PCSI

Room Redondo - Session PCSI-MoA1

Semiconductor Discovery/Interface/Surface Characterization

Moderator: Dorothee Sophie Rosenzweig, Technische Universität Berlin

2:00pm **PCSI-MoA1-1 (Al,Gd)N as a Novel Material for Neutron Detection: Materials Discovery and Interface Design**, ***Nancy Haegel,*** National Renewable Energy Laboratory **INVITED**

Ultra-wide bandgap nitrides, with their exceptional optoelectronic and charge transport properties, have already delivered transformative impact for light emitting diodes ((Al,Ga)N) and cell phone resonators ((Al,Sc)N), with potential for future impact for power electronics, sensors, and other optoelectronic/magnetic applications. This class of pseudo-binary alloys and ternary nitrides is rapidly expanding due to advances in high-throughput computational discovery and non-equilibrium synthesis [1]. In this work, Al1-xGdxN alloys have been synthesized and characterized [2]. These new materials offer exciting integration opportunities for thin film devices leveraging significant concentration of the ferromagnetic and strongly neutron absorbing 157Gd constituent in an AlN wide bandgap host.

Metastable Al1-xGdxN alloys have been synthesized using non-equilibrium combinatorial thin film deposition via radio frequency co-sputtering. First-principles calculations show that the limiting critical composition for a wurtzite to rocksalt phase transition is xc = 0.82. However, theory also suggests that at temperatures below 1000 K there is a large miscibility gap limiting Gd incorporation in AlN to only a few percent. By higher effective temperature through non-equilibrium growth we have achieved the highest Gd3+ incorporation into the wurtzite phase reported to date. Single-phase compositions up to x ≈ 0.25 are confirmed by high resolution synchrotron grazing incidence wide angle X-ray scattering and transmission electron microscopy.

Integration of these materials into devices will require electrical contact functionality and interface control. We will discuss needs and opportunities for detailed understanding and synthesis control strategies at incommensurate interfaces between rocksalt and wurtzite structures for device integration.

[1] S.R. Bauers et. al., "Ternary nitride semiconductors in the rocksalt crystal structure," Proc. of the National Academy of Sciences, 116, 14829-14834, 2019.

[2] R.W. Smaha, K. Yazawa et al., "Prediction and Synthesis of Gd-rich Al1−xGdxN Alloys," DOI:10.26434/chemrxiv-2022-k32j0

2:40pm **PCSI-MoA1-9 Surface Calibrated Electron Holography: Anomalous Strain Relaxation and Minimization of Polarization Changes at III-Nitride Hetero-Interfaces**, ***Michael Schnedler,*** *Y. Wang, Q. Lan, F. Zheng, L. Freter, Y. Lu, U. Breuer,* Forschungszentrum Jülich GmbH, Germany*; H. Eisele,* Otto-von-Guericke-Universität Magdeburg, Germany*; J. Carlin, R. Butté, N. Grandjean,* EPFL, Switzerland*; R. Dunin-Borkowski, P. Ebert,* Forschungszentrum Jülich GmbH, Germany

Polarization and electron affinity changes at $Al_{0.06}Ga_{0.94}N$/GaN and $In_{0.05}Ga_{0.95}N$/ $Al_{0.06}Ga_{0.94}N$ interfaces are quantified by off-axis electron holography (EH) in transmission electron microscopy (TEM), in conjunction with scanning tunneling microscopy and spectroscopy, as well as self-consistent simulations of the electrostatic potential and electron phase maps. The central problem of quantitative EH is that at the surfaces of the thin TEM lamellae a defect-induced pinning occurs, which alters the phase contrast. Therefore, we calibrated the electron optical phase maps using a d-doped layer at the GaN buffer/substrate interface by determining the energy of the pinning level at the surface to 0.69 eV above the VBM (consistent with pinning by nitrogen vacancies). The such calibrated EH provides quantification of the key interface properties: The biaxially relaxed $In_{0.05}Ga_{0.95}N$/ $Al_{0.06}Ga_{0.94}N$ interface exhibits polarization and electron affinity changes as theoretically expected. However, at the $Al_{0.06}Ga_{0.94}N$/GaN interface anomalous lattice relaxations and vanishing polarization and electron affinity changes occur, whose underlying physical origin is anticipated to be total energy minimization by the minimization of Coulomb interactions between the polarization-induced interface charges. [1]

[1] Y. Wang *et al.*, Phys. Rev. B **102**, 245304 (2020)

2:45pm **PCSI-MoA1-10 Surface Carrier Density in 2D and 3D Indium Nitride Structures**, ***Fernando Maia de Oliveira,*** *A. V. Kuchuk,* Institute for Nanoscience and Engineering, University of Arkansas*; C. Romanitan,* National Institute for Research and Development in Microtechnologies, Romania*; H. V. Stanchu,* Institute for Nanoscience and Engineering, University of Arkansas*; M. E. Ware,* Department of Electrical Engineering, University of Arkansas*; Y. Mazur, G. J. Salamo,* Institute for Nanoscience and Engineering, University of Arkansas

Narrow-bandgap materials have gained increased attention due to their great applicability in infrared systems. [1] In particular, indium nitride (InN) offers extraordinary advantages to the industry of ultra-fast high-power electronics due to its high mobility, low effective electron mass, and widely tunable plasmonic activity. But, the challenging fabrication of InN-based devices makes it difficult to explore its benefits. The accumulation of electrons at the surface of indium nitride structures has been previously reported for 2D and 3D materials. However, the control of such charge accumulation using growth parameters is yet to be explored. [2] In this study, we investigate the morphology, structure, and optical features of a series of 2D and 3D InN structures grown using different In/N flux ratios. By evaluating the longitudinal optical phonon-plasmon coupled modes of InN using Raman spectroscopy, we measure the surface carrier concentration increasing from approximately 10^{17} to 10^{18} cm^{-3} as the surface-to-volume ratio decreases. By simulating the InN structures using the k.p method we show that the morphological evolution from 3D to 2D structures modifies the electron occupation near the surface, as shown in Figure 1. Our key finding shows that the charge profile along the InN structure is influenced by its structural features, such as porosity, surface-to-volume ratio, in-plane strain, and roughness of the material by modifying the bending of the conduction and valence bands along the InN material.

2:50pm **PCSI-MoA1-11 Structure and Chemistry of $ZnGeN_2$ Quantum Wells in GaN for use in Green LEDs**, *M. Tellekamp,* National Renewable Energy Laboratory*;* ***Moira Miller,*** Colorado School of Mines*; A. Rice,* National Renewable Energy Laboratory*; D. Diercks,* Colorado School of Mines*; A. Tamboli,* National renewable Energy Laboratory

Hybrid II-IV-N_2/III-N heterostructures, based on current commercialized (In,Ga)N light-emitting diodes (LEDs), are predicted to significantly advance the design space of highly efficient optoelectronics in the visible spectrum, specifically in the green to amber regions where LED efficiencies are orders of magnitude lower than other colors. Yet, there are few epitaxial studies of II-IV-N_2 materials. $ZnGeN_2$, a ternary analogue of GaN, is explored as a potential green-to- amber emitter which can be integrated into existing GaN LED heterostructures due to structural similarity. $ZnGeN_2$ is wurtzite when disordered, and is structurally and electronically similar to GaN, possessing a lattice mismatch of ~0.8%. Previous work by this group has demonstrated epitaxial growth of $ZnGeN_2$ on GaN and AlN via molecular beam epitaxy (MBE) [1-2]. Here we present the growth of abrupt quantum wells (QW) of $ZnGeN_2$ within GaN by nitrogen plasma-assisted MBE, including successful five-layer multiple quantum well (MQW) structures.

Detailed structural and elemental analysis of the heterostructures was performed, including X-ray diffraction (XRD), scanning transmission electron microscopy (STEM), energy dispersive X-ray spectroscopy (STEM-EDS), and atom probe tomography (APT). These methods demonstrate high-quality and abrupt interfaces in the heterostructures after multiple repeating heterointerfaces and some compositional nonidealities in each layer. Through changes in growth methodology, we demonstrated methods to improve unintentional impurities including associated improvements in structural quality. We also investigated conduction band offset using X-ray photoelectron spectroscopy (XPS) in the GaN/$ZnGeN_2$ heterostructures, important for LED design. Together, these data demonstrate both the promise of heteroepitaxially integrated hybrid ternary/binary nitride systems along with the challenges associated with growing such systems, including an outlook on methods to improve the materials and eventual devices.

[1] M. B. Tellekamp et al 2020, Crys. Growth Des. 20, 3, 1868–1875.

[2] M. B. Tellekamp et al 2022, Crys. Growth Des. 22, 2, 1270–1275.

Author Index

Bold page numbers indicate presenter