

NAMBE

Room Tamaya DE - Session NAMBE-MoP

NAMBE Poster Session

NAMBE-MoP-1 A Simple Method of SrTiO₃ Growth on GaAs by Molecular Beam Epitaxy, *Maria Baskin*, Technion Israel Institute of Technology, Israel; *Sergey Shay Shusterman*, *Doron Cohen-Elias*, *Noam Sicon*, The Israel Center for Advanced Photonics, Israel; *Lior Kornblum*, Technion Israel Institute of Technology, Israel

The growth of functional oxides on semiconductors holds significant potential for various electronic and optoelectronic devices. Gallium arsenide is one of the toughest platforms for the integration of functional oxides, due to interface stability and lattice mismatch. Current strategies require multi-step growth schemes which take time and are hard to automate.

In this work we present a simple new method for the functional oxide epitaxy on GaAs. We demonstrate it with the growth of SrTiO₃ on GaAs, and compare the structural characteristics of the resulting films to films grown using the conventional growth scheme.

X-ray diffraction (XRD) and transmission electron microscopy (TEM) analysis of SrTiO₃ films grown by conventional method and new one are comparable. However, the new method is simpler, faster and easier to implement. We further demonstrate doping of the oxide films using the new method.

The work therefore offers comparable results using a highly-simplified molecular beam epitaxy (MBE) process, opening routes for automation and scalable production of functional oxides/GaAs heterostructures.

This work was supported by the Pazy Foundation and the PMRI – Peter Munk Research Institute – Technion.

NAMBE-MoP-2 Computational Design of Metal-Organic Precursors for Controlled Metal Oxide Growth, *Benazir Fazlioglu*, Harvard University; *Cem Sanga*, Istanbul Technical University, Turkey; *Adri van Duin*, Penn State University; *Roman Engel-Herbert*, *Nadire Nayir*, Paul Drude Institute, Germany

The hybrid molecular beam epitaxy (HMBE) technique for oxide growth has opened access to a self-regulated growth regime for complex oxide thin films with a wide range of chemistries, including titanates, vanadates, stannates, and ruthenates. While the favorable growth kinetics is often linked to the volatility of metalorganic (MO) precursors, their thermal decomposition and surface reaction mechanisms remain intricate and not yet fully elucidated. For instance, the widely used metalorganic precursor titanium(IV)-isopropoxide (TTIP), essential for titanate growth via HMBE, is generally believed to decompose thermally through C–O bond dissociation via the β -hydride elimination mechanism. However, alternative reaction pathways may also play a significant role. We present a hybrid computational framework of quantum mechanics (QM) calculations, ReaxFF reactive force field molecular dynamics (ReaxFF-MD) and metadynamics simulations that challenge this conventionally assumed scenario for thermal pyrolysis of TTIP. Utilizing the newly developed QM-informed ReaxFF force field, this study introduces a complete reaction scheme for TTIP decomposition, along with the statistical analysis and the reaction barriers for the various ligand liberation steps obtained from ReaxFF-MD and metadynamics simulations, respectively. Our combined approach show that the initial organic ligand separation step is spontaneous and occurs pre-dominantly via C–O bond dissociation, albeit not always via β -hydride elimination. Additionally, there is non-negligible contribution from the pathway of Ti–O bond breaking. During the thermal decomposition, the oxidation state of Ti plays a crucial role in directing the reaction pathways, along with other contributing factors; reactants with Ti in its equilibrium oxidation state are prone to undergo β -hydride elimination via H-transfer reactions to stabilize Ti's oxidation state in a degraded molecule, which is also confirmed by the lower activation barriers extracted from Metadynamics. Thenew MOdesign strategy presented here constitutes a predictive and cost-effective framework for molecular design of MO precursors with engineered decomposition and tailored reaction pathways, thus affording rapid and cost-effective advancements in the existing and future applications for chemical vapor deposition-based thin film growth and coating processes.

NAMBE-MoP-3 Fully Relaxed, Ultra-Thin (Si)GeSn Epilayers on Insulating Substrates with Large-Scale Direct Transfer Technique, *Suho Park*, *Haochen Zhao*, *Chandan Samanta*, *Tuofu Zhama*, University of Delaware; *Jifeng Liu*, Dartmouth; *Shui-Qing Yu*, University of Arkansas; *Yuping Zeng*, University of Delaware

We present fully relaxed, ultra-thin (Si)GeSn epilayers on insulating substrates achieved through a large-scale direct transfer technique. (Si)GeSn, a group IV compound material, exhibits quasi-direct bandgap properties with the potential for direct bandgap transition, resulting in enhanced carrier radiative recombination and higher mobility due to its favorable effective mass. However, the (Si)GeSn epitaxial layer is often grown on Ge virtual substrate due to the high lattice mismatch, which presents significant challenges for it to be used in optoelectronic devices. This is because that such growths typically induce biaxial compressive strain that suppresses the desired direct bandgap properties. In order to release the strain, a transfer process is needed. The conventional transfer techniques which rely on adhesive stamps such as polydimethylsiloxane (PDMS) cause material loss during multiple stamping steps, disrupt crystal orientation, and yield insufficient characterization areas. Here, our method provides an optimal solution for achieving full relaxation of semiconductor thin films by directly transferring thin films onto insulating handling substrates without adhesive intermediaries. This direct transfer achieves high-yield transfer areas while preserving crystalline orientation. The weak van der Waals forces between the thin film and insulating substrate, which would typically be compromised due to increasing surface free energy during transfer and etching processes, are successfully maintained by strategically fixing the edge regions using a photoresist. Raman spectroscopy confirms the strain relaxation in the transferred films, while atomic force microscopy (AFM) measurements demonstrate excellent surface quality after transfer. Moreover, photoluminescence (PL) spectroscopy reveals extended emission radiation from the transferred (Si)GeSn thin films, confirming their fully relaxed state and direct-bandgap behavior. Our large-scale transfer technique enables reliable characterization of pristine (Si)GeSn properties without substrate-induced artifacts such as threading dislocations and current leakage pathways typically associated with virtual substrates. This advancement has allowed us to pioneer comprehensive material analysis through various characterization techniques, including high resolution X-ray diffraction (XRD) and Fourier Transform infrared (FTIR) measurements, revealing intrinsic (Si)GeSn properties previously obscured by substrate effects and opening new pathways for numerous additional material characterization approaches.

NAMBE-MoP-4 Spectroscopic Ellipsometry and Optical Constants of MBE-Grown Quinary GaInAsSbBi Alloys for Mid-Wavelength Infrared Detectors, *Sonam Yadav*, New Mexico State University; *Rigo A. Carrasco*, *Preston T. Webster*, Air Force Research Laboratory; *Stefan Zollner*, *Jan Hrabovsky*, New Mexico State University

Mid-wavelength infrared (MWIR) materials, such as GaInAsSbBi alloys, are gaining attention for next-generation infrared applications due to their tunable band gaps that can, in principle, reach very long wavelengths ($E_g < 0.125$ eV) while lattice matching to GaSb substrates. In this study, we investigated the optical properties of a GaInAsSbBi quinary grown by molecular beam epitaxy (MBE). The sample consists of a 3 μm thick $\text{Ga}_{0.141}\text{In}_{0.859}\text{As}_{0.774}\text{Sb}_{0.223}\text{Bi}_{0.003}$ epilayer grown on a 20 nm $\text{InAs}_{0.91}\text{Sb}_{0.09}$ buffer layer on an n-GaSb substrate. The optical characterization was performed using two J.A. Woollam variable angle spectroscopic ellipsometers (IR-VASE and UV-VASE) covering the spectral range from 0.03 eV to 6.5 eV.

The IR-VASE data indicate strong absorption above ~ 0.25 eV, while below this energy, the epilayer remains transparent, exhibiting prominent interference oscillations in the 0.1–0.25 eV range. Initial fitting using an exciton absorption model did not yield an accurate match with the experimental data. We therefore used a B-spline fit of the pseudo-dielectric function for improved modeling. Additionally, depolarization effects peaked at approximately 6% in the 0.2–0.25 eV range, with notable effects across 0.1–0.28 eV.

To eliminate backside reflections, backside roughening was performed via sandblasting, followed by remeasurement of the quinary sample. The data showed an improvement where depolarization was reduced to 4% in the 0.2–0.25 eV range, and approached zero above this energy, confirming the effectiveness of the roughening process.

For UV-VASE analysis, a second-derivative fit of the pseudo-dielectric function was performed using MATLAB, identifying critical point transitions, (E_1 , $E_1 + \Delta_1$, E_0 , and E_2) characteristic of typical zincblende materials.

However, achieving an optimal fit in the UV range remained challenging due to surface-related effects. To address this, AFM measurements were conducted to quantify surface roughness (~1nm), followed by sample cleaning to reduce the oxide layer, and then UV-VASE measurements were repeated to improve the agreement of the model with data.

These findings provide valuable understanding of the optical properties of MBE-grown GaInAsSbBi alloys and highlight their potential for MWIR detector applications and modeling for quantum efficiency assessments.

NAMBE-MoP-5 Optical and Electrical Properties Study of Transferred Ge_{0.82}Sn_{0.18} Flakes Based on Layer Transfer Process, Yuping Zeng, Haochen Zhao, Suho Park, Shedrack Dafe, Tuofu Zhama, Chandan Samanta, Zijun Chen, University of Delaware

GeSn alloys with high Sn content have garnered significant interest in optoelectronic and semiconductor applications due to their tunable direct bandgap and improved carrier transport properties. In this study, we investigate the optical and electrical properties of Ge_{0.82}Sn_{0.18} flakes using a layer transfer process. GeSn was epitaxially grown on an InP substrate and subsequently released. The exfoliated Ge_{0.82}Sn_{0.18} flakes were first transferred onto a KBr substrate to facilitate small-area transmission and reflection measurements, enabling the extraction of optical properties such as absorption and bandgap characteristics. The optical analysis confirms strong absorption, reinforcing the potential of GeSn for infrared photonic applications. To evaluate the electrical properties, the GeSn layers were transferred onto SiO₂/Si substrates, where transmission line method (TLM) and Hall bar structures can be fabricated. Electrical characterization reveals enhanced carrier mobility, highlighting the suitability of GeSn for high-performance electronic devices. This study demonstrates a scalable and effective approach for integrating GeSn onto insulator substrates, providing valuable insights into its fundamental optical and electronic behavior. These findings pave the way for future advancements in CMOS-compatible optoelectronics and high-speed transistor technologies.

NAMBE-MoP-6 Growth and Characterization of Single Crystal Cubic TaN and Hexagonal Ta₂N Films on C-Plane Sapphire, Anand Ithepalli, Cornell University; Amit Rohan Rajapurohita, Arjan Singh, Rishabh Singh, John Wright, Farhan Rana, Valla Fatemi, Huili (Grace) Xing, Cornell University; Debdeep Jena, Cornell University

Two single crystal phases of tantalum nitride were stabilized on c-plane sapphire using molecular beam epitaxy. The phases were identified to be δ -TaN with a rocksalt cubic structure and γ -Ta₂N with a hexagonal structure. Atomic force microscopy scans revealed smooth surfaces for both the films with root mean square roughnesses less than 0.3 nm. Phase-purity of these films was determined by x-ray diffraction. Raman spectrum of the phase-pure δ -TaN and γ -Ta₂N obtained will serve as a future reference to determine phase-purity of tantalum nitride films. Further, the room-temperature and low-temperature electronic transport measurements indicated that both of these phases are metallic at room temperature with resistivities of 586.2 $\mu\Omega\cdot\text{cm}$ for the 30 nm δ -TaN film and 75.5 $\mu\Omega\cdot\text{cm}$ for the 38 nm γ -Ta₂N film and become superconducting below 3.6 K and 0.48 K respectively. The superconducting transition temperature reduces with applied magnetic field as expected. Ginzburg-Landau fitting revealed a 0 K critical magnetic field and coherence length of 18 T and 4.2 nm for the 30 nm δ -TaN film and 96 mT and 59 nm for the 38 nm γ -Ta₂N film. These tantalum nitride films are of high interest for superconducting resonators and qubits.

NAMBE-MoP-7 Impact of Ga on Incorporation Properties of Bi Evaluated with Time-Resolved and Steady State Photoluminescence Characterizations of Lattice-Matched GaInAsSbBi on GaSb, Alexander Duchane, Preston Webster, Rigo Carrasco, Alexander Newell, Air Force Research Laboratory; Marko Milosavljevic, Arizona State University; Shane Johnson, University of Arizona; Julie Logan, Diana Maestas, Christian Morath, Air Force Research Laboratory

Currently, HgCdTe focal plane arrays provide exceptional performance at the intersection of low dark current, radiation tolerance, and wavelength cutoff tunability. However, HgCdTe suffers in manufacturability; specifically, large format HgCdTe arrays struggle with total thickness variation leading to poor yield following hybridization to the readout integrated circuit, a problem that is not prevalent in III-V focal plane array technologies. Metamorphic InAsSb and type-II superlattices are attractive alternatives for large format focal plane arrays but ultimately do not deliver the same level of performance (in terms of dark current, radiation tolerance, and cutoff tunability) as state-of-the-art HgCdTe, due in large part to the fact that the HgCdTe solution is a random alloy with a lattice-matched (albeit *bespoke*)

substrate. Incorporation of Bi (notably the group-V analog to Hg) in random alloys of InAsSbBi offers a means of tuning this random alloy's cutoff across the mid and long-wave infrared with a lattice-matched GaSb substrate, however, III-V-Bi alloys have historically been plagued by degraded optoelectronic quality due to the difficulty in incorporating Bi into the alloy.

In recent work demonstrating the synthesis of mid-wave infrared GaInAsSbBi alloys with smooth surface morphologies and long minority carrier lifetimes, Bi's tendency to incorporate in clusters was found to be suppressed with the inclusion of Ga in the quinary GaInAsSbBi. With this new-found link offering a means to suppress Bi clustering and a large set of bright photoluminescence test structures exhibiting long minority carrier lifetimes, there is now great potential to gain insight into the nature of Bi incorporation and clustering, and its effect on minority carrier lifetime. This work focuses on examination of the low temperature photoluminescence, where localization effects are dominant, to characterize Bi clustering through its impact on the density of tail states below the bandgap and minority carrier lifetime. The density of tail states are characterized by the Urbach energy slope of the low energy side of the photoluminescence, the temperature-dependence of which yields an evaluation of the frozen-in lattice disorder. The lifetime is evaluated with time-resolved photoluminescence down to 4 K where localization acts to increase the lifetime, and its effect is characterized with a 3-state recombination model. Materials with varying Ga content and with heavy, moderate, and sparse Bi droplet coverage are compared to gain insight into what growth conditions are most conducive to producing the highest optoelectronic quality GaInAsSbBi.

[1] J. Appl. Phys. **137**, 065702 (2025).

NAMBE-MoP-8 Examining Magnetic Depth Profiles of Oxide MBE Grown PdCoO₂ Delafossite Thin Films with Post-Growth Helium Implantation, Sangsoo Kim, Oak Ridge National Laboratory

The delafossite PdCoO₂ consists of alternating layers of highly conductive palladium and Mott insulating octahedral cobalt oxides. While PdCoO₂ is diamagnetic in bulk crystals, both Co and Pd layers exhibit magnetic metastability. We have recently demonstrated [1] that small perturbations, such as strain, can induce itinerant magnetism in helium-implanted thin films. This positions PdCoO₂ as a promising material for future spintronics, serving as a platform for itinerant and emergent magnetism through helium microscope patterning [2] of the surface. A key question remains regarding the locality of the emergent magnetization relative to the helium implantation sites, in thin films of finite depth: after helium is implanted, are there other extrinsic effects that may affect the magnetism, such as vacancies or micro-strain distortions [3]? In this talk, we examine data from muon spectroscopy measurements alongside simulated depth profiles from TRIM [4] calculations, correlating the helium implantation depth profile with the muon magnetic volume fraction. Our analysis reveals extraneous magnetic sites located 10 to 30 nm from the surface that cannot be accounted for by helium implantation alone. This suggests that helium implantation does not fully explain the induced magnetization in PdCoO₂, necessitating additional surface-sensitive measurements to characterize the remaining magnetization.

[1] Brahlek, M. *et al.* Emergent Magnetism with Continuous Control in the Ultrahigh-Conductivity Layered Oxide PdCoO₂. *Nano Letters* **23**, 7279–7287 (2023).

[2] Toulouse, C. *et al.* Patterning enhanced tetragonality in BiFeO₃ thin films with effective negative pressure by helium implantation. *Physical Review Materials* **5**, 024404 (2021).

[3] Das, S., Liu, W., Xu, R. & Hofmann, F. Helium-implantation-induced lattice strains and defects in tungsten probed by X-ray micro-diffraction. *Materials and Design* **160**, 1226–1237 (2018).

[4] Ziegler, J. F., Ziegler, M. D., & Biersack, J. P. Srim – the stopping and range of ions in matter. *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* **268** (11–12), 1818–1823 (2010). <https://doi.org/10.1016/j.nimb.2010.02.091>

NAMBE-MoP-9 Investigation of Interface Electric Fields of GaAs/AlGaAs Quantum Dots Grown by Droplet Epitaxy, Taein Kang, Jong Su Kim, Yeungnam University, Republic of Korea; Sang Jun Lee, Korea Research Institute of Standards and Science, Republic of Korea; Jin Dong Song, Korea Institute of Science and Technology (KIST), Republic of Korea

In this work, we investigate interface electric field of GaAs/AlGaAs quantum dot (QD). The annealing temperature effects on interface electric for low-temperature growth (LTG) GaAs/AlGaAs QD. The LTG GaAs QDs were

annealed at temperature of 650, 700 and 750 °C. From the photoluminescence (PL) results, we found that the PL intensity were enhanced as increasing the annealing temperature and the emission wavelength became blue shift with increasing the annealing temperature. We confirm that the crystal quality of LTG QD could be improved due to the thermal quenching effect and the GaAs QD size could be smaller due to the Ga out-diffusion and Al inter-diffusions during the thermal annealing process. In photoreflectance (PR) spectra, the Franz-Keldysh oscillations (FKO) above GaAs band gap are getting stronger with increasing annealing temperature. The interface electric field strength also increases due to the decreasing of the defect density. As the results, we found that the defect density could be decreased as increasing the annealing temperature increased.

NAMBE-MoP-11 Eu-Doped ZnO-Based Short-Period Multi-Quantum Well Structures, *Juby Alphonsa Mathew, Piotr Dłuzewski, Aleksandra Wierzbicka, Anastasiia Lysak, Jacek M Sajkowski, Yaroslav Zhydashkevsky, Adrian Kozanecki*, Institute of Physics Polish Academy of Sciences, Poland

Co-introducing Mg in rare earth (RE)-doped host matrices is known to enhance the RE luminescence activity. Recently, we reported that Mg enhances Eu^{3+} red emission and activates higher energy radiative transitions of Eu^{3+} in Eu-doped ZnMgO matrices¹⁻³. In this work, Oxygen plasma-assisted molecular beam epitaxy was utilised to grow $30 \times (\text{ZnMgO}/\text{ZnO}:\text{Eu})/\text{ZnMgO}$ and also $30 \times (\text{Zn}_{1-x}\text{Mg}_x\text{O}/\text{Zn}_{1-y}\text{Mg}_y\text{O}:\text{Eu})/\text{Zn}_{1-x}\text{Mg}_x\text{O}$ ($x > y$) multi-quantum-well structures (MQWs) on $\alpha\text{-Al}_2\text{O}_3$ and c-ZnO substrates. Two Mg effusion cells were used to grow ZnMgO barriers with a high Mg concentration. The barrier and well thicknesses were varied in the range of 9 to 1 nm. The structural quality of crystals was investigated by high-resolution X-ray diffraction (HR-XRD) and transmission electron microscopy (TEM) techniques. Luminescence characteristics were analyzed via photoluminescence (PL), low-temperature cathodoluminescence (CL) and PL excitation (PLE) measurements. Intra 4f transitions from Eu^{3+} ions were readily visible in $\{\text{Zn}_{1-x}\text{Mg}_x\text{O}/\text{Zn}_{1-y}\text{Mg}_y\text{O}:\text{Eu}\}$ MQWs. However, Eu^{3+} luminescence in $\{\text{ZnMgO}/\text{ZnO}:\text{Eu}\}$ MQWs was weak and recovered using post-growth rapid thermal annealing at 800°C in oxygen ambient. Nevertheless, PL and PLE analysis show the excitation of Eu^{3+} centers via exciton trapping in the quantum wells and subsequent energy transfer to Eu^{3+} ions. The optical coupling of Eu^{3+} ions with both quantum barrier excitons and quantum well excitons leads to multiple energy transfers, amplifying the dopant luminescence.

References:

1. Mathew, J. A., et al. *Journal of Luminescence* 251 (2022): 119167.
2. Mathew, J. A., et al. *ACS Applied Optical Materials* 1.9 (2023): 1575-1585.
3. Mathew, J. A., et al. *Materials Research Bulletin* (2025): 113403.

Acknowledgement: This work was supported in part by the Polish National Science Centre, Grant No. 2019/35/B/ST8/01937.

NAMBE-MoP-12 Identifying Detector and Material Properties for Optimizing Mid-Wave Infrared Event Based Sensor Performance, *Zinah Alsaad, Julie Logan, Christian Morath, Diana Maestas*, Air Force Research Laboratory; *Payman Zarkesh-Ha*, University of New Mexico; *Preston Webster*, Air Force Research Laboratory

Event-based sensors have sparked a revolution in space-surveillance, offering an innovative solution to the constraints of traditional frame-based systems where power consumption is an ever-worsening constraint as arrays get larger and temporal resolution demands increase. In addition to reduced power consumption, low latency, and wide dynamic range, the event-based sensor fundamentally only produces data when there is a change in illumination from which events are generated; no data is produced if the scene remains static. With their event-based datastream being inherently focused on the dynamic information of the scene, they are particularly well-suited to machine vision and autonomous sensing applications. These sensors have many compelling advantages, however, there are presently no commercial event-based sensors made to cover the mid-wave infrared spectral range. Since many space-based sensing applications are primarily concerned with this waveband to see through the 3 - 5 μm atmospheric transmission window, there is great motivation to investigate how mid-wave infrared III-V detectors will function with the event-based sensor unit cell to assess their performance and potential utility for space-based sensing missions.

In this work, the event-based sensors pixel unit cell of is implemented on a printed circuit board and interfaced with various molecular beam epitaxy grown mid-wave infrared III-V photodetectors to facilitate rapid prototyping

of these novel infrared event-based sensors. Measurements of variable area detector device sizes packaged in process evaluation chips allows for detailed analysis of the sensitivity and noise contribution on the event-based sensor's nominal contrast threshold and other event-based sensor performance metrics, and provides insight into possible limitations on using III-V mid-wave photodetectors. Additionally, their performance is characterized as a function of proton irradiation to evaluate how the event-based sensor's sensitivity degrades with displacement damage to the detector array; a characterization that is made uniquely possible by separating the detector element from the unit cell (due to the fact that the latter is not rad-hard). The characterizations of the different detector structures will be presented at the conference, demonstrating how dark current, quantum efficiency and minority carrier lifetime affect event-based operation, and in what way it translates into paradigms of event based sensitivity and the noise equivalent irradiance of a typical photodetector.

NAMBE-MoP-13 Temperature-Dependent X-Ray Diffraction of Single-Crystal, Epitaxial Films, *Arnold Kiefer, Charles Reyner*, Air Force Research Laboratory

Non-ambient stages for measuring epitaxial films with x-ray diffraction enable temperature-dependent characterization of epitaxial films not otherwise available in bulk form or as powders. To demonstrate the strain evolution and thermal properties of epitaxial films at different temperatures, we use an Anton-Paar DCS 350 stage on a PAN'alytical Empyrean diffractometer to measure antimonide-based strained-layer superlattices (SLS) and epitaxially stabilized $\alpha\text{-Sn}_{1-x}\text{Ge}_x$ films.

For SLSs we discuss methods for modeling strain in multilayer films under temperature changes whose composite diffraction patterns qualitatively behave differently than those for single-layer films. The modeled diffraction pattern evolves in a predictable fashion as the substrate and layers thermally expand or contract. This modeling includes the estimation of the lattice parameters, coefficients of thermal expansion, and elastic properties of ternary compounds that may not be experimentally known and remains a limitation in creating accurate structural models.

We also investigate films that are difficult or impossible to produce in bulk or powder form. As an example, we measure some thermal properties of single-crystal, $\alpha\text{-Sn}_{1-x}\text{Ge}_x$ films. In bulk form, Sn and Ge are practically insoluble (<1 at%), and Sn undergoes the $\alpha \rightarrow \beta$ phase transition at 13°C. Despite these apparent limitations on film stability, we produce films with up to 6% Ge compositions and phase stability over 100°C by pseudomorphically growing these alloys on nearly lattice-matched substrates of CdTe and InSb. We exploit our ability to grow these films on two different substrates with sufficiently different coefficients of thermal expansion to determine the relaxed lattice constants, thermal expansion coefficients, and biaxial relaxation constants.

We address basic challenges in calibrating a non-ambient stage without established standards and make recommendations for standards based on our methodology.

NAMBE-MoP-14 Dual Channel 2DEG Micro Hall Effect Sensor, *Satish Shetty, Yuriy I. Mazur, H. Alan Mantooth, Gregory J. Salamo*, University of Arkansas

We present a dual-channel two-dimensional electron gas (2DEG) micro-Hall effect sensor, made using a dual-barrier $\text{AlN}/\text{GaN}/\text{AlN}/\text{GaN}$ heterostructure designed for application in Harsh environmental space explorations. The efficiency of the 2DEG Hall sensor is evaluated based on supply voltage-related sensitivity, and supply current-related sensitivity, yielding values of 0.058 T^{-1} and 37.1 $\text{VA}^{-1}\text{T}^{-1}$ at room temperature, respectively. This sensor maintains a linear response across temperatures ranging from -193°C to 407°C and magnetic fields between -0.25 T to +0.25 T, regardless of whether it is biased with a current of up to 12 mA or a voltage of up to 10 V. The temperature coefficient of sheet resistance is 1.1 $\text{ohm}/^\circ\text{C}$, which can enable additional functionality to Hall sensor to detect temperatures at the spatial location of high-power modules. The frequency bandwidth of the dual-channel sensor is approximately 6.3 MHz at a 60 mT magnetic field, and also provided an physics explanation for the correlation between Hall rise time and magnetic field strength.

NAMBE-MoP-15 Molecular Beam Epitaxy of Uranium Nitrides, Kevin Vallejo, Idaho National Laboratory; Zach Cresswell, University of Minnesota; Ahmed Mustakim, Krzysztof Gofryk, David Hurley, **Brelon May**, Idaho National Laboratory

Actinide-based compounds exhibit unique physics due to the presence of 5f electrons and serve as important technological materials. The thermophysical, magnetic, and topological properties of actinide systems have been studied in a range of chemistries, albeit far fewer than most classes of materials due to limited source material availability and associated safety constraints. Thin film synthesis of actinides has been performed by various techniques and enabled the study of the unique electron configuration, strong mass renormalization, and nuclear decay in actinide metals and compounds. However, the synthesis of monocrystalline actinide compounds with high purity, low defect and controllable dopant densities, high surface smoothness, and potential epitaxial integration with other materials could enable deeper understanding and exploitation of complex physics and strongly spin-orbit coupled (SOC) systems for novel technologies. This work presents the molecular beam epitaxy of single crystal, epitaxial uranium and uranium nitride thin films. The actinide films are not stable in ambient environments, necessitating the employment of an in-situ capping layer to protect against oxidation. Structural properties of the as-grown films are investigated using reflection high energy electron diffraction and X-ray diffraction. This work provides a platform for detailed investigation into actinide behavior and epitaxial integration of high SOC materials with other systems.

NAMBE-MoP-16 Adsorption-controlled Growth and Influence of Stacking Disorder in van der Waals GaSe Films on GaAs (111)B, **Joshua Eickhoff**, University of Wisconsin - Madison; Wendy Sarney, Ibrahim Boulares, Sina Najmaei, DEVCOM ARL; Daniel Rhodes, Jason Kawasaki, University of Wisconsin - Madison

Gallium selenide (GaSe) is a layered semiconductor with potential applications for single photon emission and ultrathin field effect transistors. A fundamental challenge for layered materials is to control stacking disorder, which can limit carrier mobility and optical properties. Here we map the adsorption-controlled growth window for GaSe films grown by molecular beam epitaxy on GaAs (111)B substrates, as a function of Se/Ga flux ratio and sample temperature. We observe broad windows of adsorption-controlled growth for GaSe, and compare the regions of stability to the bulk Ellingham diagrams. Using a combination of magnetotransport, photoluminescence, Raman spectroscopy, and transmission electron microscopy, we correlate changes in the carrier mobility and optical properties with changes in layer stacking disorder. Our work is an essential step towards controlling phase purity for GaSe, and for future devices based on these materials.

Josh Eickhoff^{1,2}, Wendy Sarney², Ibrahim Boulares², Sina Najmaei², Daniel Rhodes¹, Jason Kawasaki¹

¹University of Wisconsin Madison-Materials Science and Engineering

²DEVCOM Army Research Laboratory

This work was supported by NSF QLCI HQAN and ARL

NAMBE-MoP-17 Thermal Modulation Spectroscopy for Bandgap Determination in PAMBE-Grown AlN, **Edgar Agustin Contreras**, CINVESTAV-IPN Unidad Zacatenco, Mexico; Jesus Roberto Millan-Almaraz, Universidad Autónoma de Sinaloa, Mexico; Yenny Lucero Casallas-Moreno, UPIITA-IPN, Mexico; Salvador Gallardo-Hernandez, Raul Trejo-Hernández, CINVESTAV-IPN Unidad Zacatenco, Mexico; Cristo Manuel Yee-Rendón, Universidad Autónoma de Sinaloa, Mexico; Máximo López-López, CINVESTAV-IPN Unidad Zacatenco, Mexico

AlN is wide bandgap material commonly used as a buffer but also as part of the active layer of heterostructure for the UVC applications. However, the absence of native substrates limits the crystalline quality of AlN films and, consequently, the overall performance of heterostructure that relays on its optical properties. Since III/V flux ratio and the substrate temperature are the two key growth parameters that significantly affect film properties even with small variations, identifying optimal conditions is challenging. In this work, we investigated the influence of these parameters on the structural, morphological, and optical properties of AlN/Si(111) thin films deposited by plasma assisted molecular beam epitaxy. Growth temperature varied from 790°C to 850°C, and the aluminum cell flux was adjusted between 1.91×10^{-7} and 2.4×10^{-7} Torr. Optical characterization was performed using a thermal modulation spectroscopy technique. Unlike more traditional methods, such as photoreflectance, which employ lock-in amplifiers to measure $\Delta R/R$ our approach determined $\Delta R/R$ by simply subtracting

reflectance signals, using a perturbation light at 785 nm. The 785 nm laser is not absorbed by the film but by the substrate, as the substrate heats up, changes the refractive index of AlN and leads to changes in the reflectance spectrum that allows the bandgap identification. Our measurements indicate a bandgap of approximately 6eV at room temperature, which is consistent with literature values. X-ray diffraction (XRD) diffractograms confirm the formation of the wurtzite phase, with an average FWHM of 820 arcseconds for the main (002) peak. AFM and SEM analyses reveal a uniformly planar morphology with a root-mean-square (rms) roughness of 1nm. Optimal growth was achieved at 850 °C with an aluminum cell flux of 1.91×10^{-7} Torr having the best structural and optical quality of the film.

Acknowledgement: This work was partially supported by CONACYT under project CF-2023-G-426.

NAMBE-MoP-18 Growth, Defect Creation, and Passivation in 2D MoSe₂, **Collin Maurtua**, University of Delaware

2D semiconducting monolayer transition metal dichalcogenides (TMDs) have multiple applications in the growing field of quantum information science. In particular, monolayer TMDs are a promising platform for single-photon emitters due to their low dimensionality and high controllability. In this work, we utilize molecular beam epitaxy (MBE) to grow monolayer MoSe₂ with the goal of creating and controlling defects for single-photon applications. We aim to systematically investigate defect creation and passivation in these materials, comparing the defect properties and emission characteristics with those of exfoliated and CVD-grown monolayers. Additionally, we will grow MoSe₂ using MBE in bulk and few-layer forms and investigate the role of defects in emission properties after passivation in these materials. We will be looking at the interplay between the inherent defects in the grown monolayer and external processes.

NAMBE-MoP-20 Influence of the Growth Temperature and Surface Reconstruction on the Performance of Intermediate-Band Solar Cells Based on InAs Submonolayer Quantum Dots, **Ahmad Alzeidan**, Lucas A. T. de Souza, Alain A. Quivy, Institute of Physics, University of São Paulo, Brazil

The submonolayer technique is an alternative method for growing quantum dots (QDs) in a flexible manner, achieving high surface density without the presence of a wetting layer, which is typical of conventional quantum dots obtained in the Stranski-Krastanov (SK) growth mode. InAs/GaAs submonolayer quantum dots (SMLQDs) are formed through the cyclic deposition of a fractional monolayer of InAs (typically 30–70%), followed by the growth of a few monolayers (MLs) of GaAs. The small two-dimensional (2D) InAs islands that nucleate in successive InAs submonolayers tend to vertically stack due to the local strain field caused by lattice mismatch, eventually forming individual QDs, the height of which depends on the number of cycle repetitions. Our recent studies [1, 2] indicate that growing InAs/GaAs SMLQDs in the presence of a (2x4) surface reconstruction at a higher temperature than usually (525 °C instead of 480-510 °C) enhances the performance of infrared photodetectors, when compared to the common c(4x4) reconstruction obtained at lower temperature.

In the present work, we used these new conditions to check their influence on the performance of solar cells. Five p-i-n junctions were grown by molecular beam epitaxy (MBE), processed, and tested. Sample A was a reference device consisting of GaAs only, without any quantum dots. Samples B, C, and D contained ten layers of InAs/GaAs QDs embedded in the intrinsic layer of sample A, and differing solely in their growth conditions. Sample B had conventional InAs SKQDs obtained by depositing 2.0 MLs of InAs at 515 °C. Sample C had SMLQDs formed in the presence of a c(4x4) reconstruction of the GaAs(001) surface by repeating ten times a basic cycle consisting of 0.5 ML of InAs followed by 2.5 MLs of GaAs at 490 °C. Sample D was identical but was grown at higher temperature (525 °C) in order to keep a (2x4) reconstruction that is supposed to provide better 2D InAs islands than the c(4x4) reconstruction [3,4]. Finally, Sample E contained ten InGaAs quantum wells having the same nominal width, average In composition, and silicon doping as the SMLQDs. The experimental results of all devices will be presented and interpreted on the basis of the internal strain, amount of InAs material inside the QDs, and segregation of In atoms in the InAs/GaAs system.

[1] R. S. R. Gajjala *et al.*, Physical Review Materials 4, 114601, (2020).

[2] A. Alzeidan *et al.*, Sensors and Actuators: A. Physical 374, 115464, (2024).

[3] G. R. Bell *et al.*, Physical Review B 61, R10551, (2000).

[4] J. G. Belk *et al.*, Surface Science 387, 213, (1997).

NAMBE-MoP-21 Influence of Deposition Rate on Twinning in MBE Grown Bi₂Se₃ Nucleation Layers, Trent Johnson, Air Force Research Laboratory

The 3D topological insulator Bi₂Se₃ has attracted considerable interest due to the potential to exploit its topological surface states in various devices, including polarization sensitive photodetectors. However, implementation by using MBE-grown films is limited by the presence of crystalline defects. In particular, axially rotated twin domains may generate photocurrents that effectively cancel one another. The quality of epitaxial growth is often facilitated by a two-step process involving deposition at higher temperatures on a nucleation layer grown at relatively low temperature. The suppression of twinning in films grown via a two-step method should be aided by the reduction of twins in the nucleation layer.

We investigated the influence of relative deposition rate on twinning in Bi₂Se₃ films grown at a low temperature, as for a nucleation layer. The films were co-deposited from a conventional thermal effusion source for Bi and a valved cracking source for Se, on pre-annealed Al₂O₃ (0001) substrates. The fluxes for both materials were measured prior to deposition using a beam flux monitor and a series of films were grown by varying the Bi beam flux while maintaining a constant flux of Se and adjusting the deposition time accordingly to maintain consistent thickness. Films were annealed in Se flux at 270 °C to obtain a film consistent with preparation for a primary layer growth as in a two-step process. The twinning ratio of the low temperature films was characterized by x-ray diffraction phi-scans and atomic force microscopy. The results indicate that the absolute rate of Bi₂Se₃ growth plays a significant role in twin formation.

NAMBE-MoP-22 Epitaxial ScAlN/GaN Ferroelectric Transistors with a Subthreshold Sway of <50 mV/dec from 0.0017 to 38 mA/mm for both VGS Scan Directions, Shizhao Fan, Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences, China

Ever since the first demonstration of ferroelectric switching in ScAlN,^[1] the III-nitride research community has devoted tremendous efforts into the development of ScAlN/GaN ferroelectric high mobility electron transistors (HEMTs). Two generally pursued research targets are: 1) reduction of subthreshold sway (SS) in transfer characteristics by taking advantage of the negative capacitance effect during ferroelectric flipping, and 2) reconfigurable Enhance-/Depletion-mode HEMTs enabled by the large residual polarization charge density. J. Casamento et al. reported SS=28.1mV/dec for I_{DS} changing from 0.1 to 0.001 mA/mm during backward scan of V_{GS}, while a very high SS was observed during forward scan.^[2] Similar phenomenon was demonstrated by P. Wang et al., with a SS<50 mV/dec for I_{DS} changing from 0.004 to 1×10⁻⁵mA/mm during backward scan and a SS>100 mV during forward scan.^[3] To date, ferroelectric reduction of SS was widely observed in “OFF” state, *i.e.*, for I_{DS} in the μA/mm range. Herein, we demonstrate a ScAlN/GaN ferroelectric transistor with a SS<30 mV/dec for backward scan and a SS<50 mV/dec for forward scan. The ON/OFF state I_{DS} is 38/0.0017 mA/mm, respectively, and the ON/OFF transition occurs within 0.1V, promising drastic reduction of power consumption during HEMT ON/OFF switching.

In Fig. 2(a), unambiguous ferroelectric switching current peaks were observed at applied voltage of ±9.7V, corresponding to a coercive field of 0.97 MV/cm. P-E curves in Figs. 2(b) and (c) demonstrate a clear wake-up process in the first 20 scans, and afterwards, the residual polarization (P_r) stabilized at 54μC/cm². Several groups have reported different values of P_r,^[1-5] which could be related to ScAlN deposition method, defects and even interaction between ferroelectric flipping with the underlying 2DEG as unintentionally doped GaN buffer was grown in this case. Further investigation on the discrepancy in P_r is ongoing. The transfer characteristics of HEMT in Fig. 2(d) demonstrates hysteresis curves, with sharp turn off gate voltage (V_{GS}) at -11.6 V and sharp turn on V_{GS} at -5.2V while V_{DS} is 10V. We found that the threshold voltage turning range shrinks as V_{DS} decreases. At V_{DS}=0.5V, almost no hysteresis was observed. This work paves path towards ‘digital’ GaN HEMTs without a subthreshold zone.

NAMBE-MoP-23 Heteroepitaxial Growth of GaN on AlN Towards RF Device Applications, Haiyang Zhao, Yihao Yin, Zhichao Wang, Shizhao Fan, Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences, China

GaN promises significant application in high power RF devices. It is critical to reduce dislocation density in GaN epilayers for reliable HEMT device operation. This study investigates the epitaxial growth of GaN on AlN buffer layers by MBE. The growth started with a 100-nm thick AlN buffer layer on SiC substrate. For sample 240812B(S1), only an AlN buffer layer was grown. Two methods were utilized for the subsequent growth of GaN at 780°C. For Sample 240815A (S2), 640nm GaN was grown under a Ga/N flux ratio of

1.8, while for Sample 240822A(S3), 70nm GaN buffer layer was first grown at Ga/N flux ratio of 0.9 prior to the growth of 540nm GaN at Ga/N flux ratio of 1.8. For both samples, an AlGaIn barrier layer and a GaN cap layer were grown on top.

XRD study reveals that FWHMs of AlN(002) in S1 and S3 are comparable, much lower than that of Sample S2 (130 vs. 530 arcsec), indicating severe nucleation of screw-type or mixed-type dislocations in AlN buffer layer upon Ga-rich growth of GaN. The FWHMs of GaN (002)/(102) in Sample S3 (228/1109 arcsec) are significantly improved vs. those of S2(860/1360 arcsec). Pits were observed in AFM of S2, potentially due to higher density of c-component dislocations. For heteroepitaxial growth of GaN on AlN, it has been widely studied that 3D nucleation of GaN together with subsequent transition to 2D growth of GaN is an effective approach for strain relaxation and dislocation annihilation in GaN. However, we identified that, for the first time, Ga-rich growth of GaN on AlN has a detrimental effect on the underlying AlN buffer layer.

TEM study reveals that excessive screw-type and mixed-type dislocations nucleate at the GaN/AlN interface, extending across the interface downwards into AlN and upwards into GaN. We postulate that the liquid metallic Ga bi-layer on AlN at the start of GaN growth could facilitate misfit dislocation nucleation and inject point defects into the underlying AlN buffer layer, leading to threading dislocation propagation both upwards and downwards. T-dependent Hall measurement reveals that the carrier mobilities of S3 at RT and T<100K are 1050 cm²/V·s and 2420 cm²/V·s, much higher than those of S2(782 and 1470 cm²/V·s). Improvement in carrier mobility is related to the reduction of dislocation density and surface pits. This work provides crucial insights into interfacial engineering for GaN RF device applications.

NAMBE-MoP-24 Evidence of a Charged Defect Layer in the AlGaAsSb Barrier of MWIR nBn Photodetectors and its Influence on Detector Performance, Alexander Newell, Rigo Carrasco, Julie Logan, AFRL; Chris Hains, Blue halo; Diana Maestas, AFRL; Darryl Shima, Ganesh Balakrishnan, UNM; Christian Morath, Preston Webster, AFRL

Years of the MBE community working to improve the optoelectronic quality of mid-wave infrared strained layer superlattice material has recently paid off with its transition into the F-35's EODAS system [1]. However, while superlattice material is now routinely produced with relatively long minority carrier lifetimes and higher absorption, the gains in these parameters have diminished over time and the performance of mid-wave infrared nBn detectors is now largely limited by the properties of the barrier layer. Specifically, while typical nBn detectors are diffusion-limited at higher temperatures, their performance below ~130 K is often limited by depletion and tunneling dark currents. Elimination of these current mechanisms would reduce noise and improve sensitivity under low temperature operation, as is typical of space-born sensors. This motivates a more comprehensive study of the barrier properties.

In this work, 5.5 μm cutoff InGaAs/InAsSb superlattice nBn photodetectors with different barrier-absorber configurations are grown by molecular beam epitaxy, and the presence of a charged defect layer near the “barrier on active region” interface of nBn photodetectors is evidenced by electrical and optical characterizations. Three nBn structure configurations are evaluated: a *conventional* nBn (barrier on active region), an *inverted* nBn (active region on barrier), and a *symmetric* nBn where an active region is grown on both sides of the barrier (active region on barrier on active region). For the *symmetric* structure, a positive bias depletes the top layer while the negative bias depletes the bottom layer. In each structure, a sizeable depletion region is exhibited near the “active region on barrier” junctions (*inverted* nBn and top layer of the *symmetric* nBn) but not for the conventional “barrier on active region” junctions (*conventional* nBn and bottom layer of the *symmetric* nBn). As a result, the *inverted* and *symmetric* nBn (under positive bias) exhibit significantly higher dark currents that are dominated by the depletion current mechanism compared to the *conventional* and *asymmetric* nBn (under negative bias), which is dominated by diffusion current. Silvaco TCAD modeling is used to demonstrate that these observed effects are consistent with the presence of a positive sheet charge density near the “barrier on active region” interface.

The origin of this charged interface is investigated via transmission electron microscopy imaging, which shows that the “barrier on active region” interface giving rise to this effect exhibits an abrupt region of AlAs-like material, which may source this behavior.

[1] <https://www.rtx.com/raytheon/what-we-do/air/eodas>

NAMBE-MoP-25 Real-Time Multi-Wavelength Edge Detection Using Mbe-Grown GaAs/Alas Thin Films, Sina Mohammadi, City College of New York, City University of New York; **Matthew Markowitz Markowitz,** Queens College of the City University of New York; **Francesco Monticone,** Cornell University; **Mohammad Ali Miri,** Queens College of the City University of New York; **Maria Tamargo,** City College of New York, City University of New York

We present an MBE-grown GaAs/AlAs multilayer structure optimized for optical edge detection at multiple wavelengths. This 20-layer aperiodic stack is designed to selectively manipulate spatial frequency components of incident light, enhancing high-frequency features while suppressing low-frequency intensity variations. The fabrication via molecular beam epitaxy ensures precise layer thickness, high-quality interfaces, and minimal deviations from the design thicknesses. Simulated and experimental angle-resolved reflectance measurements confirm a strong numerical aperture (NA)-dependent reflectance transition, demonstrating the feasibility of high-contrast edge enhancement in imaging applications. The multilayer interference structure provides an energy-efficient, real-time optical processing solution with multi-wavelength operation, scalable for integration into advanced imaging and computational optics. Our findings underscore the potential of MBE-grown multilayer stacks as compact, hardware-based alternatives to conventional digital and metasurface-based edge detection techniques.

NAMBE-MoP-26 The Role of Nanostructures in the Ferromagnetism of Mn-Doped AlN, J. F. Fabian-Jacobi, M. A. Zambrano-Serrano, Y. Kudriavtset, CINVESTAV, Mexico; **L. E. López-González,** C. A. Corona-García, J. Guerrero Sánchez, UNAM, Mexico; **M. López-López,** CINVESTAV, Mexico

Ferromagnetic properties of materials hold significant promise for spintronic devices. This is the case of Diluted Magnetic Semiconductors (DMS), such as AlN doped with Mn. This study focuses on the growth of AlN by molecular beam epitaxy with variations on growth temperature and Mn concentration. All samples were grown on Si (111) substrates using a buffer layer grown at 850 °C. Samples were created employing an alternating Al and Mn growth approach to study magnetic and structural properties. The origin of magnetism in Mn-doped AlN was investigated through first principles calculations within the framework of periodic density functional theory (DFT). The study analyzed the conditions under which greater magnetism is induced, considering the Mn adsorption process on AlN (0002) and its incorporation into the crystal lattice.

Various characterizations were performed to analyze the samples, including Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM), Secondary Ion Mass Spectrometry (SIMS), Reflection High-Energy Electron Diffraction (RHEED), Raman Spectroscopy, Vibrating Sample Magnetometry (VSM), and X-ray Diffraction (XRD).

Our results show that ferromagnetism in the samples is enhanced when the samples exhibit nanostructured features, with a more pronounced effect at smaller particle sizes, consistent with theoretical calculations

In conclusion, this study provides a detailed understanding of the magnetic behavior of Mn-doped AlN. Experimental characterizations and theoretical calculations showed that magnetism is more pronounced in smaller particle sizes. The analysis of the Mn adsorption process on AlN (0002) helped identify the conditions under which magnetism increases, which has implications for the design of magnetic materials at the nanoscale, especially in spintronic applications.

Acknowledgment: This work was partially supported by CONACYT under project CF-2023-G-426.

NAMBE-MoP-27 Growth of Ge-Sn Digital Alloys Towards Group-IV Topological Materials, Adelaide Bradicich, Sandia National Laboratories; **Ram Joshi,** University of Arkansas; **Yunfan Liang,** Rensselaer Polytechnic Institute; **Fisher Yu,** University of Arkansas; **Jifeng Liu,** Dartmouth; **Damien West,** Shengbai Zhang, Rensselaer Polytechnic Institute; **Hiro Nakamura,** University of Arkansas; **Ezra Bussmann,** Sandia National Laboratories

Topological states are predicted to exist in Ge-Sn digital alloys composed of atomically-controlled, monolayer-digitized structures of α -Sn and Ge grown on Ge (111). However, realizing these structures is nontrivial. The Ge-Sn system is metastable at Sn compositions above 1.1 % due to the difference in the two constituent elements' lattice constants of 14.7 %. Additionally, α -Sn, the diamond crystal lattice phase of Sn, is unstable at temperatures above 13.2 °C. Here, we demonstrate the monolayer-by-monolayer growth of Ge-Sn digital alloys using low-temperature molecular beam epitaxy, which enables growth of the metastable α -Sn phase near the critical temperature for the crystal-amorphous transition and allows atomically

precise control of layering within the structure. We investigate the progression of the surface morphology of these structures via scanning tunneling microscopy, from which we find that Sn forms quasi-2D island structures at thicknesses beyond a wetting layer. We quantify the extent of interdiffusion of the atomic layers through cross-sectional transmission electron microscopy and atom probe tomography. As the structure grows, we provide insight into the breakdown of epitaxial growth, driven by both the metastability of the Ge-Sn system and slow growth kinetics at the low growth temperatures. Finally, we measure the band structure of select digital alloy materials through angle-resolved photoelectron emission spectroscopy. This work exhibits the feasibility of digital alloy growth in the Ge-Sn system, emphasizing the growth kinetics and morphology of metastable Ge-Sn digital alloys.

NAMBE-MoP-28 Continuum Model of Self-Organizing Epitaxial Structures Through Augmented Cahn–Hilliard Equations, Lawrence Qiu, Tufts University; **Arkadz Kirshtein,** Texas A&M University; **T. Pan Menasuta,** Chanita Tubthong, Thomas E. Vandervelde, Tufts University

Step meandering and step bunching are two common morphological phenomena observed in epitaxial growth of semiconductor materials. Computational studies suggest that the Ehrlich-Schwoebel (ES) potential is responsible for these formations—an energetic barrier limiting adatom diffusion between adjacent layers of the epitaxial growth surface. Depending on the location of the barrier relative to the terrace, the ES potential can limit diffusion on to or off of layers, resulting in different morphologies. Studies exploring this effect primarily utilize kinetic Monte Carlo (kMC) simulations [1, 2, 3], although variants such as a hybrid kMC and continuum model [4] and a cellular automata-based model [5] have also been proposed. However, kinetic Monte Carlo-based methods have limitations, including the difficulty of implementing the kinetics as well as computational demand that scales with adatom density.

We propose a purely continuum model based on extending the Cahn-Hilliard equations, which have been successfully applied in modeling a variety of phase separation problems, for multilayer epitaxial growth. Here, the presence and absence of adatoms are considered the two phases, replicating the effects of interatomic interactions. By introducing an interlayer stepping term into the simulation model, we are able to replicate the effects of an ES potential and produce step meandering and step bunching structures. Finally, we show that our simulation matches empirical growths where the ES potential is present, such as Bismuth surfactancy studies on GaSb grown via MBE [6].

[1] F. F. Leal, S. C. Ferreira, S. O. Ferreira, *J. Phys.: Condens. Matter.* **23**, 292201 (2011).

[2] J. G. Amar, F. Family, *MRS Online Proceedings Library.* **440**, 229–240 (1996).

[3] M. Rost, P. Šmilauer, J. Krug, *Surface Science.* **369**, 393–402 (1996).

[4] J. P. DeVita, L. M. Sander, P. Smereka, in *Multiscale Modeling in Epitaxial Growth*, A. Voigt, Ed. (Birkhäuser, Basel, 2005), pp. 57–66.

[5] M. Zaluska-Kotur, H. Popova, V. Tonchev, *Crystals.* **11**, 1135 (2021).

[6] T. P. Menasuta, K. A. Grossklaus, J. H. McElearney, T. E. Vandervelde, *Journal of Vacuum Science & Technology A.* **42**, 032703 (2024).

NAMBE-MoP-29 Wafer-Scale Etch-Free Transfer of Carbon Nanostructures from Metal Thin Films to Diverse Substrates, Kentaro Yumigeta, Muhammed Yusufoglu, University of Arizona; **Mamun Sarker,** University of Nebraska-Lincoln; **Franco Daluisio,** Richard Holloway, Howard Yawit, Thomas Sweepe, Julian Battaglia, Shelby Janssen, Alex Welch, University of Arizona; **Alexander Sinitskii,** University of Nebraska-Lincoln; **Zafer Mutlu,** University of Arizona

Bottom-up synthesized carbon nanostructures, particularly graphene nanoribbons (GNRs), possess atomically precise architectures and tunable electronic properties, making them promising candidates for next-generation electronic devices and advanced technologies. On-surface synthesis of atomically precise GNRs has been demonstrated using molecular beam epitaxy (MBE), which involves the deposition of monomer precursors and subsequent polymerization on the surface. However, their synthesis typically relies on metal substrates (e.g., Au, Cu, and Ag), which must be transferred to insulating substrates to enable device integration. Conventional transfer methods, such as chemical etching and hydrogen bubble delamination, face significant challenges in maintaining the structural and functional integrity of the materials. Chemical etching often introduces irreversible chemical damage, degrading material quality, while hydrogen bubble delamination is problematic for metal thin films due to

weak adhesion and mechanical fragility. These limitations restrict the scalability and reliability of current transfer techniques. Here, we present a wafer-scale, etch-free transfer method using low-melting-point metals (LMPMs), Field's metal (51% In, 32.5% Bi, 16.5% Sn), to address these challenges. This method provides robust mechanical support for metal thin films during hydrogen bubble delamination, enabling the transfer of carbon nanostructures without the use of harsh etchants while preserving their structural integrity. As a demonstration, 7-armchair graphene nanoribbons (7-AGNRs) were synthesized on Au(111)/mica substrates and successfully transferred onto SiO₂/Si substrates using this method. Raman spectroscopy confirmed the preservation of structural uniformity and minimal defect density after transfer. The scalability of this method was further validated through wafer-scale transfer of Au thin films from 100-mm sapphire substrates. Additionally, field-effect transistors (FETs) fabricated using transferred GNRs exhibited stable electronic performance. This work establishes LMPM-assisted transfer as a versatile and scalable platform for integrating carbon nanostructures into various technological applications.

NAMBE-MoP-30 Molecular Beam Epitaxy Growth of InAs/Nb Heterostructures, *Ido Levy, Jacob Issokson, Patrick Strohhoben, Tyler Cowan, Krishna Dindial, William Strickland, Lukas Baker, Melissa Mikalsen*, New York University; *Salva Salmani-Rezaie*, The Ohio State University; *Javad Shabani*, New York University

Heterostructures of a 2-dimensional electron gas (2DEG) semiconductor and a superconductor are prime candidates for various applications including quantum computing and topological superconducting circuits [1,2]. It is required that the 2DEG layer will be in close proximity to the superconductor and the layers will have an Ohmic contact. A high 2DEG mobility as well as high quality interface are often needed for device applications. The system of near-surface InAs (InGaAs/InAs/InGaAs) quantum well (QW) is a prime candidate. It has a narrow bandgap with the Fermi level close to the conduction band. Typically, a thin epitaxial Al layer is grown above the QW. However, Al superconduct at 1.2K, and in order to use it in a qubit, it is necessary to cool the structure to 30mK to limit unwanted thermal population of states. Another material to take into consideration is Nb that superconducts at 9K and can possibly used in a structure at a higher temperature of 1K.

In this work, we aim to use Nb as the superconductor in the structure. The common way to grow today is by ex-situ sputtering Nb on InAs/Al structure. MBE growth of Nb is not as well studied as Al, and we will show our approach to use Nb in growth and fabrication. We will review the differences between the methods and review the effect of As capping on the InAs layer prior to Nb sputtering. The growth process and characterization of the samples will be presented.

[1] H. Kroemer, Physica E 20, 196 (2004)

[2] J. A. del Alamo, Nature 479, 317 (2011)

NAMBE-MoP-31 Scanning Tunneling Microscopy for the Exploration of the SRO in GeSn Grown on Ge(001) using MBE, *Dinesh Baral, Nirosh M. Eldose, Ram Joshi, Diandian Zhang, Hryhorii Stanchu, Fernando Maia de Oliveira, Wei Du, Hiroyuki Nakamura, Shui-Qing Yu, Gregory J. Salamo*, University of Arkansas

Experimentally, GeSn has been reported to possess a direct band gap when the Sn content exceeds 8% [1,2], creating exciting possibilities for optics on silicon platform. More recently, growth of GeSn on Ge substrates has attracted added interest due to the potential impact of short-range ordering between Ge and Sn on the GeSn band structure [3]. Scanning Tunneling Microscopy and Spectroscopy (STM/S) and MBE serves as an ideal tools for observing the quality of the Ge buffers at the atom scale and potentially for directly observing short-range ordering. In this presentation, we will discuss optimizing the growth conditions for a Ge buffer using MBE and STMS, monitored in real-time via in situ RHEED. STM/S analysis confirms the atomic scale quality of the Ge buffer, which serves as a template for the subsequent growth of high-quality GeSn layers. Observed atomic-resolution STM/S reveals well-defined surface reconstructions in both the Ge buffer and the overlying GeSn layer, confirming their quality. Additionally, XRD-RSM analysis verifies the high structural quality of the bulk material, while ARPES studies reveal sharp and well-defined electronic bands, further corroborating the excellent crystalline quality of the material. We will also address strategies to mitigate surface oxidation, a critical challenge even under UHV conditions due to residual oxygen. Understanding and controlling surface structure is discussed as a key feature for the study of ordering using STM/S.

References:

[1] S. A. Ghetmiri et al., *Direct-Bandgap GeSn Grown on Silicon with 2230 nm Photoluminescence*, Appl. Phys. Lett. **105**, 151109 (2014).

[2] N. von den Driesch et al., *Direct Bandgap Group IV Epitaxy on Si for Laser Applications*, Chem. Mater. **27**, 4693 (2015).

[3] B. Cao, S. Chen, X. Jin, J. Liu, and T. Li, *Short-Range Order in GeSn Alloy*, ACS Appl. Mater. Interfaces **12**, 57245 (2020).

NAMBE-MoP-32 Development of High-Quality SiSn and SiGeSn Alloys for Optoelectronic and Photonic Applications, *Diandian Zhang, NIROSH ELDOSE, Dinesh Baral, Hryhorii Stanchu, Fernando Oliveira, Wei Du, Gregory Salamo, Shui-Qing Yu*, University of Arkansas

SiSn and SiGeSn alloys have emerged as promising candidates for next-generation electronic and optoelectronic devices due to their tunable band structures, enhanced carrier mobility, and potential compatibility with Si-based platform. In fact, SiGeSn presents the special opportunity for synthesis of strain-free SiGeSn on a Ge substrate or Ge/Si substrate creating the opportunity for strain-free Ge/SiGeSn and GeSn/SiGeSn structures. This advancement holds great potential for the development of devices such as Si-based light sources and quantum cascade lasers. While the growth of SiGeSn is still challenging due to issues such as phase separation, strain relaxation, defect formation.

In this study, we report the successful growth of SiSn with Sn content up to 5.5% on Si substrates using molecular beam epitaxy (MBE). X-ray diffraction (XRD) 004 rocking curves revealed the crystalline structure with a well-defined peak corresponding to the SiSn alloy. Atomic force microscopy (AFM) measurements indicated an atomically smooth surface with minimal roughness, further validating the high-quality epitaxial growth. We pursued the growth of SiSn as a first step followed by the growth of lattice-matched Si_{0.42}GeSn_{0.10} bulk materials and Si_{0.25}GeSn_{0.09}/Ge superlattice structures by MBE. XRD supports lattice-matched strain-free growth for both SiGeSn and Ge/SiGeSn on Ge. Meanwhile, SIMS demonstrates high Si and Sn composition up to 42%Si and 10%Sn and 25%Si and 10%Sn respectively. Additionally, a strong PL peak around 1850 nm is observed in the Ge/SiGeSn SLs structure, which demonstrates its high quality.

This study establishes a robust framework for high-quality SiSn and SiGeSn epitaxy, addressing critical challenges in material growth by MBE. The demonstrated material quality and optoelectronic performance provide a foundation for advancing Si-integrated photonic devices, such as lasers, detectors, and quantum systems.

NAMBE-MoP-33 Templated Growth of Screw Dislocations in Epitaxial Nanomembranes, *Ruhin Chowdhury, Emma J. Renteria*, University of New Mexico; *Sadhivakas J. Addame*, Sandia National Laboratories; *Darryl M. Shima, Divya J. Prakash, Jordan P. Neely, Francesca Cavallo*, University of New Mexico

Recent theoretical studies suggest that screw dislocations (SDs) could be repurposed as one-dimensional topological matter [1,2], with promising applications in quantum information science. Inspired by these prospects, our work focuses on scalable synthesis of SDs in single-crystalline semiconductors.

Here we present our recent results on the controlled synthesis of screw dislocations (SDs) in epitaxially grown (001) GaAs nanomembranes (NMs) or ultra-thin sheets where the lateral size-to-thickness ratio exceeds 10². Our approach to SDs' synthesis involves stacking GaAs NMs at a non-zero twist angle to form twisted bicrystals (TBICs). This configuration generates an array of twist boundaries at the interface, which act as seeds for the growth of SDs along the thickness direction in the bonded crystals. The propagation of SDs from the interfacial twist boundary is driven by thermal energy during annealing.

We used 200 nm GaAs NMs epitaxially grown onto Al_{0.8}Ga_{0.2}As-coated (001) bulk GaAs substrates. The 500 nm Al_{0.8}Ga_{0.2}As layer served as a sacrificial layer during the release process of the NMs. GaAs NMs were patterned into 2D arrays of 250 × 250 μm² square pixels and released in place by selective etching of the Al_{0.8}Ga_{0.2}As layer in diluted HCl. Pixelated NMs were then transferred at a non-zero twist angle onto unpatterned NMs. The resulting TBICs were annealed at 500°C for 40 hours in Ar atmosphere. We counteracted degassing during annealing by capping the TBICs with bulk GaAs substrates.

High-resolution cross-sectional transmission microscopy (TEM) showed gap- and oxide-free interfaces within the annealed TBICs, which are vital to the templated growth of SDs. Plan-view TEM detected arrays of SDs in weak-beam conditions. The measured spacing between the line defects was 13.23 nm, corresponding to a twist angle of 1.6° between the two

bonded GaAs crystals, as measured by selected area electron diffraction (SAED).

[1] L. Hu, H. Huang, Z. Wang, W. Jiang, X. Ni, Y. Zhou, V. Zielasek, M. G. Lagally, B. Huang and F. Liu, "Ubiquitous Spin-Orbit Coupling in a Screw Dislocation with High Spin Coherency", *Phys. Rev. Lett.*, 121, 066401 (2018).

[2] Y. Ran, Y. Zhang, and A. Vishwanath, "One-Dimensional Topologically Protected Modes in Topological Insulators with Lattice Dislocations", *Nat. Phys.* 5, 298 (2009). + Author for correspondence: ruhin@unm.edu

ACKNOWLEDGEMENT. Work at the University of New Mexico was supported by NSF CAREER award No. 2144944. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or the United States Government.

NAMBE-MoP-34 Synthesis and Nitrogen-Vacancy Magnetometry of ferromagnetic MnSb, Nurul Azam, Jeff Rable, Syed M. Shahed, Northeastern University; Sugata Chowdhury, Howard University; Alberto De la Torre, Northeastern University

MnSb exhibits ferromagnetism with a high Curie temperature ($T_c = 587$ K) and a notably large magneto-optical Kerr rotation, making it a promising candidate for spintronic applications. Here, we demonstrate the synthesis of MnSb on the GaAs (111) surface using molecular beam epitaxy (MBE). We then characterize the nanoscale magnetic ordering and spin fluctuations in the films using a scanning nitrogen-vacancy magnetometer. Additionally, detailed ex-situ crystallographic investigations, including transmission electron microscopy (TEM) and X-ray diffraction (XRD), are performed to assess the structural integrity of the grown crystals. The results of detailed experimental characterizations will be presented, along with analysis of the new observations within advanced theory and modeling. Overall, this study highlights the potential of MnSb for future quantum technology applications. Authors acknowledge support from the Massachusetts Technology Collaborative (award number 22032), and the National Science Foundation (award number OSI 2329067).

Keywords: Ferromagnetic MnSb, Molecular Beam Epitaxy, Momentum Microscopy, NV Magnetometry, Quantum Materials.

NAMBE-MoP-35 Metamorphic InAs 2DEGs for Quantum Computation Platforms, Giorgio Biasiol, Davide Curcio, Oyut Batchuluun, Luca Sbulzel, Magdhi Kirti, CNR IOM, Italy; Mate Suto, Endre Tóvári, Peter Makk, Tamas Prok, Szabolcs Csonka, Budapest University of Technology and Economics, Hungary

The development of quantum computing still relies on the development of advanced material platforms. Among the most promising candidates are semiconductor-superconductor hybrid systems, such as Andreev quantum bits and Kitaev transmons. These systems are based on high-quality superconducting thin films with transparent interfaces to low-dimensional semiconductors, offering the potential for extended coherence times and robust qubit-qubit coupling [1].

To this end, a metamorphic growth protocol has been employed, and low-temperature electron mobilities up to $8 \times 10^5 \text{ cm}^2/\text{Vs}$ have been achieved in undoped deep InAs/ $\text{In}_{0.81}\text{Ga}_{0.19}\text{As}$ two-dimensional electron gases (2DEGs) grown on GaAs (001) [2]. Additionally, superconducting proximity effects have been observed in Josephson junctions between shallow InAs 2DEGs and epitaxial Al layers [3]. Optimal mobilities were achieved by tuning the thickness t of a strain-relieving $\text{In}_{0.84}\text{Al}_{0.16}\text{As}$ layer beneath the quantum well (QW) region [2].

Here, we discuss the strain relaxation dynamics for varying t and their impact on electron scattering mechanisms in the InAs 2DEGs. Two-dimensional XRD reciprocal space maps of the (004) and (224) reflections (Fig. 1) reveal how increasing t from 50 nm to 300 nm leads to near-complete strain relaxation and a reduction in mosaicity in both the InAs QW and the surrounding barriers. Mobility measurements from gated Hall bars (Fig. 2) reveal striking gains in electron mobility and a reduced anisotropy between the [110] and [-110] orientations as t grows. This improvement stems from diminished anisotropic scattering mechanisms, linked to the cross-hatch roughness pattern—a memory of the buried dislocation network in the buffer layer (see insets of Fig. 2). These features, shaped by strain and composition fluctuations, highlight the interplay between structural engineering and electronic properties.

[1] J. S. Lee et al. *Nano Lett.* **19**, 3083 (2019)

[2] A. Benali et al., *J. Cryst. Growth* **593**, 1267681 (2022)

[3] M. Sütő et al. *Phys. Rev. B* **106**, 235404 (2022)

NAMBE-MoP-36 Atomically Precise Graphene Nanoribbon Transistors with Long-Term Stability and Reliability, Muhammed Yusufoglu, Zafer Mutlu, University of Arizona

Atomically precise graphene nanoribbons (GNRs) synthesized from the bottom-up exhibit promising electronic properties for high-performance field-effect transistors (FETs). The feasibility of fabricating FETs with GNRs (GNRFETs) has been demonstrated, with ongoing efforts aimed at further improving their performance. However, their long-term stability and reliability remain unexplored, which is as important as their performance for practical applications. In this work, we fabricated short-channel FETs with nine-atom-wide armchair GNRs (9-AGNRFETs). We revealed that the on-state (ION) current performance of the 9-AGNRFETs deteriorates significantly over consecutive full transistor on and off logic cycles, which has neither been demonstrated nor previously considered. To address this issue, we deposited a thin ~ 10 nm thick atomic layer deposition (ALD) layer of aluminum oxide (Al_2O_3) directly on these devices. The integrity, compatibility, electrical performance, stability, and reliability, of the GNRFETs before and/or after Al_2O_3 deposition were comprehensively studied. The results indicate that the observed decline in electrical device performance is most likely due to the degradation of contact resistance over multiple measurement cycles. We successfully demonstrated that the devices with the Al_2O_3 layer operate well up to several thousand continuous full cycles without any degradation. Our study offers valuable insights into the stability and reliability of GNR transistors, which could facilitate their large-scale integration into practical applications.

NAMBE-MoP-37 Growth of InSb Quantum Dots in InAs Matrix for Infrared Emitters, Molly McDonough, Eric Welp, Qihua Zhang, Stephanie Law, Pennsylvania State University

The infrared wavelength range is relevant to several technology areas, including biosensing, trace gas sensing, environmental monitoring, defense, security, and wireless communication. A wide range of molecular species have rotational and vibrational absorbance in the infrared, allowing for infrared emitters to enable the identification and monitoring of these species for industrial applications and environmental monitoring. In order to enable these technologies to be realized, there is a need for compact, high efficiency emitters.

One potential pathway to create compact, low-cost emitters in the infrared wavelength range is using InSb quantum dots in an InAs matrix. Here, we present our recent work on growth of InSb quantum dots on InAs on GaSb(100) substrates via molecular beam epitaxy. First, we examine the changes in height, size, and density as a function of InSb deposition time. We also studied the changes in height, size, and density as a function of Sb/In beam equivalent pressure (BEP) ratio at a fixed thickness. Lastly, we examine changes in the dot morphology as a function of substrate temperature at fixed Sb/In BEP ratio and fixed InSb deposition time. For all samples, we also look at peak photoluminescence wavelength and intensity as a function of growth conditions. The results demonstrate in-depth mapping of the growth parameter space of InSb quantum dots and serve as a jumping off point to integrate these structures into emitter devices.

NAMBE-MoP-38 AlInN/AIn Quantum Wells Grown on Si(111) Substrates by Metal Modulated Epitaxy, Luis Vargas Hernández, CINVESTAV-IPN Unidad Zacatenco, Mexico; Jorge Ivan Hernández Martínez, CINVESTAV-IPN Unidad Guadalajara, Mexico, Mexico; Mario Alberto Zambrano Serrano, CINVESTAV-IPN Unidad Zacatenco, Mexico; Yenny Lucero Casallas Moreno, UPIITA - IPN, Mexico; Salvador Gallardo Hernández, Máximo López López, CINVESTAV-IPN Unidad Zacatenco, Mexico

The AlInN alloys hold significant potential for various device applications such as high electron mobility transistors, vertical-cavity surface-emitting lasers, and deep-UV LEDs. However, challenges arise due to the substantial difference in surface mobility between Al and In atoms, leading to distinct optimal growth temperatures for AlN and InN. Moreover, the presence of a large lattice mismatch and In segregation further complicates the growth process of AlInN alloys. In this work, we report the first successful demonstration of growing InAlN/AIn quantum well structures on Si(111) substrates, a particularly challenging platform due to thermal and lattice constraints. To address the difficulties associated with In incorporation and segregation, we employed the metal-modulated epitaxy (MME) technique to grow AlInN alloys by MBE. The MME approach, involving the alternate supply of Al and In while maintaining a steady N flux, proved essential in

minimizing indium segregation and enabling the formation of more defined quantum wells. AlInN quantum wells (QWs) with AlN barriers were grown on Si(111) substrates using a Riber C21 MBE system. Active nitrogen species were generated via an RF-plasma source at 190 W with a N flux of 0.2 sccm, while beam equivalent pressures for In and Al were 1.4×10^{-7} and 2.8×10^{-7} Torr, respectively. Three distinct QWs (QW1, QW2, QW3) with varying In concentrations were grown on Si (Fig. 1). RHEED patterns remained streaky throughout, though 3D spots appeared during QW3 growth, indicating increasing surface roughness (Fig. 2). AFM confirmed this with an RMS roughness of 8 nm (Fig. 3). SIMS profiles revealed three In peaks, consistent with QWs of different composition, and a surface-leaning In shoulder in QW3, likely linked to In segregation at higher In content (Fig. 4). HRXRD curves exhibited satellite peaks near the AlN(0002) reflection (Fig. 5), evidencing the presence of AlInN layers and interference effects. Finally, room-temperature CL spectra showed a strong emission centered at 3.27 eV, presumably from the superposition of emissions from all three QWs (Fig. 6).

Acknowledgments: Rogelio Fragoso Soriano (AFM), Marcela Guerrero (XRD). This work was partially supported by SECIHT under project CF- 2023-G-426.

NAMBE-MoP-39 Quantum and Classical Supervised Learning-Based Design Rules for Radio Frequency Nitrogen Plasma, Andrew Messecar, Clifford Aidoo-Mensah, Western Michigan University; Steven Durbin, University of Hawai'i at Mānoa; Robert Makin, Western Michigan University Radio frequency (RF) nitrogen plasma sources are of great interest for the molecular beam epitaxy (MBE) synthesis of nitride thin film materials. The energetics as well as the relative concentrations of the various active species within the plasma have a significant impact on the quality and properties of a grown material sample. Therefore, controlling the characteristics of these plasmas is important for refining nitride material growth processes and producing high quality, precisely designed samples in both manufacturing and research and development contexts. Furthermore, control over the relative concentrations of active nitrogen species that are found in RF plasma can lead to an enhanced understanding of the influence that the various species have on the growth and processing of thin film material samples and devices.

RF plasma source operating parameters are traditionally optimized through an iterative process of Edisonian trial-and-error. This iterative approach towards process refinement can be expensive in terms of both material resources and the time spent developing, implementing, and optimizing experiments. Prior investigations into a more informed selection of operating parameters for RF nitrogen plasmas has involved calculating the ratio of active molecular to atomic nitrogen species under various combinations of operating parameters and interpolating between the recorded data points; this approach yields plotted processing spaces from which operating parameters can be selected, but it is limited by the range of operating parameters spanned by the data points. Machine learning algorithms present a top strategy for recognizing complex patterns and generalizing beyond recorded data points to forecast novel, unobserved information. To date, machine learning technologies have been implemented to predict electron density and electron temperature in RF nitrogen plasma from optical emission spectroscopy (OES) data. In the present study, we use supervised machine learning models, including those which incorporate quantum computers, to study the relationships between RF nitrogen plasma operating parameters and optical emission spectra features that are of interest for thin film deposition applications, including the ratio of active molecular to active atomic nitrogen species.

For a RF plasma source operated within a MBE chamber, we have acquired OES data and measured the relative concentrations of the active nitrogen species for nearly 2000 different combinations of RF plasma source operating parameters spanning large portions of the parameter space not previously studied. Each data point includes the full set of operating parameters as well as the resulting chamber pressure and the ratio of molecular to atomic active nitrogen species as measured via OES. The relationships between these variables were first investigated by calculating matrices of both Pearson's correlation coefficients and p-values for all possible pairings of the variables within the data set. These analyses were in agreement in describing the RF nitrogen plasma processing space as one defined by coupled variables that are highly interdependent upon one another. The splitting rules of regression tree models fit to the data further corroborated this assessment. Quantum and classical supervised learning models, including tree-based algorithms, quantum support vector machines, and artificial neural systems, were trained upon the data and compared for generalization performance. The trained and tuned

algorithms exhibiting superior generalization performance were used to predict features such as the ratio of molecular to atomic active nitrogen for combinations of RF plasma operating parameters not contained within the recorded training data. This mapping displays trends that agree with experimental insight developed from prior studies while also describing areas of the RF nitrogen plasma processing space that have not been previously investigated.

*This work was supported in part by the United States Department of Energy (award number DE-SC0025835) as well as the National Science Foundation (grant number DMR-2003581).

NAMBE-MoP-40 Modeling Processing Spaces of Epitaxially Grown Nitrides with Quantum and Classical Machine Learning Algorithms, Andrew Messecar, Western Michigan University; Kevin Vallejo, Idaho National Laboratory; Steven Durbin, University of Hawai'i at Mānoa; Brelon May, Idaho National Laboratory; Robert Makin, Western Michigan University

The design of thin film material synthesis processes occurs within multi-dimensional, highly complex growth spaces that are defined by sets of multiple experiment design parameters. Identifying the desired values for each synthesis parameter is conventionally performed through an iterative, Edisonian, trial-and-error approach to experiment design that is often costly in terms of resources as well as operating time. Therefore, considerable interest exists in the development of machine learning-based techniques for the rapid and accurate identification of optimal materials designs and growth recipes yielding thin film samples exhibiting target properties of interest.

In this work, synthesis records detailing several hundred individual plasma-assisted molecular beam epitaxy (PAMBE) thin film crystal growth experiments of transition metal as well as group-III nitride compounds have been organized into distinct, material composition-specific data sets. For each growth record, the complete set of experiment parameters (substrate temperature, growth duration, element source conditions, etc.) are associated with material properties of interest, including binary measures of crystallinity (1 for monocrystalline, 0 for polycrystalline) as well as surface morphology (1 for atomically-flat, 0 for three-dimensional growth) as determined by *in-situ* reflection high-energy electron diffraction (RHEED) patterns. A Bragg-Williams derived measure of lattice ordering ($0 \leq S^2 \leq 1$) is also investigated as a continuous, structural figure of merit for investigation.

Calculations of p-values, Pearson's correlation coefficient, decision tree splitting rules, and SHAP values are utilized to identify the PAMBE operating parameters which are most statistically influential upon each material characteristic of interest. Quantum as well as conventional supervised machine learning algorithms – including linear models, neural systems, tree-based algorithms, and quantum support vector machines – are trained on the data to investigate the relationships between the PAMBE synthesis process parameters and the resulting sample properties, including crystallinity, surface morphology, and measured S^2 . Multi-output models, hybrid quantum-classical algorithms, and ensemble learning techniques are also of interest for the maximization of both algorithm flexibility and the accuracy of the relationship learned from the available training data. When predicting the occurrence of monocrystalline PAMBE-grown GaN, supervised learning algorithms designed to incorporate quantum computing display notable generalization advantage over their classical statistical learning counterparts. The class conditional probabilities of obtaining monocrystalline and atomically-flat thin film crystals are predicted across broad processing spaces that are defined by the two PAMBE synthesis parameters determined to be most statistically significant by statistical inference metrics, and S^2 is also forecasted across the same growth spaces. These predictions are compared to conventional experimental best practices as well as the results described within published literature regarding the PAMBE synthesis of these materials. The predictions indicate that different growth conditions are of interest depending on whether a single crystalline sample, a flat surface, or a well-ordered lattice (as measured by S^2) is the prioritized outcome. The improved prediction performance displayed by the quantum-aware machine learning models when predicting GaN crystallinity implies the potential for quantum machine learning algorithms to be beneficial for studies of synthesis-structure-property relationships in other material systems.

*This work was supported in part by the United States Department of Energy (award number DE-SC0025835) as well as the National Science Foundation (grant number DMR-2003581).

NAMBE-MoP-41 Photonic Crystal Surface Emitting Lasers (PCSELS) based on InAs Quantum Dots-in-a-Well, Thomas Rotter, Subhashree Seth, Mega Frost, Andrei Sharma, Carter Heinrich, Samiha Nuzhat, Center for High Technology Materials, UNM; Chhabindra Gautam, University of Texas at Arlington; Sadhvikas Addamane, Center for Integrated Nanotechnologies, Sandia National Laboratories; Weidong Zhou, University of Texas at Arlington; Ganesh Balakrishnan, Center for High Technology Materials, UNM

Lasers based on self-assembled quantum dot (QD) gain media have attracted considerable attention due to their low sensitivity to operating temperature and low threshold current densities. Several laser architectures based on InAs QD have been demonstrated with excellent performance, e.g. edge emitting lasers (EELs), including distributed feedback (DFB) lasers, vertical cavity surface emitting lasers (VCSELS) or vertical external cavity surface emitting lasers (VECSELS). In this study, we demonstrate a photonic crystal surface emitting laser with a QD active region (QD-PCSEL). The PCSEL fabrication is based on epitaxial regrowth, which facilitates the photonic crystal (PC) to be located in the laser's waveguide near the upper clad layers. The structure is grown using elemental source molecular beam epitaxy (MBE). In the first epitaxial step the bottom AlGaAs cladding layer and the GaAs waveguide including the QD active region are grown. Subsequently, the wafer is removed from the MBE reactor and the PC is fabricated into the GaAs waveguide using electron beam lithography (EBL) patterning and etching by inductively coupled plasma (ICP) dry etching. This is followed by a second epitaxial step, the regrowth, where the top AlGaAs cladding layer and a top contact layer are grown on the sample. One of the main challenges is the surface preparation including the removal of the native oxide before the regrowth. This is accomplished by an acid etch prior to loading the sample into the vacuum chamber and a thermal surface treatment with arsenic supply prior to growth. The thermal step at $>600^{\circ}\text{C}$ can alter the QD gain medium, i.e. cause a blueshift and narrowing of the emission spectrum of the self-assembled QDs [1-3]. Alternatively, the regrowth can be performed by MOCVD at comparable high temperatures, where hydrogen is available for surface preparation. In our study the InAs QDs are embedded in a InGaAs quantum well (QW), a dot-in-a-well (DWELL) design. Our experiments indicate that the DWELL active region remains unchanged during the regrowth process, i.e. there is no significant alteration to the emission wavelength. This is key to the realization of this laser. We present characterization data of the QD-PCSEL and compare regrowth options.

Photonics 2018, 5(3), 27

Journal of Lightwave Technology, vol. 35, no. 20, 4547-4552, 2017

Crystal Growth & Design 2021, 21, 6, 3521-3527

NAMBE-MoP-42 High-Performance Core-Shell GaAsSb Nanowires on Functionalized Graphene via MBE for NIR Photodetection, Yugwini Deshmukh, Hirandeep Reddy Kuchoor, Rashmita Baruah, Joshua White, Jia Li, Shanthi Iyer, North Carolina A&T State University

This work presents the growth of high-performance, self-assisted n-i-p core-shell (C-S) GaAsSb nanowires (NWs) on surface-functionalized monolayer graphene using molecular beam epitaxy (MBE). The vertical yield of core GaAsSb NWs was carefully examined in relation to essential growth factors, including substrate temperature, Ga droplet flux, opening duration, V/III ratio, and oxygen plasma treatment duration. With an intrinsic GaAsSb section at the top to improve optical absorption, a hybrid n-i core/i-p shell architecture was designed utilizing an axial n-core Sb composition gradient design that varied from 40 at. % to 20 at. %. 4K Photoluminescence (PL) peak revealed PL emission at $\sim 1.5\ \mu\text{m}$ on graphene. Raman spectroscopy exhibited the longitudinal optical (LO) phonon mode of GaAs at $282\ \text{cm}^{-1}$, the transverse optical (TO) phonon mode of GaAs at $261\ \text{cm}^{-1}$, and the TO phonon mode of GaAsSb at $237\ \text{cm}^{-1}$. Additional confirmation of Sb's inclusion in the core-shell structure came from X-ray diffraction investigation. At a wavelength of 860 nm, electrical tests utilizing conductive atomic force microscopy (C-AFM) on a single nanowire device showed a photocurrent of $2 \times 10^{-9}\ \text{A}$ and a dark current of $10^{-11}\ \text{A}$. This led to a detectivity of $3.6 \times 10^{13}\ \text{Jones}$ at -1 V and a responsivity of 0.11 A/W. Higher responsivity ($> 10^3\ \text{A/W}$) and detectivity ($> 10^{14}\ \text{Jones}$) were attained for ensemble nanowire photodetectors on graphene, with spectral response extending beyond $1.5\ \mu\text{m}$ at -1 V. Furthermore, low cut-off frequencies and temperature-independent features were found in the photodetector's low-frequency noise and temperature-dependent capacitance-voltage (C-V) investigations, respectively. The potential of combining photodetectors with 2D platforms to improve device performance is highlighted by this work.

Bold page numbers indicate presenter

— A —

A. Carrasco, Rigo: NAMBE-MoP-4, 1
 A. Quivy, Alain: NAMBE-MoP-20, 4
 Addamane, Sadhvikas: NAMBE-MoP-41, 10
 Addame, Sadhivakas J.: NAMBE-MoP-33, 7
 Aidoo-Mensah, Clifford: NAMBE-MoP-39, 9
 Alsaad, Zinah: NAMBE-MoP-12, **3**
 Alzeidan, Ahmad: NAMBE-MoP-20, **4**
 Azam, Nurul: NAMBE-MoP-34, **8**

— B —

Baker, Lukas: NAMBE-MoP-30, 7
 Balakrishnan, Ganesh: NAMBE-MoP-24, 5;
 NAMBE-MoP-41, 10
 Baral, Dinesh: NAMBE-MoP-31, **7**; NAMBE-MoP-32, 7
 Baruah, Rashmita: NAMBE-MoP-42, 10
 Baskin, Maria: NAMBE-MoP-1, **1**
 Batchuluun, Oyut: NAMBE-MoP-35, 8
 Battaglia, Julian: NAMBE-MoP-29, 6
 Biasiol, Giorgio: NAMBE-MoP-35, **8**
 Boulares, Ibrahim: NAMBE-MoP-16, 4
 Bradicich, Adelaide: NAMBE-MoP-27, **6**
 Bussmann, Ezra: NAMBE-MoP-27, 6

— C —

Carrasco, Rigo: NAMBE-MoP-24, 5; NAMBE-MoP-7, 2
 Casallas Moreno, Yenny Lucero: NAMBE-MoP-38, 8
 Casallas-Moreno, Yenny Lucero: NAMBE-MoP-17, 4
 Cavallo, Francesca: NAMBE-MoP-33, 7
 Chen, Zijun: NAMBE-MoP-5, 2
 Chowdhury, Ruhin: NAMBE-MoP-33, **7**
 Chowdhury, Sugata: NAMBE-MoP-34, 8
 Cohen-Elias, Doron: NAMBE-MoP-1, 1
 Contreras, Edgar Agustin: NAMBE-MoP-17, **4**
 Corona-García, C. A.: NAMBE-MoP-26, 6
 Cowan, Tyler: NAMBE-MoP-30, 7
 Cresswell, Zach: NAMBE-MoP-15, 4
 Csonka, Szabolcs: NAMBE-MoP-35, 8
 Curcio, Davide: NAMBE-MoP-35, 8

— D —

Dafe, Shedrack: NAMBE-MoP-5, 2
 Daluisio, Franco: NAMBE-MoP-29, 6
 De la Torre, Alberto: NAMBE-MoP-34, 8
 de Souza, Lucas. A. T: NAMBE-MoP-20, 4
 Deshmukh, Yugwini: NAMBE-MoP-42, **10**
 Dindial, Krishna: NAMBE-MoP-30, 7
 Dluzewski, Piotr: NAMBE-MoP-11, 3
 Du, Wei: NAMBE-MoP-31, 7; NAMBE-MoP-32, 7
 Duchane, Alexander: NAMBE-MoP-7, **2**
 Durbin, Steven: NAMBE-MoP-39, 9; NAMBE-MoP-40, 9

— E —

Eickhoff, Joshua: NAMBE-MoP-16, **4**
 ELDOSE, NIROSH: NAMBE-MoP-32, 7
 Eldose, Nirosh M.: NAMBE-MoP-31, 7
 Engel-Herbert, Roman: NAMBE-MoP-2, 1
— F —
 Fabian-Jocobi, J. F.: NAMBE-MoP-26, **6**
 Fan, Shizhao: NAMBE-MoP-22, **5**; NAMBE-MoP-23, 5
 Fatemi, Valla: NAMBE-MoP-6, 2
 Fazlioglu, Benazir: NAMBE-MoP-2, 1
 Frost, Mega: NAMBE-MoP-41, 10

— G —

Gallardo Hernández, Salvador: NAMBE-MoP-38, 8
 Gallardo-Hernandez, Salvador: NAMBE-MoP-17, 4
 Gautam, Chhabindra: NAMBE-MoP-41, 10
 Gofryk, Krzysztof: NAMBE-MoP-15, 4
 Guerrero Sánchez, J.: NAMBE-MoP-26, 6

— H —

Hains, Chris: NAMBE-MoP-24, 5
 Heinrich, Carter: NAMBE-MoP-41, 10
 Hernández Martínez, Jorge Ivan: NAMBE-MoP-38, 8
 Holloway, Richard: NAMBE-MoP-29, 6
 Hrabovsky, Jan: NAMBE-MoP-4, 1
 Hurley, David: NAMBE-MoP-15, 4

— I —

Issokson, Jacob: NAMBE-MoP-30, 7
 Ithepalli, Anand: NAMBE-MoP-6, **2**
 Iyer, Shanthi: NAMBE-MoP-42, 10

— J —

Janssen, Shelby: NAMBE-MoP-29, 6
 Jena, Debdeep: NAMBE-MoP-6, 2
 Johnson, Shane: NAMBE-MoP-7, 2
 Johnson, Trent: NAMBE-MoP-21, **5**
 Joshi, Ram: NAMBE-MoP-27, 6; NAMBE-MoP-31, 7

— K —

Kang, Taein: NAMBE-MoP-9, **2**
 Kawasaki, Jason: NAMBE-MoP-16, 4
 Kiefer, Arnold: NAMBE-MoP-13, **3**
 Kim, Jong Su: NAMBE-MoP-9, 2
 Kim, Sangsoo: NAMBE-MoP-8, **2**
 Kirshstein, Arkadz: NAMBE-MoP-28, 6
 Kirti, Magdhi: NAMBE-MoP-35, 8
 Kornblum, Lior: NAMBE-MoP-1, 1
 Kozanecki, Adrian: NAMBE-MoP-11, 3
 Kuchoor, Hirandeep Reddy: NAMBE-MoP-42, 10
 Kudriavtset, Y.: NAMBE-MoP-26, 6

— L —

Law, Stephanie: NAMBE-MoP-37, 8
 Lee, Sang Jun: NAMBE-MoP-9, 2
 Levy, Ido: NAMBE-MoP-30, **7**
 Li, Jia: NAMBE-MoP-42, 10
 Liang, Yunfan: NAMBE-MoP-27, 6
 Liu, Jifeng: NAMBE-MoP-27, 6; NAMBE-MoP-3, 1
 Logan, Julie: NAMBE-MoP-12, 3; NAMBE-MoP-24, 5; NAMBE-MoP-7, 2
 López López, Máximo: NAMBE-MoP-38, 8
 López-González, L. E.: NAMBE-MoP-26, 6
 López-López, M.: NAMBE-MoP-26, 6
 López-López, Máximo: NAMBE-MoP-17, 4
 Lysak, Anastasiia: NAMBE-MoP-11, 3

— M —

Maestas, Diana: NAMBE-MoP-12, 3; NAMBE-MoP-24, 5; NAMBE-MoP-7, 2
 Makin, Robert: NAMBE-MoP-39, 9; NAMBE-MoP-40, 9
 Makk, Peter: NAMBE-MoP-35, 8
 Mantoath, H. Alan: NAMBE-MoP-14, 3
 Markowitz, Matthew Markowitz: NAMBE-MoP-25, 6
 Mathew, Juby Alphonsa: NAMBE-MoP-11, **3**
 Mautua, Collin: NAMBE-MoP-18, **4**
 May, Brelon: NAMBE-MoP-15, **4**; NAMBE-MoP-40, 9
 Mazur, Yuriy I.: NAMBE-MoP-14, 3
 McDonough, Molly: NAMBE-MoP-37, **8**
 Menasuta, T. Pan: NAMBE-MoP-28, 6
 Messecar, Andrew: NAMBE-MoP-39, **9**; NAMBE-MoP-40, 9
 Mikalsen, Melissa: NAMBE-MoP-30, 7
 Millan-Almaraz, Jesus Roberto: NAMBE-MoP-17, 4
 Milosavljevic, Marko: NAMBE-MoP-7, 2
 Miri, Mohammad Ali: NAMBE-MoP-25, 6
 Mohammadi, Sina: NAMBE-MoP-25, **6**
 Monticone, Francesco: NAMBE-MoP-25, 6
 Morath, Christian: NAMBE-MoP-12, 3;
 NAMBE-MoP-24, 5; NAMBE-MoP-7, 2

Mustakim, Ahmed: NAMBE-MoP-15, 4
 Mutlu, Zafer: NAMBE-MoP-29, 6; NAMBE-MoP-36, 8

— N —

Najmaei, Sina: NAMBE-MoP-16, 4
 Nakamura, Hiro: NAMBE-MoP-27, 6
 Nakamura, Hiroyuki: NAMBE-MoP-31, 7
 Nayir, Nadire: NAMBE-MoP-2, **1**
 Neely, Jordan P.: NAMBE-MoP-33, 7
 Newell, Alexander: NAMBE-MoP-24, **5**; NAMBE-MoP-7, 2
 Nuzhat, Samiha: NAMBE-MoP-41, 10

— O —

Oliveira, Fernando: NAMBE-MoP-32, 7
 Oliveira, Fernando Maia de: NAMBE-MoP-31, 7

— P —

Park, Suho: NAMBE-MoP-3, **1**; NAMBE-MoP-5, 2
 Prakash, Divya J.: NAMBE-MoP-33, 7
 Prok, Tamas: NAMBE-MoP-35, 8

— Q —

Qiu, Lawrence: NAMBE-MoP-28, **6**

— R —

Rable, Jeff: NAMBE-MoP-34, 8
 Rajapurohita, Amit Rohan: NAMBE-MoP-6, 2
 Rana, Farhan: NAMBE-MoP-6, 2
 Renteria, Emma J.: NAMBE-MoP-33, 7
 Reyner, Charles: NAMBE-MoP-13, 3
 Rhodes, Daniel: NAMBE-MoP-16, 4
 Rotter, Thomas: NAMBE-MoP-41, **10**

— S —

Sajkowski, Jacek M: NAMBE-MoP-11, 3
 Salamo, Gregory: NAMBE-MoP-32, 7
 Salamo, Gregory J.: NAMBE-MoP-14, 3; NAMBE-MoP-31, 7
 Salmani-Rezaie, Salva: NAMBE-MoP-30, 7
 Samanta, Chandan: NAMBE-MoP-3, 1; NAMBE-MoP-5, 2
 Sanga, Cem: NAMBE-MoP-2, 1
 Sarker, Mamun: NAMBE-MoP-29, 6
 Sarney, Wendy: NAMBE-MoP-16, 4
 Sbuels, Luca: NAMBE-MoP-35, 8
 Seth, Subhashree: NAMBE-MoP-41, 10
 Shabani, Javad: NAMBE-MoP-30, 7
 Shahed, Syed M.: NAMBE-MoP-34, 8
 Sharma, Andrei: NAMBE-MoP-41, 10
 Shetty, Satish: NAMBE-MoP-14, **3**
 Shima, Darryl: NAMBE-MoP-24, 5
 Shima, Darryl M.: NAMBE-MoP-33, 7
 Shusterman, Sergey Shay: NAMBE-MoP-1, 1
 Sicron, Noam: NAMBE-MoP-1, 1
 Singh, Arjan: NAMBE-MoP-6, 2
 Singh, Rishabh: NAMBE-MoP-6, 2
 Sinitskii, Alexander: NAMBE-MoP-29, 6
 Song, Jin Dong: NAMBE-MoP-9, 2
 Stanchu, Hryhorii: NAMBE-MoP-31, 7; NAMBE-MoP-32, 7
 Strickland, William: NAMBE-MoP-30, 7
 Strohbeen, Patrick: NAMBE-MoP-30, 7
 Suto, Mate: NAMBE-MoP-35, 8
 Sweeper, Thomas: NAMBE-MoP-29, 6
— T —
 T. Webster, Preston: NAMBE-MoP-4, 1
 Tamargo, Maria: NAMBE-MoP-25, 6
 Tóvári, Endre: NAMBE-MoP-35, 8
 Trejo-Hernández, Raul: NAMBE-MoP-17, 4
 Tubthong, Chanita: NAMBE-MoP-28, 6
— V —
 Vallejo, Kevin: NAMBE-MoP-15, 4; NAMBE-MoP-40, **9**
 van Duin, Adri: NAMBE-MoP-2, 1
 Vandervelde, Thomas E.: NAMBE-MoP-28, 6
 Vargas Hernández, Luis: NAMBE-MoP-38, **8**

Author Index

— W —

Wang, Zhichao: NAMBE-MoP-23, 5
Webster, Preston: NAMBE-MoP-12, 3;
NAMBE-MoP-24, 5; NAMBE-MoP-7, 2
Welch, Alex: NAMBE-MoP-29, 6
Welp, Eric: NAMBE-MoP-37, 8
West, Damien: NAMBE-MoP-27, 6
White, Joshua: NAMBE-MoP-42, 10
Wierzbicka, Aleksandra: NAMBE-MoP-11, 3
Wright, John: NAMBE-MoP-6, 2

— X —

Xing, Huili (Grace): NAMBE-MoP-6, 2

— Y —

Yadav, Sonam: NAMBE-MoP-4, 1
Yawit, Howard: NAMBE-MoP-29, 6

Yee-Rendón, Cristo Manuel: NAMBE-MoP-
17, 4
Yin, Yihao: NAMBE-MoP-23, 5
Yu, Fisher: NAMBE-MoP-27, 6
Yu, Shui-Qing: NAMBE-MoP-3, 1; NAMBE-
MoP-31, 7; NAMBE-MoP-32, 7
Yumigeta, Kentaro: NAMBE-MoP-29, 6
Yusufoglu, Muhammed: NAMBE-MoP-29, 6;
NAMBE-MoP-36, 8

— Z —

Zambrano Serrano, Mario Alberto: NAMBE-
MoP-38, 8
Zambrano-Serrano, M. A.: NAMBE-MoP-26,
6
Zarkesh-Ha, Payman: NAMBE-MoP-12, 3

Zeng, Yuping: NAMBE-MoP-3, 1; NAMBE-
MoP-5, 2
Zhama, Tuofu: NAMBE-MoP-3, 1; NAMBE-
MoP-5, 2
Zhang, Diandian: NAMBE-MoP-31, 7;
NAMBE-MoP-32, 7
Zhang, Qihua: NAMBE-MoP-37, 8
Zhang, Shengbai: NAMBE-MoP-27, 6
Zhao, Haiyang: NAMBE-MoP-23, 5
Zhao, Haochen: NAMBE-MoP-3, 1; NAMBE-
MoP-5, 2
Zhou, Weidong: NAMBE-MoP-41, 10
Zhydachevskyy, Yaroslav: NAMBE-MoP-11, 3
Zollner, Stefan: NAMBE-MoP-4, 1