Advanced Characterization Techniques
Room Bansal Atrium - Session AC-TuP

Advanced Characterization Techniques Poster Session II

AC-TuP-1 Photoluminescence Spectroscopy of Cr^{3+} in β-Ga_2O_3 and $(Al_{0.1}Ga_{0.9})_2O_3$, ***Cassandra Remple,*** Materials Science & Engineering Program, Washington State University*; L. Barmore,* Dept. of Physics and Astronomy, Washington State University*; J. Jesenovec, J. McCloy,* Institute of Materials Research, Materials Science & Engineering Program, Washington State University*; M. McCluskey,* Dept. of Physics and Astronomy, Washington State University

Alloying β-Ga_2O_3 with Al_2O_3 to create $(Al_xGa_{1-x})_2O_3$ enables ultra-wide bandgap material suitable for applications deep into the ultraviolet. In this work, photoluminescence (PL) spectra of Cr^{3+} were investigated in monoclinic single crystal β-Ga_2O_3:Cr, and 10 mol.% Al_2O_3 alloyed with β-Ga_2O_3, denoted β-$(Al_{0.1}Ga_{0.9})_2O_3$ or AGO. Temperature-dependent PL properties were studied for Cr^{3+} in AGO and β-Ga_2O_3 from 295 K to 16 K. For both materials at room temperature, the red-line emission doublet R_1 and R_2 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). The linewidths for AGO are larger for all temperatures due to alloy broadening. For both materials, the *R*-lines blue-shift with decreasing temperature. The (lowest energy) R_1 line is dominant at low temperatures due to the thermal population of the levels. For temperatures above ~50 K, however, the ratio of R_2 to R_1 peak areas is dominated by nonradiative combination. Additionally, Hall data was taken at low and elevated temperatures which demonstrated n-type behavior.

AC-TuP-2 Determining the Effects of Traps on the Effective Mobility of β-Ga_2O_3 MOSFETs using the Split C-V Method in Dark and Illumination Conditions and Pulsed I-V*,* ***Ory Maimon,*** George Mason University*; N. Moser,* Air Force Research Lab*; D. Chamria,* Colgate University*; K. Liddy, A. Green, K. Chabak,* Air Force Research Lab*; S. Pookpanratana, P. Shrestha,* National Institute of Standards and Technology (NIST)*; Q. Li,* George Mason University

Beta-gallium oxide (β-Ga_2O_3) high power and RF device performance is rapidly increasing due to the improved growth and fabrication methods developed in the last few years. Investigation of traps at and near the β-Ga_2O_3 and gate dielectric interface is critical for improving reliability and performance of β-Ga_2O_3 MOSFETs. Trap state energies can vary in the β-Ga_2O_3 bandgap, and their occupation can change with device bias. The trap states can also act as scattering sites, reducing the mobility. Here, we report on a study of effective mobility degradation due to traps at the Al_2O_3/β-Ga_2O_3 interface in lateral depletion-mode β-Ga_2O_3 MOSFETs using the split C-V method in dark and illumination conditions with wavelengths from 730 nm (1.7 eV) to 265 nm (4.7 eV) and pulsed I-V is used to further characterize the traps

The MOSFETs are fabricated on a (010) semi-insulating β-Ga_2O_3 substrate. A 50 nm Si-doped epi layer is grown as the channel with a target doping concentration of 2.4 x 10^{18} cm^{-3}. The ohmic contacts are formed using a Ti/Al/Ni/Au metal stack and annealed at 470 °C for 1 min in nitrogen. A 20 nm Al_2O_{-3} gate dielectric is deposited using plasma-assisted atomic layer deposition (PE-ALD). The transistors are fabricated with a constant L_G and L_{GS} of 2 µm and 0.5 µm, respectively, while L_{GD} varies between 0.5 µm, 5.5 µm, and 10.5 µm. Most FETs have a threshold voltage of -4 V, good linearity, and I_{ON}/I_{OFF} ratios between $10^7 – 10^9$.

A D_{it} of 3 x 10^{11} eV^{-1} cm^{-2} up to 0.44 eV below the conduction band is determined using the conductance method. Using illumination gives deep trap concentrations 1.7 eV below the conduction band. We observe little change for wavelengths above 455nm (2.7 eV) but see increasingly larger flatband voltage shifts as wavelength decreases, indicating a larger D_{it} 2.7 eV below the conduction band. We observe an approximate 1.8x increase in the effective mobility under 265nm (4.7 eV), indicating that it is considerably lowered due to filled traps throughout the bandgap. We will present the analysis of the split C-V method in dark and illumination conditions, with a focus on the impact of traps on the mobility, and use pulsed I-V to analyze traps in comparison to the split C-V measurement.

AC-TuP-3 Advanced Characterization Methods for Scale-up and Improvement of β-Ga2O3 Substrates*,* ***Robert Lavelle****, D. Snyder, W. Everson, D. Erdely, L. Lyle, A. Balog, N. Alem,* Penn State University

Advanced characterization methods are required to scale-up and improve the quality and uniformity of β-Ga2O3 substrates. In addition to developing these methods, one of the key challenges is implementing characterization techniques at each stage of processing and combining these data to understand the interdependency of these steps and, ultimately, the impacts on device performance. PSU/ARL is uniquely positioned to help establish this vertically integrated feedback loop based on its β-Ga2O3 substrate processing experience and relationships with crystal and epi growers. PSU/ARL has characterized β-Ga2O3 crystals grown by multiple methods, including edge-defined film-fed growth (EFG) and Czochralski (Cz), and mapped full 2” substrates following chemi-mechanical polishing (CMP). In this poster, we will share these results focused on understanding the quality and uniformity of the substrates as well as advanced characterization methods, such as high-resolution x-ray diffraction (HRXRD) and transmission electron microscopy (TEM), for understanding the impacts of processing on defects and the fundamental material properties of the substrates. In this poster, we will highlight our recent progress on etch pit density (EPD) and defect mapping of full β-Ga2O3 substrates. This includes investigating the propagation of defects such as nanopipes and impacts on epi growth. As part of this work, we have utilized a variety of characterization methods from optical mapping of full 2” substrates to performing TEM of individual defects. We will also discuss how we implemented characterization methods, including HRXRD, white light interferometry (WLI), and atomic force microscopy (AFM), for improving the surface finish and minimizing subsurface damage during CMP of β-Ga2O3 substrates. These advanced characterization methods have been essential in producing high-quality, uniform substrates during the scale-up process. Finally, we will share our recent work on characterizing off-cut/off-axis substrates and different alloy compositions in collaboration with groups focused on researching crystal and epi growth methods.

AC-TuP-4 Vacancies in Electron Irradiated β-Ga_2O_3 Probed with Positrons*,* ***Marc Weber****, C. Halverson,* Washington State University*; B. Dutton, C. Remple,* Washington State University, United States Minor Outlying Islands (the)*; M. McCluskey,* Washington State University, US, United States Minor Outlying Islands (the)*; M. Scarpulla,* University of Utah*; J. McCloy,* Washington State University, United States Minor Outlying Islands (the)

Positron annihilation spectroscopy is a powerful tool to evaluate vacancies and vacancy-related defects. To extract absolute defect concentrations data on reference samples or from other techniques must be available. We have examined bulk grown and epi-layer β-Ga_2O_3 material before and after high dose electron irradiation. Pre-existing and generated defects are probed by depth resolved positron Doppler Broadening and FTIR. Compared to other semiconducting materials, the anisotropic electron momentum distribution of β-Ga_2O_3 poses challenges. Data from samples oriented in the [100], [010], and [001] direction are examined and compared to earlier experiments on oxygen annealed β-Ga_2O_3[1] and recent theoretical work.[2] Subsequent annealing studies will further assist in the identification of the created defects. This work generously supported by the Air Force Office of Scientific Research under award number FA9550-18-1-0507 monitored by Dr. Ali Sayir.

References:

1. “Gallium vacancy formation in oxygen annealed β-Ga_2O_3“, Jesenovec J. et al., J. Applied Physics 129, 245701 (2021).
2. “Split Ga vacancies and the unusually strong anisotropy of positron annihilation spectra in β-Ga_2O_3“, Karjalainen A., et al. Physical Review B 102, 195207 (2020).
3. “Defect identification in complex oxides: Positron annihilation spectroscopy of β-Ga_2O_3 and $SrTiO_3$“, Karjalainen A, PhD thesis, Dept. of Applied Physics, Aalto University, Helsinki, Finland 2021.

AC-TuP-5 Artificial Intelligence Assisted Vacancy Detection via 3D Microscopy in Doped and Undoped Ga_2O_3*,* ***Prachi Garg****, J. Sarker,* Department of Materials Design and Innovation, University at Buffalo*; A. Uddin Bhuiyan, L. Meng,* Department of Electrical and Computer Engineering, The Ohio State University*; H. Zhao,* Department of Electrical and Computer Engineering & Department of Materials Science and Engineering, The Ohio State University*; K. Reyes, B. Mazumder,* Department of Materials Design and Innovation, University at Buffalo

Recently, gallium oxide (Ga_2O_3) has attracted attention in high-power electronics and Schottky barrier diodes, due to their wide bandgap of ~4.8eV and critical breakdown strength of ~8 MV/cm. However, the low electron mobility of Ga_2O_3 makes it crucial to dope with group IV elements (Si, Sn or Ge) in order to achieve desired electrical conductivity. This dopant incorporation in Ga_2O_3 contributes to the formation of Ga vacancies. While the inherent O vacancies in Ga_2O_3 does not contribute to the electrical conductivity, the formation of Ga vacancies upon doping tends to trap the dopant atoms resulting in charge compensation effect in the material. To further improve semiconductor properties, defects like vacancies are introduced in a controlled manner, which have significant effect on its optical/charge transfer properties. Therefore, identifying and detecting these cationic vacancies are impactful for transport properties, however it is very challenging to detect vacancies from an atomic perspective using nano-analytical tools. Atom probe tomography (APT) is the only characterization tool that is capable of providing atomic resolution in 3D space. However, the latent features remain hidden in the tool complexities and large dimensional data, making it difficult to detect vacancies and distinguish them from missing atoms using APT alone. In this work, we developed a unique approach by integrating artificial intelligence with microscopic data to map the vacancy position in real atom probe data. Here, we applied a deep learning model named U-net for vacancy extraction on the 3D microscopic APT data. U-net is the image segmentation model which works in an end-to-end setting. A raw image is fed to the model, that goes within carefully tuned architecture and results in a segmented image i.e. feature map in this case. This model is trained on the synthetically generated Ga_2O_3 structure using MD simulation software named LAMMPS (Large scale Atomic/Molecular Massively Parallel Simulator. Large structure is generated and sliced into voxels, fed into U-net model to train it on vacancy identification in each slice. Once the U-net model is trained, we use the APT data, slice it and feed into the model to detect the vacancies in real dataset. The trained U-net model will automatically analyze the APT data to learn and predict the local structure including vacancies to understand the vacancy distribution in doped and undoped Ga_2O_3 structure. This work will provide an advancement in understanding the effect of Ga vacancies in Ga_2O_3. This work can also be expanded to study similar materials systems for developing future high-power transistors and optical devices.

AC-TuP-6 Silicon Ion Implantation in β-Ga_2O_3: Effect of Temperature on Atomic Damage and Recovery, ***Naomi Pieczulewski***, *K. Gann,* Cornell University*; T. Asel, B. Noesges,* Air Force Research Laboratory*; K. Heinselman,* National Renewable Energy Laboratory*; M. Thompson, D. Muller,* Cornell University

Si implantation is a promising strategy to reduce contact resistance and improve Ga_2O_3 device performance.[1] Recent reports have shown a variety of phase transformations into Ga_2O_3 polymorphs from the β phase upon ion implantation.[2,3] Previously our group has found that by using high angle annular dark field (HAADF) and annular bright field (ABF) scanning transmission electron microscopy (STEM) imaging, we can accurately identify γ-phase of Ga_2O_3.[4] Here, we present a systematic study of high Si implant doses over a range of implant temperatures from liquid nitrogen temperature to 600°C to investigate the limits of damage recovery. We found that the kinetically favored defect structure is γ- Ga_2O_3 under the investigated implant conditions and the implanted films retain β-Ga_2O_3 resulting in fast and clean recovery.

MBE grown UID β-Ga_2O_3 [010] film was implanted with Si over a 100nm profile targeting a total carrier concentration of $5x10^{19}$ to $1x10^{20}cm^{-3}$. The implanted films were characterized by STEM to probe defects at the atomic scale, supplemented by X-ray diffraction (XRD) and Rutherford Back Scattering (RBS). We observe implantations performed at both room temperature and low temperature cause a phase transformation into γ-Ga_2O_3 as well as interstitial Ga defects in β-Ga_2O_3, but also retain significant β-Ga_2O_3. Crystallinity in the low temperature implant indicate significant dynamic annealing either during implantation or during warming back to room temperature. Implantation performed at a high temperature shows significantly less lattice damage and retains complete β-Ga_2O_3. Thermal activation by post-annealing heat treatment is required on all samples to electrically activate carriers.

Finally, lattice recovery and Si activation was investigated after annealing the Si implanted films at 950°C for 20 minutes under high purity nitrogen. Carrier activation was observed in the control implant starting only after a couple minutes, indicating the retained β-Ga_2O_3 enables fast recrystallization into recovered film.All films showed good recovery and significant dopant activation, indicating the limits of damage recovery can be still pushed.

Citations:

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2. Alexander Azarov et al. Phys. Rev. Lett. 2022, **128**, 015704
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AC-TuP-8 Kinetics of Compensation in Sn-doped Ga_2O_3 During O_2 Annealing Revealed by FTIR and Modelling*, J. High, H. Yang, N. Rock,* ***Mike Scarpulla,*** University of Utah

It is well known that annealing n-type doped β-Ga2O3 in air or O_2 produces insulating surface layers on the micron scale; however the microscopic mechanisms remain a mystery. Besides the identity of the defects involved, the locations of generation and transport are unknown.

At this time, V_{Ga}, V_O and their complexes are believed to be the dominant stable native defects but the mechanisms of their formation are unknown. Do V_{Ga} form at structural defects and interfaces then diffuse to permeate the material, or do Frenkel pairs nucleate homogeneously and the Ga_i diffuse away to sinks? How is the information about oxygen richness imposed transmitted from the surfaces inwards to the bulk; do O_i play any transient role in mediating these processes? Such details still have not been addressed, and can not be distinguished by their effects on net charge alone; some orthogonal data such as formation or migration barriers must also constrain hypotheses in order to determine the most likely.

We have been utilizing FTIR transmission through wafers approximately 500 µm thick to reveal the kinetics of the conducting-to-insulating transition during annealing. In thick samples, a mechanism with diffusion constant many orders of magnitude faster than that found near the surface (up to ~ 1 µm) using electrical methods would be required. Put more concretely, if only the previously-determined mechanism is present, the insulating transition would take centuries in wafers while only days to weeks are required near 1000 °C in pure O_2.

We developed a coupled defect diffusion, carrier density, dielectric function, multilayer optics model of the samples with which we can test hypotheses for the kinetics of compensating defect formation and transport. Our model spans from the bandgap near 5 eV to the limiting 2-phonon absorption at 1500 cm^{-1} and, after inclusion of POP phonon-limited momentum scattering lifetime in the Drude component, reproduces the data extremely well. With this level of modelling, we show with high confidence that at least two diffusion-mediated processes are required to reproduce the data. We review possible mechanisms and provide evidence on the kinetic barriers for what is presumably a native defect driven process. Fortunately, the fidelity and predictiveness of computations of defect energetics and migration barriers now allow differentiation between possible mechanisms; we hope that these experiments will motivate detailed studies to uncover the detailed mechanisms of defect processes in Ga_2O_3 and beyond.

AC-TuP-9 Cation Vacancy and Dopant Diffusion in β-Ga2O3*,* ***Nathan David Rock****, A. Levin,* University of Utah*; A. Bhattacharyya,* University of California Santa Barbara*; H. Yang, B. Eisner,* University of Utah*; S. Krishnamoorthy,* University of California Santa Barbara*; M. Scarpulla,* University of Utah

Mechanistic understanding of native and impurity defect diffusion and reaction processes in Ga2O3 is necessary for advanced fabrication of devices and for the long-term reliable operation of those devices.The diffusion of native and impurity atoms and their incorporation into various point defects and complexes is mediated by native defects.Thus, understanding the diffusion of native defects is fundamental to understanding all diffusion processes.Unlike impurities, vacancies are difficult to study because of the difficulty of measuring their concentration.Additionally, the mechanisms of formation of native defects are unknown; for example, cation vacancies may be introduced at surfaces and diffuse inwards, or interstitial-vacancy pairs may form in the bulk with interstitials diffusing outwards.

We introduced superlattices (SLs) of alternating $(Al,Ga)_2O_3/Ga_2O_3$ grown by OMVPE in order to make visible the flux of cation vacancies using Al as a tracer.We demonstrate that in the case of SLs grown on Sn-doped substrates, the diffusion of Al is mediated by the transient diffusion of a large concentration of mediating defects (presumed to be VGa or complexes thereof) from the substrate into the epilayers.This results in faster diffusion near the Sn-doped substrate and slower near the free surface indicating that the introduction of VGa from the free surface is insignificant at the at% level compared to the supply in the substrate.In the case of SLs grown on Fe-doped substates, the diffusion of Al is much slower and spatially-uniform indicating a uniform density of meditating defects vs depth.Additionally, we document the co-diffusion of Sn and Fe out of the substrates and through the SLs – this implies that VGa is not diffusing alone but rather as complexes or with high-correlation with Fe or Sn.This implies that the rates measured are not those of the VGa itself but rather a slowed rate from the mutual effects of solute drag.The role of oxygen is also investigated – annealing in O2 is generally needed for dopants to diffuse, however the role of O in the diffusion of pre-existing VGa in the substrate is not clear.In addition to the model of vacancy-mediated diffusion introduced last year, we also report on coupled drift-diffusion-reaction-Poisson models for simultaneous diffusion of V_{Ga}, Sn, and Fe.We also have documented the presence and diffusion of various other impurities which has implications for device stability.We estimate the contributions of chemical and electrical potential gradients (e.g. surface fields and dopant concentration steps) in the mass transport.

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