Novel Materials
Room Ballroom A - Session NM-MoM1
Oxide Semiconductors

Moderator: Bharat Jalan, University of Minnesota

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

8:00am **NM-MoM1-2 Art Gossard MBE Innovator Awardee Talk: Setting a New Quality Standard for Both Holes and Electrons in GaAs Ultra-High Mobility Quantum Wells***, **Loren N. Pfeiffer**,* Princeton University **INVITED**

8:30am **NM-MoM1-4 Silicon-doped β-Ga$_2$O$_3$ Films Grown at 1 µm/h by Suboxide Molecular-Beam Epitaxy***, **Kathy Azizie**, F. Hensling, C. Gorsak,* Cornell University*; Y. Kim,* Air Force Research Laboratory*; N. Pieczulewski,* Cornell University*; D. Dryden,* Air Force Research Laboratory*; M. Senevirathna, S. Coye,* Clark Atlanta University*; S. Shang,* Penn State University*; J. Steele, P. Vogt, N. Parker, Y. Birkhölzer,* Cornell University*; Z. Liu,* Penn State University*; M. Williams,* Clark Atlanta University*; K. Chabak,* Air Force Research Laboratory*; D. Muller,* Cornell University*; A. Neal, S. Mou,* Air Force Research Laboratory*; D. Schlom,* Cornell University

We report the use of suboxide molecular-beam epitaxy (*S*-MBE) to grow β-Ga$_2$O$_3$ at a growth rate of ~1 µm/h with control of the silicon doping concentration from 5x10^{16} to 10^{19} cm^{-3}. In *S*-MBE, pre-oxidized gallium in the form of a molecular beam that is 99.98% Ga$_2$O, i.e., gallium suboxide, is supplied. Directly supplying Ga$_2$O to the growth surface bypasses the rate-limiting first step of the two-step reaction mechanism involved in the growth of β-Ga$_2$O$_3$ by conventional MBE. As a result, a growth rate of ~1 µm/h is readily achieved at a relatively low growth temperature ($T_{sub} \approx 525$ °C), resulting in films with high structural perfection and smooth surfaces (rms roughness of < 2 nm on ~1 µm thick films). Silicon-containing oxide sources (SiO and SiO$_2$) producing an SiO suboxide molecular beam are used to dope the β–Ga$_2$O$_3$ layers. Temperature-dependent Hall effect measurements on a 1 µm thick film with a mobile carrier concentration of 2.7x10^{17} cm^{-3} reveal a room-temperature mobility of 124 cm^2 V^{-1} s^{-1} that increases to 627 cm^2 V^{-1} s^{-1} at 76 K; the silicon dopants are found to exhibit an activation energy of 27 meV. We also demonstrate working MESFETs made from these silicon-doped β-Ga$_2$O$_3$ films grown by *S*-MBE at growth rates of ~1 µm/h.

8:45am **NM-MoM1-5 Improving Si Dopant Control in n-type β-Gallium Oxide***, **Brenton Noesges**, Y. Kim, A. Neal, S. Mou, T. Asel,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

Ultra-wide band gap materials such as β-gallium oxide (β-Ga$_2$O$_3$) are promising for high power electronic devices since breakdown voltage scales with band gap. Within this material class, β-Ga$_2$O$_3$ is unique since β-Ga$_2$O$_3$ can be grown from the melt and demonstrates n-type conductivity with carrier concentration controllable between 10^{16} -10^{20} cm^{-3} with low donor activation energies.[1] However, oxidation of dopant material affects source vapor pressures which can impact dopant profile uniformity in β-Ga$_2$O$_3$ grown via PAMBE.[2,3] This work is focused on optimizing uniform dopant profiles in the low Si doping regime (<10^{18} cm^{-3}) of β-Ga$_2$O$_3$ films since Si doping concentrations show a gradient, increasing toward the surface of the thin films. SIMS and C-V measurements both show Si concentrations of ~3x10^{17} cm^{-3}. We also examine another aspect of Si incorporation in β-Ga$_2$O$_3$ that needs consideration when using traditional effusion cells as a Si dopant source. Previous work in PAMBE β-Ga$_2$O$_3$ growth demonstrated the importance of oxygen plasma power and Si cell temperature on the background amount of Si present in β-Ga$_2$O$_3$ films.[4] In this work, we continued to explore sources of unintentional Si accumulation during the PAMBE growth process from sources like the quartz plasma bulb and Si effusion cell. The presence of Si at the interface between β-Ga$_2$O$_3$ substrate and film provides a parasitic conduction channel which is problematic for device performance. Attempts have been made to remove Si at β-Ga$_2$O$_3$ interfaces via etching. Our results indicate that removing interfacial Si may not be as simple since Si can re-accumulate during PAMBE, thus limiting the effectiveness of pre-growth surface treatments. Exposing a clean β-Ga$_2$O$_3$ surface to a quartz plasma bulb alone did not produce Si accumulation at the surface. On the other hand, a growth interrupt exposing a fresh β-Ga$_2$O$_3$ surface to a hot Si cell with shutter closed for several minutes produced Si accumulation equal to that of the interfacial Si between substrate and film. These results demonstrate that removing Si prior to loading into PAMBE may be inadequate to remove interfacial Si since Si can be re-introduced from the Si dopant cell during pre-deposition stages. These results point toward important challenges and potential solutions when growing Si-doped β-Ga$_2$O$_3$ thin films.

1 Neal, A. T. et al., *Appl. Phys. Lett.***113**, 062101 (2018).

2 Kalarickal, N.K., et al., *Appl. Phys. Lett.***115**, 152106 (2019).

3 McCandless, J.P., et al. *Appl. Phys. Lett.***121**, 072108 (2022).

4 Asel, T. J., et al., *J. Vac. Sci. Technol. A***38**, 043403 (2020).

9:00am **NM-MoM1-6 The Effect of Gallium Beam Flux on Electron Transoport in β-Ga$_2$O$_3$ Grown via Plasma Assisted Molecular Beam Epitaxy***, **Thaddeus Asel**, B. Noesges, Y. Kim, A. Neal, S. Mou,* Air Force Research Laboratory, Materials and Manufacturing Directorate

β-Ga$_2$O$_3$ has been of interest due to its large bandgap and high critical electric field, making it an excellent candidate for power electronic and RF applications [1]. The community has made significant improvements in the growth of β-Ga$_2$O$_3$ via several techniques including molecular beam epitaxy (MBE). However, there has not been a study of the relationship between the β-Ga$_2$O$_3$ growth parameters and their effects on the defects present in the crystal and their impact on the electronic transport properties. Utilizing temperature dependent Hall Effect measurements and a self-consistent fitting of the temperature dependent carrier density and mobility data, we are able to quantify the concentration defect states, including compensating acceptors, deep level impurities, and unintentional donors, present in the epitaxial films. The Ga beam flux can control the oxygen to Ga ratio present in the chamber as our oxygen is held constant for each growth run. This allows for growths that occur in the “oxygen rich” regime where the amount of Ga supplied limits the growth rate and the “gallium rich” regime where the amount of O supplied limits the growth rate. In both regimes the formation of the volatile suboxide Ga$_2$O occurs, but in the gallium rich regime, the desorption of Ga$_2$O causes a lower growth rate than that seen in the oxygen rich regime, due to the excess of Ga presence preventing the second reaction step in Ga$_2$O$_3$ growth. Two preliminary samples were grown in the gallium rich (Ga Beam Flux = 1 × 10^{-7} Torr) and oxygen rich (Ga Beam Flux = 6 × 10^{-8} Torr) regimes. The samples had different doping densities of 4.25 × 10^{17} cm^{-3} in the gallium rich sample and 2.60 × 10^{17} cm^{-3} in the oxygen rich sample, this discrepancy is due to an inaccuracy in the Si doping source. The acceptor concentration in the gallium rich sample was calculated to be 7.26 × 10^{16} cm^{-3} and 4.50 × 10^{15} cm^{-3} in the oxygen rich sample, a factor of 16 difference based on the Ga beam. This is likely due to Ga vacancies that can form during desorption of Ga$_2$O during growth. These results indicate that there is significant impact on the electron transport properties of β-Ga-$_2$-O$_3$ with a change in the Ga to O ratio during growth, and that optimization of growth parameters is needed to optimize the electronic properties of MBE grown β-Ga-$_2$-O$_3$.

9:15am **NM-MoM1-7 Growth of α-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ by Suboxide Molecular-Beam Epitaxy***, **Jacob Steele**, K. Azizie, N. Pieczulewski, J. McCandless,* Cornell University*; I. Matara Kankanamge, M. D. Williams,* Clark Atlanta University*; H. Xing, D. Jena, D. Muller,* Cornell University*; T. Onuma,* Kogakuin University, Japan*; D. Schlom,* Cornell University (USA) and Leibniz-Institut für Kristallzüchtung (Germany)

Ga$_2$O$_3$ has attracted significant interest due to its ultra-wide bandgap, high electron mobility, and large breakdown field. These properties exceed the current benchmarks set by materials such as SiC and GaN, making Ga$_2$O$_3$ optimal for next-generation power devices. Still, it has been proposed that the properties of Ga$_2$O$_3$can be extended further by alloying with Al to form (Al$_x$Ga$_{1-x}$)$_2$O$_3$ which can raise the bandgap to 8.6 eV. This goal presents a challenge for the most researched phase, β, as β-Ga$_2$O$_3$thermodynamically prefers a monoclinic structure and α-Al$_2$O$_3$ is stable in the corundum structure. This structural mismatch limits the compositional range and the range of attainable bandgaps. In contrast, α-Ga$_2$O$_3$ occupies the corundum structure and has been shown to alloy over the full compositional range, enabling bandgaps from 5.3 - 8.6 eV. One method of growing α-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ is molecular-beam epitaxy (MBE). MBE is a powerful and highly controllable growth technique for α-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ thin films with drawbacks being slow growth rates of a few hundred nm/h and narrow adsorption-controlled growth windows. One method to increase the growth rate is the technique of suboxide MBE, which allows growth of β-Ga$_2$O$_3$thin films at rates exceeding 1 µm/h with large adsorption-controlled growth regimes.

We show that suboxide MBE can be used for the epitaxial growth of high quality α-(Al$_x$Ga$_{1-x}$)$_2$O$_3$ thin films on A plane sapphire substrates over the full range of x at greater than 1 µm/h. For our study, gallium suboxide, Ga$_2$O, and elemental Al are the MBE sources. The oxidant is 80% distilled ozone which is held at constant pressure (5 x 10-6 Torr) while the Ga_2O and Al fluxes are varied to control composition. We measure the composition of our films with XRD and confirm that we cover the full range of $0 < x < 1$ with vacuum ultraviolet transmittance measurements showing that the bandgaps of our films shift from α-$Ga_2O_3$to α-Al_2O_3. We show that the film composition can be controlled directly by the relative ratios of the Ga_2O and Al fluxes. Our films have high structural quality as revealed by the full width at half maximum (FWHM) of rocking curves of the α-$(Al_xGa_{1-x})_2O_3$ films ranging from 11 - 15 arcseconds; these FWHMs are identical to the underlying sapphire substrates. The surfaces of the films are also smooth with RMS roughnesses measured by atomic force microscopy ranging from 0.3 - 1.1 nm on α-$(Al_xGa_{1-x})_2O_3$ films with thicknesses in the 17.8 - 47.8 nm range. We also show our progress with growing α-$(Al_xGa_{1-x})_2O_3$ films over 100 nm thick and with doping our films.

9:30am **NM-MoM1-8 Electrostatic Gating of $SrSnO_3$ Thin Films with Improved Mobilities**, ***Zhifei Yang**, F. Liu, T. Truttmann, B. Jalan,* University of Minnesota, USA

Ultra-wide-bandgap (UWBG) semiconducting oxides are becoming more crucial in sustainable technologies due to their promising use in applications including transparent electronics and power switching. Among them, alkaline earth stannates such as $SrSnO_3$ with the perovskite crystal structure have gained much interest in recent years. However, the room-temperature mobility of $SrSnO_3$ thin films has been shown to be limited by defective surface scattering. By using a 4 nm undoped $SrSnO_3$ capping layer on 19 nm La-doped $SrSnO_3$ thin film, the measured room temperature mobility has been shown to improve. In this structure, charge spill over from the doped layer to the undoped layer is expected to happen as Fermi levels equilibrate. Here, we demonstrate a reversible and electrostatic doping of $SrSnO_3$ thin films grown by Hybrid molecular beam epitaxy with tunable carrier densities using electric-double-layer transistor (EDLT) configuration with ion gels. Using modeling and a discrete two-channel model, we show that the modulation due to gating is confined within 4 nm at the top capping layer and the modulation leads to an increase of mobility in $SrSnO_3$ up to 130 $cm^2V^{-1}s^{-1}$ at 250 K. A detailed growth study combined with temperature-dependent Hall effect measurements and transport analysis will be presented.

Novel Materials
Room Ballroom A - Session NM-MoM2
Nitrides

Moderator: Dr. Lutz Geelhaar, Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin

10:15am **NM-MoM2-11 Molecular Beam Epitaxy of Binary and Ternary Manganese and Chromium Nitrides**, *K. Vallejo, K. Gofryk,* Idaho National Laboratory*; S. Gutierrez-Ojeda,* Universidad Nacional Autónoma de México*; G. Cocoletzi,* Benemérita Universidad Autónoma de Puebla, Mexico*;* ***Brelon May**,* Idaho National Laboratory

Transition metal nitrides have exceptional properties and are used in a wide variety of electrochemical, structural, photochemical, and plasmonic applications. Among these compounds Mn- and Cr- nitrides have shown exceptional potential for magnetic sensing and spintronics. The Mn_xN_y system is complex with several different metastable phases both predicted and experimentally realized. Cr_xN_y has two primary phases, cubic (CrN) and hexagonal (Cr_2N), which exhibit desirable mechanical, thermal, wear, anti-corrosion, thermoelectric properties. Recent studies have provided valuable insights into the growth and formation of phases of both materials using various vapor deposition techniques. However, there are conflicting reports on the electrical and magnetic properties of Cr_xN_y which could be attributed to impurities, nitrogen vacancies, substrate effects, and strain. This controversy calls for a more detailed study and preparation of high-quality monocrystalline CrN to investigate he intrinsic physical properties. This study uses molecular beam epitaxy to synthesize epitaxial thin films of different Mn-N and Cr-N phases. The electrical and magnetic properties of these films are investigated with the rocksalt MnN and CrN both showing metallic behavior, with the latter showing a magnetic transition ~280K. However, when combining these materials at similar growth conditions, instead of maintaining the rocksalt structure, a new ternary cubic phase of Mn_xCr_yN is obtained which shows narrow-gap semiconducting behavior. This work presents an avenue for the epitaxial integration of metallic, magnetic, and semiconductor materials.

10:30am **NM-MoM2-12 Achieving Atomically Ordered GaN/AlN Quantum Heterostructures: The Role of Surface Polarity**, ***Yuanpeng Wu**, P. Zhou, Y. Xiao, K. Sun, D. Wang, P. Wang, Z. Mi,* University of Michigan, Ann Arbor

A central goal of modern material physics and nanotechnology is the control of materials and their interfaces to atomic scales. However, for interfaces between polar layers, this goal is thwarted by the atomic substitution process among cations with different ionicities. In traditional semiconductor heterostructures, such as InAs/GaAs, Si/Ge, AlGaN/GaN and ABO_3 perovskites, diffusive interfaces have been widely observed, which deteriorates the performance of electronic and optoelectronic devices. Interfacial diffusion also prohibits achieving atomically ordered quantum heterostructures for applications such as quantum light sources and sensors. The studies on the origin of interfacial diffusion are often compounded by factors such as various synthesis parameters, available epitaxial substrates, strain distribution and surface reconstruction while a vital solution for achieving a perfect heterointerface remains elusive.

In this work, we discovered a strong dependence of interfacial diffusion on surface polarity in GaN/AlN quantum heterostructures. Atomically ordered quantum interface can be readily synthesized on the semipolar plane instead of the conventional c-plane of GaN/AlN heterostructures. The underlying mechanism of this dependence is explored through first-principles density functional theory calculations and it is found that the chemical bonding configurations at the semipolar plane can effectively eliminate the cation substitution process, which leads to an atomic sharp interface. The near-perfect interface quality ensures extreme quantum confinement and superior optical properties including record-high internal quantum efficiency of ~75% in the deep ultraviolet wavelength regime. We developed a scalable and robust fabrication method and demonstrated that electroluminescence energies of interdiffusion-free GaN are free from the quantum-confined Stark effect. In addition, we demonstrated a unique strategy of controlling surface polarities through different strain relaxation mechanisms in a core-shell nanostructure platform. This work provides, for the first time, a viable path for the synthesis of interdiffusion-free polar quantum heterostructures, which is paramount for high-performance devices across various material platforms.

10:45am **NM-MoM2-13 Epitaxial Cubic Boron Nitride Grown by Ion Beam-Assisted Molecular-Beam Epitaxy on Diamond**, ***David Storm**, S. Maximenko, A. Lang, N. Nepal, T. Feygelson, B. Pate, D. Meyer,* US Naval Research Laboratory

Cubic boron nitride (c-BN) shares several properties with diamond, including high mechanical hardness; high thermal conductivity, second only to diamond; and an ultra-wide band gap (E_g ~ 6.2 eV, indirect). In addition, c-BN can be doped both *n*- and *p*-type, and the lattice mismatch between c-BN and diamond is only ~1.3%. These similarities suggest the potential for novel electronic devices based on c-BN/diamond heterostructures for high temperature and high power applications. However, the growth of device-quality layers of c-BN is challenging: boron nitride occurs in multiple phases; the desired cubic phase is metastable at pressures and temperatures typical of vapor-phase growth; and the absence of large-area bulk c-BN crystals necessitates heteroepitaxial growth on non-native substrates.

Single crystal epitaxial cubic boron nitride films were grown on (100) oriented IIa diamond substrates by ion beam-assisted molecular-beam epitaxy (MBE) in a custom MBE system equipped with an Ar ion source, a N_2 plasma source, and an electron beam evaporator for supplying elemental boron. The films are fully cubic, as indicated by Fourier transform infrared spectroscopy and corroborated by x-ray photoelectron spectroscopy. Transmission electron microscopy reveals an epitaxial c-BN film with the presence of isolated misfit dislocations but no indication of h-BN. The interface between the c-BN layer and the diamond substrate is structurally abrupt, and no interlayer between the c-BN film and diamond substrate is seen. It was found that trace amounts of impurities, such has Mg, Be, and Si, facilitate the growth of c-BN on diamond by ion-assisted MBE.

11:00am **NM-MoM2-14 Optical Properties of ScN Layers Grown on Sapphire Using Plasma-Assisted Molecular Beam Epitaxy*, Duc V. Dinh,*** Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany*; F. Peiris,* Kenyon College*; J. Lähnemann, O. Brandt,* Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany

Since the report of rock-salt scandium nitride (ScN) on sapphire 50 years ago [1], ScN has been mostly used in combination with other materials. In particular, ScN has been combined with wurtzite AlN to form (Al,Sc)N for surface acoustic wave [2] and high-electron mobility transistor applications [3]. However, very recent studies have shown that ScN itself can also be used for electronic [4] and infrared opto-electronic applications [5].

Here, we report on the optical properties of (3–250)-nm-thick ScN(111) layers grown on sapphire Al2O3(0001) substrates using plasma-assisted molecular beam epitaxy. The optical properties of the layers were investigated by three different techniques, namely, spectroscopic ellipsometry, confocal Raman and photoluminescence spectroscopies. The optical constants of the layers are investigated by variable-angle spectroscopic ellipsometry covering a spectral range from far infrared to far ultraviolet (0.045–8.5 eV). Refractive indices (n, k) of the layers are determined by fitting ellipsometry data using a parametric semiconductor model, taking into account the effects of surface roughness. Fits of ellipsometry data return the energies of four oscillators representing the band-to-band transitions. These correspond to the high-symmetry points in the band structure of ScN including 2.03 eV at the X point and three transitions (3.89, 5.33, and 6.95 eV) at the Γ point. These three oscillators are associated with direct transitions that occur between the degenerate heavy and light hole-bands and the first, second and third conduction bands at the Γ point, respectively. These energy transition values and refractive indices are consistent with theoretical studies previously reported for ScN [6]. Despite the rocksalt structure of ScN, Raman spectra of all the layers reveal several first-order phonon modes with an LO(L) mode at 675–680 cm-1. The appearance of these first-order modes is attributed to defects and impurities in the layers. Room-temperature photoluminescence measurements of the layers are dominated by a band with a peak energy decreasing from 2.3 to 2.2 eV, attributed to a reduction of the oxygen concentration in the thicker layers.

References

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[2] M. Akiyama et al, Adv. Mater., 21, 593 (2009).

[3] D.V. Dinh et al, Appl. Phys. Lett. 122, 152103 (2023).

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[5] K.C. Maurya et al, Nano Lett. 22, 5182 (2022).

[6] R. Deng et al, Phys. Rev. Lett., 91, 045104 (2015).

11:15am **NM-MoM2-15 Epitaxial Growth of High ScN Fraction ScAlN on NbN and SiC*, Matthew Hardy,*** *A. Lang, E. Jin, N. Nepal, B. Downey, V. Gokhale, S. Katzer, V. Wheeler,* U.S. Naval Research Laboratory

ScAlN thin films have attracted significant attention due to their factor of five increase in piezoresponse over AlN for $Sc_{0.43}Al_{0.57}N$. Integration of metallic epitaxial NbN with ScAlN using molecular beam epitaxy (MBE) enables a pathway towards a highly conductive lower electrode while preserving high crystal quality even in relatively thin ScAlN films suitable for use at or above X-band frequencies. Maintaining phase-pure and high crystal quality $Sc_xAl_{1-x}N$ at high x is critical to improve resonator bandwidth and reduce insertion loss.

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 MBE-grown ScAlN films on SiC and NbN/SiC. With the inclusion of a 5-nm AlN interlayer, the $Sc_{0.32}Al_{0.68}N$ XRD FWHM decreases from 2.0° to 1.13°. An AlN interlayer is also critical to growth of ScAlN on NbN thin films. A two-step AlN growth process can effectively encapsulate the NbN layer while providing a smooth surface on which to nucleate ScAlN growth, and is critical to maintaining high crystal quality for ScAlN grown on NbN.

The ScAlN initiation steps also have a strong impact on the final quality of the film. Instead of a two-step ScAlN growth we previously demonstrated, 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, as well as elimination of remaining ring-like character in the final RHEED pattern after an additional 40 nm of growth, and a XRD FWHM as low as 1.22° for ScAlN films grown on SiC. Transmission electron micrographs show near elimination of cubic grains that otherwise form in the initial layers of the $Sc_{0.40}Al_{0.60}N$. The graded sample has the same average ScN fraction and thickness as the two-step sample. 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, increasing the average ScN fraction from 0.373 to 0.393. Finally, a 500-nm-total-thickness sample (100 nm $Sc_{0.32}Al_{0.68}N \rightarrow Sc_{0.40}Al_{0.60}N$, 400 nm $Sc_{0.40}Al_{0.60}N$) was grown to show the impact of defect annihilation in thicker films, resulting in a reduction of XRD FWHM to 0.89°. Employing the same 25-nm grade followed by 125-nm of $Sc_{0.40}Al_{0.60}N$ grown on AlN/NbN/SiC results in a FWHM of 1.97°. The improved layer initiation shows that more gradual changes in surface energy and strain reduces the nucleation of undesirable cubic grains, and may point to a general strategy for elimination of anomalous grains in high ScN fraction ScAlN.

11:30am **NM-MoM2-16 High Efficiency Micrometer Scale Green and Red Light Emitting Diodes*, Yixin Xiao,*** *R. Maddaka, Y. Wu, Y. Malholtra, Y. Guo, S. Yang, J. Liu, K. Sun, A. Pandey, J. Min, Z. Mi,* University of Michigan

High efficiency light emitting diodes (LEDs) with characteristic length scales on the order of microns or less, also known as µLEDs, have been under intense investigations for their immense promise in various display and communications scenarios. Among the many material systems investigated for µLEDs, the III-nitride family possesses many desirable material properties such as comparatively low surface recombination velocities and excellent wavelength tunability. To date, however, it has remained a challenge to achieve efficient green and red emitting µLEDs, largely due to the enhanced surface recombination and poor p-type doping related to the top-down etching. Moreover, it has remained difficult to achieve the high levels of indium incorporation required for a red emitting indium gallium nitride (InGaN) active region. Here we demonstrate that the efficiency bottleneck of µLEDs can be fundamentally addressed by utilizing bottom-up III-nitride nanostructures. We report on the demonstration of micrometer scale green and red LEDs with an external quantum efficiency of 25% and 8%, respectively, which are the highest values ever reported to the best of our knowledge. We employ selective area plasma-assisted molecular beam epitaxy as the material synthesis platform. Due to efficient strain relaxation, such bottom-up nanostructures are largely free of dislocations. By exploiting the large exciton binding energy and oscillator strength of quantum-confined InGaN nanostructures, we show that the external quantum efficiency of a green-emitting micrometer scale LED can be dramatically improved from ~4% to >25%. The dramatically improved efficiency is attributed to the utilization of semipolar planes in strain-relaxed nanostructures to minimize polarization and quantum-confined Stark effect and the formation of nanoscale quantum-confinement to enhance electron-hole wavefunction overlap. We have further developed a new approach that included an InGaN/GaN short period superlattice together with an InGaN quantum dot active region to achieve high efficiency red emission. A maximum quantum efficiency of >7% was measured. Our studies offer a viable path to achieve high efficiency micrometer scale LEDs for a broad range of applications including mobile displays, virtual/augmented reality, biomedical sensing, and high-speed optical interconnects, that were difficult for conventional quantum well based LEDs.

11:45am **NM-MoM2-17 AlN/AlGaN Short Period Superlattices With Sub 2 nm Layers Grown by MME*, Alexander Chaney,*** Azimuth Corporation*; C. Bowers, K. Mahalingam,* UES INC*; S. Mou, K. Averett, T. Asel,* Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

In this work we present a method for creating AlN/$Al_xGa_{1-x}N$ short period superlattices (SPSL) with individual layer thicknesses down to 3-4 ML. By taking advantage of the oscillatory nature of metal modulated epitaxy (MME), the formation of alternating AlN and $Al_xGa_{1-x}N$ layers can be achieved through the introduction of a constant Ga overpressure during the MME growth of AlN. However a typical MME process results in SPSLs with periods between 5 and 6 nm. In order to reduce the thickness of the AlN and $Al_xGa_{1-x}N$ layers, the shutter timings are reduced in order to limit the total amount of Al deposited on the surface. Initial results with this shortened shutter timing showed 0th order SL peak with Pendellosung fringes in an XRD coupled scan. Such behavior is typically indicative of a high quality SPSL. However, TEM imaging showed a strong intermixing of between the AlN and $Al_xGa_{1-x}N$ layers, leading to a structure that more resembles a random $Al_xGa_{1-x}N$ alloy than a well ordered SPSL. In order to prevent intermixing at the interface layers, 3 altered growth processes were investigated: alternating Al and Ga shutters, inclusion of a N plasma only exposure step and reduction of the Ga flux. The goal with each of these changes was to limit the interaction of the Ga and Al during the final stages of the AlN layer formation. TEM examination of each growth's layer structures showed a significant reduction in layer intermixing for all samples. Alternating the Al and Ga shutter resulted in a SPSL with high order in its layer structure, with AlN and $Al_xGa_{1-x}N$ thicknesses of 4 ML and 3 ML respectively. Introduction of the plasma only step resulted similarly improved interfaces however the thicknesses of AlN and $Al_xGa_{1-x}N$ layers had changed to be 3 ML and 4 ML respectively. Finally, reducing the Ga flux led to a layer structure almost identical to what was obtained using alternating shutters. XRD coupled scans each sample showed Pendellosung fringes centered on a 0th order peak. Fitting of the peaks enabled determination of the average Al composition for the SPSL, which ranged from a low of 84% for alternating shutters to a high of 90% for lower Ga flux. Because these 2 samples showed the same layer thicknesses in TEM, reducing the Ga flux resulted in higher Al content $Al_xGa_{1-x}N$ layers. A coupled scan of the N pause sample showed a broad peak to the left of the main alloy peak. The cause of this is a section of growth where the layered structure had non uniformity which can be seen in TEM indicating further optimization is needed. Based on these results, MME shows promise as method for forming digital alloys.

Novel Materials
Room Ballroom A - Session NM-MoA2
Strong Spin-Orbit Oxides

Moderator: Prof. Ryan Comes, Auburn University

3:30pm **NM-MoA2-9 Atomic Scale Modeling of the Hybrid Molecular Beam Epitaxy Growth Process Using Reactive Force Field Simulations***, B. Yalcin, D. Yilmaz, A. van Duin,* Pennsylvania State University*;* ***Roman Engel-Herbert****,* Pennsylvania State University, USA, Paul-Drude-Institute for Solid State Electronics, Berlin, Germany

The hybrid molecular beam epitaxy approach for the growth of oxides – i.e. the co-supply of atomic and molecular species in their elemental and metalorganic form – has allowed accessing a self-regulated growth window for complex oxides thin films with a range of chemistries, including titanates, vanadates, stannates, and ruthenates. While it is widely accepted that the favorable growth kinetics is enabled by the volatility of the metalorganic molecules supplied, their thermal decomposition and surface reaction kinetics is complex and far from understood. For example, while it is generally assumed that the thermal decomposition of the widely employed metalorganic molecule titanium(IV)-isopropoxide (TTIP) used for the growth of titanates by hybrid MBE takes place by dissociating C-O bonds via the β-hydride elimination process, alternative reaction pathways, in particular in proximity of solid surface with different chemistries, such as SrO and TiO_2 terminated growth fronts, might be relevant as well.

In this talk, we present reactive force field molecular dynamics (ReaxFF-MD) and metadynamics simulations to shed light on the reaction kinetics of TTIP at the atomic scale. While the initial organic ligand pyrolysis step was spontaneous and occurred exclusively by breaking a C-O bond, albeit not always via β-hydride elimination in subsequent thermal decomposition stages, C-O bond dissociation events typically occurred with incomplete hydronation of the remaining Ti-containting fragment. In addition, Ti-O bond dissociation events were observed for Ti-containing molecule fragments at subsequent stages of the thermal decomposition process, challenging the simplistic picture of β-hydride elimination. The complete reaction scheme for the thermal decomposition of TTIP will be presented along with the reaction barriers and thermodynamic driving force for the different bond dissociation events and the role of the formal titanium oxidation state on the decomposition kinetics will be discussed, which offer a simple explanation to understand the different decomposition behavior of TTIP when interacting with the different terminations of $SrTiO_3$ surfaces. The computational approach provides a predictive and computationally inexpensive framework to identify chemical reaction pathways relevant to MBE film growth processes at the atomic scale under realistic, while experimentally relevant conditions. It can be easily expanded to different metalorganic precursor molecules, therefore allowing to develop a computationally informed engineering strategy to design MO molecules for hybrid MBE beyond the currently established chemistries.

3:45pm **NM-MoA2-10 Engineering Metal Oxidation Towards Epitaxial Growth of Complex Iridates using Molecular Beam Epitaxy***,* ***Sreejith Nair****, Z. Yang, D. Lee, S. Guo,* University of Minnesota, USA*; J. Sadowski,* Brookhaven National Laboratory*; S. Johnson,* Auburn University*; A. Saboor,* University of Delaware*; Y. Li, H. Zhou,* Argonne National Laboratory*; R. Comes, W. Jin,* Auburn University*; K. Mkhoyan,* University of Minnesota, USA*; A. Janotti,* University of Delaware*; B. Jalan,* University of Minnesota, USA

The platinum group metals like Ir and Ru have captured significant interest in the condensed matter physics and materials science community due to the exotic electronic and magnetic properties that they exhibit when combined with oxygen. The oxides of these metals provide a unique platform to study and leverage the delicate interplay between electron correlations, crystal field and spin-orbit coupling energies. High quality thin films of complex platinum group metal oxides are hence, critical to realizing new phenomena such as the predicted unconventional superconductivity in Sr_2IrO_4. However, the platinum group metals have extremely low vapor pressures and low oxidation potentials. These factors make it challenging to synthesize their oxide thin films using an ultra-high vacuum (UHV) technique like Molecular Beam Epitaxy (MBE). Here, we have addressed these challenges using a novel solid-source metal-organic MBE approach [1,2]. We demonstrate atomically precise synthesis of binary IrO_2 using $Ir(acac)_3$ as the metal-organic Ir source at substrate temperatures as low as 250 °C. The use of the metal-organic precursor allows Ir supply at source temperatures less than 200 °C and enables easy oxidation due to the +3 Ir oxidation state in the precursor. Further, by combining epitaxially strained IrO_2 thin film growth on different substrates, x-ray diffraction, electron microscopy, spectroscopy techniques, and DFT calculations, we demonstrate a vital role of epitaxial strain in Ir oxidation. Thus, epitaxial strain can be an additional tuning knob to engineer metal oxidation which can aid the conventional thermodynamic and kinetic driving forces [3].

However, the true test of metal oxidation in UHV occurs at high growth temperatures where oxidation becomes increasingly thermodynamically unfavorable. Hence, in order to examine the efficacy of the solid-source metal-organic MBE approach and to realize the elusive unconventional superconducting state, we study the synthesis of Sr_2IrO_4 thin films, which is favored at growth temperatures greater than 600-700 °C. We will present a detailed growth study, structural characterization, electrical and magneto-transport in epitaxial Sr_2IrO_4 films, along with alternative ways to tackle the Ir oxidation challenge in UHV synthesis.

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4:00pm **NM-MoA2-11 Solid Source Metal-Organic Molecular Beam Epitaxy for Epitaxial $SrRuO_3$ Films***,* ***Anusha Kamath Manjeshwar****, S. Nair, A. Rajapitamahuni, R. James, B. Jalan,* University of Minnesota

The investigation of the electrical and magnetic properties of $SrRuO_3$ and its associated $Sr_{n+1}Ru_nO_{3n+1}$ Ruddlesden-Popper phases requires a high degree of control over the isolation of the desired phase and its defect density. The growth of ruthenates is fundamentally challenging because ruthenium (Ru) resists scalable evaporation and oxidation. This bottleneck complicates the growth of $SrRuO_3$ films with low defect densities using inherently low-energy, ultra-high vacuum deposition techniques such as molecular beam epitaxy (MBE). Special modifications to conventional MBE such as electron-beam assisted evaporation and ozone-assisted oxidation of Ru have, so far, enabled the best defect control or the highest residual resistivity ratios (RRR = ρ_{300K}/ρ_{2K}) in $SrRuO_3$ films among all physical vapor deposition techniques. However, these modifications are expensive and require additional interlocks to ensure safe operating conditions.

We outline a novel technique called solid source metal-organic MBE to supply a solid metal-organic precursor with pre-oxidized ruthenium with an effusion cell at $T < 200$ °C, a drastic decrease from the ~ 2000 °C required to produce comparable fluxes with elemental Ru. With this technique, we demonstrate the growth of phase pure, epitaxial, and stoichiometric $SrRuO_3$ films with robust ferromagnetism below 150 K on $SrTiO_3$ (001) substrates. We simplify the route to an adsorption-controlled growth window in $SrRuO_3$ films, growth conditions where the films can self-regulate their stoichiometry, which is a key ingredient for successful defect control in electron-beam and ozone-assisted MBE-grown $SrRuO_3$ films. We discuss the intricate relationship between cation stoichiometry, magnetic domains, and RRR in epitaxial $SrRuO_3$ films and outline new pathways for achieving low defect densities in $SrRuO_3$. Using these guidelines to optimize stoichiometry and film thickness within a growth window, we achieve a RRR = 87 for a 50 nm-thick $SrRuO_3$ film, the highest for any $SrRuO_3$ film on $SrTiO_3$ (001) substrates. We will also illustrate how solid source metal-organic MBE is a simple and cost-effective method to enhance the capabilities of conventional MBE for the defect-controlled growth of ruthenates.

4:15pm **NM-MoA2-12 Growth of Ruddlesden-Popper Ruthenates via Thermal Laser Epitaxy***,* ***Brendan D. Faeth****, F. Hensling, V. Harbola, L. Majer,* Max Planck Institute for Solid State Research, Germany*; H. Boschker,* Epiray GMBH, Germany*; W. Braun, J. Mannhart,* Max Planck Institute for Solid State Research, Germany

Thermal laser epitaxy (TLE) is a novel technique for thin film deposition which employs continuous wave lasers to simultaneously heat both the substrate and elemental sources.This laser heating approach allows for evaporation or sublimation of nearly all elements from the periodic table, ultrahigh substrate temperatures exceeding 2000 C, and broad compatibility with process gases at a wide range of pressures from UHV up to 1 Torr, among other benefits.As a result, TLE dramatically expands the parameter space available for thin film synthesis compared to existing epitaxy techniques.However, to date it has been experimentally challenging to achieve simultaneous control of multiple laser based elemental sources with the flux stability and systematic fidelity necessary for the growth of ternary or multernary systems of interest such as complex oxides.

In order to establish the capabilities of TLE for the growth of such complex oxides, we demonstrate here the successful epitaxial synthesis of several Ruddlesden-Popper phases of the Sr-Ru-O ternary oxide system via TLE. Near instant thermalization of both source elements and substrates from laser heating allows the process of thermodynamic phase control to be achieved rapidly during film deposition without the need for physical shuttering of sources.Additionally, we find that the “n=1” phase Sr_2RuO_4 can be reliably synthesized at substrate temperatures in excess of 1200 C and in a background environment of pure molecular oxygen, within an adsorption-controlled growth window that is inaccessible to conventional MBE systems.We show that films grown under these conditions demonstrate high structural, electronic, and chemical quality comparable to that of MBE-grown films.A detailed accounting of the experimental approach, growth thermodynamics, and film characterization will be discussed.

This work not only demonstrates the feasibility of TLE for the synthesis of high-quality complex oxide thin films, but also suggests new routes to achieving thin film growth in other materials systems that remain as-yet inaccessible to conventional epitaxy techniques.

4:30pm **NM-MoA2-13 Growing Clean Crystals from “Dirty” Precursors in MBE***, **Rashmi Choudhary,*** University of Minnesota, USA*; Z. Liu, J. Cai, X. Xu, J. Chu,* University of Washington*; B. Jalan,* University of Minnesota, USA

Ultra-high purity elemental sources have long been considered a prerequisite for obtaining low impurity concentration in compound semiconductors in the world of molecular beam epitaxy (MBE). Furthermore, to realize intrinsic properties, the material needs to be nearly free of intrinsic and extrinsic defects. For this reason, the use of ultra-high-purity elemental sources has been the historical practice in MBE, perhaps, for the fear that impurity elements might get incorporated into the film, making it “dirty”.

In this work, we challenge this conventional MBE wisdom by presenting an extension of the hybrid-MBE approach, known as solid-source metal-organic MBE, for growing superconducting Sr_2RuO_4 films using a solid organometallic precursor, ruthenium acetylacetonate, as a source of Ru. We grew 100 nm thick (001) Sr_2RuO_4 films on (001) LSAT substrate at 900°C substrate temperature using co-deposition of Sr, ruthenium acetylacetonate, and oxygen plasma. These films are phase-pure, single-crystalline, fully coherent, and superconducting. The superconducting transition temperature of the film is 0.85 K. In contrast to the conventional MBE, which employs ultra-pure Ru metal evaporated at ~ 2000°C as a Ru source, along with reactive ozone to obtain $Ru \rightarrow Ru^{4+}$ oxidation, the use of ruthenium acetylacetonate precursor requires significantly lower temperature for Ru sublimation (less than 200°C) and eliminates the need for ozone.

This is the first-time realization of superconducting Sr_2RuO_4 films using ozone-free MBE. By combining our results with the recent developments in hybrid-MBE, we argue that leveraging precursor chemistry will be necessary to realize next-generation breakthroughs in the synthesis of atomically precise quantum materials. Our results establish hybrid-MBE as a viable method for growing highest quality crystals and put this technique at the forefront of vacuum deposition technologies despite the use of a “dirty” chemical precursor.

4:45pm **NM-MoA2-14 MBE Growth of $BaCo_2Ru_4O_{11}$: A Metallic Ferromagnetic Hexaferrite***, **Yilin Evan Li,*** Department of Materials Science and Engineering, Cornell University*; M. Brützam,* Leibniz-Institut für Kristallzüchtung, Germany*; R. Cava,* Department of Chemistry, Princeton University*; C. Guguschev,* Leibniz-Institut für Kristallzüchtung, Germany*; D. Schlom,* Department of Materials Science and Engineering, Cornell University

Multiferroics with coupled magnetic and electric orders, although rare, hold potential for low-energy-consumption materials for logic and memory capable of electric-field control of magnetism. Barium hexaferrite ($BaFe_{12}O_{19}$) is the leading seller in today’s multi-billion-dollar magnetic ferrite market and is predicted to gain electric polarization order at room temperature in addition to its robust ferrimagnetism under in-plane, biaxial, compressive strain [1]. Epitaxial strain engineering has achieved significant success in modifying materials’ electric and magnetic ground states. For instance, the tensile strain exerted by a $DyScO_3$ substrate transforms $EuTiO_3$, an antiferromagnetic paraelectric material, into a ferroelectric ferromagnet [2]. The recent realization of single-crystal substrates of $Sr_{1.03}Ga_{10.81}Mg_{0.58}Zr_{0.58}O_{19}$(SGMZ) [3], an insulator that is isostructural to $BaFe_{12}O_{19}$, enables straining $BaFe_{12}O_{19}$ as SGMZ has a ~1.1% smaller in-plane lattice constant. In addition to strain, to induce the ferroelectric state, an epitaxial bottom electrode is needed to control the electric state for this hexaferrite multiferroic candidate. $BaCo_2Ru_4O_{11}$ is a metallic ferromagnetic oxide [4], belongs to the same hexaferrite family as $BaFe_{12}O_{19}$, and has small (~0.3%) in-plane lattice mismatch to the SGMZ substrate. Consequently, a coherent $BaCo_2Ru_4O_{11}$ epitaxial thin film on the SGMZ substrate would be ideal for straining $BaFe_{12}O_{19}$and serving as the bottom electrode of a metal-insulator-metal structure to test for ferroelectricity in this predicted strain-induced multiferroic.

Epitaxial $BaCo_2Ru_4O_{11}$thin films have not previously been reported, perhaps due to the lack of hexagonal ferrite substrates and the synthesis challenges associated with the growth of complex ruthenate epitaxial thin films. Films of $BaCo_2Ru_4O_{11}$ were grown by MBE on (0001) SGMZ substrates in an adsorption-controlled regime, similar to the way that films of $SrRuO_3$ and $CaRuO_3$ films with high resistivity ratios have been grown by MBE [5]. With matching substrates and adsorption-controlled growth, we have grown epitaxial $BaCo_2Ru_4O_{11}$thin films with resistivity ratios comparable to $BaCo_2Ru_4O_{11}$ single crystals [4].

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5:00pm **NM-MoA2-15 Hybrid Molecular Beam Epitaxy of $SrIrO_3$ Films and Heterostructures***, **Gaurab Rimal**, T. Tasnim, J. Ahammad,* Auburn University*; G. Sterbinsky,* Argonne National Lab*; J. Sadowski,* Brookhaven National Laboratory*; M. Boebinger,* Oak Ridge National Laboratory*; R. Comes,* Auburn University

The iridiates form a fascinating class of oxides. The high spin-orbit coupling of Ir has been predicted to lead to novel physics such as topological phases and superconductivity in ternary iridate films and heterostructures. For investigating these effects, high quality materials, including epitaxial films, are needed. The low vapor pressure of Ir, however, precludes the use of effusion cells for MBE growth using elemental iridium. Recent progress in solid-source hybrid MBE, in which metalorganic precursors are used as a cation source, has evolved for high-quality MBE growth of films containing similar low vapor-pressure elements. In this study, we use MBE with a metalorganic iridium acetylacetonate source to grow the high-quality films of $SrIrO_3$ and heterostructures of $SrIrO_3$ with $SrCoO_3$. Specifically, we discuss the role of different substrates on film properties via temperature-dependent transport, X-ray absorption and scanning transmission electron microscopy. We examine interfacial phenomena in $SrIrO_3/SrCoO_3$ heterostructures for charge transfer and novel topological magnetic behavior.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

References

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

Micro LEDs have emerged as a strong contender for next generation display devices due to their high efficiency, fast response, high brightness, and extended lifetime. For practical applications, it is highly desired that full color LEDs can be monolithically integrated on the same chip, which, however, has remained extremely challenging to achieve via the conventional quantum well based approach. In recent years, N-polar indium gallium nitride (InGaN) based light emitting diodes on the (sub)micron scale, also known as µLEDs, that are synthesized via selective area plasma assisted molecular beam epitaxy, have achieved record levels of efficiency at the (sub)micrometer device scale, with 25% external quantum efficiency (EQE) for green emission and 8% EQE for red. Such advances are enabled by selective area plasma assisted molecular beam epitaxy, in which, unlike thin film epitaxial growths, local kinetics can be controlled by substrate mask patterning. Moreover, the selective area openings on the substrate mask naturally lead to the formation of a photonic crystal. Here, we demonstrate the effect of pattern opening diameters on the InGaN photoluminescence (PL) wavelength. We show that, for a multiple-quantum-disk structure designed for green emission, given a certain photonic crystal lattice constant, the PL peak wavelength can vary over nearly 100 nm as the opening diameter varies over 60 nm, thereby enabling the achievement of multi-color emission for LED structures grown on a single chip in a single epitaxial step. More importantly, we have demonstrated strong coherent emission over a wide wavelength range for such nanowire photonic crystal LED structures. Their emission wavelengths can be precisely controlled and tuned by varying the design and processing parameters. Such nanowire photonic crystal devices not only enable a wide range of wavelength tuning but also lead to high efficiency and highly directional emission which is desired for future near-eye display applications. By further optimizing the design and epitaxial process, the realization of full-color emission for such unique N-polar III-nitride photonic nanostructures can be potentially realized. Work is currently in progress to demonstrate high efficiency micrometer scale green and red LEDs that can exhibit strong coherent emission.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Acknowledgment

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

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

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

Alloying Bismuth into GaAs has been shown to produce a marked alternation of the valence band structure. The increased spin orbit splitting energy in $Ga_{1-x}AsBi_x$ has been shown to dramatically reduce the excess noise of GaAs APDs[1]. Higher performing III-V APDs could yet be achieved by Bi alloying with $Al_{0.8}Ga_{0.2}As$ potentially promising a new family of ultra-low-noise, photodetectors. Isolating the effect that Al may have on the incorporation of Bi will be of benefit opening up other potential material systems. This could include telecommunication APDs based on the inclusion of Bi into InAlAs, lattice matched to InP.

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

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

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

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

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

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

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

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

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

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

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

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

In this work, we report the growth of modulation doped $In_{0.81}Ga_{0.19}As/In_{0.81}Al_{0.19}As$ quantum wells grown on semi-insulating InP (001) substrates. The quantum wells are characterized utilizing low temperature magnetotransport, which is performed using gated Hall bars and the van der Pauw geometry structures. Quantum wells with electron mobilities in excess of 380,000 cm^2/Vs have been grown. The electron mobility of the $In_{0.81}Ga_{0.19}As$ quantum wells is comparable to that of the current state of the art $In_{0.75}Ga_{0.25}As$ quantum wells. The role of growth parameters on electron mobility is discussed. The low temperature electron mobility and carrier density of the quantum wells is modeled to extract the dominant scattering mechanisms that limit the mobility. The influence of an InGaAs digital alloy on the electron mobility and alloy scattering of the quantum well is investigated.

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NM-MoP-19 Light-enhanced Gating Effect at Conducting Interface of Laser MBE Grown EuO-KTO₃, ***Manish Dumen****, S. Chakraverty,* Institute of Nano Science and Technology, India

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Semiconductor quantum dots fabricated via filling of local droplet etched nanoholes in Al$_x$Ga$_{1-x}$As with GaAs are excellent candidates for on-demand sources of entangled photon pairs due to their low exciton fine structure splitting. However, photon emission in the GaAs/Al$_x$Ga$_{1-x}$As system is limited to wavelengths below 800 nm and long-haul quantum communication via the global fiber network requires sources emitting photons in the optical C-band, i. e., ca. 1550 nm. One way to tackle this challenge, is to transfer the approach of local droplet etching and re-filling to the In$_{0.53}$Ga$_{0.48}$As/In$_{0.52}$Al$_{0.48}$As-system lattice matched to InP. In this study we report on the influence of various growth parameters, as etching temperature, metal species and residual As pressure on the shape, areal density and size of the nanoholes, as these properties play an important role for the later quantum dot's emission characteristics. We present detailed statistical analysis of the nanohole morphology and densities that were obtained by analyzing measurements performed via atomic force microscopy and scanning electron microscopy. The areal density decreases strongly with increasing etching temperature (see Fig. 1) and the hole depth and diameter increase with increasing etching temperature. With increasing etching temperature, the nanoholes also become more and more elongated along the [011]-direction. Overgrowth of the nanoholes with In$_{0.52}$Al$_{0.48}$As under As$_2$-atmosphere preserves the holes (see Fig. 2) and we observed that a moderate overgrowth with 50 nm In$_{0.52}$Al$_{0.48}$As notably improved the number of symmetric nanoholes for samples etched at 410°C and 435°C. We found that filling the nanoholes with In$_{0.53}$Ga$_{0.48}$As is possible either under As$_2$- or under As$_4$-atmosphere but it works significantly better under As$_4$-atmosphere. We also observed that the shape of the etched holes strongly depends on the metal species used for etching. Under the same etching conditions, the holes etched with pure Al tend to be significantly more elongated than those etched with In, as can be clearly seen in Fig. 3. Photoluminescence measurements on overgrown filled holes show that the emission wavelength shifts with the filling level of the nanoholes and QD emission in the optical C-band can be achieved when filling holes generated at etching temperatures above 435°C (see Fig. 4).

NM-MoP-25 Heteroepitaxial growth of (111)-oriented SrTiO$_3$ on ScAlN/GaN*, E. Jin, A. Lang, B. Downey, V. Gokhale, **Matthew Hardy**, N. Nepal, S. Katzer, V. Wheeler,* Naval Research Laboratory

Ultra-wide bandgap (UWBG) semiconductor materials have been highly studied in recent years, owing to their attractive materials properties for high power and RF electronics. In particular, ScAlN has been an UWBG material that not only possesses a large bandgap, but also exhibits very high piezoelectric and spontaneous polarization coefficients, making it an appealing material for telecommunications and non-volatile memory applications. High quality epitaxial ScAlN films demonstrated by molecular beam epitaxy (MBE) have enabled high power density GaN field effect transistors utilizing ScAlN as a barrier layer. Heterogeneous integration of epitaxial oxides with ScAlN could realize novel hybrid electronics that can couple the added functionalities observed in oxides with this emergent semiconductor platform. For example, high-permittivity oxides such as SrTiO$_3$ (STO) could be used to greatly improve electric field management in RF high-electron-mobility transistors (HEMTs).

Integration of epitaxial STO with ScAlN comes with several challenges, including the lattice and crystal structure mismatch between a cubic and wurtzite material. In our previous work, we demonstrated that (111)-oriented STO films can be grown on AlGaN/GaN HEMT structures via a thin rutile TiO$_2$ buffer layer that mitigates the strain between the two different materials. We leverage that approach in this work to demonstrate the growth of STO on ScAlN/GaN HEMT structures via RF-plasma-assisted oxide MBE.

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

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

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

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

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NM-MoP-27 Growth and Characterization of GaAs (111) on 4H-SiC for Infrared Sensor

Subhashis Das, *N. M Eldose, H. Stanchu, F. Maia de Oliveira, C. Li, M. Benamara, Y. I. Mazur, G. Salamo,* University of Arkansas

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

NM-MoP-28 Growth and Conductivity Control of AlN by Plasma Assisted MBE

Neeraj Nepal, *M. Hardy, B. Downey, A. Lang, D. Katzer, E. Jin, D. Storm, V. Gokhale, T. Growden, D. Meyer, V. Wheeler,* U.S. Naval Research Laboratory

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

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

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

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NM-MoP-29 Molecular Beam Epitaxy Grown Group-IV Alloys for Infrared Photodetector and Quantum Transport Applications

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

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

For thin film α-Sn(Ge) samples, InSb substrates were chosen for lattice match conditions. The thermal oxide desorption was done under excess Sb flux at a pyrometer temperature of 480 ℃ after which temperature was lowered to 390 ℃ for Sb-rich InSb buffer growth. To separate from the conducting InSb substrate while maintaining lattice match conditions, a semi-insulating Cd-rich CdTe buffer was grown at 280 ℃. Samples were cooled overnight via contact with LN$_2$ shroud and thin films of α-Sn and dilute Ge-containing SnGe alloys were grown. Due to heating by the thermal radiation from the Sn and Ge effusion cells during growth, there is a temperature creep on the sample surface. Therefore, to maintain the substrate at a temperature below the α- to β-Sn phase transition, a short-pulse modulated technique, shutter cycles open for 2 seconds and shut for 10 seconds, was employed to grow the pure α-Sn samples but not for the SnGe films.

Ge-rich SiGeSn alloys with thermalization barrier between 0.4k_BT and 3k_BT were grown on Ge and GeSn virtual substrates. Ge substrate surfaces were cleaned using HF and HCl solutions prior to UHV outgas at 550 ℃, GeSn virtual substrates used HF and H$_2$O$_2$. A Ge buffer was grown at a substrate temperature of 500 ℃ before cooling down to 200 ℃ for SiGeSn growth. The Ge cell was held constant while Sn and Si fluxes were altered to obtain designed composition.

NM-MoP-30 Transport of Rare-Earth Nitrides Deposited via Molecular Beam Epitaxy

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

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

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

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

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

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

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

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

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

NM-MoP-34 Molecular Beam Epitaxy of Kagome-Structured Antiferromagnetic FeSn Grown on LaAlO$_3$ (111), ***Tyler Erickson**, S. Upadhyay, H. Hall, D. Ingram, S. Kaya, A. Smith,* Ohio University

Iron and tin can be alloyed to form different structures of alternating stackings of Kagome Fe$_3$Sn and honeycomb Sn$_2$ (stanene) layers. This alternating sequence results in either Fe$_3$Sn$_2$ or FeSn depending on whether there are Fe$_3$Sn bilayers or Fe$_3$Sn monolayers separating the stanene layers [1,2]. Fe$_3$Sn$_2$ and FeSn provide interesting avenues for spintronics with flat bands arising from geometrical frustration leading to novel topological phases [3]. Fe$_3$Sn$_2$ and FeSn have both been grown using molecular beam epitaxy on various substrates. [2, 4, 5] In this study, we grow FeSn by MBE following the method described by Hong et al. [2] Namely, we grew our FeSn on LaAlO$_3$ substrates at a temperature of 500 °C. The choice of using LaAlO$_3$ is based on the relatively good lattice match with difference of only 1%. Four samples have been grown with Fe:Sn flux ratios of 0.8:1, 1:1, 1.2:1, and 1.5:1. We compare the results of the 4 samples by means of RHEED, XRD, RBS, and AFM. In all cases, smooth streaky RHEED patterns are observed, and from the streak spacing we calculate the in-plane lattice constants which are then complemented by the lattice constants calculated from the XRD spectra. For the case of the 1:1 flux ratio, using RHEED we find an a = 5.290 Å as compared to the expected a_for FeSn = 5.297 Å [2] and using XRD we find c = 4.56 Å as compared to the expected c for_FeSn = 4.481 Å [2]. In this presentation, we will discuss the lattice parameters as functions of the incident flux ratios as well as the phases and phase purity of the resultant samples. We will also present results for the surface smoothness as a function of flux ratios as measured by the AFM images, and we will also address the resultant film stoichiometry as a function of incident flux ratios.

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

The structural adaptability of transition-metal oxides allows for designing different heterostructures emerging unique physical properties at interfaces[1]. High-temperature interface superconductivity takes place at the interface between overdoped (metallic) and undoped (insulating) La$_2$CuO$_4$ layers grown by oxide molecular beam epitaxy (MBE)[2]. In addition to homo-epitaxial systems[3,4], multilayers of La$_2$CuO$_4$ combined with La$_{2-x}$Sr$_x$NiO$_4$[5], LaNiO$_3$[6], and LaSrMnO$_3$[7] layers revealed the impact of the interface sharpness on the occurrence of superconducting[5], thermoelectric[6], and magnetic[7] properties, respectively. In this work, we designed new *cuprate–manganite* interfaces using oxide MBE[7,8] and focused on the interface sharpness and superconducting properties compared to *cuprate–cuprate* interfaces.

We probed the interfaces using scanning transmission electron microscopy (STEM) techniques, including high-angle annular dark-field (HAADF), annular bright-field (ABF) imaging, and electron energy-loss spectroscopy (EELS).

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

References

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

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

In this research, we investigate the growth and transformation of ultrathin Pt-telluride van der Waals (vdW) compounds by vacuum annealing and Pt-vapor exposure. We find that molecular beam epitaxy readily grown PtTe2 thin films can be converted into Pt3Te4- and furthermore Pt_2Te_2-bilayers through vacuum-induced Te-loss. Using scanning tunneling microscopy, x-ray, and angle resolved photoemission spectroscopy, we find that Pt_3Te_4 remains thermally stable up to 350℃ while achieving Pt_2Te_2 requires a higher annealing temperature of 400℃. Interestingly, bilayer Pt_2Te_2 can be re-tellurized by exposure to Te-vapor. This causes the topmost Pt_2Te_2 layer to transform into two layers of $PtTe_2$ and, thus synthesis of Pt_2Te_3.

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

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

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

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

A standard inversion technique was used to model the ellipsometry spectra by specifying a three layer model (i.e., sapphire substrate, $ZrTe_2$ layer and the Te capping layer) to fit the final ellipsometry spectra. The thicknesses obtained from X-ray reflectivity allowed us to obtain the precise dielectric function of the final $ZrTe_2$ layer (i.e., 12 u.c.). Subsequently, we fit the remaining ellipsometry spectra obtained for 11 u.c. through 1 u.c. $ZrTe_2$ and obtain their dielectric functions. Clearly, the dielectric functions show a noticeable change with the thickness of the $ZrTe_2$ layers, where the absorption depicted by the imaginary part of the dielectric function increases with the thickness of $ZrTe_2$. Additionally, the layer-dependent dielectric functions were analyzed by incorporating a Drude oscillator to account for the free electrons and two Kramers-Kronig-consistent oscillators to represent the band-to-band transitions. Interestingly, we find that the Drude contribution reduces as the thickness of $ZrTe_2$ gets smaller, suggesting that its metallic character diminishes as the thickness reduces. Further analysis of the optical conductivity verifies this observation.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Novel Materials
Room Ballroom A - Session NM-TuM1

Novel Materials, Optoelectronics

Moderator: Prof. Jason Kawasaki, University of Wisconsin - Madison

7:45am **NM-TuM1-1 Welcome and Sponsor Thank Yous***,*

8:00am **NM-TuM1-2 NAMBE Young Investigator Awardee Talk: Dislocation Dynamics in InGaSb Graded Buffers on GaSb Grown by MBE***, **Stephanie Tomasulo**, M. Twigg, S. Maximenko, I. Vurgaftman, J. Nolde,* U.S. Naval Research Laboratory **INVITED**

Conventional III-V materials possess a large range of bandgap energies (E_g) enabling their use in a wide variety of applications. However, researchers are typically constrained to the few lattice-constants available in commercial binary substrates, which greatly restricts access to the lowest-E_g (0.05-0.35 eV) options. Graded buffers can and have been used to bridge the gap between an available substrate and a bulk-like material with the desired E_g while mitigating excessively high threading dislocation densities (TDD). However, the dislocation dynamics in III-Sb materials is still poorly understood. Here, we explore the effects of substrate temperature (T_{sub}) on surface morphology and dislocation dynamics in $In_xGa_{1-x}Sb$ graded buffers. We grew two identical samples at T_{sub}=455 and 495 °C (pyro). These had 8 × 365 nm steps, increasing *x* by ~0.03 per step and capped with 1 µm of $In_{0.28}Ga_{0.72}Sb$ (grading rate of=0.58%/µm). Nomarski microscopy shows the lower T_{sub}=455 °C results in a rough surface, while T_{sub}=495 °C has a smooth, cross-hatched appearance as expected for a graded buffer. We then measured x-ray reciprocal space maps (RSMs) with the x-ray beam incident along both [110] and [1-10] to assess potential asymmetric strain relaxation. Such relaxation has been observed in other III-V graded buffers and explained by different dislocation formation energies/glide velocities along each direction, which results from the core structure of the dislocation being terminated with either a group-III (beta core) or a group-V (alpha core) element [1]. Thus, asymmetries in RSMs can be linked to dislocation glide behavior. We previously observed asymmetry in InAsSb graded buffer RSMs, finding minimal tilt when measured along [110] and significant tilt when measuring along [1-10], suggesting a preference for beta dislocation cores [2]. Interestingly, InGaSb graded buffers reveal the opposite asymmetry, i.e. measuring along [110] results in tilt while measuring along [1-10] shows little tilt, indicating alpha dislocation cores. Furthermore, in InGaSb, the tilt direction changes from positive (more glide on (111)) for T_{sub}=455 °C to negative (more glide on (-1-11)) for 495 °C revealing the significant role T_{sub} plays in dislocation dynamics. Additional samples will be explored, varying the V/III and grading rates, to build an understanding of how to control dislocation dynamics and TDD in InGaSb graded buffers. Etch pit density and transmission electron microscopy will be used to quantify TDD and supplement the understanding of dislocation dynamics gained from RSMs. [1] France et al. JAP 107, 103530 (2010). [2] Tomasulo et al., NAMBE 2019.

8:30am **NM-TuM1-4 Emergent Ferromagnetism in Altermagnetic Candidate MnTe Films Grown on InP (111)***, **Matthew Brahlek**,* Oak Ridge National Laboratory

To push into new generations of spintronic devices requires understanding new magnetic phenomena and also how to control both known and emerging material platforms as high-quality epitaxial thin films. Specifically, altermagnets are a new phase that is predicted to exhibit a strong spin splitting of the band structure, which can form the basis for new spintronic applications. MnTe, a candidate altermagnet, is a room-temperature antiferromagnet (TN ≈ 310 K) semiconductor (energy gap of order 1 eV) with a NiAs structure. Here, we present results on the molecular beam epitaxy growth and properties of MnTe/InP(111). Using polarized neutron reflectivity and magnetotransport, we find that there is emergent ferromagnetic behavior likely driven by a combination of charge transfer and strain. The ferromagnetic component is likely a slight canting of the bulk-like A-type antiferromagnetic state, as seen by neutron diffraction. This high level of tunabililty of MnTe opens the door to tailoring interlayer magnetic interactions in this layered material system. Together these results provide a potential mechanism of tuning antiferromagnetic ordering for applications in high-speed, next-generation spintronics.

8:45am **NM-TuM1-5 Growth Parameters Impact on Electronic and Optical Properties of ErAs:InGaAlBiAs Materials***, **Wilder Acuna**, W. Wu, J. Bork, M. Jungfleisch, L. Gundlach, J. Zide,* University of Delaware

We present our work on the growth of ErAs:InGaAlBiAs through a digital alloy approach where a superlattice of thin layers of the quaternary InGaBiAs and InAlBiAs, behave as a quinary and allows tuning the bandgap with the gallium and aluminum composition just with layer thickness variation. We target InGaAlBiAs for 1550 nm optical excitation for photoconductive switches (PCS) that can generate and detect terahertz (THz) pulses. Semiconductors implemented in PCS need high dark resistance, subpicosecond carrier lifetime, and a high carrier mobility is desirable. Incorporating erbium above the solubility limit creates ErAs nanoparticles, decreasing the material's carrier lifetime. At the same time, ErAs nanoparticles have a strong pinning effect of the effective Fermi level on the material. In this narrow bandgap semiconductor, the Fermi level is close to the conduction band, i.e., there is a high electron concentration, which decreases the dark resistivity. Other authors have found that the size of ErAs nanoparticles affects the electron concentration in InGaAs, where bigger nanoparticles cause a lower electron concentration. Er can be co-deposited, forming nanoparticles at the same time the matrix is grown, which saves growth time; however, while the usual 490°C growth temperature could give enough adatom mobility to create sizeable nanoparticles, our structure of interest is a dilute bismuthide that requires lower temperature growth (~280°C). At this low temperature, we use interrupt growth and migration-enhanced epitaxy, which allows us to have lower carrier concentration. All these samples are characterized by different techniques to determine relevant properties. Dark resistance is obtained from Hall effect and Van der Pauw measurements, carrier lifetime from optical pump THz probe spectroscopy, optical band gap from spectrophotometry, material quality from high-resolution x-ray diffraction, and composition through Rutherford backscattering spectrometry.

9:00am **NM-TuM1-6 Heteroepitaxial Growth of Site-determined Quantum Emitters in 2D GaSe Films***, **Mingyu Yu**,* University of Delaware*; S. Law,* Pennsylvania State University

GaSe is an attractive van der Waals (vdW) material due to its intriguing bandgap behavior and is an ideal choice for quantum photonic technology. We will grow GaSe films on patterned substrates by molecular beam epitaxy (MBE) to obtain wafer-scale films with site-controlled localized quantum emitters (QEs). A proper substrate is critical as the substrate pattern is used to funnel electrons and holes to a local minimum to form emission. Unlike traditional epitaxy, vdW materials may grow on substrates with large differences in lattice constant/structure as the weak interlayer bonds make them less affected by substrate. However, it also means less control over the crystal structure and surface morphology of the deposited film. To achieve the goal—GaSe films with strain-localized QEs—we first need flat atomically-thin GaSe films with minimal twin boundaries. Our previous work[1] proved that Al_2O_3 was not suitable for the growth of GaSe films due to the poor wettability of Ga, so we turned to GaAs(111)B, which has the same cation as GaSe and a relatively small lattice mismatch (6%).

Typically, vdW materials cannot grow heteroepitaxially on 3D substrates unless the dangling bonds are terminated. We developed a process—annealing in Se at 680°C—to deoxidize GaAs(111)B in an As-free MBE while generating a Se-terminated surface smooth enough for subsequent growth (Fig. S1). Preliminary work has resulted in GaSe films with somewhat rough surfaces (Fig. S2a, 2d). Additional annealing of the substrate prior to growth can notably promote film coalescence and reduce roughness (Fig. S2b, 2e), probably because it facilitates a fully Se-terminated GaAs surface. Fig. S2e shows a surface comprised of twinned triangular domains, and the reflection high energy electron diffraction (Fig. S2g) confirms the coexistence of two GaSe orientations. In addition, the 2-step method (low-temperature nucleation followed by high-temperature growth) facilitates film coalescence (Fig. S2c, 2f), since high substrate temperature can enhance adatom mobility. Moreover, fresh GaAs(111)B wafers lead to more directional nucleation of GaSe (Fig. S3), implying that additional oxidation due to air exposure is detrimental to the growth of high-quality GaSe. We also found that the quality of vdW films had an opposite dependence on growth conditions (temperature and rate) in 2D/2D and 2D/3D growth modes. The next challenge is to achieve uniform coverage and unidirectional nucleation. The effects of growth parameters, substrate pretreatment, and uncracked/cracked Se will be examined to better understand the growth mechanics and morphology evolution of GaSe.

9:15am **NM-TuM1-7 Evaluating (001) and (111)A InAs Quantum Emitters at Telecommunication Wavelengths Grown by Droplet Epitaxy***, **Margaret Stevens**,* US Naval Research Laboratory*; W. McKenzie, G. Baumgartner,* Laboratory for Telecommunication Sciences*; J. Grim, A. Bracker,* US Naval Research Laboratory

Droplet epitaxy is a versatile growth method that can produce nanostructures with emission in the telecommunication wavelength ranges. The MBE growth conditions have a significant impact on the morphology of the nanostructures, and as a result, the emission of the quantum dots. Due to the low surface diffusion of In on InAlAs surfaces, conventional growth conditions in MBE lead to rings of small quantum dots on (001) surfaces that limit the emission to shorter wavelengths. Previously, we have shown that we can manipulate the crystallization stage of droplet epitaxy to create new morphologies on (001) surfaces and shift the resulting emission to 1300-1550 nm at 4 K [1]. By utilizing a two-stage As flux exposure, including a low flux exposure immediately after metal droplet deposition followed by a high flux exposure with a temperature ramp [2], we can create clusters of larger quantum dots at densities ~ 1/μm^2 surrounded by a higher density of smaller quantum dots. Further understanding of why the different morphologies form, and how we can better control quantum dot density, is needed.

In this work, we have expanded on the two-stage As flux exposure to further manipulate the morphology and density of InAs QDs grown on InAlAs/InP (001). We grew samples with different temperature ramps and different low-flux conditions to change the density and size of the different QD features that form. Atomic force microscopy (AFM) is used to study the quantum dot morphology and density and photoluminescence spectroscopy (PL) is used to study the resulting emission. Additionally, we grew InAs QDs via droplet epitaxy on InAlAs/InP (111)A surfaces to compare quantum dot size, density, and resulting emission to samples grown by the two-stage flux technique on (001) substrates. Finally, we incorporate our telecommunication range emitting quantum dots in diode structures to tune the QD charge state and study resulting emission properties.

[1] M. A. Stevens et al., JVST A, 41, 032703 2023

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

9:30am **NM-TuM1-8 Growth of InSb Quantum Well on InAs Using AlInSb Buffer Layer Assisted by Interfacial Misfit Dislocation Arrays***, **Fatih Furkan Ince**, A. Newell, T. Rotter, G. Balakrishnan,* University of New Mexico*; M. McCartney, D. Smith,* Arizona State University

Mid-wave infrared (MWIR) detectors are widely used in various fields, such as medical devices, remote sensing, and spectroscopy. InSb-based infrared focal plane arrays (FPAs) have emerged as a popular choice for their affordability, scalability, and temporal stability, as well as their spatial uniformity. However, achieving fully relaxed tunable absorber to cover MWIR and LWIR is challenging due to lack of binary substrates. Thus, type-II superlattices and metamorphic buffers are employed to cover the MWIR spectrum and extend into the long-wave infrared (LWIR) region [1], [2]. In this study, we propose using interfacial misfit dislocations to grow fully relaxed InSb on an InAs substrate, combined with direct growth of $Al_xIn_{1-x}Sb$ buffer layers on InAs, to develop tunable InAsSb absorbers for MWIR and LWIR applications. This approach is expected to lead to the production of high-performance MWIR and LWIR detectors, potentially opening new avenues for future applications.

We will discuss using interfacial misfit dislocations to form instantly relaxed buffer layers on InAs substrates, and analyze the directly grown AlInSb and InSb epilayers using HR-XRD ω-2θ scans and reciprocal space mapping. TEM analysis showed misfit dislocation arrays at the AlInSb/InAs interface. We investigated InSb quantum wells grown with different AlxIn1-xSb barrier layers using PL and present a detailed analysis of the InSb quantum wells based on PL and TRPL results. These findings provide a better understanding of the properties of these materials and their potential for MWIR and LWIR applications.

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[2] A. Rogalski, "Next decade in infrared detectors," in Electro-Optical and Infrared Systems: Technology and Applications XIV, Warsaw, Poland, 2017.

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9:45am **NM-TuM1-9 Molecular Beam Epitaxy of Kagome Antiferromagnetic Mn_3GaN grown on MgO(001)***, **Ali Abbas**, A. Shrestha, A. Smith,* Ohio University

There have been very few studies of antiperovskite structure Mn_3GaN in general and it was seen in MBE growth mainly as a second-phase precipitate when growing MnGaN [4]. However, this material is very interesting since it can support the Kagome antiferromagnetic spin structure [3]. And so, we grow thin films of Mn_3GaN on cubic MgO(001) substrates using rf N–Plasma MBE. In our work, Mn_3GaN is deposited at 250 ±10°C with a Mn:Ga:N flux ratio of 3:1:1. We keep the Ga:N ratio fixed using an RF plasma nitrogen source. The sample surface is continuously monitored throughout the growth using reflection high energy electron diffraction. During the growth, the RHEED pattern was observed to be highly streaky, indicating an atomically smooth surface. In addition, we observed half-order fractional streaks (2x pattern) in the [100] direction. The calculated *in-plane* lattice constant based on RHEED is 3.89 ±0.06 Å. This value is very close to the lattice constant *a* of Mn_3GaN according to theory (3.898 Å) [1] and with the *in-plane* experimental value for sample growth by sputtering (3.896 Å); and in that work, the authors also observed a 2x pattern [2]. We also measure the *out-of-plane* lattice constant using X-ray diffraction. For the major 002 peak, the value calculated is 3.84 ±0.06 Å which also agrees well with the theoretical value (3.898 Å) [1] and with the experimental reported *c* value [2] (3.881 Å). Since we did not observe significant second-phase peaks, the phase purity of the sample is quite high, and Rutherford backscattering confirms a stoichiometry of 3:1:1.

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

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Novel Materials
Room Ballroom A - Session NM-TuM2

Thin Film Membranes

Moderator: Dr. Roman Engel-Herbert, Paul Drude Institute

10:30am **NM-TuM2-12 Doping the Undopable: Hybrid Molecular Beam Epitaxy Growth, n-type Doping, and Field-Effect Transistor using $CaSnO_3$***, **Fengdeng Liu**, P. Golani, T. Truttmann,* University of Minnesota, USA*; I. Evangelista,* University of Delaware*; M. Smeaton,* Cornell University*; D. Bugallo,* Drexel University*; J. Wen, A. Kamath Manjeshwar,* University of Minnesota*; S. May,* Drexel University*; L. Kourkoutis,* Cornell University*; A. Janotti,* University of Delaware*; S. Koester,* University of Minnesota*; B. Jalan,* University of Minnesota, USA

ABSTRACT: The alkaline earth stannates are touted for their wide band gaps and the highest room-temperature electron mobilities among all the perovskite oxides. $CaSnO_3$ has the highest measured band gap in this family and is thus a particularly promising ultra-wide band gap semiconductor. However, discouraging results from previous theoretical studies and failed doping attempts had written off this material as "undopable". Here we redeem $CaSnO_3$ using hybrid molecular beam epitaxy (hMBE), which provides an adsorption-controlled growth for the phase-pure, epitaxial and stoichiometric $CaSnO_3$ films. By introducing lanthanum (La) as an n-type dopant, we demonstrate the robust and predictable doping of $CaSnO_3$ with free electron concentrations, *n*, from 3.3×10^{19} cm^{-3} to 1.6×10^{20} cm^{-3}. The films exhibit a maximum room-temperature mobility of 42 cm^2 V^{-1}s^{-1} at *n* = 3.3×10^{19} cm^{-3}. Despite having a smaller radius than the host ion, La expands the lattice parameter. Using density functional calculations, this effect is attributed to the energy gain by lowering the conduction band upon volume expansion. Finally, we exploit the robust doping by fabricating the $CaSnO_3$ -based field-effect transistors. The transistors show promise for $CaSnO_3$'s high-voltage capabilities by exhibiting low off-state leakage below 20 pA/µm at a drain-source voltage of 100 V and on-off ratios exceeding 10^6. This work opens the door to future studies on the semiconducting properties of $CaSnO_3$ and the many devices that could benefit from $CaSnO_3$'s exceptionally wide band gap.

10:45am **NM-TuM2-13 Controlling the Balance between Remote, Pinhole, and van der Waals Epitaxy of Heusler Films on Graphene/Sapphire***, **Taehwan Jung**, Z. LaDuca, D. Du, S. Manzo, K. Su, X. Zheng, V. Saraswat,* University of Wisconsin - Madison*; J. McChesney,* Argonne National Lab*; M. Arnold, J. Kawasaki,* University of Wisconsin - Madison

Remote epitaxy is promising for the synthesis of lattice-mismatched materials, exfoliation of membranes, and reuse of expensive substrates. However, clear experimental evidence of a remote mechanism remains elusive. Alternative mechanisms such as pinhole-seeded epitaxy or van der Waals epitaxy can often explain the resulting films. Here, we show that growth of the Heusler compound GdPtSb on clean graphene/sapphire produces a 30° rotated (R30) superstructure that cannot be explained by pinhole epitaxy [1]. With decreasing temperature, the fraction of this R30 domain increases, compared to the direct epitaxial R0 domain, which can be explained by a competition between remote versus pinhole epitaxy. Careful graphene/substrate annealing and consideration of the relative lattice mismatches are required to obtain epitaxy to the underlying substrate across a series of other Heusler films, including LaPtSb and GdAuGe. The R30 superstructure provides a possible experimental fingerprint of remote epitaxy, since it is inconsistent with the leading alternative mechanisms.

This work was supported by the Air Force Office of Scientific Research FA9550-21-0127

[1] D. Du, et. al. *Nano Lett.*2022, 22, 21, 8647–8653

11:00am **NM-TuM2-14 Synthesis of Flexomagnetic GdAuGe Membranes via Van Der Waals Epitaxy on Graphene Terminated Germanium***, **Zachary LaDuca**, S. Manzo, T. Jung, T. Samanta, K. Su, M. Arnold, J. Kawasaki,* University of Wisconsin - Madison

The ability to synthesize freestanding membranes of crystalline materials is critical for advancing the understanding of strain and strain gradient effects on materials properties. A common approach for the synthesis of freestanding membranes is epitaxial growth on graphene terminated substrates, where direct bonding between the film and substrate is prevented, allowing for exfoliation of the film from the substrate. However, challenges with wetting on the low surface energy graphene frequently prevents the growth of smooth epitaxial films. Here we demonstrate high quality growth of the flexomagnetic Heusler compound GdAuGe on graphene terminated germanium substrates using a cold-seeded growth approach. Scanning electron microscopy, atomic force microscopy, and x-ray diffraction experiments illustrate the tradeoffs resulting from growth at high and low temperatures and confirm that multistep growth approach comprised of a few-nanometer, amorphous deposition at room temperature followed by an anneal and subsequent growth at elevated temperature result in smooth, highly ordered films. This improved morphology and crystallinity enhances the ability to control the strain state in rippled GdAuGe membranes.

11:15am **NM-TuM2-15 Flexomagnetism and Strain Induced Superconductivity in Rippled GdAuGe Heusler Membranes***, **Tamalika Samanta**, Z. LaDuca, D. Du, T. Jung, S. Manzo, K. Su, M. Arnold, J. Kawasaki,* University of Wisconsin - Madison

Rare earth-based Heuslers are prospective materials platforms for magnonics, topological spin texture, superconductivity, THz spintronics, etc. [1, 2]. The magneto-mechanical coupling in these materials allows for better control and manipulation of the primary order parameter and magnetic flexibility [3]. Here, we demonstrate novel flexomagnetic responses i.e., the coupling between strain gradient and magnetism, and strain-induced superconductivity, in GdAuGe Heusler membranes. The thin films of GdAuGe Heusler composition have been grown on monolayer Graphene/ Ge (111) by molecular beam epitaxy (MBE). GdAuGe films are then mechanically exfoliated to form free-standing rippled membranes.

GdAuGe shows an antiferromagnetic ordering below ~17 K, which is sustained when a homogeneous strain is applied. However, the application of strain gradient dramatically alters the magnetic ground state of GdAuGe in the rippled membranes. A phase diagram of the rippled GdAuGe membranes is shown in Fig. 1(a). Notably, a moderate strain gradient of a few tenths of a percentage transforms the ground state from antiferromagnetic to unconventional ferrimagnetic phases. These ferrimagnetic ground states in the rippled membranes offer the possibility of discovering spin reorientation and other unique magnetic phenomena; the most exciting observation is the emergence of superconductivity in GdAuGe membranes when a very large strain gradient is applied, with superconducting transitions occurring at low temperatures below ~3.5 K. Figure 1(b) shows the magnetic characterization of a superconducting GdAuGe rippled membrane.

At present, the microscopic origin of flexomagnetism and its effects on the thermodynamics of spin reorientation and phase transitions in these membranes remain unclear. Advanced spectroscopic measurements and magneto-transport experiments, combined with theoretical modeling, are planned to further investigate the phenomena in these rippled membranes.

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11:30am **NM-TuM2-16 Growth Mechanism of $SrTiO_3$ on a Graphene-covered Substrate Using Hybrid MBE***, **Sooho Choo**,* University of Minnesota, Republic of Korea*; H. Yoon,* University of Minnesota, USA, Republic of Korea*; B. Matthews,* Pacific Northwest National Laboratory*; S. Sharma,* University of Minnesota, USA*; S. Spurgeon, S. Chambers,* Pacific Northwest National Laboratory*; R. James, B. Jalan,* University of Minnesota, USA

Epitaxial films grown on a substrate covered with two-dimensional (2D) materials offer many exciting possibilities: reusability of the substrate; ability to obtain a freestanding membrane; and opportunity to reduce misfit dislocations. Three growth mechanisms are argued to be responsible for epitaxial growth on 2D material-covered substrate: (1) Remote epitaxy; (2) Van der Waals epitaxy; and (3) pinhole-assisted epitaxy. It is, however, still unclear which of these three mechanisms is responsible for epitaxial growth. In this talk, we will first present the successful growth of epitaxial $SrTiO_3$ nanomembranes on $SrTiO_3$ (001) substrates covered with bilayer graphene. Titanium tetraisopropoxide (TTIP) was used as a source of titanium and oxygen. No additional oxygen was used to avoid graphene oxidation. By varying Sr/TTIP beam equivalent ratios, we reveal a wide MBE growth window for adsorption-controlled growth of stoichiometric $SrTiO_3$ membranes [1]. Bulk-like lattice parameter of 3.905 Å was obtained for nanomembranes. By combining heteroepitaxial growth, high-resolution X-ray diffraction, atomic force microscopy, transmission electron microscopy, and Raman spectroscopy, we discuss all three growth mechanisms highlighting the role of graphene thickness, pinholes, and the substrate's ionicity on epitaxial growth.

11:45am **NM-TuM2-17 Synthesis of Free-Standing Membranes Using a Sacrificial Layer Method Grown by Hybrid MBE***, **Shivasheesh Varshney**, S. Choo, Z. Yang, J. Wen, S. Koester, B. Jalan,* University of Minnesota, USA

Free-standing membranes have broad applications in the creation of symmetry-mismatched, non-equilibrium, and artificial heterostructures. We use sacrificial layer method to synthesize phase-pure epitaxial $SrTiO_3$ membranes. In this study, we will discuss the growth of strain-engineered $SrTiO_3$ films using different sacrificial layer(s) grown by hybrid MBE. We characterize the as-grown films using x-ray diffraction (XRD) and atomic force microscopy (AFM). We show exfoliation and transfer of films onto dissimilar substrates, followed by their structural characterization. Finally, we use impedance spectroscopy to characterize the dielectric properties and show a bulk-like dielectric constant of ≈300 for $SrTiO_3$ membranes transferred on Au coated Si substrate.

Novel Materials
Room Ballroom A - Session NM-TuA2
Novel Oxides and Superconductors

Moderator: Dr. Matthew J. Brahlek, Oak Ridge National Laboratory

3:30pm **NM-TuA2-9 TaO_2 - The New Kid on the 5*d* Block***, Yorick Birkhölzer, A. Park, M. Barone, D. Schlom,* Cornell University

For the realization of the next generation of fast, energy-efficient nanoelectronics, there is a great need for new materials whose electrical and optical conductivities can be sensitively tuned between high (on) and low (off) states by altering a thermodynamic control parameter, e.g., strain or temperature. Unfortunately, most materials are either metallic or insulating and their conductivities cannot be changed substantially. Materials exhibiting a metal-insulator transition (MIT) at or above room temperature are quite rare, limiting their applicability in devices. The archetypical compound displaying an MIT is VO_2 with a transition temperature of 65 °C. Shortly after the discovery of the MIT in $3d^1$ VO_2[1], a similar effect was discovered in $4d^1$ NbO_2 albeit at a much higher temperature of 807 °C[2]. Thus far, the $5d^1$ analog TaO_2 has remained elusive.

Here, we show the growth of epitaxial thin films of phase-pure, rutile-like $5d^1$ TaO_2 using suboxide MBE. This recently developed flavor of MBE makes use of the TaO_2 molecular vapor emanating from a Ta_2O_5 charge in an effusion cell heated to temperatures around 1700 °C[3]. This approach avoids the notoriously unstable electron-beam evaporation of Ta metal and need for subsequent oxidation using a background gas or plasma. The latter is particularly challenging to control in the quest for TaO_2 as the stable bulk phase of tantalum oxide is the $5d^0$ compound Ta_2O_5, a band insulator without an MIT, similar to the case of $3d^0$ V_2O_5 and $4d^0$ Nb_2O_5. In the suboxide MBE approach, the Ta^{4+} is delivered to the substrate from a pre-oxidized molecular beam of TaO_2.

Unlike VO_2 that can be formed at back-end-of-line-compatible temperatures below 400 °C[4], we find that exceptionally high substrate temperatures above 1000 °C are needed to crystallize TaO_2 by suboxide MBE. Such high temperatures exceed the range of typical MBE systems but are attainable at the PARADIM Thin Film Facility, an NSF-supported national user facility[5], thanks to a recently installed CO_2 laser-based substrate heater.

Ongoing efforts entail the detailed investigation of the effect of epitaxial strain on the structural and spectroscopic properties of TaO_2 thin films on various substrates. To this end, we are employing an ensemble of X-ray, optical, and electrical transport techniques, searching for signs of a structural and electronic phase transition in this candidate $5d^1$ MIT compound.

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[5] www.PARADIM.org

3:45pm **NM-TuA2-10 Growth of $KTaO_3$, $KNbO_3$ and $KNb_xTa_{1-x}O_3$ solid solutions by Suboxide Molecular-Beam Epitaxy***, Tobias Schwaigert,* Cornell University*; S. Hazra,* Penn State University*; S. Salmani-Razaie,* Cornell University*; T. Kuznetsova,* Penn State University*; S. Ganschow,* Leibniz-Institut für Kristallzüchtung, Germany*; H. Paik,* Oklahoma State University*; D. Muller,* Cornell University*; R. Engel-Herbet,* Paul Drude Institute, Germany*; V. Gopalan,* Penn State University*; D. Schlom,* Cornell University*; K. Ahadi,* North Carolina State University

Strain-engineering is a powerful means to tune the polar, structural, and electronic instabilities of ferroelectrics. $KTaO_3$ is an incipient ferroelectric, with a very large spin-orbit coupling, in which highly anisotropic superconductivity emerges near a polar instability in electron doped samples[1, 2]. Growth of high-quality epitaxial films provides an opportunity to use epitaxial strain to finely tune electronic and polar instabilities in $KTaO_3$. $KNbO_3$ is a well-known ferroelectric with multiple structural transitions[3]. Using a molecular beam of the suboxides TaO_2 and NbO_2 emanating from effusion cells containing Ta_2O_5 or Nb_2O_5 in combination with a molecular beam of potassium emanating from an indium-potassium intermetallic in an oxidant (~10% O_3 + 90% O_2) background pressure of 1x10^{-6} Torr, $KTaO_3$, $KNbO_3$ and $KNb_xTa_{1-x}O_3$ films are grown under conditions of excess potassium in an absorption-controlled regime. Biaxial strains ranging from -0.1 % to -2.1 % are imposed on the commensurately strained $KTaO_3$ films by growing them upon $SmScO_3$, $GdScO_3$, $TbScO_3$, $DyScO_3$ and $SrTiO_3$ substrates, all with the perovskite structure. Reciprocal space mapping shows the epitaxial thin films are coherently strained to the underlying perovskite substrates provided the films are sufficiently thin. Cross-sectional scanning transmission electron microscopy does not show any extended defects and confirms that the films have an atomically abrupt interface with the substrate. X-ray diffraction rocking curves (full width at half maximum < 30 arc sec on all of the above substrates) are the narrowest reported to date for $KTaO_3$, $KNbO_3$ and $KNb_xTa_{1-x}O_3$

films grown by any technique. Laue fringes confirm that the films are smooth with a well-defined thickness. Atomic force microscopy reveals atomic steps at the surface of the grown films. SIMS measurements confirm that the films are free of indium contamination.

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4:00pm **NM-TuA2-11 Studying Electronic Structures of Pure $SrCoO_X$ Thin Films, Ordered Phases, and Heterostructures***, Jibril Ahammad, G. Rimal,* Auburn University*; J. Sadowski,* Brookhaven National Laboratory*; G. Sterbinsky,* Argonne National Laboratory*; M. Boebinger,* Oak Ridge National Laboratory*; R. Comes,* Auburn University

$SrCoO_x$ (SCO) exhibits contrasting crystalline, electronic, and magnetic states with varying oxygen content. While in brownmillerite (BM) phase, $SrCoO_{2.5}$ is anantiferromagnetic insulator with ordered oxygen vacanices, $SrCoO_3$ is a ferromagnetic metal with the cubic perovskite (P) structure. Although SCO has been a relatively well-studied system, its growth using molecular beam epitaxy (MBE) has remained very limited. P-phase SCO films show high sensitivity to cation stoichiometry and oxygen chemical potential, with secondary phases present depending on growth conditions. In this work, we grew $SrCoO_x$ using MBE- via both shuttered and co-deposition methods- in oxygen plasma, with $2.5 \le x \le 2.87$ as suggested by X-ray diffraction (XRD). X-ray absorption study (XAS) of Co L and O K edges confirms Co^{3+} or higher cobalt oxidization states. In-situ reflection high-energy electron diffraction (RHEED) indicates excellent quality and highly epitaxial growth of our films. Stoichiometry ratios between Co and Sr were determined using in-vacuo X-ray photoelectron spectroscopy (XPS), followed by Rutherford backscattering (RBS). We grew our films on three different substrates: $LaAlO_3$ (LAO), $La_{0.3}Sr_{0.7}Al_{0.65}Ta_{0.35}O_3$ (LSAT), and $SrTiO_3$ (STO) which have lattice mismatches of - 1.0%, 1.0% and 2.0% with P-SCO respectively. Therefore, our study also provides a scope to explore strain-induced oxygen vacancies in the SCO films and their impacts on phase stability. Measurements of these phases were performed using temperature dependent transport property measurements and Scanning transmission electron microscopy (STEM). An evolution of electronic structure of 3d SCO films when coupled with 5d Ir/ Ta based systems in superlattice/double-perovskite structures can provide a further scope to study charge transfer in metastable oxide perovskites.

4:15pm **NM-TuA2-12 Synthesizing Metastable Ruddlesden-Popper Titanates by Mbe in Pursuit of Next-Generation Millimeter-Wave Tunable Dielectrics***, Matthew Barone,* Cornell University*; Z. Tian,* University of California at Berkeley*; M. Papac,* National Institute of Standards and Technology, Boulder*; B. Goodge, E. Fleck, G. Olsen,* Cornell University*; K. Lee,* Hongik University, Republic of Korea*; L. Kourkoutis,* Cornell University*; N. Orloff,* National Institute of Standards and Technology, Boulder*; L. Martin,* University of California at Berkeley*; D. Schlom,* Cornell University

While paraelectric $(Ba,Sr)TiO_3$ films were once used as tunable dielectrics in radio frequency (RF) circuits, dielectric loss above 10 GHz renders $(Ba,Sr)TiO_3$ incompatible with the high frequency future of RF electronics.[1]The related Ruddlesden-Popper titanates—$(A\mathrm{TiO_3})_nA\mathrm{O}$ with A = (Ba,Sr)—have demonstrated low loss up to 100 GHz, but these experiments have used interdigitated capacitors compatible with the in-plane dielectric tunability of these phases,[2,3] rather than commercially preferable[1] metal-insulator-metal (MIM) capacitors requiring out-of-plane dielectric tunability. To achieve out-of-plane tunability in a Ruddlesden-Popper film, first-principles calculations indicate the concentration of barium and the series member, *n*, should both be maximized,[3,4] but synthesizing such films is extremely challenging. Here, we refine existing synthesis techniques to grow a high-*n* Ruddlesden-Popper (*n* = 20), containing the highest concentration of barium ever accomplished in a Ruddlesden-Popper (*A* = $Ba_{0.6}Sr_{0.4}$) as shown in Fig. 1(b).[5] With a firm grasp on the synthesis, we have demonstrated epitaxially strained heterostructures of $(ATiO_3)_nAO$ dielectric layers with metallic $SrRuO_3$ electrodes (Fig. 1(b)). Measurements confirm that such Ruddlesden-Popper films are, in fact, ferroelectric (Fig. 1(c)) and that the dielectric constant is highly tunable at room temperature (Fig. 1(d)). To assess their relevance to the future of tunable dielectrics for GHz electronics, it remains to evaluate the dielectric loss of these new phases at frequencies greater than 10 GHz.

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4:30pm **NM-TuA2-13 MBE Synthesis and UV Raman Characterization of hexagonal $ScFeO_3$ films**, ***Nicholas Parker***, *D. Schlom,* Cornell University*; D. Tenne,* Boise State University*; M. Barone,* Cornell University

Hexagonal $ScFeO_3$ films synthesized by molecular beam epitaxy on (0001) oriented Al_2O_3 were studied by variable temperature ultraviolet Raman spectroscopy. Films were grown in a monolayer controlled method by shuttering of the MBE fluxes as well as by a co-deposition method so that properties of the resulting films could be compared. In addition, thin films were characterized by X-ray diffraction as well as atomic force microscopy. $ScFeO_3$ in the hexagonal phase is theorized to be multiferroic at near room temperature while being isostructural to $YMnO_3$ and other rare-earth ferrites. This multiferroicity is a combination of ferroelectricity and antiferromagnetic behavior often seen in the family of rare-earth ferrites, but at significantly higher temperatures in hexagonal $ScFeO_3$. The Raman spectra of hexagonal $ScFeO_3$ at room temperature are indicative of the polar hexagonal $P6_3cm$ structure. Furthermore, the x-ray diffraction spectra of the films are correlated with hexagonal $ScFeO_3$. Atomic force microscopy provided detailed images of the surface layers of the films allowing for roughness estimates in the range of 1.5-10 nm depending on thickness and growth procedure. The temperature evolution over the range of 10-1450 K of the Raman spectra for hexagonal $ScFeO_3$ to a non-polar phase, and fitting the Raman intensities as a function of temperature provides a transition temperature of 950 K ± 50 K.

4:45pm **NM-TuA2-14 Growth and Characterization of Complex Nickelates with High Sr Concentration**, *B. Paudel, L. Wang, Z. Yang, M. Bowden,* Pacific Northwest National Laboratory*; J. Liu,* Shanghai Institute of Microsystem and Information technology, China*; K. Koirala, T. Kaspar, P. Sushko, S. Chambers,* ***Yingge Du***, Pacific Northwest National Laboratory

Complex nickelates $(R/A)NiO_3$ (where *R* denotes lanthanide and *A* denotes alkaline earth metals) are of great interests owing to their diverse structures and functionalities. Dynamic tunability of Ni valence states in nickelate thin films (from 1+ to 4+) has offered emergent properties such as superconductivity, enhanced electrocatalytic activity, quantum confinement effect, and metal insulator transitions. Despite many efforts, stabilization of the quadrivalent (Ni^{4+})state through Sr doping in rare earth nickelates has been proven difficult. In this talk, I will present our effort in growing perovskite $La_{1-x}Sr_xNiO_3$ in thin film and superlattice forms by oxygen-plasma assisted molecular beam epitaxy. We show that it is difficult to achieve high-quality single-phase epitaxy at higher Sr concentration (x>0.5) as bulk $SrNiO_3$ has a hexagonal phase. Phase segregation ($SrNiO_x$ to $SrNi_2O_3$ + Sr_2NiO_3) and phase transition (perovskite to hexagonal) are revealed for the end member at different growth and strain conditions by XPS, XRD, and STEM.

5:00pm **NM-TuA2-15 Sharpening the Superconducting Transition of $Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$ Films with *n*=1–3 Grown by MBE**, ***Y. Eren Suyolcu***, *Y. Li, D. Schlom,* Cornell University

In bulk, the $Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$ (i.e., Bi-cuprate) family provides the highest superconducting transition temperature—up to 105 K [1]—without highly toxic constituents like thallium or mercury. When prepared as epitaxial films, however, the superconducting transitions of this family are broad and depressed for as-grown epitaxial films, with the highest zero-resistance T_c reported to date of 97 K [2]. In this work, we use ozone-assisted MBE to grow $Bi_2Sr_2Ca_{n-1}Cu_nO_{2n+4}$ (*n*=1–3) single-layers and bi-layers on (100) $SrTiO_3$ substrates, where weuse a non-superconducting $Bi_2Sr_2CuO_6$ (Bi-2201, *n*=1) buffer layer to reduce disorder caused by the underlying substrate. We demonstrate that combining adsorption-controlled *co-shuttered* growth and the initial precise flux calibration provides the best structural and superconducting properties for Bi-cuprate films formed at growth rates of 0.1 µm/hr or higher.

In-situ reflection high-energy electron diffraction exhibits incommensurate structural modulation and also proves the absence of any secondary phases. The structural quality of the samples is confirmed using a combination of four-circle x-ray diffraction, atomic force microscopy, and transmission electron microscopy. The superconducting properties are studied by resistivity vs temperature measurements. Bi-2201/Bi-2212 bilayers exhibit the smoothest reported surfaces with subnanometer root-mean-square (rms) roughness of ~0.4 nm and the sharpest superconducting transition width (ΔT_c) ~10 K, similar to Bi-2212 single crystals. While the $T_{c(R=0)}$ for the as-grown bilayer is low, i.e., ~50 K, this is a matter of oxygen content and can be modified via a post-growth process. This presentation focuses on achieving the high-structural and surficial quality and the sharp ΔT_c of the as-grown samples. We conclude that combining the *co-shuttered* growth and the initial precise flux calibration provides the best structural and superconducting properties [3].

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5:15pm **NM-TuA2-16 High-Temperature Superconductor FeSe Films Enabled Through Temperature and Flux Ratio Control**, ***Maria Hilse***, *H. Yi, C. Chang, N. Samarth,* The Pennsylvania State University*; R. Engel-Herbert,* Paul-Drude-Institut für Festkörperelektronik, Germany

FeSe, a bulk superconductor with a T_C of 9K has attracted a high level of attention since a skyrocketing boost in T_C was reported for a single unit cell (UC) layer of FeSe grown on $SrTiO_3(001)$ by molecular beam epitaxy (MBE) to as high as 100K. FeSe-$SrTiO_3$ heterostructures have since been fabricated by many groups but the record T_C proved difficult to reproduce and thus the mechanism behind it remains concealed. After extensive work in the past, the field appears to agree on certain key “ingredients” in the sample preparation that are believed essential for the boost in T_C. Those are; 1. an ultra-clean substrate surface of a double TiO_2 termination realized by a chemical and thermal *ex-situ* and/or thermal *in-situ* substrate preparation; 2. ultra-thin – one UC thickness – limit of FeSe; 3. a high number of Se vacancies in the FeSe film ensured through post-growth annealing steps in ultra-high vacuum (UHV) for several hours; 4. followed by a capping layer growth protecting FeSe against oxidation during *ex-situ* characterization. We present our findings on FeSe thin film growth by MBE and present a roadmap for high-T_C - 222% higher than the reported bulk value in *ex-situ* transport measurements - circumventing above mentioned steps 1, 2, and 3 by simple *in-situ* Se/Fe flux ratio and temperature control during FeSe growth. FeSe films of 20-UC-thickness grown at varying temperatures and Se/Fe flux ratios and the structural and morphological properties of the obtained uncapped FeSe films were analyzed. The morphology of the films showed a sensitive dependence on the growth temperature and flux ratio spanning from perfectly smooth and continuous films with atomic terraces at 450 °C growth temperature and a low flux ratio of 2.5 to exclusively disconnected island growth of large height but smooth top surfaces at lower temperatures and/or higher flux ratios. Surprisingly, the tetragonal P4/nmm crystal structure of FeSe was maintained for all investigated films and the *in-situ* observed diffraction pattern in reflection high energy diffraction also maintained the streaky pattern characteristic for smooth FeSe films even for the samples with the most pronounced island growth resulting in a root mean square atomic force microscopy roughness of more than 18nm. Smaller flux ratios than 2.5 resulted in mixed - FeSe/elemental Fe - phase samples. FeSe films grown under optimized conditions at 450°C and a flux ratio of 2.5 (but without any post-growth UHV anneal) and capped with the commonly used FeTe (300°C) and elemental Te (room temperature) layers yielded superconducting onset temperatures of about 30K and a T_C of 20K.

Novel Materials
Room Ballroom A - Session NM-WeA

Low Dimensional and Topological Materials

Moderator: Prof. Dr. Joshua Zide, University of Delaware

12:15pm **NM-WeA-1 Piezo- and Flexoelectricity Arising from Extreme Strain Gradients in Bent GaAs Nanowires***, F. Marin, O. Brandt,* ***Lutz Geelhaar****,* Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin, Germany

Strain induced by lattice mismatch can be employed to engineer the electronic properties of semiconductors and enhance device performance. Conventionally, only homogeneous strain is considered, but in nanostructures strain gradients can be relevant. In particular, our group has demonstrated for freestanding GaAs nanowires (NWs) controlled bending resulting in extreme strain gradients [1]. Here, we analyze the effect of such gradients on charge carrier recombination.

GaAs NWs are grown under Ga droplets by molecular beam epitaxy on pre-patterned Si substrates under conditions that lead to an exceptionally low degree of polytypism so that their low-temperature photoluminescence spectra exhibit only two transitions characteristic for zincblende GaAs [2]. Spectra with multiple transitions as observed in typical GaAs NWs would prohibit the subsequent analysis. Bending is induced by the growth of a lattice-mismatched asymmetric (Al,In)As stressor shell on only one NW side.

Even moderate bending induces a substantial red-shift of the free-exciton transition that cannot be explained by the change in band gap due to strain alone but indicates the presence of internal electric fields. These fields arise from both piezo- and flexoelectricity. We emphasize that flexoelectricity is an effect occurring in all dielectric materials under strain gradients but whose influence on the electronic transitions of semiconductors has not been studied experimentally.

For further analysis, systematic variations in NW diameter and bending curvature are needed. The former is modified by symmetric (Al,Ga)As shell growth or thinning by thermal evaporation. The latter is affected by the diameter and stressor shell thickness. We can predict the resulting experimental curvature variations by analytical strain calculations following linear elasticity.

In bent NWs with the same diameter, the free-exciton transition red-shifts with increasing curvature. For NWs with similar curvature but different diameter, we systematically observe a stronger red-shift with larger diameter. Since, for a given curvature, the strength of the piezoelectric field depends on the diameter but the flexoelectric one does not, these experimental data allow to disentangle the piezo- and flexoelectric effect on the electronic transitions of inhomogeneously strained GaAs.

More generally, our study has the potential to elevate the concept of strain engineering in semiconductors to a new level, exploiting spatially inhomogeneous instead of homogeneous strain.

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12:30pm **NM-WeA-2 InAs Quantum Dot Nucleation on Finite Surface for Scalable Quantum Light Sources***,* ***Chen Shang****, Y. Pang, M. Kennedy,* University of California Santa Barbara*; G. Moody, J. Bowers,* University of California at Santa Barbara

The development of quantum photonic technologies will fuel a paradigm shift in data processing and communication protocols. A controlled generation of non-classical states of light is a challenging task at the heart of such technologies. Epitaxially grown self-assembled semiconductor quantum dots (QDs) offer the advantages of deterministic generation of single photons and prospects of device integration. Even though self-assembled QDs on planar substrates have demonstrated superior single deterministic single photon emission, the random distribution of the QDs limits the scalability of the emitters. In this work, we realize site-controlled nucleation of InAs QDs in SiO_2 pockets patterned on unetched GaAs substrates. Pockets with various dimensions aligned to the <1 1 0> directions of the III-V crystal were fabricated with the anticipation that the QD nucleation process would depend on the dimensions of the finite nucleation surface.

The initial 1.5 µm SiO_2 was deposited on GaAs with PECVD. To protect the surface of epi-ready GaAs substrate, the oxide pockets were formed by ICP dry etching for the first 1.3 µm oxide followed by BHF dip for the remaining oxide. After calibrating the growth temperature offset induced by the oxide patterns, InAs QDs were deposited in the pockets with both buried dots and exposed surface dots for photoluminescent (PL) and AFM characterizations, respectively. The reference QD structures grown on planar GaAs substrate have an areal density of 5×10^{10} cm^{-2}, a typical dot height of 8 to 9 nm, and an emission wavelength of 1292 nm. However, a blue shift of the emission wavelength and a significant reduction of density have been observed for QDs nucleated in the pockets on finite surfaces. The smaller the pocket dimensions, the fewer and bluer the dots, with no observable dots in pockets smaller than certain dimensions. Compared to the dots grown in rectangular pockets, dots grown in square pockets with the same width are generally bluer and sparser. This is attributed to indium adatom diffusion onto the edge of the finite surfaces and adatom evaporation at the corners. Square pockets provide an additional diffusion path to the surface edge. At the same time, the surviving indium adatoms would diffuse onto the fewer nucleation centers in smaller, yet not too small, pockets resulting in larger dot sizes. Thus, in combination with the growth conditions, one could control the location and the structure of the dots by simply adjusting the pocket dimensions without etching the substrate. Such QD nanoparticles could potentially function as scalable on-chip quantum light sources for on demand single photon streams.

12:45pm **NM-WeA-3 Epitaxial Cd_3As_2 Heterostructures for Vertical Device Architectures***,* ***Anthony Rice****, J. Nelson, A. Norman, K. Alberi,* National Renewable Energy Laboratory

Dirac semimetals provide exciting opportunities in a number of applications, owing to their gapless band structures, high electron mobilities, broadband light absorption, and fast carrier dynamics. Cd_3As_2 is a particularly promising example due to it's similarity to a number of existing III-V and II-VI technologies. A significant limiting factor to date has been its high vapor pressure, leading to growth temperatures as low as 115 °C, also significantly limiting the ability to grow epitaxial layers on top. While there have been successful reports of device structures incorporating, among others, Al_2O_3, pentacene, and metallic layers, more sophisticated devices taking advantage of band structure engineering would require higher quality, epitaxial layers.

Here, we present the first demonstration of a fully epitaxial vertical heterostructure containing Cd_3As_2 layers. Starting from existing growth approaches to high quality Cd_3As_{2-}(112) growth on II-VI/GaAs(111)B structures [1], CdTe capping layers were nucleated at Cd_3As_2 $_{-}$growth temperatures. While underlaying Cd_3As_2 layers survived temperatures much higher than possible without a capping layer, the low energy Cd_3As_2(112) surface results in visible pinholes and makes conformal layers <50nm thick impossible. Combining previously mentioned growth approaches, and demonstration of growth on GaSb(001), Cd3As2(001) is grown on GaAs(001). By moving to a higher energy (001) surface, smooth CdTe capping layers as thin as 5nm are achieved, while preserving Cd_3As_2 film quality, with electron mobilities >10,000 cm^2/V-s. Subsequent deposition of a p-type Zn_3As_2 layer creates in a p-b-n structure, as measured with C-V and I-V measurements [2]. Photodiode behavior is demonstrated up to 1000 nm. This work sets the foundation of future epitaxial devices containing Dirac semimetals.

This work was performed by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding was provided by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Sciences and Engineering, Physical Behavior of Materials Program under the Disorder in Topological Semimetals project.

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1:00pm **NM-WeA-4 Closing Remarks and Thank Yous***,*

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