Novel Materials
Room Hall of Ideas E-J - Session NM-MoP
Novel Materials Poster Session

NM-MoP-1 A Study of the Effect of Substrate Misorientation on the Strain Relaxation of InSb Grown on GaAs (001), ***Trevor Blaikie**, M. Tam, Y. Shi,* University of Waterloo, Canada*; A. Rahemtulla, N. Appathurai, B. Moreno,* Canadian Light Source, Inc., Canada*; Z. Wasilewski,* University of Waterloo, Canada

High quality growths of InSb crystals are vital for advancing the fabrication of subwavelength plasmonic nanostructures for Terahertz (THz) applications. InSb is uniquely suited to applications with THz plasmonics because it is the only semiconductor that intrinsically supports the excitation of surface plasmons at THz frequencies.

GaAs (001) is chosen as the substrate because of its low cost and availability. Naturally, the high lattice mismatch between InSb and GaAs of 14.6% leads to high dislocation densities. The effects of substrate misorientation were studied by using substrates with two different offcuts. Sample A was grown with 0° misorientation from the (001) planes, while sample B has a 2° misorientation towards the [010] crystallographic direction.

A synchrotron X-ray beamline, a standard diffractometer, and a scanning electron microscope were used to characterize the two samples of InSb grown by molecular beam epitaxy on GaAs substrates. X-ray diffraction (XRD) and electron channeling contrast imaging (ECCI) were used to, independently, estimate threading dislocation density (TDD) in both samples.

TDD estimates from XRD and ECCI are nearly matched and show that there are significant differences in TDD between the two samples. The TDD of sample B was 63-74% of the TDD in sample A. This reduction in TDD is linked to the substrate misorientation.

ECCI also revealed that a high density of microtwin defects were created during the growth of sample A. From XRD, three-dimensional reciprocal space maps (3D RSMs) were created for both samples. The 3D RSMs for sample A revealed that these microtwins significantly broaden the full width at half maximum (FWHM) of the 004 InSb Bragg peak, but only if the direction of the X-ray beam is parallel to the microtwin boundary lines. Evidence of such microtwin defects was not present in the ECCI or XRD of sample B.

Additionally, a novel method is proposed to visualize the 3D RSMs, allowing for the effects of strain and tilt caused by defects to be independently studied. Measurements from the standard diffractometer revealed that the FWHM of the Bragg peak is anisotropic for both samples. This effect could not be explained by the occurrence of microtwins alone. It is proposed that the anisotropic FWHM is a result of two different types of dislocations, α and β, that form in {111} glide planes. Glide velocities and nucleation energies are not equal in perpendicular directions. This leads to higher densities of β dislocations compared to the density of α dislocations.

NM-MoP-2 2DEG Transport at the Interface of $SrNbO_3/BaSnO_3$, ***Brian Opatosky**, S. Thapa, T. Tasnim, G. Rimal, P. Gemperline,* Auburn University*; S. Mahatara,* New Mexico State University*; H. Paik,* University of Oklahoma*; R. Vukelich, M. Giri, D. Hilton,* Baylor University*; B. Kiefer,* New Mexico State University*; R. Comes,* Auburn University

Following confirmation of a high carrier concentrated 2D electron gas (2DEG) at the interface of $SrNbO_3/BaSnO_3$ (SNO/BSO) via interfacial Nb 4d to Sn 5s injection, we investigate the transport properties of this 2DEG. As there can be transport contributions from the BSO 2DEG and the depleted SNO layer, we measure the carrier mobility via both temperature-dependent electronic transport and magnetic THz spectroscopy to decouple the contributions of the conducting pathways. In order to stabilize the material for measurement, we cap the $SrNbO_3$ film with a layer of $SrHfO_3$ (SHO), which provides an inert interface in terms of charge transfer. In establishing the transport properties of SNO/BSO, we provide a framework for future SNO interfacial studies.

NM-MoP-3 $SrIrO_3$ Films and Heterostructures Grown by Hybrid Molecular Beam Epitaxy, ***Tanzila Tasnim**,* Auburn University, Bangladesh*; G. Rimal, B. Opatosky,* Auburn University*; G. Sterbinsky,* Argonne National Laboratory*; M. Boebinger,* Oak Ridge Natinal Laboratory*; R. Comes,* Auburn University

The 5d iridium-based transition metal oxides have sparked considerable recently due to their ability to host unusual and exotic quantum states, originating from strong spin-orbit coupling, electron correlations, and octahedral rotations. We utilized hybrid molecular beam epitaxy to grow semi-metallic $SrIrO_3$ films and heterostructures on different substrates such as $SrTiO_3$, Nb-doped $SrTiO_3$, and LSAT. The iridium was supplied through a metalorganic precursor, iridium acetylacetonate [$Ir(acac)_3$]. The growth of the films was closely monitored using Reflected High Energy Electron Diffraction while the stoichiometry was characterized using in-situ X-ray Photoelectron Spectroscopy (XPS). To confirm the ideal growth window for the material, we used Rutherford Backscattering for comparison with XPS results. High-resolution X-ray Diffraction was used to determine the thickness of the films, lattice parameters, and in-plane coherence to the substrate. Scanning transmission electron microscopy studies were performed to investigate the strain-induced distortions and interfacial phenomena in the films. Ongoing work focuses on the synthesis of multilayer films with $SrNbO_3$ donor layers within $SrIrO_3$ films for interfacial charge transfer to produce novel electronic phases in the material.

NM-MoP-4 Characterization of MBE Grown $Fe_{0.75}Co_{0.25}$ in Composite Multiferroics, ***Katherine Robinson**,* Ohio State University*; M. Newburger, M. Page,* Air Force Research Laboratory*; R. Kawakami,* Ohio State University

Composite multiferroics contain both ferromagnetic and ferroelectric layers and are promising candidates for future magnonics applications. These materials have generated much interest recently because they present the opportunity to efficiently control magnon generation and propagation via electrical methods. The ferromagnet $Fe_{0.75}Co_{0.25}$ has many attractive properties, such as a low growth temperature and metallic behavior, making it easier to detect magnetic properties of the material electrically. $Fe_{0.75}Co_{0.25}$ has low ferromagnetic damping, allowing for more straightforward study of magnon propagation, as well as a relatively high magnetoelastic constant.[1–3] This work studies the growth and properties of epitaxial $Fe_{0.75}Co_{0.25}$ on ferroelectric materials by Molecular Beam Epitaxy and using Ferromagnetic Resonance (FMR), Brillouin Light Scattering (BLS), and Magneto-Optical Kerr Effect (MOKE). FMR and MOKE are utilized to determine the magnetic properties including damping parameters and coercivity while BLS illuminates the magnon dynamics and interactions. Leveraging the magnetoelastic nature of $Fe_{0.75}Co_{0.25}$, the multiferroic coupling is investigated by applying a voltage to the ferroelectric substrate, causing a strain unto the magnetic film, and altering the magnetic properties.

References

1. Edwards, E. R. J., Nembach, H. T. & Shaw, J. M. $Co_{25}Fe_{75}$ Thin Films with Ultralow Total Damping of Ferromagnetic Resonance. *Phys. Rev. Appl*. **11**, 054036 (2019).

2. Lee, A. J. et al. Metallic ferromagnetic films with magnetic damping under 1.4×10^{-3}. *Nat Commun* **8**, 234 (2017).

3. Schwienbacher, D. et al. Magnetoelasticity of $Co_{25}Fe_{75}$ thin films. *J Appl Phys* **126**, https://doi.org/10.1063/1.5116314 (2019).

NM-MoP-5 Multicolor Micrometer Scale Light Emitting Diodes Monolithically Grown on the Same Chip, ***Yifu Guo**, Y. Xiao, Y. Malholtra, Y. Wu, S. Yang, J. Liu, A. Pandey, Z. Mi,* University of Michigan

Micro LEDs have emerged as a strong contender for next generation display devices due to their high efficiency, fast response, high brightness, and extended lifetime. For practical applications, it is highly desired that full color LEDs can be monolithically integrated on the same chip, which, however, has remained extremely challenging to achieve via the conventional quantum well based approach. In recent years, N-polar indium gallium nitride (InGaN) based light emitting diodes on the (sub)micron scale, also known as μLEDs, that are synthesized via selective area plasma assisted molecular beam epitaxy, have achieved record levels of efficiency at the (sub)micrometer device scale, with 25% external quantum efficiency (EQE) for green emission and 8% EQE for red. Such advances are enabled by selective area plasma assisted molecular beam epitaxy, in which, unlike thin film epitaxial growths, local kinetics can be controlled by substrate mask patterning. Moreover, the selective area openings on the substrate mask naturally lead to the formation of a photonic crystal. Here, we demonstrate the effect of pattern opening diameters on the InGaN photoluminescence (PL) wavelength. We show

that, for a multiple-quantum-disk structure designed for green emission, given a certain photonic crystal lattice constant, the PL peak wavelength can vary over nearly 100 nm as the opening diameter varies over 60 nm, thereby enabling the achievement of multi-color emission for LED structures grown on a single chip in a single epitaxial step. More importantly, we have demonstrated strong coherent emission over a wide wavelength range for such nanowire photonic crystal LED structures. Their emission wavelengths can be precisely controlled and tuned by varying the design and processing parameters. Such nanowire photonic crystal devices not only enable a wide range of wavelength tuning but also lead to high efficiency and highly directional emission which is desired for future near-eye display applications. By further optimizing the design and epitaxial process, the realization of full-color emission for such unique N-polar III-nitride photonic nanostructures can be potentially realized. Work is currently in progress to demonstrate high efficiency micrometer scale green and red LEDs that can exhibit strong coherent emission.

NM-MoP-6 Bismuth Surfactant Enhancement of Surface Morphology and Film Quality of Low-Temperature Grown GaSb*, **Pan Menasuta**, K. Grossklaus, J. McElearney, T. Vandervelde,* Tufts University

Epitaxial growth of GaSb is critical for emerging mid-IR optoelectronics including thermal imaging, optical communications, LEDs, and thermophotovoltaic (TPV) cells [1-3]. Lower GaSb growth temperatures may be favorable for several reasons, ranging from compatibility with other layers that require low-temperature growth to lowered bulk mobility to prevent defects [4]. However, the surface of GaSb may degrade during growth at lower temperatures, leading to surface defects and device performance degradation. As the temperature decreases, the growth front transition from layer-by-layer to Stranski–Krastanov (SK) and eventually to the rough 3D-islanding regime. Furthermore, systematic characterization of homoepitaxial GaSb surfaces has not been done at temperatures beyond the range of 350°C to 450°C, not to mention in the presence of a surfactant [4-5].

We investigate the surface morphologies of two series of homoepitaxial GaSb(100) thin films grown on GaSb(100) substrates by MBE in a Veeco GENxplor system. The first series was grown at temperatures ranging from 290°C to 490°C and serves as the control. The second series was grown using the same growth parameters, with Bi used as a surfactant during the growth. We compared the two series to examine the impacts of Bi over the range of growth temperatures. AFM is used to characterize the surface morphology. The surface feature is investigated using SEM. Raman spectroscopy and ellipsometry are used to examine the films' properties. HRXRD is performed to analyze the film properties and any Bi incorporation. We found that the morphological evolution of the GaSb series grown without Bi is consistent with the standard surface nucleation theory, and we identified the 2D-3D transition temperature to be near 290°C. In contrast, the presence of a Bi surfactant during growth was found to significantly alter surface morphology and prevent undesired 3D islands at low temperatures. We observe a preference for hillocks over step morphology at high growth temperatures, anti-step bunching effects at intermediate temperatures, and the evolution from step-meandering to mound morphologies at low temperatures. This morphological divergence from the first series indicates that Bi significantly increases in the 2D Erlich-Schwöebel (ES) potential barrier of the atomic terraces, inducing an uphill adatom flux that can smoothen the surface. Our findings demonstrate that Bi surfactant can improve the surface morphology and film structure of low-temperature grown GaSb. Bi surfactant may also improve other homoepitaxial III-V systems grown in non-ideal conditions.

NM-MoP-7 Study the Temperature Effect on the Stability and Performance of III-Nitride HEMT Based Magnetic Fields Sensors *, **Satish Shetty**,* Institute for Nanoscience and Engineering, University of Arkansas*; A. Kuchuk,* 1Institute for Nanoscience and Engineering, University of Arkansas*; H. Mantooth,* Department of Electrical Engineering, University of Arkansas*; G. Salamo,* Institute for Nanoscience and Engineering, University of Arkansas

We investigated the reliability of $Al_{0.34}Ga_{0.66}N$/GaN micro-Hall-effect sensors under industry-relevant environmental conditions. The 2DEG formation heterostructure was grown on a GaN/sapphire template by molecular beam epitaxy. The performance and stability of Hall sensor was correlated by monitoring the Hall sensitivity, sheet density of two-dimensional electron gas, and contact resistance while the device was subjected to 200 °C thermal aging for a long-time duration of 2800 hours under atmospheric conditions. The stability and performance of $Al_{0.34}Ga_{0.66}N$/GaN micro-Hall sensors was evaluated by correlating electrical results with the micro-structural evolution of the $Al_{0.34}Ga_{0.66}N$/GaN Hall sensor heterostructure. Overall, we have found that the design $Al_{0.34}Ga_{0.66}N$/GaN Hall-effect sensors structure has yielded a stable response for a prolonged 2800 hours of thermal aging at 200 °C. The output result of Hall device was evaluated in terms of Hall sensitivity and ohmic contacts, data shows very stable performance without any significant degradation. However, at the early stage of thermal aging we notice a small change in performance but after subsequent aging sequence the performance was further stabilized and provided stable output Hall sensitivity for 2800 hours of thermal aging at 200 °C.

NM-MoP-8 Optimization of Heteroepitaxial $ZnGeN_2$/GaN Quantum Wells for Green LEDs*, M. Miller,* Colorado School of Mines*; A. Rice,* National Renewable Energy Laboratory*; D. Diercks,* Colorado School of Mines*; A. Tamboli, **Brooks Tellekamp**,* National Renewable Energy Laboratory

Newly theorized hybrid II-IV-N_2/III-N heterostructures, based on current commercialized (In,Ga)N light-emitting diodes (LEDs), are predicted to significantly advance the design space of highly efficient optoelectronics in the visible spectrum, specifically in the green to amber regions where LED efficiencies are orders of magnitude lower than other colors. Yet, there are few epitaxial studies of II-IV-N_2 materials. $ZnGeN_2$, a ternary analogue of the wide bandgap material GaN, is explored as a potential green-to- amber emitter which can be integrated into existing GaN LED heterostructures due to structural similarity. Cation-ordered $ZnGeN_2$ has a theoretical band gap of 3.4 eV, which is expected to be reduced with cation disorder. $ZnGeN_2$ is wurtzite when disordered, and is structurally and electronically similar to GaN, possessing a lattice mismatch of ~0.8%. Past work by this group has demonstrated epitaxial growth of $ZnGeN_2$ on GaN and AlN via molecular beam epitaxy (MBE) [1,2]. Here we present the first growth of well-defined quantum wells of $ZnGeN_2$ within GaN by nitrogen plasma-assisted MBE, including successful five-layer multiple quantum well (MQW) structures.

Detailed structural and elemental analysis of the heterostructures was performed, including X-ray diffraction (XRD), scanning transmission electron microscopy (STEM), energy dispersive X-ray spectroscopy (STEM-EDS), and atom probe tomography (APT). These methods demonstrate high-quality and abrupt interfaces in the heterostructures, even after multiple repeating heterointerfaces. Through changes in growth methodology, we also demonstrate methods to improve unintentional incorporations, including associated improvements in structural quality. We include reports of a full LED stack growth, including n- and p-type GaN for carrier injection, an InGaN/GaN short-period superlattice, the $ZnGeN_2$/GaN active region, and an AlGaN electron blocking layer. Together, this data demonstrates both the promise of heteroepitaxially integrated hybrid ternary/binary nitride systems along with the challenges associated with growing such systems, including an outlook on methods to improve the materials and devices.

References

[1] M. B. Tellekamp et al. Heteroepitaxial integration of $ZnGeN_2$ on GaN buffers using molecular beam epitaxy. Crys. Growth Des. 2020; 20, 3, 1868–1875.

[2] M. B. Tellekamp et al. Heteroepitaxial $ZnGeN_2$ on AlN: Growth, Structure, and Optical Properties. Crys. Growth Des. 2022; 22, 2, 1270–1275.

NM-MoP-9 Machine Learning Analysis and Predictions of PAMBE III–Nitride Growth*, **Andrew Messecar**, S. Durbin, R. Makin,* Western Michigan University

There is considerable interest in applying machine learning techniques to optimize the synthesis of crystalline materials. Already, Bayesian optimization has been employed to optimize the molecular beam epitaxy (MBE) synthesis of $SrRuO_3$ and TiN thin films. Also, dimensionality reduction techniques and clustering algorithms have been applied to identify significant features in reflection high–energy electron diffraction (RHEED) patterns for a broad range of material systems, and convolutional neural networks have been shown to be useful in the classification of RHEED spot patterns for arsenide materials. Here, we explore how supervised machine learning techniques can be utilized to understand the relationships between the plasma–assisted molecular beam epitaxy (PAMBE) growth parameter space and the quality of GaN and InN thin film samples.

Data from over 100 PAMBE growth runs of GaN and InN (each) have been organized into material–specific data sets, including substrate temperature, metal source effusion cell temperature, initial N_2 pressure, and RF power. These variables were selected, as they are the direct system parameters a machine learning model would control. Each run took place in a Perkin–

Elmer 430 MBE system equipped with an Oxford Applied Research HD–25 RF plasma source. RHEED was used as the primary quality metric, with crystallinity represented for the initial study by a binary numerical value (1 for monocrystalline and 0 for polycrystalline). The values of the growth variables were then mapped to this crystallinity label and other structural properties using supervised learning algorithms to perform both inference and prediction.

P–values corresponding to the growth parameters in each data set were measured with respect to the crystallinity; decision tree algorithms were fit to the same data for additional inference. Results from these two separate analyses were found to agree when deciding the most statistically significant synthesis variables: initial N_2 pressure and substrate temperature for GaN, and indium effusion cell temperature and initial N_2 pressure for InN. Supervised learning algorithms were subsequently trained on the synthesis data and used to predict the probability of growing monocrystalline and other metrics including the Bragg–Williams order parameter across a broad range of synthesis parameter values. The resulting machine learning–predicted growth maps agreed with conventional experimental wisdom while also providing new insight on the processing space for these materials.

This work was supported in part by the National Science Foundation (grant number DMR–2003581).

NM-MoP-10 Tuning the Emission Wavelength by Varying the Sb Composition in InGaAs/GaAsSb W-quantum Wells Grown on GaAs(001) Substrates, *.. Zon, S. Voranthamrong,* Department of Electrical Engineering, National Chung Hsing University, Taichung, Taiwan*; C. Cheng,* Department of Physics, National Central University, Chung-Li, Taiwan*; Z. Lee, T. Lo, C. Liu,* Department of Electrical Engineering, National Chung Hsing University, Taichung, Taiwan*; C. Chiang, L. Hung, M. Hsu,* Epileds Co., Ltd., Tainan, Taiwan*; W. Liu,* Department of Electrical Engineering, Yuan Ze University, Chung-Li, Taiwan*; J. Chyi,* Department of Electrical Engineering, National Central University, Chung-Li, Taiwan*;* ***Charles W. Tu****,* Department of Electrical Engineering, National Chung Hsing University, Taichung, Taiwan

Current vertical-cavity surface-emitting lasers (VCSELs) on cell phones for facial recognition are based on 940 nm VCSELs consisting of GaAs/AlAs distributed Bragg reflectors (DBRs) grown on GaAs(001) substrates. It is desirable to have longer-wavelength VCSELs, however, because the screen of a smart phone is transparent at longer wavelength (1380 nm) and because of eye safety. The maximum permissible exposure to the retina is higher for wavelength longer than 940 nm.

Long-wavelength lasers beyond 1300 nm is commonly fabricated on InP substrates, but InP-based VCSELs present many practical challenges. Thus, there is a great deal of interest in long-wavelength VCSELs, especially at 1550 nm, on GaAs substrates. Several approaches have been developed, including dilute nitrides, quantum dots, and antimonides. Here we explore strain-compensated GaAsP/InGaAs/GaAsSb W-quantum wells (W-QWs).

In this study, we investigate the effect of the Sb composition in GaAsSb on the photoluminescence (PL) wavelength. The tensile-strained GaAsP layer is inserted to compensate the compressive strain from the InGaAs/GaAsSb/InGaAs W-QWs. The samples are grown on GaAs(001) substrates by solid-source molecular beam epitaxy (MBE) with valved cracker cells for group-V materials.

Because of technical issues, our Sb flux is limited. We, therefore, vary the Sb composition in the range of 6-20% by controlling the growth temperature of GaAsSb, while the other parameters (thickness and composition) are kept constant for the $In_{0.3}Ga_{0.7}As$ and $GaAs_{0.66}P_{0.34}$ layers. All samples are grown at 520ºC, except during the growth of GaAsSb. The higher Sb composition is realized at lower growth temperature of GaAsSb.

X-ray rocking curve (XRC) measurements and simulations are performed to investigate the material composition and layer thickness. Low-temperature photoluminescence (PL) spectra are consistent with the XRC results. At the lowest Sb composition of 6%, the PL intensity is the strongest, and room-temperature PL is realized at ~1100 nm. By increasing the Sb composition in the GaAsSb layer, low-temperature (20 K) PL emits at longer wavelength up to ~1400 nm at 20% Sb while the PL intensity is the weakest. The XRC is also degraded.

In summary, this study shows that the composition of the GaAsSb layer, which can be controlled by its growth temperature, is an important factor to tune the PL wavelength. When the Sb composition is higher, the lattice mismatch with GaAs is larger, resulting in larger strain. To maintain the sample quality then requires adjusting the layer thickness of the GaAsP strain-compensation layer. This work is in progress.

NM-MoP-11 Strong Correlation in Two-Dimensional 1T- $NbSe_2$, ***Joy Hsu****, R. Birchmier, M. Altvater, V. Madhavan,* University of Illinois at Urbana-Champaign

Two-dimensional 1T-phase $NbSe_2$, a strongly correlated system, has drawn enormous attention since it was predicted to be a candidate to host quantum spin liquid.[1] However, the insulating mechanism of 1T-$NbSe_2$ is still unclear, and there is ongoing debate regarding whether the gap is dominated by Mott physics or charge transfer within each charge density wave (CDW).[2,3] More experimental studies need to be conducted to determine the potential of 1T-$NbSe_2$ to support a quantum spin liquid.

In this work, monolayer and bilayer 1T-$NbSe_2$ were grown with molecular beam epitaxy method and investigated with scanning tunneling microscopy (STM). During the growth, the film was monitored by *in situ* reflection high-energy electron diffraction, and a quenching treatment was applied to ensure retaining of the 1T-phase. The sample was further transferred to 4K-STM *via* a vacuum suitcase to avoid contamination. At low temperature, 1T-$NbSe_2$ experienced a CDW transition and displayed ordered triangular superlattice with start of David motifs, which were clearly shown by our 4K-STM. The density of states of monolayer and bilayer 1T-$NbSe_2$ was measured with scanning tunneling spectroscopy, and the gap character was discussed. Our measurements reveal that the gap feature is very sensitive to local perturbations, including CDW domains, defects, and interlayer coupling. In summary, we achieved controlled growth of monolayer and bilayer 1T-$NbSe_2$ and shed light on the delicate modulation of correlation-driven insulating states.

Acknowledgment

The work was supported by the National Science Foundation through grant DMR-200378, with partial support from the Gordon and Betty Moore Foundation through EPiQS grant 9465.

References

[1] G. Misguich, C. Lhuillier, B. Bernu, C. Waldtmann, *Phys. Rev. B* **1999**, *60*, 1064.

[2] M. Liu, J. Leveillee, S. Lu, J. Yu, H. Kim, C. Tian, Y. Shi, K. Lai, C. Zhang, F. Giustino, *Sci. Adv.* **2021**, *7*, eabi6339.

[3] Y. Nakata, K. Sugawara, R. Shimizu, Y. Okada, P. Han, T. Hitosugi, K. Ueno, T. Sato, T. Takahashi, *NPG Asia Mater.* **2016**, *8*, e321.

NM-MoP-12 Growth of Cobalt-containing Compounds for Back-End-of-Line Interconnects, ***Yansong Li****, G. Zhou, C. Hinkle,* University of Notre Dame

The resistivity of conventional metal interconnects increases rapidly with decreasing size, which greatly limits the performance of devices and causes high energy consumption. Electron scattering at surfaces and grain boundaries are found to be the main causes for this size effect. To solve this size effect issue, we synthesized two types of cobalt-containing materials, topological semimetal CoSi and delafossite metal PtCoO2, which could be promising candidates to replace currently used conventional metals. CoSi, a topological semimetal with multifold fermions, possesses unique topologically protected surface states that are expected to decrease resistivity at scaled dimensions where surface transport dominates. Here we demonstrate the growth of CoSi thin films and single-crystal CoSi nanowires by MBE. Multiple characterization techniques including RHEED, HRXRD, Raman microscopy, and TEM are utilized for optimizing growth conditions and realization of single-phase CoSi growth. Another candidate PtCoO2, a delafossite metal with an anisotropic 2D fermi surface and layered structure, is expected to have a very low in-plane resistivity even at ultra-downscaled dimensions. We achieved highly conductive PtCoO2 thin films by the technique combining shutter-controlled MBE growth and postgrowth annealing. Apart from the characterization techniques mentioned above, XPS and XRF are also utilized to detail chemical information and optimize the stoichiometry. We will show resistivity vs. dimension data for both CoSi and PtCoO2 and provide an outlook for using these materials as scaled interconnects.

NM-MoP-13 Development of $Al_XGa_{1-X}as_{1-Y}Bi_Y$ for the Next Generation of APDs, ***Matthew Carr****, N. Bailey,* University of Sheffield, UK*; M. Sharpe, J. England,* University of Surrey, UK*; R. Richards, J. David,* University of Sheffield, UK

Alloying Bismuth into GaAs has been shown to produce a marked alternation of the valence band structure. The increased spin orbit splitting energy in $Ga_{1-x}AsBi_x$ has been shown to dramatically reduce the excess noise of GaAs APDs[1]. Higher performing III-V APDs could yet be achieved by Bi alloying with $Al_{0.8}Ga_{0.2}As$ potentially promising a new family of ultra-low-noise, photodetectors. Isolating the effect that Al may have on the

incorporation of Bi will be of benefit opening up other potential material systems. This could include telecommunication APDs based on the inclusion of Bi into InAlAs, lattice matched to InP.

This study aims to investigate the synthesis and growth optimisation of $Al_xGa_{(1-x)}As_{(1-y)}Bi_y$ with a viewto understand how adding Bi to an Al containing alloy affects its material properties. We present a series of $Al_xGa_{(1-x)}As_{(1-y)}Bi_y$ structures, grown in an Omicron MBE STM reactor. Crystallographic and optical material quality was assessed using X-ray diffraction, photoluminescence, Rutherford backscattering and time of flightmeasurements.

Samples of $Al_xGa_{(1-x)}As_{(1-y)}Bi_y$ with between 0-80% Al and up to 6.2% Bi were synthesised successfully. The incorporation efficiency of Bi was unaffected by the group III substitution of Ga for Al. The inclusion of 2.5% of Al into the ternary $GaAs_{0.975}Bi_{0.025}$ showed an acute reduction in the optical quality with thePL intensity reduced by a factor of 36, with further degradation at increased Al concentrations up to 30% with loss of optical activity. Improvements to optical quality and wafer homogeneity were observed with annealing for 30s at temperatures between 400-600°C under N_2. Beyond 600°C optical quality decreased by a factor of 0.5. The bandgap reduction caused by Bi incorporation is strikingly similar to GaAs. There is a strong relation between Bi incorporation and the key growth parameters of temperature and Bi flux that is also akin to those observed in GaAs[2]. Growth temperature variation by 60 °C alone altered Bi content in the between 0.8 – 6.2%.

The study has been successful in the synthesis of $Al_xGa_{(1-x)}As_{(1-y)}Bi_y$. However further work remains in the optimization of the epitaxial growth. Optical quality remains limited by the increase in non-radiative recombination centres with alloying of Al. We attribute this increase in part due to the reduced bond stability between Al and Bi. It is however promising that the incorporation of Bi into the group V lattice site showed no sensitivity to the Al content. This reveals a non-trivial relationship between the Bi incorporation into Al containing III-V alloys.

NM-MoP-15 Epitaxial Growth of *a*-plane Mn_3Sn on *c*-plane Al_2O_3 using Molecular Beam Epitaxy, ***Sneha Upadhyay***, *T. Erickson,* Ohio University*; J. Moreno,* Universidad Autonoma de Puebla, Mexico*; H. Hall,* Ohio University*; K. Sun,* University of Michigan, Ann Arbor*; G. Cocoletzi,* Universidad Autonoma de Puebla, Instituto de fisica, Mexico*; N. Takeuchi,* Centro de Nanociencias y Nanotecnología, Universidad Nacional Autonoma de México*; A. Smith,* Ohio University

Noncollinear antiferromagnetic Weyl semimetal Mn_3Sn has become fascinating in the current times because it is one of the rare antiferromagnets that exhibits large anomalous Hall and Nernst effects[1]. For future device applications, it is necessary to grow high-quality crystalline films, which has been particularly challenging to achieve. Higo *et al.* reported a large perpendicular switching in an Mn_3Sn (01$\underline{1}$0) film grown on a MgO substrate with a W buffer layer by MBE[2]. Gao *et al.* reported the growth of Mn_3Sn (0001) on Al_2O_3(0001) with a Pt buffer layer, while Mn_3Sn (11$\underline{2}$0) was grown on *R*-plane Al_2O_3 and MgO (110) substrates using PLD[3]. In this work, we grew Mn_3Sn (11$\underline{2}$0) directly on Al_2O_3 (0001) without a buffer layer in our molecular beam epitaxy chamber. Compared to our previous single-step deposition at high temperature, which resulted in a crystalline but rough and discontiguous film, here the growth was carried with a two-step deposition method at room temperature. This method results in a smooth, epitaxial Mn_3Sn (11$\underline{2}$0) film having a thickness of ~220 nm. The growth is monitored *in-situ* using reflection high energy electron diffraction (RHEED) and measured *ex-situ* using X-ray diffraction, Rutherford backscattering, and cross-sectional STEM. We observe that the RHEED patterns are streaky, and the XRD shows a predominant single crystalline (11$\underline{2}$0)orientation. Additional results pertaining to the growth and structure, as well as empirical models, will be discussed.

Acknowledgment:

The authors acknowledge support from the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317. The authors would like to thank Dr. Eric Stinaff and his students for back-coating the sapphire (0001) substrates.

[1] S. S. Zhang *et al.*, "Many-body resonance in a correlated topological Kagome Antiferromagnet," *Physical Review Letters **125**, 046401* (2020).

[2] T. Higo *et al.*, "Perpendicular full switching of chiral antiferromagnetic order by current", *Nature**607**, 474 (2022).*

[3] D. Gao *et al.*, "Epitaxial growth of high quality Mn_3Sn thin films by pulsed laser deposition", *Applied Physics Letters **121**, 242403 (2022).*

NM-MoP-16 Surfactant Effect of Mn on AlN MBE Growth, ***Jesús Fernando Fabian Jocobi***, *R. Trejo Hernández, A. Martínez López,* Nanoscience and Nanotechnology Program, Center for Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV), Mexico*; Y. Casallas Moreno,* CONACYT-Interdisciplinary Professional Unit in Engineering and Advanced Technologies, National Polytechnic Institute, Mexico*; I. Koudriavysev,* Electrical Engineering Department, Solid State Electronic Section, Center for Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV), Mexico*; D. Olguin Melo,* Center for Research and Advanced Studies of the National Polytechnic Institute Querétaro Unit, Mexico*; S. Gallardo Hernández, M. López López,* Physics Department, Center for Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV), Mexico

Diluted magnetic III-N semiconductors (DMSs) have attracted significant attention due to their attractive applications for spintronic devices. The introduction of Mn atoms has been used to induce a ferromagnetic behavior in III-nitride materials [1], such as AlN. The presence of doping atoms on the surface during the MBE growth process can significantly influence the properties of the films [2]. In this study, we investigated the surfactant effects of Mn during the MBE growth of AlN.

The heterostructures were grown on Si (111) substrates employing a 200 nm-thick AlN buffer layer grown at 850 ºC. After the buffer growth, clear streak (1X1) reflection high-energy electron diffraction (RHEED) patterns were observed (Fig. 1). Subsequently, three layers of AlN were grown with increasing doping levels of Mn (BEP_{Mn}=1.9, 3.9 and $5X10^{-9}$ Torr, respectively). A set of samples were prepared by varying the growth temperature from 790 to 830 °C.

During the growth of AlN:Mn layers at 790 ºC, the streak (1X1) RHEED patterns were conserved, and the RMS surface roughness as evaluated by AFM was in the order of nanometers (Fig. 2). Employing secondary ion mass spectrometry (SIMS), we observed that the Mn concentration (Fig. 3), for the AlN layer grown at BEP_{Mn}= $5X10^{-9}$ Torr was in the order of $1X10^{19}$ atoms/cm^3. On the other hand, we observed a complete distinct behavior for the growth temperature of 830 °C. No significant Mn incorporation was observed by SIMS in the films, regardless of the Mn flux used. However, for this growth temperature, the appearance of a 3X RHEED reconstruction was observed in the AlN:Mn growth (Fig. 1). Furthermore, the surface of the AlN:Mn film showed a very flat morphology with a RMS roughness of 0.3 nm.

The absence of Mn incorporation in AlN layers at 830 ºC, coupled with the observed 3X surface reconstruction and a very flat surface morphology, suggest a surfactant behavior of Mn in AlN grown at these conditions. These findings contribute to the fundamental understanding of surfactant effects in III-nitride growth on Si substrates and may have implications for the optimization of AlN-based optoelectronic devices.

[1] R. Frazier et al., "Indication of hysteresis in AlMnN," *Appl. Phys. Lett.*, vol. 83, no. 9, pp. 1758–1760, 2003, doi: 10.1063/1.1604465.

2] T. F. Kuech, "Surfactants in semiconductor epitaxy," *AIP Conf. Proc.*, vol. 916, pp. 288–306, 2007, doi: 10.1063/1.2751920.

NM-MoP-17 Growth and Scattering Mechanisms of Metamorphic $In_{0.81}Ga_{0.19}As$ Quantum Wells, ***Jason Dong***, University of California at Santa Barbara*; Y. Gul,* University College London, UK*; A. Engel, C. Dempsey, S. Chatterjee,* University of California at Santa Barbara*; M. Pepper,* University College London, UK*; C. Palmstrøm,* University of California at Santa Barbara

$In_xGa_{1-x}As/In_xAl_{1-x}As$ quantum wells with high In content have potential advantages over the GaAs/AlGaAs structures for spintronics and topological quantum computing applications. In comparison to GaAs/AlGaAs quantum wells, $In_xGa_{1-x}As/In_xAl_{1-x}As$ quantum wells possess a lower electron effective mass, higher g-factor, and higher Rashba spin-orbit coupling. Due to a lack of latticed matched substrates, $In_xGa_{1-x}As/In_xAl_{1-x}As$ quantum wells are grown on lattice mismatched substrates such as GaAs and InP with a metamorphic buffer layers. However, the growth of high mobility $In_xGa_{1-x}As/In_xAl_{1-x}As$ quantum wells is hampered by enhanced interface roughness scattering from the metamorphic buffer layers and alloy scattering within the well [1].

In this work, we report the growth of modulation doped $In_{0.81}Ga_{0.19}As/In_{0.81}Al_{0.19}As$ quantum wells grown on semi-insulating InP (001) substrates. The quantum wells are characterized utilizing low temperature magnetotransport, which is performed using gated Hall bars and the van der Pauw geometry structures. Quantum wells with electron mobilities in excess of 380,000 cm^2/Vs have been grown. The electron

mobility of the $In_{0.81}Ga_{0.19}As$ quantum wells is comparable to that of the current state of the art $In_{0.75}Ga_{0.25}As$ quantum wells. The role of growth parameters on electron mobility is discussed. The low temperature electron mobility and carrier density of the quantum wells is modeled to extract the dominant scattering mechanisms that limit the mobility. The influence of an InGaAs digital alloy on the electron mobility and alloy scattering of the quantum well is investigated.

[1] Chen, C. et al. Journal of Crystal Growth **425**, 70–75 (2015).

NM-MoP-19 Light-enhanced Gating Effect at Conducting Interface of Laser MBE Grown EuO-KTO_3, ***Manish Dumen**, S. Chakraverty,* Institute of Nano Science and Technology, India

Light illumination and electrostatic gating field are two widely used stimuli for controlling electronic processes in low-dimension systems. $KTaO_3$(KTO)-based conducting interfaces have gained tremendous interest because its spin-orbit coupling strength is one order of magnitude higher than STO, which makes it a promising candidate for spintronics and optoelectronic devices. In this talk, I will present the combined effect of light illumination and electrostatic gate on the conducting EuO-KTO interface. An unusual illumination enhanced gating effect is observed for this metallic system at room temperature. This enormous change in conductance is observed even with visible light of very low power intensity of 0.5 mW along with the back gate. This unusual effect offers a new perspective for tuning the photoelectrical properties at the oxide interfaces, which can be helpful for designing advanced photoelectric devices with high performance and multifunctionality

NM-MoP-20 4.3 µm InAs/AlSb Quantum Cascade Detector Strain-Balanced to a GaSb Substrate, ***Stefania Isceri**, M. Giparakis, W. Schrenk, B. Schwarz, G. Strasser, A. Andrews,* Technische Universität Wien, Austria

Quantum cascade detectors (QCD) are high-speed, low-noise, photovoltaic detectors based on intersubband (ISB) transitions operating in the mid-infrared range at room temperature [1]. The active region of a QCD is composed of multiple periods of superlattice (SL) like structures. Each period includes an optical transition quantum well (QW) and an extraction cascade composed of thinner QWs. Previously, InAs/AlSb on InAs substrates was used for QCDs operating at 2.7 µm, because InAs offers a low effective electron mass of 0.023 m0, which increases the optical transition strength and improves responsivity [2]. In this study, we present the development of molecular beam epitaxy (MBE) techniques to produce high-quality InAs/AlSb layers for a QCD detecting at 4.3 µm on GaSb substrates. The advantages are that wavelengths longer than 1.7 µm (0.74 eV band gap) are not absorbed by the substrate and it enables subsequent waveguides and light coupling.

Before the superlattice, we tuned the temperature and the Sb flux to remove the native oxide and grow a GaSb buffer layer, which improves the surface roughness, as observed by the root mean square (RMS) surface roughness of 0.27 nm measured with atomic force microscopy (AFM).

We then optimized the growth temperature for the InAs/AlSb heterostructures. Due to the As-for-Sb exchange, the strain-compensated InAs/AlSb SLs growth is challenging. The bond strength of As is stronger than for Sb and excess As on the surface during growth preferentially forms AlAs, instead of AlSb, leading to growth defects and lattice mismatch. We adjusted the As flux, shutter sequences, and “soak” times in order to have sharp interfaces, as determined by high-resolution x-ray diffraction (HR-XRD) and AFM. The devices are Te-doped, since Si and Sn are amphoteric in GaSb and AlSb. As the dopant source, we use the volatile compound GaTe instead of the element itself. The current active region design results in the InAs to AlSb thickness ratio of 2.4:1. This is not strain balanced. To overcome this problem, we include InSb interlayers for strain balancing.

The grown QCD with contact layers was processed into 150×150 µm mesas with the 45º wedge-facet substrate illuminated geometry and then optically characterized with a Fourier transform infrared (FTIR) spectrometer and a Globar source. The spectrum shows a strong intersubband absorption at the designed wavelength of 4.3 µm. Device performance and comparisons will be presented.

1. F. Giorgetta et al., IEEE Journal of Quantum Electronics 45(8), 1039 (2009)
2. M. Giparakis, et al., Appl. Phys. Lett. 120, 071104 (2022)

NM-MoP-21 Growth and Surface Investigation of Antiferromagnetic $D0_{19}$–Mn_3Ga Thin Films on GaN (0001), ***Ashok Shrestha**, A. Abbas, D. Ingram, A. Smith,* Ohio University

In recent years, Mn_3Ga has garnered significant attention due to its exotic physical properties and potential applications in spintronic devices [1,2]. One of the most intriguing, yet less explored, phases is the hexagonal antiferromagnetic phase of Mn_3Ga ($D0_{19}$), which exhibits anomalous Hall effect and topological Hall effect in distinct temperature ranges [2]. In this presentation, we will delve into the growth and surface studies of a thin film of $D0_{19}$-Mn_3Ga on a Ga polar- GaN (0001) substrate.

The experiments are carried out in an ultra-high vacuum chamber equipped with a molecular beam epitaxy (MBE) system and a room-temperature scanning tunneling microscope (STM). Initially, the GaN epilayer is deposited on a GaN (0001) substrate at 700 ^{o}C under gallium-rich conditions, followed by the growth of $D0_{19}$-Mn_3Ga at 250 ^{o}C under manganese-rich conditions. Reflection high-energy electron diffraction (RHEED) is used during growth to monitor the sample, and the *in-plane* lattice constant is evaluated. Both RHEED and STM confirm that the grown sample exhibits epitaxial growth. Furthermore, STM measurements show atomic resolution images with multiple flat terraces and steps. The *ex-situ*-X-ray diffraction (XRD) clearly shows the Mn_3Ga 0002 peak, and the calculated *d*-spacing matched well with the step heights measured by STM. These measurements are consistent with the theoretically reported *c*-value of $D0_{19}$-Mn_3Ga. The concentration of manganese and gallium in the sample is confirmed to be 3.2:1.0 by Rutherford backscattering (RBS). Various *in-situ* and *ex-situ* measurements confirm the $D0_{19}$-Mn_3Ga growth. Further work is planned to refine the sample stoichiometry and investigate the non-collinear antiferromagnetism.

This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317.

References:

[1] L. Song, B. Ding, H. Li, S. Lv, Y. Yao, D. Zhao, and J. He, Appl. Phys. Lett. **119**, 152405 (2021).

[2] Z. H. Liu, Y. J. Zhang, G. D. Liu, B. Ding, E. K. Liu, H. Mehdi Jafri, Z. P. Hou, W. H. Wang, X. Q. Ma, and G. H. Wu, Scientific Reports **7**, 515 (2017).

NM-MoP-22 Guided Anisotropic Oxygen Transport in Vacancy Ordered Oxides, ***Jeffrey Dhas**, Y. Du,* Pacific Northwest National Laboratory

Understanding the transport processes of ions under external stimuli is critical as they govern the operation and failure mechanisms within energy-conversion systems and microelectronic devices. The atomically precise fabrication of materials through methods such as molecular beam epitaxy or pulsed laser deposition enables the reliable study of novel functional states, which can be probed to characterize relevant fundamental processes at play. Using *in situ* transmission electron microscopy, we show that oxygen migration in vacancy ordered, semiconducting $SrFeO_{2.5}$ epitaxial thin films can be guided to proceed in two different types of diffusion pathways. Depending on the pathway which the oxygen ions undertake, different polymorphs of $SrFeO_{2.75}$ can be achieved, which give rise to different ground electronic properties before reaching a metallic, fully oxidized $SrFeO_3$ phase. Utilization of oxygen tracer exchange experiments and time-of-flight secondary ion mass spectrometry helps probe the characteristics of oxygen ion transport in the system via determination of the oxygen depth profile. Additionally, *ab initio* calculations are implemented to reveal the diffusion steps and reaction intermediates. Ultimately, the underlying principles of controlling oxygen diffusion pathways and reaction intermediates which we demonstrate can be beneficial to advancing the design of structurally ordered oxides and novel devices for tailored applications.

NM-MoP-23 Impact of Unintentional Sb in the Tensile Electron Well of Type-II InAs/InAsSb Superlattices Grown on GaSb by Molecular Beam Epitaxy, ***Marko Milosavljevic**, Arizona State University; P. Webster,* Air Force Research Laboratory*; S. Johnson,* Arizona State University

High-performance materials that cover the mid-wave (3 to 5 µm) and long-wave (8 to 14 µm) infrared atmospheric transmission windows are essential for detection applications such as thermal sensing, gas detection, and infrared spectroscopy. Strain-balanced type-II InAs/InAsSb superlattices provide a high-quality material system with design flexibility in both the mid-wave and long-wave infrared regions that offer long lifetimes, robust absorption, and the ability to grow thick pseudomorphic layers on commercially available GaSb substrates. Despite many advantages,

InAs/InAsSb superlattice performance is hindered by the incorporation of unintentional Sb into the tensile InAs layer.

In this work, the impact of unintentional Sb in the tensile InAs electron well of type-II InAs/InAsSb superlattices is investigated. Several coherently strained mid and long wave superlattices are grown on (100) GaSb substrates by molecular beam epitaxy and examined using X-ray diffraction and temperature-dependent photoluminescence. The zero-order diffraction angle provides average strain and hence the average Sb mole fraction in a superlattice period. Analysis of higher order diffraction angles provides period thickness, which along with the individual layer growth times and the average strain, provides the tensile InAs and compressive InAsSb layer thicknesses. Analysis of the photoluminescence measurements provides the ground-state transition energy of the superlattice, which along with simulations of the ground state energies of the electrons and heavy-holes using a Kronig-Penney model, specify the distribution of Sb among the compressive hole well and the tensile electron well, which contains 1.8% (1.2%) unintentional Sb in the mid (long) wave superlattices.

A model of the Sb mole fraction profile in the compressive and tensile layers is developed and fit to the measured average Sb mole fractions of the compressive and tensile layers. The best-fit parameters provide the saturation and depletion rates of surface Sb and the Sb mole fraction. When the Sb shutter is opened, the compressive Sb mole fraction rapidly saturate at 41% in less than 1 s (1 monolayer); when the Sb shutter is closed, the tensile Sb mole fraction decays to a background of 0.6% in less than 3 s. Dilute amounts of Sb in the tensile electron well reduces the tensile strain, requiring a thicker well to achieve a strain balance. Analysis of the electron and heavy hole wavefunctions show that this increases the electron confinement, reducing the wavefunction overlap, and thus the optical absorption performance of the superlattice.

NM-MoP-24 Local Droplet Etching and Filling Behavior of Nanoholes in $In_{0.52}Al_{0.48}As$ Layers, ***Dennis Deutsch***, *V. Zolatanosha, C. Buchholz, K. Jöns, D. Reuter,* Paderborn University, Germany

Semiconductor quantum dots fabricated via filling of local droplet etched nanoholes in $Al_xGa_{1-x}As$ with GaAs are excellent candidates for on-demand sources of entangled photon pairs due to their low exciton fine structure splitting. However, photon emission in the $GaAs/Al_xGa_{1-x}As$ system is limited to wavelengths below 800 nm and long-haul quantum communication via the global fiber network requires sources emitting photons in the optical C-band, i. e., ca. 1550 nm. One way to tackle this challenge, is to transfer the approach of local droplet etching and re-filling to the $In_{0.53}Ga_{0.48}As/In_{0.52}Al_{0.48}As$-system lattice matched to InP. In this study we report on the influence of various growth parameters, as etching temperature, metal species and residual As pressure on the shape, areal density and size of the nanoholes, as these properties play an important role for the later quantum dot's emission characteristics. We present detailed statistical analysis of the nanohole morphology and densities that were obtained by analyzing measurements performed via atomic force microscopy and scanning electron microscopy. The areal density decreases strongly with increasing etching temperature (see Fig. 1) and the hole depth and diameter increase with increasing etching temperature. With increasing etching temperature, the nanoholes also become more and more elongated along the [011]-direction. Overgrowth of the nanoholes with $In_{0.52}Al_{0.48}As$ under As_2-atmosphere preserves the holes (see Fig. 2) and we observed that a moderate overgrowth with 50 nm $In_{0.52}Al_{0.48}As$ notably improved the number of symmetric nanoholes for samples etched at 410°C and 435°C. We found that filling the nanoholes with $In_{0.53}Ga_{0.48}As$ is possible either under As_2- or under As_4-atmosphere but it works significantly better under As_4-atmosphere. We also observed that the shape of the etched holes strongly depends on the metal species used for etching. Under the same etching conditions, the holes etched with pure Al tend to be significantly more elongated than those etched with In, as can be clearly seen in Fig. 3. Photoluminescence measurements on overgrown filled holes show that the emission wavelength shifts with the filling level of the nanoholes and QD emission in the optical C-band can be achieved when filling holes generated at etching temperatures above 435°C (see Fig. 4).

NM-MoP-25 Heteroepitaxial growth of (111)-oriented $SrTiO_3$ on ScAlN/GaN, *E. Jin, A. Lang, B. Downey, V. Gokhale,* ***Matthew Hardy***, *N. Nepal, S. Katzer, V. Wheeler,* Naval Research Laboratory

Ultra-wide bandgap (UWBG) semiconductor materials have been highly studied in recent years, owing to their attractive materials properties for high power and RF electronics. In particular, ScAlN has been an UWBG material that not only possesses a large bandgap, but also exhibits very high piezoelectric and spontaneous polarization coefficients, making it an appealing material for telecommunications and non-volatile memory applications. High quality epitaxial ScAlN films demonstrated by molecular beam epitaxy (MBE) have enabled high power density GaN field effect transistors utilizing ScAlN as a barrier layer. Heterogeneous integration of epitaxial oxides with ScAlN could realize novel hybrid electronics that can couple the added functionalities observed in oxides with this emergent semiconductor platform. For example, high-permittivity oxides such as $SrTiO_3$ (STO) could be used to greatly improve electric field management in RF high-electron-mobility transistors (HEMTs).

Integration of epitaxial STO with ScAlN comes with several challenges, including the lattice and crystal structure mismatch between a cubic and wurtzite material. In our previous work, we demonstrated that (111)-oriented STO films can be grown on AlGaN/GaN HEMT structures via a thin rutile TiO_2 buffer layer that mitigates the strain between the two different materials. We leverage that approach in this work to demonstrate the growth of STO on ScAlN/GaN HEMT structures via RF-plasma-assisted oxide MBE.

The preparation of the ScAlN surface prior to STO growth can also greatly impact both the crystal quality of the STO film and the channel electrical properties of the ScAlN/GAN heterostructure. To study the effects of surface pre-treatment prior to STO growth, we prepare the ScAlN surface with a series of different chemical cleans, including piranha acid, UV ozone and hydrofluoric acid, and a sulfuric-phosphoric acid mixture. We show that the a sulfuric-phosphoric solution results in the best combination of STO crystallinity (measured with x-ray diffraction) and ScAlN/GaN channel electrical properties (measured with Hall effect measurements). We also perform scanning transmission electron microscopy imaging to compare the impacts of the chemical cleans on the microstructure and find a significantly rougher oxide-nitride interface for the piranha-cleaned sample.

This work presents some of the growth and process optimization that is required to obtain high crystal quality epitaxial STO/ScAlN/GaN heterostructures, and can pave the way for subsequent perovskite oxide-UWBG semiconductor integration for the development of functional oxide-nitride electronics.

NM-MoP-26 Strain-Mediated Sn Incorporation and Segregation in Compositionally Graded $Ge_{1-x}Sn_x$ Epilayers Grown by MBE at Different Temperature, ***Nirosh M Eldose***, *H. Stanchu, S. Das, S. Shetty, C. Li, Y. I Mazur, S. Yu, G. J. Salamo,* University of Arkansas

Group IV alloys of Ge and Sn are extensively studied for various electronic and optoelectronic applications on a Si platform. $Ge_{1-x}Sn_x$ with α-Sn concentrations as low as 6% [1] allows for a transition from an indirect bandgap to a direct optical. Higher Sn content makes possible mid and even long-range infrared optical emission and detection [2]. At the same time, due to the low solid solubility of Sn in Ge (~1%), as well as the large lattice mismatch of α-Sn with Ge (~14%), the realization of high-quality Sn-rich $Ge_{1-x}Sn_x$ structures has proved challenging. In this study, we demonstrate enhanced Sn content using molecular beam epitaxy (MBE) growth of compositionally graded $Ge_{1-x}Sn_x$ on Ge (001). High-quality GeSn alloys with Sn composition reaching 6% at constant temperature. The maximal fraction of Sn was further increased to 9.0% when the growth temperature was continuously lowered while increasing the Sn flux. The analysis of surface droplets and SIMS (secondary ion mass spectrometry) profiles of elemental composition give evidence of Sn rejection during the growth, potentially associated with a critical energy of elastic strain. The intentional reduction of the coherent strain by decreasing the Sn flux near the sample surface has shown to trap a higher fraction of Sn in the $Ge_{1-x}Sn_x$ layer and lower surface segregation. Supporting data (Fig.2) shows an approach for XRD spectra simulation was developed for strain and composition characterization.

[1] S. Wirths, D. Buca, S. Mantl, Prog. Cryst. Growth Charact. Mater. 2016, 62 (1), 1–39.

[2] J. Bass, H. Tran, W. Du, R. Soref, S.-Q. Yu, Opt. Exp. 2021, 29 (19),30844-30856.

NM-MoP-27 Growth and Characterization of GaAs (111) on 4H-SiC for Infrared Sensor, ***Subhashis Das***, *N. M Eldose, H. Stanchu, F. Maia de Oliveira, C. Li, M. Benamara, Y. I. Mazur, G. Salamo,* University of Arkansas

Epitaxial growth of III-V semiconductors on 4H-SiC would potentially allow the integration of optical sensors on SiC based power devices. We report on the growth of high-quality crystalline GaAs layer on the SiC hexagonal substrate by molecular beam epitaxy (MBE). For fabrication on SiC, a 5 nm AlAs nucleation layer was grown at 700 °C followed by a 60 nm GaAs layer buffer grown at 600 °C. We will discuss the surface morphology, structural quality, and the optical properties of the MBE grown samples. The ω-2θ scan result (fig.1. (a)) corroborates the crystalline growth of GaAs (111) on 4H-SiC. The structural quality is further illustrated by the cross-sectional TEM image in fig. 1(b). It consists of a high-quality GaAs layer and a highly defected interface region between GaAs and the 4H-SiC substrate. This defect region is attributed to the lattice and crystal structure mismatch between substrate and film. Fig. 1(c) shows the temperature dependent photoluminescence properties of the grown structure. Good free-exciton (FE) emission has been observed at room temperature (300 K) and lower temperature (77 K). Excitingly, the optical results were comparable with the same structure grown on a GaAs substrate. Overall, these observations exhibit potential to achieve an optical emitter for sensors integrated on SiC based power device platform.

NM-MoP-28 Growth and Conductivity Control of AlN by Plasma Assisted MBE, ***Neeraj Nepal***, *M. Hardy, B. Downey, A. Lang, D. Katzer, E. Jin, D. Storm, V. Gokhale, T. Growden, D. Meyer, V. Wheeler,* U.S. Naval Research Laboratory

Aluminum nitride (AlN) is an ultra-wide direct bandgap semiconductor of interest due to its bandgap of ~6.2 eV, large critical electric field breakdown (>15 MV/cm), high saturation velocity (~2x10^7 cm/s) and high thermal conductivity. Compared to GaN, it provides higher Baliga's figure-of-merit for power devices and higher Johnson's figure-or-merit for RF devices. Realizing the full potential of this material in electronic device applications requires the ability to tailor the electrical conductivity in active AlN layers through impurity dopings.

Due to AlN's large bandgap, impurity doping is challenging. To-date there are only a few reports on achieving impurity doping of AlN by molecular beam epitaxy (MBE) [1], ion implantation, [2] and metal organic chemical vapor deposition (MOCVD) [3]. Recently, MOCVD was used to grow metal semiconductor field effect transistor structure with n-type AlN channel [4]. Still, there is limited understanding of how to control and implement repeatable impurity doping in AlN-based devices.

In this paper, we report the plasma-assisted MBE growth of ~500 nm thick Si doped AlN films grown on AlN/sapphire templates using a metal modulated epitaxy (MME) approach Specifically, the parameters of growth temperature (760-1060°C), growth rate (3.7-11.1 nm/min), and Si flux (1E17-5E19 cm^{-3}) were investigated and correlated with the resulting sheet resistance. All films were nucleated using an optimum *in-situ* cleaning Al-absorption and desorption technique monitoring the evolution of the growth surface with reflection high-energy electron diffraction. This was followed by a ~20 nm unintentionally doped AlN layer and ~500 nm Si doped AlN layers. Hall measurements show that sheet resistance increases with increasing growth rate, while a minimum resistance is attained at a mid-range thermocouple temperature of 860 °C (~688 °C real temperature). Additional results correlating XRD, AFM, and electrical measurements for the full parameter space will be discussed and related to potential defects limiting the conductivity in these films. Si-doping in AlN/sapphire templates will be compared with that on bulk substrates to determine the impact of threading dislocations on conductivity.

References:

1. H. Ahmad et al., J. Appl. Phys. 131, 175701 (2022) and references therein.
2. P. Bagheri et al., Appl. Phys. Lett. 122, 142108 (2023) and references therein.
3. Y. Taniyasu, Appl. Phys. Lett. 85, 4672 (2004).
4. M. Hiroki et al., IEEE Electron Dev. Lett. 43, 350 (2022).

NM-MoP-29 Molecular Beam Epitaxy Grown Group-IV Alloys for Infrared Photodetector and Quantum Transport Applications, ***Tyler McCarthy***, Arizona State University; *R. Basnet,* University of Arkansas; *Z. Ju, X. Qi, A. McMinn,* Arizona State University; *J. Hu, S. Yu,* University of Arkansas; *Y. Zhang,* Arizona State University

Group-IV alloys are an emerging material system for potential applications in quantum transport and infrared photodetectors while remaining CMOS compatible. By utilization of strain, magnetic fields, and light illumination, the zero-gap, diamond-cubic phase of Sn, α-Sn, is predicted to be a topological insulator, Dirac semimetal, or Weyl semimetal[1]. Focusing on the unexplored alloys with other Group-IV elements, Ge or Si, offers a novel tool to navigate the exciting boundaries of these topological phases. Additionally, SiGeSn is a model material system to demonstrate the momentum(*k*)-space charge separation (*k*-SCS) idea[2].Photodetectors with SiGeSn compositions near the indirect-to-direct bandgap transition have broad wavelength range of 2 to 22 μm covering multiple IR spectrum bands.

Both Sn-rich and Ge-rich SiGeSn samples were grown at Arizona State University by molecular beam epitaxy in a VG-V80 chamber equipped with elemental effusion cells of In, Sb, Cd, Te, Sn and Ge, and a Si sublimation source. Complete sample details investigated using quantum PPMS for quantum and magneto transport measurements and RHEED, XRD, SEM, AFM, XPS, FTIR, and TEM methods for optical and structural characterization to be presented at the conference.

For thin film α-Sn(Ge) samples, InSb substrates were chosen for lattice match conditions. The thermal oxide desorption was done under excess Sb flux at a pyrometer temperature of 480 ℃ after which temperature was lowered to 390 ℃ for Sb-rich InSb buffer growth. To separate from the conducting InSb substrate while maintaining lattice match conditions, a semi-insulating Cd-rich CdTe buffer was grown at 280 ℃. Samples were cooled overnight via contact with LN_2 shroud and thin films of α-Sn and dilute Ge-containing SnGe alloys were grown. Due to heating by the thermal radiation from the Sn and Ge effusion cells during growth, there is a temperature creep on the sample surface. Therefore, to maintain the substrate at a temperature below the α- to β-Sn phase transition, a short-pulse modulated technique, shutter cycles open for 2 seconds and shut for 10 seconds, was employed to grow the pure α-Sn samples but not for the SnGe films.

Ge-rich SiGeSn alloys with thermalization barrier between $0.4k_BT$ and $3k_BT$ were grown on Ge and GeSn virtual substrates. Ge substrate surfaces were cleaned using HF and HCl solutions prior to UHV outgas at 550 ℃, GeSn virtual substrates used HF and H_2O_2. A Ge buffer was grown at a substrate temperature of 500 ℃ before cooling down to 200 ℃ for SiGeSn growth. The Ge cell was held constant while Sn and Si fluxes were altered to obtain designed composition.

NM-MoP-30 Transport of Rare-Earth Nitrides Deposited via Molecular Beam Epitaxy, ***Kevin Vallejo***, *Z. Hua, Y. Zhang, K. Gofryk, B. May,* Idaho National Laboratory

Rare-earth nitrides have a variety of attractive physical properties including magnetic, semiconducting, and superconducting behaviors. These heavy elements have high spin orbit coupling, and their compounds could enable potential spintronic devices. However, the physical properties of these materials is intrinsically linked to crystalline quality. Thus, a systematic investigation of these properties requires high quality samples with minimal defects and tunable dopant density. Molecular beam epitaxy is an ideal tool for such synthesis and this work explored the effects of temperature, metal flux, and nitrogen plasma power on the synthesis of cerium, neodymium, and samarium nitrides on several substrates (silicon, yttria-stabilized zirconia, and fused silica) and orientations. The team performed structural characterization of these materials using atomic force microscopy, x-ray diffraction, and transmission electron microscopy. The thermal and electrical transport characteristics were identified using non-destructive, laser-based metrology techniques and resistivity measurements as a function of temperature and magnetic field. These results serve as a platform for understanding the growth conditions of elements with complex oxidation states, low vapor pressures, and large atomic masses, paving the way for the high-quality synthesis of other lanthanoid and actinoid compounds.

NM-MoP-31 High Al-Content AlGaN Grown on TaC Virtual Substrates with Metallic Conductivity, ***M. Brooks Tellekamp***, *D. Roberts,* National Renewable Energy Laboratory*; M. Miller,* Colorado School of Mines*; A. Rice,* National Renewable Energy Laboratory*; J. Hachtel,* Oak Ridge National Laboratory*; N. Haegel,* National Renewable Energy Laboratory

The lack of lattice matched substrates for AlGaN is the primary limitation to achieving high-performance power electronics, high-frequency electronics, and deep UV LEDs. This substrate limitation affects both material quality, through the formation of misfit-induced threading dislocations and strain-induced phase separation, and limitations to device geometry due to resistive or insulating electrical behavior. Dislocations and phase separation prevent AlGaN from reaching its full potential, and in the case of semiconducting substrates the primary loss mechanism in a vertically conductive device is resistive loss in the substrate itself. Thus, AlGaN alloys coulddrive disruptive technology iflong-standing substrate issues can be solved [1]. For $Al_xGa_{1-x}N$ there are competing effects of increasing alloy scattering, increased bandgap with increasing Al fraction, and decreasing dopant activation such that ideal compositions for power devices fall in the range $0.3 < x < 0.85$ [2]. For these compositions pseudomorphic growth on GaN and AlN is very difficult or impossible.

Recently we have reported the design of virtual substrates for $Al_xGa_{1-x}N$epitaxy consisting of (111) TaC_x grown on sapphire substrates via RF sputtering [3]. The crystallinity is subsequently improved by face-to-face annealing. These substrates offer several opportunities to improve power electronic devices through lattice and thermal conductivity matching, high electrical conductivity, high stability, and epitaxial liftoff.

In this talk we will discuss the growth of AlGaN on TaC templates by molecular beam epitaxy (MBE). Annealed TaC substrates show streaky-smooth reflection high-energy electron diffraction (RHEED) patterns and 6-fold rotational symmetry. The epilayers consist of $Al_xGa_{1-x}N$ in the range $0.7 < x < 1$. Using RHEED, X-ray diffraction, atomic force microscopy, and scanning transmission electron microscopy (STEM) we investigate the impact of nucleating conditions on the structure of the film and interface. During metal-rich growth we observe incommensurate RHEED features associated with laterally contracted bilayers of metal which are not observed in nitrogen-rich growth. For $Al_{0.7}Ga_{0.3}N$ we observe relaxed growth on TaC and strained growth on co-loaded AlN templates, and corresponding to this relaxed growth only the film on TaC exhibits a step-terrace structure in AFM observed as spiral hillocks. The impact of TaC defects on the AlGaN epilayer will be discussed, informed by aberration-corrected STEM.

[1] Kaplar *et al.*, *ECS J. Solid State Sci. Technol.*, 6 (2), p. Q3061, 2016.

[2] Coltrin et al., *J. Appl. Phys.*, 121, p. 055706, 2017.

[3] Roberts et al., arXiv, 2208.11769, 2022.

NM-MoP-32 Grafted AlGaAs/GeSn p-i-n Heterojunction for GeSn MIR Electrically Pumped Laser Application, ***Yang Liu***, *J. Zhou, D. Vincent, J. Gong, S. Haessly, Y. Li, Q. Zhang,* University of Wisconsin - Madison*; S. Yu,* University of Arkansas*; Z. Ma,* University of Wisconsin - Madison

In recent years, there has been significant progress in the development of germanium-tin (GeSn) lasers, which are promising candidates for applications in on-chip photonics, The recent advances in the growth of GeSn alloys have enabled the realization of high-performance GeSn lasers with improved efficiency, power output, and wavelength tunability. The electrically pumped GeSn laser diode is of much interest, as it presents the capacity of heterogeneous integration with the existing Si CMOS platform. However, the electrically pumped GeSn laser diode stops lasing at 90 K[1], due to increased free carrier absorption loss and competing non-radiative recombination at higher temperature. To get a higher operating temperature, introducing carrier confinement with heterostructures is desired[2]. However, the current epitaxy lattice-matched heterostructures, such as SiGeSn/GeSn and Ge/GeSn, shows insufficient electrical confinement to electrically driven GeSn laser at room temperature due to small band offset.

Here, we introduce a semiconductor grafting technology to form an AlGaAs/GeSn heterostructure to provide a viable approach to creating a larger band offset using the AlGaAs confinement layer[3],regardless of their respective lattice constant. In this grafting strategy, an ultrathin oxide (UO) layer is first deposited on the GeSn substrate, serving as a quantum tunneling layer and a double passivation layer. The formation of heterojunction is followed by transferring a single crystalline AlGaAs layer onto the passivated GeSn and finished by a thermal process to chemically bond them together. The introduction of the UO layer exhibits significantly suppressed interfacial density of states, which rivals the one obtained from epitaxy growth.

The grafted AlGaAs/GeSn heterojunction confines the electrons in the active GeSn layer due to the 0.324eV band offset between AlGaAs and GeSn(Figure 1a). It shows the well-passivated interfaces reflected from the uniform diode ideality factor IF~1.5(Figure 3a) in all of the 341 devices, which are similar to the IF obtained from the MBE growth[4]. And I-V measurement also reveals the benefits from a larger band offset with an On/Off ratio of around 4 orders(Figure 3a). Most of the capacity-voltage sweeping measurements are consistent when the frequency changes from 10kHz to 200kHz(Figure 3b). The formation of the high-quality AlGaAs/GeSn diode indicates the feasibility of semiconductor grafting. The preliminary diode performance has also manifested a great potential for room-temperature electrically pumped GeSn laser by employing AlGaAs/GeSn heterojunction with better electrical confinement.

NM-MoP-34 Molecular Beam Epitaxy of Kagome-Structured Antiferromagnetic FeSn Grown on $LaAlO_3$ (111), ***Tyler Erickson***, *S. Upadhyay, H. Hall, D. Ingram, S. Kaya, A. Smith,* Ohio University

Iron and tin can be alloyed to form different structures of alternating stackings of Kagome Fe_3Sn and honeycomb Sn_2 (stanene) layers. This alternating sequence results in either Fe_3Sn_2 or FeSn depending on whether there are Fe_3Sn bilayers or Fe_3Sn monolayers separating the stanene layers [1,2]. Fe_3Sn_2 and FeSn provide interesting avenues for spintronics with flat bands arising from geometrical frustration leading to novel topological phases [3]. Fe_3Sn_2 and FeSn have both been grown using molecular beam epitaxy on various substrates. [2, 4, 5] In this study, we grow FeSn by MBE following the method described by Hong et al. [2] Namely, we grew our FeSn on $LaAlO_3$ substrates at a temperature of 500 °C. The choice of using $LaAlO_3$ is based on the relatively good lattice match with difference of only 1%. Four samples have been grown with Fe:Sn flux ratios of 0.8:1, 1:1, 1.2:1, and 1.5:1. We compare the results of the 4 samples by means of RHEED, XRD, RBS, and AFM. In all cases, smooth streaky RHEED patterns are observed, and from the streak spacing we calculate the in-plane lattice constants which are then complemented by the lattice constants calculated from the XRD spectra. For the case of the 1:1 flux ratio, using RHEED we find an a = 5.290 Å as compared to the expected a_for FeSn = 5.297 Å [2] and using XRD we find c = 4.56 Å as compared to the expected c for_FeSn = 4.481 Å [2]. In this presentation, we will discuss the lattice parameters as functions of the incident flux ratios as well as the phases and phase purity of the resultant samples. We will also present results for the surface smoothness as a function of flux ratios as measured by the AFM images, and we will also address the resultant film stoichiometry as a function of incident flux ratios.

This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317.

References:

[1] L A Fenner et. al., J. Phys. Condens. Matter 21 452202 (2009).

[2] Deshun Hong et. al., AIP Advances 10, 105017 (2020).

[3] Yaofeng Xie et. al. Communications Physics 4:240 (2021).

[4] Shuyu Cheng et. al., APL Mater. 10, 061112 (2022).

[5] Igor Lyalin et. al., Nano Lett. 21, 16, 6975–6982 (2021).

NM-MoP-35 Tuning Interface Sharpness and Superconductivity at Oxide Heterostructures, ***Y. Eren Suyolcu***, Max Planck Institute for Solid State Research, Germany*; G. Kim,* Max Planck Institute for Solid State Research*; Y. Wu, G. Logvenov, P. van Aken,* Max Planck Institute for Solid State Research, Germany

The structural adaptability of transition-metal oxides allows for designing different heterostructures emerging unique physical properties at interfaces[1]. High-temperature interface superconductivity takes place at the interface between overdoped (metallic) and undoped (insulating) La_2CuO_4 layers grown by oxide molecular beam epitaxy (MBE)[2]. In addition to homo-epitaxial systems[3,4], multilayers of La_2CuO_4 combined with $La_{2-x}Sr_xNiO_4$[5], $LaNiO_3$[6,] and $LaSrMnO_3$[7] layers revealed the impact of the interface sharpness on the occurrence of superconducting[5], thermoelectric[6], and magnetic[7] properties, respectively. In this work, we designed new *cuprate–manganite* interfaces using oxide MBE[7,8] and focused on the interface sharpness and superconducting properties compared to *cuprate–cuprate* interfaces.

We probed the interfaces using scanning transmission electron microscopy (STEM) techniques, including high-angle annular dark-field (HAADF),

annular bright-field (ABF) imaging, and electron energy-loss spectroscopy (EELS).

Our findings demonstrate that hetero-epitaxial contacts with manganite layers can realize sharper Sr-doped La_2CuO_4 interfaces. The dopant distribution in La_2CuO_4 is affected by the elemental intermixing at the first atomic monolayer of the interfacial $LaMnO_3$ contact, and different superconducting behavior (*e.g.*, interface vs filamentary) can be customized with the interfacial design[8]. With such a design, we create interface superconductivity confined down to one monolayer thickness but with a cost of filamentary behavior due to local intermixing. We also demonstrate that structurally sharp interfaces can be chemically rough, and the chemical intermixing dominates the physical properties.[8]

References:

1. Y. E. Suyolcu *et al.*, *J. Supercond. Nov. Magn.* **33**, 107–120 (2020).
2. A. Gozar *et al., Nature* ***455***, 782–785 (2008).
3. Y. E. Suyolcu *et al.*, *Adv. Mater. Interfaces* ***4***, 1700737 (2017).
4. F. Baiutti *et al., Nanoscale* ***10***, 8712–8720 (2018).
5. P. Kaya *et al., ACS Appl. Mater. Interfaces* ***10***, 22786–22792 (2018).
6. Y.-M. Wu, Y. E. Suyolcu *et al., ACS Nano* ***15***, 16228–16235 (2021).
7. G. Kim *et al., Phys. Rev. Mater.* ***3***, 084420 (2019).
8. Y. E. Suyolcu *et al.*, submitted, 2023.

NM-MoP-37 Molecular Beam Epitaxial Growth of GaInAs, GaNAs and GaInNAs Nanowires over 2-inch Si(111) Substrate Showing Emission at Near Infrared Regime, ***Keisuke Minehisa**, H. Hashimoto, K. Nakama, F. Ishikawa,* Hokkaido University, Japan

Semiconductor nanowires are the materials with one-dimensional structures and are expected to be applied to next-generation optical and electronic devices. Besides, III-V compound semiconductor GaAs has high electron mobility and photoelectric conversion efficiency, and has been used for lasers, solar cells, and transistors. Monolithic structures of GaAs nanowires grown heteroepitaxially on Si substrates are thus promising for future device applications. Among them, dilute nitride GaNAs or GaInNAs are materials of interest since the introduction of few % of N into host matrix Ga(In)As provides efficient tunability of band gap and lattice constant, working at the near infrared wavelengths of solar spectrum. In this study, we report the molecular beam epitaxial growth and the characteristics of GaAs-related GaNAs and GaInNAs core-multishell nanowires on 2-inch Si(111) substrates.

We fabricated GaAs-related core-multishell nanowires samples having optically active GaInNAs, GaNAs, or GaInNAs shells, respectively, on 2-inch n-type Si(111) substrates by constituent Ga-induced vapor liquid solid growth using a plasma-assisted molecular beam epitaxy. We prepared several samples with different shell layers. GaInAs shell contains 20% In. GaNAs shell have its nitrogen concentration 1%. The concentration of In and nitrogen was 20% and 1%, respectively, for GaInNAs. After the nanowire growth, the substrate wafer was observed to be black, resulting from efficient light absorption. GaInAs, GaNAs, and GaInNAs nanowires showed PL peak at 1000, 1050, and 1100 nm, respectively at room temperature. The intensity of the GaInNAs was comparable with GaInAs and the peak width was smaller than that of GaInAs, considered to be induced by the mediation of strain deformation by the introduction of nitrogen. The results is promising for the realization of high quality GaInNAs material operating at near infrared regime.

NM-MoP-38 Tunable Superconductivity in Hybrid Interface $FeTe_{1-x}Se_x/Bi_2Te_3$ Grown by Molecular Beam Epitaxy, ***An-Hsi (Jane) Chen**,* Oak Ridge National Laboratory, USA*; Q. Lu, R. Moore, M. Brahlek,* Oak Ridge National Laboratory

Hybrid interfaces of topological insulators and s-wave superconductors are great candidates for realizing Majorana bound states which have been projected to have paradigm-changing possibilities in quantum computing. The epitaxial $FeTe_{1-x}Se_x/Bi_2Te_3$ platform possess the necessary parameters for topological states, high transition temperatures, and a high level of tunability available through doping and interfacial engineering. Recently, monolayer of superconducting $FeTe_{1-x}Se_x$ (x=0.25) grown on the Bi_2Te_3 was reported to exhibit emergent topological interfacial Dirac states at the Fermi energy. Pushing to lower Se levels reduces disorder which is critical for interrogating Majorana bound states, yet pure FeTe is not superconducting. Here we systematically interrogate how modifications to the molecular beam epitaxy growth of Bi_2Te_3 and the $FeTe_{1-x}Se_x$ can enable tailoring both superconductivity and topological properties at low Se doping levels. Low temperature transport measurement, angle resolved photoemission spectroscopy and X-ray diffraction are combined to unravel the roles of band structure, crystallinity, and superconductivity which can be tailored as a function of growth conditions. This study will reveal the complex relation of strain and charge at $FeTe_{1-x}Se_x/Bi_2Te_3$ interface which will hopefully create a robust platform for Majorana bounds states and advancing quantum devices.

This material was based on work supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division, and U.S. Department of Energy, Office of Science, National Quantum Information Sciences Research Centers, Quantum Science Center.

NM-MoP-39 Van Der Waals Epitaxy of 2D Ferromagnetic $Fe_{5-x}GeTe_2$ Films with Curie Temperature Above Room Temperature on Graphene, ***Joao Marcelo J. Lopes**, H. Lv, A. Kassa, A. da Silva, J. Herfort, M. Hanke, A. Trampert, R. Engel-Herbert, M. Ramsteiner,* Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin, Germany

Van der Waals (vdW) heterostructures combining layered ferromagnets and other two-dimensional (2D) crystals such as graphene and transition metal dichalcogenides are promising building blocks for the realization of ultra-compact devices with integrated magnetic, electronic and optical functionalities. Their implementation in various technologies depends strongly on the development of a bottom-up, scalable synthesis approach allowing to realize highly uniform heterostructures with well-defined interfaces between different 2D layered materials. It also requires that each material component of the heterostructure remains functional, which ideally includes ferromagnetic order above room temperature for 2D ferromagnets. In this contribution, we will present our recent results on van der Waals (vdW) epitaxy of the 2D itinerant ferromagnetic metal $Fe_{5-x}GeTe_2$ (FGT, x ~ 0) on single crystalline epitaxial graphene using molecular beam epitaxy. For the growth of FGT films (with thickness ranging from 10 to 15 nm), elemental Fe, Ge, and Te were co-supplied from conventional effusion cells, and a growth temperature of 300 °C was employed. As a substrate, epitaxial graphene on 4H-SiC(0001), synthesized via SiC surface graphitization, was employed. Morphological and structural characterization using methods such as atomic force microscopy, synchrotron-based grazing incidence X-ray diffraction, and scanning transmission electron microscopy (STEM) revealed that epitaxial FGT films exhibiting very good surface morphology, high crystalline quality, and a sharp interface to graphene could be realized. Interestingly, stacking faults related to the presence of single FGT layers with thicknesses exceeding those expected for the Fe_5GeTe_2 phase could be identified by STEM. We expect these to be novel FGT metastable phases with Fe composition higher than 5 and potentially enhanced magnetic properties. Temperature-dependent magneto-transport measurements and superconducting quantum interference device (SQUID) magnetometry were employed to assess the magnetic properties of the samples. Ferromagnetic order with a predominant out-of-plane magnetization was shown to persist above 350 K. Furthermore, magneto-transport also revealed that the epitaxial graphene continues to exhibit a high electronic quality. These results represent an important advance beyond non-scalable flake exfoliation and stacking methods, thus marking a crucial step toward the implementation of ferromagnetic 2D materials in practical applications.

NM-MoP-40 Molecular Beam Epitaxy of $MnBi_2Te_4$ and Bi_2Te_3/ $MnBi_2Te_4$ Heterostructures, ***Hyunsue Kim**,* University of Texas at Austin*; M. Liu,* Harvard University*; L. Frammolino, Y. Li, F. Zhang,* University of Texas at Austin*; W. Lee,* University of Chicago*; X. Li, A. MacDonald, C. Shih,* University of Texas at Austin

Intrinsic Magnetic Topological Insulator (MTI) has been widely recognized as an excellent platform to study topological surface state critical for understanding exotic quantum phenomena, including the Quantum Anomalous Hall effect and Axion insulator states. Using molecular beam epitaxy (MBE), we gain control of high-quality MnBi2Te4 thin films on Si (111) and epitaxial graphene substrates, and Bi2Te3/ MnBi2Te4 heterostructure. By combining several *in-situ* characterization techniques, we obtain critical insights toward atomical control of MBE growth of MnBi2Te4 and Bi2Te3/ MnBi2Te4 heterostructures. In specific, we extract the free energy landscape for the epitaxial relationship as a function of the in-plane angular distribution. Furthermore, with the optimized layer-by-layer growth, we map out the chemical potential and Dirac point of the thin film grown. Lastly, we observe Mn out-diffusion behavior across the interface on Bi2Te3/ MnBi2Te4 heterostructure with an abrupt Bi2Te3/

MnBi2Te4 heterostructure with an abrupt interface, we observe Mn out-diffusion behavior across the interface. These scientific insights secure the foundation for understanding growth dynamics and pave the way for the future applications of MBE for magnetic topological insulators and their heterostructure for emerging topological quantum materials.

NM-MoP-41 Effect of Spin-Orbit Field on the Magnetization Reversal in a Crystalline (Ga,Mn)(As,P) Ferromagnetic Layer, ***Seongjin Park***, *K. Lee, S. Lee,* Korea University, Republic of Korea*; X. Liu,* Unversity of Notre Dame*; M. Dobrowolska, J. Furdyna,* University of Notre Dame

Effect of current induced spin-orbit field (SOF) on the magnetization reversal have investigated in a crystalline (Ga,Mn)(As,P) ferromagnetic layer with perpendicular anisotropy. To study the dependence of SOFs on current direction, two types of Hall devices along the <110> and the <100> crystallographic directions, in which the Rashba-type and the Dresselhaus-type SOFs are collinear and orthogonal to each other have been fabricated. The current scan experiments clearly show magnetization switching in all devices regardless of current direction, which varies in 4 different crystal directions of the film. However, magnetization switching chirality in current scan hysteresis depends on the crystal direction of current flow. The effect of SOF was further studied external field scan experiments, in which Hall resistance hysteresis shows clear difference between current polarity (i.e., positive and negative currents) with increasing magnitude current. The observed SOT switching chirality in current scan hysteresis and the current polarity dependent shift of in field scan hysteresis are consistently explained with the Rashba-type and the Dresselhaus-type spin-orbit fields induced by tensile strain in the (Ga,Mn)(As,P) film. Furthermore, the differences of magnetization switching field between opposite current polarities show clear dependence on the direction of Hall devices (i.e., <110> and <100>). We have systematically measured crystalline dependences of magnetization switching process by varying magnitude of current and external field strength. From the magnitudes of hysteresis shifts between two opposite current polarities measured for the <110> and <100> Hall devices, we are able to quantify magnitudes of the Rashba-type and the Dresselhaus-type spin-orbit fields.

NM-MoP-42 Unraveling the Role of Dopant Clustering in Magnetic Impurity Doped Monolayers of Transition Metal Dichalcogenides, ***Rehan Younas***, *G. Zhou, C. Hinkle,* University of Notre Dame

Efforts to achieve above room temperature ferromagnetism in monolayers of transition metal dichalcogenides (TMDs) through substitutional doping with magnetic impurities are actively being pursued for energy-efficient logic and memory devices. However, the current limitations stem from phase separation and multi-layered growth at heavy doping levels, restricting the doping in monolayers to levels well below the threshold established by density functional theory (DFT) for above room temperature Curie temperature. On the other hand, room temperature magnetism has been frequently observed at significantly lower doping levels (0.1-1%), but this magnetism arises from a combination of substitutional dopants, point defects, contaminants, interstitials, or edge states. As a result, the origin of purely substitutional doping-induced ferromagnetism remains a subject of debate.

Toward this end, this study employs molecular beam epitaxy (MBE) to achieve up to 30% substitutional doping of vanadium (V) and iron (Fe) in a monolayer of tungsten diselenide, surpassing the doping requirements (>15%) indicated by DFT for room temperature ferromagnetism. Magnetometry measurements, however, reveal the absence of ferromagnetism down to a temperature of 4 K in these phase-pure films, with only the phase-separated films exhibiting any room temperature ferromagnetic behavior at Fe doping levels exceeding 30%. Structural characterization utilizing plan-view transmission electron microscopy reveals significant dopant clustering, even at modest doping levels (~5%), which serves as the primary factor responsible for the absence of ferromagnetism in phase-pure films. Remarkably, these observations align with DFT calculations, which predict a low formation energy for dopant clustering, leading to a weakened exchange interaction that subsequently suppresses ferromagnetism. The insights gained from this exploratory study offer a promising pathway to attain high doping densities in monolayer TMDs while emphasizing the influence of dopant clustering on the magnetic properties of the films.

NM-MoP-43 Atomic Layer Molecular Beam Epitaxy Growth of Kagome Ferrimagnet RMn_6Sn_6 (R = Rare Earth) Thin Films, ***Shuyu Cheng***, *W. Zhou, R. Kawakami,* Ohio State University

Materials with quasi-2D Kagome layers are an ideal platform for studying physics at the junction of non-trivial band topology and magnetism. In recent years, Kagome-structured ternary compounds RMn_6Sn_6 (R = rare earth) have drawn much attention due to their highly tunable physical properties. With different rare earth elements R, the magnetic anisotropy of RMn_6Sn_6 varies from within the Kagome plane (e.g. Gd) to perpendicular direction (e.g. Tb) [1, 2]. Especially for $TbMn_6Sn_6$, a large anomalous Hall conductance arises from gapped Dirac cones that are close to the Fermi level [1]. In this work, we synthesized (0001)-oriented thin films of $ErMn_6Sn_6$ and $TbMn_6Sn_6$ using atomic layer molecular beam epitaxy (AL-MBE). The structure of the sample was characterized by RHEED, AFM, and XRD. The magnetic properties were measured with SQUID, and the transport properties were measured with PPMS. We show that $ErMn_6Sn_6$ thin films exhibit easy-plane anisotropy up to room temperature, while $TbMn_6Sn_6$ exhibits uniaxial anisotropy at low temperatures. In general, the AL-MBE growth recipe can be applied to other materials in the RMn_6Sn_6 family. This work establishes RMn_6Sn_6 thin films as a highly tunable system for fundamental research and potential applications in the future.

References

[1]. Yin, et al. "Quantum-limit Chern topological magnetism in $TbMn_6Sn_6$." Nature 583.7817 (2020): 533-536.

[2]. Ma et al. "Rare Earth Engineering in RMn_6Sn_6 (R= Gd− Tm, Lu) Topological Kagome Magnets." Physical review letters 126.24 (2021): 246602.

NM-MoP-44 Investigating Phase Transformations and Stability of Pt-Te Van Der Waals Materials Through Pt Vapor Exposure and Post-Growth Annealing, ***Kinga Lasek***, Purdue University; University of South Florida

In this research, we investigate the growth and transformation of ultrathin Pt-telluride van der Waals (vdW) compounds by vacuum annealing and Pt-vapor exposure. We find that molecular beam epitaxy readily grown $PtTe_2$ thin films can be converted into Pt3Te4- and furthermore Pt_2Te_2-bilayers through vacuum-induced Te-loss. Using scanning tunneling microscopy, x-ray, and angle resolved photoemission spectroscopy, we find that Pt_3Te_4 remains thermally stable up to 350℃ while achieving Pt_2Te_2 requires a higher annealing temperature of 400℃. Interestingly, bilayer Pt_2Te_2 can be re-tellurized by exposure to Te-vapor. This causes the topmost Pt_2Te_2 layer to transform into two layers of $PtTe_2$ and, thus synthesis of Pt_2Te_3.

Additionally, we introduce a novel method to transform monolayer $PtTe_2$ into Pt_2Te_2, using vapor-deposited Pt atoms. This innovative process allows for well-defined metal-semiconductor junctions by nucleating the Pt_2Te_2 phase within $PtTe_2$. These compositional phase transformations hold significant potential for efficient in-plane metal contacts, particularly in materials with substantial spin-orbit coupling like $PtTe_2$.The comprehensive understanding of these processes enables the controlled synthesis of all known Pt-telluride vdW compounds in their ultrathin form by precisely managing Te removal or Pt addition.

Furthermore, we investigate the chemical stability of these materials through exposure to oxygen and air. Remarkably, even after extended air exposure, only the surface Te layer is modified by oxygen chemical bonds, leading to a 3-eV shift to the higher binding energy of the Te-3d core levels. However, these oxygen species can be effectively removed through vacuum annealing at 280 ℃, restoring the pristine state of Pt-telluride samples. This demonstrates the excellent air stability of these materials.

NM-MoP-45 Layer-Dependent Optical Properties of MBE-Grown $ZrTe_2$ Determined by in-Situ Spectroscopic Ellipsometry, *E. Houser,* ***Frank Peiris***, Kenyon College*; A. Richardella, M. Stanley, N. Samarth,* Pennsylvania State University

Two-dimensional transition metal dichalcogenides (TMDCs) are an interesting platform to interrogate fundamental physics questions as well as to advance the development of optoelectronic technologies. Both these endeavors are heavily dependent on having high-quality TMDCs, realized only after employing extensive growth optimization procedures. In this work, we investigated the growth and the optical properties of $ZrTe_2$, a candidate topological Dirac semimetal. During the growth of 12 unit cells (u.c.) of$ZrTe_2$ on a sapphire substrate, we obtained in-situ spectroscopic ellipsometry after the deposition of each u.c. After the deposition of the $ZrTe_2$, we deposited a Te capping layer to protect the TMDC film. X-ray reflectivity measurements performed subsequently indicated that the total thickness of $ZrTe_2$ and the thickness of Te to be 5.95 nm and 19 nm, respectively.

A standard inversion technique was used to model the ellipsometry spectra by specifying a three layer model (i.e., sapphire substrate, $ZrTe_2$ layer and the Te capping layer) to fit the final ellipsometry spectra. The thicknesses obtained from X-ray reflectivity allowed us to obtain the precise dielectric

function of the final $ZrTe_2$ layer (i.e., 12 u.c.). Subsequently, we fit the remaining ellipsometry spectra obtained for 11 u.c. through 1 u.c. $ZrTe_2$ and obtain their dielectric functions. Clearly, the dielectric functions show a noticeable change with the thickness of the $ZrTe_2$ layers, where the absorption depicted by the imaginary part of the dielectric function increases with the thickness of $ZrTe_2$. Additionally, the layer-dependent dielectric functions were analyzed by incorporating a Drude oscillator to account for the free electrons and two Kramers-Kronig-consistent oscillators to represent the band-to-band transitions. Interestingly, we find that the Drude contribution reduces as the thickness of $ZrTe_2$ gets smaller, suggesting that its metallic character diminishes as the thickness reduces. Further analysis of the optical conductivity verifies this observation.

The work at Kenyon is funded by DMR-2004812 and the work at The Pennsylvania State University Two-Dimensional Crystal Consortium – Materials Innovation Platform (2DCC-MIP) is supported by NSF cooperative agreement DMR-1539916 and DMR-2039351.

NM-MoP-46 Bi Heteroantisites at Ga(As,Bi)/(Al,Ga)As Interface: Role of the Surface Reconstruction?, ***Esperanza Luna**, A. da Silva, K. Biermann,* Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany*; J. Puustinen, J. Hilska, M. Guina,* Optoelectronics Research Centre, Tampere University, Finland*; P. Laukkanen, M. Punkkinen,* University of Turku, Finland*; A. Trampert,* Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany

Innovative growth strategies, including the use of (Al,Ga)As barriers, have been proposed to improve the performance of optoelectronic devices based on Ga(As,Bi) quantum wells (QWs). It is argued that the presence of Al might suppress the well-known Bi surface segregation but the exact role of Al is unclear, as well as its impact on the Ga(As,Bi)/(Al,Ga)As interface properties.

We investigate the interfaces of $GaAs_{0.96}Bi_{0.04}/Al_{0.15}Ga_{0.85}As$ QW structures using a combination of (scanning) transmission electron microscopy (S)TEM techniques. The samples were grown by solid source MBE on GaAs(001). The Ga(As,Bi) QWs, with nominal thickness of 7 nm, were grown at 370 °C, while the substrate temperature T_s was raised to 580 °C for the barriers growth. There were growth interruptions (GI) before and after the QW to adjust T_s and the V/III ratio. In addition to As-flux during the GI, Bi-flux was supplied just before the QW growth at the Ga(As,Bi)-on-(Al,Ga)As interface.

Our TEM investigations reveal that the layers grow pseudomorphically on the GaAs substrate. Whereas high-angle annular dark-field (HAADF) micrographs with Z-contrast show the expected sequence of layers with their expected thickness and compositions, diffraction-based chemically-sensitive $\mathbf{g}_{002}$ dark-field TEM images reveal the striking presence of "dark lines" at both Ga(As,Bi)-on-(Al,Ga)As and (Al,Ga)As-on-Ga(As,Bi) interfaces, precisely at the GI positions, delimiting the interfaces. The line at the Ga(As,Bi)-on-(Al,Ga)As interface is ~2 nm thick and remarkably well-defined. Formation of quaternary (Al,Ga)(As,Bi) at the interface may cause the features, but theoretical estimations of the $\mathbf{g}_{002}$ diffracted intensity I_{002} for (Al,Ga)(As,Bi) result in a much brighter contrast than observed experimentally. In the calculation Bi and Al are incorporated substitutionally at V- and III-element positions, respectively. Interestingly, Bi incorporation at III-element position, i.e., the presence of Bi antisites, Bi_{Ga}, has a remarkable impact decreasing I_{002} and 1% Bi_{Ga} would explain the observed contrast. EDX and HAADF-STEM reveal Ga depletion and Bi accumulation at the Ga(As,Bi)-on-(Al,Ga)As interface, consistent with the presence of Bi_{Ga} at this location. Furthermore, $CuPt_B$ atomic ordering is detected at the 7-nm thick Ga(As,Bi) QW but not at the GI positions before and after the QW, suggesting QW growth on (2x1) reconstruction. With support of density-functional-theory calculations, we discuss the role of the surface reconstruction and/or the impact of Al on Bi_{Ga} formation, a largely anticipated defect in Ga(As,Bi) yet challenging to detect.

NM-MoP-47 Substrate Preparation Methods for the MBE Growth of Van Der Waals Materials, ***Ryan Trice**, M. Yu, A. Richardella, M. Hilse, S. Law,* Penn State University

The growth of van der Waals thin films by MBE has exploded in recent years, including Bi_2Se_3,a popular prototypical 3D topological insulator. Despite the interest in these materials, the growth of high-quality Bi_2Se_3 films by MBE with low carrier density and high mobility remains challenging, in part due to a lack of understanding of the influence of the substrate. In this study, we investigate how the preparation of c-plane sapphire substrates influences film quality. Sapphire was chosen as the substrate of investigation due to its widespread use in van der Waals epitaxy. Although Bi_2Se_3 was used as the material of interest, these results are likely applicable to growth of any van der Waals material on c-plane sapphire.

The Bi_2Se_3 thin films were grown using MBE in a DCA Instruments R450 reactor. Bismuthand selenium were supplied using thermal evaporation from standard Knudsen effusion cells. All films showed streaky reflection high energy electron diffraction patterns and the expected x-ray diffraction patterns, indicative of good film growths. Further characterization was done with atomic force microscopy and room-temperature Hall effect measurements.

We explored three significant substrate preparation methods. The first was an ultra-high vacuum anneal of the substrate at 800°C for 10 minutes. This gave a 9.4% increase in mobility without noticeable change to the surface of the substrate. Second, we found that the previous use of Nano-strip®, a stabilized sulfuric acid and hydrogen peroxide mix, reduced the mobility of the film by 5-12%. It was previously thought that this reagent's ability to eliminate positive and negative resists, remove organic materials, and create an atomically smooth surface would be beneficial to the growth of thin films. However, the use of Nano-strip® likely resulted in a sulfur-terminated surface, as characterized by XPS. This sulfur-terminated surface was detrimental to good Bi_2Se_3 film growth. Third, we found that annealing sapphire at temperatures which formed a terrace-step morphology had approximately a 40% improvement in mobility of the film. Changes in the anneal temperature showed slight changes in the sapphire step heights following previous literature. Use of UV-light to clean the substrate surface showed mixed results with improvement of mobility and carrier density on less terraced surfaces but worse carrier density and mobility of the highly terraced surfaces. AFM characterization of the films showed no considerable changes in RMS roughness values. Further studies can focus on optimizing these step heights to better match Bi_2Se_3 growth conditions.

NM-MoP-49 Comparison of the Optoelectronic Properties of InGaAs and GaAsSb Absorbers on InP for 1.55 µm Avalanche Photodiodes, ***Nathan Gajowski**,* The Ohio State University*; P. Webster,* Air Force Research Lab*; S. Lee,* The Ohio State University*; P. Grant,* Air Force Research Lab*; S. Krishna,* The Ohio State University

The development of short-wave infrared Avalanche Photodiodes (APDs) operating at the 1.55 µm wavelength are critical for advancement of remote sensing and optical communication. APDs achieve internal gain through the impact ionization process, which yields a sensitive, high-speed detector that suppresses the system's circuit noise. The 1.55 µm wavelength is notable in optical communication for its low loss in optical fiber and can also be used in eye-safe LiDAR systems which, along with high atmospheric transmission and low solar background at this wavelength, enable detection at longer distances than conventional systems [1]. Separate Absorption, Charge, and Multiplication (SACM) APDs are specifically well suited to both applications due to the highly tunable device design. By separating the absorption and multiplication regions of the device, each can be optimized individually, resulting in devices with lower dark currents, lower excess noise factors, and higher gains. The InP substrate is well situated for SACM APD applications at 1.55 µm due to the availability of lattice-matched quaternary multipliers that exhibit extremely low excess noise as well as two lattice-matched bulk absorbers for this wavelength; $In_{0.47}Ga_{0.53}As$ and $GaAs_{0.50}Sb_{0.50}$ [2].

In this work, lattice-matched $In_{0.47}Ga_{0.53}As$ and $GaAs_{0.50}Sb_{0.50}$ alloys are grown on InP substrates by molecular beam epitaxy to compare their optoelectronic properties as a function of doping and evaluate their performance as the absorber volume in SACM APD applications. The band gap and Urbach energy are measured as a function of temperature using steady-state photoluminescence and evaluated using an Einstein single oscillator model to extract the frozen in disorder, average phonon energy, and electron-phonon coupling parameters. The minority carrier lifetime of each material is extracted from time-resolved photoluminescence to assess how doping modifies the minority carrier lifetime, providing insight into the optimal design of an effective absorber in an SACM APD.

NM-MoP-50 Transmission Electron Microscopy Studies of the Formation of In_2Se_3 Layers via Selenium Passivation of InP(111)B Substrates, ***Kaushini Wickramasinghe***, *C. Forrester,* City College of New York, City University of New York*; M. McCartney, D. Smith,* Arizona State University*; M. Tamargo,* City College of New York, City University of New York

Three-dimensional topological insulators (3d-TIs) are a new class of materials with their non-trivial topology giving rise to exotic metallic surface states protected by time reversal symmetry and an insulating bulk. However, exploiting the surface channels is often hindered by the presence of crystal defects, such as antisites, vacancies and twin domains. In particular, twinning is shown to be highly deleterious for terahertz device applications. Twinning reduces helicity dependent topological photocurrent, thus eliminating twinning can provide a path to chip-scale polarimeters, among other devices. In the past, it has been challenging to fully suppress the twin domains. In our previous study, we have demonstrated that the growth of fully twin-free Bi_2Se_3 and other 3D TIs on smooth non-vicinal InP(111)B substrates is feasible by incorporating a newly developed selenium (Se) passivation technique during the oxide removal process of the substrate[1]. This technique allows the formation of several quintuple layers of untwined In_2Se_3 on the InP surface that serve as the platform for the growth of twin-free Bi_2Se_3.

In this study, we investigate the structural details of the In_2Se_3 and Bi_2Se_3 layers formed by this novel technique using high resolution transmission electron microscopy (HR-TEM) and scanning transmission electron microscopy (STEM). The data show that well-ordered In_2Se_3 van der Walls layers form over the InP (111)B surface. The interface between the zinc blende InP lattice and the rhombohedral In_2Se_3 layers is abrupt and flat, and largely free of imperfections and defects. Similarly abrupt interfaces are evident at the Bi_2Se_3/In_2Se_3 interface. Additionally, STEM bright field (BF) and dark field (DF) images show clear evidence of significant Se diffusion into the substrate beyond the In_2Se_3/InP interface. The presence of this excess Se does not alter the crystal structure of the InP, which remains zinc blende. This observation suggests that during the In_2Se_3 formation process, the In atoms remain fixed in their lattice sites while Se diffuses into the substrate. When sufficient Se is present at the appropriate temperature, the lattice transforms into the rhombohedral In_2Se_3 lattice, maintaining its registry with the substrate and precluding the formation of twins. Once this twin-free In_2Se_3 layer is formed, it serves as a perfect template for twin-free Bi_2Se_3 layer or other 3D TI formation. This novel approach for forming a high quality twin free 2-dimensional crystal on a 3-dimensional zinc blende crystal lattice may have more general applications to other technologically important substrates.

1. Wickramasinghe et al. Crystals,**13**(4),677 (2023)

Author Index

Bold page numbers indicate presenter

Author Index