Thin Films
Room 115 - Session TF1+EM-FrM

Thin Films for Microelectronics III: Wide Band Gap Materials

Moderators: Mark Losego, Georgia Institute of Technology, **Virginia Wheeler**, U.S. Naval Research Laboratory

8:15am **TF1+EM-FrM-1 Interlayer Engineering of Heterostructure Thermal Boundary Resistance of Power Device Heat Spreader**, ***Youhwan Jo***, *T. Hwang, K. Cho,* University of Texas at Dallas **INVITED**

The needs for high power electronic devices are expanding for diverse applications including power conversion, smart grid, renewable energy generation and storage systems. The power capacity of devices is correlated to the bandgap of the semiconductors, and the current GaN power devices are expected to evolve to more powerful devices with ultra-wide bandgap semiconductors (e.g., b-Ga2O3, diamond, AlN, c-BN) in the future. As the power capacity of a device increases, the increasing waste heat generated by the operation must be removed efficiently and maintain the device temperature sufficiently low to avoid accelerated degradation and premature failure of the devices. However, even the performance of current GaN power device is limited by the capacity of waste heat removal at the device level from the hot spots. Specifically, the thermal resistance along the heat transport pathway from the GaN device hot spots to an adjacent heat spreader (e.g., diamond or AlN) is dominated by the thermal boundary resistance (TBR) of the heterostructure interfaces. To enable the full potential performance of GaN power devices, it is critically important to optimize the GaN/diamond TBR well below the previously reported values which are larger than the classically known limit of ~3 m^2K/GW based on the diffuse mismatch model (DMM) study of phonon transport at the heterostructure interfaces. In this talk, we will discuss the role of nanoscale interlayers at the heterostructure interfaces and demonstrate that the interlayer phonon engineering can enable novel phonon transport mechanisms at nanoscale leading to TBR values lower than the classical DMM limit. We envision applying the nanophononics design of interlayers to address the thermal management challenges of high-power devices.

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8:45am **TF1+EM-FrM-3 Characterization of Defects in AlN Using Deep Ultraviolet Photoluminescence**, ***Virginia Wheeler***, *N. Nepal, M. Hardy, A. Lang,* Naval Research Laboratory*; J. Hart,* Nova Research Inc*; B. Downey, D. Meyer,* Naval Research Laboratory

AlN is being explored as an ultrawide bandgap material that offers the combined possibility of higher voltage handling and better thermal management than current semiconductor technologies such as GaN, SiC, and Si. However, realizing the full potential of this material in electronic device applications requires the ability to tailor the electrical conductivity in active AlN layers through impurity doping. Due to the large bandgap and lower formation energy of native point defects, which serves as carrier compensating centers, impurity doping in AlN has been challenging and lacking in reproducibility. Deep ultraviolet photoluminescence (DUVPL) is a crucial tool to identifying near-band edge emission and radiative point defects within ultrawide bandgap materials. In this work, we use DUVPL to identify and correlate defect and band edge emission intensities with AlN substrates and films deposited by molecular beam epitaxy (MBE) to point towards approaches to achieving electrical conductivity for device applications.

Si-doped AlN films, ~300-500 nm thick, were deposited by plasma-assisted MBE on both AlN/sapphire templates and bulk AlN substrates from different vendors using a metal modulated epitaxy approach. All AlN substrates underwent an *ex-situ* chemical clean and *in-situ* Al-absorption and desorption technique to create an abrupt, pristine, oxygen-free growth interface. Resulting films were characterized using DUVPL, x-ray diffraction (XRD), atomic force microscopy (AFM) and van der Pauw resistivity measurements. Cross-sectional transmission electron microscopy (TEM) measurements were carried out on selected samples along (10-10) and (11-20) orientations to assess the epitaxial material quality and defect density.

DUVPL measurements of MBE AlN layers, using above bandgap excitation (at 6.458 eV), show that unintentionally-doped AlN films have strong band-edge emission and no impurity bands. After Si doping, an impurity band appears near 3.67 eV related to an Al-vacancy Si-complex and the band-edge emission at 6.03 eV decreases. Van der Pauw resistivity measurements show that conductive AlN:Si films can be obtained on all substrates, but minimal changes in resistivity result from varying growth parameters further. For AlN layers grown under similar conditions, conductive AlN films have lower intensity impurity bands. Results correlating DUVPL, XRD, AFM, TEM and resistivity measurements for the full parameter space will be discussed.

9:00am **TF1+EM-FrM-4 Ultrathin Tantalum Films for Silicon Carbide Schottky Barrier Diode**, ***Renato Beraldo***, *R. Reigota Cesar, J. Alexandre Diniz,* Center for Semiconductor Components and Nanotechnology - CCSNano, Brazil

The first device based on SiC released was a Schottky barrier diode (SBD), and device is basically a junction of a semiconductor and a particular metal capable of providing a rectifier contact. Therefore, instead of focusing only on the work function of the elements, it is important to pay attention to the quality of the interface between metal and semiconductor, for example, inhomogeneous levels, defects, impurities and morphology, which can cause interface states and change the factor of ideality (ideal is 1). Since then, ways of creating surface arrangements associated with better quality have been employed, including metallization techniques, annealing treatments, types of metals, geometric arrangements, and even the addition of tiny oxides, where some of these Applications can adjust SBH values and improve reliability resource results.

Among many metallization techniques, studies using ultrathin films yielded high quality junctions employing Ni onto Si and W, Ti onto SiC. So then, based on these results, the motivation of this work was the selection of tantalum to be the metal with this metallization technique, due to its low work function that could provide lower resistance of SBH and its refractory properties which could afford elevated temperature without affecting the device performance.

Initially, a double side polished SiC wafer n-type of 350 µm thick (0.015~0.028 Ω.cm) with drift layer of 3x1015 cm-3 dopants and 30 µm thick was selected. The samples were cleaned with 10 minutes in piranha bath and nitric acid 30% at 50 ºC. After the cleaning process, 2 nm of tantalum was deposited by RF sputtering at the top of the samples to form Schottky contact and then, rapid thermal annealed performed from 500 to 700ºC under 50ºC intervals. Then 100 nm of aluminum was deposited by thermal evaporation to provide electric contact for test probes. To create the ohmic contact, 100 nm of nickel was deposited by sputtering without any thermal treatment. The samples were diced in 1 cm2 and followed by lithographic pattern with squares of 30 µm side.

Each device was submitted to IxV curves to check the current response, leakage current under reverse bias, SBH, and ideality factor. At Fig. 1 it is possible to verify that the annealing treatment yielded the difference among the annealing treatments. At the Fig. 1, the best result was related to the 650ºC which showed lower values of leakage current and value of SBH around 0.74 eV and ideality factor of 1, resulting in a low resistance device addressed to power devices, combined with the lowest leakage current, as shown in Fig. 2.

9:15am **TF1+EM-FrM-5 Plasma Enhanced Atomic Layer Deposition of Hydrogen Free In_2O_3 Thin Films with High Charge Carrier Mobility**, ***Sudipta Mondal***, *I. Campbell, A. Bol,* University of Michigan, Ann Arbor

In_2O_3 has recently emerged as an alternative channel material for field effect transistors (FETs), owing to its exceptional carrier mobility preservation even when scaled down to ultra-thin layers below 10 nm. Despite the superior performance of In_2O_3-based FETs, understanding the underlying operation mechanisms is incomplete, particularly concerning the impact of native defects and doping. Hydrogen dopants in metal oxide films are often responsible for increased Hall mobility, albeit at the detriment of device stability. Herein, we have used plasma-enhanced atomic layer deposition (PEALD) to deposit highly uniform and conformal In_2O_3 thin films. A β-diketonate indium precursor tris(2,2,6,6-tetramethyl-3,5-heptanedionato) indium-(III), which is stable over a large temperature range was used as the indium source. O_2 plasma was selected for oxygen incorporation instead of hydrogen-containing precursors like H_2O to prevent unintentional hydrogen doping, while still aiming for high carrier mobility. Saturation behaviour for the PEALD process was studied using in-situ spectroscopic ellipsometry and indicated a wide ALD window from 150ºC to 500ºC. Our optimized process achieves a growth rate of 0.14 Å/cycle at 150ºC, and 0.29 Å/cycle at 500ºC. The In_2O_3 films manifest in a polycrystalline Bixbyite cubic phase, as confirmed by grazing incidence X-ray diffraction (GIXRD). The chemical composition of the films was investigated using X-ray photoelectron spectroscopy (XPS), which revealed a rising

number of oxygen vacancies with increasing deposition temperature. Diverse analytical methods, including UV-vis spectroscopy, scanning electron microscopy (SEM), and Hall measurements, were employed to elucidate the influence of oxygen vacancies on the film properties. Our n-type In_2O_3 films showed a Hall mobility value of 84.1 cm^2/V-s at a deposition temperature of 150°C, which is among the highest reported for ALD In_2O_3 thin films, making them an ideal candidate as a channel material in FET devices. Through Elastic Recoil Detection Analysis (ERDA), we have excluded the presence of hydrogen dopants by comparing the relative hydrogen concentration in the substrate and the sample, (detection limit ≥0.01 atomic %), cementing the role of oxygen vacancies as the principal contributor to the exceptional electrical behaviour in our films. Moreover, we explored post-deposition annealing in air and argon atmospheres as a strategy to modulate oxygen vacancies and, by extension, the electrical properties of the films. We observed that air annealing increases resistivity by eliminating oxygen vacancies, while vacuum annealing enhances conductivity by creating oxygen vacancies.

9:30am **TF1+EM-FrM-6 Epitaxial Integration of Transition-Metal Nitrides with Cubic Gallium Nitride***, **Zachery Cresswell**, N. Fessler, T. Garrett, K. Vallejo, B. May,* Idaho National Laboratory

GaN is ubiquitous in the optoelectronics industry in its thermodynamically stable wurtzite structure, but it also has a metastable zinc blende allotrope that is less explored and more difficult to synthesize. One of the potential advantages of cubic-GaN (c-GaN) is the simplified interfacial symmetry with the other cubic transition metal nitrides, which are of interest for an assortment of applications requiring high chemical and thermal stability, high hardness, superconductivity, or plasmonic properties. The shared cubic symmetry would allow for easier integration of the nitrides with a wide-bandgap semiconductor.

This work will discuss the synthesis of epitaxial c-GaN on 3C-SiC substrates and its integration with known superconducting nitrides via molecular beam epitaxy. The hexagonal-free nature of the c-GaN, and the epitaxial relationship of it and the transition metal nitrides, are confirmed via *in-situ* reflection high energy electron diffraction, *ex-situ* X-ray diffraction, photoluminescence, and transition electron microscopy. The electrical transport of the transition metal nitrides grown on c-GaN(001) is compared to growth directly on 3C-SiC(001) and c-plane hexagonal GaN. Epitaxial synthesis of cubic wide-bandgap and superconducting metallic nitrides under similar growth conditions opens a new world of possibilities in band engineering, as well as the ability to create new device structures for areas such as metamaterials, quantum computing, and condensed matter physics.

9:45am **TF1+EM-FrM-7 Comparison of AlScN Thin Films Grown via Pulsed Laser Deposition and Sputtering***, **John Wellington-Johnson**,* Georgia Institute of Technology

$Al_xSc_{1-x}N$ (AlScN) is a promising material for piezoelectric micro-electro-mechanical systems (MEMS) applications, due to its high coupling coefficient (k_t^2 > 15.5%) , large piezoelectric coefficient (>27 pC/N), and CMOS compatibility [1,2]. However, large variability in film crystallinity, orientation, composition, and grain morphology still limit the full potential of AlScN [2]. The majority of literature focuses on the sputtering growth on AlScN but and there is great variability in the film quality, with multiple deposition parameters influencing the resultant film composition, morphology, and crystallinity - there are limited reports on the impact of pulsed laser deposition on AlScN film quality. This presentation will compare the impact of thin film growth by sputtering and PLD to determine the impact on the resultant AlScN films' crystalline, compositional, and morphological features.

AlScN thin films were deposited on (111) platinized silicon by PLD and RF or DC sputtering. In PLD, thin films are deposited from a single stoichiometric $Al_{70}Sc_{30}N$ target, whereas two independent AlN and Sc targets are used in sputtering. X-ray reflectivity (XRR) and diffraction (XRD) studies are used to characterize film thickness and phase. XRD scans reveal the films maintain the desired (0002) orientation over a range of temperatures and laser fluences. Compositional analysis and depth profiling reveals the nature of surface and bulk oxygen through the film, with discussions on the differing oxidation states and bonding environments of the O1s spectra, with respect to each growth method. Grain size, surface roughness, and surface morphology of the films will also be presented through SEM and AFM studies – with R_a ranging from 1.3 to 5 nm. These results illustrate and compare the PLD growth of c-axis oriented AlScN thin films under CMOS conditions.

References

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10:00am **TF1+EM-FrM-8 Exploring the Impact of [Si-C] and [N=C] Bonds in SiCN Films by First Principles Calculation: A Study of Composition, Structure, and Properties***, **Tsung-Hsuan Yang**,* Tokyo Electron America, Inc.*; G. Hwang,* University of Texas at Austin*; P. Ventzek, J. Zhao,* Tokyo Electron America, Inc.

Silicon carbon nitride (SiCN) is a dielectric material featuring a variety of desirable properties, including thermal stability, chemical resistance, and materials strength. It has been found to have better materials properties than silicon nitride (Si_3N_4) due to its potential for controlling the element compositions and microstructure. However, the relationship between SiCN microstructure and materials properties is not well understood. This simulation study aims to bridge the gap by correlating the bonding environment in SiCN with materials properties, specifically by investigating the effect of adding [Si-C] or [N=C] bonds to SiN film. We begin by constructing amorphous SiCN in two ways: replacing Si with C to create [N=C] bonds or replacing N with C to create [Si-C] bonds. The resulting films were annealed at 500K to optimize geometry and passivate defective sites with hydrogens. A wide range of Si, N and C compositions (e.g., Si_3N_4, SiC, $Si_2N_4C_1$) and different C bonding environments were examined. The film stability was tested, and properties such as dielectric constant, refractive index, band gap, bulk modulus, H content, and bond densities were calculated. The study successfully demonstrates how [N=C] and [Si-C] bonds modify the materials properties of SiCN film, providing guidelines for tailoring the materials properties of SiCN.

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