Novel Materials
Room Swan BC - Session NM-MoM1

Nitrides

Moderator: Bharat Jalan, University of Minnesota

7:45am **NM-MoM1-1 Welcome, Introductions and Sponsor Thank Yous***,*

8:00am **NM-MoM1-2 MBE Growth and Properties of Ultra-wide Bandgap Oxide Layers Spanning 5.0 - 9.0 eV Energy Gaps***, **Debdeep Jena,*** Cornell University **INVITED**

8:30am **NM-MoM1-4 Demonstration of $Sc_{0.2}Al_{0.8}N$ HEMT Structures with a Sheet Resistance of 150 Ω/□ and a Sheet Charge of $5.9x10^{13}$ cm^{-2} with Phase Pure, Metal Rich Growth***, **Zachary Engel,** K. Motoki, W. Doolittle,* Georgia Institute of Technology

ScAlN alloys are of great interest in recent years due to their high spontaneous and piezoelectric polarization and their ferroelectric properties, in addition to the fact that ScAlN is lattice matched to GaN at a composition of ~20% Sc. Due to the immense spontaneous polarization coefficients of the alloy, even in the case of being lattice matched to GaN where piezoelectric polarization will have no effect, a sheet charge as high as ~$6x10^{13}$ cm^{-2}has been predicted in literature due solely to spontaneous polarization. Thanks to these favorable properties, a number of $Sc_xAl_{1-x}N$/GaN HEMT structures have been demonstrated, achieving sheet resistances as low as 167 Ω/□ and mobilities as high as 1556 cm^2/vs most often requiring an AlN interlayer to achieve good performance. However, a number of growth issues have plagued the alloy that must be overcome to achieve the theoretical potential of the system. Previously, ScAlN was deposited via RF sputtering, which often yielded material that was polycrystalline and/or contained a high defect density, degrading device performance. MOCVD films have been grown but the limited volatility of Sc-precursors limits growth rates. In recent years, MBE growth of single phase ScAlN has been demonstrated with high crystal quality, allowing for HEMT properties to be advanced to the excellent metrics listed above. However, a challenge still remains in MBE growth of ScAlN in the form of metal rich growth. In traditional III-Nitride MBE growth, metal rich growth has led to an improvement of crystal quality and both surface and interface roughness. Thus far, attempts to grow ScAlN under metal rich conditions have faced the issue of multiple intermetallic Al_xSc_y phases being thermodynamically stable under metal rich conditions and the phase transition of ScAlN from wurtzite towards rock salt that occurs around 40% Sc, leading to the inclusion of unintended metal and rock salt phases in previous metal rich growth.

$Sc_{0.2}Al_{0.8}N$ high electron mobility transistor (HEMT) structures are grown with a simple two-layer structure and fabricated contacts, demonstrating a sheet resistance (R_s) of 150 Ω/□, a mobility of 700 cm^2/Vs, and a sheet charge of $5.9x10^{13}$ cm^{-2}. To achieve these properties, growth conditions for a metal rich form of molecular beam epitaxy (MBE) called metal modulated epitaxy of $Sc_{0.2}Al_{0.8}N$ growth was explored. While metal-rich MBE has been challenging because it normally leads to mixed wurtzite, rock salt and intermetallic phases, here phase pure, metal rich growth was demonstrated with a x ray diffraction 002 FWHM as low as 229 arcsec and an atomic force microscopy (AFM) RMS roughness as low as 0.8 nm.

8:45am **NM-MoM1-5 Influence of Nucleation Schemes on Crystal Quality of Heteroepitaxial $Sc_{0.4}Al_{0.6}N$***, **Matthew Hardy,** A. Lang, E. Jin, N. Nepal, S. Katzer, V. Wheeler,* U.S. Naval Research Laboratory

$Sc_xAl_{1-x}N$ thin films have attracted significant attention due to their very large piezoresponse for compositions up to $x = 0.43$, recent demonstrations of ferroelectric switching, and potential for improved output power in GaN-based transistors. Maintaining phase-pure and high crystal quality $Sc_xAl_{1-x}N$ at high x is critical to increase resonator bandwidth and to reduce insertion loss, coercive field strength, and leakage in ferroelectric devices.

In this work, we show the importance of layer nucleation—both an AlN interlayer, and the initial ScAlN layer—to the final crystal quality of ScAlN films grown on 4H-SiC substrates. Very thin AlN layers, grown at standard molecular beam epitaxy growth conditions (840 °C estimated substrate temperature, III/V = 1.05) have a large impact on both the surface evolution, as observed though reflection high-energy electron diffraction (RHEED), and in the final X-ray diffraction (XRD) 0002 reflection full-width at half maximum (FWHM). AlN layers grown on SiC show streaky, narrow RHEED patterns, indicating a smooth, well-ordered surface, for film thicknesses as low as 5 nm. With the inclusion of a 5-nm AlN interlayer, the $Sc_{0.32}Al_{0.68}N$ XRD FWHM decreases from 7200 arcsec to 4100 arcsec. The RHEED pattern evolution also improves, showing well a well-defined spotty pattern after only 30 nm of subsequent $Sc_{0.32}Al_{0.68}N$ growth.

In addition to the AlN interlayer, the method of initiation of the ScAlN layer also has a strong impact on the final quality of the film. Initiation using a linear composition grade from $Sc_{0.32}Al_{0.68}N$ to $Sc_{0.40}Al_{0.60}N$ over 100 nm leads to further improvements in the RHEED pattern, including a narrowing of the spots early in the growth, and elimination of remaining ring-like character in the final RHEED pattern following an additional 50 nm of $Sc_{0.40}Al_{0.60}N$ growth, resulting in an XRD FWHM as low as 4400 arcsec. The graded sample has the same average ScN fraction and thickness as the two-step sample. Surprisingly, the grade thickness can be reduced to 25 nm (with the remaining 125 nm $Sc_{0.40}Al_{0.60}N$) without degrading the XRD FWHM or RHEED pattern. Finally, a 500-nm-total-thickness sample (100 nm $Sc_{0.32}Al_{0.68}N \rightarrow Sc_{0.40}Al_{0.60}N$, 400 nm $Sc_{0.40}Al_{0.60}N$) showing a reduction in XRD FWHM to 3190 arcsec. The influence of layer initiation suggests that large abrupt changes in chemical composition (surface energy) and strain promote nucleation of thermodynamically unfavorable anomalous cubic grains, and may point to a general strategy for elimination of anomalous grains in high ScN fraction ScAlN.

9:00am **NM-MoM1-6 Realization of AlN Homojunction PN Diodes***, **Christopher M. Matthews,*** Georgia Institute of Technology*; H. Ahmad,* Georgia Institute of Technology, Pakistan*; Z. Engel, K. Motoki, S. Lee, W. Doolittle,* Georgia Institute of Technology

With a direct band gap of 6.1 eV, aluminum nitride (AlN) has traditionally been classified as an insulator. Prior to this work, difficulty doping AlN proved to be the main obstacle preventing the use of AlN beyond structural or insulating layers in semiconductor devices. P-type conductivity of AlN has been a major challenge with the only success being reports of surface conductivity via carbon doping, but no substantial bulk doping [1]. N-type AlN has only been reported in near surface regions or as limited to ~10^{15} cm^{-3} in bulk films [2].

Our recent success in bulk doping of AlN could open the door to AlN-based deep ultraviolet emitters, high performance power electronics, radio frequency devices, and extreme environment devices. In this work, we will demonstrate (1) substantial bulk p-type AlN ($p = 3.1 \times 10^{18}$ cm^{-3}), (2) the highest reported Si-doped n-type AlN ($n = 6 \times 10^{18}$ cm^{-3}, nearly 6000 times the prior state-of-the-art), and (3) the first homojunction PN AlN diode with a nearly ideal turn-on voltage of ∼6 V and current rectification of ~6 orders of magnitude.

Low temperature metal-modulated epitaxy (MME) was used to reduce the number of compensating impurities introduced during growth. This low temperature growth yields a lower impurity flux from heated structural components of the growth chamber. Additionally, we theorize that less thermal expansion of the lattice during growth inhibits the formation of compensating Si-DX and O-DX centers in the n-type AlN. The dopant elements (Be and Si) were chosen to reduce compensation (via undesired interstitial configurations) by providing candidates for substitutional impurities that closely match aluminum in size.

Semiconducting AlN requires highly crystalline material. However, a dense layer of stacking faults can form due to the presence of surface oxides on AlN and initiate threading dislocations at the fault edges. Using Al-flashing [3], we have removed the surface oxides and defects as seen with TEM. The effects of varying the number Al-flashing cycles on device performance will be presented by comparing current-voltage-temperature behavior with TEM.

References

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[3] Y. Cho, C.S. Chang, K. Lee, M. Gong, K. Nomoto, M. Toita, L.J. Schowalter, D.A. Muller, D. Jena, and H.G. Xing, Appl. Phys. Lett. 116, 172106 (2020).

9:15am **NM-MoM1-7 MBE AlScN/GaN Heterostructures Showing High-K, Ferroelectricity, and High Mobility 2DEGs***, **Joseph Casamento**, H. Lee, V. Gund, T. Maeda, K. Nomoto,* Cornell University*; S. Mu,* University of California, Santa Barbara*; W. Turner,* University of Notre Dame*; L. van Deurzen, Y. Shao, T. Nguyen, B. Davaji, M. Javad Asadi, J. Wright,* Cornell University*; P. Fay,* University of Notre Dame*; C. Van de Walle,* University of California, Santa Barbara*; A. Lal, D. Muller, H. Xing, D. Jena,* Cornell University

Epitaxial $Al_{1-x}Sc_xN$ with compositions near 18% Sc (x=0.18) of ~100 nm thickness grown on metal polar GaN by plasma-assisted molecular beam epitaxy (MBE) is found to exhibit enhanced relative dielectric permittivity (ε_r) and signs of ferroelectric behavior. The measured ε_r for $Al_{1-x}Sc_xN$ reaches a value of ~21 at x=0.25, which is larger than a 2x enhancement relative to AlN (ε_r~9). Ferroelectric behavior, with measured remnant polarization (P_r) and coercive field (E_c) values ranging from 10 to 15 μC/cm^2 and 0.7 to 1.2 MV/cm, respectively. In addition, epitaxial integration strategies and insight into the electron transport mechanisms of AlScN/AlN/GaN based 2DEGs with room temperature electron mobilities of ~1600 cm^2/Vs are discussed.

Currently wide-bandgap, gallium nitride semiconductor based high electron mobility transistors (HEMTs) use AlGaN/GaN or AlN/GaN heterojunctions to generate high density 2D electron gases due to the polarization discontinuity. The combination of 2DEGs with mobilities greater than silicon channels and a wider energy bandgap than silicon has established the Al(Ga)N/GaN semiconductor system as the leading contender for energy-efficient power electronics and microwave applications for 6G and beyond.[1]

Alloying AlN with transition metals such as scandium (Sc) introduces new physical phenomena into the nitride semiconductor family by increasing bond ionicity. This allows for enhanced piezoelectricity,[1] and an enhancement in the relative dielectric permittivity is attributed to local bond distortions and bond softening along the c-axis.[2]With softer out-of-plane bonds, an electric field along the *c* axis induces larger atomic displacement and polarization change, giving rise to the enhanced dielectric response. These structural distortions are also related to the metastable nature of the ternary alloy system and the traversal through a ferroelectric phase transition.[3] Epitaxial AlScN barrier layers in AlN-GaN heterostructures show 2DEG room temperature electron mobilities of ~1600 cm^2/Vs. The epitaxial integration of the dielectric and ferroelectric properties of AlScN with nitride semiconductors aims to enhance the performance and increase the functionality of nitride electronic and photonic devices.

References

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9:30am **NM-MoM1-8 Realizing GaN/AlN Short Period Superlattices (SPSLs) Through Ga Surfactant Enhanced MME Growth of AlN***, **Alexander Chaney**,* Azimuth Corporation*; C. Bowers,* UES*; K. Mahalingam,* UES*; S. Mou,* Materials and Manufacturing Directorate, Air Force Research Laboratory*; K. Averett,* Materials and Manufacturing Directorate, Air Force Research Laboratory

We present a novel method for obtaining GaN/AlN short-period superlattices (SPSL's) by introducing Ga into the metal modulated epitaxy (MME) growth of AlN. During the MME process, the growth alternates between metal accumulation and metal consumption, with the end of the consumption regime resulting a metal deficient surface. By ensuring that Ga is present during this portion of the MME growth of AlN, it is possible to oscillate between the epitaxy of AlN and GaN in a controlled manner. This presents an advantage over more common methods of forming GaN/AlN SL's in MBE such as relying on periodic growth interrupts or migration enhanced epitaxy (MEE), both of which can lead to surface roughening. For our study, Ga partial pressures ranging from 1x10^{-7} Torr to 1x10^{-6} Torr were used along with a growth temperature of 825 ^{o}C. XRD analysis using coupled ω-2Θ scans found that at this growth temperature, Ga partial pressures greater than 3x10^{-7} Torr resulted in the formation of a GaN/AlN SPSL, with higher Ga pressures resulting thicker GaN films. These results indicate that the impinging Ga flux plays a dominate role in the resulting GaN layer thickness. TEM analysis showed that GaN layers as thin as 2 ML were formed. At the same time, wide angle TEM imaging indicated that the GaN/AlN SPSL layer thicknesses were maintained over 1 µm of total thickness without degradation of the interface quality. AFM scanning showed an improvement of the surface morphology with increasing Ga overpressure, characterized by a reduction in the RMS roughness and reduction in the diameters of hillocks on the surface. A minimum RMS roughness of 0.46 nm was found for a Ga partial pressure of 1x10^{-6} Torr. Based on this data, it is possible that the presence of Ga on the surface during the growth of AlN is creating a surfactant effect for the Al adatoms. Finally, this modified MME growth technique was used to attempt to create an AlGaN digital alloy with a target of 75% Al composition. Initial UV-Vis absorption measurements showed a prominent increase in the absorption at 225 nm, which correlates to a DA with 75% Al composition. This closely to the 78% Al content obtained from a coupled XRD scan. The UV-Vis data shows 2 additional peaks near 225 nm whose origins are currently being investigated. These results highlight the validity of introducing Ga into the MME growth of AlN as a practical method for obtaining high quality GaN/AlN SPSL'swith the potential for realizing DA's.

9:45am **NM-MoM1-9 Cubic Boron Nitride Grown by Mg-Catalyzed MBE***, **David Storm**, S. Maximenko, A. Lang, N. Nepal, T. Feygelson, B. Pate, D. Meyer,* U.S. Naval Research Laboratory

We report on the role trace amounts of Mg performs in facilitating the growth of c-BN on single-crystal diamond (100) by ion beam-assisted MBE. We have grown c-BN in a custom III-N MBE system equipped with an Ar ion source, a N_2 plasma source, and an electron beam evaporator for supplying elemental boron. Growth is initiated using a flux of Mg from a dual filament effusion cell (Φ_{Mg} ~ 8×10^{10} cm^{-2}s^{-1}), which facilitates the growth of c-BN. [1] Even trace amounts of Mg are sufficient to facilitate the growth of the cubic phase; however, neither Mg catalysis nor ion beam assistance alone appear sufficient to enable the growth of c-BN on diamond. Fourier transform infrared (FTIR) spectroscopy indicates that ion-assisted growth of BN under a Mg flux results in films which are fully cubic without any hexagonal phase (Figure 1).Transmission electron microscopy confirms the presence of an epitaxial c-BN film; the interface between the c-BN layer and the diamond substrate is structurally abrupt, and stacking faults comprise the nearly all of the visible defects. Electron energy loss spectroscopy indicates the film is >99% cubic, and while sp^2-bonded BN is detected near the layer surface, the regrowth interface, and at isolated misfit dislocations, no h-BN is detected.

[1] D.F. Storm et al., phys status solidi-RRL, https://doi.org/10.1002/pssr.202200036]doi.org/10.1002/pssr.202200036 (2022).

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