MBE-Grown Devices
Room Swan BC - Session GD-MoM2

Devices

Moderator: Jason Kawasaki, University of Wisconsin - Madison

10:30am **GD-MoM2-12 High Equivalent Quantum Efficiency InAs Avalanche Photodiode with Lattice Matched AlAsSb Layer**, ***Nathan Gajowski***, *M. Muduli, S. Lee, H. Jung,* The Ohio State University*; T. Basko, E. Cho,* SK Infrared*; D. Hollingshead,* The Ohio State University*; E. Fuller,* SK Infrared*; S. Krishna,* The Ohio State University

There is a growing interest in developing avalanche photodiodes (APDs) in the short-wave infrared region (SWIR, 1-3 μm). One of the primary applications for SWIR APD receivers is for eye-safe Light Detection and Ranging (LiDAR) with increased range due to the low absorption. In this work, we are developing high Equivalent Quantum Efficiency (EQE), low dark current InAs APDs for this wavelength range. InAs has a favorable bandstructure for single carrier impact ionization that leads to low excess noise. We have grown InAs APDs on InAs substrate using solid source molecular beam epitaxy. The design included a 6 μm undoped multiplication layer, a 700 *nm* *p*–type absorber with a $1x10^{17}\ cm^{-3}$ doping concentration, and a 3 μm graded absorber. The growth temperature, V/III ratio and growth rate were optimized to get low background doping. We report background doping below $1x10^{15}\ cm^{-3}$ for InAs layer as measured by capacitance voltage (CV) measurements. We have included a lattice matched AlAsSb electron blocking layer to reduce the dark current. We have fabricated single element and 4x4 arrays using standard lithography techniques. At the 2 μm operating wavelength, the devices exhibited a high equivalent quantum efficiency of 581% at the maximum voltage of 36 *V*. We are undertaking further work to understand the role of the AlAsSb layer in the impact ionization process.

10:45am **GD-MoM2-13 A High-Performance Epitaxial Transparent Oxide Thin-Film Transistor Fabricated at Back-End-of-Line Temperature (< 450 °C) by Suboxide Molecular-Beam Epitaxy**, ***Felix V.E. Hensling***, *J. Park, P. Vogt,* Cornell University*; D. Schlom,* Cornell University / Kavli Institute at Cornell for Nanoscale Science / Leibniz-Institut für Kristallzüchtung

Utilizing a recently developed variant of molecular-beam epitaxy (MBE) called suboxide MBE (S-MBE),[1] In_2O_3 films of unmatched crystalline quality are achieved as is evident from reflective high energy electron diffraction (RHEED) Fig. 1(a), root mean square roughness of the surface measured by atomic force microscopy (AFM) Fig. 1(b) and the rocking curve shown in Fig. 1(c), even at temperatures below the threshold for back-end-of-line (BEOL) fabrication, T_{sub} < 450 °C. This is based on the remarkable advantages of S-MBE for the deposition of epitaxial In_2O_3 films in comparison to conventional MBE. For conventional MBE the growth of In_2O_3 can be described by the two-step reaction: 2 In +3 O → In_2O + 2 O → In_2O_3, where the first reaction is the rate limiting step.[2] Heating a source of a carefully chosen mixture of In + In_2O_3 results in the generation of a molecular beam containing >90% In_2O molecules, thus bypassing the first step in the aforementioned two-step formation reaction of In_2O_3. In addition to eliminating this first step, supplying a molecular beam of In_2O has a second major advantage that it is a volatile species, ushering the possibility for adsorption-controlled growth. From In_2O_3 films grown by S-MBE at BEOL temperatures, transparent oxide thin film transistors (TFTs) were fabricated. It is well-established that epitaxial active layers result in TFTs with superior properties,[4] however, the epitaxial deposition of high-mobility channel layers usually requires high substrate temperatures that greatly exceed the BEOL limit. A comparison of our initial results on In_2O_3-based transparent transistors with those of the best transparent transistors in the literature (many of which are prepared at temperature above the BEOL temperature limit or are not fully transparent) is impressive as seen in Fig. 1(d). Further fine-tuning of the device architecture and film growth are expected to improve the TFT further and will be presented.

References

[1] P. Vogt, *et al.*, *APL Materials* **9**(2021) 031101

[2] P. Vogt, O. Bierwagen, *Phys. Rev. Mat.***2** (2018) 120401

[3] K.M. Adkison, *et al.*, *APL Materials***8** (2020) 081110

[4] J. Park, *et al.*, *APL Materials***8** (2020) 011110

11:00am **GD-MoM2-14 Low Temperature Crack Formation in III-V Quantum Dot Lasers Epitaxially Grown on Silicon**, ***Rosalyn Koscica***, *C. Shang, K. Parto, G. Moody, J. Bowers,* University of California, Santa Barbara

Monolithic integration of III-V films on silicon presents a scalable approach to combining high performance III-V lasers with existing silicon photonics platforms. When III-V films are epitaxially grown on Si substrate, the mismatch between coefficients of thermal expansion (CTE) causes formation of misfit dislocations (MD) and threading dislocations (TD), limiting device performance. Recent efforts in reducing TD density (TDD) for GaAs on (001) Si have resulted in levels as low as 1.5×10^6 cm^{-2}. In such low-TDD films, stress from the CTE mismatch is not relieved through dislocation formation or glide. This results in wafer bowing or film cracking, which hinder device fabrication and reduce performance. Here, we examine bowing and cracking of monolithic III-V quantum dot laser films on Si over a temperature range of 4 K to 294 K.

The structure consists of GaAs/AlGaAs grown on a GaP/(001) Si template by molecular beam epitaxy (MBE). The active region contains five InGaAs quantum wells with InAs quantum dots. Samples of varied TDD between 1×10^6 cm^{-2} and 4×10^8 cm^{-2} are investigated with different post-growth cooling rates, either slow or rapid. Additionally, different thickness stacks, thicker with lower (40%) Al content or thinner with higher (70%) Al content in AlGaAs layers, are considered. The deformation of these epitaxial structures was recently examined at temperatures between MBE growth at 540 °C and room temperature, where cracks were only found in a rapidly cooled sample with TDD 1×10^6 cm^{-2}. Here, films are further inspected from 294 K to 4 K, in the regime where samples are expected to experience no stress relief from plastic deformation through dislocation glide. At low temperature, additional cracking occurs in quenched samples of all TDD levels. The low-TDD slow-cooled sample also shows cracking at lower temperatures. However, slow-cooled samples with higher TDD remain crack-free. This identifies structural stress cases that border the critical cracking stress at room temperature, but are pushed beyond that threshold by additional CTE mismatch when cooled. Wafer curvature measurements taken at 294 K before and after cooling to 4 K indicate elastic deformation outside of cracking: macroscopic sample bowing is unchanged by local crack effects. Identifying the stress threshold that results in sample cracking is critical for the development of monolithic III-V on Si structures that capitalize on the performance advantages of low TDD without trading off structural integrity of the epitaxial film.

11:15am **GD-MoM2-15 Thin Film Engineering in Er-Doped CeO_2 for Quantum Memory**, *K. Sautter,* ***Gregory Grant***, Argonne National Laboratory; Pritzker School of Molecular Engineering, University of Chicago*; S. Sullivan,* Argonne National Laboratory*; P. Nittala, C. Ji, M. Singh, F. Heremans, S. Guha,* Argonne National Laboratory; Pritzker School of Molecular Engineering, University of Chicago

Developing a commercially available quantum memory device is essential for building wide-area ground-based quantum networks, which will yield applications like guaranteed cryptographic security that uses existing telecommunication infrastructure.However, a functional quantum memory requires the discovery of the optimal materials for these devices, and the optimization of their processing parameters. Researchers have investigated a multitude of materials that could be useful, especially diamond nitrogen-vacancy centers, silicon carbide, and rare-earth doped oxides. A particularly promising candidate for quantum memory is erbium-doped ceria (Er:CeO_2), which theoretically could yield long quantum coherence times of up to 47 ms [1]. Er:CeO_2 is also favorable due to erbium's $^4I_{15/2}$ to $^4I_{13/2}$ optical transition in the telecom-C band (~1.5 µm), which would allow for direct incorporation of Er:CeO_2 quantum memory into already-existing telecom optical fiber infrastructure with minimal signal attenuation. Recent research on MBE-grown Er:CeO_2 on Si(111) suggests that the emission lifetime of Er:CeO_2 can be further improved through thin film engineering and the reduction of Er^{3+} concentration below 1% [2].

We build on this research by doping CeO_2(111) with low Er^{3+} concentrations (<1%). We use Raman spectroscopy, atomic force microscopy (AFM), and photoluminescence excitation (PLE) spectroscopy to investigate the effects of MBE growth parameters, grown host material quality, and low Er^{3+} concentrations on Er:CeO_2 optical linewidths and emission lifetime. We expand this investigation from Si(111) to two additional substrates, GaAs(111)A and yttria-stabilized zirconia(111) (YSZ), to identify the effects of different substrates and compressive/tensile strain on PLE spectra.

[1] Kanai *et al*., arXiv:2102.02986 [quant-ph], (2021).

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11:30am **GD-MoM2-16 Hybrid MBE Growth of Metastable $SrNbO_3$ for High Mobility 2DEGs**, *S. Thapa,* Auburn University, Department of Physics*; S. Mahatara,* Department of Physics, New Mexico State University*; P. Gemperline,* Department of Physics, Auburn University*; B. Kiefer,* Department of Physics, New Mexico State University*;* ***Ryan Comes****,* Auburn University, Department of Physics

Two-dimensional electron gases (2DEGs) in complex oxide interfaces offer great promise for high-speed electronics. $BaSnO_3$ (BSO) is well known for its high mobility due to an availability of unoccupied 5s bands in Sn. $SrNbO_3$ (SNO) is a 4d transition metal oxide serving as a good donor material in interfacial oxide systems. Synthesis is challenging, however, due to the metastable nature of the d^1 Nb^{4+} cation and the challenges of delivery of refractory Nb. To that end, SNO thin films were grown using hybrid MBE (hMBE) for the first time using a tris(diethalamido)(tert-butylimido) niobium (TDTBN) precursor for Nb and an elemental Sr source on $GdScO_3$ substrates. Varying thicknesses of $SrHfO_3$ (SHO) capping layers were deposited using a precursor for Hf on top of SNO films to preserve the metastable surface. Grown films were transferred *in vacuo* for X-ray photoelectron spectroscopy studies to quantify elemental composition and Nb oxidation state. *Ex situ* studies by XANES illustrates the SHO capping plays vital role in preserving the Nb $4d^1$ metastable charge state in atmospheric conditions.

Heterostructures of SNO were also prepared on high mobility semiconductor $BaSnO_3$ (BSO) thin film surfaces to examine charge transfer between SNO and BSO across the interface. Using a combination of density functional theory (DFT) modeling of the BSO/SNO interface and *in vacuo* XPS, we find sheet carrier densities ~10^{14} e-/cm^2, which are the largest observed for SNO heterostructures. Angle-resolved XPS measurements are in agreement with the DFT model and show that the interfacial BSO layer receives ~0.3 e- per Sn ion and that there is significant electron diffusion farther into the BSO layer due to the low effective mass and highly dispersive bands of BSO. These results demonstrate that SNO can serve as a strong donor material for future 2DEG structures.

11:45am **GD-MoM2-17 Vertical AlGaN Deep-UV LEDs Grown on Si Using Nanowire-Assisted AlN Template by Molecular Beam Epitaxy**, ***Qihua Zhang****, H. Parimoo, S. Zhao,* McGill University, Canada

Aluminum gallium nitride (AlGaN) deep ultraviolet (UV) light emitting diodes (LEDs) are the ideal candidates to replace the conventional bulky, poisonous mercury lamps for deep UV light emitting in various applications. In addition, given the advantages of uniform current injection, reduced joule heating, and easy chip packaging process, fabricating vertically injected AlGaN deep UV LEDs have been an interest of research. Hitherto, existing AlGaN deep UV LEDs rely mainly on lateral injection, hindered by the insulating substrates and the difficulty of substrate removal. In this context, silicon (Si) is a promising substrate choice, given its excellent conductivity and easy removal by wet etching. Nonetheless, owing to the large lattice and thermal mismatches between AlGaN and Si, thick AlN buffer layers and costly substrate patterning processes are required in order to realize high quality AlGaN thin films on Si.

In this work, we present a new path to realize vertical AlGaN deep UV LEDs on Si by plasma-assisted molecular beam epitaxy, which exploits a nanowire-assisted AlN buffer layer [1]. By using such a technique AlGaN epilayers over a wide Al content range have been obtained. Moreover, such as-grown AlGaN epilayers can possess a surface roughness as low as 0.4 nm (rms value). Further studies suggest that such AlGaN epilayers are metal-polar. As initial device demonstration, AlGaN double-heterojunctions (DH), schematically shown in Figure 1, are used. Such devices are able to emit light from 298 nm to down to 247 nm (Figure 2). Moreover, I-V characteristics as a function of device size indicate uniform current injection, due to the use of vertical injection scheme. Current progress on optimizing the growth of AlGaN epilayers as well as the device performance will be presented as well.

12:00pm **GD-MoM2-18 Long Lifetime Mid-Wave InGaAs/InAsSb Superlattice Photodetectors with a 2× Reduction in Proton Radiation Induced Quantum Efficiency Degradation**, *A. Newell, G. Balakrishnan,* Center for High Technology Materials, University of New Mexico*; R. Carrasco,* Air Force Research Laboratory, Space Vehicles Directorate*; Z. Alsaad,* A-Tech, LLC, a BlueHalo company (ATA BlueHalo)*; J. Logan, C. Morath,* Air Force Research Laboratory, Space Vehicles Directorate*; C. Hains, M. Milosavljevic,* A-Tech, LLC, a BlueHalo company (ATA BlueHalo)*; S. Johnson,* Center for Photonics Innovation & Electrical, Computer, and Energy Engineering, Arizona State University*; J. Duran, G. Ariyawansa,* Air Force Research Laboratory, Sensors Directorate*; D. Maestas,* ***Preston T. Webster****,* Air Force Research Laboratory, Space Vehicles Directorate

In the years to come, manufacturable sensors tolerant of the space radiation environment will be critically important to outfit increasingly larger networks of satellites that our society has come to depend on. III-V materials have long been the workhorse of the telecom industry due to their high yield of manufacturing and performance in the short-wave infrared, thus there could be great value in leveraging the manufacturing capability built up in this industry if one could extend their operability to longer wavelengths. In one III-V solution discussed here, InAs/InAsSb superlattices already in use today can be significantly improved by the inclusion of Ga in an InGaAs/InAsSb superlattice. Work in 2021 demonstrated that these materials can be produced with minority carrier lifetimes exceeding 1 µs, and since then lifetimes in the range of 0.8-2.5 µs have been demonstrated, depending on the active region doping.

In this work, the lifetime, quantum efficiency (QE), and dark current of 5.3 µm wavelength cutoff InGaAs/InAsSb *n*B*n* photodetectors are examined as a function of *n*-type doping and proton radiation. Undoped InGaAs/InAsSb *n*B*n*'s exhibit the longest lifetime of 2.5 µs, maximizing QE but at the expense of higher diffusion dark current enhanced by its smaller lifetime×doping product. Doping degrades the *n*B*n*'s lifetime with a slight negative impact on QE, but yields an overall higher signal-to-noise ratio. A doping grade offers the best performance, as it offers the lower dark current of doped material while imparting an electric field across the detector's active region that enhances carrier collection. This graded *n*B*n* exhibits the same signal-to-noise as its constant-doped counterpart, but its QE degrades at half the rate when subjected to proton irradiation, resulting in a more radiation-tolerant detector.

The minority carrier lifetime, QE, and dark current are examined as a function of temperature and voltage before and after 64 MeV proton irradiation, and as a function of proton fluence up to 7.5×10^{11} cm^{-2}. The lifetime and device samples are held at operating temperature and evaluated as a function of step-wise proton dose throughout radiation experiments to eliminate thermal annealing effects that would not occur in space, which would compromise the proton damage analyses. Characterizing all of these metrics on the same materials provides insight into the fundamental physics governing these detector's operation in the space environment. The performance of these detectors are compared to the aggregate of over 30 III-V *n*B*n*'s that have been evaluated in our lab.

Novel Materials
Room Swan BC - Session NM-MoM1
Nitrides

Moderator: Bharat Jalan, University of Minnesota

7:45am **NM-MoM1-1 Welcome, Introductions and Sponsor Thank Yous**,

8:00am **NM-MoM1-2 MBE Growth and Properties of Ultra-wide Bandgap Oxide Layers Spanning 5.0 - 9.0 eV Energy Gaps**, ***Debdeep Jena****,* Cornell University **INVITED**

8:30am **NM-MoM1-4 Demonstration of $Sc_{0.2}Al_{0.8}N$ HEMT Structures with a Sheet Resistance of 150 Ω/□ and a Sheet Charge of 5.9×10^{13} cm^{-2} with Phase Pure, Metal Rich Growth**, ***Zachary Engel****, K. Motoki, W. Doolittle,* Georgia Institute of Technology

ScAlN alloys are of great interest in recent years due to their high spontaneous and piezoelectric polarization and their ferroelectric properties, in addition to the fact that ScAlN is lattice matched to GaN at a composition of ~20% Sc. Due to the immense spontaneous polarization coefficients of the alloy, even in the case of being lattice matched to GaN where piezoelectric polarization will have no effect, a sheet charge as high

as ~6x10^{13} cm^{-2}has been predicted in literature due solely to spontaneous polarization. Thanks to these favorable properties, a number of $Sc_xAl_{1-x}N$/GaN HEMT structures have been demonstrated, achieving sheet resistances as low as 167 Ω/□ and mobilities as high as 1556 cm^2/vs most often requiring an AlN interlayer to achieve good performance. However, a number of growth issues have plagued the alloy that must be overcome to achieve the theoretical potential of the system. Previously, ScAlN was deposited via RF sputtering, which often yielded material that was polycrystalline and/or contained a high defect density, degrading device performance. MOCVD films have been grown but the limited volatility of Sc-precursors limits growth rates. In recent years, MBE growth of single phase ScAlN has been demonstrated with high crystal quality, allowing for HEMT properties to be advanced to the excellent metrics listed above. However, a challenge still remains in MBE growth of ScAlN in the form of metal rich growth. In traditional III-Nitride MBE growth, metal rich growth has led to an improvement of crystal quality and both surface and interface roughness. Thus far, attempts to grow ScAlN under metal rich conditions have faced the issue of multiple intermetallic Al_xSc_y phases being thermodynamically stable under metal rich conditions and the phase transition of ScAlN from wurtzite towards rock salt that occurs around 40% Sc, leading to the inclusion of unintended metal and rock salt phases in previous metal rich growth.

$Sc_{0.2}Al_{0.8}N$ high electron mobility transistor (HEMT) structures are grown with a simple two-layer structure and fabricated contacts, demonstrating a sheet resistance (R_s) of 150 Ω/□, a mobility of 700 cm^2/Vs, and a sheet charge of 5.9x10^{13} cm^{-2}. To achieve these properties, growth conditions for a metal rich form of molecular beam epitaxy (MBE) called metal modulated epitaxy of $Sc_{0.2}Al_{0.8}N$ growth was explored. While metal-rich MBE has been challenging because it normally leads to mixed wurtzite, rock salt and intermetallic phases, here phase pure, metal rich growth was demonstrated with a x ray diffraction 002 FWHM as low as 229 arcsec and an atomic force microscopy (AFM) RMS roughness as low as 0.8 nm.

8:45am **NM-MoM1-5 Influence of Nucleation Schemes on Crystal Quality of Heteroepitaxial $Sc_{0.4}Al_{0.6}N$**, ***Matthew Hardy***, *A. Lang, E. Jin, N. Nepal, S. Katzer, V. Wheeler,* U.S. Naval Research Laboratory

$Sc_xAl_{1-x}N$ thin films have attracted significant attention due to their very large piezoresponse for compositions up to x = 0.43, recent demonstrations of ferroelectric switching, and potential for improved output power in GaN-based transistors. Maintaining phase-pure and high crystal quality $Sc_xAl_{1-x}N$ at high x is critical to increase resonator bandwidth and to reduce insertion loss, coercive field strength, and leakage in ferroelectric devices.

In this work, we show the importance of layer nucleation—both an AlN interlayer, and the initial ScAlN layer—to the final crystal quality of ScAlN films grown on 4H-SiC substrates. Very thin AlN layers, grown at standard molecular beam epitaxy growth conditions (840 °C estimated substrate temperature, III/V = 1.05) have a large impact on both the surface evolution, as observed though reflection high-energy electron diffraction (RHEED), and in the final X-ray diffraction (XRD) 0002 reflection full-width at half maximum (FWHM). AlN layers grown on SiC show streaky, narrow RHEED patterns, indicating a smooth, well-ordered surface, for film thicknesses as low as 5 nm. With the inclusion of a 5-nm AlN interlayer, the $Sc_{0.32}Al_{0.68}N$ XRD FWHM decreases from 7200 arcsec to 4100 arcsec. The RHEED pattern evolution also improves, showing well a well-defined spotty pattern after only 30 nm of subsequent $Sc_{0.32}Al_{0.68}N$ growth.

In addition to the AlN interlayer, the method of initiation of the ScAlN layer also has a strong impact on the final quality of the film. Initiation using a linear composition grade from $Sc_{0.32}Al_{0.68}N$ to $Sc_{0.40}Al_{0.60}N$ over 100 nm leads to further improvements in the RHEED pattern, including a narrowing of the spots early in the growth, and elimination of remaining ring-like character in the final RHEED pattern following an additional 50 nm of $Sc_{0.40}Al_{0.60}N$ growth, resulting in an XRD FWHM as low as 4400 arcsec. The graded sample has the same average ScN fraction and thickness as the two-step sample. Surprisingly, the grade thickness can be reduced to 25 nm (with the remaining 125 nm $Sc_{0.40}Al_{0.60}N$) without degrading the XRD FWHM or RHEED pattern. Finally, a 500-nm-total-thickness sample (100 nm $Sc_{0.32}Al_{0.68}N$ → $Sc_{0.40}Al_{0.60}N$, 400 nm $Sc_{0.40}Al_{0.60}N$) showing a reduction in XRD FWHM to 3190 arcsec. The influence of layer initiation suggests that large abrupt changes in chemical composition (surface energy) and strain promote nucleation of thermodynamically unfavorable anomalous cubic grains, and may point to a general strategy for elimination of anomalous grains in high ScN fraction ScAlN.

9:00am **NM-MoM1-6 Realization of AlN Homojunction PN Diodes**, ***Christopher M. Matthews***, Georgia Institute of Technology*; H. Ahmad,* Georgia Institute of Technology, Pakistan*; Z. Engel, K. Motoki, S. Lee, W. Doolittle,* Georgia Institute of Technology

With a direct band gap of 6.1 eV, aluminum nitride (AlN) has traditionally been classified as an insulator. Prior to this work, difficulty doping AlN proved to be the main obstacle preventing the use of AlN beyond structural or insulating layers in semiconductor devices. P-type conductivity of AlN has been a major challenge with the only success being reports of surface conductivity via carbon doping, but no substantial bulk doping [1]. N-type AlN has only been reported in near surface regions or as limited to ~10^{15} cm^{-3} in bulk films [2].

Our recent success in bulk doping of AlN could open the door to AlN-based deep ultraviolet emitters, high performance power electronics, radio frequency devices, and extreme environment devices. In this work, we will demonstrate (1) substantial bulk p-type AlN ($p = 3.1 \times 10^{18}$ cm^{-3}), (2) the highest reported Si-doped n-type AlN ($n = 6 \times 10^{18}$ cm^{-3}, nearly 6000 times the prior state-of-the-art), and (3) the first homojunction PN AlN diode with a nearly ideal turn-on voltage of ~6 V and current rectification of ~6 orders of magnitude.

Low temperature metal-modulated epitaxy (MME) was used to reduce the number of compensating impurities introduced during growth. This low temperature growth yields a lower impurity flux from heated structural components of the growth chamber. Additionally, we theorize that less thermal expansion of the lattice during growth inhibits the formation of compensating Si-DX and O-DX centers in the n-type AlN. The dopant elements (Be and Si) were chosen to reduce compensation (via undesired interstitial configurations) by providing candidates for substitutional impurities that closely match aluminum in size.

Semiconducting AlN requires highly crystalline material. However, a dense layer of stacking faults can form due to the presence of surface oxides on AlN and initiate threading dislocations at the fault edges. Using Al-flashing [3], we have removed the surface oxides and defects as seen with TEM. The effects of varying the number Al-flashing cycles on device performance will be presented by comparing current-voltage-temperature behavior with TEM.

References

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9:15am **NM-MoM1-7 MBE AlScN/GaN Heterostructures Showing High-K, Ferroelectricity, and High Mobility 2DEGs**, ***Joseph Casamento***, *H. Lee, V. Gund, T. Maeda, K. Nomoto,* Cornell University*; S. Mu,* University of California, Santa Barbara*; W. Turner,* University of Notre Dame*; L. van Deurzen, Y. Shao, T. Nguyen, B. Davaji, M. Javad Asadi, J. Wright,* Cornell University*; P. Fay,* University of Notre Dame*; C. Van de Walle,* University of California, Santa Barbara*; A. Lal, D. Muller, H. Xing, D. Jena,* Cornell University

Epitaxial $Al_{1-x}Sc_xN$ with compositions near 18% Sc (x=0.18) of ~100 nm thickness grown on metal polar GaN by plasma-assisted molecular beam epitaxy (MBE) is found to exhibit enhanced relative dielectric permittivity (ε_r) and signs of ferroelectric behavior. The measured ε_r for $Al_{1-x}Sc_xN$ reaches a value of ~21 at x=0.25, which is larger than a 2x enhancement relative to AlN (ε_r~9). Ferroelectric behavior, with measured remnant polarization (P_r) and coercive field (E_c) values ranging from 10 to 15 μC/cm^2 and 0.7 to 1.2 MV/cm, respectively. In addition, epitaxial integration strategies and insight into the electron transport mechanisms of AlScN/AlN/GaN based 2DEGs with room temperature electron mobilities of ~1600 cm^2/Vs are discussed.

Currently wide-bandgap, gallium nitride semiconductor based high electron mobility transistors (HEMTs) use AlGaN/GaN or AlN/GaN heterojunctions to generate high density 2D electron gases due to the polarization discontinuity. The combination of 2DEGs with mobilities greater than silicon channels and a wider energy bandgap than silicon has established the Al(Ga)N/GaN semiconductor system as the leading contender for energy-efficient power electronics and microwave applications for 6G and beyond.[1]

Alloying AlN with transition metals such as scandium (Sc) introduces new physical phenomena into the nitride semiconductor family by increasing bond ionicity. This allows for enhanced piezoelectricity,[1] and an enhancement in the relative dielectric permittivity is attributed to local bond distortions and bond softening along the c-axis.[2]With softer out-of-plane bonds, an electric field along the *c* axis induces larger atomic displacement and polarization change, giving rise to the enhanced dielectric response. These structural distortions are also related to the metastable nature of the ternary alloy system and the traversal through a ferroelectric phase transition.[3] Epitaxial AlScN barrier layers in AlN-GaN heterostructures show 2DEG room temperature electron mobilities of ~1600 cm^2/Vs. The epitaxial integration of the dielectric and ferroelectric properties of AlScN with nitride semiconductors aims to enhance the performance and increase the functionality of nitride electronic and photonic devices.

References

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9:30am **NM-MoM1-8 Realizing GaN/AlN Short Period Superlattices (SPSLs) Through Ga Surfactant Enhanced MME Growth of AlN***, **Alexander Chaney,*** Azimuth Corporation*; C. Bowers,* UES*; K. Mahalingam,* UES*; S. Mou,* Materials and Manufacturing Directorate, Air Force Research Laboratory*; K. Averett,* Materials and Manufacturing Directorate, Air Force Research Laboratory

We present a novel method for obtaining GaN/AlN short-period superlattices (SPSL's) by introducing Ga into the metal modulated epitaxy (MME) growth of AlN. During the MME process, the growth alternates between metal accumulation and metal consumption, with the end of the consumption regime resulting a metal deficient surface. By ensuring that Ga is present during this portion of the MME growth of AlN, it is possible to oscillate between the epitaxy of AlN and GaN in a controlled manner. This presents an advantage over more common methods of forming GaN/AlN SL's in MBE such as relying on periodic growth interrupts or migration enhanced epitaxy (MEE), both of which can lead to surface roughening. For our study, Ga partial pressures ranging from $1x10^{-7}$ Torr to $1x10^{-6}$ Torr were used along with a growth temperature of 825 ^oC. XRD analysis using coupled ω-2Θ scans found that at this growth temperature, Ga partial pressures greater than $3x10^{-7}$ Torr resulted in the formation of a GaN/AlN SPSL, with higher Ga pressures resulting thicker GaN films. These results indicate that the impinging Ga flux plays a dominate role in the resulting GaN layer thickness. TEM analysis showed that GaN layers as thin as 2 ML were formed. At the same time, wide angle TEM imaging indicated that the GaN/AlN SPSL layer thicknesses were maintained over 1 µm of total thickness without degradation of the interface quality. AFM scanning showed an improvement of the surface morphology with increasing Ga overpressure, characterized by a reduction in the RMS roughness and reduction in the diameters of hillocks on the surface. A minimum RMS roughness of 0.46 nm was found for a Ga partial pressure of $1x10^{-6}$ Torr. Based on this data, it is possible that the presence of Ga on the surface during the growth of AlN is creating a surfactant effect for the Al adatoms. Finally, this modified MME growth technique was used to attempt to create an AlGaN digital alloy with a target of 75% Al composition. Initial UV-Vis absorption measurements showed a prominent increase in the absorption at 225 nm, which correlates to a DA with 75% Al composition. This closely to the 78% Al content obtained from a coupled XRD scan. The UV-Vis data shows 2 additional peaks near 225 nm whose origins are currently being investigated. These results highlight the validity of introducing Ga into the MME growth of AlN as a practical method for obtaining high quality GaN/AlN SPSL'swith the potential for realizing DA's.

9:45am **NM-MoM1-9 Cubic Boron Nitride Grown by Mg-Catalyzed MBE***, **David Storm**, S. Maximenko, A. Lang, N. Nepal, T. Feygelson, B. Pate, D. Meyer,* U.S. Naval Research Laboratory

We report on the role trace amounts of Mg performs in facilitating the growth of c-BN on single-crystal diamond (100) by ion beam-assisted MBE. We have grown c-BN in a custom III-N MBE system equipped with an Ar ion source, a N_2 plasma source, and an electron beam evaporator for supplying elemental boron. Growth is initiated using a flux of Mg from a dual filament effusion cell (Φ_{Mg} ~ $8×10^{10}$ $cm^{-2}s^{-1}$), which facilitates the growth of c-BN. [1] Even trace amounts of Mg are sufficient to facilitate the growth of the cubic phase; however, neither Mg catalysis nor ion beam assistance alone appear sufficient to enable the growth of c-BN on diamond. Fourier transform infrared (FTIR) spectroscopy indicates that ion-assisted growth of BN under a Mg flux results in films which are fully cubic without any hexagonal phase (Figure 1).Transmission electron microscopy confirms the presence of an epitaxial c-BN film; the interface between the c-BN layer and the diamond substrate is structurally abrupt, and stacking faults comprise the nearly all of the visible defects. Electron energy loss spectroscopy indicates the film is >99% cubic, and while sp^2-bonded BN is detected near the layer surface, the regrowth interface, and at isolated misfit dislocations, no h-BN is detected.

[1] D.F. Storm et al., phys status solidi-RRL, https://doi.org/10.1002/pssr.202200036]doi.org/10.1002/pssr.202200036 (2022).

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Novel Materials
Room Swan BC - Session NM-MoA2

Chalcogenides
Moderator: Maria Tamargo, City College of New York

3:30pm **NM-MoA2-9 Growth of Ultrathin $PtSe_2$ using Molecular Beam Epitaxy**, ***Maria Hilse***, *K. Wang,* The Pennsylvania State University; *R. Engel-Herbert,* Paul-Drude-Institut für Festkörperelektronik, Germany

$PtSe_2$ was recently proposed as promising material for low-power, high-performance, and ultra-thin-body electronic application because of its sizeable band gap up to 1.2 eV, high carrier mobility in the order of 1,000 cm^2/Vs, stability in air, and possibility of low-temperature fabrication compatible with CMOS back-end-of-line (BEOL) processing. First experimental values of its high carrier mobility of 210 cm^2/Vs, that outperforms other 2-dimensional materials such as black phosphorus, MoS_2 and WSe_2, demonstrate the great potential of optimizing the deposition process in order to grow high-quality $PtSe_2$ material. This work employed molecular beam epitaxy (MBE) to take advantage of its excellent in-situ control and monitoring capabilities to shine light on the kinetic processes involved and to optimize material properties, a strategy that is proven to produce high-quality and large size layers of various transition metal chalcogenides.

In a first growth approach, we optimized deposition parameters for 3-layer (L), and 3-nm thick Pt layers on c-plane Al_2O_3, which we subsequently exposed to a Se flux at medium temperatures to drive a selenization conversion of the Pt film into $PtSe_2$. A detailed investigation of reflection high-energy electron diffraction (RHEED) and Raman spectroscopy revealed that the thickness of the so formed $PtSe_2$ is limited to the mono/few-layer regime regardless of the selenization temperature and the Se flux exposure time. Even for the very thin 3-L thick Pt film, the $PtSe_2$ transformation rate was smaller than 100 %. We conclude that the reason for the observed self-limited selenization process in the MBE environment is the compared to other physical vapor deposition techniques extremely small Se flux accessible within MBE.

In a second growth approach, we deposited Pt and Se simultaneously with the goal to form $PtSe_2$ directly from the gas phase on the Al_2O_3 substrate surface. This approach proved unlimited in the film thickness and enabled crystalline $PtSe_2$ formation with a close to ideal wetting behavior, and nucleation starting at the atomic Al_2O_3 step edges at 200 °C to 300 °C growth temperature with an optimal Se overpressure of 10 to 15 times the Pt flux judged by atomic force microscopy, RHEED, X-ray diffraction, and Raman investigation. A $PtSe_2$ film conversion from a three- to a two-dimensional layered microstructure alongside with a significant enhancement of the crystallinity of the material was however observed only after a post-growth annealing process in Se atmosphere confirmed by Raman and transmission electron microscopy investigation.

3:45pm **NM-MoA2-10 Ultra-thin Bi_2Se_3 Films Grown by Molecular Beam Epitaxy**, ***Saadia Nasir***, *S. Law,* University of Delaware

Bi_2Se_3 (BS) is a widely studied 3D topological insulator material which has potential applications in optics, electronics, and spintronics. Below the critical thickness of approximately 6 nm, the bandgap opens and BS transitions into the trivial insulator. Investigation of different optical or electronic phenomenon around the critical thickness can provide us with some interesting information that can be useful for device applications. Growing continuous ultra-thin BS films with a thickness of few nanometers and good morphology is challenging. To obtain good-quality ultra-thin films, we tried growing BS films using a variety of different growth recipes and conditions on sapphire (0001) substrates using a Veeco GENxplor MBE system. We started with the two-step method in which after growing a few nanometers of the film, the rest of the sample is grown at a comparatively higher temperature. Growing directly on un-treated sapphire substrates using a two-step growth method resulted in a fragmented non-coalesced film, and we did not observe the usual triangular domain morphology. We next tried a substrate pre-treatment recipe in which we grew 5nm of BS then heated the substrate to 470°C and kept it there for 30 minutes to thermally decompose the film. Decomposition was confirmed by the reflection high energy electron diffraction pattern that showed only the sapphire Kikuchi lines. We then tried the direct growth and the two-step growth on the pre-treated sapphire substrates using different growth rates and substrate temperatures. The samples grown on sapphire after treatment showed better substrate coverage indicating improvement in domain coalescence. We also explored the effects of substrate temperature and growth rate on the films grown on pre-treated substrates. We observed that for direct growth, higher growth rates resulted in films with an improved RMS surface roughness (SR), whereas for two-step growth the SR stayed comparable for different growth rates. For higher growth temperatures, the bismuth and selenium ions do not wet the substrate well,resulting in a film morphology comprising non-coalesced columns. Decreasing the substrate temperature suppressed the columnar growth which drastically improved the SR for both growth recipes. We also observed that the two-step growth on the pre-treated substrate resulted in the typical triangular domain morphology. Improvement of the SR and the film morphology with higher growth rates and lower substrate temperatures contrasts with what we usually see for the epitaxial growths. Overall, the flatter ultra-thin films with lower surface roughness makes them reliable for thickness-dependent studies.

4:00pm **NM-MoA2-11 Molecular Beam Epitaxy Growth of Site-determined Wavelength-tunable Quantum Emitters in Atomically-thin Semiconductors**, ***Mingyu Yu***, *S. Law,* University of Delaware

Two-dimensional (2D) van der Waals (vdW) materials have emerged as a promising platform to develop quantum photonics technology, where site-controlled localized quantum emitters (QEs) can be created at a wafer-scale. The weak interlayer vdW interaction along the c-axis allows various materials to be stacked together or transferred to different substrates. The strain-induced QEs on vdW materials have the advantage of long coherence time and position-controllability. Ga_2Se_2 is an advanced vdW material with exceptional bandgap tunability and favorable synthesis conditions. We aim to obtain an atomically-thin Ga_2Se_2 film to create strain-localized QEs.

A QEs system based on 2D vdW materials is a highly anticipated but immature technology because most existing fabrication methods for 2D material devices are hard to employ at the wafer-scale. We use molecular beam epitaxy in a Veeco GENxplor system to obtain extremely-high sample quality at the wafer scale. The first challenge is to obtain a flat, single-orientation Ga_2Se_2 monolayer (ML) with minimal twin boundaries. The Se overpressure, growth rate, and growth temperature are critical factors affecting the film quality.

To date, we have optimized the growth window for bulk Ga_2Se_2 film (30 nm thickness). The sample scan shows a root mean square roughness as low as 1.83 nm with a (002)-oriented crystal structure (Fig.S1). The growth rate is found to significantly affect the Se overpressure. A slow growth needs a substantially reduced Se flux, otherwise the excess Se will lead to Ga_2Se_3 (Fig.S2). Contrary to expectation, a higher growth rate caused better crystallinity (Fig.S3). We are now focusing on the growth of MLs. Since Ga and Ga_2Se_2 do not wet sapphire well, films tend to show 3D features instead of a flat, continuous film when the film is thin. A 2-step growth mode is proposed as a potential solution. Step 1 is to deposit an initial Ga_xSe_y film, then thermally decompose it at high temperature, aiming to improve film wettability by changing the substrate surface chemistry. We expect that this is achieved via atomic substitution at the substrate surface and/or by forming a reaction interlayer. Step 2 is to grow a Ga_2Se_2 film on the reacted substrate. A streaky reflection high energy electron diffraction pattern and characteristic X-ray diffraction peaks both confirm a much-improved film crystallinity compared to the sample grown directly, and the atomic force microscopy image shows a continuous film (Fig.S4). Further study will focus on this 2-step growth method and further improvement of film quality.

4:15pm **NM-MoA2-12 Epitaxial Growth of PbSnSe Ternary Alloys on III-V Substrates**, ***Pooja Reddy***, Stanford University; *B. Haidet,* Univesity of California Santa Barbara; *K. Mukherjee, L. Nordin,* Stanford University

The IV-VI semiconductor family of PbSe-SnSe alloys is a rich system to explore for electronic and optoelectronic applications. It spans narrow direct bandgap materials and topological crystalline insulators in the Pb-rich cubic rocksalt phase, and indirect bandgap semiconductors with useful thermoelectric and optoelectronic properties in the Sn-rich layered orthorhombic phase [1,2,3]. Importantly, this layered phase is only a slightly distorted rocksalt structure, making the study of structural phase transitions between the two systems very interested towards the end of harnessing contrasts in the electronic properties between the two phases. Heteroepitaxy of PbSe-SnSe materials provides a route to access these diverse set of properties for a range of thin film devices. In our work, we describe the growth of PbSnSe alloys in both the cubic and layered phases on technologically relevant (001) GaAs substrates by molecular beam epitaxy.

In order to grow PbSnSe alloys on GaAs, we used a PbSe buffer layer [4]. The structural similarity between the cubic and orthorhombic phases

allows for quasi-van der Waals epitaxial growth of SnSe and PbSnSe alloys on PbSe. A Riber Compact 21 MBE system with compound PbSe and SnSe cells was used to grow films. (001)-oriented semi-insulating GaAs substrates were prepared either by a regrowth and arsenic capping process, or by desorbing the oxide under a Se overpressure. Once the arsenic cap or oxide layer was thermally desorbed, the GaAs substrate was dosed with a PbSe flux at 400 °C, transforming the (2 x 4) reconstruction to a (2 x 1) reconstruction. A thin nucleation layer of PbSe was then grown at 330 °C which templates the sample for single-oriented growth resulting in a (1 x 1) reconstruction [4]. The PbSnSe alloy or SnSe was grown at temperatures ranging from 200-300 °C, where the composition was determined by the relative fluxes of the PbSe and SnSe compound cells. The structural quality of SnSe and the PbSnSe alloys clearly improved with the PbSe dosing and nucleation growth steps.

While the properties of cubic PbSnSe in the bulk and thin film limits are better known, here we will present electronic property trends as a function of composition for the orthorhombic phase of PbSnSe thin films. We will also explore the effect that PbSe dosing and nucleation has on these trends, thus discerning the role structure has to play on such properties.

[1]P. Dziawa et al. ...T. Story, Nature Mater., **11,** 1023, (2012).

[2]L. Zhao et al. ... M. Kanatzidis, Nature, **508,** 373, (2014).

[3]Y. Jhon et al. ... J. Lee, Adv. Optical Mater., **7,** 1801745 (2019).

[4]B. Haidet et al. ... K. Mukherjee, Phys. Rev. Mater., **4,** 033402 (2020).

4:30pm **NM-MoA2-13 Bi_2Se_3 Growth on III-V Substrates**, ***Yongchen Liu***, *W. Acuna,* University of Delaware*; H. Zhang,* National Institute for Science and Technology (NIST)*; D. Ho, R. Hu, Z. Wang, A. Janotti,* University of Delaware*; G. Bryant, A. Davydov,* National Institute for Science and Technology (NIST)*; J. Zide, S. Law,* University of Delaware

Terahertz (THz) technologies have been in the spotlight for several decades due to the variety of applications in this frequency range. Although significant research regarding THz applications has been conducted, combining different THz components into one device for a THz integrated system has not yet been achieved. In this paper, we will present the van der Waals (vdW) epitaxy of the topological insulator Bi_2Se_3, which can serve as a THz plasmonic waveguide, on the technologically-important GaAs (001) substrate using a variety of substrate pretreatment conditions in order to understand how to best combine vdW materials with traditional semiconductor substrates.

We conducted the following pre-treatments and growth in a dual Veeco GENxplor system. Three pre-treatments have been used before the synthesis of 50nm Bi_2Se_3 films on (001)-oriented GaAs substrates: GaAs oxide desorption under a Se-overpressure, GaAs oxide desorption under an As-overpressure, or a 100nm GaAs/AlAs smoothing superlattice (SL) and a 50nm GaAs buffer layer grown on it. After growth, scanning transmission electron microscopy (STEM), atomic force microscopy (AFM), x-ray diffraction (XRD), and room-temperature Hall effect measurements were used to characterize the samples. STEM shows two different orientations of Bi_2Se_3 grains in the Se-desorbed and As-desorbed samples: the desired (0001) and the undesired (10-15) orientation. As opposed to these two samples, a smooth Bi_2Se_3/GaAs interface was attained in the SL sample. AFM scans show similar morphology in all three samples; the root mean square roughness of the SL sample is smaller than the others. The XRD scans confirm the presence of the undesired (10-15) orientation in the Se-desorbed and As-desorbed samples. From the AFM images, we also observed antiphase domains: two sets of domains rotated 60 degrees with respect to each other. We performed x-ray pole scans to quantify the ratio of the antiphase domains. The SL sample has a slightly better antiphase domain ratio compared with the other two samples. Finally, DFT calculations determined that a Se-terminated interface is most likely, which is consistent with previous experimental analyses. In summary, this work demonstrates the importance of substrate pretreatment for the growth of the van der Waals material Bi_2Se_3 on a GaAs (001) substrate, which lays a concrete foundation for future THz integrated devices.

4:45pm **NM-MoA2-14 Structural and Optical Properties of CdSe Grown on InAs**, ***Zheng Ju***, *S. Schaefer, A. McMinn, X. Qi, D. Smith, Y. Zhang,* Arizona State University*; S. Grover,* First Solar, Inc.

Structural and Optical Properties of CdSe Grown on InAs

Zheng Ju [2] **, Stephen Schaefer** [1] **, Allison McMinn** [1] **, Xin Qi** [1] **, David Smith** [2] **, Sachit Grover** [3] **and Yong-Hang Zhang** [1]

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CdSe is an ideal candidate material for the top cell in tandem applications with a Si bottom cell. Its bandgap energies are 1.68 eV and 1.71 eV in the zincblende (ZB) and wurtzite (WZ) structures, respectively, enabling a theoretical power conversion efficiency of the tandem cell as high as 40%. The ZB InAs (111) crystal plane has an in-plane lattice constant of 4.28 Å, offering a suitable substrate for the epitaxial growth of monocrystalline WZ CdSe with lattice constant a = 4.30 Å. However, the growth of single-phase monocrystalline CdSe with perfect crystallinity, high electron mobility and long carrier lifetimes remains challenging. This abstract reports the molecular beam epitaxial growth of CdSe bulk thin films on InAs substrates for solar cell applications.

Bulk CdSe layers have been grown on (100)-, (111)A- and (111)B-oriented InAs substrates indium-mounted to Si wafers in a dual-chamber III-V and II-VI MBE system at different growth temperatures, Cd/Se flux ratios, and growth rates. InAs buffer growth is carried out in the III-V chamber first, followed by transferring under UHV to the II-VI chamber for CdSe overgrowth. RHEED patterns for the growths on (100) show steaky 2×1 surface reconstruction, while on (111)-oriented substrates show a transition from a streaky 1×1 surface reconstruction with four-fold symmetry to a spotty 1× reconstruction with six-fold symmetry, which indicates growth of WZ CdSe. XRD and PL measurements indicate that CdSe films grown on InAs (100) substrates consist primarily of the ZB phase, while CdSe films grown on (111) substrates exhibit characteristics of mixed ZB and WZ phases. SEM images provide additional clues about the mixed-phase nature of CdSe layers grown on (111) substrates, with some preliminary evidence of a transition from ZB to WZ phase as growth progresses on top of the ZB InAs (111) substrate. TRPL experiments of unpassivated bulk CdSe indicate minority carrier lifetimes of 1-5 ns, with ZB material exhibiting longer lifetime than WZ material. It is anticipated that proper or novel control of the growth conditions will yield desired single-phase CdSe thin films, which are necessary for device applications.

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5:00pm **NM-MoA2-15 Measuring and Then Eliminating Twin Domains in SnSe Thin Films Using a Fast Optical Metrology and Molecular Beam Epitaxy**, ***Wouter Mortelmans***, MIT*; M. Hilse,* Penn State University*; Q. Song, S. Jo, K. Ye,* MIT*; D. Liu, N. Samarth,* Penn State University*; R. Jaramillo,* MIT

Van der Waals (vdW) layered chalcogenides have strongly direction-dependent properties that make them interesting for certain photonic and optoelectronic applications. Orthorhombic tin selenide (α-SnSe) is a triaxial vdW material with strong optical anisotropy within layer planes, which has motivated studies of optical phase and domain switching. As with every vdW material, controlling the orientation of crystal domains during growth is key to reliably making wafer-scale, high-quality thin films, free from twin boundaries. Here, we demonstrate a fast and easy optical method to quantify domain orientation in SnSe thin films made by molecular beam epitaxy (MBE). The in-plane optical anisotropy results in white-light being reflected into distinct colors for certain optical polarization angles and the color depends on domain orientation. We use our method to confirm a high density of twin boundaries in SnSe epitaxial films on MgO substrates, with square symmetry that results in degeneracy between SnSe 90° domain orientations. We then demonstrate that growing instead on a-plane sapphire, with rectangular lattice-matched symmetry that breaks the SnSe domain degeneracy, results in single-crystalline films with preferred orientation, with twin domains all-but-eliminated. Our SnSe bottom-up film synthesis by MBE is enabling for future applications of this vdW material that is particularly difficult to process by top-down methods. Our optical metrology is fast and easy and can apply to all triaxial vdW materials.

Science and Technology of MBE
Room Swan BC - Session ST-MoA1

MBE Technology

Moderator: Paul Simmonds, Boise State University

1:30pm **ST-MoA1-1 NAMBE Innovator Awardee Talk: Physics and Technology of Antimonide Based Short Wave Infrared Avalanche Photodiodes on InP Substrates***, Sanjay Krishna*[1]*,* Ohio State University **INVITED**

There are a variety of applications ranging from greenhouse gas detection, 3D topographic mapping and light detection and ranging (lidar) are limited by the sensitivity of the receiver system. In particular, there is a needed for high sensitivity photonic detectors in the short wave infrared (1.5-3 microns) A low noise linear mode avalanche photodiodes (LmAPDs) is a critically enabling component for eye-safe long range LiDAR and remote sensing applications. Unlike PIN diodes, APDs provide internal gain that can lead to increased signal to noise ratio and suppress downstream circuit noise. The highest performing infrared APDs are based on interband transitions in mercury cadmium telluride (MCT, HgCdTe). State of the art (SoA) MCT diodes have large multiplication gains and low excess noise factors due to the favorable bandstructure that promotes single carrier impact ionization. However, their dark currents are high (3-5e-4A/cm2 at a gain of 10 at 125K) that requires cryogenic cooling. Commercial APDs use an InGaAs absorber with an InAlAs or InP multipliers. We are investigating two antimonide based multipliers, AlGaAsSb and AlInAsSb, on InP substrates. We have recently demonstrate GaAsSb/AlGaAsSb separate absorber charge and multiplier (SACM) heterostructures[i] [file:///C:/Users/Yvonne/AppData/Local/Microsoft/Windows/INetCache/Content.Outlook/C2N18W2U/Krishna%20OSU%20NAMBE%20Invited%20Talk%20Sept%202022.doc#_edn1] . We will discuss the technical challenges associated with the design, growth, fabrication and test of these LmAPDs and the potential for the development of these critical APD arrays for active 3D sensing and imaging systems.

[i] S. Lee et al " High Gain, Low Noise, Room Temperature 1550 nm GaAsSb/AlGaAsSb Avalanche Photodiodes", Manuscript under preparation (2022).

2:00pm **ST-MoA1-3 Overview of Virtual Substrate Technologies for 6.3 Angstrom Lattice Constant***, S. Svensson,* Army Research Laboratory*; N. Mahadik,* Naval Research Laboratory*; G. Kipshidze, **Dmitri Donetski**, G. Belenky,* SUNY at Stony Brook

Over the years the approaches to lattice mismatch have ranged from ignoring the problem, to brute force growth of very thick layers, to application of various schemes to engineer a strategy for gradually changing the lattice constant to ideally form a dislocation free virtual substrate (VS) with the desired properties.

A specific lattice constant range of interest is that between GaSb and InSb, in which no other substrate exists, which imposes limitations on our ability to exploit the (Al,Ga,In)(As,Sb) alloy system. This is of great interest primarily because of InAsSb, the III-V alloy with the smallest bandgap among compounds that can be grown with sufficient quality. The minimum energy gap occurs around 6.3 Å, which is why we focus specifically on this value.

InAsSb was set aside in the early 1990's since measurements seemed to indicate that its bandgap was not small enough to reach the long-wavelength infrared wavelength band. The decision was mainly based on investigations of defect-dominated materials. By using a VS approach based on the theoretical work by Tersoff we have been able to improve the quality of InAsSb so that its intrinsic properties could be investigated and the results show a material that closely resembles HgCdTe, the current LWIR performance standard.

Even though our VS approach allows determination of basic materials and device properties, it remains to be determined if it, or indeed any VS, is good enough for large array development. IR detector arrays are some of the largest devices made from semiconductors and are usually sensitive to crystalline defects. The first question that needs to be addressed then is what the density of threading dislocations needs to be. Even for the well-studied case of HgCdTe, there is no publically available information on what density allows what technical application to be addressed, although a general consensus seems to be that a density of 1E5 cm-2 or better is a minimum.

A significant related problem is to find a suitable tool for determining crystalline defect densities at this order of magnitude. However, recent progress in X-ray topology (XRT) is now enabling such investigations. We have been able to apply XRT on thick InAsSb-layers and determine promising defect densities that are close to the target value.

We will further discuss the strategies for designing grades, ongoing programs for modeling VS, summarize the materials properties of InAsSb, compare it with competing materials and discuss other hetero-structures enabled by the VS technique.

2:15pm **ST-MoA1-4 Measurement of Low Semiconductor Substrate Temperatures Using Reflectance Tracking of High Energy Critical Points***, **Kevin Grossklaus**, J. McElearney, A. Lemire, T. Vandervelde,* Tufts University

Small bandgap semiconductor alloys, including the $Si_{1-x-y}Ge_ySn_x$ and III-V-Bi alloy families, are in development for a range of infrared photonic applications.When produced by molecular beam epitaxy (MBE) these alloys are, out of necessity, grown at low temperatures to ensure Sn or Bi solute incorporation and produce films of good epitaxial quality.Those growth temperatures can be less than 200°C in some cases, far below the optimal epitaxial growth temperatures used for their base materials.Accurate measurement of substrate and buffer temperature before alloy film growth is critical for ensuring film quality and process repeatability.However, measurement is difficult using common non-contact techniques such as optical pyrometry at very low growth temperatures, and difficult for band-edge thermometry in the case of indirect or small bandgap substrates.

In this work we examine in-MBE temperature measurement of some common semiconductor substrates using a reflectance thermometry technique to track above bandgap, higher energy critical points in the dielectric function of those materials.This approach uses a broad spectrum, unpolarized UV-NIR light reflected specularly off the target substrate.The spectrum of reflected light is measured, processed, and then the locations of peaks corresponding to above band-gap critical points are identified in the reflectance data.The locations of those peaks can then be compared to reference reflectance data generated ex-situ at known temperatures, here collected by temperature varying spectroscopic ellipsometry, to determine in-situ process temperature.Temperature measurement by this method is relatively insensitive to background and stray light sources in the MBE system, and by optical system adjustment can be made insensitive to substrate rotation.Data will be presented showing successful temperature measurement of Ge, InAs, and GaSb from approximately room temperature up to or near the higher growth temperatures commonly used for these materials.The sensitivity and accuracy of the technique as shown by this data will be examined.The applicability of this temperature measurement technique to alloy buffer layers, heavily doped substrates, and MBE at cryogenic temperatures will also be discussed.Finally, the shortcomings of the present technique and optical system as employed will be reviewed, with discussion of how those issues may be overcome to enable temperature measurement of other materials, including InSb, InP, GaAs, and Si.

2:30pm **ST-MoA1-5 Perovskite Hetero-Chalco-Epitaxy Enabled by Self-Assembled Surface Passivation and Gas-Source MBE***, **Ida Sadeghi**, R. Jaramillo,* MIT

Chemical intuition, first-principle calculations, and recent experimental results suggest that chalcogenide perovskites feature the large dielectric response familiar in oxide perovskites, but also have band gap in the VIS-IR and strong light absorption [1]. Preliminary results suggest that chalcogenide perovskites feature excellent excited-state charge transport properties familiar in halide perovskites, while also being thermally-stable and comprised of abundant and non-toxic elements. Nearly all experimental results on chalcogenide perovskites to-date were obtained on powders and microscopic single-crystals. Advances in fundamental understanding and development for applications hinges on the availability of high-quality thin films.

[1] **NAMBE Innovator Award**

We recently reported the first epitaxial synthesis of chalcogenide perovskite thin films by MBE: $BaZrS_3$ films on (001)-oriented $LaAlO_3$ substrates [2]. The films are atomically-smooth, and scanning transmission electron microscopy (STEM) data show an atomically-abrupt substrate/film interface. The sulfide perovskite film has a pseudo-cubic lattice constant more than 30% larger than the oxide perovskite substrate. This strain is fully accommodated by a remarkable, self-assembled interface buffer layer that enables epitaxial growth of strain-free films, and that the propensity for buffered epitaxy can be controlled by the H_2S gas flow during growth.

We further demonstrate control of the band gap by making layered (Ruddleden-Popper) phases, and by alloying $BaZrS_3$ with Se. We have made the first epitaxial $BaZrS_{(3-y)}Se_y$ films with varying Se composition, up to and including a pure selenide perovskite $BaZrSe_3$. $BaZrSe_3$ is theoretically predicted to be stable in a non-perovskite, needle-like phase with very low band gap. We instead find two distinct phases, which we can control by choice of growth conditions. On non-lattice-matched substrates, $BaZrSe_3$ forms textured films in a hexagonal phase with surprisingly high band gap above 2 eV. On a perovskite $BaZrS_3$ buffer layer, we achieve pseudomorphic epitaxy of $BaZrSe_3$ in the perovskite phase with band gap in the near-infrared. We support these findings with experiments including high-resolution STEM, high-resolution X-ray diffraction, and photocurrent spectroscopy.

This work sets the stage for developing chalcogenide perovskites as a family of semiconductor alloys with properties that can be tuned with strain and composition in high-quality epitaxial thin films, as has been long-established for other semiconductor materials.

[1] R. Jaramillo, J. Ravichandran, APL Materials 7(10) (2019) 100902.

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2:45pm **ST-MoA1-6 Molecular Beam Epitaxy of Monocrystalline GaAs on Water Soluble NaCl Thin Films**, ***Brelon May***, National Renewable Energy Laboratory*; J. Kim,* Shell International Exploration and Production*; H. Moutinho, P. Walker, W. McMahon, A. Ptak, D. Young,* National Renewable Energy Laboratory

The high cost of III-V substrates for growth can be cost-limiting for technologies that require large area semiconductors. Thus, being able to separate device layers and reuse the original substrate is highly desirable, but many existing techniques to lift off a film from a substrate have substantial drawbacks. This work discusses some of the complexities with the growth of water-soluble NaCl as sacrificial layers for removal of GaAs thin films from GaAs (100) substrates. Much of the difficulty stems from the growth of the GaAs overlayer on the actively decomposing NaCl surface at elevated temperatures. We investigate a wide range of growth temperatures and the timing of the impinging flux of both elemental sources and high energy electrons at different points during the growth. We show that an assortment of morphologies (discrete islands, porous material, and fully dense layers with sharp interfaces) and crystallinity (amorphous, crystalline, and highly textured) occur depending on the specific growth conditions, driven largely by changes in GaAs nucleation. Interestingly, the presence of the reflection high energy electron diffraction (RHEED) beam incident on the NaCl surface, prior to and during GaAs deposition, affects the nucleation of GaAs islands, as well as the resultant crystallinity, and morphology of the III-V overlayer. By utilizing careful exposure of the NaCl to the RHEED beam and a low temperature GaAs nucleation layer, single-crystalline and epitaxial GaAs templates on continuous NaCl layers are realized. The low temperature GaAs layer functions as a template for subsequent single crystalline GaAs homojunction cell deposition by MBE or hydride vapor phase epitaxy. The GaAs cells are removed nearly immediately from the substrate via dissolution of the NaCl layer. However, fusion of as little as a few nanometers of the overlayer to the substrate results in holes that prove detrimental to fabrication of working devices. The frequency of fused locations can be reduced by engineering the early nucleation stages of GaAs on NaCl. Atomic force microscopy between these defects reveals that this process results in an increase in a rms surface roughness of the original wafer of only 0.2 nm. Therefore, combination of these systems could be well-suited for heteroepitaxial liftoff with further reduction of the density of fused locations.

3:00pm **ST-MoA1-7 Thermal Laser Epitaxy of Refractory Metals**, ***Lena Nadine Majer***, *H. Wang, W. Braun, P. van Aken, J. Mannhart, S. Smink,* Max Planck Institute for Solid State Research, Germany

Thermal laser epitaxy is a promising method for the production of epitaxially grown, refractory-metal layers, which may open up exciting perspectives, e.g., for solid state quantum computing devices. In thermal laser epitaxy, high-power continuous-wave lasers heat both the substrate and the individual evaporation sources, very similar to a MBE process. This method combines the advantages of MBE and PLD, allowing the efficient thermal evaporation and epitaxial deposition of practically any combination of elements from the periodic table, because there are practically no limits on substrate and source temperatures. Our setup has a liquid-nitrogen-cooled shroud, which allows us to grow layers with background pressures below 10^{-10} mbar. Moreover, in many cases crucibles can be replaced by free-standing cylinders of source material, which possibly contain a melt within the solid. Both of these factors allow producing very clean layers with low impurity levels.

We demonstrate and discuss the epitaxial growth of refractory metals on c-plane sapphire. As examples we present and discuss Ru and Ta films. We have optimized the growth parameters to obtain epitaxial films of superior quality, which are apparently devoid of defects over large areas. These films grow in a single phase, with a low surface roughness and an atomically sharp interface between the layer and the substrate.

MBE-Grown Devices
Room Swan A & Sandpiper - Session GD-MoP
MBE-Grown Devices Poster Session

GD-MoP-1 High Power Sb-Based Mid-Wave Infrared Diode Laser Arrays, ***Andy Lu***, *C. Yang,* Air Force Research Laboratory

High power diode laser source in the 2-3µm spectral range are critical for numerous applications, including defense infrared countermeasures, remote gas sensing, and as pump source for solid state lasers. In this paper, we present high power diode laser arrays using antimonide-based diode laser architectures spanning the 2.0-2.7µmwavelength range. The diode laser structure used was designed for 2.0µm, 2.4µm, and 2.7µm emission and grown using molecular beam epitaxy on GaSb substrates. The active region consists of lattice-matched quinary alloy for 2.7µm and quaternary alloy for 2.0µm and 2.4µm waveguide and four compressively strained, InGaAsSb quantum wells laced at the center with an inter-well spacing of 50 nm. The n-type bottom-clad and the p-type top-clad layers were both 1.5µm-thick lattice-matched AlGaAsSb alloy layers doped with Te and Be, respectively. Four-bar stack arrays were processed, fabricated, and packaged with water-cooled microchannel cooler. We demonstrated continuous wave operation of these diode array stacks with output power of 25 Watts at 2.0µm, 15 Watts at 2.4µm, and >7 Watts at 2.7µm.

GD-MoP-2 High Performance Diluted III-V Multijunction Solar Cell Grown by MBE for Space Application, ***Prashant Tyagi***, Orbit Engineering, LLC, India; *M. Sheldon,* Orbit Engineering, LLC; *T. Tabbakh, A. Albadri,* King Abdulaziz City for Science and Technology, Saudi Arabia

The III-V semiconductor materials have proven to be the most versatile group of materials due to direct and tunable band gap, robust, and radiation hardness properties.These versatile physical properties with relatively low mass-to-power ratio make III-V material an excellent candidate for space power application.Among all the space power technologies, compound semiconductor-based multijunction solar cells (MJSC) have demonstrated the highest efficiency of photovoltaic conversion.Most of the III-V semiconductor solar cells are based on heterostructure of InGaP/InGaAs/Ge.These solar cells are the core of satellite solar energy production [1-3]. Moreover, lattice-matched triple-junction III-V solar cell offers efficiencies of over 30% along with excellent performance and reliable stability for space missions [4]. The triple junction III-V is a well-established technology that has fulfilled numerous space applications over the past two decades. Currently, the highest conversion efficiency of solar cells is 47.1% achieved by six-junction inverted metamorphic solar cells exposed to 143 suns [5]. Our six junctions dilute III-V solar cell hybrid technology, which is an approach to further enhance the performance of III-V MJSC. Our aim is to develop the dilute MJSC technology which gives 36% conversion efficiency at AM0. Dilute nitrides are III-V compounds that incorporate small amounts of nitrogen (below 5%). The dilute nitrides exhibit excellent optical and electrical properties such as tunable band gap, which could be engineered to cover the entire range from 0.8 to 1.4 eV maintaining lattice matching to Ge. During our first on grown characterization, we achieved 20.6% efficiency under 1 Sun illumination and a current density of 7.2 mA/cm^2 with 79% fill factor. The details of growth and characterization would be presented at the conference.

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GD-MoP-3 Annealing Effect on the Magnetic Anisotropy of P Composition Graded GaMnAsP Layers, ***Seul-Ki Bac***, Korea University; *S. Lee,* Korea University, Republic of Korea; *X. Liu, M. Dobrowolska,* Physics Department,; *J. Furdyna,* Physics department

We have investigated annealing effect on the magnetic anisotropy properties of $GaMnAs_{1-y}P_y$ thin film, in which phosphorus content ***y*** varies from 0 % to 24 % along the growth direction. The Hall effects measurement revealed that the portion of magnetic layers having either only in-plane easy axes, both in-plane and out-of-plane easy axes, or only out-of-plane easy axis in the sample to be 80 %, 10 %, and 10 %, respectively, in as-grown sample. Such gradual change of the magnetic anisotropy in the film from the in-plane to the out-of-plane anisotropy with increasing P concentration is in accordance with the continuous variation of the strain from compressive to tensile toward the film surface. However, thermal annealing significantly changes magnetic anisotropy of the graded $GaMnAs_{1-y}P_y$ film. In particular, the intermediate region having both in-plane and out-of-plane easy axes nearly disappears in the film after thermal annealing and the film is divided into two types of layers having either only in-plane or only out-of-plane anisotropy. This investigation shows that thermal annealing significantly changes the magnetic anisotropy of graded $GaMnAs_{1-y}P_y$ film and thus one can strategically use the process to realize orthogonal magnetic bilayer consisting of in-plane and out-of-plane easy axes.

Novel Materials
Room Swan A & Sandpiper - Session NM-MoP
Novel Materials Poster Session

NM-MoP-1 Slow Photoluminescence Lifetime of Heavily Be-doped GaAsN, ***Takashi Tsukasaki***, Waseda Univ., Japan; *H. Sumikura,* NTT Basic Laboratories, Nippon Telegraph and Telephone Corp., Japan; *T. Fujimoto,* Waseda Univ., Japan; *M. Fujita,* NIT Ichinoseki College, Japan; *T. Makimoto,* Waseda Univ., Japan

The GaAsN alloy has been receiving increasing attention owing to its drastic band gap reduction property in a dilute nitrogen composition ([N]) [1]. Therefore, a heavily doped p-type GaAsN system alloy such as (In)GaAsN is expected to be applicable for a tunnel diode inserted to a multi-junction solar cell with GaAs system alloys [2]. In this multi-junction solar cell, the recombination mechanism is needed to be revealed for increasing its efficiency. For undoped GaAsN and lightly Si-doped n-type GaAsN, the recombination mechanisms were systematically discussed using both continuous and time-resolved photoluminescence (PL) measurements [3, 4]. However, it was only partially discussed for heavily doped p-type GaAsN using the continuous PL measurement [5]. Therefore, in this study, temperature dependence of PL lifetime is evaluated using the time-resolved PL measurement to reveal the recombination mechanism for heavily Be-doped p-type GaAsN.

Be-doped GaAsN layers were grown by radio-frequency plasma-assisted molecular beam epitaxy on semi-insulating GaAs (001) substrates using nitrogen RF plasma. The Be impurity concentrations ([Be]) were designed at 1×10^{19}, 6×10^{19}, and 3×10^{20} cm^{-3}, and [N] was fixed at about 0.8 %. The time-resolved PL measurement unit consisted of a picosecond Ti-sapphire laser with a photon energy of 1.80 eV and time-correlated photon counting module using superconducting single photon detector.

PL decay curves are well fitted by the bi-exponential decay function for Be-doped GaAsN independent of [Be] and temperature, meaning that two distinct PL lifetimes coexist as well as undoped GaAsN and lightly Si-doped GaAsN [3, 4]. Especially, the slow PL lifetimes are slightly less than 1 ns for Be-doped GaAsN independent of [Be] and temperature, which correspond to the optical transition from inherent localized levels in dilute GaAsN [3, 4, 6]. This result also shows that these localized levels are formed for ultra-heavily Be-doped GaAsN with extremely high [Be] of 3×10^{20} cm^{-3}. In contrast, the fast PL lifetimes tend to decrease with increasing [Be] for Be-doped GaAsN. This is due to increasing density of nonradiative recombination centers with increasing [Be] for Be-doped GaAsN. On the basis of these discussions of two distinct PL lifetimes, the recombination mechanism is revealed for heavily Be-doped GaAsN.

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NM-MoP-2 A Route Towards Actinide Heterostructure Synthesis and Science, ***Brelon May**, K. Vallejo, C. Dennett,* Idaho National Laboratory*; P. Simmonds,* Boise State University*; D. Hurley, K. Gofryk,* Idaho National Laboratory

Actinide-based materials possess unique physics due to the presence of 5*f* electrons, yet their study has been primarily focused on nuclear fuel applications, leaving aspects of their fundamental physics largely open for investigation. Effective examination of the unique quantum phenomena in these materials requires high purity monocrystalline samples. However, thin film synthesis of actinide compounds is particularly underexplored relative to other material systems because of limited source availability and safety regulations due to radioactivity. We will discuss the promises, challenges, and synthesis routes for these actinide-bearing heterostructures. Molecular beam epitaxy (MBE) presents an attractive avenue for the study of actinide heterostructures because of the high degree of control over dimensionality, strain, and interfaces. Idaho National Laboratory has recently installed an MBE chamber with the specific goal of studying uranium, cesium, and thorium containing compounds. To facilitate deposition of these low vapor-pressure elements, the chamber is outfitted with a quad-pocket electron beam source, several high temperature cells, and a nitrogen plasma source. Introductory studies on transition metals with complex oxidation states (Zr, Nb, Mn, Ni, and Cr) will function as early-stage surrogates for actinide-based nitride compounds. These new capabilities will create unrivaled opportunities for the exploration of functional and energy materials with complex electron correlations and provide important experimental validation for computational models of these systems.

NM-MoP-3 Epitaxial Growth of Antimony Selenide on Bismuth Selenide, ***Zhengtianye Wang**, S. Law,* University of Delaware

In addition to being a traditional thermoelectric material, Sb_2Se_3 has recently been investigated as a candidate for next generation photovoltaic devices, such as solar cells. Under ambient conditions, Sb_2Se_3 has orthorhombic crystal structure. It has recently been shown that rhombohedral Sb_2Se_3 can be stable up to five quintuple layers (5QL≈5nm) when grown on top of Bi_2Se_3, a topological insulator. In rhombohedral Sb_2Se_3, a quintuple layer refers to vertical stacking of atomic layers of 'Se-Sb-Se-Sb-Se' which make up one monolayer. Angle-resolved photoemission spectroscopy measurements on the Sb_2Se_3-Bi_2Se_3 heterostructure indicate that the rhombohedral Sb_2Se_3 is a topologically trivial material at ambient pressure. Beyond 5QL thickness, Sb_2Se_3 films tend to form in the thermodynamically stable orthorhombic phase.

To grow heterostructures of Sb_2Se_3 and Bi_2Se_3 that take advantage of the Sb_2Se_3 photovoltaic properties and the topological properties of Bi_2Se_3, we have investigated growth of 50nm Sb_2Se_3 on a 10nm Bi_2Se_3 seed layer on sapphire via direct co-deposition in a Veeco GENxplor R&D molecular beam epitaxy system. Instead of the 'worm-like' structure that is normally obtained when Sb_2Se_3 is directly grown on sapphire, we see a hexagonal mesh of orthorhombic Sb_2Se_3 nanoneedle structure. The surface roughness of the Sb_2Se_3 film decreases as the substrate temperature decreases from 300°C to 150°C. From the x-ray diffraction (XRD) pattern, we conclude that the Sb_2Se_3 growth plane is (021), and its crystallinity is enhanced by adding a Bi_2Se_3 seed layer instead of growing directly on sapphire. A high index plane of Bi_2Se_3 is obtained when we grow it on the mesh of Sb_2Se_3 nanoneedles rather than the standard (001) orientation. This research has paved the way for investigations of Sb_2Se_3 heterostructures with novel quantum materials like Dirac/Weyl semimetals and topological insulators.

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NM-MoP-4 Defect Free Ingaas/Inalas Superlattice on a Inp(111)B Substrate, ***Ida Sadeghi**,* MIT*; A. Pofelski,* Brookhaven National Laboratory*; H. Farkhondeh, A. Tam, K. Leung,* University of Waterloo, Canada*; G. Botton,* McMaster University, Canada*; Z. Wasilewski,* University of Waterloo, Canada

Epitaxial growth on (111) substrates, using molecular beam epitaxy (MBE), was mainly studied in the 1970s, 1980s and 1990s with the focus on GaAs [1-3]. However, since most of the growth conditions resulted in a defective and rough surface, McFee et al. [4] concluded that growth on (111) substrates is too difficult; therefore, efforts should focus on (001) surfaces for reproducible device quality epitaxial layers. In recent years, growth on the polar (111) surfaces has generated renewed interest due to the emergence of new applications. Prime examples are devices based on spin transport [5] and novel tensely strained quantum dots for quantum computing applications [6].

InGaAs/InAlAs grown on (001) InP substrates has application in optoelectronics. Also, MBE-grown InGaAs/InAlAs superlattices (SLs) on (001) InP have been successfully used for terahertz (THz) transmitters (Tx) and receivers (Rx) in photoconductive antennas for THz time-domain spectroscopy systems [7]. Unlike the more established MBE-grown low-temperature GaAs (LT-GaAs), InGaAs can be excited over fiberoptics at a wavelength of 1.55 μm using compact and relatively inexpensive telecom lasers. However, MBE growth conditions must be separately optimized for Tx and Rx structures, adding to cost and complexity. Recently, InGaAs/InAlAs SLs grown on InP(111) substrates were proposed as a next-generation material system, combining advantages of LT-GaAs and non-polar InGaAs/AlGaAs material systems. However, attempts resulted in defective growth [8]. Additional tailoring of strain in (111) InGaAs and InAlAs SL layers can embed strong piezoelectric fields in the material, bringing further enhancement of the Tx and Rx antennas performance without the need for individual MBE growth optimization.

With the use of density functional theory calculations and extensive scanning transmission electron microscopy (STEM) analysis along with the STEM Moiré Geometrical Phase analysis, we showed the first defect-free epitaxial growth of InGaAs/InAlAs heterostructures on InP (111)B substrates. Our work sets the stage for developing InGaAs/InAlAs/InP(111) photoconductive antennas for THz-TDS system with properties tuned by the embedded piezoelectric fields.

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NM-MoP-5 Site-Controlled InAs Quantum Dot Columns for Templating Self-Assembled Quantum Dots, *L. McCabe,* ***Nazifa T. Arony**, J. Zide,* University of Delaware

We present on the growth of low-density, site-controlled InAs quantum dot columns (QDCs) for templating high optical quality, self-assembled InAs quantum dots (QDs) and quantum dot molecules (QDM). The epitaxial formation of InAs QDs has been extensively studied[1] and have largely been considered as possible qubits[2]. However, a scalable platform to produce large arrays of identical QDs for integration into semiconductor devices is still being refined[3]. It is a challenge to produce high-optical quality site-templated QDs due to the presence of defects at the regrowth interface. We have previously shown a molecular beam epitaxy (MBE) grown low-density site-templated InAs QD platform[4]. Using this initial site-controlled growth, we are exploring the growth and morphology of InAs QDCs to serve as templated buffer layers for self-assembled QDs. This method maintains the spatial location of our patterns while obtaining QDs with optical qualities of self-assembled structures.

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NM-MoP-6 Characterizing SiGeSn Stability by Temperature Varying Spectroscopic Ellipsometry, ***Amanda Lemire**, K. Grossklaus, T. Vandervelde,* Tufts University

Tin-containing group IV alloys are being developed for infrared photonic devices. $Si_{1-x-y}Ge_xSn_y$ alloys grown by molecular beam epitaxy, particularly high tin content films with direct bandgaps, require low substrate temperatures during growth. The resulting layers are metastable, so additional heat exposure for subsequent layer growth or device processing may induce strain relaxation and tin segregation within or to the surface of the film. A complex set of material and temperature factors contribute to the relative degrees of defect formation and tin segregation. Each mechanism has different implications for device design, processing methods, and working lifetime at elevated temperatures such as those experienced by thermophotovoltaic cells.

In this work, we show studies of the thermal stability and annealing behaviors of $Si_{1-x-y}Ge_xSn_y$ films performed by temperature varying spectroscopic ellipsometry (SE). Heating was carried out on a Linkam heating stage mounted to a JA Woollam VASE instrument under a nitrogen atmosphere. Changes in strain state and material uniformity present as changes in the location and shape of the bandgap absorption edge and

critical points in the dielectric function, and overall shifts in optical properties of the films. Findings and additional evidence of film changes are confirmed by Nomarski optical microscopy, high-resolution x-ray diffraction, and atomic force microscopy. We collect data at room temperature after in-situ rapid thermal anneals to approximate thermal effects from device processing, and take continuous SE measurements at elevated temperatures for lifetime assessment. Tin content, film thickness, and strain state are varied to examine the effects of these properties on breakdown behaviors and to demonstrate the flexibility of the SE technique.

NM-MoP-7 Band Structure and Strain Distribution of InAs Quantum Dots Encapsulated in (Al)GaAs Asymmetric Matrixes, ***Pablo Olvera Enríquez****, C. Mercado Ornelas,* Center for the Innovation and Application of Science and technology, UASLP, Mexico*; L. Espínoza Vega,* Facultad de Ciencias, Universidad Autónoma de San Luis Potosí (UASLP). Center for the Innovation and Application of Science and technology, UASLP, Mexico*; I. Cortes Mestizo,* CONACYT-Center for the Innovation and Application of Science and technology, UASLP, Mexico*; F. Perea Parrales, A. Belio Manzano,* Center for the Innovation and Application of Science and technology, UASLP, Mexico*; C. Yee Rendón ,* Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Sinaloa, Mexico*; V. Méndez García ,* Center for the Innovation and Application of Science and technology, UASLP. Facultad de Ciencias, Universidad Autónoma de San Luis Potosí (UASLP), Mexico

Quantum dots (QDs) based devices often requires for their functionality to successfully stack several layers barrier/QD/barrier structures. Nevertheless, the growth gets more challenging as each layer of QDs is added, since diffusion, segregation, alloy intermixing, and strain effects intrinsically appear along the process. In this work, the strain distribution, and the electronic band structure of InAs QDs embedded in (Al)GaAs matrixes are investigated by numerical analysis based on finite element method.As input data, experimental parameters from MBE grown samples such as the QDs morphology, wetting layer (WL) thickness and the composition of the materials were employed. The biaxial (ε_{xx}) and hydrostatic (ε_{hydro}) strain tensors were calculated for pyramidal and truncated pyramidal QDs shapes, considering that capping usually flattens the apex of the islands [1]. The results revealed that ε_{xx} resulted more affected with the variations of InAs QDs geometry, which is correlated with changes in the heavy hole (HH) and light hole (LH) band structure behavior of the simulated heterostructures. Differences of the maximum and minimum values of ε_{xx} and ε_{hydro} tensors above islands, which carry information about the vertical pairing probability, for each type of heterostructure geometry were observed. The electronic confinement states and eigenfunctions probability distributions were calculated for the QD well. Higher energy states and lower number of eigenfunctions can be confined in truncated pyramids, as compared with non-modified shape QDs. This work shows a clear picture of the strain fields and their consequences on the band structure of InAs/(Al)GaAs multi-stacked heterojunctions found in actual QDs devices.

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NM-MoP-8 High Temperature Growth of Thick AlN on Si, ***Rohith Allaparthi****, M. Ware,* University of Arkansas*; C. Taylor, H. Edwards,* Texas Instruments*; Y. Mazur, F. Maia de Oliveira, M. Refaei,* University of Arkansas

Direct wide bandgap (WBG) III-Nitride (III-N) semiconductor material is promising alternative to silicon (Si) technology for high-power density, high-frequency, and high-voltage applications. However, native substrate material for most WBG semiconductors is not yet commercially available at low cost.One inexpensive alternative is to use standard Si wafers as substrates due to their extremely mature development.This has been relatively well developed for GaN on Si, with several commercial examples of well-developed devices. Here, we investigate the growth of the ultra-WBG semiconductor, AlN, on Si(111) in a high-temperature regime by plasma-enhanced MBE. For thick films, the low surface roughness and monocrystalline quality is characterized by the AFM and XRD respectively. Additionally, metal Al (111) signal is seen in the XRD, which corresponds to Al droplets resulting from the metal rich growth. Optical microscopy, however, reveals the presence of two distinct regions on the surface. Further investigation using micro-Raman spectroscopy identifies one region as high-quality, relaxed, crystalline Si and the other region as relaxed AlN.Analysis of the Raman spectra reveals week AlN peaks alongside the Si peaks, indicating that the Si exists as a film on the surface. AFM on the AlN regions is extremely smooth with surface roughness of less than 0.4 nm, while the Si regions are slightly rougher. In addition, it is found that small, three-dimensional crystals of Si have started to nucleate out of the Al droplets.All elemental conclusions are confirmed by electron dispersive x-ray (EDX) spectroscopy performed in a scanning electron microscope. Piezoresponse force microscopy has been performed on the free AlN regions and demonstrates that the AlN is single domain and metal polar. Thinner films, in stark contrast to the thick films, reveal only AlN domains with no areas of Si apparent.These results along with the findings from cross-sectional material analysis demonstrate a complicated diffusion effect between Al, Si, and AlN, occurring during the material growth, which will be discussed.

NM-MoP-9 Correlating Charge Carrier Profiles and Elemental Compositions in MBE-grown GaN/AlGaN Stacks, ***Stefan Schmult****,* TU Dresden, Germany*; P. Appelt, C. Silva, A. Großer, A. Wachowiak,* NaMLab gGmbH, Germany*; T. Mikolajick,* TU Dresden, Germany

Capacitance vs. voltage (C(V)) measurements represent a common way to trace levels of free charge carriers in semiconductors and semiconductor heterostructures. Concentration profiles of free charges obtained from C(V) measurements are widely accepted to reflect residual impurity background levels in GaN/AlGaN layer stacks. Particularly when the material is grown by MBE on highly compensated (insulating) GaN substrates, free carrier concentrations reaching levels below 10^{15} cm^{-3} are often reported for GaN buffer layers [1]. The growth of GaN/AlGaN stacks, hosting a 2-dimensional electron gas (2DEG), on insulating substrates is essential to probe the intrinsic 2DEG transport properties and to enable lateral HEMT functionality.

We realized a strong discrepancy in such GaN/AlGaN layer stacks - grown by MBE on highly compensated GaN substrates - between the concentrations of free charges extracted from C(V) data and the elemental donor background observed in secondary ion mass spectroscopy (SIMS) runs [2]. The conversion of the C(V) data into depth profiles relies on a model assuming a parallel plate capacitor geometry with defined top and bottom electrodes. The low level of free charges $<10^{15}$ cm^{-3} compared to the unintentional oxygen donor background of $>2\cdot10^{16}$ cm^{-3} is attributed to the experimental details of the measurement. A gate metal layer serves as the top electrode, while a defined bottom electrode is missing once the 2DEG is completely depleted and the C(V) data become unreliable for charge profiling.

Such a defined bottom electrode can be introduced by either growing GaN/AlGaN stacks on conductive substrates or – as implemented here - by making use of atmospheric silicon adhesion at the surface of unintentionally-doped (uid) substrates, which leads to parasitic conductivity at the substrate/MBE regrowth interface [3]. This parasitic channel is detrimental for investigating the intrinsic 2DEG transport properties and for HEMT functionality. On the other hand, the free charge carrier and donor background concentrations both agree well at a level of $4\cdot10^{16}$ cm^{-3}. Here, the bottom electrode is preserved after the 2DEG is depleted.

In summary, a parasitic channel in GaN/AlGaN heterostructures is a building block for a parallel plate capacitor, as it represents a defined bottom electrode for C(V) measurements. Consequently, free charge carrier concentrations extracted from C(V) data agree well with the elemental donor concentrations determined by SIMS.

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NM-MoP-10 Thin-film Growth of ζ- Mn_2N on MgO (001) Using Molecular Beam Epitaxy, ***Ashok Shrestha****, A. Smith,* Ohio University

The growth and structure of the cubic manganese nitride, namely θ - MnN, η- Mn_3N_2(010), η- Mn_3N_2(001), and ε- Mn_4N have already been investigated intensively on MgO (001) substrate [1,2]. However, the hexagonal ζ- Mn_2N has remained unexplored. The thin films of hexagonalζphase Mn_2N were grown successfully on MgO (001) using molecular beam epitaxy (MBE) under manganese-rich conditions. Multiple samples were grown by varying the Mn: N flux ratio from 0.6:1 to 0.9:1, and the ζphase is observed at the flux ratio of 0.9:1 at 455 ± 30 ^{o}C growth temperature. The sample growth process was monitored by *in-situ* reflection high energy electron diffraction (RHEED). During the sample growth, the streaky RHEED pattern with reduced streak spacing compared to MgO substrate was observed. The chemical composition of the samples was determined by *in-situ* Auger

electron spectroscopy (AES) at different locations of the sample. The stoichiometric ratio of Mn: N on the film is nearly 2:1 which is consistent with the ζ- phase Mn_2N. The experimentally measured *in-plane* lattice constant, based on the RHEED, is 2.86 ± 0.02 Å, and the *out-of-plane* lattice constant, measured using X-ray diffraction (XRD), is 4.56 ± 0.02 Å, which agrees with the *a* (2.82 Å)and *c* (4.54 Å) value of Mn_2N reported by Aoki *et al.* (2004) [3]. Furthermore, the room temperature scanning tunneling microscopy (STM) studies show some steps with a step height of 4.50 Å and atomic resolution of hexagonal arrays. This research was 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.

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NM-MoP-11 Impurity Doping of β-Ga_2O_3 Thin Films, ***Neeraj Nepal***, *. Downey, V. Wheeler, D. Katzer, E. Jin, . Hardy, V. Gokhale, T. Growden,* US Naval Research Laboratory*; K. Chabak,* Air Force Research Laboratory*; D. Meyer,* US Naval Research Laboratory

Ultra-wide bandgap (UWBG) semiconductors with a bandgap greater than 3.4 eV, such as c-BN, AlN, high Al content AlGaN, β-Ga_2O_3, anddiamond, have higher figures of merit values than GaN and SiC for power and rf devices making them candidates for next generation high-power/high-temperature electronic materials [1-4]. Higher operating frequency and power density enable smaller transformers and better power quality filter components, which mitigate Navy architecture space/weight/power (SWaP) issues, and also allow smaller size, higher-speed for future ship payloads and electric propulsion systems [1].

The availability of inexpensive large-area bulk substrates synthesized by melt growth techniques at atmospheric pressure provides a scaling advantage for β-Ga_2O_3 over other UWBG semiconductors [2]. In addition, homoepitaxial growth on bulk substrates offers the potential for low defect density films for vertical power devices. Further, controlled n-type doping with a shallow donor level (15-50meV [5]) is another advantage of β-Ga_2O_3 compared to AlN and high Al-content AlGaN. For these reasons, homoepitaxial growth of unintentionally- and impurity-doped Ga_2O_3 films and their electrical and structural properties is of great interest.

In this talk, we will present advances in MBE growth homoepitaxial of β-Ga_2O_3 thin films. First, the growth rate was increased approximately from 1 to 3 nm/min by optimizing the growth conditions such as Ga flux, plasma conditions and growth temperature (T_g). At optimal conditions with a T_g of 725 °C, surface roughness and X-ray rocking curve full-width at half maximum were 0.36 nm and 20 arc-sec, respectively, for 390 nm thick films. Optimal growth conditions that resulted in high structural and surface quality were used to explore doping parameter space using Sn and Si impurity. Hall effect measurements were carried out doped layers. For Sn-doped layers, the free carrier density can be controlled in the range $1x10^{16}$ to $3x10^{19}$ cm^{-3}. A mobility of 49 cm^2/V-s with free carrier density of $3x10^{19}$ cm^{-3} was measured which is comparable to the previously reported values for Sn-doped β-Ga_2O_3 [6]. We will also present the data on Si doped homoepitaxial β-Ga_2O_3 thin films.

This work was funded by the Office of Naval Research and the Office of the *Secretary of Defense*.

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NM-MoP-12 MBE Synthesis of Single-Crystal $LiMn_2O_4$ Thin Films as Li-Ion Battery Cathode Model Systems, *B. KC,* University of Illinois - Chicago*; G. Evmenenko, B. Buchholz,* Northwestern University*; **Robert Klie**,* University of Illinois - Chicago

To address the increasing demand for energy storage technology, model thin films Li-ion battery cathode systems are highly desirable since they avoid the complexity associated with polycrystalline or nano-sized powders which make detailed study of surfaces and interfaces difficult. However, the electro-chemical behavior of thin films depends on defect concentration, grain boundaries, and surface terminations. An ideal way to study the material and interface properties is by isolating a particular crystallographic orientation and investigate the orientation dependent performance.

To study such behavior, we have developed novel thin film MBE synthesis of single-crystal Li transition metal oxide spinels, such as $LiMn_2O_4$, to serve as Li-ion battery cathode model systems, where the thin film orientation and surface termination can be carefully controlled.We will discuss the modification necessary to synthesize fully stoichiometric, single crystal $LiMn_2O_4$ thin films that show Li de/intercalation properties similar to that seen in bulk Li-ion battery cathodes. These thin films are characterized using a suite of approaches, including XPS, XRD, and analytical electron microscopy. We will utilize these thin films to study the interfacial ion diffusion and structural evolution as the result of electro-chemical cycling against a graphite anode. These model thin film cathode frameworks will not only be used for monovalent Li^+ ions but also for divalent Mg^{2+} ion intercalation to quantify the the role of bulk orientation, surface termination and ion valence on the interfacial ion mobility.

The authors acknowledge funding from the Joint Center for Energy Storage Research (JCESR), funded by U.S. Department of Energy (DoE). The acquisition of the JEOL JEM-ARM200CF was supported byMRI-R^2 grant from the National Science Foundation (DMR-0959470) and the Gatan Quantum GIF acquisition by an MRI grant (DMR-1626065).

NM-MoP-13 Tunable Electronic States and Instabilities in PbSnTe Heterostructures, *A. Al-Tawhid, A. Gonzalez, S. Poage,* NCSU*; **Kaveh Ahadi**,* NC State University

Combination of broken inversion symmetry and spin-orbit coupling gives rise to a wide range of exotic superconducting states, such as mixed-parity superconductivity, superconducting Weyl state, and superconducting diode effect. Incipient ferroelectrics e.g., PbTe, are near a polar instability. The emergence of superconductivity has been reported in some of these incipient ferroelectrics upon doping. Many unconventional superconductors, such as the cuprates, pnictides, and heavy fermion systems, occur in close proximity to magnetic fluctuations or magnetic orders, suggesting that these are important ingredients in the superconductivity in these materials. Here, ferroelectricity and superconductivity could be connected or accidental neighbors. Furthermore, the intersection of superconductivity and topologically nontrivial states is a fertile landscape for exciting quantum phenomena, including non-abelian excitations.

IV-VI compounds show a wide range of electronic and polar instabilities. $Pb_{1-x}Sn_xTe$ demosntrates a highly tunable superconductivity and ferroelectricity which are dependent on carrier density and Sn(Pb) concentration. Furthermore, a topological phase transition is expected at x~0.4, which inverts the conduction and valence bands for Sn rich compounds. I will report on our recent growth efforts of high quality $Pb_{1-x}Sn_xTe$ heterostructures,using a chalcogenide molecular beam epitaxy (Veeco 930) near the topological phase transition (x~0.4). The cross-sectionhigh-angle annular dark-field (HAADF) imaging in scanning transmission electron microscopy (STEM) shows abrupt interfaces. X-ray diffraction demonstrates single oriented films. The sheet resistancev.s. temperature demosntrates a metallic-like behavior, dR/dT >0, in doped samples extending to 2 K. The Hall carrier density was measured at various temperatures, resolving the carrier mobility. The carrier mobility is inversely proportional to doping concentration. We report on superconductivity in electron and hole doped $Pb_{1-x}Sn_xTe$ heterostructures and its relation to neighboring ferroelectric and topological phase transitions.

NM-MoP-15 Controlling the Size and Density of InN QDs formed on Sapphire Substrate by Droplet Epitaxy, ***Malak Refaei***, *A. Kuchukc, R. Allaparthid, M. Sarollahiad, M. Maruf , M. Ware,* University of Arkansas

The growth of InN quantum dots (QDs) on c-plane sapphire by droplet epitaxy (DE) using radiofrequency plasma-assisted molecular beam epitaxy (MBE) was reported. The QD growth process from liquid In droplets to the InN QDs was described with a focus on the effect of RF-plasma on the formation of In droplets size and density as a function of substrate temperatures. Two nitridation procedures were used to investigate the crystallization of In droplets in order to understand the process. The variation in the shape and size of InN QDs was explained in terms of the In atom migration of droplets and surface diffusion. The growth of InN QDs

using the DE method has many advantages over the classical Stranski-Krastinow technique, including the ability to control a wide range of QD shapes, sizes, and densities.

NM-MoP-16 Selective-area Growth of GaN and AlGaN Nanowires on N-polar GaN Template with 4° Miscut by Plasma-assisted Molecular Beam Epitaxy, ***Kamruzzaman Khan***, *A. Jian,* University of Michigan, Ann Arbor*; J. Li,* University of California at Santa Barbara*; E. Ahmadi,* University of Michigan, Ann Arbor

In this study, selective area growths (SAGs) of AlGaN/GaN nanowires on miscut N-polar GaN templates were studied and was compared with that grown on Ga-polar templates. The SAG of N-polar AlGaN/GaN nanowires demonstrated higher growth rate and more selectivity than that of Ga-polar AlGaN/GaN nanowires. Additionally, Lateral growth rate of N-polar nanowires was shown to be significantly lower than Ga-polar nanowires. Moreover, as opposed to top surface of Ga-polar NWs which have pyramidal shape, the N-polar GaN NW have a flat head. The combination of higher growth selectivity, larger growth window, negligible lateral growth, and flat head, makes N-polar (Al,Ga)N nanowires attractive for a variety of applications including UV LEDs and detectors as well as quantum sensing applications.

NM-MoP-17 Molecular Beam Epitaxy Grown Group-IV Alloys: Ideal Candidate for Momentum(*k*)-Space Carrier Separation Photodetectors, ***Tyler McCarthy***, *Z. Ju, S. Schaefer, X. Qi, A. McMinn,* Arizona State University*; S. Yu,* University of Arkansas*; Y. Zhang,* Arizona State University

Recently, we proposed the momentum(*k*)-space carrier separation (*k*-SCS) concept that combines the advantages of both direct and indirect bandgaps for light detection/conversion devices. The basic principle is to have a direct bandgap in a semiconductor that has a slightly larger bandgap than the indirect fundamental bandgap, giving a thermalization barrier, $D_{G\text{-}L}$, such as $3k_BT$, for electrons at the conduction band edge. In this example, the Γ-valley minimum is $3k_BT$ higher in energy than the *L*-valley minimum. The sharp absorption edge of the direct bandgap energy, $E_{g,\Gamma}$, appears at just slightly ($3k_BT$) higher in energy than the slow onset of the absorption edge at the indirect bandgap, $E_{g,L}$. Under light illumination, electrons are excited to the direct *Γ*-valley in the conduction band while leaving holes in the valence band edge at the symmetry point of *Γ*. The large majority of photogenerated electrons in the direct *Γ*-valley will quickly thermalize at a sub-picosecond time scale to the lower energy indirect *L*-valley. These electrons in the *L*-valley will recombine with the holes in the valence band at a time scale of tens of microseconds to milliseconds. Both carriers, electrons and holes, are transported in real space but with different momentums, i.e. separately in *k*-space, to their corresponding contacts with negligible recombination. This clever design not only improves photogenerated carrier lifetime, similar to indirect bandgap semiconductors, but also offers a large absorption coefficient, similar to direct bandgap semiconductors.

Group-IV alloys such as GeSn are a model material system to demonstrate the novel idea as photodetectors with Sn compositions near the indirect-to-direct bandgap transition are predicted to have greater detectivity than conventional IV-VI and III-V compound photodetectors at room temperature, and comparable detectivity to InAs detectors operating at 77 K. GeSn samples with $D_{G\text{-}L}$ between $0.4k_BT$ and $3k_BT$ were grown by MBE on Ge substrates for MWIR (2 to 5 µm). Substrate surfaces were first cleaned using HF and HCl solution prior to a UHV outgas at 550 ˚C. A Ge buffer was grown at a substrate temperature of 500 ˚C before cooling down to 200 ˚C for GeSn growth. Ge effusion cell was held constant while Sn effusion cell was varied between 825 to 900 ˚C to obtain designed composition. RHEED showed a streaky (2x1) surface reconstruction pattern that transitions to a (1x1) with increasing Sn. Introducing Si expands the wavelength coverage range to 2 ~ 22 µm, making it ideal for MWIR, LWIR and VLWIR applications. More details of the theory and experiments will be reported at the conference.

Science and Technology of MBE
Room Swan A & Sandpiper - Session ST-MoP
Science and Technology of MBE Poster Session

ST-MoP-1 Cryo-MBE: Ultra Low (<20k) Growth Temperatures for High Quality Metal Epitaxy, ***Nils-Eike Weber***, Scienta Omicron, Germany*; D. Beaton,* Scienta Omicron*; M. Heiss,* Scienta Omicron, Germany

Superconductor-semiconductor nanowires enable the route to quantum information devices, like topological qubits [1]. Such hybrid nanowires can be grown in a bottom-up approach by Molecular Beam Epitaxy (MBE). Low-temperature evaporation of the superconductor was demonstrated to promote a continuous and flat film morphology growth and thereby assist the fabrication of disorder-free hardgap superconductor/semiconductor epitaxial hybrids [2]. As pristine surfaces and interfaces are key, eliminating post-growth etch processes by the employment of “shadow epitaxy” is seen as a promising approach [3].

We present a new MBE system that combines an ultra-low temperature manipulator with optimized chamber geometry for shadow epitaxy which enables exploration of so far uncharted growth parameters. The closed-cycle ULT manipulator with base temperature of < 20 K can be precisely positioned in the azimuthal and polar rotation axis allowing defined growth of half-shell or full-shell structures.

Our system and manipulator geometry allows to reach grazing incidence as well as normal incidence for an up to 2” sample cryogenic sample with respect to any of the 10 source ports (including e-beam sources needed for some promising material combinations). This allows to speed up the research of a wide range of possible epitaxial hybrid material systems for a full range of low temperature nucleation conditions. We demonstrate experimental data of the sample temperature at standby as well as when exposed to a hot effusion cell surface as a proof of the excellent manipulator cooling performance.

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ST-MoP-2 Vertical Cation Segregation in During $A_xB_{1-x}N$ Epitaxy, ***Christopher M. Matthews***, *Z. Engel, W. Doolittle,* Georgia Institute of Technology

III-nitrides represent the possibility to realize high efficiency electronics in many different areas, from power electronics to light emitters to photovoltaics and more. However, many optoelectronic devices are limited by indium gallium nitride’s (InGaN) tendency to phase separate. Phase separation is one of the key challenges preventing further progress in III-nitride electronics, but the driving mechanisms for this phenomenon are not fully understood. Based on experimental success in limiting phase separation in AlInN and InGaN, we suggest that surface kinetics drive this phase separation during growth, rather than a bulk diffusion mechanism that has traditionally been credited as the cause. We propose that vertical cation segregation (VCS), lateral cation separation (LCS), and thermal decomposition and desorption are the main drivers of phase separation. In this work, we present a comprehensive dynamic growth model to examine the role of VCS in phase separation of ternary III-nitrides, and we compare modeled and experimental films.

A critical dose of excess metal exists for InGaN [1] and AlGaN [2], beyond which diffusion of the larger cation away from the growth surface occurs – a process defined as VCS. Metal-modulated epitaxy (MME) can be used to eliminate VCS or to alter the way VCS manifests in thin films (as compared to metal-rich MBE). VCS can result in self-assembled super lattices (SASL), which are used to evaluate the model presented here. MME’s low temperatures and high growth rates can be used to inhibit thermal effects and LCS, respectively, leaving VCS as the lone phase separation driver.

We have built a dynamic growth model to describe the accumulation and consumption of metal adatoms during epitaxy of III-nitrides. These processes are modeled by a system of coupled differential equations that use growth parameters extracted from state-of-the-art III-nitride epitaxy to calculate rates of growth, exchange, decomposition and more. This model is solved numerically to compute the time-evolution of each surface adlayer and a composition profile of the resultant crystalline film. We matched measured XRD to simulated diffraction patterns and composition profiles to TEM for experimental and simulated AlGaN SASLs. The general nature of this dynamic model makes it applicable to most variants of MBE.

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ST-MoP-3 Non-amphoteric N-type Doping with Sn of GaAs(631) Layers Grown by Molecular Beam Epitaxy, ***Alan Cano Rico,*** Facultad de Ciencias, Universidad Autónoma de San Luis Potosí (UASLP), Mexico*; L. Espiinosa Vega ,* Facultad de Ciencias, Universidad Autónoma de San Luis Potosí (UASLP). Center for the Innovation and Application of Science and technology, UASLP, Mexico*; I. Cortes Mestizo,* CONACYT-Center for the Innovation and Application of Science and technology, UASLP, Mexico*; R. Pinson Ortega ,* Facultad de Ciencias, Universidad Autónoma de San Luis Potosí (UASLP), Mexico*; F. Perea Parrales,* Center for the Innovation and Application of Science and technology, UASLP, Mexico*; P. Olvera Enríquez,* Center for the Innovation and Application of Science and technology, UASLP, Mexico*; M. Villareal Faz,* Facultad de Ciencias, Universidad Autónoma de San Luis Potosí (UASLP), Mexico*; L. Hernandéz Gaytán , A. Belio Manzano,* Center for the Innovation and Application of Science and technology, UASLP, Mexico*; V. Méndez García ,* Center for the Innovation and Application of Science and technology, UASLP. Facultad de Ciencias, Universidad Autónoma de San Luis Potosí (UASLP), Mexico

The molecular beam epitaxial (MBE) growth and doping of III-V semiconductor compounds on high-index crystallographic orientations (HICO) opens a vast number of possibilities to investigate new physical properties and to develop optoelectronic devices that overcome the currently technology. The peculiar HICO surface anisotropy can conduce to a natural arrangement of unidimensional nanostructures under appropriated growth conditions. Recently, the formation of self-assembled corrugation on GaAs(631) conducted to the formation of 1D multi-quantum well heterostructures, and the modulation of the confined state eigenstates has been achieved, attaining quasi-one-dimensional or fractional dimension eigenstates [1]. Further applications in electrical and optoelectronic devices demand of the realization doped layers preserving the 1D order. Although Si is widely used as an n-type dopant for GaAs (100) the growth of Si doped GaAs on (631)A surfaces results in amphoteric behavior, p-type and n-type conduction depending on the growth parameters [2]. In this work the Sn doping effects on the electronic conduction and optical properties of GaAs(631)A layers grown by MBE are investigated. We found that the conduction type conversion is avoided when Sn-doping is implemented instead. The maximum carrier concentration was $2x10^{19}$ cm^{-3}, which is an order of magnitude higher than previously reported for Si, and it is within the same order of magnitude as compared with the growth of GaAs(100). The electron mobility was $4x10^3$ cm^2/Vs ($1x10^3 cm^2/Vs$) for carrier concentration of $1x10^{17}$ cm^{-3} ($1x10^{19}$ cm^{-3}), suitable for many optoelectronic applications. Raman spectroscopy (RS) of highly Sn-doped (100) samples showed that the TO mode completely dominates the spectrum, indicating low crystalline quality. Conversely, the selection rules for the (631) indicate that the TO mode is allowed, and according to the experimental data it was found to increase with Sn-doping. In general, the incorporation of Sn in HICO-GaAs follows a completely different process as in singular (100)-planes, which was also supported by HRXRD and AFM measurements on the films.

[1] J. Appl. Phys. 128, 244302 (2020); https://doi.org/10.1063/5.0029103

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ST-MoP-4 Uniformity: A Phenomenon That Arises from Anisotropy and De-Relaxation During Growth, ***Felipe Perea Parrales,*** *C. Mercado Ornelas, A. Belio Manzano,* Center for the Innovation and Application of Science and technology, Universidad Autónoma de San Luis Potosí (UASLP), Mexico*; I. Cortes Mestizo,* CONACYT-Center for the Innovation and Application of Science and technology, Universidad Autónoma de San Luis Potosí (UASLP), Mexico*; L. Vega Espinosa,* Center for the Innovation and Application of Science and technology, Universidad Autónoma de San Luis Potosí (UASLP), Mexico*; D. Valdez Perez,* Instituto de Física, Universidad Autónoma de San Luis Potosí, Instituto Politécnico Nacional, UPALM, Mexico*; C. Yee Rendón ,* Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Sinaloa, Mexico*; A. Cano Rico,* Facultad de Ciencias, Autonomous University of San Luis Potosí, Mexico*; V. Mendez Garcia ,* Center for the Innovation and Application of Science and technology, Universidad Autónoma de San Luis Potosí (UASLP), Facultad de Ciencias, Autonomous University of San Luis Potosí, Mexico

Recently, the set of advantages of assembling quasi-one dimensional quantum wire (QWR) heterostructures by molecular beam epitaxy (MBE) over high-indexcrystallographicorientations(HICO)has been exhibited. Some of them include the wave function's in-plane symmetry break, allowing transitions that, in principle, must be forbidden and the induction of blue shifts or red shifts to theQWR energy spectrumdepending on the lateral(L_p)and vertical(H_p) QWRperiodicities(see the inset of Figure 1.(a)). Overall, merging the benefits of both integer-dimension extremes while ruling out their flaws [1], (Figure 1.(a)) and exhibiting the presence of a lateral confinement system(Figure 1.(b)). Although the growth processes over HICO are far from being fully understood, the GaAs (631) has proven to be an ideal substrate to grow QWR heterostructures before, owing to its unparalleled uniformity length [2]. One can assert that until now, there has been scarceor nonexistent *in situ* characterization that could bring us to grasp an overview of the real-time growth process performed over HICOs. This work expands the basis of the GaAs (631) faceting uniformity in terms of the anisotropic diffusion dynamics (Figure 2.(a)) and surface (1x1) buckling-like reconstruction (Figure 2.(b)) together with their dependence on the macroscopic constraints ∏=As/Ga BEP relation and growth temperature. The discussion is supported by experimental results, kinetic Monte Carlo simulations, a proposed inverse W-RHEED method and a thorough reciprocal space analysis. A new perspective for the free energy surface minimization apparatus is introduced.

[1] J. Appl. Phys. 128, 244302 (2020); https://doi.org/10.1063/5.0029103

[2] Applied Physics Letters 101, 073112 (2012); doi: 10.1063/1.4746423

ST-MoP-5 Feature-Independent Molecular Beam Epitaxy Selective Area Regrowth Towards Embedding High Aspect Ratio Microstructures, ***Ashlee Garcia,*** *A. Skipper, D. Ironside, S. Bank,* University of Texas at Austin

A molecular beam epitaxy (MBE) approach to selective area epitaxy (SAE) of III-V semiconductors has the potential to advance optoelectronic structures through seamless integration of metals, dielectrics and high-quality crystalline semiconductors. While SAE by metal organic chemical vapor deposition has been widely successful due to its high deposition selectivity, an all-MBE method could enable access to non-equilibrium growth conditions and high layer precision[1,2].

SAE is difficult to achieve with conventional MBE due to III-V nucleation on the amorphous mask. As a result, Allegretti et al. developed periodic supply epitaxy (PSE), a method to inhibit polycrystal deposition by cycling group III deposition under a constant group V flux[2-4]. While an all-MBE approach has enabled the embedding of features 2µm wide and 300nm tall, applications requiring high aspect ratio microstructures such as mid- and long-wave infrared high-contrast photonics[5-7] and aspect ratio trapping of threading dislocations for metamorphic growth[8], are challenging to selectively regrow due to low adatom surface diffusion[1,3].

To expand the accessible applications, a numerical 1D model was developed to describe PSE selectivity and determine selective growth regimes by fitting adsorption, desorption, and diffusion constants to GaAs growth on SiO_2 films at 600˚C [9-12]. The model identified a desorption-limited growth regime under an 18% PSE cycle, in which only thermal desorption off the mask is required to achieve selectivity. The selective growth regime was verified experimentally by observing no polycrystal formation on the mask surface after 100nm of 10% PSE GaAs growth (Ga open 6s, closed 54s) on a SiO_2 film and patterned gratings varying from 1 to 10µm wide, indicating the ability overgrow any arbitrary set of SiO_2 features and motivating its use for embedding high aspect ratio microstructures.

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Novel Materials
Room Swan BC - Session NM-TuM1

Novel Materials

Moderator: Debdeep Jena, Cornell University

8:00am **NM-TuM1-1 Navigating MBE Growth of Atomically Precise Complex Oxides of Stubborn Metals Using Source Chemistry***, **Bharat Jalan,*** University of Minnesota, USA **INVITED**

Molecular-beam epitaxy (MBE) has come to the forefront for the thin film synthesis of materials with an exceptionally high structural quality, and with the best figures of merits whether it is related to their electrical or optical properties. From its beginnings as a successful method for III–V semiconductor growth to today for the growth of many contenders for next-generation electronics and spintronics devices, several new synthesis challenges have however emerged. For instance, it has been notoriously difficult to grow metal oxides, in an atomically precise manner, of metals having ultra-low vapor pressures and difficulty of oxidation.

In this talk, we will review these issues and will present our group's effort to address these challenges using a novel solid-source metal-organic MBE approach. We show, for the first time, controlled synthesis of metal and metal oxides of these "stubborn" elements with the ***same ease and control*** as afforded by III-V MBE. We will present detailed growth study utilizing chemistry of source materials as a controlling knob to navigate synthesis. With the goal to understand and control electronic ground states in defect-managed complex oxide films and nano-membranes, we will discuss how chemistry of source materials can be used to navigate synthesis on-demand.

8:30am **NM-TuM1-3 Pinhole-Seeded Lateral Epitaxy and Exfoliation on Graphene-Terminated Surfaces***, **Sebastian Manzo**, P. Strohbeen,* University of Wisconsin - Madison*; Z. Lim,* University of Wisconsin - Madison, Malaysia*; V. Saraswat,* University of Wisconsin - Madison, India*; D. Du, S. Xu,* University of Wisconsin - Madison, China*; N. Pokharel,* University of Wisconsin - Madison, Nepal*; K. Su, L. Mawst, M. Arnold , J. Kawasaki,* University of Wisconsin - Madison

Remote epitaxy is a promising approach for synthesizing exfoliatable crystalline membranes and enabling epitaxy of materials with large lattice mismatch. However, the atomic scale mechanisms for remote epitaxy remain unclear. Here we experimentally demonstrate that GaSb films grow on graphene-terminated GaSb (001) via a seeded lateral epitaxy mechanism, in which pinhole defects in the graphene serve as selective nucleation sites, followed by lateral epitaxy and coalescence into a continuous film. Remote interactions are not necessary in order to explain the growth. Importantly, the small size of the pinholes permits exfoliation of continuous, free-standing GaSb membranes. Due to the chemical similarity between GaSb and other III-V materials, we anticipate this mechanism to apply more generally to other materials. By combining molecular beam epitaxy with in-situ electron diffraction and photoemission, plus ex-situ atomic force microscopy and Raman spectroscopy, we track the graphene defect generation and GaSb growth evolution a few monolayers at a time. Our results show that the controlled introduction of nanoscale openings in graphene provides a powerful route towards tuning the growth and properties of 3D epitaxial films and membranes on 2D material masks.

8:45am **NM-TuM1-4 Molecular Beam Epitaxial Growth of Cr-Sn Thin Films on Al2O3***, **Tyler Erickson**, S. Upadhyay, A. Abbas, D. Ingram, A. Smith,* Ohio University

The suggestion of a spin liquid state in spin-1/2 Kagome antiferromagnetic materials poses interesting possibilities for investigating Kagome materials[1]. The confirmation of spin liquid states in the $ZnCu_3(OD)_6Cl_2$ spin-1/2 Kagome lattice antiferromagnet[2] and recent demonstration of a large anomalous Hall effect present in Mn_3Sn fims[3] demonstrate interesting magnetic properties valuable for future developments in spintronics and quantum materials. With a recent theoretical investigation into the Cr-Sn system that predicts an antiferromagnetic alloy[4], we now pursue the growth and characterization of this system. We investigate the growth of the Cr-Sn system on Al_2O_3 using molecular beam epitaxy with precise control over the flux ratio of Cr to Sn (from 1.7:1 to 5.1:1) and substrate growth temperature (650 °C - 850 °C). Growths for 1.7:1 and 5.1:1 Cr:Sn ratios were performed at 750 °C, and growths for 3.4:1 ratios have been performed at 650 ≥°C, 750 ≥°C, and 850 ≈°C. Reflection high energy electron diffraction patterns give *in-situ* characterization of the *in-plane* lattice, while X-ray diffraction characterizes the *out-of-plane* lattice. Preliminary analysis of RHEED patterns for Cr-Sn flux ratios of 3.4:1 and 5.1:1 give two distinct ranges of *in-plane* lattice constants. These ranges are 3.11 Å - 3.29Å and 3.98 Å - 4.06 Å. The second range gives good agreement with the *in-plane* lattice constant a = 4.054 Å calculated by Senthur Pandi Rajasabai *et al*[4]. We are currently in the process of further characterizing our Cr-Sn samples using Rutherford backscattering and XRD. This research was 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.

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9:00am **NM-TuM1-5 Growth of Mn_3Sn on Sapphire Using Molecular Beam Epitaxy***, **Sneha Upadhyay,*** Ohio University*; T. Erickson , D. Ingram ,* Ohio University*; K. Sun,* University of Michigan, Ann Arbor*; A. Smith,* Ohio University

The kagome antiferromagnet Mn3Sn has become fascinating in the current times because it's one of the rare antiferromagnets that exhibits large anomalous Hall and Nernst effects. This opens a new area of research using functional antiferromagnets[1], but for future device applications, it requires fabricating high-quality thin films. There are reports of the controlled growth of Mn_3Sn on substrates like m-plane sapphire,[2] Pt/Al2O3 (0001)[3] and others using sputtering growth, but this often can result in polycrystalline films. In this work, the goal is to grow a crystalline high quality Mn_3Sn film using molecular beam epitaxy. Effusion cells are used for Mn and Sn sources which are calibrated using a quartz crystal thickness monitor. 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. The samples are grown at 500 ± 9°C and 416 ± 9 °C with Mn: Sn atomic flux ratio of 3.2: 1 on c-plane sapphire for 60 mins. We observed that, for both temperatures, the RHEED patterns are streaky; however, the resulting orientations of the films are different. Additional results pertaining to surface morphologies, film orientations, chemical compositions, as well as empirical models will be discussed in detail.

Acknowledgement:

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. Stinaff and his students for back coating the sapphire substrates, as well as Ashok Shrestha for useful discussions and help.

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9:15am **NM-TuM1-6 Relaxed Epitaxial Constraints for Semi-freestanding Shape Memory Alloy Ni_2MnGa Films Grown on Graphene/MgO***, **Zachary LaDuca**, S. Manzo, D. Du, K. Su, M. Arnold, J. Kawasaki,* University of Wisconsin - Madison

Ferromagnetic shape memory alloys such as Ni_2MnGa have great potential as microelectronic actuators due to their ability to reversibly transform between multiple crystalline phases. However, epitaxial growth of shape memory alloys can prevent their ability to undergo structural phase transformations through substrate clamping effects, especially in nanometer scale films below their relaxation thickness. Here, we demonstrate interfacial decoupling between the ferromagnetic shape

memory alloy Ni_2MnGa and MgO via the introduction of a graphene interlayer. X-ray diffraction experiments of Ni_2MnGa films grown by molecular beam epitaxy on bare and graphene terminated MgO(001) show that the constraints of epitaxy are relaxed on graphene terminated surfaces, allowing for multiple epitaxial relationships between substrate and film. This decoupling from graphene allows the Ni_2MnGa to be exfoliated, providing an etch-free method to produce free-standing membranes. Finally, we will discuss the similarities and differences between the three sample types based on magnetization, transport, and structural measurements.

9:30am **NM-TuM1-7 Ferroelectricity at 900 °C in a 1 Unit-Cell-Thick Film***, **Yilin Evan Li**, R. Steinhardt, M. Holtz,* Cornell University*; P. Silva,* University of California, Berkeley*; Z. Xiao,* Lawrence Berkeley National Laboratory*; R. Ozgur,* University of California, Berkeley*; C. Brooks,* Cornell University*; D. Tenne,* Boise State University*; D. Muller,* Cornell University*; P. Shafer, E. Arenholz,* Lawrence Berkeley National Laboratory*; J. Mundy,* Cornell University*; R. Ramesh,* University of California, Berkeley, Lawrence Berkeley National Laboratory*; D. Schlom,* Cornell University, USA, Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Ferroelectric and multiferroic materials are of great importance for functional devices including low-power non-volatile memories and logic. Proper ferroelectrics, in which spontaneous polarization drives the ferroelectric phase transition, have attracted broad interest in the past few decades. Both theoretical and experimental studies indicated that critical thicknesses exist for proper ferroelectrics. For example, a synchrotron X-ray study revealed that, at room temperature, $PbTiO_3$ films can be structurally ferroelectric with thicknesses down to 3-unit cells [1], which agrees well with theoretical predictions [2]. Unfortunately, far less is known about improper ferroelectrics, where an ordering other than polarization (e.g., structural, charge or spin ordering) drives a phase transition that results in ferroelectricity.

To explore the intrinsic properties of improper ferroelectrics, we have investigated a model system, hexagonal $LuFeO_3$. Phase-pure films of this improper ferroelectric are grown on epitaxial iridium bottom electrodes on YSZ (111) substrates by MBE. Atomic force microscopy (AFM) shows that *h*-$LuFeO_3$ films grow smoothly on the iridium bottom electrode in a layer-by-layer fashion with an RMS roughness of 0.55 nm. X-ray ω-rocking curves are measured to assess the structural quality. The full width at half maximum (FWHM) of 111 Ir peak is 29 arc sec (0.008°) and of the 002 *h*-$LuFeO_3$ peak is 0.12°, narrower than any prior reports [3,4] by factors of about 60 and 2, respectively. Our results show that *h*-$LuFeO_3$ films as thin as 1-unit cell are still ferroelectric at ~900 °C.

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9:45am **NM-TuM1-8 Strange Metal $Ybrh_2Si_2$ Grown by Molecular Beam Epitaxy***, **Stefania Isceri**,* Institute of Solid State Electronics, Technische Universität Wien, Austria*; M. Giparakis,* Institute of Solid-State Electronics, Technische Universität Wien, Austria*; E. Bakali,* Insitute of Solid-State Physics, Technische Universität Wien, Austria*; R. Svagera,* Institute of Solid-State Physics, Technische Universität Wien, Austria*; M. Waas,* Institute of Solid State Physics, Technische Universität Wien, Austria*; D. Nguyen,* Institute of Solid-State Physics, Technische Universität Wien, Austria*; H. Detz, W. Schrenk,* Institute of Solid State Electronics, Technische Universität Wien, Austria*; S. Buehler-Paschen,* Insitute of Solid-State Physics, Technische Universität Wien, Austria*; G. Strasser, A. Andrews,* Institute of Solid-State Electronics, Technische Universität Wien, Austria

$YbRh_2Si_2$ is a heavy fermion material [1, 2] crystallizing in the tetragonal $ThCr_2Si_2$-type structure (space group I4/mmm). It has a well-defined quantum critical point [2, 3], a linear-in-temperature strange metal behavior resulting from a dynamical electron localization-delocalization transition [1] and shows superconductivity below 10 mK [4]. $YbRh_2Si_2$ crystal thin films have been recognized as promising for novel applications, such as THz transmission spectroscopy and shot noise detection.

In this work, we study the growth of $YbRh_2Si_2$ on Ge(001) substrates by molecular beam epitaxy (MBE). The substrate chosen is Ge (fcc, a=5.658 Å [5]), due to the low lattice mismatch between its nearest neighbor distance a'=(a√2)/2= 4.001 Å and the a lattice parameter of $YbRh_2Si_2$ (a= 4.007 Å, c= 9.860 Å [6]). The thickness of the deposited films is around 60 nm.

Complementary characterization techniques, *in situ* reflection high-energy electron diffraction (RHEED), *ex situ* atomic force microscopy (AFM), x-ray diffraction (XRD), and energy-dispersive x-ray (EDX) spectroscopy, demonstrate that epitaxial crystalline films are obtained.

The crystal structure analysis highlights that small changes in the out-of-plane lattice parameter correlate with the Rh content. In particular, larger values are directly related to higher Rh concentration. XRD φ-scans show that the films have a four-fold symmetry and are rotated by 45° with respect to the substrate. Resistivity measurements show that the 60 nm thin film $YbRh_2Si_2$ exhibit similar characteristics to bulk single crystals.

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Novel Materials
Room Swan BC - Session NM-TuM2
Infrared Materials

Moderator: Ida Sadeghi, MIT

10:30am **NM-TuM2-11 Strain-Engineered MBE Growth of InAs Quantum Dots Emitting at Telecom Wavelengths***, **Bianca Scaparra**, A. Ajay, H. Riedl, G. Koblmueller, J. Finley , K. Mueller,* Walter Schottky Institut, Technische Universität München, Germany

In recent years, there has been a great interest in the search of solid-state spin-photon interfaces that couple flying photonic qubits at telecom wavelengths and stationary matter qubits [1,2]. Operating at telecom wavelengths is strongly desired to benefit from the low propagation losses that occur in the commonly employed, industry compatible silica fibers. Deterministically charged semiconductor quantum dots (QDs) are a very promising platform for spin-photon interfaces, due to their fast emission rates and fast optical spin manipulation [1]. However, the most widely studied QDs, InAs QDs embedded in a GaAs matrix, have their transition wavelength mainly centered in the near infra-red region.

In this work, we describe our recent progress on the optimization of two epitaxial growth methods that lead to QDs with emission wavelength in the O and C telecom bands. First, in order to shift the emission wavelengths of the QDs towards the O-band, the study of the growth of a high crystal quality InGaAs strain-reducing layer (SRL) above the QDs is presented [3].

Reciprocal space maps show how, by carefully tailoring the growth conditions of the SRL, the degree of relaxation and alloy composition are affected, thus leading to the expected redshifted QDs photoluminescence emission.

With the goal to further shift the emission wavelength towards the C-band, an In-graded InGaAs metamorphic buffer layer (MBL) is grown beneath the QDs, leading to further strain reduction [3].

With the aim to achieve a deeper understanding of the influence of growth parameters on the material quality of the MBL, reciprocal space maps of $In_xGa_{1-x}As$ MBLs grown with different grading profiles are presented. In particular, the samples studied consist of linearly graded $In_xGa_{1-x}As$ buffers with different constant slopes of the In content. These results are combined with compositional EDX mappings for further proving the variation of the In content distribution with different grading profiles.

Finally, in order to understand how the QDs formation arises on the MBL, we discuss how the density and shapes of InAs QDs are correlated to the different In grading profiles and growth conditions.

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10:45am **NM-TuM2-12 InP-based InAs Quantum Dot/dash Lasers Emitting in the O-band***, **Sadhvikas Addamane**,* Center for Integrated Nanotechnologies, Sandia National Laboratories*; S. Seth,* Center for High Technology Materials, University of New Mexico*; S. Hawkins, N. Collins,* Sandia National Laboratories*; C. Shang, Y. Wan,* University of California Santa Barbara*; G. Balakrishnan,* Center for High Technology Materials, University of New Mexico*; J. Klem,* Sandia National Laboratories*; R. Venables,* Intel Corp.*; J. Bowers,* University of California Santa Barbara

Epitaxially-grown quantum dot (QD) lasers are emerging as the ideal candidate for on-chip sources in fiber-optic communication applications. QDs exhibit 3-dimensional carrier confinement which translates to several advantages over traditional quantum well (QW) lasers: low threshold current density, high temperature-stability, reduced linewidth enhancement factor, and increased tolerance to defects[1]. In the O-band (1260-1360nm), most QD-related laser work has been limited to GaAs-based structures and recent advances have demonstrated exceptional device properties including epitaxial integration on Si substrates[1]. The case for exploring InP-based QD lasers in the O-band can be made from both material and device perspectives. The lattice mismatch between InAs and InP is lower (3.2%) compared to the InAs/GaAs system (7.2%); this could lead to improved reliability of lasers. Further, strain compensation is more straightforward on InP and could facilitate stacking of multiple QD layers without accumulating strain. On the device side, InP-based QD lasers in the C-band have been shown to yield higher modal gain (per QD layer) values compared to 1.3µm InAs/GaAs lasers. If this advantage extends to the O-band, higher modal gain would alleviate limitations to device geometry. In this work, we present results from a study focused on realizing 1.3µm QD lasers based on InP.

Methods: The samples described in this study were grown on InP substrates using molecular beam epitaxy (MBE).Short structures consisting of 5x QD layers embedded in InGaAlAs barriers were first grown for photoluminescence (PL) measurements. Each QD layer consists of an asymmetric dot-in-a-well (DWELL) region and the surrounding InGaAlAs QW composition is varied between the different PL samples. Starting from the well-established C-band (1.55µm), increasing the bandgap of the QW slowly moved the emission wavelength towards 1.3µm. Atomic force microscopy (AFM) measurements carried out on uncapped QD layers reveal elongation of the QDs along a preferred crystalline direction (quantum dashes). The optimized active region is integrated into a laser structure with AlInAs cladding and InGaAs (both lattice-matched to InP) p- and n-contact layers. Laser characterization results (I-V, L-I and spectrum) will also be presented.

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This work was performed, in part, at CINT, an Office of Science User Facility operated for the U.S. DOE. Sandia National Labs is a multimission laboratory managed and operated by NTESS, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. DOE's NNSA under contract DE-NA-0003525.

11:00am **NM-TuM2-13 Photonic Crystal Surface Emitting Lasers (PCSELs) grown by Molecular Beam Epitaxy***, **Thomas J Rotter**, S. Seth, K. Reilly, F. Ince,* University of New Mexico*; A. Kalapala, Z. Liu, W. Zhou,* University of Texas at Arlington*; G. Balakrishnan,* University of New Mexico

Photonic crystal surface emitting lasers (PCSELs) based on InGaAs quantum wells emitting near 1040nm are fabricated by molecular beam epitaxy (MBE). PCSELs achieve vertical emission with high beam quality while avoiding the complexity associated with DBR growth for VCSELs. The epitaxial structure of a PCSEL is similar to that of an edge emitting laser. Vertical emission is achieved by a photonic crystal, which is realized as a pattern of holes near the waveguide core. PCSELs can be power scaled with area while maintaining coherent emission.

The fabrication process starts with MBE growth of a part of the laser structure. This includes the lower clad and waveguide core with the active region. Next, in the top surface of the waveguide (PC layer) a pattern consisting of periodically spaced voids is fabricated using electron-beam lithography and ICP etch. In the third step, the regrowth, the top clad and contact layers are grown on the patterned surface, which completes the laser structure.

Epitaxial regrowth is challenging due to infilling of the voids and because obtaining a clean surface for regrowth is difficult. Thermal and chemical treatment options to prepare the patterned surface for regrowth are explored.

For the PC design, it is important to match its resonance to the photoluminescence of the active region. Relevant parameters such as void shape and PC fill factor are influenced by the regrowth. SEM characterization of the voids before and after regrowth shows that pre-regrowth void radius influences the growth dynamics, i.e. growth at the sidewalls versus at the bottom of the void. Regrown PCSEL devices are demonstrated by optical pumping and electrical injection.

In addition to PCSEL fabrication by regrowth, non-regrowth methods are explored. The advantages include significantly reduced fabrication complexity and time. Here the entire laser structure is epitaxially grown and the PC fabricated on the surface of the top contact, which requires etching of very deep voids. Non-regrowth PCSELs are compared to edge-emitters from the same epitaxial structure.

11:15am **NM-TuM2-14 Low Growth Temperature Epitaxial PbSe for Heterogeneous Mid-Infrared Emitters***, **Leland Nordin**, J. Meyer, P. Reddy, K. Mukherjee,* Stanford University

The mid-infrared (MIR) wavelength range is vital for an abundance of sensing, health/biological monitoring, security and defense, and fundamental science applications. For compact solid-state sources of MIR light, III-V semiconductor heterostructures, such as quantum cascade lasers (QCL), interband cascade lasers (ICL), or type-II superlattice light emitting diodes (SLED), are often used. However, QCL, ICL, and SLED structures all suffer from substantial growth complexity. Recently, thin films of PbSe grown epitaxially on III-V GaAs (001) substrates have shown high internal quantum efficiency (IQE) at room temperature and comparatively low growth temperatures of 300 °C, compatible with back end of line processes [1].

In this work, we show that the growth window for high optical-quality PbSe/III-V extends to substantially lower temperatures than previously demonstrated and investigate the recombination dynamics of the low growth temperature films. A high temperature (300 °C) PbSe film [Figure 1(a)] and a lower temperature (170 °C) PbSe film [Fig. 1(b)] were grown on oxide-desorbed and arsenic-capped GaAs (001) substrates in a molecular beam epitaxy (MBE) system using a compound PbSe source. Both growths started with a PbSe dose procedure and nucleation layer [2]. Following the nucleation layer, the growth temperature was lowered to the either 300 °C or 170 °C, and 80 nm of PbSe was grown. Room temperature MIR photoluminescence (PL) was measured on both films and is shown in Fig. 1(c). Notably, the magnitude of PL is nearly identical for both the high and low growth temperature films. To better understand the impact of growth temperature on luminescence efficiency we performed power dependent PL (PDPL) measurements, shown in Figure 2. Remarkably, we do not see a substantial deviation in PL magnitude for lower pump powers, suggesting similar SRH recombination rates.

We have grown PbSe films on GaAs substrates at 300 °C and 170 °C and investigated their luminescence properties. PL is not dramatically impacted by the lower growth temperature, corroborated by both the magnitude of spectral dependent PL and power dependent PL. Most importantly, the low growth temperatures investigated are compatible with back end of line processes, likely extend the accessible crack-free film thicknesses, and possess bright PL. Additionally, these low growth temperatures enable the investigation of more esoteric ternaries, such as PbGeSe, which require extremely low growth temperatures.

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11:30am **NM-TuM2-15 Structural Properties of MBE-grown PbSnSe on GaAs (001) Films for Mid-infrared Optoelectronics Investigated by X-ray Diffraction***, **Jarod Meyer**,* Stanford University*; E. Hughes,* University of California at Santa Barbara*; L. Nordin, K. Mukherjee,* Stanford University

The narrow gap IV-VI semiconductor PbSe is an intriguing material for heterogeneously integrated mid-infrared light emitters in the 3 – 5 um wavelength range. The combination of an anomalously low Auger recombination coefficient and high tolerance of minority carriers to crystal defects suggests the potential for mid-infrared light emission with high quantum efficiency. Recently, we showed that bare, epitaxial thin films of PbSe on (001)-oriented GaAs emitted brightly despite an 8% lattice

mismatch, indicating a high internal quantum efficiency of luminescence at room-temperature.

Moving beyond binary PbSe, the bandgap may be tuned across the mid- and far-IR via alloying with Sn in the ternary $Pb_{1-x}Sn_xSe$.[2] This motivates us to explore how alloying Sn alters the microstructure and luminescence properties of PbSe films. Strain-induced structural distortions, stemming from lattice and thermal-expansion mismatches with GaAs, are also important for understanding the optoelectronic properties of these thin films.

We grew $Pb_{1-x}Sn_xSe$ epitaxial films on (001)-oriented GaAs substrates by molecular beam epitaxy at 280–330 °C using PbSe and SnSe compound source effusion cells, following a 400 °C surface pretreatment with PbSe flux that we find essential for good photoluminescence. High resolution x-ray diffraction was used to extract alloy compositions and structural properties. Across a Sn composition range of x = 0–0.31, full-width-at-half-maximums of (004) and (224) rocking curves were in the range of 370 – 510 and 700 – 840 arcseconds, respectively, indicating only minor differences in structural quality. For the x = 0.41 sample, however, structural quality was significantly degraded, likely due to the presence of both rock-salt and orthorhombic phases in the film. In-plane residual tensile strains of 0.25–0.50% at room-temperature were also found for the $Pb_{1-x}Sn_xSe$ films, in agreement with the predicted thermal mismatch strain between PbSe and GaAs upon cooldown from growth temperature.[1,3]

Preliminary room-temperature photoluminescence of dilute $Pb_{1-x}Sn_xSe$ ternaries shows redshifted peak wavelengths out to 4.6 µm for x = 0.03, but with significantly decreased intensity compared to PbSe. We will present results investigating and comparing loss mechanisms in PbSe and $Pb_{1-x}Sn_xSe$ to understand whether these are fundamental or may be overcome by engineering.

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11:45am **NM-TuM2-16 MBE Growth and Characterization of an InAs/$AlAs_{0.16}Sb_{0.84}$ Quantum Cascade Detector at 2.7 µm***, M. Giparakis, H. Knötig, S. Isceri, M. Beiser, H. Detz, W. Schrenk, B. Schwarz, G. Strasser,* ***Aaron Maxwell Andrews,*** Technische Universität Wien, Austria

We present the molecular beam epitaxy (MBE) growth, design, and characterization of an InAs/$AlAs_{0.16}Sb_{0.84}$ quantum cascade detector (QCD) grown lattice-matched to an InAs substrate detecting at 2.7 µm (0.459 eV), which is above the band gap energy of the InAs substrate of 0.345 eV (3.5 µm) [1] and in the center of a CO_2 absorption line.

The InAs/$AlAs_{0.16}Sb_{0.84}$ material system was chosen because it combines two important characteristics for improved optical absorption strength, low noise, high detectivity, and a broad designable wavelength range – one of the lowest effective electron masses m^*_e in III-V semiconductors of m^*_e = 0.023 m_0 and second the highest cubic conduction band offsets of 2.1 eV [2].

The growth of this material system is challenging due to the mixed group V compound in the barrier. The As and Sb fluxes must be precisely controlled, especially when growing in lattice-matched conditions. Additionally, QCDs designed for short wavelength absorption, like the one presented here, need thin wells and barriers – which were ranging from 1.38 to 3.85 nm for this QCD. The precise layer thickness control necessary for this structure was achieved by implementing special shutter sequences to reduce intermixing at the interfaces and growth rate variations caused by shutter operations were taken into consideration. Lattice matching well and barrier materials to the substrate improves the growth quality and more degrees of freedom exist, because strain balancing does not have to be considered.

The QCD was fabricated into mesas with a diffraction grating on top that allows top-side illumination, which is normally forbidden by the selection rule of intersubband devices, such as QCDs. It also allows for a detection wavelength above the band gap energy of the InAs substrate. To find the optimal parameters for the grating-period, grating-duty, and grating-depth simulations were performed using COMSOL.

The absorption spectrum was measured using a Fourier-transform infrared spectrometer together with a Globar and a longpass filter with a cut-on wavelength of 2.4 µm. The designed absorption wavelength of 2.7 µm was confirmed. The QCD shows a peak responsivity at room temperature of 5.63 mA/W and a specific detectivity of 1.14×10^8 Jones.

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12:00pm **NM-TuM2-17 Substrate Preparation and MBE Growth of High Quality α-Sn Topological Insulator Thin Films on InSb(001) Surfaces***, **Aaron Engel**, C. Dempsey,* University of California, Santa Barbara*; S. Nishihaya, Y. Chang,* University of California, Santa Barabara*; M. Hashimoto, D. Lu,* Stanford Synchrotron Radiation Lightsource*; C. Palmstrøm,* University of California, Santa Barabara

α-Sn is one of the only elemental materials that shows multiple topological phases. Of high interest is the conversion from a Dirac semimetal state under compressive strain to a topological insulator state under both compressive strain and confinement. When in this topological insulator state, α-Sn has been calculated to have a large band gap and measured to have Dirac surface states with high Fermi velocity, making it attractive for spintronics applications [1]. α-Sn does not suffer from stoichiometry, uniformity, and disorder issues to the degree seen in compound topological materials. Unfortunately, interactions with the substrate have made clean studies into this system difficult. Particularly, the typical sputter cleaning and annealing preparation of InSb results in poor crystal quality at the interface and significant hole doping of the α-Sn films [2]. Here we present the combination of *in-situ* atomic hydrogen cleaning and Sb-termination of the InSb(001) substrates in an interconnected growth and characterization system to 1) prepare high quality α-Sn(001) by MBE and 2) limit the effects of hole doping. These methods, along with a UHV vacuum suitcase, allowed the α-Sn electronic bands to be studied at high resolution using synchrotron-based angle-resolved photoelectron spectroscopy (ARPES). We confirm that the 3D Dirac semimetal state transitions to a topological insulator under confinement. A two-dimensional electron gas is found to coexist with the Dirac surface state after electron doping the Sn surface. Magnetotransport measurements will be performed and compared with the ARPES spectra. Our work paves the way for deeper studies into pristine α-Sn prepared on a larger scale.

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Novel Materials
Room Swan BC - Session NM-TuA1

Bismuthides

Moderator: Kevin Grossklaus, Tufts University

1:30pm **NM-TuA1-1 NAMBE Young Investigator Awardee Talk: Why do we Bother Using Costly MBE for Semiconductor Nanowires?**, ***Songrui Zhao***[1], McGill University, Canada **INVITED**

Low-dimensional semiconductor nanowires has been an attractive material platform for both novel electronic and photonic devices as well as exploring new physics at low dimensions. Back to more than two decades ago, low-cost chemical vapor deposition (CVD) techniques had already been able to demonstrate devices based on single Si, Ge, InP, and GaN nanowires. Comparing to CVD, the operational cost of MBE is dramatically higher. So why do we bother using costly MBE for semiconductor nanowires? In this talk, I will discuss III-nitride nanowires grown by MBE as well as applying such nanowires to photonic devices. I will show that using such nanowires, quite a few underlying material challenges for III-nitride photonic devices can be greatly addressed, e.g., p-type doping into InN and AlN. This enables devices that were not possible previously, such as 207 nm emitting AlN LEDs with turn-on voltage only limited by the bandgap energy and a rectification ratio of more than 10^6, electrically injected AlGaN deep ultraviolet (UV) lasers down to 239 nm. Moreover, I will further show that such nanowires can be a useful template for the wafer-scale integration of ultrawide bandgap III-nitride epilayers (AlN and Al-rich AlGaN) on Si, and greatly relax the substrate requirement for the development of ultrawide bandgap III-nitride electronic and photonic devices. Vertical semiconductor deep UV LEDs down to 247 nm are demonstrated using such an approach.

2:00pm **NM-TuA1-3 Electrical Characterization of Doped GaSbBi Films Using High Resistivity AlGaSb Underlayers**, ***John McElearney***, *K. Grossklaus, T. Vandervelde,* Tufts University

Dilute III-V-Bi alloys, such as $GaSb_{1-x}Bi_x$, have garnered interest in recent years as useful materials for mid- to far-IR optoelectronic devices. This is primarily due to the dramatic reduction in bandgap energy caused by the interaction of the Bi impurity with the host valence band edge [1]. In $GaSb_{1-x}Bi_x$ specifically, reductions of up to 35 meV/%Bi [2] have been observed. Additionally, a predicted suppression of Auger recombination [3] and ability to be grown pseudomorphically on commercially available GaSb substrates makes $GaSb_{1-x}Bi_x$ a prime candidate for use in long wavelength photonics. Effective design of such devices will require a deeper understanding of the doping behavior of GaSbBi than is currently available. However, both GaSb substrates and MBE-grown GaSb buffer layers are intrinsically p-type (n_a ~ 1e16/cm^3), making the measurement of carrier concentrations or mobilities of any epilayers grown on them non-trivial. Following techniques previously employed in GaSb [4], we report on the electrical characterization of Bi-containing films grown on high resistivity Al-containing underlayers.

In this work we present carrier concentrations and mobilities for intentionally and unintentionally doped $GaSb_{1-x}Bi_x$ samples grown on highly resistive $Al_yGa_{1-y}Sb$ underlayers. Samples were grown on Zn-doped GaSb substrates (n_a ~ 1e18/cm^3) in a Veeco GENxplor system. Al, Ga and Bi, as well as dopant fluxes, were supplied by solid source effusion cells, while Sb was sourced from a valved cracker cell. Growth was monitored in-situ via RHEED and temperature was tracked by blackbody emission using a k-Space BandiT system. Hall effect measurements were conducted on Be and Te-doped GaSbBi films of low to moderate Bi-fraction, as well as on GaSb-capped AlGaSb layers to demonstrate their resistive behavior. High-resolution XRD was used to determine Bi and Al content, as well as confirm film quality and homogeneity. We also examine the effect the Al-underlayer, as well as any dopants present, has on Bi droplet formation and surface morphology via both Nomarski optical microscopy and atomic force microscopy. Results of this work will enable improved modeling and design of future GaSbBi-based optoelectronic devices.

[1] D.P. Samajdar, T.D. Das, S. Dhar, *Mater Sci Semicond Process*, **40**, 539-542 (2015).

[2] M. K. Rajpalke et al., *J. Appl. Phys*. **116**, 043511 (2014).

[3] S. Das, M. K. Bhowal, S. Dhar, *J. Appl. Phys.* **125**, 075705 (2019).

[4] M. G. Mauk, V. M. Andreev, *Semicond. Sci. Technol.* **18,** S191 (2003).

2:15pm **NM-TuA1-4 Influence of Growth Conditions on InAlBiAs Morphology and Electrical Properties**, ***James Bork***, *W. Acuna, J. Zide,* University of Delaware

We present on our recent progress in MBE-growth of InAlBiAs on (001) InP. As highly-mismatched alloys, quaternary bismuthides like InAlBiAs offer high degree of control over lattice constant, bandgap and band alignment, and spin-orbit coupling. This tuneabilty makes bismuthides of interest for use in infrared emitters and detectors, solar cells, and other (opto)electronic devices. [2,3,4,5] However, the high mismatch between the bismuthides' constituent elements make high quality, droplet-free growth difficult to achieve. [6] While previous work has explored the optical properties of InAlBiAs [7], a systematic study of the impacts of growth conditions on InAlBiAs morphology and electrical properties was still needed.

Through variation of the V/III and Bi/As flux ratios used during growth, we have constructed a growth-space diagram of Bi incorporation that demonstrates several key morphological regimes: V-rich (with droplets), III-rich (with droplets), and droplet-free. Using this diagram, we have demonstrated droplet-free growth of InAlBiAs w/ up to 5.1% Bi. The unintentional n-type doping concentration of these materials were measured to be between 10^{13}-10^{15} cm^{-3}.

[1] *Crystals.*17, 7, 63 (2017) [2] *Semicond. Sci. Technol.* 27, 094011 (2012) [3]*Appl. Phys. Lett.* 88, 201112 (2006) [4] *Sol. Ener. Mat. and Sol. Cells.* 155, 446-453 (2016) [5] *Jour. of Photovol.* 6, 1183-1190 (2016) [6] *Jour. of Appl. Phy.* 120, 125310 (2016) [7] *Jour. of Appl. Phy.* 126, 095704 (2019)

2:30pm **NM-TuA1-5 ErAs:InGaAlBiAs materials for 1.55 µm-pumped Terahertz Photoconductive Switches**, ***Wilder Acuna***, *J. Bork, J. Avenoso, L. Gundlach, J. Zide,* University of Delaware

Here, we present the study on the molecular beam epitaxy growth of ErAs nanoparticles embedded within an InP-based $(InGaBiAs)_x$ $(InAlBiAs)_{1-x}$ digital alloy for use in photoconductive switches (PCS) for terahertz (THz) generation and detection. Towards the aim of achieving PCs with desired properties, ErAs:$(InGaBiAs)_x$ $(InAlBiAs)_{1-x}$ digital alloy (henceforth: ErAs:InGaAlBiAs) offers several advantages. First, ErAs self-assembles as nanoparticles and can be incorporated by co-deposition or interrupt-growth. These nanoparticles pin the Fermi level and act as effective carrier traps, decreasing the carrier lifetime to sub-picosecond values [1]. Additionally, the InGaAlBiAs matrix allows band alignment to be engineered around the pinned Fermi level. When the matrix is InGaAs, ErAs pin the Fermi level close to the conduction band. Adding Bi and Al makes it possible to align the band to have a midgap Fermi level, thereby increasing the dark resistance while maintaining a bandgap below 0.8 eV. In the case of Bi, just a small amount narrows the bandgap by lifting the valence band due to valence band anti-crossing (VBAC) [2]; however, this increases the growth complexity as low temperatures and stoichiometric conditions are required. In addition, the semiconductor needs to be optically thick to absorb the majority of the optical pump pulse. Accordingly, the film must be lattice-matched to the InP substrate. In addition to discussing the growth, we present our progress in measuring material properties required for a high-performance PCS. [1] Appl. Phys. Lett. 75, 3548 (1999); [2] Phys. Rev. B 75, 045203 (2007).

2:45pm **NM-TuA1-6 Impact of Bi Surface Coverage During Growth on GaAsBi Diode Performance**, ***Robert Richards***, *N. Bailey, T. Rockett, M. Carr,* University of Sheffield, UK*; S. Hasegawa, H. Kawata, H. Nishinaka, M. Yoshimoto,* Kyoto Institute of Technology, Japan*; J. David,* University of Sheffield, UK

The dramatic effect of bismuth alloying on the band structure of GaAs makes GaAsBi a promising candidate material for a range of applications from telecommunication laser diodes [1] to solar cells [2]. Recently, the increased spin-orbit splitting energy in GaAsBi has been shown to dramatically reduce the "excess noise" associated with GaAsBi avalanche photodiodes [3], promising a new family of ultra-low-noise, Bi-engineered photodetectors. Further development of the MBE growth of this alloy is required to reduce dark currents and realise its potential.

In this work, the influence of growth conditions on the performance of GaAsBi diodes is investigated across a large number of p-i-n diode devices grown at the University of Sheffield and the Kyoto Institute of Technology, as well as other devices reported in the literature. The results show that increasing bismuth content leads to an increase in the device dark currents due to the resultant reduction in the device band gap. The rate of change in saturation current density with respect to band gap is broadly in line with the findings of earlier work [4]; however, the temperature dependence of

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the saturation current density is not trivial. The results suggest that growth temperature is not the only key parameter for high-quality device production and that control of the bismuth surfactant layer during growth is critical to maintaining good material quality and the attendant low dark currents. For the most heavily strained devices, low temperatures appear to reduce the effect of plastic strain relaxation on the device properties [5]. By relating the dark currents to the low temperature photoluminescence properties of GaAsBi layers, the importance of the bismuth surface coverage during growth is highlighted.

[1]S. J. Sweeney and S. R. Jin, "Bismide-nitride alloys: Promising for efficient light emitting devices in the near- and mid-infrared," J. Appl. Phys., 113(4), 043110, (2013).

[2]R. D. Richards et al., "Photovoltaic characterisation of GaAsBi/GaAs multiple quantum well devices," Sol. Energy Mater. Sol. Cells, 172, 238-243, (2017).

[3]Y. Liu et al., "Valence band engineering of GaAsBi for low noise avalanche photodiodes," Nat. Commun., 12(1), 4784, (2021).

[4]R. D. Richards et al., "Temperature and band gap dependence of GaAsBi p-i-n diode current–voltage behaviour," J. Phys. D: Appl. Phys., 54(19), 195102, (2021).

[5]N. Bailey et al., "Effect of MBE growth conditions on GaAsBi photoluminescence lineshape and localised state filling," Sci. Rep., 12(1), 1-8, (2022).

3:00pm **NM-TuA1-7 Towards Lattice-Matched Narrow Bandgap $InAs_ySb_{1-x-y}Bi_x$ Photodetectors**, ***Corey White**, M. Bergthold,* The University of Texas at Austin*; I. Okoro,* Texas State University*; Y. Wang,* The University of Texas at Austin*; L. Nordin,* Stanford University*; A. Muhowski,* Sandia National Laboratories*; D. Wasserman, S. Bank,* The University of Texas at Austin

Bismuth incorporation in III-V alloys induces a desirable bandgap reduction, however, III-V-Bi alloys have struggled to achieve high material quality due to the dramatic difference between the ideal growth temperature of the host III-V matrix and the relatively cold growth temperatures necessary for promoting significant bismuth incorporation.[1,2] In-SbBi, however, is a particularly promising material system for accessing the longwave-infrared (LWIR) with high performance optoelectronic devices due to the relatively similar ideal growth windows for InSb and III-Bi materials. Recently we demonstrated the growth of high quality InSbBiwith unity sticking Bi incorporation and demonstrated the first photoluminescence (PL) measurements from this alloy. By incorporating As into InAsSbBi, the quaternary can be lattice-matched to InSb substrates enabling the growth of thick layers, which is vital for strong absorption in photodetectors. Here we report the growth and optical properties of the first dilute-bismide films lattice-matched to InSb. Films exhibited highly substitutional bismuth incorporation enabling the first room temperature PL, as well as progress towards LWIR photodetection.

InAsSbBi films were grown on InSb substrates by solid-source MBE. Low substrate temperatures and V/III flux ratios near unity promoted high substitutional bismuth incorporation. Following similar high-quality GaAsBi growth,[3] a relatively fast growth rate was used to kinetically suppress bismuth segregation during growth.

X-ray diffraction measurements confirmed lattice-matching of InAsSbBi to InSb and Rutherford backscattering spectrometry measurements were performed to quantify the 1.3% Bi content in the film. Ion channeling measurements demonstrated highly substitutional bismuth incorporation (~95%), which is a prerequisite for high optical quality.[4] We observed room temperature PL at ~7.6 um from InAsSbBi demonstrating a considerable redshift in emission wavelength beyond InSb. To evaluate the potential of this material family for optoelectronic devices, a prototype MSM photodetector was fabricated on InSbBi and preliminary light and dark I-V characteristics demonstrated the first photodetection from InSbBi grown in the unity sticking regime.

[1]S. Francoeur et al., *Appl. Phys. Lett.* **82** (2003).

[2]S. Tixier et al., *Appl. Phys. Lett.* **82** (2003).

[3]A. Ptak et al., *J. Cryst. Growth***338** (2012).

[4]S. Spruytte et al., *MRS Internet J. Nitride Semicond. Res.* **5** (2000).

This work was performed at the UT-Austin MRC, a member of the NNCI support by the NSF (No. ECCS-1542159) and supported by Lockheed Martin, NSF (ECCS-1933836), and an NSF GRF (RCW).RBS measurements were performed at Rutgers LSM.

Novel Materials
Room Swan BC - Session NM-TuA2
Heterogenous Integration

Moderator: Vladimir Vladimirovich Protasenko, Cornell University

3:45pm **NM-TuA2-10 sub-Monolayer Surface Termination Control of Charge Transfer and Band Alignment Across a Semiconductor-Crystalline Oxide Heterojunction**, *M. Chrysler,* University of Texas-Arlington*; T. Lee, J. Gabel,* Diamond Light Source, UK*; Z. Zhu, P. Sushko, S. Chambers,* Pacific Northwest National Lab*; **Joseph Ngai**,* University of Texas-Arlington

Semiconducting heterojunctions exhibiting built-in electric fields that stem from charge transfer are the building-blocks for virtually all device technologies. While such heterojunctions are typically formed between covalent semiconductors, the epitaxial growth of SrTiO3 on Si(100) using MBE enables charge transfer and the formation of built-in fields to be studied in hybrid heterojunctions in which ionic and covalent properties are coupled. We find that the surface of SrTiO3 drives the transfer of electrons from Si to SrTiO3, and that electron transfer can be tuned by altering the composition of the terminating layer, as revealed by electrical transport and hard x-ray photoelectron spectroscopy measurements. The transferred electrons in turn create space charge across the interface which modifies the interfacial dipole that stems from epitaxial bonding. The modulation of the dipole leads to a change in band alignment from type-II to type-III, which promotes additional electron transfer. The surface driven transfer of charge across the interface is discussed within the context of surface depletion, surface adsorbates, as well as physical structure. The strong sensitivity of interfacial charge transfer to surface termination as well as the tunability of band alignment via the interfacial dipole, opens degrees of freedom by which functional behavior can be engineered in hybrid heterojunctions.

4:00pm **NM-TuA2-11 Heteroepitaxial Growth of (111)-oriented $Sr_{1-x}Ca_xTiO_3$ Thin Films on III-Nitride Semiconductors**, ***Eric Jin**, B. Downey, V. Gokhale, J. Roussos, M. Hardy, N. Nepal, D. Katzer, J. Calame, V. Wheeler, D. Meyer,* U.S. Naval Research Laboratory

Heterogeneous integration of epitaxial functional oxides with semiconductors has attracted significant interest in recent decades with the goal to couple the novel functionalities observed in these oxides—including high-temperature superconductivity, multiferroicity, tunable electronic phases, and high dielectric constants (κ)—with technologically-relevant semiconductor platforms. Advances in epitaxial growth techniques have enabled the monolithic integration of perovskite oxides with Si, Ge, GaAs, and more recently, GaN. Development of electronics based on wide and ultra-wide bandgap (UWBG) semiconductors such as AlN, AlGaN, and ScAlN is especially attractive for high frequency and power electronics applications, due to the larger breakdown electric field of these materials when compared to conventional semiconductors.

High quality epitaxial growth of perovskite oxides on wurtzite-phase III-nitrides is challenging due to both the crystal and chemical mismatches. For example, the lattice mismatch between $SrTiO_3$ (STO) and GaN is 13.3%, which leads to polycrystalline films when STO is directly deposited onto GaN. However, a thin rutile TiO_2 buffer layer can significantly reduce the lattice mismatch [1]. In this work, we demonstrate the epitaxial growth and characterization of (111)-oriented STO and $Sr_{1-x}Ca_xTiO_3$ (SCTO) thin films on AlGaN/GaN and ScAlN/GaN high-electron-mobility transistor (HEMT) heterostructures by RF-plasma-assisted oxide molecular beam epitaxy. A 1-nm-thick TiO_2 buffer layer is used to orient the SCTO film and greatly improves crystal quality [2].

As an application, we extract the dielectric constant of the oxide/III-nitride heterostructures with capacitance-voltage measurements and find a κ value as high as 290 and a fixed positive interface charge density of 2.38×10^{13} cm^{-2} at the SCTO/AlGaN interface [3]. RF characterization of interdigitated capacitors fabricated on the SCTO films show that the high κ values are maintained at 2 GHz. These results demonstrate the epitaxial integration of an “extreme κ” functional oxide with GaN that can potentially improve electric field management in RF HEMTs [4]. Moreover, the epitaxial connection between a perovskite and wurtzite crystal structure can pave the way for perovskite oxide-UWBG semiconductor integration to realize next-generation multifunctional oxide/nitride hybrid electronics.

This work is supported by the Office of Naval Research.

[1] W. Tian et al., *Appl. Phys. Lett.* (2007)
[2] E. N. Jin et al., *J. Appl. Phys.* (2020)

[3] E. N. Jin et al., *APL Mater.* (2021)
[4] N. K. Kalarickal et al., *IEEE Trans. Electron Devices* (2021)

4:15pm **NM-TuA2-12 MBE Growth and Electronic Properties of Epitaxial $SrNiO_3$-based Heterostructures**, ***Le Wang***, *P. Sushko, S. Spurgeon, Y. Du, S. Chambers,* Pacific Northwest National Laboratory

The rich phase diagrams of nickelates RNiO$_3$ (R denotes the lanthanide) are of critical importance for both material physics and oxide electronics. The recent discovery of superconductivity in infinite-layered $R_{1-x}Sr_xNiO_2$ further motivates the synthesis of other related nickelates in searching for high-T_c materials and should provide new insights into the origin of high-temperature superconductivity. However, Sr substitution in $RNiO_3$ solid solutions has been shown to induce local defects and structural instabilities, presumably because bulk $SrNiO_3$ exhibits a hexagonal phase and is not stable. Thus, it is important to understand how to stabilize perovskite structured $SrNiO_3$ and how the local charges are distributed in the lattice.

One of our recent efforts to stabilize $SrNiO_3$ thin films on perovskite substrates by oxide molecular beam epitaxy (MBE) led to spontaneous phase segregation. Two co-existing oxygen-deficient Ruddlesden-Popper (RP) phases, Sr_2NiO_3 and $SrNi_2O_3$, are formed to balance the stoichiometry and stabilize the energetically preferred Ni^{2+} cation.[1] We envision that this kind of spontaneous phase segregation and RP faults may occur during the synthesis of Sr doped $RNiO_3$ when the Sr doping level is high.On the other hand, by fabricating epitaxial $(SrNiO_3)_m/(ABO_3)_n$ superlattices, we show that normally hexagonal-structured $SrNiO_3$ can be stabilized as a perovskite at the single unit cell level (m = 1).[2,3] Spectroscopy reveals that the Ni valence can exceed Ni^{3+} and can be also tuned by controlling the magnitude of the BO_6 octahedral rotations. In-plane transport data are consistent with variable-range hole hopping conductivity for these superlattices, whereas hole hopping along the c-axis direction can be tuned by changing n. Our results offer exciting opportunities to generate novel ground-states unobtainable in bulk crystals and will inspire the epitaxial synthesis of $(SrNiO_3)_1/(RNiO_3)_n$ superlattices. Measurements of the associated properties may open new avenues for studying superconductivity in nickel-based oxides.

[1] L. Wang *et al.* Sci. Adv. 7, eabe2866 (2021).

[2] L. Wang *et al.* Adv. Mater. 32 (45), 2005003 (2020).

[3] L. Wang *et al.* Phys. Rev. Mater. submitted (2022)

4:30pm **NM-TuA2-13 Controlling Dislocation Formation and Dynamics in GaAs-Based Films on Silicon via Indium Alloying**, ***Eamonn Hughes***, *M. Dumont, J. Selvidge, J. Norman,* University of California, Santa Barbara*; Y. Hu,* Hewlett-Packard Labs*; C. Shang, D. Jung, A. Taylor, M. Kennedy,* University of California, Santa Barbara*; R. Herrick,* Intel Corporation*; D. Liang, R. Beausoleil,* Hewlett-Packard Labs*; J. Bowers,* University of California, Santa Barbara*; K. Mukherjee,* Stanford University

Much dislocation research sensibly focuses on growth strategies to reduce dislocation densities and thereby improve device performance and reliability, but one often overlooked stage of growth is the cooldown phase. In many III-As films on silicon, this phase is especially important because dislocations continue to evolve due to (1) thermal stress generated by thermal expansion mismatch between film and substrate and (2) the lack of obstacles to glide particularly in (Al)GaAs. For a GaAs-based film grown on silicon at a typical molecular beam epitaxy temperature of 580 °C, cooling to room temperature leaves about 0.15% residual thermal tensile strain. We have recently shown that alloying such a film with just 5% indium can effectively halt dislocation glide under these low stress conditions. Here, we detail two cases where we leverage this indium alloy-hardening effect to mitigate certain undesirable dislocation formations.

In one application involving regrowing GaAs-based films on a thin GaAs template bonded to silicon for integrated photonics, we explore the potential for thin indium-alloyed layers to reduce threading dislocation (TD) densities, which nucleate due to thermal expansion mismatch. We find that the initial compressive stress is relaxed efficiently by a small density of dislocations nucleated at the bond interface, but during cooldown when the stress state reverses, the dislocation density rises sharply. We block the propagation of these latter dislocations by inserting strained indium-alloyed 'trapping' layers and reduce dislocation densities in the remainder of the film by 40×.

In a separate application, misfit dislocations (MDs) are seen to form during cooldown in InAs QD lasers directly above and below the active region due to TD pinning and thermal stress. These MDs cannot pass through the active region because, in addition to pinning, they experience a strong repulsive force due to the tensile-to-compressive stress reversal at the interface. To address this, we displace the network of MDs away from the active region by inserting a thin indium-alloyed trapping layer a short distance on either side of the active region to extend the region of TD pinning. By placing the trapping layers outside the depletion region, the MDs are starved of minority carriers, rendering them largely benign during device operation and yielding up to two orders of magnitude improvement in reliability.

These studies showcase a method to engineer around cooldown-generated dislocations rather than eliminate them entirely, particularly useful when doing so is exceedingly difficult or comes with unwanted side effects such as cracking.

4:45pm **NM-TuA2-14 Grafted Si/GaN, AlN/Si, and GaAs/GeSn PN Junctions with Epitaxy-Like Interface Qualities**, ***Jie Zhou***, University of Wisconsin - Madison*; P. Wang, D. Wang,* University of Michigan, Ann Arbor*; T. Ng,* King Abdullah University of Science and Technology, Saudi Arabia*; H. Wang, S. Xu,* National University of Singapore*; S. Ojo,* University of Arkansas*; Z. Mi,* University of Michigan, Ann Arbor*; B. Ooi,* King Abdullah University of Science and Technology, Saudi Arabia*; X. Gong,* National University of Singapore*; S. Yu,* University of Arkansas*; T. Grotjohn,* Michigan State University*; Z. Ma,* University of Wisconsin - Madison

Semiconductor heterojunction-based devices have revolutionized modern human society. Epitaxy growth employing MBE, MOCVD, MOVPE, etc. has been the only approach to form abrupt semiconductor heterojunctions. The essential requirement to form abrupt heterojunctions using the epitaxy techniques is lattice match (or a close match for pseudomorphic growth) between two different semiconductors. Lattice-mismatched heterojunctions can open much broader applications than the lattice-matched ones, however, cannot be realized easily with heteroepitaxy growth. Metamorphically grown interface of such heterojunctions retains a large quantity of density of interface states (Dit). While wafer bonding/fusion techniques have offered limited applications in tunnel junction devices, they cannot be generally used to fabricate abrupt interface with low defect densities [1][2].

Here, we present a novel semiconductor grafting technology as a strategy to overcome the lattice-mismatched constraints faced by epitaxy growth communities. By grafting single-crystalline epitaxially grown semiconductors with a quantum-tunneling gluing layer in between any two semiconductors, high-quality semiconductor heterojunctions, exhibiting significantly suppressed Dit (10^{10}-10^{11} /cm^3.eV) at their interfaces, have been formed. The interface quality reflected from the diode ideality factor rivals the lattice-matched epitaxy interfaces [3]. Specifically, we will report Si/GaN, AlN/Si, and GaAs/GeSn PN junctions formed via the grafting approach. The approach can be applied to any semiconductor heterojunctions that have arbitrary lattice structures and lattice constants.

[1] M. N. Hasan et al (2022). Influences of Native Oxide on the Properties of Ultrathin Al2O3-Interfaced Si/GaAs Heterojunctions. Advanced Materials Interfaces, 2101531.

[2] Y. Ohno et al (2020). Chemical bonding at room temperature via surface activation to fabricate low-resistance GaAs/Si heterointerfaces. Applied Surface Science, 525, 146610.

[3] D. Liu, et al (2018). Lattice-mismatched semiconductor heterostructures. arXiv preprint arXiv:1812.10225.

5:00pm **NM-TuA2-15 Integrating GaSb-Based Infrared Detectors with Si Substrates via Interfacial Misfit Arrays**, ***Trent Garrett***, *M. Drake ,* Boise State University*; P. Reddy,* Stanford University*; K. Mukherjee,* Stanford University*; K. Grossklaus,* Tufts University*; S. Maimon,* Netz Vision*; P. Simmonds,* Boise State University

With applications from night vision and aerial target acquisition, to space telescope operation, infrared (IR) detectors are of great interest to the defense and scientific communities alike. The functionality of these detectors hinges on achieving a high signal-to-noise ratio so that weak signals can still be resolved. Of the many IR detector designs, the nBn device has emerged as a leading choice. As the name suggests, nBn detectors comprise an electron-blocking barrier between n-type absorber and contact layers [1].

nBn-based IR detectors are typically grown on GaSb substrates, which represents perhaps their biggest disadvantage. GaSb substrates are expensive and only widely available up to 4" diameter, placing a limit on high volume manufacturing. Successfully integrating III-V based nBn detectors with Si substrates would overcome these wafer cost and size constraints. However, this approach comes with its own set of challenges, primarily due to the large lattice mismatch between GaSb and Si. GaSb deposited directly onto Si typically forms large 3D islands with a high density of threading dislocations that help relieve the strain [2].

We therefore adopt the use of interfacial misfit (IMF) arrays grown by molecular beam epitaxy (MBE) to manage strain at the III-Sb/Si heterointerface. IMFs consist of the spontaneous formation of a 2D array of 90º dislocations that lie in the plane of the heterointerface. Previous studies show that thin initiation AlSb layers between the GaSb and Si are critical. Compared with GaSb grown directly on Si, GaSb deposited onto an AlSb/Si IMF heterostructure has dramatically improved material quality and lower threading dislocation density (TDD) [3]. To ensure the growth of GaSb-on-Si virtual substrates with the highest possible quality for subsequent nBn growth, perfecting the growth of this AlSb/Si IMF layer is fundamentally important.

We will discuss how choices regarding AlSb growth initiation, substrate temperature, annealing, AlSb thickness, and AlSb growth rate affect the quality of GaSb overlayers. By optimizing these MBE growth parameters, initial results suggest that we can grow GaSb layers with quality comparable to the current state-of-the-art, giving us a benchmark against which to measure further improvements. We will also discuss the use of dislocation filtering superlattices above the IMF to further reduce TDD.

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[1] S. Maimon and G.W. Wicks, Applied Physics Letters 89, (2006).

[2] S.H. Vajargah, S. Ghanad-Tavakoli, J.S. Preston, R.N. Kleiman, and G.A. Botton, Journal of Applied Physics 114, 113101 (2013).

[3] K. Akahane, N. Yamamoto, S.-ichiro Gozu, and N. Ohtani, Journal of Crystal Growth 264, 21 (2004).

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5:15pm **NM-TuA2-16 Epitaxial Growth of Highly Mismatched Antimonide-Based Alloys Using Imf and Defect Filter Layers***, **Fatih Ince**, T. Rotter, A. Mansoori,* University of New Mexico*; S. Addamane,* Sandia National Laboratories*; D. Shima, G. Balakrishnan,* University of New Mexico

Antimonide-based alloys have the capability to detect medium and long-wavelength infrared ranges of the EM spectrum. However, realizing fully relaxed lattice constants between 6.09 Å and 6.47 Å remains a challenge due to the lack of substrates. This limitation can be overcome by using interfacial misfit dislocation (IMF) array growth mode and it has been shown that fully relaxed GaSb growth on GaAs with dislocation density of ~108 dislocations/cm2 is possible [1]. In this presentation, it will be shown that further reduction of the dislocation density to ~107 dislocations/cm2 is possible using AlSb defect filter layers that bend dislocations due to the strain at the AlSb/GaSb interface.

The IMF growth of GaSb on GaAs involves the exchange of the group V element. The same principle is applied to the growth of In0.53Ga0.47Sb on In0.53Ga0.47As in order to further extend the lattice constant to ~6.3 Å. The latter can be grown on an InP substrate, since it is lattice matched. TEM images show the formation of the interfacial misfit dislocation array at the interface similarly to GaSb on GaAs. Defect filter layers can be realized in this case by varying the composition of InGaSb or using InAlSb. However, XRD indicates low crystalline quality of In0.53Ga0.47Sb. This might be due to phase segregation in In0.53Ga0.47Sb.

To reduce the complexity associated with ternaries, the growth of InSb on InAs substrates is investigated. XRD results indicate that InSb can be grown fully relaxed on InAs as in the case of GaSb on GaAs. Studying the direct growth of InSb on InAs helps to identify parameters to improve the growth of the ternary In0.53Ga0.47Sb on In0.53Ga0.47As/InP. In this presentation, our current efforts to optimize the growth quality of InSb and InGaSb alloys as well as the use of antimonide-based defect filter layers to reduce dislocation density will be presented.

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5:30pm **NM-TuA2-17 Controlling the Balance between Remote, Pinhole, and van der Waals Epitaxy of Heusler Films on Graphene/Sapphire***, D. Du, S. Manzo, T. Jung, X. Zheng, M. Arnold, **Jason Kawasaki**,* University of Wisconsin - Madison

Remote epitaxy on monolayer graphene is promising for synthesis of highly lattice mismatched materials, exfoliation of free-standing membranes, and re-use of expensive substrates. However, clear experimental evidence of a remote mechanism remains elusive. In many cases, due to contaminants at the transferred graphene/substrate interface, alternative mechanisms such as pinhole-seeded lateral epitaxy or van der Waals epitaxy can also explain the resulting exfoliatable single-crystalline films. Here, using Heusler film growth on clean graphene on sapphire substrates, we observe a 30 degree rotated epitaxial superstructure that cannot be explained by pinhole or van der Waals epitaxy. With decreasing growth temperature the volume fraction of this 30 degree domain increases compared to the direct epitaxial 0 degree domain. We further show that careful graphene/substrate annealing (T ~ 700 C) and consideration of the film/substrate vs film/graphene lattice mismatch are required to obtain epitaxy to the underlying substrate. The 30 degree rotated superstructure provides the first experimental fingerprint of remote epitaxy that cannot be explained by the other mechanisms.

5:45pm **NM-TuA2-18 Improved-Quality of 3D Semiconductors at Low Temperature Using Intermediate 2D Materials***, **Guanyu Zhou**, R. Younas, T. Sun, G. Harden, Y. Li, A. Hoffman, C. Hinkle,* University of Notre Dame

Low-temperature growth of materials with high-quality is of great importance as it will enable advanced technologies such as monolithic three-dimensional (3D) integration and flexible electronics. However, low growth temperature prohibits sufficient atomic diffusion and directly leads to poor growth quality, as described by the exponential decay of atomic diffusion D with growth temperature T in classic nucleation theory[1] $D \propto exp(-V_s/k_BT)$, where V_s is the potential-energy barrier for adatom diffusion. To enhance atomic diffusion at low T, V_s must be reduced. Here we show, using a thin layer of 2D materials to separate the adatom and the substrate spatially, V_s is significantly reduced based on a Lennard-Jones potential diagram. Simultaneously, the 2D materials behave like a "transparent layer", that permit the adatom-substrate interactions such that the 3D materials can retain epitaxial growth, which have been demonstrated by the novel growth method "remote epitaxy".[2] The maintained, but reduced, potential field through the 2D layer, coupled with the inert surface of the 2D materials, enables long-distance atomic diffusion and enhanced growth quality at lower growth temperatures. As model systems, GaN and ZnSe using WSe_2 and graphene as intermediate layers, exhibit larger grains, preferred orientation, reduced strain, and improved carrier mobility, all at temperatures lower by >200 °C compared to direct growth as characterized by diffraction, X-ray photoelectron spectroscopy (XPS), Raman, and Hall measurements. Moreover, the impact of thickness and grain-size of the WSe_2 on the 3D materials' growth quality was also studied taking advantage of molecular beam epitaxy that can realize excellent uniformity and thickness control. We further demonstrate an improved method to obtain band alignment of the ZnSe/WSe_2 heterostructure using XPS, taking advantage of the easy exfoliation of the grown 2D/3D heterostructure, eliminating quantum confinement issues caused by needing to use thin overlayers to remain photoelectron transparent in conventional methods.

Our results reveal the benefits of a reduced potential field through atomically thin 2D layers, showing promise for reducing the growth temperature of 3D semiconductors and other materials as a solution to severe thermal budget constraints. Moreover, the 2D/3D heterostructures could also enable promising new heterostructures for novel device designs.

This work was supported in part by NEWLIMITS, a center in nCORE, an SRC program sponsored by NIST through award number 70NANB17H041.

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Novel Materials
Room Swan BC - Session NM-WeM1

Quantum-confined Structures
Moderator: Joseph Ngai, University of Texas-Arlington

8:00am **NM-WeM1-1 Ultra-Strong Light-Matter Coupling in the THz with Continuously Graded $Al_xGa_{1-x}As$ Parabolic Quantum Wells***, Chris Deimert,* University of Waterloo (currently at National Research Council Canada), Canada*; P. Goulain, M. Jeannin,* CNRS, Université Paris-Saclay, France*; W. Pasek,* University of Waterloo (currently at University of Campinas), Canada*; A. Bousseksou, R. Colombelli, J. Manceau,* CNRS, Université Paris-Saclay, France*; Z. Wasilewski,* University of Waterloo, Canada

Conventional THz optoelectronic devices operate in the regime where the coupling between light and matter is weak. As an alternative, the strong coupling regime has attracted considerable study in recent years – one can envision the development of coherent light sources based on parametric oscillation and sources of non-classical states of light [1,2]. For such devices, the typical square quantum well struggles above cryogenic temperatures or at frequencies below 3 THz [3], largely due to electron-electron interactions in the well. Parabolic quantum wells (PQWs), on the other hand, are effectively immune to such interactions, providing a strong unified absorption line in situations where square wells cannot be employed [4].

PQWs can be grown with molecular beam epitaxy using digital alloys, but this technique only approximates the parabolic potential and it also generates many interfaces. We instead generate a smooth composition gradient, employing a linear dynamical model of our aluminum effusion cell to smoothly vary the flux at standard growth rates (up to 2.5 Å/s) [5].

Using this technique, we have grown arrays of PQWs in $Al_xGa_{1-x}As$ with composition in the 2–30% range. THz multipass absorption measurements on samples with different transition frequencies and doping levels reveal clear absorption peaks between 2 and 3 THz. The linewidths observed in these samples are remarkably small for THz intersubband (ISB) transitions – at 2.2 THz, we observe a 69 GHz linewidth, which represents a record-small 3.2% fraction of the centre frequency.

We fabricate several of these samples into metal-insulator-metal microcavities, which are designed to be resonant with the ISB mode of the PQWs. Strong coupling (heralded by the appearance of Rabi splitting) is measured via angle-dependent reflectivity. In one sample, we observe a lower polariton branch centered at 1.8 THz, which is the lowest-frequency ISB polaritonic mode to date. Further, we observe ultrastrong coupling (defined as a Rabi splitting greater than 10% of the central frequency) up to 200 K. Further development of these PQW samples could be of great interest for strong-coupling studies and devices with reduced numbers of electrons or at smaller THz operating frequencies.

[1] S. De Liberato and C. Ciuti, Phys Rev Lett **102**, 136403 (2009).
[2] C. Ciuti, G. Bastard, and I. Carusotto, Phys Rev B **72**, 115303 (2005).
[3] Y. Todorov *et al.*, Phys Rev Lett **105**, 196402 (2010).
[4] C. Deimert *et al.*, Phys Rev Lett **125**, 097403 (2020).
[5] C. Deimert and Z.R. Wasilewski, J Crys Growth, **514**, 103-108 (2019)

8:15am **NM-WeM1-2 Molecular Beam Epitaxy and Characterization of Bi_2Se_3 and Sb_2Te_3 on In_2Se_3 Layers via Selenium Passivation of InP(111)B Substrates***, Kaushini Wickramasinghe, C. Forrester, I. Levy, M. Tamargo,* City College of New York, City University of New York

Topological Insulators (TI) have attracted a great deal of interest in the past decade due to their non-trivial topology giving rise to metallic surface states protected by time reversal symmetry and an insulating bulk. A wide variety of applications in thermoelectrics, spintronics, twistronics, and quantum computation are being considered. Also, they provide a fundamental platform to explore novel physics. However, there is a large unintentional background doping that conceals their surface channels, and crystal defects such as twin domains are frequently observed. Although these are van der Waals materials, the influence of the substrate on the molecular beam epitaxy (MBE) grown material properties has been shown to be non-negligible. InP(111)B has been used before and reported by some to produce good material properties, although the reports vary and there are few details of the growth conditions. In practice, most materials are grown on sapphire substrates.

In this study, we propose and explore the quality of epitaxial Bi_2Se_3, Sb_2Te_3 and Sb_2Te_3 on Bi_2Se_3 structures on In_2Se_3 layers grown by a selenium passivation technique during the oxide desorption of the InP(111)B substrates. The crystallinity of the samples is measured using high-resolution X-ray diffraction (HR-XRD). Surface morphology is explored using atomic force microscopy (AFM). Here we present the process of growth and optimization with detailed analysis of the quality of the samples.

First, the surface is prepared with a self-grown 5 nm layer of In_2Se_3 which is formed during the oxide removal process in the presence of excess selenium. After that, the substrate is cooled down to the required growth temperature. No low temperature seed layer is grown. AFM shows the formation of a smooth In_2Se_3 layer and the HR-XRD shows its high crystallinity, with the presence of satellite peaks from which the thickness could be extracted. Morphology of Bi_2Se_3 samples grown at different substrate temperatures exhibits smooth surfaces with large terraces. Φ scans of the (015) plane of the Bi_2Se_3 layers show complete suppression of twin domains. AFM of Sb_2Te_3 layers grown on the In_2Se_3 layer show planes with steps, with a larger roughness than Bi_2Se_3, yet the Φ scan of the (015) plane of Sb_2Te_3 also shows complete suppression of twin domains. The surface morphology of Sb_2Te_3 on Bi_2Se_3 structure shows three fold symmetry with varying domain sizes. Again, twin suppression is evident in this sample. Thus, our results show that growth of the materials on the In_2Se_3 interfacial layer results in full suppression of the twin domains compared with samples grown on sapphire, GaAs, or vicinal InP substrates.

8:30am **NM-WeM1-3 Structural and Optical Properties of GaNAs Highly Mismatched Alloys Multi-Quantum Well Heterostructures.***, Rolando Pinson Ortega,* Universidad Autónoma de San Luis Potosí, Mexico*; L. Espinosa Vega, E. Espinoza Figueroa , A. Belio Manzano , P. Olvera Enríquez , M. Villareal Faz, L. Hernandéz Gaytán , F. Perea Parrales ,* Universidad Autónoma de San Luis Potosí (UASLP), Mexico*; C. Yee Rendón ,* Universidad Autónoma de Sinaloa, Mexico*; I. Cortes Mestizo ,* CONACYT-Universidad Autónoma de San Luis Potosí (UASLP), Mexico*; V. Méndez García ,* Universidad Autónoma de San Luis Potosí (UASLP), Mexico

In recent years, novel materials, and new designs of solar cells (SC_s) have been proposed with the aim of contributing to the universal attempt to retrieve solar energy more efficiently. Up to now, the highest conversion efficiencies have been achieved with tandem or multi-junction SCs, a technology that comprise the simultaneous absorption of photons of different wavelengths. This mechanism allows to capture a wider region of the solar spectrum, as compared to simple pn junctions. An alternative approach to achieve the multi-wavelength photon absorption is throughout the utilization of highly mismatched alloys (HMA) where the decoupling in electronegativity and size of the atomic radii of the constituting elements, generates a splitting of the host material conduction band (CB). The lower and higher energy CBs after splitting are called as E_- and E_+, respectively. Thus, in a single layer three different transitions are allowed: i) valence band – E_-, ii) E_- – E_+ and iii) VB –E_+. Presumably, a larger number of transitions can be obtained if quantum confinement effects are added like in any other quantum well system. In this work, the physical and optical properties of multi-quantum well heterostructures of GaNAs are investigated. The GaNAs alloy, with nitrogen mole fraction x_N of 1.1%, was inserted between AlGaAs barriers with $x_{Al}$from 0 to1 to selectively achieve the confinement of E_+ and/or E_-. Theoretically both GaNAs' bands may contribute to the localization of carriers, which certainly depends on x_{Al}. There is not clear evidence of quantum confined states related with E+, suggesting that E- is the sole energy band that contributes to the electron confinement. According to HRXRD measurements the Al concentration in the alloys partially relieves the strain of the multi-quantum well heterostructures. The Raman LO phonon can be related to the residual strain in films. In spite that this technique gets information only from those layers laying within the laser excitation source penetration length and that the heterostructures are capped with GaAs, the LO peak shifts to higher vibrating frequency with respect to the natural LO frequency of homoepitaxial GaAs (291.9cm^{-1}), which is indicative of a reduction of tensile strain in the heterostructures.

8:45am **NM-WeM1-4 Strained Ge Quantum Wells by Molecular Beam Epitaxy for Superconducting Quantum Circuits***, Patrick Strohbeen, M. Hatefipour, W. Strickland, I. Levy, J. Shabani,* New York University

Superconducting quantum circuits utilizing superconductor-semiconductor (S-Sm) Josephson Junctions (JJs) enable rapid gate-tunability of qubit frequency and are an extremely promising avenue for future quantum computing devices [1,2]. However, these systems utilizing InAs 2D electron systems (2DESs) suffer from strong dielectric losses in the substrate they are grown on, resulting in significantly reduced qubit lifetimes [1,3]. To this end, it is highly advantageous to develop a new materials platform for gate-tunable superconducting qubits that are not limited by substrate dielectric loss.

In this talk, I will discuss our work on the molecular beam epitaxy (MBE) growth of a 2D hole system (2DHS) in shallow strained Ge quantum wells as an alternative structure to InAs 2DESs. Samples are grown in an MBE system via electron-beam evaporation to enable rapid deposition of group IV species. Shallow Ge quantum wells are proximitized via in-situ deposition of a superconducting metal enabling higher quality S-Sm interfaces than can be achieved via ex-situ metal deposition. Use of the 2DHSs in strained Ge quantum wells for superconducting quantum circuitry will also be discussed.

[1] L. Casparis, M. R. Connolly, M. Kjaergaard, et. al., Nat. Nanotechnol.13, 915-919 (2018).

[2] M. C. Dartiailh, W. Mayer, J. Yuan, et. al., Phys. Rev. Lett. 126, 036802 (2021).

[3] J. O'Connell Yuan, K. S. Wickramasinghe, W. M. Strickland, et. al., J. Vac. Sci. Technol. A 39, 033407 (2021).

9:00am **NM-WeM1-5 Vertical Transport in Bulk InAsSb and InAs/InAsSb and InGaAs/InAsSb Superlattices Grown on GaSb is Investigated using Photoluminescence Spectroscopy and Compared to Magnetoresistance Measurements***, **Marko Milosavljevic,*** Arizona State University*; R. Carracso, A. Newell,* Air Force Research Laboratory, USA*; J. Love,* New Mexico State University*; S. Zollner,* University of New Mexico*; C. Morath, P. Webster,* Air Force Research Laboratory, USA*; S. Johnson,* Arizona State University

Due to strong carrier confinement in type-II superlattices, vertical transport is much smaller than lateral transport.This asymmetry in carrier mobility affects the performance of type-II superlattice photodetector devices, is complicated to evaluate, and has been determined using temperature and magnetic field dependent magnetoresistance measurements on Van der Pauw structures [1].On the other hand, photoluminescence spectroscopy provides a noninvasive method to investigate carrier transport in bulk and superlattice materials.In which case, photoexcited carriers generated in a mid-wave absorber diffuse into a long-wave well.The ratio of the long to mid wave photoluminescence intensity strongly depends on the diffusion rate of photoexcited carriers into the long-wave well, providing carrier mobility for the mid-wave region.In this work, temperature dependent steady state photoluminescence measurements are performed on samples containing 800 to 2100 nm thick mid-wave absorber regions that are bulk InAsSb or superlattice InAs/InAsSb or InGaAs/InAsSb on top of 130 nm thick long-wave InAs/InAsSb superlattice wells.

In the analysis, the relative luminescence intensity from the long-wave well depends on its carrier lifetime and radiative coefficient, and most significantly on the diffusion rate of the carriers from the mid-wave absorber into the long-wave well.The ratio of the long to mid wave luminescence is proportional to the ratio of the respective photon extraction factors (~1), radiative coefficients (~0.1), and integrated carrier densities squared.The carrier density term has a strong power law dependence on the carrier diffusion length in the mid-wave region, providing the desired sensitivity to vertical transport. The optical constants of the mid and long wave materials are measured using spectroscopic ellipsometry to accurately determine the radiative coefficients.The extracted vertical hole mobility for the mid-wave InAs/InAsSb superlattices are consistent with those reported for magnetoresistance measurements [1]. There are methods of analysis that do not require knowledge of the material optical constants, as they assume that the external quantum efficiency ratio, and hence radiative lifetime ratio, are approximately unity.For the samples investigated here, this approximation underestimates the hole mobility by two orders of magnitude and is not utilized.

[1] L.K. Casias, C.P. Morath, E.H. Steenbergen, G.A. Umana-Membreno, P.T. Webster, J.V. Logan, J.K. Kim, G. Balakrishnan, L. Faraone, S. Krishna, Vertical carrier transport in strain-balanced InAs/InAsSb type-II superlattice material, Appl. Phys. Lett. **116**, 182109 (2020).

9:15am **NM-WeM1-6 Tensile-Strained InGaAs Quantum Dots With Interband Emission in the Mid-Infrarred***, **Kevin Vallejo,*** Idaho National Laboratory*; T. Garrett,* Boise State University*; C. Cabrerara-Perdomo,* Autonomous University of the State of Morelos, Mexico*; M. Drake,* Boise State University*; B. Liang,* University of California, Los Angeles*; K. Grossklaus,* Tufts University*; P. Siimonds,* Boise State University

We determined a robust set of growth conditions for the self-assembly of tensile-strained $In_{1-x}Ga_xAs$ quantum dot (QD) nanostructures on GaSb(111)A surfaces. During molecular beam epitaxy (MBE), $In_{1-x}Ga_xAs$ QDs form spontaneously on GaSb(111)A seemingly with less than 1 ML deposited, indicating a Volmer-Weber growth mode. We characterized these nanostructures using atomic force microscopy, transmission electron microscopy and energy-dispersive X-ray spectroscopy to understand InGaAs/GaSb(111)A QD structure as a function of the MBE conditions. A combination of photoluminescence spectroscopy and computational modeling shows that residual tensile strain in the QDs reduces the InGaAs band gap energy to produce band-to-band emission at 3.5-3.9 µm. When coupled with quantum size effects, the use of tensile strain to red-shift QD emission offers an attractive way to create highly tunable mid-IR light sources.

9:30am **NM-WeM1-7 High Quality Quantum Dot Formation on 300 Mm Si Photonic Wafers for Monolithic on-Chip Light Source***, **Chen Shang,*** *E. Hughes,* UC Santa Barbara*; A. Clark,* IQE Inc.*; R. Koscica, K. Feng,* UC Santa Barbara*; G. Leake, D. Harame,* SUNY Polytechnic Institute*; J. Bowers,* UC Santa Barbara

Monolithic integration via direct epitaxial growth III-V gain material onto Si substrates is the ultimate solution for laser integration with silicon photonics. High reliability has been achieved in InAs quantum dot (QD) lasers grown on (001) blanket Si substrate. However, the required thick buffer layers for the defect reduction makes the evanescent light coupling to the underneath Si waveguides difficult. Growing the III-V gain materials in pockets in a butt-coupled configuration is a more promising approach. Transferring the QD active region from the blanket Si substrate into the pockets on the patterned Si template has proven to be nontrivial. In this work, we have successfully realized high quality QD nucleation in pockets after identifying the growth challenge introduced by the template architecture. Pockets are aligned to either the [1 1 0] or the [1 -1 0] crystal orientation.

Since most of the template is covered with the oxide mask, the use of RHEED as the *in-situ* monitor for QD nucleation is completely forbidden. We observed that the sample with the oxide mask gives a lower pyrometer reading compared to that measured on blanket GaAs/GaP/Si. Once the oxide mask is covered with polycrystalline III-V from the non-selective growth, the pyrometer reading is higher than that measured on blanket GaAs/GaP/Si, depending on the thickness of the polycrystal. The consequence of the temperature uncertainty results in either an over- or under-estimated actual growth temperature. Sample heater power calibrated on a blanket GaAs/GaP/Si template was then used for the pocket growth instead of using the pyrometer, resulting in a blanket-substrate-level low defect III-V film with no QD contrast observed. This is attributed to the much lower heat conductivity of the oxide mask than the III-V material in the pockets. Thus, even though the sample was heated to the same temperature as if it were a blanket GaAs/GaP/Si piece, less heat is radiated from the oxide mask, resulting in a hotter-surface that evaporates the InAs dots. Arbitrary lowering of the heater power was then carried out at 5 °C intervals and QD nucleation was realized after an approximately 30 C° decrease with respect to the temperature profile obtained on blanket GaAs/GaP/Si template. Room temperature photoluminescent and cross-section TEMs were obtained from materials grown in pockets aligned to either [1 1 0] or the [1 -1 0] crystal orientation. Clear differences were observed, potentially attributed to the asymmetric surface diffusion. Further investigation is required to understand the underlying cause of the material asymmetry and to provide guidance to future template and growth designs.

9:45am **NM-WeM1-8 Manipulating Surface Diffusion for InAs Quantum Emitters at Telecommunication Wavelengths by Droplet Epitaxy***, **Margaret Stevens,*** NRC Postdoctoral Fellow residing at the Naval Research Laboratory*; W. McKenzie, G. Baumgartner,* Laboratory for Telecommunication Sciences*; J. Grim, S. Carter, A. Bracker,* Naval Research Laboratory

Droplet epitaxy (DE) is a useful growth technique to achieve light emitters that span the near-infrared wavelengths, including ranges important for telecommunication applications. The two-step growth process, including nucleation of group-III droplets in a group-V depleted environment, followed by crystallization under group-V overpressure, enables tuning of the quantum dot size, density, and morphology without being constrained by strain. DE can also yield quantum dots with very low fine structure splitting [1], an important quality to achieve entangled photon pairs. InAs DE quantum emitters are typically grown by (1) metal organic chemical vapor deposition on (001) surfaces or (2) molecular beam epitaxy on (111)A or (311)A surfaces. InAs DE structures grown on (001) surfaces often yield "ring" shapes, unless the droplet deposition temperature is near room temperature. These ring shapes form due to the high surface diffusion of indium adatoms. While these remaining rings, often made up of smaller

clusters of quantum dots, have interesting optical properties, quantum dots for telecommunication sciences require symmetric, isolated dots with low areal density.

In this study, we explored methods of manipulating indium surface diffusion to achieve symmetric, hemispherical quantum dots on (001) InP surfaces grown by MBE. We explored deposition temperature and group-III coverage, the impact of strained underlayers, and a two-step group-V flux technique, previously demonstrated for InAs droplets on GaAs [2], to discourage indium from diffusing away from the center of the droplet faster than it can crystallize. We used atomic force microscopy to characterize the droplet morphology, and photoluminescence spectroscopy of capped samples to characterize the optical properties. Ultimately, we showed that controlling indium surface diffusion is critical to achieving quantum dots that are suitable for telecommunication sciences experiments.

[1] J. Skiba-Szymanska et al., Phys. Rev. Appl, **8,** 014013, 2017

[2] S. V. Balakirev et al.,Appl. Surf. Sci. **578**, 152023, 2022

Novel Materials
Room Swan BC - Session NM-WeM2
Topological Insulators

Moderator: Kunal Mukherjee, Stanford University

10:30am **NM-WeM2-11 Structure-Property Relationship of the Magnetic Properties of Molecular Beam Epitaxy Grown $(Sb_2Te_3)_{1-x}(Mnsb_2Te_4)_x$ Magnetic Topological Insulators***, **Ido Levy,*** City College of New York, City University of New York*; C. Forrester,* Graduate Center of CUNY and CIty College of New York and Lehman College*; X. Ding, K. Wickramasinghe,* City College of New York*; C. Testelin,* Sorbonne Université, CNRS*; D. Smith,* Arizona State University*; L. Krusin-Elbaum,* City College of New York, City University of New York*; M. Tamargo,* City College of New York

Magnetic topological insulators such as $MnBi_2Te_4$ and $MnSb_2Te_4$ are of great interest due to their promise for realizing exotic physical phenomena and for potential applications in quantum science and quantum computing. However, the control and understanding of the materials properties are still far from adequate. Molecular beam epitaxy (MBE) promises higher control and improved materials properties due to its far from equilibrium conditions and its layer-by-layer growth. Addition of Mn during growth of Sb_2Te_3 results in the formation $MnSb_2Te_4$ septuple layers (SL). Although the individual SLs are ferromagnetic (FM), when SLs stack to form a crystal, their spins align opposite each other, resulting in net antiferromagnetic properties, not conducive to the desired exotic phenomena. It has also been shown that depending on the amount of Mn added, the structure self-assembles into layered QL:SL stacks of the form $(Sb_2Te_3)_{1-x}(MnSb_2Te_4)_x$.

Our group is investigating the MBE growth of the $MnSb_2Te_4$ system. We recently reported the growth of layered QL:SL structures ranging in composition from 100% QL to 100% SLs**.**We showed that modification of the growth conditions by incorporation of a preannealing step and increased growth temperatures leads to samples with varying amounts of SL for the same Mn flux ratios. This suggests that Mn incorporates both as a structural component in SLs and as antisite defects, affecting the magnetic properties of the resulting structures.

Here we present the detailed magnetic properties of the materials using Hall Effect and remanent magnetization measurements. We show that under our MBE growth conditions, all layers with at least a few SLs are FM. Furthermore, their Curie temperatures (T_C) vary as a function of the %SLs in the structure. Results show that: 1) Samples with low %SLs (< 70%) exhibit a single T_C value of 15-20K. 2) Samples with nearly 100% SLs (>90%) also exhibit a single Tc, with a higher value of 35-40K. 3) Samples with intermediate values of 70-85% SLs exhibit unusual T_C behavior, with evidence for two T_C components in the structure (T_{C1} and T_{C2}). For these, the T_{C1} value is ~40K, similar to the value for samples with >90% SLs, while the T_{C2} values are as high as 80K, higher than values reported to date for these materials. We interpret these results on the basis of the distribution of SL and QL layers within the structure, and the excess Mn contained in the layers. We propose that the structures with two T_C values consist of two distinct regions: regions of mostly SLs, that behave as materials with >90%SLs, and regions of SLs surrounding isolated QLs which lead to the higher T_{C2} values.

10:45am **NM-WeM2-12 High Curie Temperature $(Mnsb_2Te_4)_x(Sb_2Te_3)_{1-x}$ Magnetic Topological Insulator Structures Growth by Molecular Beam Epitaxy***, **Candice Forrester,*** The Graduate Center (CUNY), The City College of New York, Lehman College*; I. Levy,* The Graduate Center (CUNY), The City College of New York*; G. Lopez-Morales,* The Graduate Center (CUNY), Lehman College*; X. Ding, K. Wickramasinghe,* The City College of New York*; C. Testelin,* Sorbonne Université, CNRS, Institut des NanoSciences de Paris*; D. Smith,* Arizona State University*; G. Lopez,* The Graduate Center (CUNY), Lehman College*; M. Tamargo,* The Graduate Center (CUNY), The City College of New York

The interaction between magnetic impurities and topological electronic states of 3D topological insulators (TIs) has attracted many studies of predicted exotic phenomena, which may lead to the observance of quantum anomalous hall effect (QAHE) and realizations of quantum computing, among others.[1]

Mixing of Mn, Sb and Te during crystal growth by bulk growth or epitaxial techniques forms a new crystal phase, $MnSb_2Te_4$, with septuple layer (SL) units rather than typical quintuple layer (QL) units of the undoped TIs. These magnetic TIs display antiferromagnetic (AFM) behavior in bulk, which is not conducive for QAHE, and typically have high bulk conductivity, which limits the ability to detect the surface states and their possible applications. Our group has shown that controlling the Mn incorporation into crystal led to the design of QL:SL structures.[2] These structures exhibit ferromagnetic (FM) behavior and a reduced bulk conductivity depending on the %SLs in the structure. Our group has also recently observed that, for some QL:SL layer ratios, samples exhibit mixed magnetic behaviors, with two distinct Curie temperature (Tc) components (Tc1 and Tc2), and Tc2 values as high as 75-80K.

Here we report the further enhancement of the Tc2 values by modification of the MBE growth conditions. In particular, growth rates and the Mn beam equivalent pressure (BEP) ratios were varied in this study. Samples with a lower growth rate of about 0.5-0.6 nm/min, compared to ~0.9-1.0 nm/min used previously, and with Mn BEP ratios between 0.07 and 0.09, resulted in structures having 79-89% SLs that also exhibit two distinct Tc values, one Tc value (Tc1) at ~40-50K and a high Tc value (Tc2) of 100K and above. (Fig. 1) These high Tc values are significantly higher than any values reported to date for these materials. Reducing the Mn BEP ratio to levels of 0.04-0.06 led to the observation of a single Tc value of ~30K and evidence for the coexistence of FM and AFM phases, suggesting the approach to stoichiometric $MnSb_2Te_4$ growth, with little excess Mn. (Fig. 2) We will present these results as they relate to the $(MnSb_2Te_4)_x(Sb_2Te_3)_{1-x}$ structural properties and the details of the growth mechanism. We will perform first-principle calculations using the Ising model to describe and understand the possible magnetic interactions that lead to samples with such high Curie temperatures.

1. R. Yu, et al., *Science* 2010, 329, 61−64.
2. I. Levy et al., *Crystal Growth & Design* 2022 https://doi.org/10.1021/acs.cgd.1c01453 (Published Online)

11:00am **NM-WeM2-13 Structural and Magnetotransport Properties of $MnBi_2Te_4$-based Heterostructure Grown by Molecular Beam Epitaxy***, **Seul-Ki Bac,*** *K. Koller, J. Wang, L. Riney, M. Zhukovskyi, T. Orlova, X. Liu, B. Assaf,* University of Notre Dame

The intrinsic magnetic topological insulators get enormous attention due to the interplay of the topological nontrivial electronic states and the magnetic order, which produces quantum phenomena, such as the quantum anomalous Hall effect and the axion insulator state. Although most research has been accomplished in exfoliated $MnBi_2Te_4$ thin flakes, it remains a big challenge to prepare high-quality thin films with well-controlled compositions and thicknesses. Here, we grow three different types of $MnBi_2Te_4$-based films by molecular beam epitaxy (MBE) and analyze structural and magnetotransport properties. Three samples are spontaneously obtained during the growth depending on growth conditions: a single $MnBi_2Te_4$ (1-phase), a composite structure with $MnBi_2Te_4$ and Bi_2Te_3 (2-phase), and a composite structure with $MnBi_2Te_4$, Bi_2Te_3, and MnTe (3-phase). We distinguish each phase using structural analysis, Raman spectroscopy and x-ray diffraction, and magnetotransport measurement. Our studies disclose insights on optimizing the MBE growth conditions and differentiating the types of $MnBi_2Te_4$-based films.

11:15am **NM-WeM2-14 MBE Growth and Thermo-/Magneto-Transport Properties of Ternary $(Bi,Sb)_2(Te,Se)_3$ Films with High Mobility**, ***Patrick Taylor,*** US Army Research Laboratory*; H. Chi,* Massachusetts Institute of Technology*; B. Wooten, J. Heremans,* Ohio State University*; H. Hier, O. Vail,* US Army Research Laboratory*; J. Moodera,* Massachusetts Institute of Technology

We report the results from the exploration of the MBE growth and characterization of ternary *p*-type $(Bi,Sb)_2Te_3$ and *n*-type $Bi_2(Te,Se)_3$. Comprehensive temperature, field and angular dependent magnetotransport measurements of these ternary $(Bi,Sb)_2(Te,Se)_3$films show band-insulator behavior and display low carrier density on the order of 10^{18} cm^{-3} and a record high mobility exceeding 10^4 cm^2 V^{-1} s^{-1} at 2 K. The remarkable manifestation of strong Shubnikov–de Haas (SdH) quantum oscillation under 9 T at liquid helium temperatures, as well as the analyses therein, has allowed direct experimental investigation of the epitaxial layer electronic structure. Thermal phenomena including the Seebeck and Nernst coefficients are found to be consistent with the understanding obtained from magneto-transport measurements.The primary significance of these results is a path forward for topological spintronics with low bulk carriers and unprecedented magnetoelectric functionalities.

11:30am **NM-WeM2-15 MBE Growth of High Mobility Topological Crystalline Insulators in Proximity with a Magnetic Insulator**, *J. Wang,* University of Notre Dame*; M. Ozerov,* National High Magnetic Fields Lab*; T. Wang, M. Zhukovskyi, T. Orlova,* University of Notre Dame*; D. Smirnov,* National High Magnetic Fields Lab*; V. Lauter,* Oak Ridge National Laboratory*; X. Liu,* ***Badih Assaf,*** University of Notre Dame

Topological insulators (TIs) are promising materials for spintronic and quantum devices due to the fact that they host Dirac fermions with spin-momentum locking. Spintronic devices based on TIs generally consist in a TI proximitized with a magnetic insulator. But the Dirac fermions in the TI can be gapped by magnetism. The magnetic proximity induced gap has never been measured but is important to quantify to properly evaluate the impact of the magnetic layer on the TI. Here, report an MBE synthesis scheme of a topological crystalline insulator (TCI) in proximity with a magnetic insulator that yields very high mobilities needed to evaluate this gap. The mobility is high enough (~$1m^2$/Vs at 4.5K) to allow us to extract the gap using magnetoinfrared spectroscopy. Our measurements allow us to conclude that the magnetic proximity gap cannot be larger than 20meV. Considering the size of the Fermi surface in TIs and TCIs, such a small gap likely preserves the helicity of topological states, making TIs ideal for spintronic devices, despite their fragility to magnetic exchange interactions.

11:45am **NM-WeM2-16 Closing Remarks and Thank Yous**,

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