures were measured for $(Al_xGa_{1-x})_2O_3$ films (with 0<x<0.3) and a commercially available (-201) β-Ga_2O_3 substrate as a reference. XRD (-401) pole figure for the (-201) β-Ga_2O_3 reference substrate shows both (-401) at χ = ~23° and (-400), at χ = ~50° (the 2θ angle difference is less than 0.5°) with no symmetry. However, the pole figures from the $(Al_xGa_{1-x})_2O_3$ thin films grown on sapphire (0<x<0.3) all show six-fold symmetry for both (-401) and (-400). We believe the six-fold symmetry is a result of three sets of twins (120° away from each other), plus the existence of anti-parallel domains (0° and 180° pairs). On the other hand, additional 12 spots at χ = ~58° were observed in the $(Al_xGa_{1-x})_2O_3$ films on sapphire. These do not

correspond to any planes with (-201) surface orientation, suggesting grains with different orientation exist. We speculate that the anisotropy of the monoclinic structures, the surface energy differences associated with the miscut substrate, and step edge features impact the formation of the composition striations.

5:00pm **TM-MoA-14 Plasmon-phonon Coupling in Electrostatically Gated *β*-Ga_2O_3 Films with Mobility Exceeding 200 $cm^2V^{-1}s^{-1}$**, *A. Rajapitamahuni, A. Manjeshwar,* University of Minnesota, USA*; A. Kumar, A. Datta,* University at Buffalo*; P. Ranga,* University of California Santa Barbara*; L. Thoutam,* SR University, Warangal, India*; S. Krishnamoorthy,* University of California Santa Barbara*; **Uttam Singisetti,*** University at Buffalo*; B. Jalan,* University of Minnesota, USA

Monoclinic β-Ga_2O_3, an ultrawide-bandgap semiconductor, has seen enormous activity in recent years. However, the fundamental study of the plasmon-phonon coupling that dictates electron transport properties has not been possible due to the difficulty in achieving higher carrier density (without introducing chemical disorder). In this talk, we present a highly reversible, electrostatic doping of β-Ga_2O_3 films with tunable carrier densities using ion-gel-gated electrical double layer transistor configuration. Combining temperature dependent Hall effect measurements, transport modeling and comprehensive mobility calculations using ab-initio based electron-phonon scattering rates, we demonstrate an increase in the room-temperature mobility to 201 $cm^2V^{-1}s^{-1}$ followed by a surprising decrease with an increasing carrier density is due to the plasmon-phonon coupling. The modeling and experimental data further reveal an important “anti-screening” (of electron-phonon interaction) effect arising from dynamic screening from the hybrid plasmon-phonon modes. Our calculations show that a significantly higher room-temperature mobilities of 300 $cm^2V^{-1}s^{-1}$ is possible if high electron densities (> 10^{20} cm-3) with plasmon energies surpassing highest energy LO mode can be realized. As Ga_2O_3 and other polar semiconductors play an important role in several device applications, the fundamental understanding of the plasmon-phonon coupling can pave the way to enhance the mobility by harnessing the dynamic screening of the electron-phonon interactions.

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