

NAMBE

Room Cummings Ballroom - Session NAMBE1-MoM

Low Dimensional Materials

Moderator: **Badih A. Assaf**, University of Notre Dame

8:00am **NAMBE1-MoM-1 Welcome & Sponsor Thank You**,

8:15am **NAMBE1-MoM-2 Art Gossard MBE Innovator Awardee Talk: How MBE Enabled Polarization Doping in Ultrawide Bandgap Semiconductor Heterostructures for Photonics and Electronics**, *Debdeep Jena*, Cornell University **INVITED**

The story of each semiconductor is intertwined with the story of its doping, so much so that a modern definition of an insulator may well be: "An insulator is a semiconductor that has not been successfully doped yet". In this presentation, I shall discuss the early discovery of chemical doping of semiconductors of Ge and Si at Bell Labs, the dramatic impact of MBE in modulation doping in GaAs, followed by the discovery of new forms of doping in polar nitride semiconductors enabled and perfected by MBE. I will discuss how the new method of *abrupt* polarization doping produces dopant-free 2D electron and hole gases in semiconductor quantum heterostructures. Then I will discuss how the new method of *distributed* polarization doping creates dopant-free mobile 3D electron and hole gases which enable new forms of vertical photonic and electronic devices with ultrawide bandgap semiconductors. In this light, I will discuss how polarization-induced doping has only recently enabled the first p-channel HFET RF power amplifiers, and the first electrically injected deep-UV lasers, and the exciting new frontiers coming up in the future.

8:45am **NAMBE1-MoM-4 Site-Templated MBE Grown InAs/GaAs Quantum Dot Platforms with Spectral Homogeneity and Tunability**, *Nazifa Tasnim Arony*, University of Delaware; *L. McCabe*, University of Delaware (Now working at Yale University); *J. Rajagopal*, *L. Murray*, *L. Mai*, *P. Ramesh*, *T. Long*, *M. Doty*, *J. Zide*, University of Delaware

Epitaxially grown semiconductor quantum dots (QDs) have been well studied in the past few decades and have shown great promise as single photon emitters, and as a basis for potential qubits. These features of quantum dots grown on a semiconductor matrix make it a desirable platform/building block for quantum devices which has a wide-range of applications in quantum information, quantum sensing and quantum computing. For a complete epitaxially grown quantum device, spatial, spectral, and structural homogeneity, and scalability are the key requirements. Recent work from our group has shown a method for site controlled QD growth where InAs/GaAs quantum dots are grown on nanofabricated substrates with site-templated arrays of nano-pits.[1] However, achieving good quality of optical emission from these QDs is still a big challenge due to the impurities introduced in the regrowth surface from the nanofabrication process. These aforementioned challenges are addressed in this work and three different objectives are being explored, first one being the domain of quantum dot columns (QDCs) as a buffer layer for the topmost QD-arrays of interest while burying defects underneath the QDCs. Additionally, initial experiments on spectral control of InAs/GaAs QDs by 'cap and flush' are discussed and the concept of quantum dot molecules is introduced for optical tunability.

[1] *J. Vac. Sci. Technol. B* 38, 022803 (2020)

9:00am **NAMBE1-MoM-5 Site Controlled InAs/GaAs Quantum Dots for Photonic Integration**, *Ian Farrer*, *C. Chan*, *A. Verma*, *A. Trapalis*, *C. Ovenden*, *D. Hallett*, *E. Clarke*, *M. Skolnick*, *J. Heffernan*, University of Sheffield, UK

Controlling the position of quantum dots (QDs) is desirable for nanophotonic devices due to their potential as single photon emitters for quantum technology applications.[1] Challenges that are associated with forming site-controlled (SC) QDs include single QD occupation, planarisation, narrow linewidths and controllable wavelength. For Stranski-Krastonov growth, QDs nucleate preferentially in local minima in the surface chemical potential.[2] In this study, we use ex-situ fabrication of arrays of nanoholes to form preferential nucleation sites, investigating the effects of nanohole size, nanohole density and other parameters on the emission wavelength of single QDs for undoped and doped structures.

Initial development focused on good site-selectivity of QD arrays, which allowed for optimisation of growth parameters to control emission wavelength and QD linewidth. Planarisation on the patterned surface was also crucial: during the GaAs buffer layer, preservation of the nanoholes is important to allow them to function as preferential nucleation sites, but

after QD formation, planarisation of the capping layer is important for good optical properties, for example in waveguides. This is a crucial step for doped structures, as insufficient planarisation can result in optically inactive QDs due to close proximity to the doped layer. Each sample contains different arrays with variations in nanohole size and spacing, allowing for direct investigation of the effects of these parameters on the emission wavelength and linewidth of nucleated quantum dots using site-specific photoluminescence (PL) measurements.

We observe a shift in emission in the range of 900 to 1000nm, which is compatible with high-efficiency Si detectors. Clusters of uniform single-line emissions are obtained from micro-PL measurements. These conditions resulted in nucleated QDs with a minimum linewidth of 22 μ eV (resolution limited) and an average linewidth of \sim 87 μ eV measured using non-resonant excitation. In addition, we demonstrate the emission and tuning of groups of QDs for doped diode structures with good site selectivity.

References

[1] Carter, S., Sweeney, T., Kim, M. et al. *Quantum control of a spin qubit coupled to a photonic crystal cavity*. *Nature Photon* 7, 329–334 (2013)

[2] Srolovitz, D.J., *On the stability of surface of stressed solids*, *Acta Metallurgica*, 37, 621-625, (1989)

9:15am **NAMBE1-MoM-6 Commercializing Nanowire LEDs**, *David Laleyan*, *B. Le*, *G. Frolov*, NS Nanotech Canada; *M. Stevenson*, *S. Coe-Sullivan*, NS Nanotech

MicroLED display technology consists of many carefully arranged microscopic light-emitting diodes (LEDs) to directly create color pixels. MicroLED displays thus have the potential brightness, efficiency, and response time of inorganic LEDs, but suffer from the high cost of epitaxy, as well as the challenges of creating red, green, and blue materials on a single material and substrate. Furthermore, conventional approaches of growing planar LEDs and then etching them into micron scale devices causes a fundamental loss of efficiency, especially for the smallest devices. In this regard, nanowire-based LEDs for microLED applications have been of great interest and a topic of extensive research for over a decade. This is due to their unique ability to maintain high efficiencies even as the LED size becomes quite small, even into the sub-micron regime, contrary to conventional thin-film LEDs. Another valuable benefit is the ability to form photonic crystal arrangements, such that the formation of a photonic bandgap leads to highly directional and narrow bandwidth emission. More recently, reports have shown nanowire LEDs in the green with >25% external quantum efficiency (EQE) and red with >8% EQE, competitive with the best direct green and InGaN red LEDs ever fabricated – despite being sub-micron in size. These structures were obtained by molecular beam epitaxy (MBE) using a selective area epitaxy (SAE) technique, where nanostructures can be controllably grown on a thin-film template. Novel development and engineering efforts are required for such nanowire LEDs to become commercially viable. This work presents a pathway towards the wafer-scale production of nanowire LEDs for displays. This talk will explain how breakthrough academic research can be made manufacturable by studying run-to-run variability, understanding the process windows, targeting yield-limiting steps, and ensuring process scalability. Focusing on the reproducibility and uniformity of nanowire growth by SAE is the first critical step toward the large-scale deployment of these highly efficient LED that are perfectly suited for the next generation of microLED displays.

9:30am **NAMBE1-MoM-7 Epitaxial Ge Membranes Detachment via Porous Ge Layer and Adhesion Force Engineering**, *Ahmed Ayari*, *T. Hanuš*, *N. Paupy*, *F. Zouaghi*, 1-Institut Interdisciplinaire d'Innovation Technologique (3IT), Université de Sherbrooke, 2-Laboratoire Nanotechnologies Nanosystèmes (LN2)-IRL3463, CNRS, Université de Sherbrooke., Canada; *B. Illahi*, 1-Institut Interdisciplinaire d'Innovation Technologique (3IT), Université de Sherbrooke, 2-Laboratoire Nanotechnologies Nanosystèmes (LN2)-IRL3463, CNRS, Université de Sherbrooke., Canada 3-DistriQ - Zone d'Innovation Quantique, Canada; *J. Cho*, *K. Dessen*, Umicore Electro-Optic Materials, Belgium; *D. Machon*, 1-Institut Interdisciplinaire d'Innovation Technologique (3IT), Université de Sherbrooke, 2-Laboratoire Nanotechnologies Nanosystèmes (LN2)-IRL3463, CNRS, Université de Sherbrooke., Canada

Recently, there has been an increasing interest in single-crystal germanium (Ge) membranes for lightweight, low-cost solar cells and flexible optoelectronic devices. A viable solution for the large-scale fabrication of

such Ge membranes, appears to be the direct growth of Ge on porous Ge (PGe) template [1-3], allowing the detachment and substrate reuse [4].

After creating a PGe template, a low-temperature buffer layer is grown to maintain the voids in the sealed surface. Then, a high temperature Ge layer is grown, ensuring a good crystallinity for the membrane, and allowing to the porous structure to transform into a weak layer that facilitates later detachment as shown in Fig 1 a-b. However, there is a lack of studies focusing on the Ge membrane detachment, the adhesion of the membrane to the parent substrate, and how it can be modulated by morphological changes of the porous structure underneath.

In this work, we demonstrate the adhesion force engineering of the Ge membranes by controlling the morphological transformations of the PGe layer, from porous structure to well-defined pillars, through thermal budget adjustments and variations in PGe porosity and thickness. Scanning electron microscopy (SEM) analysis reveals the evolution of pillar diameter and density with post-growth thermal annealing at temperatures between 650°C and 850°C as shown in Fig. 2 a-e. The membrane's adhesion strength can be successfully tailored through the control of this pillar transformation (Fig. 2 f). Moreover, with increasing PGe layer thickness and/or porosity, the membrane adhesion force is found to significantly change from a highly adhesive to easily detachable.

The high-quality Ge membranes on PGe substrates offer the possibility of detachment from the substrate using the weak nanostructured interface. By controlling the weak interface nanostructure through the thermal annealing and PGe substrate physical properties, allowing the tailoring of the adhesion force of the membrane for specific applications. This includes a high-temperature growth of III-V heterostructures, paving the way for lightweight and flexible photovoltaic and optoelectronic applications.

[1] N. Paupy et al., *Nanoscale Adv.*, **2023**, vol. 5, no. 18, pp. 4696–4702.

[2] T. Hanuš et al., *Materials Today Advances*, **2023**, vol. 18, p. 100373.

[3] V. Daniel et al., *Solar RRL*, **2024**, vol. 8, no. 1, p. 2300643.

[4] A. Chapotot et al., *Materials Science in Semiconductor Processing*, **2023**, vol. 168, p. 107851.

9:45am **NAMBE1-MoM-8 Synthesis of InSe Thin Films on Sapphire using Molecular Beam Epitaxy**, *Emily Toph*, *C. Voigt*, Georgia Institute of Technology; *B. Wagner*, Georgia Tech Research Institute; *E. Vogel*, Georgia Institute of Technology

InSe is a monochalcogenide two-dimensional (2D) semiconducting material¹ with a high room-temperature electron mobility of approximately $10^3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ for encapsulated devices.² InSe is a promising material for high-sensitivity Hall sensors³, ballistic transistors,⁴ and non-volatile memory applications.⁵ The In-Se system contains many different stable phases⁶ including selenium rich In_2Se_3 and the selenium deficient phase In_4Se_3 . One challenge in synthesizing InSe is that the stoichiometry of this phase is stable only in a narrow range on the phase diagram. Therefore, synthesizing high-quality InSe requires a detailed understanding of how the synthesis parameters affect the structure and stoichiometry of In_xSe_y thin films near and within the narrow range of stability for InSe.

Recently, the effect of precursor fluxes and substrate temperature on the synthesis of InSe on Si(111) substrates was explored, with differences found in morphology and stoichiometry across a range of synthesis parameters.⁷ However, using InSe for device applications often requires using an insulating substrate for electrical isolation of the devices. Sapphire is a widely used insulating substrate for epitaxial synthesis of transition metal dichalcogenides, another 2D material system. This work investigates the impact of substrate temperature and precursor flux on the structure and stoichiometry of InSe thin films on sapphire substrates. The chemical bonding, crystalline structure, and morphology of the thin films are characterized with X-ray Photoelectron Spectroscopy, Raman spectroscopy, and Atomic Force Microscopy, respectively.

References

¹Camara, M., et al., *Physical Review B* (2002) **65** (12), 125206

²Li, M., et al., *Advanced Materials* (2018) **30** (44), 1803690

³Bandurin, D. A., et al., *Nature Nanotechnology* (2017) **12** (3), 223

⁴Jiang, J., et al., *Nature* (2023) **616** (7957), 470

⁵Lu, Y.-Y., et al., *ACS Applied Materials & Interfaces* (2021) **13** (3), 4618

⁶Bergeron, H., et al., *Applied Physics Reviews* (2020) **7** (4)

⁷Liu, D. S. H., et al., *ACS Applied Nano Materials* (2023) **6** (16), 15029

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Room Cummings Ballroom - Session NAMBE2-MoM

III-Vs

Moderator: Eric Jin, Naval Research Laboratory

10:30am **NAMBE2-MoM-11 Exploring MBE Growth Parameters and Material Quality of III-V Topological Insulators Grown on GaSb(111)A Substrates**, *James R Rushing*, *L. Qui*, Tufts University; *X. Xie*, Tufts University; *T. Menasuta*, *J. Mcelearney*, *P. Simmonds*, Tufts University

Since the discovery of the Quantum Spin Hall effect (QSHE), topological insulators have received significant attention for their novel uses in electronic devices. Spin-momentum locking in the surface states of a Quantum Spin Hall Insulator (QSHI) offers electron transport without scattering. These topological surface states arise due to strong spin-orbit coupling and band inversion. The QSHE was proposed for HgTe/CdTe heterostructures in 2006 and was experimentally realized in 2007 [Bernevig 2006] [König 2007]. In our work, we focus on QSHI's based on InAs/GaSb-based quantum well heterostructures. Creating robust QSHI's out of extensively studied III-V materials is highly desirable. Doing so would allow for an ease of integration with existing III-V devices such as 2DEG's. Quantum size effects should enable one to tune the device in and out of the topological insulating phase by adjusting the quantum well widths. Furthermore, we can tune the strain and confined hole state energy by altering the indium percentage in the ternary GaInSb layer [Irie 2020]. The other nice feature of these structures is that the electrons and holes are strongly localized in the InAs and GaInSb wells, respectively. This spatial separation allows for additional tunability of the topological phase using top- and bottom-gates.

Accessing the rich topological phases of these materials requires precise control of quantum well thickness [Schmid 2022]. This is best achieved with molecular beam epitaxy (MBE). To our knowledge, research into these structures has been limited to III-V quantum wells grown on (001) surfaces. Our calculations show that quantum wells with a (111) orientation are likely to exhibit distinct electronic behavior, for example a larger hybridization energy gap than on (001). However, growth on (111) surfaces is typically more difficult and the literature available for optimal growth parameters is sparse. Furthermore, the growth of even relatively simple structures is complicated by the mismatched lattice constants and the need to switch group V species between the quantum wells.

We will present our results exploring the growth and subsequent material quality of InAs/GaInSb double quantum wells grown on GaSb(111)A substrates as a function of growth parameters that include: group V flux, substrate temperature, and growth rate. We mirror these results with control quantum well structures grown on the (001). From the result of AFM, XRD, and SEM characterization, we will describe how the variation in the above growth methods effect material quality, with an eye to exploring emergent topological states in these quantum wells.

10:45am **NAMBE2-MoM-12 Molecular Beam Epitaxy Growth and Regrowth of InAs/Al Heterostructures**, *Ido Levy*, New York University; *J. Issokson*, New York University; *A. Danilenko*, *P. Strohbeen*, *T. Cowan*, New York University; *W. Strickland*, New York University; *L. Baker*, *M. Mikalsen*, *J. Shabani*, New York University

Heterostructures of a 2-dimensional electron gas (2DEG) semiconductor and a superconductor are prime candidates for various applications including quantum computing and topological superconducting circuits [1,2]. It is required that the 2DEG layer will be in close proximity to the superconductor and the layers will have an Ohmic contact. A high 2DEG mobility as well as high quality interface are often needed for device applications. The system of near-surface InAs (InGaAs/InAs/InGaAs) quantum well (QW) is a prime candidate. It has a narrow bandgap with the Fermi level close to the conduction band and a thin epitaxial Al layer grown above it. The high mobility of the 2DEG embedded in the InAs QW and the compatibility between the QW and epitaxial Al makes this heterostructure a promising candidate. However, the close proximity of the QW to the surface hinders the mobility and limits it to low values of $100,000 \text{ cm}^2/(\text{V s})$. While QWs that are not close to the surface (buried) show greater mobility, there is no way to couple them with a superconductor due to the distance between them.

In this work, we aim to bridge the gap between buried and surface InAs QWs and grow buried, fabricated, semiconductor/superconductor heterostructures by molecular beam epitaxy. We present a newly developed 2-stage growth procedure which aims to enhance 2DEG

mobilities while keeping the proximity to the Al. The first step includes growth of surface InAs and an epitaxial Al layer. After growth, we remove the sample and fabricate our structure as usual, and then reintroduce the sample back to the chamber and regrow a thick (~100nm) layer of In_{0.81}Al_{0.19}As in order to bury the structure. By burying the structure we aim to improve transport by reducing the effects of surface scattering, which normally limits mobilities in these near-surface QWs. We compare surface morphology and magnetotransport characterization data for buried and unburied structures, as well as for varying growth conditions. The growth process and characterization of the samples will be presented.

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

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

11:00am **NAMBE2-MoM-13 Engineering MBE Structures for Ultraclean 2D Hole Systems with Mobilities Exceeding 10^7 cm²/Vs**, *Adbhut Gupta, C. Wang, S. Singh, K. Baldwin*, Princeton University; *R. Winkler*, Northern Illinois University; *M. Shayegan, L. Pfeiffer*, Princeton University

Two-dimensional (2D) carrier systems confined to modulation-doped semiconductor structures provide a nearly ideal testing ground for exploring new physical phenomena. The advances in molecular beam epitaxy (MBE) has substantially elevated the quality of these systems, notably reflected in the emergence of plethora of many-body states stemming from electron-electron interactions, for instance, the fractional quantum Hall (FQH) liquid, the Wigner solid, and the newly discovered striped and bubble phases in the higher Landau levels. Following innovations in MBE growth chamber design, and purification of source materials, we achieved a recent breakthrough in mobility of 2D electrons in GaAs quantum wells with the peak mobility $\sim 60 \times 10^6$ cm²/Vs at a 2D density $\sim 1.55 \times 10^{11}$ /cm². This implies an incredibly low number $<10^{13}$ /cm³ of background charged impurities. Building up on the already extreme levels of vacuum and source material purity in our MBE growth chamber, we present an alternative way our achieving new world-record mobilities for 2D hole systems (2DHSs) by optimizing the sample structure design. 2DHSs in GaAs quantum wells host many unique properties as compared to their electron counterparts – large effective mass, strong and tunable spin-orbit coupling, heavy-hole and light-hole coupling in the valence band, and a complex energy-band and Landau level fan diagram. We systematically grew 60 GaAs 2DHS samples, optimizing two structural parameters, the alloy fraction x of the Al_xGa_{1-x}As barriers near the GaAs quantum well, and the quantum well width. For the first time, in a 2DHS in any material, we obtain peak mobility $\approx 10 \times 10^6$ cm²/Vs at density of only $\approx 3.8 \times 10^{10}$ /cm², at 300 mK which rises to $\approx 18 \times 10^6$ cm²/Vs (a mean-free-path ≈ 57 μ m) when measured at 30 mK. Low-temperature magnetotransport data exhibit a numerous delicate FQH states, the collection of which has never been seen before in any 2D system. The achievement of mobilities up to 18×10^6 cm²/Vs in 2D hole systems represents a giant, 10-fold, leap, considering that the highest recorded mobilities, until two years ago, were only $\approx 2 \times 10^6$ cm²/Vs. The quality improvement and concomitant new FQH states evince a bright future for exploring interaction driven physics in GaAs based 2D systems.

11:15am **NAMBE2-MoM-14 Selective Area Regrowth of High Aspect Ratio Microstructures for Mid-Infrared Optoelectronics**, *Ashlee Garcia, B. Aguilar, W. Doyle*, University of Texas at Austin; *Y. Wang*, University of Illinois at Urbana-Champaign; *D. Ironside, A. Skipper, M. Bergthold*, University of Texas at Austin; *M. Lee*, University of Illinois at Urbana-Champaign; *D. Wasserman, S. Bank*, University of Texas at Austin

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

MBE SAE has been historically difficult to achieve under conventional growth conditions due to its poor III-V deposition selectivity. This leads to an aggregation of adatoms on the amorphous mask which results in the formation of polycrystalline material on the mask surface.²⁻⁵ Despite many efforts to improve selectivity²⁻⁵, the accessible growth window remains narrow necessitating high temperatures and low growth rates. Mask surface roughness further restricts the selective growth regime by lowering the barrier for nucleation.⁶ This limits applications requiring microns-tall high aspect ratio dielectric structures, such as mid-wave infrared high-contrast photonics⁷⁻⁸ and aspect ratio trapping for metamorphic growth⁹,

due to the innately rough surfaces produced by plasma-enhanced chemical vapor deposition of thick films.

Here we demonstrate hydrogen silsesquioxane (HSQ) planarization^{10,11} as an effective solution to aid MBE regrowth selectivity for the design of novel device and optical structures by mitigating the surface roughness of micron-scale dielectric features. By restoring the surface of 2 μ m tall SiO₂ features with 100 nm HSQ, a 4x decrease in RMS roughness was demonstrated. GaAs selective regrowth of the 2 μ m tall SiO₂ features saw significant improvement in selectivity as compared to the un-planarized features with no polycrystalline formation on SiO₂ bars <10 μ m wide alongside a 30x increase in achievable feature aspect ratio. Experiments are underway to extend this approach to InAs regrowth for accessing applications in the mid-wave infrared regime. This work was supported by NASA (Award 80NSSC22K0287), NSF (ECCS-1926187), and Lockheed Martin.

[1] D.J. Ironside et al., *J. Cryst. Growth*, 2019. [2] F.E. Allegretti et al., *J. Cryst. Growth*, 1995. [3] S.C. Lee et al. *J. of Appl. Phys.*, 2002. [4] S. Yokoyama et al. *J. Cryst. Growth*, 1989. [5] Aseev et al. *Nano Lett.*2019. [6] M. Ohring, *The Material Science of Thin Films*, Academic Press, 1992. [7] J. Wang et al. *Laser Phys. Lett.*, 2017. [8] C.J. Chang-Hasnain et al. *Adv. Opt. Photon.*, Sep 2012. [9] J.Z. Li et al. *Appl. Phys. Lett.*, 2007. [10] F. Salmassi et al, *Appl. Opt.*, 2006. [11] C.-C. Yang et al., *J. Mater. Chem.*, 2002.

11:30am **NAMBE2-MoM-15 Shadow Mask Molecular Beam Epitaxy**, *S. Mukherjee, R. Sitaram, X. Wang*, University of Delaware; *Stephanie Law*, Penn State University

Shadow mask molecular beam epitaxy (SMMBE) is a form of selective area epitaxy (SAE) which uses a mask either directly fabricated on or placed in contact with the substrate. During film deposition, epitaxial layers are grown on the substrate through apertures in the mask. In addition to selective area growth, SMMBE also produces a shadowing effect near the mask edges in which elemental fluxes vary as a function of position. This results in a gradient of film thickness and/or composition near the mask edges. The steepness of the gradient can be controlled by varying the mask thickness and/or the angle of the mask edges. In this paper, we demonstrate the potential of the SMMBE technique to create in-plane gradient permittivity materials (GPMs) by taking advantage of the shadowing effect. A GPM is a material in which the permittivity varies as a function of location. Our aim is to synthesize in-plane GPMs, in which the permittivity varies in the lateral in-plane direction rather than in the vertical growth direction. In an in-plane GPM, different wavelengths of light can be confined at different in-plane locations on the chip. We are interested in creating an infrared GPM, so we chose Si:InAs as our material. To create our GPMs, we use the SMMBE approach: by creating flux gradients of both indium and silicon near the edges of the mask, we can control the doping density and thus the permittivity of Si:InAs in the lateral in-plane direction. We started with reusable Si masks that are 200 mm thick and 1 cm \times 1 cm in dimension. Each mask has an aperture at its center which has a dimension of 0.5 cm \times 0.5 cm at the top and ≈ 0.528 cm \times 0.528 cm at the bottom. Nano-FTIR spectra obtained via s-SNOM using a mid-IR nano-FTIR module demonstrates that we successfully synthesized infrared GPMs. The GPM grown using a 200 mm mask can confine light with wavenumbers ~ 650 cm⁻¹ to 900 cm⁻¹ over an in-plane distance of ~ 13 mm. In this talk, I will discuss the influence of several growth parameters in controlling the in-plane permittivity of the GPMs, including the growth temperature, mask thickness, and As:In ratio. In particular, the 500 mm mask provides a larger shadowing effect in comparison to 200 mm mask. This leads to a larger gradient in permittivity over a longer in-plane distance in the GPM: light with wavenumbers ~ 650 cm⁻¹ to 1400 cm⁻¹ can be confined over an in-plane distance of ~ 30 mm. This provides a larger surface area for the construction of an ultracompact spectrometer. Tailored mask designs can be employed to synthesize in-plane GPMs with tailored permittivity gradients in the future.

11:45am **NAMBE2-MoM-16 Electron Microscopy Characterization of GaSb islands on Silicon substrates grown via Molecular Beam Epitaxy**, *Mega Frost, S. Seth, F. Ince*, University of New Mexico; *N. Arony, L. Mai*, University of Delaware; *D. Shima, T. Rotter*, University of New Mexico; *M. Doty, J. Zide*, University of Delaware; *G. Balakrishnan*, University of New Mexico

GaSb quantum dots (QDs) grown on III-V substrates provide a promising alternative to the typical InAs QDs for emission in the NIR. This material system has shown that QDs can be grown strained under the typical Stranski-Krastanov (SK) growth mode or fully relaxed under the Interfacial Misfit dislocation array (IMF) growth mode. GaSb QDs are implemented in a variety of devices, with publications demonstrating their use in lasers, photovoltaics, detectors, and memory devices. Growing these GaSb QDs on Silicon substrates instead would enhance the fields of Silicon photonics and

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quantum computing. In this study we investigate the growth of GaSb grown on Silicon (100) and conduct characterization through Transmission Electron Microscopy (XTEM), Scanning Electron Microscopy (SEM), and Energy-Dispersive X-Ray Spectroscopy (EDS) analysis.

GaSb is grown on Si (100) using solid-source molecular beam epitaxy (MBE). The native oxide is removed from the Silicon substrate with a 49% HF etch, producing a hydrogen-passivated surface. This is verified in the MBE by observation of its reflection high energy electron diffraction (RHEED) pattern. Four samples are grown with thicknesses of 3 MLs, 5 MLs, 10 MLs, and 50 MLs. Imaging and investigation of the surface is performed using SEM and analysis of the crystallographic structure is performed using XTEM. The growth of GaSb on Silicon is compared to AlSb on Silicon, which has been well understood and documented in the literature [1].

These samples demonstrate no coalescence of the GaSb islands into a planar layer, whereas AlSb has been shown to planarize when 50 MLs has been reached. Instead, the samples display two distinct distributions of island growths: smaller islands that are grown via the direct nucleation of Ga and Sb atoms on the Silicon surface and noticeably larger islands which appear to be catalyzed under the Vapor-Liquid-Solid (VLS) growth mode. This occurs due to the presence of liquid Ga on the Silicon surface, which acts as a trap for Sb atoms to facilitate the GaSb growth, thereby allowing the islands to grow visibly larger than those that are directly nucleated. Electron microscopy images show the highly-faceted, equilibrium crystalline structure of the islands and fully relaxed crystals with no observable threading dislocations. Furthermore, we will present a peculiar observation of Silicon diffusion from the substrate into the metallic droplet during growth, verified through EDS. We will also describe a growth method we are developing to take advantage of the faceted islands and the VLS growth mode to control the size and distribution of the GaSb QDs.

[1] *Appl. Phys. Lett.* 86, 034105 (2005)

NAMBE

Room Cummings Ballroom - Session NAMBE1-MoA

Small Bandgap Materials: Bismuthides and SiGeSn

Moderator: Kevin A. Grossklau, MIT Lincoln Laboratory

1:30pm **NAMBE1-MoA-1 Determination of the Temperature Dependent Complex Refractive Index of GaSbBi Films by Variable Angle Spectroscopic Ellipsometry**, John McElearney, K. Grossklau, T. Vandervelde, Tufts University

III-V-Bi alloys, such as $\text{GaSb}_{1-x}\text{Bi}_x$, offer a slew of advantages for use in infrared optoelectronics. An anti-crossing interaction between the Bi impurity state and the host valence band dramatically reduces the film's bandgap energy [1], opening up new lattice constant and bandgap combinations. A second interaction in the split-off band [2] has recently been shown [3] to increase the spin-orbit splitting energy (Δ_0), potentially leading to a suppression of Auger recombination [4]. Finally, it has been predicted that increasing Bi fraction should reduce the bandgap energy temperature dependence as the film moves towards the semi-metal GaBi [5]. These effects can be observed by tracking critical points in the complex refractive index as functions of temperature and film composition [6, 7]. As many target applications for GaSbBi-based optoelectronics are operated either cooled, such as IR photodetectors, or at elevated temperature, such as thermophotovoltaic cells, a deeper understanding of this material's temperature dependent optical properties will improve device design and modelling.

In this work, we determine the optical constants of GaSbBi alloys as functions of wavelength, Bi fraction, and temperature using variable angle spectroscopic ellipsometry (VASE). Specifically, we measure the refractive index (n), the extinction coefficient (k), and the absorption coefficient (α) for GaSbBi films with Bi fraction $x \leq 4.2\%$, over a spectral range of 0.5 to 6.2 eV, at temperatures ranging from 78 to 473.2 K. Samples were grown on unintentionally doped, (100) GaSb substrates in a Veeco GENxplor MBE, with Sb supplied by a valved cracker cell, and Ga and Bi by high temperature effusion cells. Scans were taken using a J.A. Woollam VASE with samples mounted and held under vacuum in a JANIS cryostat. The energies of key interband transitions, such as the bandgap (E_0) and split-off band energy ($E_0 + \Delta_0$), were determined by critical point analysis of the second derivative of k with respect to energy. Finally, the temperature dependence of these transitions, including each film's Varshni parameters, were extracted.

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1:45pm **NAMBE1-MoA-2 Interplay of Al and Bi Incorporation in AllnSbBi**, Amberly Ricks, R. White, University of Texas at Austin; H. Hijazi, Rutgers University; S. Bank, University of Texas at Austin

InSb-based alloys are widely explored as an alternative to HgCdTe for mid-wave infrared operation.^{1,2} While InSb alone cannot access the long-wave infrared (LWIR), incorporating small amounts of Bi can decrease the bandgap energy, and photoluminescence has recently been demonstrated out to 7.6 μm at 230K from InSbBi.³ Because narrow-gap materials are required for extended infrared operation, parasitic dark currents often arise to the detriment of device performance.² While nBn structures are shown to suppress sources of high dark current, AllnSb barriers in InSb-based nBn detectors introduce a tradeoff between a desirably large conduction band offset and an undesirably large valence band offset.⁴ This tradeoff is exacerbated for InSbBi absorbers as experimental evidence suggests that the bandgap energy of InSb is expected to decrease by 29 meV/% Bi incorporated,³ and most of this bandgap change is expected to manifest in the valence band.⁵ To break this tradeoff in InSb-based nBn detectors, small amounts of Bi can be incorporated into the AllnSb barrier to independently decrease the valence band offset while maintaining a sufficiently high conduction band offset. In this work, we explore the interplay of Al and Bi incorporation in AllnSbBi.

AllnSbBi films were grown on InSb substrates under similar growth parameters to those used for high quality InSbBi:³ a 300°C substrate temperature, 0.975x V/III flux ratio, and $\sim 1 \mu\text{m/hr}$ growth rate. At low Al concentrations, Bi incorporation was limited to $\sim 0.4\%$ and the excess Bi precipitated out into droplets on the surface. However, we found that higher concentrations of Bi could be incorporated as the Al concentration was increased; this may be due to the shorter AlBi bond being more energetically favorable than that of InBi.⁶ Rutherford backscattering spectrometry measurements demonstrated that AllnSbBi films containing 25 and 32% Al enabled incorporation of 3.2 and 4.2% Bi, respectively. Atomic force microscopy scans revealed the presence of Bi droplets, indicating Bi saturation was reached under these growth conditions. Future work on optimizing the AllnSbBi growth regime and experimentally measuring the band offsets in these materials is underway to better understand the efficacy of Bi in an AllnSb barrier layer for LWIR devices. This work was supported by the NSF (Award Nos. ECCS-1933836).

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2:00pm **NAMBE1-MoA-3 Growth of GaBi Thin Films via Molecular Beam Epitaxy**, Molly McDonough, S. Law, Pennsylvania State University

Like the well-known arsenides, antimonides, and phosphides, the bismides are part of III-V semiconductor class. Bismides include the ternaries $\text{GaSb}_{1-x}\text{Bi}_x$, $\text{GaAs}_{1-x}\text{Bi}_x$, $\text{InSb}_{1-x}\text{Bi}_x$, and the binary compounds AlBi, GaBi, and InBi. The ternary bismides are relatively well-studied due to their applications in infrared sensing: their bandgaps can be decreased significantly with the inclusion of a relatively small amount of bismuth. Density functional theory (DFT) calculations indicate that the binary bismides should be topologically non-trivial materials, converting to topological insulators or semimetals upon the application of a small amount of strain. The ternary compounds $\text{GaSb}_{0.5}\text{Bi}_{0.5}$, $\text{GaAs}_{0.5}\text{Bi}_{0.5}$, and $\text{InSb}_{0.5}\text{Bi}_{0.5}$ have also been predicted by DFT to be metastable Dirac semimetals. Despite the long-standing interest in bismides, progress in the synthesis of high-Bi content-containing alloys has been slow due to the surfactant behavior of bismuth, making the growth of defect-free coalesced films with high-Bi content challenging. There have only been two reported attempts of growth of the binary bismides via molecular beam epitaxy (MBE). In 2014, the growth of InBi on GaAs(100) resulted in large droplet formation and uncoalesced films. This attempt was likely unsuccessful due to the large lattice mismatch between the substrate and the bismide films. In 2019, a paper was published on the growth of InBi on Si(111), showing coalesced InBi films in the tetragonal structure with some remaining crystalline bismuth in x-ray diffraction (XRD) measurements.

Here, we present the successful synthesis of coalesced GaBi films using MBE. The GaBi films were grown with a Ga:Bi beam equivalent pressure (BEP) ratio of 1:1 on InSb(100) substrates. The choice of InSb(100) for GaBi growth is due to the near-perfect (-0.34%) lattice matching between the substrate and the predicted lattice constant of GaBi. Using XRD and energy dispersive spectroscopy (EDS) measurements, we demonstrate that we can stabilize the zinc-blende structure of GaBi and grow this material as a thin film. We show that substrate temperatures below 100C, as measured by thermocouple, result in droplet formation. Substrate temperatures exceeding 200C result in phase segregation of the Ga and Bi. However, within the substrate temperature window of 100-200C, crystalline GaBi thin films will form. These results are promising for further study of GaBi and have the potential to inform future work on InBi and AlBi for applications in infrared detectors and topological materials.

2:15pm **NAMBE1-MoA-4 Long-Wave Infrared Sensing via InSb-Based Dilute-Bismide Alloys**, Corey White, M. Berghold, A. Ricks, F. Estévez, D. Wasserman, S. Bank, The University of Texas at Austin

Due to the significant bandgap reductions induced by bismuth incorporation in III-V alloys,^{1,2} dilute-bismide alloys present a unique opportunity to access technologically significant operating wavelengths for optoelectronics. Specifically, long-wave infrared (LWIR) detectors are of critical importance for chemical sensing and thermography, but the corresponding narrow bandgap energies have proven challenging to reach with III-V alloys. By incorporating small concentrations of bismuth^{3,4} and arsenic⁵ into InSb, the quaternary alloy InAsSbBi can be grown lattice-

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matched to InSb substrates with tunable narrow bandgap energies, thus highlighting a route to LWIR detectors that do not suffer from the fabrication, growth, and toxicity challenges plaguing the current state-of-the-art material, HgCdTe. Here we report the first InSbBi nBn detector showing a significant bismuth-induced extension in cutoff wavelength. Building on this, we will show how arsenic incorporation can be leveraged to lattice-match to InSb substrates enabling the growth of thick absorbers for strong absorption.

Epitaxial In(As)SbBi alloys were grown on InSb substrates. To impose a kinetically-limit growth regime,⁵ low substrate temperatures, Sb/In flux ratios near stoichiometry, and fast growth rates were employed to encourage significant bismuth incorporation. From these alloys, we observed room temperature photoluminescence (PL) with significant wavelength extension into the LWIR indicating high optical quality, which is promising for high-performance detectors. Furthermore, by incorporating arsenic and bismuth in ~1:3 proportions, we grew InAsSbBi lattice-matched to InSb and observed that the arsenic incorporation assisted in reducing the alloy's bandgap as expected due to the band bowing between InAs and InSb.⁵

To demonstrate a prototype InSbBi detector, an nBn detector was grown with an InSbBi absorber and an AlInSb barrier. Comparing this detector to an identical device with no bismuth, we observed a significant extension in cutoff wavelength at 79K from 5.5 μm for InSb to 6.6 μm with 1% bismuth incorporation. Building on this, growth of optimized detectors with thicker InAsSbBi absorbers are underway and results will be presented at the conference.

This work was supported by the NSF (Award No. ECCS-1933836) and an NSF Graduate Fellowship (RCW). The work was performed at the UT MRC, a member of NNCI.

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2:30pm **NAMBE1-MoA-5 GePb Alloys Grown using Molecular Beam Epitaxy for Infrared Photodetector Applications**, *Tyler McCarthy, A. McMinn*, Arizona State University; *X. Liu, R. Hossain, X. Qi*, Arizona State University; *Z. Ju*, Arizona State University; *Y. Zhang*, Arizona State University
The Group-IV material system, Si, Ge and their alloys, has been one of the most widely used and researched material families in the semiconductor industry for over half a century. The addition of α -Sn, the diamond cubic semiconducting form of Sn, over the last couple of decades has fostered new research into IR materials and novel techniques such as momentum(k)-space charge separation (k -SCS) for devices. The next evolution of Group-IV alloys is the inclusion of Pb as an exciting new alternative route for IR detectors, quantum materials, and high-speed electronic devices. GePb alloys are an especially promising candidate for k -SCS and as an alternative materials for high-speed field effect transistors, due to the indirect to direct bandgap crossover predicted to occur at approximately 1 to 3.4 % Pb and their higher electron mobility, respectively. Short-range order (SRO) effects are also predicted to occur in GePb alloys, altering their optical and electrical properties for a given composition.

DFT modeling has predicted that like the other Group-IV elements, Pb can have the tetrahedral sp^3 hybrid bonding required for diamond lattice structure formation, with an estimated lattice constant of 6.83 \AA . Similarly to Sn in the Ge-Sn system, there is low solid solubility of Pb in the Ge-Pb system (< 0.5 at.%). Due to this, obtaining single crystal alloys with high Pb concentrations has been challenging and will require non-equilibrium growth conditions, such as MBE.

Single crystal GePb alloys with Pb concentrations between 0.2 % to 7.2 % have previously been grown by pulsed laser-induced epitaxy (PLIE), magnetron sputtering, and a layer inversion thermal evaporator method, but there has not yet been work done by MBE. The MBE growth of single crystal GePb alloys on Ge(100) substrates is reported here. Effusion cells of Ge and Pb are used to control the flux ratio independently in a VG-V80 MBE system. The optimal substrate temperature is found to be near the thermocouple temperature of 300 $^\circ\text{C}$ based on HRXRD and RHEED characterization of the grown films. The RHEED pattern changes from the (2 x 2) of Ge to a (1 x 1) for GePb growths at 400 and 500 $^\circ\text{C}$. At 300 $^\circ\text{C}$ the

pattern changes to a streaky pseudo(4 x 2) that remains throughout the epilayer growth and for samples at 200 $^\circ\text{C}$ and lower, this pattern becomes spotty. SEM images show a large volume of Pb islands on the surface that form into either long trapezoidal rods or uniform droplets that coalesce as growth progresses. Raman spectrometry gives an estimated Pb composition near 1 % with only minimal change in Pb incorporation for a large change in the Ge:Pb BEP ratio.

2:45pm **NAMBE1-MoA-6 Temperature Dependent Optical Constants of Germanium-Tin Alloys**, *Amanda Lemire*, Tufts University; *K. Grossklaus*, MIT Lincoln Laboratory; *T. Vanderveelde*, Tufts University

Mid-infrared materials are desirable for applications in imaging, spectroscopy, telecommunications, and lasing. $\text{Ge}_{1-x}\text{Sn}_x$ alloys, which have a bandgap tunable by compositional changes and are compatible with existing Si processing techniques, are being developed for photonic devices providing infrared emission and detection. It is necessary for designing such devices to have accurate information on the optical properties of the material, including changes in response to composition and temperature. In this work, we present properties for alloys between 3.6% and 8.4% Sn at temperatures between liquid nitrogen and 200 $^\circ\text{C}$.

Three samples were grown on a custom-designed, dual-chamber, VG-90 MBE system. Approximately 100 nm films were deposited on Ge (001) wafers, using an effusion cell for Sn and electron beam gun for Ge. Film compositions were determined by high-resolution x-ray diffraction. The three samples contain 3.6%, 6.5%, and 8.4% Sn respectively. Optical properties were measured by a J.A. Woollam UV-visible spectroscopic ellipsometer fitted with a CRV-725V cryostat. Samples were cleaved and cleaned in dilute hydrofluoric acid to remove surface oxidation before insertion into the cryogenic stage. Data were collected at 50K intervals from 78K to 475K at energies between 0.39 eV and 4.12 eV. Scans were also taken of Ge for modeling purposes. The complex index of refraction was calculated from each data set. Band transition energies are found to decrease in energy as Sn content increases.

NAMBE

Room Cummings Ballroom - Session NAMBE2-MoA

Advances in In Situ Characterization

Moderator: *Zachary LaDuca*, University of Wisconsin - Madison

3:30pm **NAMBE2-MoA-9 Principal Component Analysis of Rheed as an Indicator of Process Change During Molecular Beam Epitaxial Growth**, *Kurt Eyink, Y. Zhang, K. Mahalingam, R. Bedford*, Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

Reflection high energy electron diffraction (RHEED) is a ubiquitous sensor used in the epitaxial growth of materials. It is routinely used to determine the surface phase present during growth but has also been used to extract many additional features such as: QD facet structures, surface roughness and strain relaxation to name a few. In addition to surface features, RHEED also possesses bulk components in the Kikuchi lines and therefore potentially linked to bulk material quality. In this presentation, we discuss Principle Component Analysis (PCA) applied to RHEED movies acquired during the growth of molecular beam epitaxy of GaAs(001). In particular we use of PCA on a series of images from a section of the growth and show the components determined in this section allow growth to be followed in subsequent images of the growth. In addition, we show these same components can be used to follow growth on a different wafer. We discuss changes which occur in RHEED due to the unique orientations every wafer has relative to the chamber/electron beam as well as the inability to exactly reproduce conditions such as focus, angle of incidence, and wafer orientation. Correction for these modifications need to be applied prior to projection onto existing PCA components however after application we demonstrate the ability to track growth under similar conditions to the first analysis. We also show that growths which deviates from this region cause an increase in residual using the projected images and show that this is a simple method to indicate when new processes are occurring.

3:45pm **NAMBE2-MoA-10 Automated Machine Learning of in-Situ RHEED Data Provides Real-Time Guidance for Materials Growth Optimization**, *Christopher Price, J. Munro*, Atomic Data Sciences; *G. Zhou, Y. Li, C. Hinkle*, University of Notre Dame

Achieving fine control of process feedback during bottom-up synthesis is critical to achieve repeatable synthesis of materials using commercially scalable methods. Composition is controlled by adjusting synthesis

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parameters, but the relationships between these adjustments and the resulting sample characteristics are only established after sample growth with ex-situ characterization such as XPS, and vary between individual hardware installations. Using automated feature extraction for in-situ reflective high-energy electron (RHEED) patterns, we show that quantitatively predictive relationships can be established between in-situ and ex-situ characterization (XPS measurements) based on small sets of labeled training points within a specific material system. Non-obvious but straightforward correlations are shown to be predictive in quantitatively estimating composition on par with expert XPS analysis. The compositional estimates from RHEED data collected during growth can be delivered fast enough to make real-time adjustments to materials processing and influence the synthetic output. In this work, we outline the workflow and show that this strategy generalizes across two different materials systems without retraining of the core feature extraction models. A reduction in ex-situ experiments and quasi-real-time feedback to offer more precise synthetic control is demonstrated. These relationships provide guidance to develop hardware-specific recipe adjustments to unlock fine-tuned control of materials synthesis.

4:00pm NAMBE2-MoA-11 On-the-Fly Analysis of RHEED Images During Deposition Using Artificial Intelligence, Tiffany Kaspar, Pacific Northwest National Lab; *J. Pope, S. Akers, H. Sprueill, A. Ter-Petrosyan, D. Hopkins*, Pacific Northwest National Laboratory

Modern synthesis methods enable the fabrication of an ever-expanding array of novel, non-equilibrium, and/or metastable materials and composites that may possess unique and desirable functionality. Thin film deposition by molecular beam epitaxy (MBE) can produce atomically precise (or nearly so) materials with a wide range of functional electronic, magnetic, ferroelectric/multiferroic, optical, and/or ion-conducting properties. We are working to employ artificial intelligence (AI)-accelerated analysis of in situ and ex situ data streams for on-the-fly feedback control of the MBE deposition process that will enable targeted synthesis of novel materials with desired structure, chemical stability, and functional properties. Here we present a machine-learning-enabled framework for analysis of reflection high energy electron diffraction (RHEED) pattern images in real time (one image per second). Our approach utilizes pre-trained neural networks for image preprocessing, statistical analysis to identify change points in the images over time, and network graph analysis methods to precisely identify and classify changes. We demonstrate this framework using RHEED images collected from the deposition of epitaxial oxide thin films such as anatase TiO_2 on $\text{SrTiO}_3(001)$. Advantages and disadvantages of our approach will be discussed, as well as its potential use as the basis for on-the-fly feedback control of deposition parameters.

4:15pm NAMBE2-MoA-12 The Development of Order and Interfaces During Oxide MBE Growth: Real Time X-Ray Diffraction Measurements, Hawoong Hong, *D. Fong, A. Bhattacharya*, Argonne National Laboratory

While the atomic structure of interfaces in complex oxide heterostructures created by epitaxial growth has been investigated extensively, few studies have been conducted on how interfaces form at the initial stage of film growth. The dynamic aspects of the growth behavior can strongly influence the final interfacial atomic structure, which may lead to the emergence of interface-specific properties. Here, the structural development of La_2CuO_4 thin films grown by molecular beam epitaxy on a LaSrAlO_4 substrate is investigated by X-ray diffraction measurements with rapid scans over a volume of reciprocal space in addition to fixed-point measurements. The results show that the atomic structure of the interface becomes fully established after just a single unit cell growth; afterwards, changes occur only within the topmost half- to one unit cell of the growing film. However, diffraction intensity oscillations from simultaneous reflection high energy electron and X-ray measurements stabilize only after the growth of two unit cells, indicating that the growth front morphology continues to evolve until the start of the third unit cell. Our multimodal investigation provides new insights into the atomic processes of layered oxide interface formation, such information can be relevant to the engineering and optimization of functional layer structures.

NAMBE

Room Cummings Ballroom - Session NAMBE3-MoA

Late News I

Moderator: John McElearney, Tufts University

4:30pm NAMBE3-MoA-13 James S. Harris MBE Scientific Discovery Awardee Talk: MBE Growth of GaN: From Novel Growth to Record Performance Materials and Devices, James Speck, University of California, Santa Barbara

By the mid-to-late 1990s, growth of GaN by MBE was in disarray with little promise of realization of materials with quality comparable to those already developed MOCVD. In this presentation, we provide an overview of the progression of plasma-assisted MBE (PAMBE) and NH_3 growth of GaN. The highest quality materials in PAMBE growth are typically realized with a saturated chemisorbed metal adlayer ($\sim 2 - 2.5$ ML of Ga) on the surface. Challenges with metal droplet formation can be suppressed by metal modulated growth in which periodic growth interrupts or reduced Ga flux suppress the formation of large Ga droplets. Record electron mobilities were realized by higher temperature growth in the intermediate growth region. Many of features of today's GaN HEMTs were developed by PAMBE including the widely used AlN interlayer at the AlGaN/GaN interface to reduced alloy scattering and compositional grading to realize three dimension electron gases (3DEGs) on gradients in electrical polarization. NH_3 MBE has been extensively for both lateral and vertical devices. Highlights of NH_3 work include record electron mobilities, outstanding pn junctions with record low ideality factor.

5:00pm NAMBE3-MoA-15 Interfacial Misfit Arrays in Ternary III-V Compounds for Virtual Substrates on Si with Arbitrary Lattice Constant, Trent Garrett, Boise State University; *J. Rushing*, Tufts University; *J. Tenorio*, Boise State University; *P. Simmonds*, Tufts University

Lattice constants of the III-V semiconductors range from 5.45 Å (GaP) to 6.48 Å (InSb). III-V semiconductors are grown on commercially available substrates made from binary III-V materials (e.g., GaAs, InP, and GaSb), or group IV materials (e.g., Si or Ge). These substrates offer very high quality, but only offer access to a small number of specific lattice constants. Given this constraint, it is desirable to develop growth methods that allow the grower to modulate from the substrate lattice constant into the lattice constant of the material structure under investigation.

Structures lattice-mismatched to these substrates can be challenging to grow due to the deleterious effects of strain relaxation on their electronic and optical properties. One way to overcome this limitation uses metamorphic buffers to gradually adjust the lattice constant from that of the substrate to that of the desired III-V compound. Metamorphic buffers are frequently much thicker than the device structure grown on top, adding time and expense to the overall growth.

An alternative way to accommodate lattice mismatch involves interfacial misfit (IMF) arrays. These 2D networks of 90° misfit dislocations lie in the substrate/III-V interface and efficiently relieve the strain. Careful control of this process can limit the density of 60° threading dislocations extending away from the interface, helping protect the quality of layers grown above. To date, the IMF process has been studied in only a few "virtual substrate" systems, notably GaSb on GaAs and on Si, which crucially both still only offer access to a fixed lattice constant of ~ 6.1 Å.

Motivated by producing virtual III-V substrates with any lattice constant, we have expanded the IMF approach to enable growth of ternary compounds. Due to the benefits of Si substrates (availability, cost, scalability, and ease of integration with Si electronics) we chose as a starting point the GaSb-on-Si IMF system. For lattice constants > 6.1 Å we have explored IMF-based MBE growth of ternary $\text{Al}_{1-x}\text{In}_x\text{Sb}$ and $\text{Ga}_{1-x}\text{In}_x\text{Sb}$ compounds directly on Si substrates. Similarly, for lattice constants < 6.1 Å we have explored IMF-based $\text{AlSb}_{1-x}\text{As}_x$ and $\text{GaSb}_{1-x}\text{As}_x$ grown on Si. By varying their composition, we have grown ternary buffers with lattice constants ranging from 6.05 – 6.4 Å. We will present preliminary results discussing their structural properties.

We believe this approach will produce high quality, ternary III-V-on-Si virtual substrates. By choosing the lattice constant in advance, these virtual substrates will enable users to grow a wide range of III-V structures without strain, impacting device applications from LiDAR to LWIR.

NAMBE

Room Cummings Lobby - Session NAMBE-MoP

NAMBE Poster Session

NAMBE-MoP-1 Synthesis and Characterization of Molybdate Pyrochlore Thin Films, Kyeong-Yoon Baek, M. Anderson, C. Brooks, J. Mundy, Harvard University

The molybdate pyrochlore oxides, $R_2\text{Mo}_2\text{O}_7$ (R = rare earth), form a series of compounds where there is a transition from a ferromagnetic metal to a spin glass insulator as a function of the R^{3+} radius [1]. To date, most of the work on this family of materials has been on bulk polycrystalline samples [2]. In this work, we synthesized pyrochlore $\text{Gd}_2\text{Mo}_2\text{O}_7$ and $\text{Tb}_2\text{Mo}_2\text{O}_7$ in thin-film form using reactive oxide molecular-beam epitaxy; in the bulk samples, $\text{Gd}_2\text{Mo}_2\text{O}_7$ and $\text{Tb}_2\text{Mo}_2\text{O}_7$ are a metallic ferromagnet and an insulating spin glass, respectively, both sitting adjacent to the phase boundary. The crystal structure of our films is confirmed through X-ray diffraction and scanning transmission electron microscopy. Electric transport measurements exhibit the insulating behavior of both films and magnetic ground states are confirmed through SQUID measurements. Our work continues to explore phase boundary of molybdate pyrochlore oxides by thin-film deposition.

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NAMBE-MoP-2 Growth of InGaBiAs for Extended Short Wave Infrared Photodetectors, Mrudul Parasnis, J. Bork, M. Islam, A. Razi, N. Babikir, J. Phillips, J. Zide, University of Delaware

Dilute bismuthides are a class of highly mismatched alloys consisting of small amounts of bismuth incorporation in III-V semiconductors.¹ This incorporation of bismuth, due to its larger size compared to other elements within the host matrix, induces valence band anticrossing, thereby reducing the bandgap.² For this reason, dilute bismuthides are explored as a class of materials in optoelectronic devices such as infrared photodetectors.^{2,3,4}

Previous studies have shown that InGaAs based photodetectors have a wavelength of 1.7 μm . Bi incorporation in InGaAs reduces bandgap by 56meV/%Bi.³ In our work, we aim at optimizing InGaBiAs to establish it as a promising material in the intrinsic region of shortwave infrared photodetectors and extend the wavelength beyond 1.7 μm . Growth of dilute bismuthides is a challenging process. Hence, we are using molecular beam epitaxy to grow InGaBiAs at low temperatures of 265 $^\circ\text{C}$ (as measured by band-edge thermometry) and near-stoichiometric conditions. Be:InGaAs as a capping p-type layer and Si:InGaAs as a n-type layer are grown at 490 $^\circ\text{C}$ for infrared photodetectors. In our work, we show that 1.5%Bi incorporation in InGaBiAs extends the wavelength up to 1.8 μm . We are also studying the recombination lifetime of the carriers in InGaBiAs using optical pump terahertz probe spectroscopy. The optimization of Bi in InGaBiAs to give longer wavelengths and higher recombination lifetimes is currently ongoing research.

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NAMBE-MoP-3 Investigating the Influence of Bismuth Surfactant on InSb Thin Films for Mid-Infrared Devices Applications, Pan Menasuta, J. McElearney, Tufts University; K. Grossklauss, Lincoln Lab; T. Vandervelde, Tufts University

Indium antimonide (InSb) possesses a narrow direct bandgap, 0.17eV at 300K, facilitating efficient absorption and conversion of infrared photons in the mid-wave infrared (MWIR) spectrum. Consequently, InSb detectors demonstrate high sensitivity in thermal imaging, spectroscopy, and astronomical observation. Recently, there has been notable interest in employing bismuth as a surfactant during the epitaxial growth of many III-V material systems. A very low bismuth flux can modify the ad-layer surface and eventually desorb, leading to improved surface morphologies across multiple materials. However, no studies on Bi surfactancy have been conducted on MBE-grown InSb thin films. This work aims to document the effects of Bi surfactancy on InSb growth across a range of temperatures. We have recently shown that the Bi surfactant can substantially modify the morphology of GaSb thin films over a broad spectrum of growth temperatures. Given the significance of surface morphology control in multilayer epitaxial growth, especially those that require high-quality InSb

layers, understanding its influence is crucial. Additionally, the systematic characterization of homoepitaxial InSb surfaces holds value for the MBE community.

Two series of homoepitaxial InSb(100) thin films are grown via molecular beam epitaxy (MBE) on an InSb(100) substrate over a range of growth temperatures. All other growth parameters remain identical. The first set serves as a control, while the second are grown under Bi surfactancy. Surface characterization is conducted using atomic force microscopy (AFM), and scanning electron microscopy (SEM) coupled with energy-dispersive X-ray spectroscopy (EDS) to analyze large features and elemental distribution. Raman spectroscopy and variable-angle spectroscopic ellipsometry (VASE) are employed to detect alterations in lattice and optical properties induced by the surfactant. Finally, high-resolution X-ray diffraction (HRXRD) is performed to detect any potential Bi incorporation. This study seeks to assess the effects of Bi surfactancy on the surface morphology and material properties of InSb thin films, potentially contributing to the advancement of next-generation MWIR detectors with improved performance for diverse applications.

NAMBE-MoP-5 Si / TiN Backside Thermal Absorbers for MBE Growth on Transparent Substrates, D. Scott Katzer, M. Hardy, N. Nepal, E. Jin, D. Meyer, V. Wheeler, US Naval Research Laboratory

Efficient, controlled absorption of thermal radiation from the MBE system substrate heater into the growth substrate continues to be a technological challenge [1]. This problem is especially difficult for the case of wide- and ultra-wide bandgap (WBG and UWBG) semiconductors where near IR absorption is low and growth temperatures exceeding 1000 $^\circ\text{C}$ may be required for high quality epitaxy. UWBG semiconductors are attracting increased attention for high power density RF electronics and other applications, so addressing the practical MBE growth temperature issues is important. In addition, a commonly-used method to increase IR absorption by using thick, opaque, specular backside metal layers can be detrimental to substrate temperature monitoring with diffuse reflectance [1,2], so a different approach is needed.

Woltersdorff [3] showed that in the far IR where the optical constants n and k are both large for metals, the maximum absorption is 50% for a thin metal film that has a sheet resistance of half that of the characteristic impedance of free space, namely $377/2 = 188.5$ ohms/sq. Thus, one would expect that the ideal thickness of a thermal absorbing layer to depend on the wavelength range and the absorbing layer properties, and that thick layers may be counter-productive for efficient heating.

Here we report our recent work in modeling and experiments using thin stacks of silicon (Si) on titanium nitride (TiN) to greatly increase the thermal absorption of WBG SiC substrates during MBE growth. Modeling with the Python software package WPTherml [4] indicates that a 100 nm thick Si layer on a 9 nm thick TiN layer increases the peak absorbance of IR from a 1000 $^\circ\text{C}$ blackbody substrate heater to over 58%. We used a similar thin layer stack on a 4H-SiC substrate and a substrate heater temperature of 1100 $^\circ\text{C}$ to efficiently heat the substrate to a real temperature of ~ 1000 $^\circ\text{C}$ (hundreds of degrees hotter than bare SiC [1]) as revealed by a bright $\text{Ö}3 \times \text{Ö}3$ R30 $^\circ$ RHEED pattern [5], showing the value of this approach.

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NAMBE-MoP-6 Verification of Epitaxially Grown InAs/GaSb Topological Insulators using Spectroscopic Ellipsometry, Lawrence Qiu, P. Simmonds, J. Rushing, X. Xie, Tufts University

The theoretical and practical implications of topological materials have captured intense research interest. Topologically nontrivial phases emerge from the crossing of electron and hole band energies, resulting in novel phenomena like topologically protected surface states. Established topological insulators like Bi_2Se_3 rely on spin-orbit-coupling to induce band crossing, limiting configurability and requiring exotic materials. Topological insulators based on widely used III-V materials would simplify the creation of hybrid topological/semiconductor devices. Topologically nontrivial

phases have already been demonstrated in the broken gap InAs/GaSb material system. We hope to achieve a tunable topological phase change in III-V quantum wells by carefully adjusting their widths to tailor the confined electron and hole states and inducing band inversion.

Quantum well behavior is sensitive to aspects of the epitaxial growth process, such as growth rate variations, composition inaccuracy, impurity contamination, and poor interface quality. Topological insulators based on quantum wells are especially sensitive to thickness imperfections because they emerge from the configuration of relative and absolute electron and hole energies. Single digit variations of the monolayer count can induce topological phase change, so confirming that the intended structure was grown is an essential step in understanding the behavior of novel quantum well-based topological insulators.

Spectroscopic ellipsometry is an established method of confirming sample structure and composition through the nondestructive survey of device optical properties. We report the use of spectroscopic ellipsometry in characterizing InAs/GaSb quantum well structures. These structures consist of a GaSb buffer that includes a superlattice for improved active region quality, an AlSb bottom barrier, a GaInSb quantum well, an InAs quantum well, an AlSb top barrier and a GaSb cap. Such a complex structure increases the degrees of freedom for an ellipsometer thickness measurement, and makes single layer changes subtle and unpredictable. Additional difficulties for these measurements include the use of a previously uncharacterized GaInSb ternary compound and variations between samples grown on (001) and (111) substrates. We will show how the careful use of ellipsometry can give us useful information about these growths without the need for costly and time consuming tunneling electron microscopy.

NAMBE-MoP-7 Investigation of Tunable Parameters Influence in InAs/GaSb Quantum Wells Heterostructure, Xikai Xie, P. Simmonds, Tufts University

Quantum spin Hall insulators (QSHIs) are advanced materials with topologically protected surface states that allow electronic transport without scattering from defects. QSHIs with a large energy gap in the topological phase are of great interest for development of both quantum and electronic devices. The ability to control the topological phase transition in a QSHI would represent a functional improvement for applications that require in-situ tunability of the material's topological properties such as spintronics and fault-tolerant quantum computing.[1]

It is possible to induce topological states in III-V semiconductor quantum wells with a brokengap band alignment and use quantum well width to adjust the size of the hybridization energy gap. We are therefore interested in investigating the topological phase transition in InAs/GaSb quantum well heterostructures varying different structural parameters. By simulating band topology and topological invariants we can observe changes in wavefunction in k-space and control the quantized responses of the material.[2] Two key parameters that shape a material's band structure are symmetry and strain. We compare (001)- and (111)-oriented III-V semiconductor quantum well heterostructures under both compressive and tensile strain to explore their effects on the emergent topological states.

QSHIs consisting of InAs/GaSb quantum well heterostructures are considered since by changing the well widths and gate voltage we can control the degree of band inversion and corresponding topological properties.[3] The ability to tune the strain in these structures by varying the composition of the ternary GaInSb quantum well can enhance the size of the hybridization gap energy between the topological states compared to QSHIs based on binary InAs/GaSb QWs.[3]

We have therefore carried out computational simulation to investigate InAs/GaSb double quantum well heterostructures with both (001) and (111) crystalline orientations.[4] We will present our results that show the influence of tunable parameters such as quantum well width and strain on topological band structure.

Furthermore, given the result of our computational work, we can create these structures with molecular beam epitaxy (MBE) down to monolayer precision. This precise control enables us to adjust the quantum well widths and strain levels, to influence topological properties of the InAs/GaSb quantum wells. We anticipate that MBE's high degree of control over the deposition of our simulation parameters will lead to the realization of QSHIs with optimized performance for applications in spintronics and quantum computing.

NAMBE-MoP-8 Exploring In situ Aluminum Deposition Kinetics on InSb Substrates for Hybrid Superconductor/Semiconductor Materials Systems, A. Elbaroudy, Alan Tam, University of Waterloo, Canada

Hybrid Superconductor/Semiconductor (SP/SE) structures play an important role in condensed matter and mesoscopic physics, particularly in topological quantum computing aimed at realizing Majorana Zero Modes. Aluminum growth on InAs or InSb quantum wells using Molecular Beam Epitaxy emerges as the most promising direction due to the high electron mobility and strong spin-orbit interactions within these wells. Nevertheless, achieving a thin, continuous Al layer (~10 nm) poses challenges in standard MBE systems due to Al's high surface mobility in ultra-high vacuum environments and its tendency for 3D nucleation.

We have demonstrated that a thin, continuous Al layer can be successfully grown on an InGaAs surface at temperatures above room temperature using a high Al-growth rate of 3 Å/s [1]. In the current study, we compare this process with the growth of Al on a homomorphic epitaxial InSb surface. In-situ RHEED studies reveal similar Al behaviors on both surfaces. Regardless of the semiconductor surface used, 3D nucleation occurs after the initial Al monolayers for both growth rates tested (0.1 and 3 Å/s). With a growth rate of 0.1 Å/s, the 3D growth mode dominates throughout the deposition of the nominal 10 nm of Al. In contrast, at the Al growth rate of 3 Å/s, the initial 3D nucleation RHEED pattern quickly transitions to a streaky pattern, indicating the coalescence of Al islands and a shift to 2D growth for both InSb and InGaAs surfaces.

Surface morphology inspections with SEM and AFM of the samples grown at 0.1 Å/s reveal a similar discontinuous layer of Al islands, regardless of the semiconductor surface type. For InGaAs surface, faster deposition rates consistently result in a 2D Al layer. However, for the InSb surface, 2D morphology is preserved only for Al deposition on InSb with Sb-rich surface reconstruction, while growth on Sb-depleted reconstruction, despite showing 2D growth mode during deposition, was found to have a distinct 3D morphology when inspected with SEM. Most likely, the dewetting process took place at some point after finishing Al deposition, before moving the wafer out of the MBE system.

For both InSb and InGaAs surfaces, the 3D to 2D growth mode transition is abrupt and is governed by the interplay between the wafer's thermal trajectory and the Al deposition rate. We will discuss the temperature evolution during and after Al deposition, as monitored with band-edge thermometry. Detailed surface morphology and interface characterization using SEM, AFM, and STEM will also be addressed during the presentation.

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NAMBE-MoP-9 Phases Control of Epitaxial MnTe through Buffer Layers, Yuxing Ren, H. Huang, L. Tai, Q. Tao, K. Wang, University of California at Los Angeles

MnTe is one of the 3D semiconductors that can exhibit anomalous Hall effect. The potential edge states correlated with the alter-magnet properties in the α -phase MnTe is also under study these days. The epitaxial growth becomes one method to tune the electronic structure. In this work we have grown both α -phase and β -phase MnTe by Molecular Beam Epitaxy on GaAs (111) and sapphire (0001) substrates with different buffer layers.

While in bulk crystal MnTe α -phase is the most stable state at room temperature, in the epitaxial structure β -phase MnTe can also be achieved in the as-grown thin films without post-growth annealing. On GaAs (111) substrates α -phase MnTe are naturally favored without any buffer layer. When using Bi₂Te₃ series TI (topological insulators) the buffer layers on sapphire (0001) substrates, we found out that β -phase MnTe are favored over pure Bi₂Se₃ due to the smaller lattice mismatch. However, when we add some alloy effect to the buffer layer, though the lattice mismatch is still smaller in β -phase, α -phase is actually grown. This unveil the role of the entropy effect and the changed in the surface potential. The nanorods structure in MnTe α -phase can also be controlled by buffer layer control and a CrSe_x layer under it.

NAMBE-MoP-10 Self-Bias Bi-Directional Photocurrent Switching Effect in Epitaxial GaN-NWn, PARGAM VASHISHTHA, RMIT University, Australia; G. Gupta, CSIR-National Physical Laboratory, India; S. Walia, RMIT University, Australia

Conventional optoelectronic devices face limitations when serving as a single detector for broadband and narrow-band applications due to their one-way photocurrent, restricting their potential uses in photodetection.

Monday Evening, July 22, 2024

However, a promising solution is emerging: bi-directional photocurrent switching. This advancement opens doors to unique functions like optical logic operations. We design an epitaxial GaN nanowall network-based ultraviolet bidirectional photocurrent photodetector. By introducing the different surface potential-induced photocurrent switching effects, the photocurrent direction can be switched in response to the wavelength of incident light at 0V bias. In particular, the photocurrent direction exhibits negative when the irradiation wavelength is less than 285 nm, but positive when the wavelength is longer than 285 nm. Special logic gates in response to different dual UV light inputs are proposed via a single bipolar PD, which may be beneficial for future multifunctional UV photonic integrated devices and systems.

NAMBE-MoP-11 Systematic Study on Synthesis of High Quality SnTe Layers by Molecular Beam Epitaxy, Qihua Zhang, M. Hilsse, J. Gray, M. Stanley, N. Samarth, S. Law, Pennsylvania State University

Tin telluride (SnTe) is a narrow bandgap semiconductor which has many attractive properties, such as in-plane ferroelectricity, good thermoelectric performance, and a topological crystalline insulator (TCI) band structure.¹ In addition to these properties, SnTe also serves as an important buffer layer for developing Te-based heterostructures for magneto-transport devices.² Despite such promises, there have been few investigations focused on understanding the optimal epitaxial growth conditions for SnTe layers, which has led to poor surface morphologies and/or low crystallinity in synthesized films.³ A major challenge in the growth of thin film SnTe is the lack of suitable substrates, owing to the rock-salt crystal structure of SnTe and the large lattice mismatch with common substrates.

In this study, we report on the molecular beam epitaxy (MBE) growths of SnTe(111) layers on InP(111)A substrates. We have conducted a detailed investigation of the surface morphology and film crystal quality based on growth parameters including substrate temperature, Te/Sn flux ratio, and film growth rate. Despite the 7.4% lattice mismatch between the film and substrate, we found that a narrow substrate temperature range from 300 °C to 340 °C, a Te/Sn flux ratio of ~3, and a growth rate of 0.48 Å/s yield both smooth and single-crystalline SnTe(111) layers with thicknesses ranging from 10 nm up to 800 nm. Using these conditions, fully coalesced and smooth SnTe layers with root-mean-square (rms) roughness as low as 0.3 nm (Fig. 1a) can be obtained. The as-grown SnTe layer is free of rotational twin domains (Fig. 1b) and has exceptional crystal quality, including a full-width-at-half-maximum (FWHM) value as narrow as 0.06° from x-ray diffraction (XRD) rocking curves (Fig. 1c). Reciprocal space mapping confirms that thin (15 nm) SnTe layers are fully relaxed. Detailed transmission electron microscopy (TEM) imaging suggests that formations of In-Sn-Te nanoclusters during substrate annealing in a Te environment prior to growth aids strain relaxation as well as improves crystalline quality (Fig. 1d). Finally, preliminary angle-resolved photoelectron spectroscopy further indicates the three-fold symmetry of SnTe (111) layer at the Γ point, as well as Fermi level located 0.19 eV below the Dirac point. These promising results lay the foundation for employing SnTe on InP as a platform for developing all-telluride heterostructures integrated with III-V semiconductor devices.

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[2]DOI:10.1038/ncomms11623.

[3]DOI:10.1002/pssa.202200555.

NAMBE-MoP-14 In Situ Curvature Measurement: A Great Breakthrough for MBE Growth Monitoring, Romain Bruder, Y. Rousseau, RIBER, France

As a long-known high performance epitaxial technique, Molecular Beam Epitaxy has experienced several major innovation across the past 50 years. Epitaxy recipes complexity has gradually increased to obtain advanced structures and devices thanks to the unique MBE capabilities. To cover this complexity, numerous monitoring probes and communicating devices (pumps, valves, gauges, thermocouples,...) have gradually been used on the reactors.

Nowadays, the MBE process is integrating additional class of optical in situ real time measurement techniques, including curvature / bowing monitoring.

Based on Magnification Inferred Curvature principle, Riber developed a dedicated curvature instrument on the basis of a CNRS-LAAS Toulouse patent. Named EZ-CURVE®, this instrument aims at giving insight in real-time about the growth process: it enables investigations at the growth mechanisms level for fundamental and applied research purposes, or

alternatively, it can help evaluating process repeatability and stability without requiring detailed knowledge of all growth parameters.

This talk will give recent examples of EZ-CURVE users' cases for different class of materials (arsenides, antimonides, phosphides, others,...), and highlight the capability of such an approach to quickly converge on process optimization and monitoring.

NAMBE-MoP-15 Synthesis and Transport Properties of Doped Samarium Nitride Thin Films, Kevin Vallejo, Z. Cresswell, B. May, V. Buturlim, S. Regmi, K. Gofryk, Idaho National Laboratory

Lanthanide-based nitride compounds are an understudied group of materials compared to lanthanide oxides. Their 4f electron shell gives rise to a variety of interesting physics such as unconventional superconductivity. Samarium nitride (SmN) has been recently identified as a material where ferromagnetic order and p-type superconductivity coexist. Our team will present results on the growth conditions of pure and doped SmN using molecular beam epitaxy, and its electronic transport properties as a function of temperature and magnetic field. The team used an yttria-stabilized zirconia (YSZ) substrate in the (001) crystallographic direction. After outgassing and removal of the native oxide, substrates were heated to 600°C and Sm and N were deposited for 60 minutes. Sm films deposited under similar conditions oxidized immediately upon contact with the air, while optimized SmN films avoided these samarium oxide peaks. Substrate temperature during growth of SmN films heavily influences the level of oxidation upon removal from the vacuum environment. The films have so far not been confirmed to be single crystalline due to the presence of SmN(111) peaks. AC magnetic susceptibility studies have shown the oxidized sample to be mostly paramagnetic, with a potential superconductive transition around ~10 K. Doping effects on crystal structure and electronic properties are characterized.

NAMBE-MoP-16 Tunable Ordering of 2D Tin on Silicon, Caitlin McCowan, S. Misra, Sandia National Laboratories

The atomic site-to-site correlations of a binary alloy can determine its optical and electronic properties. A direct bandgap is theoretically expected to occur in group IV alloys composed of silicon, germanium, and tin. However, an indirect bandgap is observed experimentally, which is thought to be caused by short range order (SRO). The atomic organization of thin films is determined by a combination of deposition rates, temperature, and templating effects of the substrate. The characterization needed for visual representation is made further arduous due to the atomic-scale nature of these factors. Here, using scanning tunneling microscopy (STM), we visualize step-by-step growth of Sn on Si *in situ* by separately controlling sub-monolayer growth and sample heating.

This work aims to understand the impact that SRO has on a material's electronic properties through systematic characterization. While long-range ordering of monolayers of Sn has been observed on Si and Ge substrates in both 100 and 111 orientations, the impact of temperature and film thickness on SRO remain unknown. Additionally, surface segregation of Sn depends strongly on annealing, which is expected to influence SRO. We use *in situ* STM to analyze growth in a series of steps that include Sn deposition, Si deposition, and various annealing stages to probe the dynamics of thin film growth at the substrate interface. By discretizing the growth process, we create regions of metastable ordering that can be dynamically tuned throughout investigations, improving our ability to relate growth conditions to SRO and, correspondingly, to a material's optical and electronic properties.

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NAMBE-MoP-17 Continuous Wave Lasing from Individual InAs Nanowires, Steffen Meder, Technical University Munich, Germany

Extending the emission wavelengths of monolithically integrated nanowire (NW) lasers to longer wavelengths and even the mid-infrared (MIR) spectral range, shows great promise for optical on-chip communication and sensing applications using the mature silicon photonic circuit platform. Strong absorption within the visible range in silicon waveguides necessitates the integration of lasers with wavelengths in the near- or mid-IR for low-loss optical transmission. While examples of NW lasers have been shown with emission in the near [1] to mid-infrared [2], few operate under continuous wave operation necessary for on-chip processors.

In this work, we report on the mid-infrared continuous wave lasing of individual InAs nanowires at cryogenic temperatures. Figure 1a shows finite difference time domain simulations of the diameter dependent threshold

gain, that allow us to determine the optimal nanowire geometry. Catalyst-free InAs NWs are grown site-selectively and with high homogeneity on SiO₂-templated Si(111) substrates via molecular beam epitaxy, whereby the diameter and length is tuned from 160-745nm and 6-28µm by varying the pitch and growth durations (Fig 1c). Under optical pumping with a 976nm continuous wave laser, stimulated emission is demonstrated for individual NWs transferred on a sapphire substrate with diameters of 745±55 nm and nanowire resonator lengths between 10-30 µm (Fig 1b). Typical lasing thresholds are found to range from 2-30 kW/cm² with emission wavelengths of 2.4-2.7µm (0.455-0.515eV).

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NAMBE-MoP-18 Impact of Growth Temperature on the Formation of AlGa_N During the MME Growth of AlN/AlGa_N Short Period Superlattice Structures, *Alexander Chaney, S. Mou, K. Averett, T. Asel*, Air Force Research Laboratory, Materials and Manufacturing Directorate, USA

We have previously shown that AlN/Al_xGa_{1-x}N short period superlattices (SPSL's) can be formed through the introduction of a constant Ga overpressure during the metal modulated epitaxy (MME) growth of AlN. It was found that when a growth temperature of 830 °C was used, the incorporation of Ga into the layer structure was limited due to the final stages of Al consumption due to Ga adatom desorption. As a result, the lowest Al composition in the Al_xGa_{1-x}N layers obtained was 72% for a Ga BEP of 1x10⁻⁶ Torr. For this work, the impact of Ga adatom desorption on the formation of the AlGa_N layer was investigated in order to realize the growth of AlN/GaN SPSL's. In this study, a series of 3 growths was done where substrate temperatures of 800 °C, 760 °C or 730 °C were used. Outside of the variations in substrate temperature, Al, Ga and N fluxes were kept constant for each sample. Shutter conditions were chosen such that the Ga shutter opened only after complete consumption of Al on the surface had occurred. This removes any potential influence that Al adatoms have on Ga. Comparing XRD coupled scans of each sample showed that the 0th order peak shifted to lower ω-2θ angle as the growth temperature was lowered. However, the position of the higher order peaks remained mostly unchanged. Therefore, while there was a reduction in the Al composition of the Al_xGa_{1-x}N layers, the overall SPSL period remained mostly unchanged. This was confirmed by STEM imaging, which found that for all 3 samples, the AlN had a thickness of ~ 5 nm while the Al_xGa_{1-x}N had a thickness of ~3 ML. By inserting the thickness values determined by STEM into XRD simulations it is possible to determine the Al content in the Al_xGa_{1-x}N layers. For the growth temperatures of 800 °C, 760 °C, and 730 °C, the resulting Al composition was calculated to be 84.3%, 66% and 52.5% respectively. These results represent the lowest Al content we have achieved using MME to date. However, the fact that no GaN formed serves to highlight that the current model explaining the formation of Al_xGa_{1-x}N is incomplete. Fully fleshing out this model will be the focus for continuation of this work.

NAMBE-MoP-19 Buffer Layer Approach for Smooth GaSe Epitaxial Films on GaAs (111) B, *Joshua Eickhoff*, University of Wisconsin; *M. Yu, M. Hilse, S. Law*, Penn State University; *D. Rhodes, J. Kawasaki*, University of Wisconsin - Madison

GaSe is a layered semiconductor with potential applications for single photon emission and for ultrathin field effect transistors. The quality of epitaxially grown GaSe critically depends on the roughness and chemical termination of the starting surface. Previous work reports improved GaSe film morphology on GaAs (111)B using a pre-growth surface selenization treatment of the de-oxidized GaAs (111)B (1). Here I will show that an epitaxially grown buffer layer of GaAs (111) B in conjunction with the surface selenium treatment results improved GaSe film quality, as determined by X-ray diffraction, Raman spectroscopy, and cross sectional TEM.

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NAMBE-MoP-20 Incorporating ErAs Into InGaAlBiAs Material by Interrupted Growth: Effects on Optical and Electronic Properties Targeting Terahertz Pulse Emitters and Detectors for Telecom Wavelength Excitation, *Wilder Acuna, W. Wu, J. Bork, M. Doty, M. Jungfleisch, L. Gundlach, J. Zide*, University of Delaware

Our study focuses on the growth of ErAs:InGaAlBiAs thin films using a digital alloy approach to achieve a bandgap of 0.8 eV suitable for telecom

wavelength excitation (1550 nm). This semiconductor thin film is the active layer within a photoconductive switch (PCS) designed for terahertz (THz) pulse generation and detection. Key to the performance of such PCSs are several intrinsic semiconductor properties, such as dark resistivity, carrier lifetime, and carrier mobility. The incorporation of ErAs nanoparticles within the InGaAlBiAs matrix significantly influences these properties. Beyond the solubility limit, erbium incorporation leads to the formation of ErAs nanoparticles, resulting in a decrease in the material's carrier lifetime. Additionally, ErAs nanoparticles exert a pronounced pinning effect on the effective Fermi level of the material, thereby impacting carrier concentration and, consequently, dark resistivity. The size of these nanoparticles impacts the position of the Fermi level, a parameter controlled through interrupted growth and migration-enhanced epitaxy due to constraints posed by the bismuthide matrix, necessitating lower growth temperatures.

Despite the requirement for relatively low growth temperatures (~280°C) for the bismuthide matrix, this system offers enhanced flexibility in tuning bandgap and band alignment while ensuring the growth of high-quality lattice-matched films on an InP substrate. The ability to manipulate band alignment facilitates positioning the Fermi level deep in the bandgap, thereby reducing carrier concentration and elevating dark resistivity. Moreover, the positioning of the Fermi level with respect to the band edges plays a pivotal role in carrier lifetime, affecting the efficacy of nanoparticles in trapping free carriers.

Different characterization techniques are employed to assess these pertinent properties comprehensively. Dark resistance is determined through the Hall effect and Van der Pauw measurements, while carrier lifetime is evaluated via optical pump THz probe spectroscopy. Optical bandgap measurements are conducted using spectrophotometry, and material quality is scrutinized through high-resolution X-ray diffraction analysis.

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NAMBE-MoP-21 Ferromagnetic Nanostructures Formation by Metal Modulated Epitaxy of AlN:Mn, *Jesús Fernando Fabian Jacobi, S. Gallardo Hernández, A. Conde Gallardo*, CINVESTAV, Mexico; *D. Olguin Melo*, CINVESTAV-Queretaro, Mexico; *Y. Casallas Moreno*, UPIITA - Unidad Profesional Interdisciplinaria en Ingeniería y Tecnologías Avanzadas IPN, Mexico; *M. Zambrano Serrano, M. López López*, CINVESTAV, Mexico

Diluted magnetic III-N semiconductors (DMSs) are promising for spintronic devices. Incorporating Mn atoms induces ferromagnetic behavior in III-nitride materials, notably AlN. Doping atoms during molecular beam epitaxy (MBE) growth process can significantly impact film properties. This study delves into the growth technique of AlN:Mn films using alternating Al and Mn atom fluxes, a technique known as metal modulated epitaxy (MME).

Samples were grown on Si (111) substrates utilizing a 200 nm thick AlN buffer layer grown at 850°C (Figure 1(a)) by MBE. Al and Mn atom fluxes were supplied from Knudsen-type effusion cells. Active Nitrogen (N) flux was provided by a rf-plasma source operating at 150 W with a N₂ flow of 0.25 sccm. The first set of samples employed a continuous growth method, simultaneously supplying fluxes of Al and Mn atoms along with Nitrogen. The second set of samples was grown using an alternating method, with the Al shutter opened for 5 s followed by Mn shutter for 1 s, with a 3 s pause in between, while the Nitrogen flux was constant. The alternated shutters sequence during the growth process are depicted in Figure 1(b). The continuous growth utilized a growth temperature of 750°C, while the alternating method employed 720°C. In both samples, the Al flux was set at BEP_{Al}=2×10⁻⁷ Torr and the Mn flux at BEP_{Mn}=5×10⁻⁹ Torr.

Reflection High-Energy Electron Diffraction (RHEED) patterns revealed that continuous growth process yielded a surface with flat regions with some 3D features, evident from the combination of linear and spotty patterns (Fig. 2(a)). In contrast, the alternating growth process resulted in a completely spotty RHEED pattern, indicating nanostructure formation, as depicted in Fig 2(b). This observation was corroborated by AFM micrographs (Fig. 3), showcasing flat regions in the continuous growth method, and nanostructures formation for the alternating growth process. From AFM measurements we estimated the size of the AlN:Mn nanostructures of 30 nm in height with a base of 80 nm. Moreover, we confirmed that Mn atoms induced ferromagnetic behavior in the material. As illustrated in Fig. 4, magnetization curves exhibited clear hysteresis at 300K, with no

diamagnetic signal in either case, and stronger magnetic moments observed in nanostructured samples.

In conclusion, supplying alternating fluxes of Al and Mn atoms facilitates the formation of AlN:Mn nanostructures exhibiting ferromagnetic behavior at room temperature, with higher magnetic moment intensity compared to samples prepared by the continuous growth process. Thus, an alternative approach for forming ferromagnetic nanostructures is presented.

NAMBE-MoP-22 Ultralow Threshold Surface Emitting Ultraviolet Lasing by Low-Temperature Selective Area Epitaxy of GaN Nanowires, *M. Vafadar, Songrui Zhao*, McGill University, Canada

Surface emitting lasers have become indispensable in our everyday life, with applications in a wide range of fields from optical communications and data transmission to medical diagnostics and therapeutics. While surface emitting lasers in the near-infrared (NIR) range are relatively mature, progress in the development of GaN based surface emitting lasers operating in the ultraviolet (UV) range has been sluggish. To mitigate various issues related to conventional vertical cavity surface emitting lasers (VCSELs) such as material quality, mirror reflectivity, and so on, nanowire photonic crystals (NPCs) have received increasing attention over the past few years for surface emitting lasers. NPCs offer a promising approach by simplifying the design of the lasing cavity in which utilizing the photonic band edge mode at the Γ point in a photonic crystal structure can produce optical gain through the formation of slow light and further achieve light emission from top surface when proper diffraction condition is satisfied. However, for these lasers, the formation of NPCs often requires selective area epitaxy (SAE) at high substrate temperatures on patterned substrates. Such a high substrate temperature could affect the NPC formation and lasing performance.

Herein, we demonstrate ultralow threshold surface emitting lasing in the UV range by exploiting molecular beam epitaxy (MBE) grown GaN NPCs using low-temperature SAE regime, which offers an unprecedented controllability of nanowire formation on patterned substrates (Figure S1a). Utilizing GaN NPC arranging in a square lattice with a center-to-center spacing (a) of 200 nm and a nanowire diameter (d_{nw}) of 173 nm, UV SE lasing at ~ 367 nm is measured with a threshold of merely 7 kW/cm² (Figure S1b), a 100 \times reduction compared to the conventional AlGaAs UV VCSELs at a similar wavelength (Figure S1c). Further developments on such GaN based surface emitting UV lasers will also be reported in the conference.

NAMBE-MoP-23 Trade-Off between Hall Sensitivity and Frequency Limit of Two-Dimensional Electron Gas III-Nitride Hall Effect Sensor, *Satish Shetty*, Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, AR, 72701, USA; *A. Hassan*, Department of Electrical Engineering, University of Arkansas, Fayetteville, AR, 72701, USA; *Y. Mazur*, Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, AR, 72701, USA; *H. Mantooth*, Department of Electrical Engineering, University of Arkansas, Fayetteville, AR, 72701, USA; *G. Salamo*, Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, AR, 72701, USA

We investigated the tradeoff between Hall sensitivity and frequency limit of an AlGaIn/GaN two-dimensional electron gas Hall effect sensor. For this study, we utilized three different heterostructure designs that had variations in sheet carrier density, carrier mobility, sheet resistance, and capacitance. The heterostructure designs used for fabricating Hall sensors are capable of operating at high temperatures. The efficiency of Hall sensor quantified in terms of supply voltage-related sensitivity (SVRS) is 0.024, 0.044, and 0.051 T⁻¹, while the supply current-related sensitivity (SCRS) is 101, 48, and 67 VA⁻¹ T⁻¹, similarly supply power related sensitivity (SPRS) is measured to be 57, 92, and 103 VW⁻¹ T⁻¹, at room temperature respectively. By varying the Hall device carrier velocity, carrier density, and inbuilt capacitance, we investigate in detail the tradeoff between Hall sensitivity and frequency limit in terms of Hall signal rise time and phase shift. In addition, we have proposed a method to address the frequency limitation that arises from the current spinning technique. This method involves measuring the induced voltage at the Hall measurement terminal, which results from the time-variable magnetic field, without applying any external bias to the Hall sensor.

NAMBE-MoP-24 Photonic Crystal Surface Emitting Lasers (PCSELs) based on InAs Quantum Dots-in-a-Well, *Thomas J Rotter, S. Seth, K. Reilly, F. Ince*, Center for High Technology Materials, The University of New Mexico, Albuquerque, NM; *A. Kalapala, C. Gautam, Z. Liu*, Department of Electrical Engineering, The University of Texas at Arlington, Arlington, TX; *S. Addamane*, Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, NM; *W. Zhou*, Department of Electrical Engineering, The University of Texas at Arlington, Arlington, TX; *G. Balakrishnan*, Center for High Technology Materials, The University of New Mexico, Albuquerque, NM

Lasers based on self-assembled quantum dot (QD) gain media have attracted considerable attention due to their low sensitivity to operating temperature and record-low threshold current densities. InAs QD based edge emitting lasers (EELs), vertical cavity surface emitting lasers (VCSELs) or vertical external cavity surface emitting lasers (VECSELs) have been demonstrated with excellent performance. In this study, we demonstrate a QD based optically-pumped photonic crystal surface emitting laser (QD-PCSEL). The PCSEL fabrication process includes epitaxial regrowth, which enables the photonic crystal (PC) to be buried in the laser's waveguide near the upper clad layers. The structure is grown using elemental source molecular beam epitaxy (MBE). In the first epitaxial step the bottom AlGaAs cladding layer and the GaAs waveguide including the QD active region are grown. In the next step, the wafer is removed from the MBE reactor and the PC layer is fabricated by electron beam lithography (EBL) patterning and etching into the GaAs waveguide using inductively coupled plasma (ICP) dry etching. Subsequently the top AlGaAs cladding layer and a top contact layer are grown on the sample. One of the most crucial steps is the removal of the native oxide before growing the top clad layer. This is accomplished by an acid etch prior to loading the sample into the vacuum chamber and a thermal surface treatment with arsenic supply prior to growth. The thermal step at >600°C can alter the QD gain medium, i.e. cause a blue shift and narrowing of the emission spectrum of self-assembled QDs [1-3]. This study employs a dot-in-a-well (DWELL) design as the active region, where the InAs QDs are embedded in a InGaAs quantum well (QW). Our experiments indicate that the DWELL active region is stable during the regrowth process, i.e. there is no significant change to the emission wavelength. This is key to the realization of this laser. The PCSEL is tested by optical pumping and we present measurements of both light-input light-output (LL) and optical spectrum.

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NAMBE-MoP-25 Determination of Optical Properties and Band Structure Parameters of MBE-grown InAs and InAsSb Bulk and InAs/InAsSb and InGaAs/InAsSb Superlattices from Photoluminescence Lineshape, *Marko Milosavljevic*, Arizona State University; *P. Webster*, Air Force Research Lab; *S. Johnson*, Arizona State University

The development of sensors that operate in the mid (3-5 μ m) and long (8-14 μ m) wavelengths are essential for space-based sensing applications. Many Sb-based, III-V material solutions exist ranging from random alloys to superlattices. Furthermore, the growth of high-quality coherently-strained materials is required to achieve the desired long (1-10 μ s) lifetimes for sensor applications. Yet, performance is limited by alloy and interface disorder and also band structure. The impact of disorder on the performance and band structure of MBE-grown InAs, InAsSb, InAs/InAsSb, and InGaAs/InAsSb is examined using the temperature and excitation dependent photoluminescence lineshape.

The excitation and temperature-dependent measurements are analyzed using a lineshape model that is sensitive to the band structure parameters, including bandgap energy, characteristic energy of Urbach tail states, and the electron-hole effective mass ratio and Coulomb interaction. The model also captures the quasi-Fermi level separation, which is the chemical potential of the photoexcited electron-hole population. As a result, the model predicts an excitation induced blue-shift in the lineshape peak position as the chemical potential approaches the bandgap energy. Furthermore, the lineshape model predicts the so-called S-shape behavior of the peak position as a function of temperature and excitation for materials with large Urbach tails. The S-shape behavior typically occurs at low temperatures, where in disordered materials, the width of the electronic Urbach tail states exceeds the width of the thermal Fermi occupation tail. This causes the lineshape to red shift as the electron-hole chemical potential is reduced and the occupied tail states dominate emission. As the temperature is reduced further, the chemical potential for

a given excitation density increases, thereby blue-shifting the lineshape peak back towards the bandgap, thus completing the S-shape.

In the experiment, the various materials listed above are grown by MBE and examined using excitation and temperature dependent photoluminescence spectroscopy. The measurement temperatures range from 12 to 295 K and the pump powers range from 0.4 to 200 mW. The lineshape model is fit to the resulting families of spectra from each material. From the results, i) the lineshape peak position and the chemical potential of the photoexcited electron-hole population is determined as a function of both pump power and temperature, ii) the bandgap and Urbach tail width are determined as a function of temperature, and iii) the effective mass ratio is determined as a single global parameter for all temperatures and excitations measured.

NAMBE-MoP-27 Mbe Epitaxy Solution of the Quantum Well Heterostructure: Atomistic Tnl-Epigrow Simulator, Praveen Kumar Saxena, Tech Next Lab, Lucknow, India; *P. Srivastava, A. Srivastava,* Tech Next Lab, India

The use of standard manufacturing techniques based on highly uniform and well controlled MBE growth on GaAs wafers paves the way for the development of quantum well heterostructure-based semiconductor device technologies, e.g., infrared sources and detectors, memories, lasers, solar cells, HEMT, etc. In order to create a high-quality quantum well, the layers of semiconductor material must be grown with extremely high precision, with thicknesses that are accurate down to the atomic scale. This requires sophisticated equipment and expertise. Even a small variation in the growth process can lead to defects in the material that can significantly impact its electronic properties. The substrate temperature and flux are important factors that affect the growth. A small fluctuation in the substrate temperature, or flux, during the growth process generates several defects. The intensity of the atomic/molecular beam current depends not only on the temperature of the beam source furnace, but also on other influencing factors, such as the shape of the crucible opening and the surface area of the source material. So, it is difficult to extract the right values of flux. The calibration of the flux requires a hit-and-trial. It results in the waste of various costly raw materials, manpower consumption, time, etc., with no guarantee of reproducibility of similar results due to the occurrence of various unpredicted events during growth [1 -2].

In the present paper, the authors have attempted to provide a solution through atomistic simulation to reduce the experimentation cost and the technology development time cycle. To demonstrate the capabilities of the TNL-EpiGrow™ simulator, the MBE growth simulation example used GaSb substrate to simulate the three periods of InAs and AlSb epitaxy, respectively, at atomistic scale. The input conditions used in the simulation are given in Table I. The capabilities to extract the position of each atom on the lattice provide direct access to the various details of the growth morphology, along with defects generated in each monolayer. [2 - 5].

The optimization of the flux is carried out by variations in the effusion cell temperature under the MBE reactor environment. The GaSb/InAs/AlSb quantum well structure is depicted in Fig.1, and the other data are tabulated in Table II. The results are matched with the experimental results [6].

TNL-EpiGrow™ simulator shows great promise for epitaxial growth of II-VI and III-V materials based on various reactor geometries, with potential capabilities to understand the underlying atomistic process inside the reactor [2-5].

NAMBE-MoP-28 Room Temperature Extended Shortwave Infrared Light Emitting Diode, M. Benker, Applied NanoFemto Technologies LLC; *G. Gu,* Stonehill College; *Xuejun Lu,* University of Massachusetts - Lowell

High efficiency infrared light emitting diode (LED) are needed in numerous sensing and imaging applications. In this paper, we report an extended shortwave infrared (e-SWIR) LED capable of working at room temperature (RT). To extend the detection wavelength, the e-SWIR is based on a higher indium (In) composition, i.e. In_{0.3}Ga_{0.7}As_{0.25}Sb_{0.75}/GaSb/AlGaSb multiple quantum well (MQW) heterostructures. The strong carrier confinement allows the e-SWIR LED to work at RT. Detailed analysis and experimental results will be presented.

NAMBE-MoP-29 Infrared Plasmon-Polariton Modes in Hyperbolic Metamaterials Made from Patterned Doped/Undoped InAs Multilayers, E. Caudill, University of Oklahoma; *M. Lloyd,* US Naval Research Laboratory; *K. Arledge, T. Mishima, C. Cailide,* University of Oklahoma; *J. Nolde, C. Ellis,* US Naval Research Laboratory; *P. Weerasinghe, T. Golding,* Amethyst Research Inc; *J. Murphy,* US Naval Research Laboratory; **Michael Santos, J. Tischler,** University of Oklahoma

In *k*-space, the iso-frequency surface of an electromagnetic wave in a hyperbolic material is a hyperboloid, in contrast to the spherical or elliptical surface for an ordinary dielectric material. This unusual property arises when one principal component of the dielectric tensor has the opposite sign to the other two principal components. Hyperbolic materials are expected to exhibit a range of distinctive behaviors, including negative refraction and enhanced superlensing effects [1]. Ionic crystals with anisotropic optical-phonon frequencies provide natural low-loss infrared hyperbolic resonances through the excitation of phonon polaritons. However, the operational bandwidth of these materials is limited to a few hundred wavenumbers (cm⁻¹) or tens of millielectronvolts. A promising route to a wider infrared bandwidth is the excitation of plasmon polaritons in homoepitaxial material engineered to have alternating layers of high- and low-carrier concentration [2,3].

In this work, we implement a low-loss Type-II hyperbolic metamaterial covering a wide spectral bandwidth of 2000 cm⁻¹ for wavelengths above 5.3 μm. We produced the hyperbolic metamaterial with a stack of intercalated heavily-doped InAs and undoped InAs epilayers grown by molecular beam epitaxy. Electron concentrations of 7×10¹⁹ cm⁻³ were obtained by Tellurium doping of InAs epilayers and the optical properties of this stack were measured by infrared ellipsometry. These materials were then dry etched to form one-dimensional square gratings (with periods from 2 to 10 μm) and modeled by finite-element electromagnetic calculations (COMSOL). The models agree with measurements, showing the formation of hyperbolic plasmon polaritons at the same frequencies where experimental features were observed. Additionally, we have identified an Epsilon Near Zero mode associated with long-range surface plasmon polaritons contained in the dielectric layers. This work demonstrates that highly subdiffractional light confinement can be achieved with a III-V metamaterial that can be integrated with III-V semiconductor infrared devices such as photodetectors and emitters at a large scale.

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NAMBE-MoP-30 Impact Ionization Coefficients in Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92} Lattice Matched to Gasb, Jingze Zhao, E. Portyankin, L. Sheterengas, D. Donetski, G. Kipshidze, G. Belenky, Stony Brook University/Brookhaven National Laboratory

There is a demand for mid-wave infrared (MWIR) photodetectors capable of detecting single photons for advanced industrial, military, and biomedical applications. This goal can be realized with cooled avalanche photodiodes (APD) operating in Geiger-mode for single photon counting. The development of the APDs with InAsSb absorption and AlGaAsSb multiplication regions grown lattice matched to GaSb was pursued. Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92} alloys are reported to have high hole impact ionization coefficients compared to electrons in these materials as well as greater than the corresponding coefficients in other semiconductors^[1]. Following the procedure in Ref. 1 we determined the hole and electron multiplication coefficients in Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92} separately using p-i-n and n-i-p diodes within the field range of 140 to 600 kVcm⁻¹. The structures were grown in Veeco GEN-930 solid-source MBE system. The p-i-n diode structures for measurements of the hole impact ionization coefficient were grown on p-type GaSb substrates consisting of a 500-nm-thick Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92} Be-doped contact layer, a 300-nm-thick nominally undoped Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92} hole multiplication region, and a 1.2-mm thick Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92} Te-doped top contact layer capped with a 50-nm-thick Te-doped GaSb. The n-i-p diode structures for electron impact ionization measurements were grown on n-type GaSb with Te-doped, undoped and Be-doped Al_{0.9}Ga_{0.1}As_{0.08}Sb_{0.92} layers of similar thicknesses. The wafers were processed into diodes with mesa diameters in the range from 80 μm to 320

mm. CV measurements confirmed that the 300-nm-undoped multiplication regions were fully depleted. Temperature dependences of I-V characteristics showed that above 140 K the dark current was limited by thermal generation of excess carriers in the depletion region with the activation energy of 0.3 eV. The carrier multiplication coefficients were determined by measuring photocurrent versus bias voltage. For a nearly complete absorption of photons in the top layer and multiplication dominated by one type of carriers the excess carriers were generated at 532 nm. Preliminary experimental data show that the hole ionization coefficients are up to 100 times greater than the electron ionization coefficients.

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NAMBE-MoP-31 High-Mobility III-V Core-Shell Nanowire Heterostructures for Thermoelectric Energy Conversion, Genet Bacha Hirpessa, Technical University of Munich, Germany; *S. Fust*, R. Maier, Technical University Munich, Germany; *F. Del Giudice*, J. Finley, Technical University of Munich, Germany; *G. Koblmüller*, Technical University Munich, Germany

Thermoelectric energy conversion offers widespread applications in waste heat recovery for power generation but requires suitable materials with large thermoelectric conversion efficiency. To aim at high efficiency with large figure-of-merit $ZT = \sigma S^2 T / \kappa$, relevant parameters such as electrical conductivity (σ), thermoelectric power factor (σS^2), and thermal conductivity (κ) need to be optimized for any given Seebeck coefficient S and operating temperature T . Due to the interdependence between thermal and electrical properties, modification of parameters for high ZT is limited in bulk materials, but in nanostructures, the properties can be decoupled^[1].

The aim of our research is to demonstrate independent control of these parameters by exploiting the 1D density of states in very high mobility III-V nanowires (NWs). First proof-of-principle studies were performed on modulation-doped GaAs-AlGaAs core-shell NWs grown by MBE, where we found enhanced thermopower in 1D-subbands at substantially lowered κ ^[2]. While these initial studies were limited to cryogenic temperatures, studying more suitable low-bandgap III-V materials with lower electron effective mass are more appealing for enhanced 1D-thermoelectric transport at higher temperatures. Here, we show our recent progress towards InAs/AlAsSb core-shell NW heterostructures^[3], where both contact formation establishment and electrical characterization were performed up to elevated temperatures. Using NW-field effect transistor (NW-FET) test structures, the DC output characteristics were confirmed and transfer characteristics up to temperatures >100 K demonstrated clear 1D sub-band quantization, with transmission probabilities of ~ 0.4 for 700-nm long channel devices.

To further introduce n -type modulation-doping (Si- δ doping) into the InAs/AlAsSb core-shell NW-system, two strategies are illustrated: first, δ -doping of a very thin (<2nm-thin) InAs quantum well (QW) embedded in the AlAsSb shell to overcome the otherwise p -type nature of amphoteric Si-dopants in Al(As)Sb^[4]. Secondly, we also developed quaternary InAlAsSb shell layers to enable direct Si- δ doping without the need of InAs QWs. By guiding the design via band-profile calculations (nextnano-3), first results of the MBE growth and structural characterization of the desired InAs-InAlAsSb core-shell NW heterostructures are demonstrated^[5].

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NAMBE-MoP-32 Wafer Scale GaAs/AlGaAs Core-Shell Nanowires on 2-inch Si Substrate Showing Efficient Light Emission/Absorption with High Thermal Stability, Keisuke Minehisa, H. Hashimoto, K. Nakama, Research Center for Integrated Quantum Electronics, Hokkaido University, Japan; *H. Kise*, *S. Sato*, *J. Takayama*, *S. Hiura*, *A. Murayama*, *F. Ishikawa*, Faculty of Information Science and Technology, Hokkaido University, Japan

Semiconductor nanowires (NWs) are promising materials for nanoscale devices with diameters of less than several hundred nanometers. GaAs has a high electron mobility and direct bandgap, and is used in lasers, solar cells, and transistors through heterojunctions with related compounds. In addition, the integration of III-V semiconductor NWs on Si can integrate superior electrical and optical properties to mature Si technology, which is expected to be applied to the next generation optical and electronic

devices. However, the surface recombination velocity of GaAs is several orders of magnitude higher than that of other III-V semiconductors, and the effect is further exacerbated by the large surface-to-volume ratio in NWs. To suppress the effect of non-radiative recombination, surface passivation on the GaAs core with an AlGaAs shell is known to be effective.^[1] Besides, preserved material properties at temperatures higher than room temperature is desirable for the practical device applications.

We here report wafer scale growth of GaAs/Al_{0.8}Ga_{0.2}As core-shell NWs on the 2-inch Si(111) wafer by constituent Ga-induced vapor-liquid-solid growth using molecular beam epitaxy (MBE).^[2] The sample is investigated by the optical reflectance, photoluminescence (PL) and time-resolved PL measurements from 300 to 400 K. The nature of the light scattering induced by the complex NWs structure on the Si substrate enables the measurement of diffuse reflectance, making the Kubelka-Munk (K-M) transformation^[3] to be applicable, obtaining the absorption characteristics of the sample. The sample shows a low optical reflectance less than 2% at energies higher than GaAs absorption edge in the visible to near-infrared region at 300 K, resulting in the dark observation of the sample wafer. That band gap of the sample is estimated to be 1.41 eV from the K-M plot, and it's deviation between the PL peak energy suggests that the Stokes shift is close to be negligible. The carrier lifetime obtained from the time-resolved PL measurement is longer than 1 ns between 300 and 400 K. That indicates the effective passivation of the GaAs core by the AlGaAs shell, suppressing the surface non-radiative recombination. From these results, we obtain wafer scale GaAs/AlGaAs core-shell nanowires on 2-inch Si(111) substrate showing efficient light emission/absorption with high thermal stability.

NAMBE-MoP-33 Optimizing Growth on GaAs (111)B for Enhanced Parametric Downconversion Efficiency in Quantum Optical Metasurfaces, Trevor Blaikie, University of Waterloo, Canada; *S. Stich*, Walter Schottky Institut, Technische Universität München, Germany; *M. Tam*, University of Waterloo, Canada; *M. Belkin*, Walter Schottky Institut, Technische Universität München, Germany; *M. Chekhova*, Max-Planck-Institut für die Physik des Lichts, Germany; *Z. Wasilewski*, University of Waterloo, Canada

Quantum optical metasurfaces (QOMs) hold promise for generating entangled photons and engineering complex quantum states. To generate entangled photon pairs, QOMs leverage spontaneous parametric downconversion (SPDC). Despite SPDC being the leading method for generating entangled photon pairs in quantum optics, QOMs dependent on SPDC face limitations due to low conversion efficiency. This project aims to enhance SPDC efficiency in QOMs by utilizing GaAs (111)B substrates for the growth of the bulk GaAs material from which the QOMs are fabricated.

GaAs is appropriate for QOMs because of its very high second-order susceptibility. It is predicted that the nonlinear response of GaAs in the (111) orientation is even stronger than it is in the typically used (001) orientation. Calculations indicate a potential 1-3 orders of magnitude increase (pump frequency dependent) in QOM conversion efficiency for GaAs with (111) surface orientation as compared to (001).

Growth on (111) oriented GaAs substrates is challenging and requires a very different set of growth parameters for optimized deposition than growth on (001) surface; therefore, precise in-situ monitoring and control are necessary.

In the pursuit of optimized growth parameters, we have grown GaAs and AlGaAs on GaAs (111)B substrates with an intentional 2° surface misorientation towards [11-2]. In-situ reflection high-energy electron diffraction (RHEED) is monitored to observe changes in surface reconstruction. Desorption mass spectrometry is used to monitor the group V/III ratio. A laser light scattering system has been implemented to measure the diffuse scatter from the wafer during the epitaxial process. The latter is a sensitive probe of the onset of roughening of the growth front.

Ex-situ, the growth surface morphologies are studied with Nomarski interference contrast microscopy and atomic force microscopy. Surface morphologies resulting from different growth conditions will be compared, and their effect on QOM fabrication and operation will be discussed.

NAMBE-MoP-34 Magnetization Switching Behavior in Anisotropy Gradient GaMnAsP Film Grown by Molecular Beam Epitaxy, Kyung Jae Lee, Korea University, Canada; *S. Lee*, Korea University, Germany; *X. Liu*, University of Notre Dame, Canada; *M. Dobrowolska*, *J. Furdyna*, University of Notre Dame, Germany

Magnetization switching behavior of GaMnAsP ferromagnetic semiconductor (FMS) films with magnetic anisotropy gradient along the growth direction has been investigated. To achieve such magnetic anisotropy gradient in the GaMnAsP film, the phosphorus concentration

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was gradually decreased from 24% to 3% with step of about 5 % during the growth of 62.5 nm film by molecular beam epitaxy. The continuous adjustment of phosphorus results in a change of strain from tensile to compressive in the film. Such strain gradation leads a progressive change of the magnetic anisotropy of the film from out-of-plane to an in-plane direction. In order to perform the spin-orbit torque (SOT) magnetization switching experiments, a Hall device was fabricated along the [110] crystal direction where the Rashba-type and Dresselhaus-type spin-orbit fields are antiparallel to each other. The SOT magnetization switching experiment was performed at a temperature of 2.5 K by applying a pulsed current of 10 ms duration in the presence of an in-plane bias field. The magnetization state was monitored by Hall resistance (HR) measurement, in which a small direct current of 10 uA was used for sensing magnetization. We observed that the chirality of magnetization switching changes depending on the strength of the external field. Specifically, the SOT switching chirality changes from clockwise at a small external field (e.g., 200 Oe) to counterclockwise as the field increases (e.g., 1000 Oe), and then back to clockwise again at a strong field (e.g., 2500 Oe). This unusual dependence of SOT switching chirality on the strength of an in-plane external field can be explained by the coexistence of the in-plane and out-of-plane magnetization components, which vary with strength of in-plane external fields.

NAMBE-MoP-35 Growth, Electrical and Optical Properties of SrMoO₃ Grown by Suboxide Molecular Beam Epitaxy, Roman Engel-Herbert, Paul - Drude-Institute for Solid State Electronics, Leibniz Institute within the Forschungsverbund Berlin, Germany; T. Kuznetsova, J. Roth, J. Lapano, A. Pogrebnyakov, Penn State University

Correlated metals with perovskite structure have generated much interest due to their intriguing combination of electrical and optical properties rendering them as alternative transparent conductor material to degenerately doped wide band gap oxide semiconductors, such as ITO. While SrVO₃ and CaVO₃ have been reported to outcompete ITO, SrNbO₃ has been shown unparalleled performance of electrical conductivity while maintaining a high optical transparency deep into the UV range to show unparalleled performance in the UV range. SrMoO₃ is yet another candidate material, which meets the requirement of the new transparent conductor design paradigm.

In this talk we will discuss the growth of SrMoO₃ thin films by suboxide molecular beam epitaxy. We will show that optically transparent and electrically conductive SrMoO₃ films can be grown by supplying elemental strontium via a conventional effusion cell and thermally evaporating MoO₃ pellets as a molybdenum source. The direct supply of a molecular oxygen flux to the MoO₃ charge was found critical to prevent Mo reduction to lower oxidation states and to ensure congruent evaporation. Optimal growth conditions were found by varying the Sr to MoO₃ flux ratio resulting in SrMoO₃ films being optically transparent with transmission between 75 to and 91% throughout the visible spectral range, and electrically conducting with a room temperature resistivity of $5.0 \times 10^{-5} \Omega \cdot \text{cm}$.

NAMBE-MoP-36 Modeling and Characterization of GaAsSb/InGaAs 'W'-Quantum Wells with GaAsP Strain Compensated Layers, Z. Li, T. Lo, Charles W. Tu, National Chung Hsing University, Taiwan

Vertical-cavity surface-emitting lasers (VCSELs) have applications in facial recognition in smart phones, 3D sensing for augmented reality/virtual reality, etc. The current VCSELs emitting at 940 nm for cell phones are manufactured on GaAs substrates, utilizing the well-established GaAs/AlGaAs distributed Bragg reflectors (DBRs). However, long-wavelengths, 1300 nm to 1550 nm, are desirable for eye-safety and transparency to cell phone screens.

Here we explore strain-compensated GaAsP/InGaAs/GaAsSb W quantum wells (W QWs), grown by MBE, for long-wavelength emission on GaAs substrates. The tensile-strained GaAsP compensates for the compressive-strained InGaAs and GaAsSb layers. Three cycles (samples A-D) and one cycle (samples E and F) of GaAs_{1-z}P_z/In_yGa_{1-y}As/GaAs_{1-x}Sb_x/In_yGa_{1-y}As/GaAs_{1-z}P_z 'W' QWs were grown with $y = 0.3$ and $z = 0.3$. The Sb composition ($x = 0.06-0.21$) of GaAs_{1-x}Sb_x QW in all samples was controlled by the QW growth temperature in the range of 410-520 °C. X-ray rocking curve (XRC) analysis and 20K photoluminescence (PL) measurement are performed.

The W QW with different Sb contents are modelled by the energy band-diagram simulations. The input parameters, QW thicknesses and material compositions, are extracted by the XRC analysis. The one-cycle of 15 nm-GaAs_{1-z}P_z/3.5 nm-In_yGa_{1-y}As/16 nm-GaAs_{1-x}Sb_x/3.5 nm-In_yGa_{1-y}As/15 nm-GaAs_{1-z}P_z W QW structure is designed as shown in Fig. 1. The strained bandgap energies of QWs are obtained from the bulk bandgap using

various bowing parameters as the fitting parameters and energy shifts due to strain using various deformation potentials.

where b_i is the bowing parameters, and $i = g, c, v_{hh}, v_{lh}$ for bandgap, conduction and heavy hole/light hole valence bands, respectively. The material parameters are taken from the literature for the end compounds of InAs, GaSb, GaP and GaAs. In our calculations, the bandgap bowing parameters b_g of GaAs_{1-x}Sb_x and InGa_{1-y}As are set as the fitting parameters to our experimental results. The experimental PL peak positions can be fit well by b_g of -1.58 and -1.1 for the strained GaAs_{1-x}Sb_x and In_yGa_{1-y}As QWs, respectively. The one-band time-independent Schrödinger equation with Hamiltonian in the effective mass approximation is solved by COMSOL Multiphysics, enabling us to obtain the electron and hole wavefunctions, the energy levels of electrons in conduction band and holes in valence band, and the estimated emission wavelengths.

In summary, in consideration of strain effect in band alignment simulation, the PL peak positions as a function of Sb composition (samples A-C) are well fitted by the simulated transition wavelength of strained WQWs at 20 K

NAMBE

Room Cummings Ballroom - Session NAMBE1-TuM

Magnetism, Superconductivity, and Quantum Computing

Moderator: Patrick Strohbeen, New York University

8:15am NAMBE1-TuM-1 Welcome & Sponsor Thank Yous,

8:30am NAMBE1-TuM-2 NAMBE Young Investigator Awardee Talk: Epitaxial Integration of Dissimilar Semiconductors for Infrared Optoelectronics, Kunal Mukherjee, Stanford University INVITED

Integrating dissimilar semiconductors on a single crystal platform can power the next generation of electronics and photonics applications. In such a platform, semiconductors like III-V and IV-VI materials bring exciting new properties to the table and leverage the scale and functionality of conventional silicon technology. The synthesis of high-quality semiconductor thin films while mediating this dissimilarity, however, is quite the materials science challenge. These very differences in properties also lead to unusual interfaces and crystal defects such as dislocations that severely degrade device performance. In this talk, we update our understanding of how dislocations are bad for epitaxially-integrated telecom lasers on silicon using new microscopy and microanalysis tools, and we present on our progress in engineering dislocation tolerance in such devices using MBE-grown III-V (InAs) quantum dots. With an eye towards materials and devices naturally more tolerant to dislocations, we will show new opportunities that arise from MBE-grown IV-VI (PbSe-SnSe) mid-infrared light emitters and crystalline-crystalline phase change materials grown epitaxially on III-V substrates

9:00am NAMBE1-TuM-4 MBE Synthesis of Altermagnetic MnTe Exhibiting an Anomalous Hall Effect, S. Bey, X. Liu, University of Notre Dame; A. Ievlev, Oak Ridge National Laboratory; S. Bennett, Naval Research Laboratory; M. Zhukovskiy, T. Orlova, Badih A. Assaf, University of Notre Dame

Altermagnets are a new class of magnetic materials that host a spin polarization texture on the Fermi surface despite being antiferromagnetic [1]. An anomalous Hall effect (AHE) can result from this spin texture under specific conditions dictated by the magnetic anisotropy of the material. Hexagonal α -MnTe is an altermagnet where the AHE has already been reported but is not understood [2] [3]. We have successfully synthesized MnTe by molecular beam epitaxy on GaAs (111) and SrF₂ (111) and doped with In. The lattice mismatch between MnTe and the two substrates is +3.8% and +1.2% however in both cases, a heteroepitaxial growth is achieved with [11 -2 0] direction of MnTe aligning with the [1-10] direction of the substrate. We reveal this by carrying out systematic high-resolution x-ray diffraction in the specular and off-specular direction. On both substrates, MnTe hosts an anomalous Hall effect, generally unexpected in collinear antiferromagnets. The conductivity of MnTe is found to be higher when it is grown on GaAs. We find that In doping alters the carrier density to below 10¹⁹ holes/cm³ without significantly changing the conductivity. We exploit this tuning of the transport parameters to study the scaling law relating the anomalous Hall and longitudinal conductivity in this prototypical altermagnet. [4]

[1] L. Šmejkal, J. Sinova, and T. Jungwirth, *Beyond Conventional Ferromagnetism and Antiferromagnetism: A Phase with Nonrelativistic Spin and Crystal Rotation Symmetry*, Phys Rev X **12**, 031042 (2022).

[2] R. D. Gonzalez Betancourt et al., *Spontaneous Anomalous Hall Effect Arising from an Unconventional Compensated Magnetic Phase in a Semiconductor*, Phys Rev Lett **130**, 036702 (2023).

[3] K. P. Kluczyk et al., *Coexistence of Anomalous Hall Effect and Weak Net Magnetization in Collinear Antiferromagnet MnTe*, ArXiv 2310.09134 (2023).

[4] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, *Anomalous Hall Effect*, Rev Mod Phys **82**, 1539 (2010).

9:15am NAMBE1-TuM-5 Lateral Strain and Magnetism Patterning in Flexomagnetic GdAuGe Thin Films via Helium Ion Implantation, Zachary LaDuca, T. Samanta, T. Jung, University of Wisconsin - Madison; M. Brahlek, T. Ward, A. Chen, Oak Ridge National Laboratory; N. Hagopain, F. Fei, T. Xi, K. Su, M. Arnold, P. Voyles, J. Xiao, J. Kawasaki, University of Wisconsin - Madison

Strain gradients provide a new degree of freedom to precisely tune the ferroic properties of quantum materials. However, studying the effects of strain gradients on materials properties has proven to be a great challenge, as it is difficult to control strain gradients in bulk crystals and epitaxial films.

Here, using patterned helium ion implantation, we demonstrate top-down control of strain gradients and flexomagnetism ($M \propto \nabla \epsilon$) in epitaxial GdAuGe thin films on Graphene/Ge (111). Unstrained GdAuGe is antiferromagnetic, with a Néel temperature of 17K. Uniform strain up to 4.5% along the c-axis suppresses the Néel temperature to 8K yet preserves antiferromagnetic ordering in GdAuGe. Remarkably, patterned strain gradients induce a transition to ferro/ferrimagnetic ordering around 100K, subsequently followed by an antiferromagnetic transition at approximately 8K. These results confirm the presence of flexomagnetism rather than piezomagnetism ($M \propto \epsilon$) or magnetostriction ($M^2 \propto \epsilon$). Furthermore, the presented results underscore the efficacy of patterned helium ion implantation as a novel and versatile method for controlling strain, strain gradients, and their impact on material properties.

This work was supported by the Air Force Office of Scientific Research and the National Science Foundation via the Wisconsin MRSEC.

9:30am NAMBE1-TuM-6 Synthesis and Fabrication of Superconducting Germanium Alloys for Quantum Information, Patrick Strohbeen, J. van Dijk, I. Levy, M. Mikalsen, A. Danilenko, W. Schiela, J. Shabani, New York University

Germanium as a platform for quantum information has been rapidly gaining interest in the last five years due in large part to drastic improvements in 2D hole gas quality (2DHG) [1]. As a result, there is immediate interest in using the Ge 2DHG in superconductor-semiconductor (S-Sm) hybrid platforms for quantum information [2]. Indeed, recent experimental works have shown a hard superconducting gap in a Ge quantum well [3] as well as long parity lifetimes [4]. However, the Josephson junctions created thus far have required direct contact to the quantum well region which is likely to drastically reduce carrier mobilities within the junction region [5]. In addition, growth of superconducting materials compatible with group IV semiconductors enables the growth of buried superconducting layers for more complex devices, such as the merged-element transmon [6]. In this talk I will discuss our recent work on the growth of superconducting binary germanium alloys and their promise for quantum information applications. This work will be discussed in the context of both planar and out-of-plane device architectures and the utility afforded by germanium alloys.

[1] M. Myronov et al., Small Sci. 3, 2200094 (2023).

[2] G. Scappucci et al., Nat. Rev. Mater. 6, 926-943 (2021).

[3] A. Tosato et al., Commun. Mater. 4, 23 (2023).

[4] M. Hinderling et al., arXiv:2403.03800 (2024).

[5] D. Laroche et al., AIP Adv. 5, 107106 (2015).

[6] R. Zhao et al., Phys. Rev. Applied 14, 064006 (2020).

9:45am NAMBE1-TuM-7 Molecular Beam Epitaxy Growth of Al and Ta Multilayers for Superconducting Qubits, Kevin A. Grossklaus, D. Miller, L. Burkhardt, A. Sabbah, M. Gingras, B. Nidezielski, C. O'Connell, H. Stickler, D. Calawa, A. Melville, MIT Lincoln Laboratory; A. Goswami, Massachusetts Institute of Technology; D. Kim, J. Yoder, M. Schwartz, MIT Lincoln Laboratory; W. Oliver, Massachusetts Institute of Technology; K. Serniak, MIT Lincoln Laboratory

Superconducting qubits have advanced from proof-of concept demonstrations to broad deployment of a variety of qubit designs into many-qubit quantum processors. Reducing materials- and processing-induced losses in superconducting qubit circuits remains a critical focus in the effort to reduce qubit decoherence and improve overall performance. For the superconducting base metal used in a qubit, the metal's microstructure, the interfaces between the metal and its surroundings, crystalline defects, and the presence of contaminants in the metal interior or on its surface may all be expected to play a role in the performance of a final device. Because loss may come from a variety of sources, it is often difficult to unambiguously link changes in specific superconducting material properties and structure to changes in qubit performance. For this reason, deposition of superconducting metals by molecular beam epitaxy (MBE) may serve as a valuable method for understanding and isolating the material factors that affect their performance in superconducting qubits. As an approach, MBE allows for careful control of source material quality, vacuum conditions, deposition rate, layer thicknesses, and interface sharpness. Thus, MBE allows for deposition of superconducting materials with very low contamination and deposition conditions that can be known with a high degree of precision.

In this work we will present results from the low temperature MBE deposition of Al and Ta/Al multilayers on silicon substrates. Superconducting co-planar waveguide (CPW) resonators will be used to probe expected

material performance for qubit applications. Characterization of the as-deposited metals and data from CPW resonators fabricated using them will be shown. Materials characterization of epitaxial Al layers by AFM, XRD, XPS, RHEED, and TEM will be shown and discussed in terms of both the benefits of deposition by MBE and implications for superconducting device performance. Similarly, characterization of Ta/Al bilayers will be shown and the impacts of bilayer deposition on the structure of both Ta and Al layers will be discussed. Finally, the possible impacts of Ta/Al bilayers on the material sources of qubit loss and next steps in improving the quality of MBE grown Ta/Al multilayer structures will be considered.

This material is based upon work supported under Air Force Contract No. FA8702-15-D-0001. Any opinions, findings, conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the U.S. government or the U.S. Air Force.

10:00am **NAMBE1-TuM-8 Electrical, Magnetic, and Thermoelectric Characterizations of Strange Metallicity in Epitaxial Thin Film Kagome Intermetallics**, *Minyong Han, C. John, J. Zheng, S. Fang, J. Checkelsky*, Massachusetts Institute of Technology

The observation of strange metallicity in a paramagnetic kagome intermetallic Ni_3In has demonstrated the role of hopping-frustration-induced d -electron flat band in generating Kondo-like behaviors even in the absence of f -electrons in the lattice [1]. A number of bulk single crystal experiments consistently suggest the potential presence of a quantum critical point in a proximate phase space. This calls for a platform that enables versatile materials tunings along various non-thermal control axes. In this talk, we present successful stabilization of Ni_3In in epitaxial thin film form using Molecular Beam Epitaxy. We discuss key aspects of the synthesis which are critical in attaining high crystallinity and flat morphology at the same time. Electrical transport under a wide temperature range reveals that quantum fluctuation is strongly influencing the electronic conduction even when the system is confined in thin film structure. Magnetoresistance and magneto-Seebeck responses suggest the relevance of spin fluctuation in generating such a behavior. We also present high precision magnetometry suitable for probing those spin fluctuations in our films – the task that is typically nontrivial in paramagnetic thin films with dramatically reduced sample volume. In the end, we will propose useful post-synthesis thin film engineering techniques for controlling the quantum criticality in Ni_3In . (ref: [1] L. Ye et al., Nat. Phys. (2024), doi.org/10.1038/s41567-023-02360-5)

NAMBE

Room Cummings Ballroom - Session NAMBE2-TuM

Chalcogenides and Topological Materials

Moderator: **Stephanie Law**, Penn State University

10:45am **NAMBE2-TuM-11 Rhombohedral-to-Cubic Phase Transition in $\text{Ge}_{1-x}\text{In}_x\text{Te}$ Thin Films Grown by MBE**, *Xinyu Liu, K. Yoshimura, S. Bey, M. Abdu Karim, J. Wang, L. Riney, M. Zhukovskiy, T. Orlova, B. Assaf*, University of Notre Dame

Topological superconductors are the subject of intense research due to their potential to harbor Majorana boundary modes, which hold promising applications in quantum computing. Superconductors that lack inversion symmetry host singlet-triplet mixing and are a precursor of topological superconductivity. GeTe , a non-centrosymmetric semiconductor, has been observed to undergo a semiconductor-superconductor transition above 1K when doped with In at a critical level ($x \approx 0.12$).¹ The transition to superconductivity is accompanied by a structural phase transition to a centrosymmetric cubic phase. This study introduces the first synthesis of $\text{Ge}_{1-x}\text{In}_x\text{Te}$ films via MBE, motivated by recent findings that quantum confinement promotes the stabilization of the non-centrosymmetric structure of IV-VI materials.

Structural analyses of 120nm $\text{Ge}_{1-x}\text{In}_x\text{Te}$ thin films ($0 \leq x \leq 0.4$) on BaF_2 (111) substrates show distinct characteristics not observed in single crystals. The process begins with the deposition of a 40nm GeTe buffer layer to facilitate initial layer nucleation. We then co-deposit Ge, In, and Te from separate elemental sources, maintaining a Ge to Te flux ratio of 0.1. The growth is monitored via in situ RHEED, revealing that only a specific growth temperature range (220–270°C) is suitable for high-quality epitaxial growth.² We observe that In atoms tend to migrate into the GeTe buffer

layer, confirmed by TEM and EDX mapping.

The samples undergo comprehensive analysis using both SEM and XRD techniques. To evaluate the crystal orientation along the growth axis, specular ω -2 θ scans were conducted. To investigate the films' strain relaxation, reciprocal space maps were acquired for both symmetric rhombohedral- GeInTe (0006) and asymmetric rhombohedral- GeInTe (01-18) Bragg peaks. Both SEM and XRD show a rhombohedral-to-cubic phase transition at In level of $x=0.19$ in MBE grown $\text{Ge}_{1-x}\text{In}_x\text{Te}$ films, higher than what is found in single crystals. We also observe the coexistence of strained and unstrained cubic $\text{Ge}_{1-x}\text{In}_x\text{Te}$ phases for high In content films.

Growing non-centrosymmetric $\text{Ge}_{1-x}\text{In}_x\text{Te}$ films with high In content enables deeper exploration of its unconventional superconductivity through thin-film-specific devices. Upcoming magnetotransport studies will examine the connection between its phase transitions and superconductivity. Additionally, cubic $\text{Ge}_{1-x}\text{In}_x\text{Te}$'s compatibility with topological crystalline insulators positions it as a key material for creating heterostructures that could support topological superconductivity.

Work was supported by DOE-BES-Award DE-SC0024291.

11:00am **NAMBE2-TuM-12 Coherent strain through quasi van der Waals Epitaxy of magnetic topological insulators Cr: $(\text{Bi}_x\text{Sb}_{1-x})_2\text{Te}_3$ on a GaAs (111) substrate and the influence from growth windows**, *Yuxing Ren, K. Pan, Y. Chen, J. Kang, B. Regan, C. Wong, M. Goorsky, K. Wang*, University of California at Los Angeles

Quasi van der Waals Epitaxy (qvWE) has been realized for decades at the interfaces between 3D and 2D materials or van der Waals materials. The growth of magnetic topological insulators (MTI) Cr: $(\text{Bi}_x\text{Sb}_{1-x})_2\text{Te}_3$ (CBST) on GaAs (111) substrates for Quantum Anomalous Hall Effect (QAHE) is actually one of the examples of qvWE, which is not well noticed despite the fact that its advantages have been used in growth of various MTI materials. This is distinguished from the growth of MTIs on other substrates. The specific surface potential and ionicity determines the nature of a quasi van der Waals growth, which has the same advantage of van der Waals epitaxy of getting rid of surface roughness while at the same time maintaining a uniform grain orientation as traditional epitaxy. Despite many reports, there are still no clear conclusions on the root cause of qvWE and the features of qvWE have not been well recognized. The typical features are coherent interface and the existence of a strain within a short period of distance. While coherency is much more widely observed for qvWE, the existence of strain is generally hard to be demonstrated due to the small thickness of strained layers in the van der Waals materials. Our goal in this work is to demonstrate both coherency and the existence of strain at the interface of epitaxial CBST on GaAs (111) substrate.

Here in this work, we have for the first time shown the features of both coherent interfaces and the existence of strain originating from qvWE at the same time. To show the coherently strained interface, we have grown samples with thickness of 1 QL (quintuple layer), 2QL and 6 QL under the same conditions respectively to compare the relaxed layers and strained layers. X-ray pole figures and Reciprocal Space Mapping (RSM), in-situ Reflective High Energy Electron Diffraction (RHEED), STEM (Scanning Transmission Electron Microscope) and EDS (Energy Dispersive X-ray Spectroscopy), and a Raman measurement are used to demonstrate the coherently strained interface.

Growth window of quantization regime is also studied in this work. By controlling source flux and substrate temperatures, we have identified the growth of samples with quantum anomalous Hall effect at the boundary of mass-transport flow and adsorption-control mode on GaAs (111) substrates.

11:15am **NAMBE2-TuM-13 Epitaxial Hexagonal BaZrSe_3 Thin Films with Strong Birefringence in-Plane**, *Ida Sadeghi, V. Kamboj*, MIT; *T. Simonian*, College Green, Ireland; *J. Van Sambeek, M. Xu*, MIT; *V. Nicolosi*, College Green, Ireland; *J. LeBeau, R. Jaramillo*, MIT

Systems of ternary chalcogenides – such as the Ba-Zr-Se system - have a rich diagram of stable and metastable phases, including perovskite, needle-like, and hexagonal structures that vary in the connectivity of octahedra (e.g. ZrSe_6), and are predicted to vary widely in their opto-electronic properties.^{1,2} We previously demonstrated synthesis of BaZrSe_3 thin films in the corner-sharing perovskite phase,^{3,4} which has a band gap of 1.5 eV and is theoretically predicted to be thermodynamically unstable.^{5,1} Others have reported that powder synthesis results in a hexagonal phase with very small

band gap and possible defect ordering.^{6,7} These results highlight the strong dependence of phase and properties on synthesis conditions for ternary chalcogenides.

Here we demonstrate synthesis of face-sharing hexagonal BaZrSe₃ (h-BaZrSe₃) thin films by MBE. We can make the hexagonal phase via two routes: (1) by aggressive selenization of a thin film of BaZrS₃ in the corner-sharing perovskite phase on LaAlO₃ (LAO), or (2) by direct deposition on YAlO₃ (YAO) (001) substrates. The kinetics of transformation from perovskite to hexagonal phase depend on the processing temperature and H₂Se gas flux.

The hexagonal structure is highly anisotropic and is expected to feature giant optical birefringence, similar to the iso-structural compound BaTiS₃.⁸ LAO is pseudo-cubic, and h-BaZrSe₃ films form on LAO in two domain types, with the optic axis rotated by 90° in-plane; this renders the birefringence difficult to measure and use. In contrast, YAO is orthorhombic and (001) substrates feature rectangular symmetry. As a result, h-BaZrSe₃ films on YAO (001) have a dominant domain orientation with the optic axis in-plane; this enables more direct measurement and use of the optical anisotropy.

To demonstrate the effect of epitaxial control over film phase and orientation, we report measurements of optical transmission versus incident polarization angle, demonstrating a large modulation with a period of ~ 180° at near-infrared wavelengths. We also find using measurements of photoconductivity spectroscopy that the band gap is 1.79 ± 0.1 eV, which is many times larger than theoretically predicted. Our results indicate that epitaxial h-BaZrSe₃ may be uniquely useful for free-space modulation of mid-wave and near infrared light.

1. *Nano Lett.* **15**, 581, 2015.
2. *Chem. Mater.* **34**, 6894, 2022.
3. *Adv. Funct. Mater.* **33**, 2304575, 2023.
4. *arXiv:2403.09016*, 2024.
5. *J. Appl. Phys.* **125**, 235702, 2019.
6. *Russ. J. Inorg. Chem.* **9**, 1090, 1964.
7. *J. Am. Chem. Soc.* **120**, 7639, 1998.
8. *Photonics* **12**, 392, 2018.

11:30am **NAMBE2-TuM-14 Quasi-Van Der Waals Epitaxial Growth of Thin γ -GaSe Films**, *Mingyu Yu*, University of Delaware; *S. Law*, Pennsylvania State University

GaSe is an advanced 2D layered semiconductor, possessing various appealing properties, such as rare p-type conductivity, nonlinear optical behavior, and high transparency in 650-180000 nm. GaSe also exhibits bandgap behavior opposite to transition metal chalcogenides, as it transitions from an indirect bandgap monolayer to a direct bandgap bulk material, with a reduction in bandgap energy. These features make GaSe rich in potential in many applications, such as quantum photonic devices, field-effect transistors, etc. GaSe has a hexagonal crystal structure composed of Se-Ga-Ga-Se quadruple layers (QLs). Each QL is bonded by weak van der Waals (vdW) interactions, enabling flexible stacking configurations. Therefore, there are multiple polymorphs for GaSe, namely ϵ -, β -, δ -, and γ -, all having identical non-centrosymmetric QL with a D_{3h} space group. In addition to the 4 extensively explored polymorphs, a new polymorph, γ' -GaSe, was proposed for the first time in 2018. γ' -GaSe is unique for its centrosymmetric D_{3d} QL and the QLs are stacked like γ -GaSe (Fig. S1). On this basis, γ' -GaSe has been predicted to show intriguing performance compared to other polymorphs. However, to date, there are only a few reports showing the observation of γ' -GaSe, and it usually coexists with other polymorphs since the formation energy of γ' -GaSe is less favorable. Moreover, the commercial applications of GaSe are limited by synthesis technology, as common methods such as exfoliation are difficult to achieve wafer-scale, high-quality production of GaSe. Obtaining a single-phase, single-polymorph GaSe is also challenging due to the coexistence of multiple stable phases and polymorphs.

We developed a quasi-vdW epitaxial growth method to obtain high-quality pure γ' -GaSe thin films on GaAs(111)B substrates at a wafer scale. The resulting films exhibit a smooth surface with a root-mean-square roughness as low as 7.2Å (Fig. S2a) and a strong epitaxial relationship with the substrate (Fig. S2b). More interestingly, we observed a pure γ' -type configuration using scanning transmission electron microscopy (Fig. S2c,d) and analyzed its formation mechanism through density-functional theory (Fig. S3). These findings contribute to the exploration of GaSe. We also investigated the unconventional 2D/3D epitaxial growth mechanism and have overcome technical challenges, benefiting the advancement of

heterogeneous integration. In the future, we will focus on developing the properties and applications of γ' -GaSe, and delving into the understanding of the epitaxial growth mechanism from a theoretical perspective.

11:45am **NAMBE2-TuM-15 Response of Topologically Protected Helical Modes in Monolayer WTe₂ to Band-gap Tuning**, *Yulia Maximenko*, Colorado State University; *Y. Chang*, Rutgers University; *M. Hirsbrunner*, *L. Wagner*, *V. Madhavan*, *T. Hughes*, University of Illinois at Urbana Champaign

Two-dimensional transition metal dichalcogenide (TMD) materials exhibit a variety of novel quantum phenomena, including topological, superconducting, magnetic, and strongly correlated phases as monolayers and homo-, hetero-, and twisted bilayers. Unlike the exfoliation method, molecular beam epitaxy (MBE) of TMDs produces organics-free atomically pristine layers allowing surface-sensitive measurements. Local atomically resolved studies of such TMD platforms are crucial for unraveling their spatially dependent electronic properties. Here, we report a study of monolayer 1T' WTe₂, a quantum-spin-Hall (QSH) insulator and a superconductor, which has been studied extensively using magnetotransport and local-probe techniques previously. We performed an STM study of epitaxially grown monolayer WTe₂ imbedded in a device with back-gating capabilities. Using local density of states (LDOS) STM measurements and density functional theory (DFT) simulations, we gained new insights into 1D helical edge modes of WTe₂ and report their asymmetric spatial response to out-of-plane displacement fields. Such tunable spatial dependence gives new insights about harvesting spin-momentum-locked 1D modes of WTe₂ for energy-efficient devices, spintronics, and topological quantum computing applications. This talk will also address technical challenges of fabricating a device suitable for MBE and gate-tuned STM and epitaxial growth of high-quality monolayer TMDs on commercial CVD graphene.

12:00pm **NAMBE2-TuM-16 Phase-selective Growth of the Topological Insulators Bi₂Te₃ and Bi₄Te₃ for Integration with the Superconductor Fe(Te,Se)**, *Matthew Brahlek*, *J. Chen*, *J. Lu*, Oak Ridge National Laboratory; *R. Moore*, Oak Ridge Natinal Laboratory

Realizing exotic forms of superconductivity by epitaxially integrating high-transition-temperature (T_c) superconductors with topological insulators can open new paths for quantum-based applications. In this talk, we will discuss how molecular beam epitaxy can be used to controllably synthesize the topological insulators Bi₂Te₃ and Bi₄Te₃ by carefully controlling the flux ratio during growth. Alternatively, high-quality Bi₄Te₃ can readily be achieved by reducing Bi₂Te₃ post-growth. It is found that both phases can be integrated them with high T_c superconductor Fe(Te,Se) with sharp interfaces. In the low Se-doping regime, measurements of the electronic and crystalline structure reveal that a large electron transfer, epitaxial strain, and novel chemical reduction processes likely affect superconductivity at the interface of Fe(Te,Se) with Bi₄Te₃ compared to Bi₂Te₃. This novel route for epitaxial phase control at topological/superconducting interfaces provides new insight into the nature of unconventional superconductivity while being a new platform for identifying and utilizing new electronic phases.

12:15pm **NAMBE2-TuM-17 Origin of the high Curie Temperature in (Sb₂Te₃)_{1-x}(MnSb₂Te₄)_x structures grown by molecular beam epitaxy**, *Candice Forrester*, The Graduate Center (CUNY); *C. Testelin*, CNRS, France; *K. Wickramasinghe*, City College of New York, City University of New York; *S. Mohammadi*, The Graduate Center (CUNY); *M. Tamargo*, City College of New York, City University of New York

Previously we reported the growth of (Sb₂Te₃)_{1-x}(MnSb₂Te₄)_x magnetic topological materials with Curie temperatures (T_c) as high as 100K, much higher than reported values for these materials. They are formed by combining Mn, Sb and Te in molecular beam epitaxy (MBE) via self-assembly, where MnSb₂Te₄ septuple layers (SLs) and Sb₂Te₃ quintuple layers (QLs) form compositions (x) that depend on the growth parameters used. By reducing the growth rate to ~ 0.5 nm/min, from the previously used 0.9 nm/min, the highest T_c values were obtained for structures with 0.7 ≤ x ≤ 0.85.¹ Derivative curves of temperature dependent Hall resistance revealed the presence of two T_c components, T_{c1} about 20-25K and T_{c2} as high as 100K. Energy dispersive X-ray spectroscopy (EDS) data as a function of x suggests that excess Mn incorporation in our samples is responsible for the high T_c values. We have proposed that the lower T_{c1} originates from the MnSb₂Te₄ SLs of the structure, while the higher T_{c2} is associated with the formation of (Mn_ySb_{1-y})₂Te₃ QLs alloys.² However, direct evidence for this proposal is difficult to obtain due to the complex nature of the materials.

Although transition metal (TM) ternary alloys like (TM_ySb_{1-y})₂Te₃, where TM = Cr or V, have been demonstrated and shown to exhibit high T_c values, Mn

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alloys of Sb_2Te_3 , with $y > 0.03$, have not been experimentally realized. However, DFT simulations have predicted $(\text{Mn}_y\text{Sb}_{1-y})_2\text{Te}_3$ to have very high T_c as the Mn content increases.³ An alloy formation equation was derived $y = 1/2 [(5+2x) \chi_{\text{Mn}} - x]$, where χ_{Mn} is the Mn fraction in the samples obtained from the EDS data. This equation assumes that excess Mn incorporates into QLs and SLs equally and all the excess Mn is substituting for Sb. The equation was employed to fit our experimental data to the predicted data for samples with $0.7 \leq x \leq 0.85$. Although a good fit was observed for samples with low Mn content, samples with high Mn content deviated significantly from the simulated data. Here we explore modifications of the alloy formation equation to better describe the observed results. Specifically, a better fit to all the data is obtained when Mn substitution is not limited to only Sb sites, as seen when χ_{Sb} is used instead of χ_{Mn} . Other scenarios, such as Mn/Te substitution or Mn incorporation in the vdW gaps are also considered. Our results are consistent with the formation of $(\text{Mn}_y\text{Sb}_{1-y})_2\text{Te}_3$ with $y > 0.35$, much higher than ever obtained before, and bring us closer to achieving magnetic topological materials with T_c values for practical applications.

1. arXiv:2311.10891 (2023)
2. Sci Rep 13, 7381 (2023)
3. Phys. Rev. B 89, 165202 (2014)

NAMBE

Room Cummings Ballroom - Session NAMBE1-TuA

Oxides I

Moderator: Matthew Brahlek, Oak Ridge National Laboratory

2:00pm NAMBE1-TuA-1 Plasma Assisted Molecular Beam Epitaxial Growth of β -Ga₂O₃ (100) Thin Films on MgO(100) Substrates, Seth Hibbert, R. Reeves, M. Allen, University of Canterbury, New Zealand

Gallium oxide (Ga₂O₃) is a transparent conducting oxide undergoing active research for its many potential uses in power electronics. It has a larger breakdown field (~8MV/cm) and a larger bandgap (4.6 – 4.9 eV) than silicon carbide, a popular material for power electronics. Currently five phases of gallium oxide have been identified, these have been labeled the α , β , γ , δ , and ϵ phases. Of these phases, β -Ga₂O₃ is the most stable and thus the most commonly grown by epitaxial methods. β -Ga₂O₃ has a monoclinic structure (figure 1a in supplemental document) and can be either conducting or insulating depending on the conditions of the crystal growth. Due to the monoclinic structure of β -Ga₂O₃, the asymmetric unit cell leads to anisotropies in the structural, electrical and optical properties. The (-201) orientation of β -Ga₂O₃ can be easily grown on a variety of materials with c-plane sapphire being a common substrate for heteroepitaxy. The (100) orientation, however, has seen little research due to a relatively slow growth rate when grown heteroepitaxially via molecular beam epitaxy. In the work presented here, β -Ga₂O₃ thin films of ~90nm thickness, were grown on MgO(100) substrates using plasma-assisted molecular beam epitaxy. The films exhibited very smooth, epitaxial surfaces as measured by in-situ RHEED and atomic force microscopy after growth (figure 2). X-ray diffraction showed crystalline thin films having the (100) orientation and figure 3 shows a comparison with a (-201) oriented film grown under similar conditions on a c-plane sapphire substrate. It is apparent the (100) oriented film has excellent crystal quality with FWHM of the (400) peak measured as 0.280 degrees compared to 0.397 degrees for the (-402) peak. The films showed high transmission in the optical region with indications the (100) oriented film has a slightly lower bandgap energy (figure 4). While it is known epitaxial strain can change bandgap values, the excellent crystal quality suggests anisotropy of lattice directions is the probable cause.

2:15pm NAMBE1-TuA-2 Progresses Towards Production-Worthy Epitaxy of BaTiO₃ and SrTiO₃ Perovskites on Si(001) Substrates, Mark O'Steen, Veeco Instruments Inc.; M. Baryshnikova, G. Croes, IMEC, Belgium; Y. Wang, S. Farrell, G. Sundaram, Veeco Instruments Inc.; C. Merckling, IMEC, Belgium

Barium titanate (BaTiO₃ or BTO) exhibits a large, linear electro-optic effect (or Pockels effect), making it potentially useful for a variety of applications including datacom/telecom, LIDAR, and quantum computing. To be practical for such applications, it is advantageous to integrate BTO to a substrate material such as Si, which is readily available in large wafer sizes at low cost. Since BTO is chemically unstable in contact with Si, this integration requires the use of an intermediate strontium titanite (SrTiO₃ or STO) template.

BTO (using an STO buffer) can be grown on Si by several techniques; however, so far, only conventional, solid-source MBE (SS-MBE) produces material exhibiting a high Pockels coefficient due to higher crystalline quality. SS-MBE has only a small process window to produce high quality material due to the challenges in maintaining cation stoichiometry in STO and BTO. Alternatively, hybrid MBE (hMBE), in which the precursor Tetrakispropoxide (TTIP) is used as the Ti source, has a much larger process window to achieve stoichiometric STO and BTO perovskites due to the presence of self-regulating growth regimes.

In this study, we investigate the epitaxy and characteristics of STO and BTO thin films on Silicon by hMBE approach. A novel precursor delivery system, designed and optimized for use in hMBE, enabled optimizing the growth processes and methodologies for consistent deposition results. Epitaxial materials are characterized using several techniques including TEM, XRD, XRF, RBS, AFM, and electro-optical measurements. Finally, SS-MBE and hMBE growth of BTO will be compared and the growth characteristics and tradeoffs of the two techniques will be discussed. In particular, the potential and challenges for scaling to large diameter substrates and to develop the robust processes needed for manufacturing will be highlighted.

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2:30pm NAMBE1-TuA-3 Epitaxial Growth of Si-doped (Al, Ga)₂O₃ Films by Hybrid MBE, Zhuoqun Wen, E. Ahmadi, University of Michigan

The oxidation of Al metal source in the conventional oxide MBE requires frequent opening of the system to reload materials. A regular crucible filled with Al element can be depleting within 10 growth cycles. Additionally, oxidation of silicon source in these systems makes controlled and uniform Si-doping of Ga₂O₃ challenging. To overcome these challenges, we are using a hybrid MBE which uses conventional effusion cells for Ga and Ge, and gas sources to supply Al and Si. In this talk, we will give an overview of our custom-built gas delivery system with diluted disilane as Si source and TTBAL as Al source, and present our latest results on achieving AlGaO films with different Al compositions (1%-25%) by controlling TTBAL flow and Ga₂O₃ films with Si doping concentrations ranging from 4×10^{16} cm⁻³ to 2×10^{19} cm⁻³ concentrations with different disilane flows. Fig.1 shows the β -(Al_xGa_{1-x})₂O₃ grown by TTBAL at different flows at 525 °C, Ga beam-equivalent pressure (BEP) at 10⁻⁸ Torr, and O plasma 410W, 2 sccm. By increasing the TTBAL beam-equivalent pressure (BEP) from 1.1×10^{-7} Torr to 4.3×10^{-7} Torr, the Al incorporation increases from 1.8% to 14.9%. The Al composition can be further increased up to 25% by controlling the TTBAL flow and increasing the growth temperature. The electron properties of Si doped β -(Al_xGa_{1-x})₂O₃ grown by disilane and TTBAL will be studied.

2:45pm NAMBE1-TuA-4 Correlated Phase Diagram Tunable by Structural Layering in Square-Planar Nickelates, Grace Pan, D. Ferenc Segedin, S. TenHuisen, Harvard University; L. Bhatt, Cornell University; H. LaBollita, Arizona State University; A. Jiang, Harvard University; Q. Song, Cornell University; A. Turkiewicz, Harvard University; H. Paik, University of Oklahoma; C. Brooks, M. Mitran, Harvard University; B. Goodge, Max Planck Institute for Chemical Physics of Solids; A. Botana, Arizona State University; J. Mundy, Harvard University

Since the discovery of superconductivity in Sr-doped NdNiO₂¹, the identification of independent tuning parameters has further expanded the materials and correlated phases in this family of nickel-based compounds. One such knob has been the structural layering, which has been used to realize a superconducting phase in the five-layer square-planar nickelate Nd₅Ni₂O₁₂². In the square-planar Nd_{n+1}Ni_nO_{2n+2} compounds the primary role of layering is to provide a nominal doping level of 1/n electrons per nickel site. Nonetheless, one might expect substantial modification of the electronic structure, correlation effects, or even nominal doping levels from intentional restructuring of the atomic lattice. Here, we present the correlated phase diagram of the layered Nd_{n+1}Ni_nO_{2n+2} compounds. We observe a superconducting dome of clear resemblance to the chemically doped infinite-layer nickelates, indicating that structural layering can generally tune the electronic doping levels. This furthermore supports the potential universality of doping-dependent superconducting phases³⁻⁶. We discuss the role of layering beyond providing rigid doping shifts, including effects on correlations, spin fluctuations, and disorder.

¹Li, D. *et al.* Superconductivity in an infinite-layer nickelate. *Nature* **572**, 624–627 (2019). ²Pan, G. A. *et al.* Superconductivity in a quintuple-layer square-planar nickelate. *Nat. Mater.* **21**, 160–164 (2022). ³Lee, K. *et al.* Linear-in-temperature resistivity for optimally superconducting (Nd,Sr)NiO₂. *Nature* **619**, 288–292 (2023). ⁴Keimer, B. *et al.* From quantum matter to high-temperature superconductivity in copper oxides. *Nature* **518**, 179–186 (2015). ⁵Johnston, D. C. The puzzle of high temperature superconductivity in layered iron pnictides and chalcogenides. *Adv. Phys.* **59**, 803–1061 (2010). ⁶Cao, Y. *et al.* Unconventional superconductivity in magic-angle graphene superlattices. *Nature* **556**, 43–50 (2018).

3:00pm NAMBE1-TuA-5 Synthesis of Layered Square-planar Lanthanum Nickelate Thin Films, La_{n+1}Ni_nO_{2n+2}, Dan Ferenc Segedin, G. Pan, A. Turkiewicz, A. Jiang, C. Brooks, J. Mundy, Harvard University

The layered square-planar nickelates, R_{n+1}Ni_nO_{2n+2} (R = trivalent rare-earth cation and n > 1), are an exciting platform to tune the properties of superconducting square-planar nickelates via dimensionality [1-2]. To date, superconducting Nd_{n+1}Ni_nO_{2n+2} films have been achieved only on NdGaO₃ due to the competing requirements for the synthesis of the precursor Ruddlesden-Popper, Nd_{n+1}Ni_nO_{3n+1}, and reduction to the square-planar phase [3]. On SrTiO₃, the high tensile strain in the precursor phase, Nd_{n+1}Ni_nO_{3n+1}, leads to a high density of stacking faults [3]. Improved crystalline quality and an enhanced superconducting transition temperature have been achieved in (Nd,Sr)NiO₂ on LSAT by lowering the tensile strain in the parent perovskite phase [4]. Here, we investigate the role of epitaxial strain in the synthesis of Lanthanum-based layered nickelates on NdGaO₃. We demonstrate a substantially higher crystalline quality in La_{n+1}Ni_nO_{3n+1} on NdGaO₃ than Nd_{n+1}Ni_nO_{3n+1}, due to the lower

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tensile strain. Finally, we discuss the reduction to the square-planar phase on NdGaO₃.

[1] Li, D. *et al.* Superconductivity in an infinite-layer nickelate. *Nature* 572, 624–627 (2019).

[2] Pan, G. A. *et al.* Superconductivity in a quintuple-layer square-planar nickelate. *Nat Mater* 1–5 (2021).

[3] Ferenc Segedin, D. *et al.* Limits to the strain engineering of layered square-planar nickelate thin films. *Nat. Commun.* 14, 1468 (2023).

[4] Lee, K. *et al.* Linear-in-temperature resistivity for optimally superconducting (Nd,Sr)NiO₂. *Nature* 619, 288–292 (2023).

*US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under award no. DE-SC0021925

NAMBE

Room Cummings Ballroom - Session NAMBE2-TuA

Oxides II

Moderator: Zach Cresswell, Idaho National Laboratory

3:45pm **NAMBE2-TuA-8 Signatures of Bosonic Coupling in Superconducting LiTi₂O₄ Thin Films**, *Zubia Hasan, G. Pan*, Harvard University; *M. Barone*, Cornell University; *C. Brooks*, Harvard University; *A. Kaczmarek*, Cornell University; *S. Sung*, Harvard University; *E. Mercer*, Northeastern University; *S. Sharma*, Arizona State University; *I. El Baggari*, Harvard University; *K. Nowack*, Cornell University; *A. Botana*, Arizona State University; *B. Faeth*, Cornell University; *A. De La Torre Duran*, Northeastern University; *J. Mundy*, Harvard University

The mechanisms behind unconventional superconductivity have been intensely studied over the past few decades. Leading this thrust has been the high T_c cuprates, whose pairing ‘glue’ has been widely debated. LiTi₂O₄, a spinel oxide material, is an unconventional superconductor that preceded the cuprates [1]. However, despite having one of the highest T_c (~13.7 K) for a non-cuprate oxide, little is known about its superconducting mechanism, with reports of both unconventional pairing [2] and traditional phonon-mediated BCS-like behavior [3]. There have also been signs of orbital and spin fluctuations persisting up to ~100 K, based on angle-dependent transport data [4]. Nevertheless, it remains unclear which mechanisms—spin fluctuations, electron-phonon coupling or mixed valency—are essential for superconductivity in LiTi₂O₄. Despite interest in this compound, the direct visualization of its band structure has been inhibited due to the difficulty of cleaving the highly three dimensional single crystals of LiTi₂O₄. Here, we utilize a novel approach to incorporate Li in a Molecular Beam Epitaxy (MBE) system and synthesize phase pure, highly crystalline LiTi₂O₄ thin films for the very first time via MBE. The atomically smooth surfaces that are enabled by MBE growth allow us to interrogate the electronic band structure via Angle Resolved Photoemission Spectroscopy (ARPES) experiments. Our work reveals the presence of strong bosonic coupling in the compound. The bands intriguingly show a kink resembling cuprate-like band renormalizations. Our data indicates strong correlations: the band centered at Γ shows a ‘kink’ at around E_g~40 meV and a quasi-particle peak and incoherent tail suggestive of coupling to a bosonic mode. We see that this mode is present at all values of k_F and k_Z and persists above T_c. We discuss the origin of the kinks in LiTi₂O₄, providing broader insight into the pairing symmetry present in this superconducting system.

[1] D. C. Johnston *et al.*, *Mater. Res. Bull.* 8, 777–784 (1973).

[2] H. Xue *et al.*, *ACS Nano* 16 (11), 19464 (2022).

[3] C. P. Sun *et al.*, *Phys. Rev. B* 70, 054519 (2004).

[4] K. Jin. *et al.*, *Nat. Commun.* 6, 7183 (2015)

*US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM). Paul & Daisy Soros Fellowship for New Americans. NSF Graduate Research Fellowship Grant No. DGE-1745303. Packard Foundation and the Gordon and Betty Moore Foundation’s EPIQS Initiative, grant GBMF6760

4:00pm **NAMBE2-TuA-9 Defect Engineering in Thin Films of the Pyrochlore Frustrated Magnet Tb₂Ti₂O₇**, *Margaret Anderson, I. El Baggari, C. Brooks, T. Powell*, Harvard University; *C. Lygouras*, Johns Hopkins University; *A. N’diaye*, Lawrence Berkeley National Laboratory; *S. Koohpayeh*, Johns Hopkins University; *J. Nordlander*, Paul Drude Institute, Germany; *J. Mundy*, Harvard University

Among the pyrochlore oxides, the frustrated magnet Tb₂Ti₂O₇ has drawn intense interest as a spin liquid candidate. Its unusual magnetic properties rely on a careful balance of interactions on the frustrated pyrochlore lattice and are exquisitely sensitive to composition. Using reactive-oxide molecular beam epitaxy, we synthesize Tb₂Ti₂O₇ thin films on (111)-oriented YSZ substrates and probe their structural and magnetic properties. Single-phase pyrochlore thin films are realized within a large growth window at up to 25% off-composition. Using both scanning transmission electron microscopy and electron energy loss spectroscopy, we investigate defect formation with varying film stoichiometry. Titanium-rich films incorporate titanium excess via antistuffing of both Ti³⁺ and Ti⁴⁺ locally along slanted <112> antiphase boundaries. In contrast, excess terbium is directly incorporated into the film through homogeneous stuffing and terbium-rich films exhibit mostly <111> antiphase boundaries. DC magnetic susceptibility measurements suggest that defects reduce the frustration index of Tb₂Ti₂O₇, with titanium and terbium excess both leading to an enhanced saturated magnetic moment and less negative Curie–Weiss temperature compared to the stoichiometric film, while all films remain paramagnetic down to 1.8K.

4:15pm **NAMBE2-TuA-10 Soft Chemical Manipulation of MBE-Synthesized Ruddlesden-Popper Nickelates**, *Abigail Jiang, A. Turkiewicz, G. Pan, D. Ferenc Segedin, C. Brooks, J. Mason, J. Mundy*, Harvard University

Recent observations of nickelate superconductivity have established the Ruddlesden-Popper (RP) Ln_{n+1}Ni_nO_(3n+1) and square-planar Ln_{n+1}Ni_nO_(2n+2) series as important comparisons to the high-T_c cuprates. Both theory and experiment suggest that lower dimensional phases may lead to higher critical temperatures. However, existing soft-chemical methods to achieve a cuprate-like d⁹ configuration (i.e. deintercalation of apical oxygens to achieve the square-planar phase) do not apply to the most dimensionally confined n=1 RP due to stoichiometric limitations, prompting alternative chemical modifications to tune electronic structure of RP nickelates. Here, we synthesize low dimensional RP nickelate thin films via atomically precise, reactive-oxide MBE with chemical doping and tunable strain states on a variety of substrates. We also demonstrate new soft-chemical, topotactic methods to modify the anion sublattice with commensurate and promising changes in electronic structure.

4:30pm **NAMBE2-TuA-11 BaTiO₃ Films for Integrated Electro-Optics**, *Larissa Little, B. Fazlioglu-Yalcin, A. Cavanagh, N. Sinclair, T. Zulu, K. Powell, C. Brooks, R. Westervelt, M. Loncar*, Harvard University; *D. Barton*, Northwestern University; *J. Mundy*, Harvard University

Barium titanate has been identified as a promising electro-optic material for wider-scale adoption of integrated electro-optic modulators and other integrated photonic devices. Currently, electro-optic modulators are often bulk crystals of lithium niobate with indiffused waveguides, limiting their size, speed, and efficiency. Although thin film lithium niobate offers improved scalability and higher bandwidth over its bulk counterpart, lithium oxides are not CMOS compatible and there is a growing need for higher bandwidth modulators with lower voltage requirements. Barium titanate is an alternative material platform which exhibits an extremely high electro-optic coefficient (r₄₂ ~ 900 pm/V), a reasonably high band gap (> 3eV), a relatively high refractive index (n = 2.4), and is compatible with traditional CMOS processing. Scalable methods for creating high quality, single ferroelectric domain films of barium titanate are therefore extremely attractive for highly efficient modulators and integrated optical devices. Here we use molecular beam epitaxy to grow barium titanate films and characterize the defects and effects that stoichiometry and strain changes have on their properties.

4:45pm **NAMBE2-TuA-12 Exploration of Erbium-Doped Oxide Thin Films on Silicon for Quantum Memory-Oriented Nanophotonics Development**, *Ignas Masulionis*, University of Chicago/Argonne National Laboratory; *G. Grant*, University of Chicago; *R. Chebrolu*, University of Chicago / Argonne National Laboratory; *A. Dibos, J. Zhang, F. Heremans, S. Guha*, Argonne National Lab

Trivalent erbium ions (Er³⁺) are promising defects for developing photon-enabled quantum communication technology due to their emission at telecom wavelengths (~1.5 μ m). Certain classes of materials present appealing conditions for hosting erbium defects for quantum

communication, such as oxides having the potential for long spin defect coherence times [1]. Titanium dioxide (TiO_2), in particular, has been investigated as an erbium host due to its ease of fabrication and well-known optical properties; certain complex oxides similarly have been chosen due to their low (<2%) in-plane lattice mismatch with silicon. Here, we discuss the growth and post-growth treatment of these materials for use in nanophotonics and eventual integration with quantum communication technologies, focusing on key metrics such as host surface roughness and Er^{3+} spectral diffusion linewidths. We identify particular optimizations that may be made, for example, that post-growth anneals at moderate temperatures can narrow Er^{3+} spectral diffusion linewidths in TiO_2 without significant roughening of the film. Additional spectroscopy (photoluminescence excitation (PLE) spectroscopy and transient spectral holeburning (TSHB)) plus traditional materials characterization (X-ray diffraction (XRD), atomic force microscopy (AFM)) allow us to ensure the crystalline host quality is suitable for ongoing quantum memory device development.

[1] S. Kanai, et al. PNAS. 119, e2121808119 (2022).

Funding Acknowledgment: This work is primarily supported by Q-NEXT, a U.S. Department of Energy Office of Science National Quantum Information Science Research Center, with additional support from the U.S. Department of Energy Office of Science Basic Energy Sciences, Materials Sciences and Engineering Division.

5:00pm **NAMBE2-TuA-13 Simultaneous Optical and Microstructural Characterization of Er-Doped CeO_2 on Silicon**, **Gregory Grant**, University of Chicago; *J. Zhang*, Argonne National Laboratory; *I. Masiulionis*, University of Chicago; *S. Chattaraj*, *K. Sautter*, Argonne National Laboratory; *S. Sullivan*, memQ; *R. Chebrolu*, University of Chicago; *Y. Liu*, *J. Martins*, *J. Niklas*, *A. Dibos*, Argonne National Laboratory; *S. Kewalramani*, Northwestern University; *J. Freeland*, *J. Wen*, *O. Poluektov*, *F. Heremans*, Argonne National Laboratory; *D. Awschalom*, University of Chicago; *S. Guha*, Argonne National Laboratory

Erbium-doped cerium dioxide ($\text{Er}:\text{CeO}_2$) is a promising defect-host combination for applications in quantum memories and single photon emitters for wide-area fiber optic-based quantum networks. This is due to the combination of the telecom-compatible ($\sim 1.5 \mu\text{m}$) 4f-4f transition of Er, the predicted long electron spin coherence time of defects in CeO_2 [1], and the small lattice mismatch between silicon and CeO_2 . Here we report on the epitaxial growth of low-doped $\text{Er}:\text{CeO}_2$ thin films on silicon using molecular beam epitaxy (MBE), with controlled Er concentration in the 1-100 ppm regime. We verify the CeO_2 host structure via thorough microstructural study, and in tandem characterize the spin and optical properties of the embedded Er^{3+} ions as a function of doping density. This allows identification of trends that can enable quantum memory technologies, and simultaneously yields insights into what improvements must be made to the thin films for these applications. Notably for quantum memories, when studying the Er^{3+} Z_1 - Y_1 optical transition near 1530 nm at liquid helium temperatures, we find spectral diffusion-limited homogeneous linewidths as narrow as 5 MHz [2], a promising result towards quantum memory technologies. Based on our study, we discuss routes towards improvement of the optical and spin linewidths via growth optimization and post-growth treatment of the $\text{Er}:\text{CeO}_2$ films.

[1] S. Kanai, et al., PNAS. 119, e2121808119 (2022).

[2] G. Grant, et al., APL Mater. 12, 021121 (2024).

Funding Acknowledgment: This work is primarily supported by Q-NEXT, a U.S. Department of Energy Office of Science National Quantum Information Science Research Center, with additional support from the U.S. Department of Energy Office of Science Basic Energy Sciences, Materials Sciences and Engineering Division.

NAMBE

Room Cummings Ballroom - Session NAMBE1-WeM

Nitrides

Moderator: Kevin Vallejo, Idaho National Laboratory

8:15am **NAMBE1-WeM-1 Welcome & Sponsor Thank You,**

8:30am **NAMBE1-WeM-2 Tunnel Junction Engineered MBE-grown Nanowires: Toward Self-Powered, Dual-Wavelength Photoelectrochemical Photodetectors for Secure and Efficient Underwater Wireless Sensors Networks, S. Zhao, Milad Fathabadi,** McGill University, Canada

The development of underwater wireless sensor networks (UWSNs) is increasingly critical for monitoring the ocean environment, where the demand for robust, secure, and energy-efficient technologies is at its highest peak. Self-powered, wavelength-distinguishable photodetectors (PDs) are appealing to meet the demands of UWSNs, offering low energy consumption and maintenance costs and enabling complex data encryption via light. The self-powered and wavelength-distinguishable photodetection can be more easily achieved with photoelectrochemical (PEC) PDs, thanks to their operating principle that leverages semiconductor-electrolyte interactions that offer greater flexibility in tuning the photoresponse. Semiconductor p-n heterojunctions with suitable bandgaps could enable wavelength-distinguishable photodetection based on photocurrent polarity (negative for p-type and positive for n-type). However, the built-in electric field at the p-n junction prevents reaching the desired dual photocurrent polarity (Figure S1a).

Herein, we designed a III-nitride nanowire p-n heterojunction embedded with a tunnel junction (TJ) to overcome this challenge, and achieved the first self-powered, wavelength-distinguishable PEC-PDs. The TJ not only reverses the direction of the unfavorable electric field but also facilitates the transport of photogenerated carriers (Figure S1b). Figure S1c shows the STEM images of high-quality n-GaN/p-InGaN nanowires with a n⁺-GaN/InGaN/p⁺-GaN TJ embedded for UV-visible wavelength detection, and the response is shown in Figure S1d. It is seen that, self-powered, wavelength-distinguishable photodetection is obtained at 405 and 302 nm. Moreover, our devices exhibit high responsivities in the mA/W range for both wavelengths, with ultrafast response times of less than 10 ms for 405 nm and 20-30 ms for 302 nm light. The ability of this PEC-PD to function without external electrical power and to distinguish between UV and blue light wavelengths paves the way for more secure data transmission in UWSNs with blue light, the most transparent wavelength in the ocean.

8:45am **NAMBE1-WeM-3 MBE Growth of n-type AlN and Defect Characterization Using Deep UV Photoluminescence, Neeraj Nepal, M. Hardy, A. Lang, B. Downey, D. Katzer, E. Jin, V. Gokhale, T. Growden, D. Meyer, V. Wheeler,** Naval Research Laboratory

AlN has a bandgap of ~6.2 eV resulting in a large critical electric field breakdown (>15 MV/cm), leading to a higher Baliga's and Johnson's figure-of-merit for power and RF devices, respectively. Further, AlN possesses a high saturation velocity (~2x10⁷ cm/s) and high thermal conductivity (~319 Wm⁻¹K⁻¹). Realizing the full potential of this material in electronic devices requires the ability to tailor the electrical conductivity in active AlN layers through impurity doping.

Due to the large bandgap and lower formation energy of native point defects, which serves as carrier compensating centers, impurity doping in AlN has been challenging, and thus there is limited understanding of how to control and implement repeatable impurity doping in AlN-based devices. Deep ultraviolet photoluminescence (DUVPL) is a crucial tool to understand and optimizing the AlN growth process for electrical applications, allowing for the correlation of impurity defects, near-bandedge emission bands and conductivity.

In this presentation, we report on the growth of ~300 to 500 nm thick Si-doped AlN films by plasma-assisted molecular beam epitaxy (MBE). The AlN thin films were grown on AlN/sapphire and bulk AlN templates from different vendors using a metal modulated epitaxy approach and studied the resulting films using room temperature DUVPL, x-ray diffraction (XRD), atomic force microscopy (AFM) and van der Pauw resistivity measurements. Cross-sectional transmission electron microscopy (TEM) measurements were carried out on selected samples along (1 0 1̄ 0) and (1 1 2̄ 0) orientations to assess the epitaxial material quality and defect density.

All AlN substrates underwent an ex-situ chemical clean and in-situ Al-absorption and desorption technique before nucleating AlN films. The evolution of the substrate surface during the in-situ clean was monitored with reflection high-energy electron diffraction and verified to be oxygen free using TEM and electron energy loss spectroscopy. DUVPL measurements of MBE AlN layers, using above bandgap excitation (at 6.458 eV), show that unintentionally-doped AlN films have strong band-edge emission and no impurity bands. After Si doping, an impurity band near 3.67 eV due to an Al-vacancy Si-complex appears and band-edge emission at 6.03 eV (for AlN/sapphire) decreases. Van der Pauw resistivity measurements show that the AlN:Si films grown at optimized growth conditions on all substrates are conductive. For AlN layers grown under similar conditions, conductive AlN films have lower intensity impurity bands. Results correlating DUVPL, XRD, AFM, TEM and resistivity measurements for the full parameter space will be discussed.

9:00am **NAMBE1-WeM-4 Evolution of AlN: from 1 nm Nitridation to 2 μm by Molecular Beam Epitaxy, M. Liao, D. Luccioni, K. Huynh, Y. Wang, L. Matto,** University of California Los Angeles; **H. Ahmad,** Georgia Institute of Technology; **Z. Zhang,** Argonne National Laboratory; **W. Doolittle,** Georgia Institute of Technology; **Mark Goorsky,** University of California Los Angeles
The structural evolution of AlN from ~1 nm nitridation on (0001) sapphire followed by up to 2 μm of molecular beam epitaxial growth at 800 °C was studied. An ~80 nm Al cap was deposited for each sample after nitridation or epitaxial growth of various AlN thicknesses. In-situ, post-growth annealing at 800 °C improved the structural characteristics of the AlN. The structures are important for understanding the role of interfacial defects on thermal transport across AlN interfaces.

The initial nitridation of the sapphire substrate surface produced a 1.6 nm AlN layer. Synchrotron X-ray measurements revealed only {0001} surface planes and a narrow (0002) rocking curve width of ~30°. The (0001) orientation was maintained during subsequent AlN growth. This contrasts with AlN growths on non-nitrided sapphire where (0001) and (101̄2) islands formed [1] initially. We show nitridation of (0001) sapphire enables only (0001) AlN formation and hinders the nucleation of other orientations, resulting in less defective AlN|Al₂O₃ interfaces. Symmetric X-ray rocking curves for all thicknesses of AlN exhibit two-peak components. Two-peak-component rocking curves have been reported by other studies [2], but the components' characteristics had not previously been determined. By observing the behavior of each rocking curve component at different orders of {0001} symmetric reflections, it is ascertained that one component is attributed to lattice tilt (~30° for 1.6 nm to 230 nm AlN films) or mosaic and the other is due to lateral coherence length (which increases with increasing AlN thickness). In situ annealing at the growth temperature resulted in further rocking curve width reduction for the broad component, which corresponds to longer coherence lengths and therefore higher quality material as well. More insightfully, the improvement in film quality is due to the time spent at elevated temperatures rather than the act of growing thicker films. For example, the broad component width of the as-grown 68 nm film was 640° and decreased to 480° after annealing at the growth temperature to match the growth time to achieve a 120 nm thick film. The annealed 68 nm film width matched the as-grown 120 nm film peak width. Studying the evolution of films from ~1 nm to μm regime is essential towards refining epitaxial growth strategies and understanding the role of structural characteristics on the thermal transport across interfaces.

The authors acknowledge support from the Office of Naval Research, grant No. N00014-18-1-2429.

[1] J.R.Heffelfinger, et al., J.Appl.Phys., 85(1) 466 (1999).

[2] J.Wang, et al., Scientific Reports, 7 42747 (2017).

9:15am **NAMBE1-WeM-5 Addressing the High Coercive Field of ScAl₂N₃ via Magnesium Doping in Molecular Beam Epitaxy, Samuel Yang, D. Wang, D. Wang, Z. Mi,** University of Michigan, Ann Arbor

Wurtzite nitride ferroelectrics have been the centre of much attention since their experimental introduction in 2019. The incorporation of rare earth elements, such as Sc and Y, into the conventional III-nitride materials AlN and GaN can transform them into ferroelectric materials by flattening the energy landscape for polarity switching between the metal-polar and nitrogen-polar states. Compared to conventional oxide ferroelectrics, these materials have been shown to offer higher Curie temperatures, larger remanent polarisations, and greater scalability. Advances in molecular

beam epitaxy (MBE) have led to demonstrations of high-quality monocrystalline $\text{Sc}_x\text{Al}_{1-x}\text{N}$ and $\text{Sc}_x\text{Ga}_{1-x}\text{N}$. Together with amplified piezoelectricity and optical activeness, these materials harbour great promise for next-generation reconfigurable electronics and optoelectronics, memory, and piezoelectric and acoustic devices. Despite these prospects, ferroelectric nitrides face numerous challenges, especially considering stringent demands within the modern semiconductor industry. Among these challenges is the high coercive field (E_c) of $\text{Sc}_x\text{Al}_{1-x}\text{N}$. Although some technologies benefit from higher E_c , the increased switching voltage can promote defect formation and accumulation, as well as exacerbate leakage currents and diminish endurance cycles. As a first step towards realising $\text{Sc}_x\text{Al}_{1-x}\text{N}$ with lower E_c , an investigation into the epitaxial growth and ferroelectric properties of Mg-doped $\text{Sc}_x\text{Al}_{1-x}\text{N}$ is performed. Samples of $\text{Sc}_{0.2}\text{Al}_{0.8}\text{N}$ doped with various concentrations of Mg are grown via plasma-assisted MBE on a GaN-on-sapphire template. Reflection high-energy electron diffraction (RHEED) and atomic force microscopy (AFM) confirm excellent crystallinity and morphology, with surface *rms* roughness of ~ 0.5 nm over $25 \mu\text{m}^2$ scan areas across multiple samples. Quasi-static J-E (current density vs electric field) measurements reveal clear reduction in E_c with Mg incorporation. Further P-E (polarisation vs electric field) measurements corroborate unambiguous ferroelectric switching and demonstrate moderate remanent polarisations of ~ 70 - $80 \mu\text{C cm}^{-2}$. The initial demonstration of Mg-doped $\text{Sc}_x\text{Al}_{1-x}\text{N}$ to ameliorate faced challenges opens exciting new avenues through which nitride ferroelectrics can be tuned and enhanced for multifarious applications via doping engineering. Further study is anticipated to optimise the effects of and unveil the mechanisms behind E_c reduction with Mg doping.

9:45am **NAMBE1-WeM-7 Epitaxial Integration of Transition-Metal Nitrides with Cubic Gallium Nitride**, *Zach Cresswell, N. Fessler, T. Garrett, K. Vallejo, B. May*, Idaho National Laboratory

GaN is ubiquitous in the optoelectronics industry in its thermodynamically stable wurtzite structure, but it also has a metastable zinc blende allotrope that is less explored and more difficult to synthesize. One of the potential advantages of cubic-GaN (c-GaN) is the simplified interfacial symmetry with the other cubic transition metal nitrides, which are of interest for an assortment of applications requiring high chemical and thermal stability, high hardness, superconductivity, or plasmonic properties. The shared cubic symmetry would allow for easier integration of the nitrides with a wide-bandgap semiconductor.

This work will discuss the synthesis of epitaxial c-GaN on 3C-SiC substrates and its integration with known superconducting nitrides via molecular beam epitaxy. The hexagonal-free nature of the c-GaN, and the epitaxial relationship of it and the transition metal nitrides, are confirmed via *in-situ* reflection high energy electron diffraction, *ex-situ* X-ray diffraction, photoluminescence, and transition electron microscopy. The electrical transport of the transition metal nitrides grown on c-GaN(001) is compared to growth directly on 3C-SiC(001) and c-plane hexagonal GaN. Epitaxial synthesis of cubic wide-bandgap and superconducting metallic nitrides under similar growth conditions opens a new world of possibilities in band engineering, as well as the ability to create new device structures for areas such as metamaterials, quantum computing, and condensed matter physics.

10:00am **NAMBE1-WeM-8 Epitaxial Growth of High ScN Fraction ScAlN on (111) Si**, *Matthew Hardy, E. Jin, N. Nepal, B. Downey, V. Gokhale, D. Katzer, V. Wheeler, V. Wheeler*, U.S. Naval Research Laboratory

ScAlN thin films have attracted significant attention due to their $5\times$ increase in piezoresponse over AlN for $\text{Sc}_x\text{Al}_{1-x}\text{N}$ compositions of $x = 0.43$ [1], leading to applications in 5G filters and RF electronics. Epitaxial growth of ScAlN on Si enables the use of mature MEMS processing technology.

In this work, we demonstrate the growth of $\text{Sc}_x\text{Al}_{1-x}\text{N}$ layers on AlN nucleation layers (NL) on 100-mm (111) Si wafers with x up to 0.40 using MBE. AlN NLs with III/V ratios of 0.5 and 0.8 show polycrystalline ring segments in reflection high-energy electron diffraction (RHEED), III/V of 0.93 gives a streaky RHEED pattern with slight spot-modulation and no apparent etching of the Si substrate, seen in AlN with III/V > 1. Subsequent growth of $\text{Sc}_{0.40}\text{Al}_{0.60}\text{N}$ layers exhibit similar features to the underlying AlN NL, with a single phase wurtzite RHEED pattern only for the AlN III/V = 0.93 sample.

Several ScAlN samples were grown at 410 °C, varying both the Sc and Al flux to allow changes in the III/V ratio for a fixed composition. At low III/V ≤ 0.8 , rings appear in the RHEED pattern suggesting the presence of polycrystalline domains. At III/V around 0.95, the ScAlN RHEED is free of extraneous features. At III/V ≥ 1.0 the RHEED pattern broadens and forms

indistinct dual-ring-segments. This is the first demonstration of both a lower and upper bound to the high ScN fraction growth space, as well as identification of characteristic RHEED patterns, and is distinct from the III/V ratio behavior at low ScN fraction ($x \leq 0.2$).

A graded ScAlN nucleation layer, previously demonstrated for ScAlN/SiC, is further investigated for ScAlN on Si. A 25-nm grade from $x = 0.3 \rightarrow 0.38$ reduces the 0002 X-ray diffraction (XRD) rocking curve full-width at half maximum (FWHM) from 0.90° to 0.73° , and reduces the film stress from 0.92 to 0.59 GPa. Increasing the grade thickness for a fixed total thickness of 133 nm leads to a small reduction in FWHM (0.71°) and stress (0.46 GPa) for a 75 nm grade, with little change for a 115 nm grade.

An optimized ScAlN/AlN/Si sample, having a 10-nm AlN NL, a 20-nm graded 0.32 to 0.40 ScAlN nucleation layer, and a 100-nm $\text{Sc}_{0.40}\text{Al}_{0.60}\text{N}$ layer, shows a clean wurtzite RHEED pattern throughout growth, a FWHM of 1.1° , and an *rms* roughness of 0.57 nm. Atomic force microscopy height and phase images show no indication of anomalously oriented grains. Such thin, high structural and phase purity films are well suited to high frequency RF MEMS applications.

[1]M. Akiyama, K. Kano, and A. Teshigahara, *Appl. Phys. Lett.*, **95**, 162107 (2009).

NAMBE

Room Cummings Ballroom - Session NAMBE2-WeM

IR Materials and Devices (and SiGeSn)

Moderator: Carolina Adamo, Northrop Grumman

10:45am **NAMBE2-WeM-11 Characterization of Random Alloy $\text{Al}_{0.85}\text{Ga}_{0.15}\text{As}_{0.07}\text{Sb}_{0.93}$ for Mid-Wave Infrared Avalanche Photodiodes**, *Nathan Gajowski, M. Muduli, T. Ronningen, S. Krishna*, Ohio State University

The success of Short-Wave Infrared (SWIR) linear mode Avalanche Photodiodes (APDs) has created a growing interest in creating Mid-Wave Infrared (MWIR) photodetectors with gain. Creating effective MWIR linear mode APDs has the potential to increase the signal to noise ratio of an infrared receiver system by reducing the effect of the read-out circuit noise. To reduce the Size, Weight, Power, and Cost (SWaP-C) of these systems, III-V solutions are being researched as an alternative to the industry standard Mercury Cadmium Telluride (MCT) devices which must operate at low temperatures that require bulky and costly cryogenic cooling. These III-V APDs implement a Separate Absorption Charge and Multiplication (SACM) design to achieve these higher operating temperatures. III-V material systems also offer the advantage of higher yield and therefore lower production cost than MCT devices. AlInAsSb on GaSb has shown promise as an electron multiplier but has a high conduction band offset electrons must overcome when transiting from the MWIR absorber to the multiplier region. This band offset requires complicated grading to enable the carrier transport. AlGaAsSb on GaSb is alternative multiplier in which hole impact ionization dominates, and there is very little valence band offset between the required absorbers. The impact ionization coefficients of high band gap AlGaAsSb on GaSb have been reported, but only for thin multiplication regions [1]. In this study, we grew 600 nm thick $\text{Al}_{0.85}\text{Ga}_{0.15}\text{As}_{0.07}\text{Sb}_{0.93}$ NIP and PIN devices to study the gain properties in thick layers of this material. One of the key parameters that we want to optimize is the background concentration. A low background concentration is required to maintain a flat electric field profile in the multiplier. We chose to study a thicker multiplier as thicker layers of AlAsSb on InP have shown reduced excess noise over thin layers despite the dead space effect [2].

The $\text{Al}_{0.85}\text{Ga}_{0.15}\text{As}_{0.07}\text{Sb}_{0.93}$ material was grown using MBE as a random alloy for simplicity with a growth rate of $1 \mu\text{m/hr}$ at 500 °C. Using ex-situ material characterization feedback, the optimal total V/III and As/Sb BEP flux ratios were determined to be 4.8 and 16.8, respectively. We achieved a background doping of $< 1 \times 10^{16} \text{ cm}^{-3}$ as extracted from capacitance measurements. Sub 2 \AA RMS surface roughness's were achieved for device growths with 20 nm GaSb caps over a $5 \times 5 \mu\text{m}$ area as measured by atomic force microscopy. Devices were fabricated and tested using dark and illuminated current-voltage (IV) measurements to extract the gain mechanics of the material.

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11:00am **NAMBE2-WeM-12 Comparison Study of InAs/InAsSb and InAs/GaSb Type-II Superlattices**, Allison McMinn, Z. Ju, X. Liu, Y. Zhang, Arizona State University

Type-II superlattices (T2SLs) have been extensively studied for their IR applications in sensing and imaging. An early T2SL of interest was InAs/GaSb, which is predicted theoretically to have superior performance to leading HgCdTe technology [1]. Utilizing conventional InAs/GaSb T2SLs in photodetector applications has become challenging due to the short carrier lifetime of ~ 90 ns [2]. An alternative, Ga-free InAs/InAsSb T2SL was discovered experimentally to have improved performance over conventional InAs/GaSb T2SLs due to its much-improved carrier lifetime [3]. To our knowledge, a direct experimental comparison of these two T2SL materials has not been reported in the literature. This abstract reports a side-by-side comparison of these two types of T2SLs to evaluate the differences in their fundamental material properties.

A Ga-free and a conventional T2SL structure were grown consecutively via MBE. Samples were designed with similar electron-hole wavefunction overlaps and bandgaps. A 1- μm thick absorber consisting of a Ga-free or a conventional T2SL with a 10 nm GaSb cap was grown on GaSb substrates with a GaSb buffer. HR-XRD patterns for the T2SLs show sharp satellite peaks, indicating uniform layer thicknesses of the SL periods and close strain balance between constituent layers. The Ga-free T2SL also showed a nearly perfect overlap between the substrate peak and the T2SL 0th order peak.

PL spectra, measured with a FTIR spectrometer, showed a peak wavelength of 4.74 μm and 4.40 μm for the Ga-free and conventional T2SL at 12 K, respectively. The slopes of the integrated-PL-intensity vs. excitation-density plots show that radiative recombination dominates under excitation over 1 W/cm² at 12 K for the conventional T2SL. Over 77 K, the PL from the conventional T2SL is weak under excitations between 0.1 ~ 1 W/cm² and SRH recombination dominates. Above 1 excitation a mixture of SRH and radiative recombination is observed. In contrast, the Ga-free T2SL shows radiative recombination dominates under excitation between 0.1 ~ 1 W/cm² and Auger recombination dominates under 1 ~ 10 W/cm² excitation, below 77K. Additionally, SRH recombination begins to dominate at 150 K below 1 W/cm² in the Ga-free T2SL and radiative recombination still dominates above 1 W/cm². These findings are consistent with previously reported results where carrier lifetime in Ga-free T2SLs was found to be longer [3] due to low non-radiative defect density [4], so the photogenerated carrier concentration is higher than conventional T2SLs, offering an advantage in device applications. A comparison of the absorption coefficients and carrier lifetimes will be reported at the conference.

11:15am **NAMBE2-WeM-13 Use of Hydrogen Plasma to Increase Minority Carrier Lifetime in InAs_xSb_yBi_{1-x-y}**, F. Estevez Hilario, M. Bergthold, University of Texas at Austin; Oleg Maksimov, H. Bhandari, Radiation Monitoring Devices; C. Morath, A. Duchane, P. Webster, Air Force Research Laboratory; D. Wasserman, University of Texas at Austin

InAs_xSb_yBi_{1-x-y} is of interest for the fabrication of mid-wavelength and long-wavelength infrared (MWIR and LWIR) detectors. It can be grown lattice-matched to commercially available large area GaSb substrates while its bandgap energy can be tuned from 0.32 eV to 0.10 eV (4 μm to 12 μm).

InAs_xSb_yBi_{1-x-y} is grown by Molecular Beam Epitaxy (MBE). However, the desired Bi incorporation into the InAs_xSb_y lattice can be accomplished only at low growth temperatures of < 400 °C, below the optimal growth temperature for III-V semiconductors [1]. The low growth temperature results in the formation of point defects in the InAs_xSb_yBi_{1-x-y} lattice degrading its optical quality and reducing the minority carrier lifetime. Hence, to realize InAs_xSb_yBi_{1-x-y} for the fabrication of MWIR and LWIR detectors, it is essential to develop strategies for improving the minority carrier lifetimes in the low temperature grown material.

Hydrogen and its radicals (plasma) are known to react in semiconductors with broken or weak covalent bonds associated with extended and localized defect centers. These interactions can shift the energy levels of the defects out of the gap resulting in electrical passivation of defects. Hydrogen passivation was shown to be effective in increasing carrier lifetime in InAs/InAsSb superlattices [2] and improving performance of HgCdTe LWIR detectors [3].

Here, we present the use of post-growth remote hydrogen plasma treatment to improve minority carrier lifetimes of MBE-grown InAs_xSb_yBi_{1-x-y} films. The process produces hydrogen concentration of 1.0 x 10¹⁶ atoms/cm³ at depth exceeding 2.5 μm . When followed by the low temperature annealing at 160 °C, it results in the 2 – 3.5 extension of the

minority carrier lifetime, from ~70 ns to 170 – 220 ns, as estimated using the time resolved photoluminescence measurements. This effect remains stable over a period of months after the treatment [4].

References:

- [1] Schaefer, S. T., Kosireddy, R. R., Webster, P. T., & Johnson, S. R. (2019). *J. Appl. Phys.*, 126(8), 083101.
- [2] Hossain, K., Höglund, ... & Gunapala, S. D. (2016). *J. Electron. Mater.*, 45(11), 5626-5629.
- [3] Boieriu, P., Velicu, S., ... & Hagler, P. (2013, February). *Quantum Sensing Nanophotonic Devices X* (8631, 284-303). SPIE.
- [4] Estévez H, F. A., Bergthold, M., ... & Wasserman, D. (2024). *Appl. Phys. Lett.*, 124(2).

11:30am **NAMBE2-WeM-14 Micro-Transfer Printing of Gasb-Based Infrared Devices Grown by Molecular Beam Epitaxy**, Margaret A. Stevens, US Naval Research Laboratory; A. Grede, J. Murphy, NRC Postdoctoral Fellow at the US Naval Research Laboratory; S. Mack, US Naval Research Laboratory; K. Schmieder, Formerly US Naval Research Laboratory; J. Nolde, US Naval Research Laboratory

III-V-Antimonide (Sb) compounds are useful for many different infrared device applications, ranging from full spectrum photovoltaics, to eye-safe photonic power converters, to light-emitting diodes for biomedical applications. The ability to remove the III-V-Sb device from its native substrate and heterogeneously integrate it with different materials would further support these technologies. For GaSb-based devices, heterogeneous integration is typically achieved by inverting the device, bonding the epitaxial surface to a new handle, and etching through the substrate. However, this method is not compatible with substrate reuse or additive manufacturing capabilities that could be provided with micro-transfer printing. Though complete substrate removal is undesirable in some aspects, it is typically the most successful method of separating a sample from its substrate due to the low etch selectivity between 6.1 Å semiconductors.

In this work, we demonstrate how solutions of citric-acid (C₆H₈O₇) and hydrogen peroxide (H₂O₂) can achieve high etch selectivities and enable micro-transfer printing of MBE-grown GaSb devices. We found mixtures of citric acid and hydrogen peroxide yield the highest etch selectivity ratio, >850, between InAs_{0.91}Sb and Al_{0.33}Ga_{0.50}Sb epilayers lattice-matched to GaSb. To monitor the lateral undercut rate, 2 μm AlGaAsSb membranes were grown on top of InAsSb sacrificial and AlGaAsSb etch-stop layers and monitored by infrared microscopy. While vertical etch tests demonstrated etch rates of InAsSb at ~554 nm/min, lateral etch rates were found to be 45% slower. To decrease the overall time required to undercut the device, the temperature of the solution can be increased without negatively impacting the etch selectivity. Using these findings, photovoltaic cells and quantum-well LEDs were grown by molecular beam epitaxy on GaSb substrates. Devices were fabricated on-substrate and immersed in a solution of 1:5 C₆H₈O₇:H₂O₂ for selective release. The importance of the thickness of the sacrificial etch layer, the tethering scheme, and the composition of the dielectric protection layer were explored to improve the etch-release yield and device performance.

[1] M. A. Stevens, et al. "Selective Etching of 6.1 Å Materials for Transfer-Printed Devices," in *IEEE 49th Photovoltaics Specialists Conference (PVSC)(2022)* 0240-0243

11:45am **NAMBE2-WeM-15 The InAsSb-based SACM APD with Hole-Initiated Multiplication**, Egor Portiankin, L. Shterengas, G. Kipshidze, J. Zhao, D. Donetski, Stony Brook University/Brookhaven National Laboratory We have designed and fabricated separate absorption, charge, multiplication (SACM) mid-infrared avalanche diodes (APD) relying on hole-initiated impact ionization. The device heterostructures were grown onto Te-doped GaSb substrates and contained 1- μm -thick nominally undoped InAs_{0.91}Sb_{0.09} absorber, ~100-nm-thick Te-doped Al_{0.9}Ga_{0.1}As_{0.07}Sb_{0.93} charge layer and 300-nm-thick nominally undoped Al_{0.9}Ga_{0.1}As_{0.07}Sb_{0.93} multiplier terminated with ~300-nm-thick p-doped contact layers. The epitaxial wafers were processed into circular shallow etched mesa devices with windows in top contact metallization. The barrier photodetector inspired APD architecture did not require etching through absorber section. The devices were indium-soldered epi-side-up onto gold-plated submounts and characterized in temperature range from 77K to 300 K. The APDs demonstrated cutoff wavelength of 3.9 μm at liquid nitrogen temperature and showed current responsivities well above 10 A/W (Figure 1). The linear mode multiplication gains exceeding 100 were observed at voltages near

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17.5 V. The dark current values of several nA have been recorded for all devices before the breakdown. The analysis of the temperature dependences of the dark current values below and above punch-through voltage confirms diffusion limited absorber operation at temperatures above 150 K (activation energy ~ 360 meV). Independently measured responsivities values above 10 A/W at bias voltages above 17 V.

NAMBE

Room Cummings Ballroom - Session NAMBE1-WeA

Heterogeneous Integration

Moderators: Rafael Jaramillo, Massachusetts Institute of Technology, John McElearney, Tufts University

1:45pm **NAMBE1-WeA-2 Superconducting (001) and (111) Metal Nitrides on GaN**, *Brelon May, Z. Cresswell, S. Regmi, V. Buturlim, K. Vallejo, K. Gofryk, D. Hurley*, Idaho National Laboratory

Group III-Nitride materials have found applications in optoelectronic, photonic, and high power devices due to many factors, including the large variation in bandgap spanning from the infrared to the deep ultraviolet. Recent research has pursued the combination of this well-established material system with transition-metal nitrides for the creation of complex heterostructures which possess interesting optical, magnetic, or superconducting functionality. While GaN research has been primarily focused on the hexagonal allotrope, the metastable zincblende phase has a direct bandgap of 3.2 eV and providing an attractive option as a wide bandgap cubic material. Many transition metal nitrides have a stable cubic rocksalt structure. This includes ZrN, NbN, and TaN which are also well-known superconductors with relatively low lattice mismatch to GaN. This work will use molecular beam epitaxy for the epitaxial integration of these metal nitrides with hexagonal (c-plane) and cubic (001) GaN and will discuss the effect of growth parameters, including growth direction, on the structural and electrical quality of the metal nitrides. Reflection high energy electron diffraction, X-ray diffraction, and transmission electron microscopy reveal the epitaxial quality of single layer films and superlattices. Temperature dependent resistivity measurements show the superconducting critical temperature is strongly dependent on the growth conditions. These results open the door for new epitaxial superconductor-semiconductor systems and provide a platform for integration with other cubic materials to enable complex heterostructures. Such atomically precise hierarchical matter could be used for metamaterials or quantum science.

2:00pm **NAMBE1-WeA-3 Epitaxial Growth of (111) BaTiO₃ Thin Films on AlGa_N/Ga_N Heterostructures**, *Eric Jin*, Naval Research Laboratory; *J. Hart*, NOVA Research; *A. Lang, M. Hardy, N. Nepal, D. Katzer, V. Wheeler*, Naval Research Laboratory

Development of GaN-based high electron mobility transistors (HEMTs) has led to significant performance improvements in solid-state power switching and RF electronics, owing to the wider bandgap and larger breakdown field strength of GaN compared to semiconductors such as Si and GaAs. Despite these enhanced material properties, GaN HEMT performance is limited by non-uniform peak electric fields that can cause premature breakdown. One field management strategy recently demonstrated leverages the high dielectric constant (κ) of a gate material such as BaTiO₃ (BTO) to both control the electrostatics and reduce the peak electric field in the gate-drain region of the HEMT [1]. These BTO dielectric layers are typically sputtered, leading to either poor crystal quality or polycrystalline films, which have lower dielectric constants than bulk or crystalline materials ($\kappa > 1000$ for bulk BTO).

In this work, we demonstrate epitaxial (111)-oriented BTO thin films grown on AlGa_N/Ga_N HEMT heterostructures by oxide and nitride molecular beam epitaxy. Key in this approach is the use of a thin SrTiO₃ (STO)/TiO₂ bilayer in between the BTO and AlGa_N to both grade the lattice mismatch between the oxide and nitride layers and to orient the BTO film. In previous work, we showed that a 1-nm TiO₂ buffer layer greatly improves crystallinity when cubic STO films are deposited on wurzite AlGa_N [2]. However, BTO has a tetragonal structure and a slightly larger unit cell volume than STO. Consequently, BTO films deposited on TiO₂-buffered AlGa_N exhibit lower crystallinity compared to films with an additional STO buffer layer.

We determine the growth window of BTO/AlGa_N films across substrate growth temperature, oxygen flow, and Ba/Ti flux, and characterize the crystal phase and structural properties with x-ray diffraction, atomic force microscopy, and reflection high-energy electron diffraction. We investigate the atomic microstructure with scanning transmission electron microscopy (STEM), which confirms the epitaxial relationship as (111)[1-10] BTO || (0001)[11-20] AlGa_N, which is similar to the observed STO/AlGa_N epitaxial relationship [2]. Additionally, the STEM imaging reveals that the BTO film is highly textured, with crystallites approximately 10 nm in size, and that the buffer layers are rougher than the BTO film. Finally, we show through van

der Pauw Hall effect measurements that the electrical properties of the GaN channel are robustly maintained, with no appreciable degradation of sheet resistance, electron mobility, or charge density.

- [1] N. K. Kalarickal et al., *IEEE Trans. Electron Devices* (2021)
[2] E. N. Jin et al., *APL Mater.* (2020)

2:15pm **NAMBE1-WeA-4 Selective Area Growth for Monolithically Integrated Quantum Dot Lasers**, *Alec Skipper, K. Feng*, University of California at Santa Barbara; *G. Leake, J. Herman*, SUNY Poly; *C. Shang, R. Koscica*, University of California at Santa Barbara; *D. Harame*, SUNY Poly; *J. Bowers*, University of California at Santa Barbara

While research on the direct growth of InAs quantum dot lasers on silicon has progressed rapidly in recent years, silicon photonic integrated circuits with heteroepitaxially-integrated lasers have not achieved the same level of success as heterogeneous wafer-bonded integration techniques. On-chip coupling between the silicon photonics passives and embedded heteroepitaxial III-V lasers has proven to be a significant challenge in the practical application of this technology with the best reported devices showing insertion losses of 7.35 dB. Heteroepitaxial integration has the potential to offer a significant manufacturing cost and throughput advantage over heterogeneous integration by allowing 300 mm wafer processing without the use of expensive III-V substrates. However, the coupling problem must be addressed for the technology to be competitive in device performance.

The large coupling losses in heteroepitaxially integrated lasers arise primarily from the air gap between the etched facets of the lasers and silicon photonics waveguides. Lasers are fabricated by first etching a pocket in a conventionally fabricated silicon photonics wafer, with the III-V laser material subsequently grown in the pocket to allow butt coupling between the active and passive regions. However, the growth at the edges of the pockets must be etched away to reduce the non-uniformity and to produce adequate facet mirrors for the III-V lasers. This results in a ~ 10 μm air gap between the laser facet and the waveguides that severely degrades coupling. In molecular beam epitaxy, these non-uniformities at the pocket edges are the result of polycrystalline III-V deposition on the silicon dioxide sidewalls. Selective area growth can reduce or eliminate this air gap by preventing the formation of polycrystalline III-V material on the sidewalls. However, selective area MBE growth is not practical for aluminum-containing alloys due to aluminum's low volatility.

We report the growth and fabrication of III-V lasers heteroepitaxially integrated with silicon photonic integrated circuits using a partial selective area growth method to reduce the coupling gap. The use of a highly selective GaAs buffer layer and non-selective laser stack mitigates the formation of polycrystalline III-V material, reducing the effective coupling gap from 11 μm to 6 μm while maintaining previously reported growth conditions in the active region. Fabricated ridge lasers exhibit scattered light output powers as high as 20 mW continuous wave with thresholds as low as 205 mA. Coupling loss measurements are in progress and will be reported at the conference.

2:30pm **NAMBE1-WeA-5 Influence of Number of Graphene Layers on Epitaxy of GdAuGe on /6H-SiC**, *Taehwan Jung*, University of Wisconsin - Madison, Republic of Korea; *N. Hagopian*, University of Wisconsin - Madison; *C. Dong, J. Robinson*, Penn State University; *P. Voyles, J. Kawasaki*, University of Wisconsin - Madison

We investigate the dependence of the number of graphene layers on the strain and epitaxial orientation of GdAuGe films, grown on graphene / 6H-SiC (0001). Whereas GdAuGe films growth directly on SiC or on few layer epitaxial graphene on SiC forms a hexagon on hexagon epitaxial alignment (GdAuGe [10-10] // SiC [10-10]), GdAuGe films grown on buffer layer graphene on SiC are rotated 30 degrees with respect to the underlying substrate. These results cannot be explained by a "remote" epitaxy mechanism, but instead may result from the highly buckled structure of buffer graphene which has strong covalent bonding to the underlying SiC. We will present a detailed analysis of the structure and strain by cross sectional STEM and reciprocal space mapping, and the impacts on magnetism in GdAuGe.

NAMBE

Room Cummings Ballroom - Session NAMBE2-WeA

Late News II

Moderator: John McElearney, Tufts University

3:15pm **NAMBE2-WeA-8 Growth and Properties of InSe Thin Films on GaAs(111)B and Si(111)**, *Maria Hilse, D. Liu, J. Rodriguez, J. Gray, J. Yao, S. Ding*, Penn State University; *M. Li, J. Young*, New Jersey Institute of Technology; *Y. Liu*, Penn State University; *R. Engel-Herbert*, Paul-Drude Institute for Solid State Electronics; *A. Lupini*, Oak Ridge National Laboratory; *J. Redwing*, Penn State University

Urgent societal and environmental needs have sparked searches for high-mobility 2D layered materials with sizeable bandgap and decent stability under ambient conditions for potential use in ultra-low power, ultra-high performance field effect transistors. With a reported carrier mobility exceeding 1000 cm²/Vs at room temperature, small electron effective mass, flat electronic band dispersions, excellent optoelectronic properties, possible ferroelectric properties and a close-to-ideal solar spectrum matched bulk bandgap of 1.26 eV, InSe shows high potential for future use in electronics.

In the presented study, InSe thin films were grown by MBE on GaAs(111)B and Si(111). The presence of many InSe phases and polytypes required a systematic and careful mapping of the growth parameters to identify conditions for single-phase, single-polytype, and single-crystal growth. Through structural characterization in- and ex-situ using reflection high-energy electron and X-ray diffraction, growth conditions for solely gamma-phase, crystalline InSe films were found. Although the structural properties of the films presented nearly unchanged over a small window of growth conditions, the film morphology was seen to sensitively depend on the Se:In flux ratio. Raman spectroscopy confirmed the phase and polytype assignment deduced from large-area structural characterization.

Microstructure analysis, however, revealed a high degree of structural defects in the films. Nano-scale domains of varying single layer stacking sequences, high-angle rotational domains as well as single layers of unusual bonding configuration resulting in a novel InSe polymorph were found in the films. The total number of defects and the general locations of the new polymorph varied in films across GaAs and Si. The highest structural homogeneity was found for InSe films grown on Si.

Density functional theory calculations for a representative selection of the experimentally observed defects confirmed that most defects, including the novel polymorph have formation energies at or below the thermal budget of the MBE synthesis process. Although the bandgaps of all InSe polytypes and polymorphs possess comparable values, large differences were found in their relative offsets. Due to the random distribution of polytypes and polymorphs in the film, our study suggests a high degree of electronic disorder in these films. Electrical transport showed a variable-range hopping-like behavior supporting the hypothesis of electronic disorder.

3:30pm **NAMBE2-WeA-9 Investigation of the Indium-flush Technique on InAs/InAlGaAs/InP (001) Quantum Dots for 1.55 μm Laser Applications**, *Calum Dear, J. Yuan, H. Jia, J. Park*, University College London, UK; *Y. Hou*, Swansea University, UK; *K. El Hajraoui*, University of York, UK; *H. Zeng, H. Deng, M. Tang*, University College London, UK; *Q. Ramasse*, University of Leeds, UK; *H. Liu*, University College London, UK

Growth of InAs/InP quantum dot (QD) materials for 1.55 μm laser applications faces two key challenges: (1) a morphological preference for elongated islands, known as quantum dashes, and (2) a large dispersion in island heights. Both issues are pronounced by the low lattice-mismatch interface of 3.2%. With respect to the optical characteristics, the former results in wire-like optical behaviour and the latter in a broadening of the photoluminescence (PL) spectra's full-width at half-maximum (FWHM). The work presented address these challenges in synchronous in pursuit of a high quality and optically active ensemble of QDs for high-performance laser applications on native and, potentially, on the important Si (001) platform.

To this end, we first optimised the island shape by reducing the indium surface migration using As₂ species [1], a V/III beam equivalent pressure (BEP) ratio of 18 [2], and an InAlGaAs buffer layer. A stable dot-like population of QDs with a high density of 4×10¹⁰cm⁻² was achieved with 5.5 monolayers (ML) of InAs. However, the deposition thickness nucleated large QDs; resulting in a room temperature (RT) PL emission wavelength greater than 1.8 μm. Additionally, a considerable dispersion in island height was presented in a ~90 meV FWHM.

Second, by employing an indium flush (IF) [3] (fig. 1), the QD heights and uniformity were reduced and improved, respectively. 4 nm of InAlGaAs was grown immediately following QD deposition to partially cap the ensemble. By raising the substrate temperature under As-pressure, indium desorption occurred in the larger exposed QDs, effectively truncating them to the height of the partial cap. Thereby resulting in a 300 nm blueshift of the emission wavelength and a substantial linewidth narrowing to 47.9 (51.0) meV for single (five)-layer structures (fig. 2(d)).

By investigating the resulting characteristics through means such as high-resolution scanning transmission electron microscopy (HR-STEM), we present key insights into the morphological changes to the QD morphology resulting from the IF technique. Furthermore, laser structures utilising the IF technique have been grown and fabricated, including additional work on enhancing the InAlGaAs buffer quality via ex-situ cyclic rapid thermal processing.

[1] C. Gilfert et al., *Appl. Phys. Lett.*, vol. 96, no. 19, May 2010.

[2] S. Banyoudeh and J. P. Reithmaier, *J. of Crys. Grow.*, vol. 425, pp. 299–302, Sep. 2015.

[3] Z. R. Wasilewski et al., *J. of Crys. Grow.*, vol. 201–202, pp. 1131–1135, May 1999.

3:45pm **NAMBE2-WeA-10 MBE Growth of Ge and GaAs on (111)-faceted V-groove Silicon**, *Makhayeni Mtunzi, H. Jia*, University College London, UK; *Y. Hou*, Swansea University, UK; *L. Bao*, University of Southampton, UK; *M. Masteghin*, University of Surrey, UK; *H. Deng, X. Yu, H. Zeng, J. Park, Y. Wang*, University College London, UK; *W. Li, A. Li*, Beijing University of Technology, China; *K. El Hajraoui*, York University, UK; *Q. Ramasse*, University of Leeds, UK; *I. Skandalos, F. Gardes*, University of Southampton, UK; *M. Tang, S. Chen, A. Seeds, H. Liu*, University College London, UK
Germanium (Ge) buffer layers on silicon (Si) substrates have long been developed for group IV and III–V devices by suppressing defect propagation during epitaxial growth. This is a key step for the development of highly efficient photonic devices on the Si platform. Patterned silicon substrates have increasingly been employed for their ability to restrict and hinder the motion of defects. In this work, we demonstrate the effectiveness of an optimised two-step growth recipe structure on a (111)-faceted V-groove silicon substrate with a 350 nm flat ridge. This strategy successfully reduces the threading dislocation (TD) density while growing a 1 μm Ge buffer layer via molecular beam epitaxy. As a result, a high-quality Ge buffer is produced with a low TD density on the order of 10⁷ cm⁻² and a surface roughness below 1 nm.

Furthermore, in order to move towards competent light emitting sources, the suppression of antiphase domains (APDs) from the polar on non-polar heterointerface of III–V GaAs on to group IV materials must also be considered. Such defect tolerant buffers are crucial for enabling highly effective GaAs based laser devices. Subsequently, we also demonstrate techniques to suppress the formation and propagation of APDs using a (113)-faceted Ge/Si virtual substrate as well as a (111)-faceted sawtooth V-groove Si substrate.

4:00pm **NAMBE2-WeA-11 Closing Remarks & Sponsor Thank You**,

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