PCSI
Room Ballroom South - Session PCSI-MoA2
Wide Band Gap Semiconductor & DUV Lithography

Moderator: Jason Kawasaki, University of Wisconsin - Madison

4:20pm **PCSI-MoA2-29 Polarization Birefringence and Surface Roughness of XeLiF + Al Mirrors**, ***Nathan Skousen***, Brigham Young University; *Sarah Loewecke,* Fordham University; *James Hilfiker,* J.A. Woollam Co., Inc.; *Luis Rodriguez de Marcos,* Catholic University of America, Spain

A new deposition method developed by Goddard Space Flight Center fluorinates the surfaces of freshly evaporated Al mirrors by exposure to XeF2. This produces an ultrathin film of aluminum fluoride which is thought to conformally coat the aluminum. This is followed by an evaporated LiF coating to create a broadband, relatively stable mirror which is termed Al+XeLiF. This in-situ, room-temperature process produces mirrors with noteworthy environmental stability and high reflectance over a broad spectral range from the FUV to the IR, including the desirable, but hard to achieve, 100 to 115 nm range. NASA may use this approach to prepare mirrors and grating coatings for the future Habitable Worlds Observatory. To accomplish its primary mission of imaging and characterizing potentially habitable exoplanets the HWO requires total extinction of the light from an exoplanet's star to capture the light of dim exoplanets without contaminating starlight. When used with an internal coronograph, however, surface roughness and polarization effects from the telescope mirrors could result in starlight leaking into the coronograph's dark pit preventing clear detection and characterization of Earth-size planets in a star's habitable zone. We studied retardance and diattenuation using variable-angle, spectroscopic ellipsometry (VASE) to better understand these effects on lithium-fluoride-coated aluminum mirrors exposed to different temperature/humidity environments.

The physical evolution of roughness on deposited fluoride surfaces is noteworthy. Fluorides, particularly LiF, are observed to roughen in moist air even at relatively low humidity. Water condenses out of the air in any small defects due to Laplace pressure. Condensed water will attack the film. Then, in an Oswald ripening-type process, larger crystals form at the expense of nanometer size crystals. This creates defects even more favorable for the condensation of moisture and the eventual destruction of the film.

4:25pm **PCSI-MoA2-30 Beyond Isotropy of Cubic Crystals**, ***Beáta Hroncová,*** Masaryk University, Czechia; *Subiao Bian, Oriol Arteaga,* Universitat de Barcelona, Spain; *Razvigor Ossikovski,* Institut Polytechnique de Paris, France

The dielectric response of cubic crystals, like Si, Ge, GaAs, InSb, and CaF_2, is commonly assumed to be isotropic. This assumption stems from the fact that, at optical frequencies, the wavelength of light is much larger than characteristic distances inside the crystal (usually of the order of interatomic distances), $a/\lambda<<1$. Within this limit, the macroscopic material response is local. This description breaks down mainly in the spectral region near excitations, where the refractive index increases and the ratio a/λ becomes non-negligible. Keeping non-local terms in the dielectric tensor explains the weak anisotropy observed in cubic crystals [1]. The intrinsic birefringence has caused many problems in the semiconductor industry, where cubic crystals are widely used as substrates for layer growth. Substrate anisotropy can make optical characterization of the layers challenging. Another example is the failure of 157nm lithography, where the crystals used for UV laser optics, CaF_2 and BaF_2, exhibit unacceptably large birefringence [2].

In this work, we utilize high-sensitivity Mueller matrix polarimetry to measure the weak anisotropy of cubic crystals. This approach has recently been shown to work well for reflection measurements on silicon [3]. We also present our transmission experimental results that show intrinsic birefringence of Si and CaF_2. In addition, we demonstrate the directional dependence of the intrinsic birefringence by examining crystals with different surface orientations. Rotational symmetries of the crystal axes are clearly visible (Fig. 1), indicating that the measured birefringence is intrinsic and not induced, e.g. by strain.

4:30pm **PCSI-MoA2-31 Investigating the Dust Mitigation Abilities of Dissociative Degradation**, ***Kira Sand,*** Brigham Young University

Particulate contamination requires dust mitigation techniques to provide low-scatter surfaces on sensitive instrumentation in space. We have previously shown that poly(olefin sulfone)s photodegrade in spacelike conditions: in vacuum and with UV light exposure. We now demonstrate that photodegradable polymers can reduce dust accumulation on optical surfaces for space applications. Our research shows that dissociative degradation of poly(olefin sulfone)s significantly decreased the number of dust particles on a dust-coated surface.

Our findings show a viable way to mitigate the collection of extraterrestrial dust on optical surfaces in space, enabling passive removal of particulate contamination without any direct human intervention.

4:40pm **PCSI-MoA2-33 Development of UV-C light Source in 180-190 nm Spectral Range using Rocksalt-structured MgZnO Alloys**, ***Takeyoshi Onuma,*** 2665-1 Nakano, Hachioji, Japan; *Kotaro Ogawa,* Kogakuin University, Japan; *Yuichi Ota,* Toyama Prefectural University, Japan; *Kentaro Kaneko,* Ritsumeikan University, Japan; *Tomohiro Yamaguchi,* Kogakuin University, Japan; *Shizuo Fujita,* Kyoto University, Japan; *Tohru Honda,* Kogakuin University, Japan **INVITED**

The Minamata Convention on Mercury is advancing the regulation of mercury products. However, low-pressure mercury lamp is exempted from the regulation. The 185 nm emission is widely utilized as a light source for oxygen dissociation, ozone generation, and OH radical production in water treatment, while the 254 nm emission is widely used for UV sterilization. Although AlGaN-based deep UV LEDs are becoming promising alternative to the 254 nm emission, almost no effort has been made to replace the 185 nm emission.Behind the background, we have studied rocksalt (RS)-structured MgZnO alloys as candidate materials for UV-C emitters in 180-190 nm spectral range. Our group has reported growth of atomically-flat single crystalline RS-MgZnO films on MgO (100) substrates by using the mist chemical vapor deposition (mist CVD) method [1-3]. Observations of deep UV cathodoluminescence (CL) have been reported [1–6]. Post-growth slow-cooling process was used to improve the crystallinity and emission properties [7]. A near-band-edge emission was eventually achieved in the 187–223 nm spectral range at 300 K. Our group also succeeded in growing RS-MgZnO polycrystalline films on quartz glass substrates using the mist CVD [8]. The achievement brought us a demonstration of RS-MgZnO-based UV-C lamp emitting in 190-220 nm spectral range using 146 nm line of Kr_2^* generated by dielectric barrier discharge as an excitation light source [9]. The progresses and recent achievements in growth of RS-MgZnO/MgO multiple quantum well structures will be discussed.This work was supported in part by Grants-in-Aid for Scientific Research Nos. 17H01263, 20H00246, 22K04952, 25K08495, and 25KJ2089 from MEXT, Japan and The Canon Foundation. T.O. would like to thank Prof. S. F. Chichibu and Dr. K. Shima of Tohoku University for their help with time-resolved photoluminescence measurements. The RS-MgZnO-based UV-C lamp was developed as a joint research project between ORC Manufacturing Co., Ltd. and Kogakuin University.[1] K. Kaneko *et al*., Appl. Phys. Express **9**, 111102 (2016). [2] K. Kaneko *et al*., J. Electron. Mater. **47**, 4356 (2018). [3] K. Ishii *et al*., Appl. Phys. Express **12**, 052011 (2019). [4] T. Onuma *et al*., Appl. Phys. Lett. **113**, 061903 (2018). [5] M. Ono *et al*., J. Appl. Phys. **125**, 225108 (2019). [6] T. Onuma *et al*., J. Appl. Phys. **134**, 025102 (2023). [7] K. Ogawa *et al*., Jpn. J. Appl. Phys. **63**, 02SP30 (2024). [8] W. Kosaka *et al*., Phys. Status Solidi B **259**, 2100354 (2021). [9] K. Ogawa *et al*., Appl. Phys. Express **17**, 121001 (2024).

5:20pm **PCSI-MoA2-41 Epitaxy of β-Ga2O3 on Highly-Offcut (>10°) Substrates**, ***M. Brooks Tellekamp,*** *Anna Sacchi, John Mangum,* National Lab of the Rockies; *Drew Haven, David Joyce,* Luxium Solutions; *Andriy Zakutayev,* National Lab of the Rockies

β-Ga_2O_3 has emerged as a leading candidate for next-generation power electronics, radio frequency (RF) switches, and extreme environment electronics due to a wide band gap (4.6 – 4.9 eV), high dopability (~40 meV activation energy for an isolated silicon donor), and melt growth characteristics resulting in commercially available 4-inch substrates and commercial demonstrations of 6-inch substrates by multiple techniques.

The (100) surface of Ga_2O_3 is highly desirable from a device and epitaxy standpoint – bulk growth of (100) material is more scalable than (010), the surface is nearly lattice-matched to p-type partner NiO, and Al_2O_3 incorporates at higher concentrations without phase separation. However, the epitaxial growth rate on (100) surfaces is less than 10% of other faces due to weak bonding and favorable desorption. Recent demonstrations have shown growth rate improvements from 0.4 nm/min to 1.5 nm/min by growing on (100) wafers that are offcut 6° in the -c direction.[1] These films show step-flow growth from (-201) step-edges and high electron mobility. Despite these exciting results, offcuts greater than 6° have not been

explored due to the waste associated with grinding and polishing large offcuts.

In this talk we will discuss the molecular beam epitaxy (MBE) growth and properties of β-Ga_2O_3 grown on (100) substrates offcut in the -c direction up to 13.4°. These large offcuts are enabled by edge-fed film-defined growth (EFG) where the offcut is grown into the surface by pulling the crystal through the EFG die with the seed crystal rotated by the desired offcut angle. We will demonstrate that 13.4° offcut substrates still exhibit a terraced (100) surface, and that a >10x increase (4.8 nm/min) in growth rate is achieved. As previously reported on lower offcuts, we observe 100% reversal of substrate twin domains around the (001) direction at the substrate-epilayer interface. We will discuss electrical properties including record-low (by MBE) unintentional doping densities of < 5E15 cm^{-3}.

5:25pm **PCSI-MoA2-42 Direct Link between Duv-Induced amorphous SiO2 Compaction and Lens Aberration Drift - From Atomic-Scale Modeling to Field Optical Validation in Photolithography***, **Kwang Hoon Lee**, Won Bo Lee,* Seoul National University, Republic of Korea

This study presents a comprehensive characterization of the dynamic interplay between atomistic interface evolution in amorphous SiO_2 projection optics and device-scale optical performance drift under deep ultraviolet (DUV, 193nm) exposure. By integrating large-scale molecular dynamics (MD) simulations with machine learning force fields and density functional theory (DFT) calculations, we unveil how DUV-induced local compaction and defect evolution at interfacial regions modulate both refractive index (n) and wavefront aberrations in operational lithography systems. Specifically, our results demonstrate a quantitative correlation between MD-tracked Si-Si bond fraction/density metrics and DFT-calculated optical constants, establishing a structure-property relationship essential for device-level transport and optical characterization.

Fleet-scale, in-field monitoring of photolithography scanners confirms that progression of Y-direction Zernike coma (WFE, Coma-Y) is aligned with simulation-predicted compaction-driven refractive index shifts, cementing the impact of interface-level atomic changes on macroscopic optical device performance. Notably, the transition from elastic to plastic compaction regimes leads to nonlinear escalation in WFE drift slopes, providing actionable thresholds for predictive maintenance and device calibration.

This work bridges atomistic simulation and high-volume manufacturing field data to deliver direct, actionable insights for the characterization and management of light transport, wavefront propagation, and functional reliability in advanced optical devices.

5:30pm **PCSI-MoA2-43 Strong Fermi-level Pinning Driven by Epitaxial Graphene Interlayer in Metal/4H-SiC Junction***, **Eunseok Hyun**, Jungjae Park,* Ulsan National Institute of Science and Technology, Republic of Korea*; Junhyung Kim,* Electronics and Telecommunications Research Institute, Republic of Korea*; Jaehyeong Jo, Jiwan Kim, Hyunjae Park, Kibog Park,* Ulsan National Institute of Science and Technology, Republic of Korea

Fermi-level pinning is a phenomenon that the Schottky barrier of metal/semiconductor junction exhibits weak dependence on the metal work-function. According to the previous study [1], the metal/graphene/Si junction exhibits strong Fermi-level pinning which is expected on an ideal metal/Si junction. It has been reported that the Fermi-level pinning of metal/SiC junction is relatively weak compared with the metal/Si junction due to the ionicity between atomic elements of crystalline structure [2]. With this background, we investigated the Fermi-level pinning in metal/graphene/4H-SiC junctions. The junction was fabricated by first epitaxially growing graphene on a 4H-SiC substrate with the metal-capping method under UHV environment [3] and then depositing circular metal (Al, Ni, Pt) electrodes onto the grown graphene layer. The Fermi-level pinning factor S was extracted from current-voltage (I-V) and capacitance-voltage (C-V) curves, signifying strong Fermi-level pinning. A theoretical model proposed by Kopylov *et al*. describing the charge transfer at the graphene/SiC interface provides a plausible explanation for the observed strong Fermi-level pinning [4].

[1]Hoon Hahn Yoon *et al*., Nano Letters **17(1)**, 44 (2017)
[2] Stephen Kurtin, T. C. McGill, and C. A. Mead, Physical Review Letters **22**, 1433 (1969)
[3] Han Byul Jin *et al*.,Scientific Reports **5**, 9615 (2015)
[4] Sergey Kopylov *et al*., Applied Physics Letters **97**, 112109 (2010)

+Author for correspondence: kibogpark@unist.ac.kr
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5:35pm **PCSI-MoA2-44 UPGRADED: (Al)GaN/High-K Oxide Interface Formation: Insight from Time-Resolved Synchrotron Studies***, Shreemoyee Chakraborty, Nishant Patel, Eleni Charitoudi, Erik Lind, Vanya Darakchieva, **Rainer Timm**,* Lund University, Sweden

The (ultra)wide bandgap semiconductors gallium nitride (GaN) and aluminum gallium nitride (AlGaN) are the materials of choice for enabling power electronic devices with very high switching frequency and superior energy efficiency. Such devices are based on metal-oxide-semiconductor (MOS) gate stacks, where downscaling and leakage control require gate oxides with high dielectric constant, so-called high-k oxides, such as HfO_2 [1]. However, device performance and especially switching frequencies are often limited by the insufficient quality of the (Al)GaN/high-k interface. Ultrathin, conformal high-k layers can be synthesized using atomic layer deposition (ALD), where the choice of oxide material, pre-ALD cleaning methods, and ALD parameters strongly influence film and interface quality. Many important details about the physics and chemistry of the interface formation still remain unknown. Furthermore, until now all efforts to explore the high-k oxide film formation have been based on ex situ approaches, meaning that film deposition and characterization of the resulting interface occur in separate steps.

Here, we present a first time-resolved investigation of the ALD reactions of HfO_2 on (Al)GaN. For this, we implemented the ALD process in a synchrotron ambient-pressure X-ray photoelectron spectroscopy (AP-XPS) setup [2]. Thus, we mapped surface chemistry and electronic properties *in situ* during subsequent ALD half-cycles, which consisted of tetrakisdimethylamido-hafnium (TDMA-Hf) and water deposition. We observed a rather inefficient first ALD cycle, compared to previous semiconductor ALD studies [2], which improved with increasing aluminum content. Thickness and chemical composition of the resulting Hf-oxide film varied strongly if the order of the precursors was changed. Both observations are against the established ligand-exchange ALD model and highlight the importance of in-depth studies for improving the quality of high-k layers on (Al)GaN.

In addition, we have used XPS to systematically investigate the electronic properties and chemical composition of the interface between different (Al)GaN substrates and HfO_2 or Al_2O_3 high-k oxide films, for different ALD temperatures, where HfO_2 resulted in less interfacial oxide. The choice of pre-ALD cleaning methods (HCl or HF etching) was also found to be of importance, which can enhance ALD efficiency but also result in interface contamination. We will discuss how our structural results can be implemented to improve device performance.

[1] P. Gribisch et al., IEEE Trans. Electron Dev. 70, 4101 (2023).
[2] G. D'Acunto et al., ACS Appl. El. Mat. 2, 3915 (2020).

5:55pm **PCSI-MoA2-48 Structure and Transport Relationships of ZrN on MgO (001)***, **Evangeline Beeching**,* Idaho National Laboratory

Combining superconducting metals with semiconductors provides the basis for many solid state devices including Josephson junctions, single electron transistors, and some photon emitters [1]. The interface between the superconductor and semiconductor can be a major source of loss in these devices, and the transport properties are highly intertwined with structural disorder and defects at various length scales. This project focuses on elucidating the role of disorder on superconductivity using thin films fabricated by molecular beam epitaxy, a deposition technique which leverages precise control of stoichiometry, temperature, and substrate preparation. Using molecular beam epitaxy, we employ a method for controlling resulting disorder at the crystalline, structural scale and atomic scale resolutions.

ZrN thin films, a known superconductor, were deposited on various substrates and orientations across a range of growth conditions. Structural disorder is characterized using high-resolution x-ray diffraction. Additionally, 4-point contact schemes are used to analyze the effects of the structural disorder and determine the relationships with electrical transport down to cryogenic temperatures and under magnetic fields. These measurements reveal that the critical temperature of films deposited on MgO are below bulk critical temperature of 10 K, and some show steps indicative of multiple superconducting phases. The transport properties of ZrN on MgO are intimately related to the structural properties, which are found to depend on the nitrogen plasma conditions moreso than variations in substrate temperature. This somewhat contrasts observations on substrates with better lattice matching, which show quite a high dependence on substrate temperature. Disorder at a structural scale and atomic scale both arise, and can be somewhat independently controlled through tailoring the growth parameters. The understanding of disorder in

epitaxial semiconductor-superconductor systems will pave the way for thin film based quantum devices.

Author Index

Bold page numbers indicate presenter