Program Overview

Room /Time	Jefferson 2-3
TuM	AC-TuM: Advanced Characterization & Microscopy

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 β-Ga_2O_3*, 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 β-Ga_2O_3. 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 interstitial-divacancy complexes in β-Ga_2O_3 and planar defects and phase transition in $(Al_xGa_{1-x})_2O_3$ 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_2O_3 (edge-defined, film-fed (EFG)-grown (001) β-Ga_2O_3 substrate) as a function of Si dose, using a combination of STEM and secondary ion mass spectrometry (SIMS). Peak Si concentrations of 10^{18}-10^{21} cm^{-3} were investigated. Different types of point defects and their complexes were observed in lower Si concentrations (< ~ 10^{19} cm^{-3}), 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^{-3}), the structure tends to transform into different Ga_2O_3 phases, including γ-Ga_2O_3 which, according to our previous investigation, has a close relationship to the extended defects in *β*-Ga_2O_3. 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_2O_3 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) $(Al_xGa_{1-x})_2O_3$ 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

$(Al_xGa_{1-x})_2O_3$ 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 $(Al_xGa_{1-x})_2O_3$ varies with growth orientation. While (010)–$(Al_xGa_{1-x})_2O_3$ is single β–phase stable till 27% Al, (-201) and (100)–$(Al_xGa_{1-x})_2O_3$ 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)–$(Al_xGa_{1-x})_2O_3$ varying Al composition was probed. From the in-plane lateral Al/O distribution, $(Al_xGa_{1-x})_2O_3$ layers with 20% Al are found to be homogeneous in (100), (-201) and (010) orientation while $(Al_xGa_{1-x})_2O_3$ 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)–$(Al_xGa_{1-x})_2O_3$ films varying Al content. The observed APT spectroscopy result reveals that the bond length of Ga–O and Al–O changes as the $(Al_xGa_{1-x})_2O_3$ 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%.

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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 κ-Ga_2O_3 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_2O_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_2O_3, namely trigonal α (corundum structure), monoclinic β, orthorhombic κ, and cubic γ (cation deficient spinel structure) phases. Of those four polymorphs, β-Ga_2O_3 has been the most investigated, as this phase is the thermodynamically stable phase from room temperature to the melting point at atmospheric pressure[1-2]. However, the lower symmetry of β-Ga_2O_3 results in anisotropic optical and electronic properties. Compared with β-Ga_2O_3, κ-Ga_2O_3 has higher symmetry and some unique properties. κ-Ga_2O_3 shows spontaneous polarization (Psp) parallel to the c-axis and thus a high-density two-dimensional electron gas can be formed at the interface without doping. The reported values of Psp are 0.23 C/m^2 [3] and 0.242 C/m^2 [4], respectively, which are about an order of magnitude higher than those of GaN and AlN. In this study, nominally phase pure κ-Ga_2O_3 films were successfully grown on vicinal c-plane sapphire (0.15° offcut toward m-plane) by low-pressure metal-organic chemical vapor deposition[5]. 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_2O_3 film grown under optimum conditions revealed the pseudomorphic growth of 3-4 monolayers of α-Ga_2O_3 at the interface, followed by a 20-60 nm transition layer containing a mixture of β- and γ-Ga_2O_3 which was covered by an ~700 nm-thick layer of phase-pure κ-Ga_2O_3. 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 ~100% κ-Ga_2O_3 and ~100% β-Ga_2O_3, depending on the growth temperature and the growth rate. XRD ϕ scans showed in-plane epitaxial relationships and the presence of the three rotational domains in the κ-Ga_2O_3. 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 κ-Ga_2O_3; whereas the β-phase is favored at higher growth temperatures and lower growth rates.

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 (β-Ga_2O_3) 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_2O_3 devices. Investigation of extended defects over large diameter Ga_2O_3 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_2O_3 wafers with 10µm 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_1 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 ~$3x10^3$ cm^{-2}. 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 micro-structure and dislocation analysis will be presented on the extended defects observed in the multiple XRT images.

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