Electronic Materials and Photonics
Room 207 A W - Session EM1+CPS+MS+PS+SM+TF-TuA

Advances in Materials and Processes for Devices and Interconnects (FEOL and BEOL)

Moderators: Moon Kim, University of Texas at Dallas, **Philip Lee**, University of Kentucky

2:15pm **EM1+CPS+MS+PS+SM+TF-TuA-1 Defect- and Strain-driven Electronic Modulations on Thin Crystals of Mo_2C**, ***Gokay Adabasi***, *Sourabh Kumar, Joshua Evans,* University of California Merced*; Eren Atli, Elif Okay, Goknur Buke,* TOBB ETU, Turkey*; Ashlie Martini, Mehmet Baykara,* University of California Merced

Thin transition metal carbides (TMCs) exhibit remarkable electrical properties combined with mechanical flexibility and environmental resistance, making them promising candidates for next-generation electronic devices. On the other hand, effective use of TMCs in such applications requires a fundamental understanding of the effect of strain and defects on local electronic properties including conductivity and work function.

Here, we utilize a multi-modal approach comprising conductive atomic force microscopy (C-AFM) and Kelvin probe force microscopy (KPFM) to investigate the electronic properties of ultrathin crystals of Mo_2C (with thicknesses below 20 nm), a prototypical TMC. Atomic-resolution C-AFM imaging under ambient conditions reveals clusters of atomic defects that strongly influence local electronic conductivity. In particular, current vs. voltage (*I-V*) spectroscopy on defective and non-defective locations highlights locally non-linear transport properties as well as changes in resistivity up to 30% induced by the defects. Additionally, KPFM measurements performed on micrometer length scales, combined with C-AFM, are employed on rippled regions of Mo_2C crystals to study the effect of strain on electronic properties. Specifically, conductivity is found to be enhanced on the ripples, and reductions in work function on the order of 100 meV are observed at tensile strains of ~0.5%. *Ab initio* calculations based on density functional theory (DFT) are utilized to investigate the interplay between mechanical strain and work function changes.

Our work provides fundamental insights into defect- and strain-driven changes in the electronic behavior of Mo_2C, highlighting the possibility of defect- and strain-engineering for rational tuning towards specific applications. Our approach also constitutes a multi-modal framework for the comprehensive characterization of local electronic properties of surfaces under ambient conditions.

2:30pm **EM1+CPS+MS+PS+SM+TF-TuA-2 Ferroelectricity in Atomic Layer Deposited Wurtzite Zinc Magnesium Oxide Zn1–xMgxO**, ***Benjamin Aronson,*** University of Virginia*; Kyle Kelley,* Oak Ridge National Laboratory*; Ece Gunay,* Carnegie Mellon University*; Ian Mercer,* Penn State University*; Bogdan Dryzhakov,* Oak Ridge National Laboratory*; Susan Trolier-McKinstry, Jon-Paul Maria,* Penn State University*; Elizabeth Dickey,* Carnegie Mellon University*; Jon Ihlefeld,* University of Virginia

Ferroelectric wurtzites have garnered interest in the scientific community since first reported in 2019. $Zn_{1-x}Mg_xO$ has shown promise due its low coercive field (2–3 MV/cm) relative to other wurtzites, integrability on flexible polymer substrates, and complementary metal–oxide–semiconductor (CMOS) and back–end–of–line (BEOL)compatible deposition temperatures as low as room temperature. However, the majority of ferroelectric wurtzite thin films – including $Zn_{1-x}Mg_xO$ – have been fabricated using physical vapor deposition (PVD) techniques, which features largely directional growth. Due to the use of high aspect ratio structures in non–volatile memory devices, the ability to conformally deposit ferroelectric wurtzites will contribute to BEOL integration. Atomic layer deposition (ALD) presents an opportunity to overcome this outstanding challenge due to its sequential, self–limiting growth. In this work, $Zn_{1-x}Mg_xO$ thin films with compositions between x = 0 and x = 0.58 were grown on platinized silicon substrates using plasma–enhanced atomic layer deposition. Films were characterized using X–ray diffraction (XRD), transmission electron microscopy (TEM), and piezoresponse force microscopy (PFM). All films deposited featured a singular out–of–plane *c*–axis textured wurtzite structure. The *c*/*a* ratio decrease with increasing Mg content indicates the increasing structural distortion. Film structure and structural distortions were further reinforced and visualized via TEM. PFM amplitude and phase hysteresis loops demonstrated polarization reversal in the x = 0.46 and x = 0.58 films. Ultimately, this finding presents opportunities to further mature the $Zn_{1-x}Mg_xO$ processing space in which ferroelectric switching is possible, as well as explore ALD of other ferroelectric wurtzites.

2:45pm **EM1+CPS+MS+PS+SM+TF-TuA-3 Harnessing Nitrogen-Rich Interfaces in AlN Ferroelectrics**, ***Ian Mercer***, *Erdem Ozdemir, Chloe Skidmore, Benjamin Debastiani, Kazuki Okamoto,* Penn State University*; Sebastian Calderon, Elizabeth Dickey,* Carnegie Mellon University*; Susan Trolier-McKinstry, Jon-Paul Maria,* Penn State University

The importance of interface preparation in the nitride semiconductor and thin film community has long been recognized as critical in controlling nucleation and properties. These AlN ferroelectrics are an enticing pathway toward integrated energy-efficient robust non-volatile memory, displaying CMOS chemical compatibility, large polarizations, and BEOL processing. Although this has not been fully realized in the relatively recent nitride wurtzite ferroelectric community, current convention stems from strictly polar systems like GaN and AlN. However, there is a clear opportunity in engineering electrode interfaces in these systems to aid in film nucleation, reduced leakage, and extended fatigue lifetimes. In this work, we discuss the influence of surface nitriding on a variety of relevant substrates prior to film deposition to enhance film texture and electrical properties. Adding the surface nitriding leads to a discussion on whether nitrogen-rich interfaces can compensate for nitrogen vacancies that migrate to electrode interfaces during cycling. By depositing top and bottom metal nitride electrodes, we investigate the benefits in the electrical properties versus metallic electrodes. Reactive RF magnetron sputtering is employed to co-sputter AlN ferroelectrics. X-ray diffraction (XRD) is used to display *c*-axis texture, while hysteresis (PE), leakage (PUND), and fatigue measurements are used to characterize the electrical properties. Etching/SEM is also used to display partial switching, exploiting the n-polar fast etch in KOH solutions, which helps visualize the effects of nitrogen-rich interfaces. Furthermore, this study reinforces the functionality of interface engineering in AlN ferroelectrics at both the top and bottom electrode interfaces. The importance of this work is that all films in this class may benefit from nitrogen-rich interfaces.

3:00pm **EM1+CPS+MS+PS+SM+TF-TuA-4 Selective Etching of GaN Over AlGaN and Monitoring via Optical Emission Spectroscopy**, ***Michael Thomas***, *Patrick Wellenius, Spyridon Pavlidis,* North Carolina State University

Achieving etch selectivity between GaN and AlGaN is critical for the repeatable fabrication of enhancement-mode AlGaN/GaN High Electron Mobility Transistors (HEMTs). The selectivity can be tuned by varying the O_2 content in a Cl_2-based etch. In this work, we explore the etch process parameter space that affects selectivity and explore how *in-situ*optical emission spectroscopy (OES) can be used as an indicator of chamber and plasma conditions over time.

Two epitaxial structures on sapphire were used. The first is a thin film of GaN (control). The second is a device-relevant AlGaN/GaN heterojunction with a GaN cap layer**.** Following photolithography,samples of each type were etched simultaneously in an Oxford Instruments Plasmapro 100 Cobra inductively coupled plasma (ICP) to eliminate run-to-run variation from the selectivity determination. The total etch time was varied by gas composition to keep the HEMT sample etch depth within the AlGaN front barrier. Etch step heights were measured via atomic force microscopy (AFM) in an Oxford Instruments Asylum Research MFP-3D Origin AFM. Using an OceanOptics USB4000 Spectrometer, OES signals were collected with 1 s integration every 60 s during chamber cleaning and conditioning, and every 30 s during the final etches for each composition.

During initial experiments, the chamber pressure, ICP power, and table RF power were all kept constant at 15 mTorr, 500 W, and 25 W, respectively. The total gas flow was kept constant at 50 sccm, and Cl_2 was further kept constant at 35 sccm. The remaining 15 sccm were split between O_2 and Ar, with three tests being done at 0/15, 2/13, and 4/11 sccm of O_2/Ar respectively. An initial peak selectivity of 3.45:1 was measured with 2 sccm O_2. The OES signalconfirms O_2 emission brightness changes as expected with flow rate. To further improve the selectivity, we will report on the etch characteristics across a wider parameter space, including varying the Cl_2 content of the plasma, the total gas flow rate, the chamber pressure, ICP power and substrate size. Moreover, we explore how the OES's utility can be leveraged to assess the effectiveness of pre-etch chamber conditioning to improve both selectivity and repeatability. The results of this study are expected to boost the yield and performance of AlGaN/GaN HEMTs.

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3:15pm **EM1+CPS+MS+PS+SM+TF-TuA-5 A Pioneer Gas Screening Technique for Cryoetching Using Graph Neural Network Potential***, **Bong Lim Suh**, Taeuk Park,* Samsung Electronics Co., Republic of Korea*; Seungwu Han,* Seoul National University, Korea*; Suyoung Yoo, Sang Ki Nam,* Samsung Electronics Co., Republic of Korea

With the ongoing drive in the semiconductor industry towards miniaturization and more compact chips having a high aspect ratio (HAR), the need for advanced etching techniques is more crucial than ever. Recently, a cryoetching technique has attracted attention as one of the approaches that can address issues commonly found in traditional etching processes, such as sidewall deformation. However, utilize the recipe of cryoetching process has limitation because of the equipment company's patent. Therefore, it is necessary to develop a novel cryoetching gas for internalization. Here, we figure out the decisive physical properties of cryoetching gas and screened the reasonable 27 kinds of gas candidate using the graph neural network (GNN) potential. From the results, the gases were selected that include the halogen atoms that easily form with effective derivatives. Moreover, we demonstrated the possibility of selected gases to act as reactant, catalyst, or adsorption enhancer in the etching process using Grand Canonical Monte Carlo(GCMC) method. Our theoretical strategy provides a blueprint to design the next generation etching gases that can operate at low temperature to expand its applicability in various equipment.

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