

Saturday Morning, August 23, 2025

Workshop on MBE for Emerging Emitter Technologies

Room Tamaya ABC - Session WME1-SaM

Photonic-Crystal Surface-Emitting Lasers (PCSELs)

Moderator: Ricky Gibson, Air Force Research Laboratory

8:00am WME1-SaM-1 Welcome & Opening Remarks, **Ganesh Balakrishnan**, University of New Mexico

8:15am WME1-SaM-2 Passively Coupled Coherent PCSEL Arrays, **Mingsen Pan**, University of Texas at Arlington; **Chhabindra Gautam**, Semergytech, Inc.; **Thomas Rotter**, **Ganesh Balakrishnan**, University of New Mexico; **Shanhui Fan**, Stanford University; **Weidong Zhou**, University of Texas at Arlington

INVITED

As a novel design of surface-emitting semiconductor lasers, photonic crystal surface-emitting lasers (PCSELs) feature in-plane optical feedback from photonic crystal (PC) modulation and vertical coupling with active region and emitted beams. For surface-normal emission, cavity mode in a PCSEL cavity is designed to operate at the Γ point in the momentum space. Such a cavity mode, originating from the guided resonances in PC, is coupled to radiation channels in the upward and downward directions. Thus, a surface-normal laser beam can be directed with low beam divergence which is, in theory, near the diffraction limit. One advantage of designing low divergence light source is its superior brightness in applications such as free-space optical communications and material processing [1]. The low beam divergence of a PCSEL device makes it hundreds of times brighter than the vertical cavity surface-emitting lasers (VCSELs) without collimation lens.

Monolithic PCSELs, also single PCSELs, have been demonstrated to possess high-power exceeding 50 W in continuous-wave (CW) operation and brightness of over $1 \text{ GW cm}^{-2} \text{ sr}^{-1}$ from a 3 mm diameter device aperture [2]. By designing the PC cavities, even higher output power can be achieved with larger cavity sizes. However, as the cavity size becomes larger, laser performance degrades due to the complex thermo-optical and electro-optical effects. At higher injection currents, the spatial hole burning effects create non-uniform gain distribution, thus reducing the lasing efficiency and distorting the mode profiles. High injection current induced thermal effects due to the produced high photon density at the cavity center also bring negative impacts and complexities for compensation design. On the other hand, semiconductor laser arrays are important to the applications of power scaling, which can be a promising solution to overcome the challenges in high-power PCSELs. PCSEL cavities are realized by the two-dimensional (2D) in-plane optical feedback by the PC modulation. Thus, the lateral coupling control between two PCSELs is achievable and such coupled PCSELs have been implemented by applying a waveguide connection in between for active coupling control using its optical gain/loss switching. [3]

In this paper, we investigate a compact design of coherent PCSEL arrays by placing PCSELs with suitable spacing to implement passive couplings. [4][5] The PCSEL arrays are designed on an InGaAs/GaAs multiple quantum well (MQW) platform for lasing wavelength of 1040 nm. We fabricated single PCSELs and up to 5x5 PCSEL arrays under the same processing parameters and conditions for comparison. To test the coherent operation of PCSEL arrays, we characterize the spectral linewidth properties and measure the coherency in emitted laser beam by self-interference experiments. Linewidth of 0.22 nm from a 2-by-2 PCSEL array and 0.08 nm from a single PCSEL was observed, indicating feasible coherent beam combining with narrow peak wavelength splitting from different PCSELs. The self-interference experiments test the visibility of the interference fringes, showing strong coherency of the emitted beam from the PCSEL array that is similar with a single PCSEL.

The authors acknowledge the support from JDETO and ARO.

References

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- [3] R. J. Taylor, D. T. Childs, P. Ivanov, B. J. Stevens, N. Babazadeh, J. Sarma, et al., "Coherently coupled photonic-crystal surface-emitting laser array," *IEEE J Select. Topic. Quant. Electron.* 21, pp. 493-499, 2015.

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[5] M. Pan, C. Gautam, Y. Chen, T. Rotter, G. Balakrishnan, and W. Zhou, "Recent Advances in Photonic Crystal Surface Emitting Lasers," *IEEE J Select. Topic. Quant. Electron.* 31, pp. 1-8, 2025.

8:45am WME1-SaM-4 Molecular Beam Epitaxy Regrowth in InP and GaSb Short-Wave Infrared PCSELs, **Bradley J. Thompson**, Air Force Research Laboratory

INVITED

Photonic crystal surface-emitting lasers (PCSELs) have been reported with high-brightness output, $1 \text{ GW cm}^{-2} \text{ sr}^{-1}$, in the near-infrared fabricated in GaAs [1]. The high-brightness is a result of the high power single-mode output for the 1 mm diameter aperture. The aperture size has been increased to 3 mm diameter with a 50 W output [2]. These impressive outputs have yet to be scaled to the short-wave infrared (SWIR) in either InP- or GaSb-based devices. Each of these material platforms offers a new set of challenges to achieve the high-brightness afforded by the PCSEL architecture due to the longer wavelength, and thus increase in lattice constant, as well as the achievable index contrast available with lattice matched materials. In this workshop techniques and challenges for fabrication of SWIR PCSELs will be presented with a focus on molecular beam epitaxy regrowth techniques including epitaxial lateral overgrowth for InP-based PCSELs [3].

References

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- [2] Noda, S., Yoshida, M., Inoue, T. et al. Photonic-crystal surface-emitting lasers. *Nat Rev Electr Eng* 1, 802-814 (2024).
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9:15am WME1-SaM-6 III-V/Si Bound States in Continuum Lasers with Quantum Well (QW) and Quantum Dot (QD) Gain, **Ashok Kodigala**, Sandia National Laboratories

INVITED

We demonstrate the integration of quantum well and quantum dot gain with a silicon photonic crystal (PhC) at telecommunication wavelengths near 1550nm resulting in optically pumped laser emission from symmetry-protected bound states in the continuum (BIC).

9:45am WME1-SaM-8 Panel Discussion,

Workshop on MBE for Emerging Emitter Technologies

Room Tamaya ABC - Session WME2-SaM

Emerging Materials and Growth Technologies

Moderator: Carolina Adamo, Northrop Grumman

10:30am WME2-SaM-11 Clean Oxides at High Temperatures, **Joseph Falson**, California Institute of Technology

INVITED

In this presentation I will discuss recent developments in the epitaxy of ultra-pure ZnO as a platform for emerging emitters. Using clean homoepitaxial layers we have investigated a range of extrinsic defects as well as implanted ions inside ZnO as the host lattice. I will provide an outlook on the current status of developing method for in-situ incorporation of the most promising varieties of defects, as well as approaches to improving their quantum lifetimes through dilution of the nuclear spin bath. If time permits, I will also discuss other novel oxides which can be grown using similar techniques to very high purity.

11:00am WME2-SaM-13 Dislocation-Tolerant Quantum Dot Light Emitters: From Growth on Silicon to Remote Epitaxy, **Minjoo Larry Lee**, University of Illinois at Urbana-Champaign

INVITED

InAs quantum dots (QDs) grown on GaAs/Si have emerged as a compelling active region for reliable monolithically integrated lasers on Si with emission around 1200-1300 nm. In 2020, my group demonstrated that InP QDs also show promise as dislocation-tolerant light emitters with tunable emission in the red visible wavelength range. Since then, we have demonstrated InP QD visible lasers on both GaP/Si templates and patterned photonic integrated circuit (PIC) templates. More recently, we have demonstrated InP QD visible light-emitting diodes on GaAs templates grown by remote epitaxy, which can also exhibit escalated dislocation

Saturday Morning, August 23, 2025

densities. In this talk, I will review these directions and also describe new results from my group on InAsP QDs, which promise tunable emission in the near-infrared spectral range from 750-1200 nm. The potential to grow dislocation-tolerant InAsP light emitters spanning from 650-1300 nm could open a range of new applications, ranging from sensing to quantum technology.

11:30am WME2-SaM-15 Thermal Laser Epitaxy for Emerging Emitter Materials, *Brendan Faeth*, epi-ray **INVITED**

As the scope of both technological demand and known material systems continues to expand, the need for greater variety and control of constituent sources has begun to strain the capabilities of conventional deposition techniques. Here, we demonstrate a new thin-film deposition technique, Thermal Laser Epitaxy (TLE), which combines IR laser heating of elemental sources with direct CO₂ laser heating of substrates. This approach allows for the evaporation of practically all elements of the periodic table in the same setup, while maintaining even extremely corrosive process gas environments up to pressures as high as 10⁻¹ mbar, and at extremely high substrate temperatures. Here, I will introduce and discuss the advantages of TLE for epitaxy, with a focus on applications for emerging emitter materials across a wide range of materials families including oxides, nitrides, and other more exotic opportunities not accessible by conventional MBE approaches.

12:00pm WME2-SaM-17 Panel Discussion,

Saturday Afternoon, August 23, 2025

Workshop on MBE for Emerging Emitter Technologies

Room Tamaya ABC - Session WME1-SaA

Emitters on Silicon

Moderator: Ganesh Balakrishnan, University of New Mexico

1:30pm WME1-SaA-1 MBE Growth of Interband Antimonide Lasers on Silicon, *Laurent Cerutti, Maëva Fagot, Daniel Diaz-Thomas, Andres Remis, IES, University of Montpellier, CNRS, France; Audrey Gilbert, University of Montpellier, France; Yves Rouillard, Jean-Baptiste Rodriguez, Eric Tournié, IES, University of Montpellier, CNRS, France*

INVITED

The evolution towards smart, compact, low power and affordable optical gas sensors to monitor our environment requires the integration of III-V optoelectronic devices with a silicon photonics-based platform. Although two approaches, bonding and direct epitaxy, are possible, the latter appears to be the most promising long-term solution. The antimonide-based compound semiconductors (ABCs), which are particularly suitable for the development of mid-infrared optoelectronics (2-5 μm), where the absorption of pollutants (CH₄, CO, HF, ...) is very strong, make them the best candidate for the realisation of monolithically integrated mid-IR lasers on silicon substrates. However, differences in crystal structure, lattice constants, thermal expansion coefficients have made this topic extremely challenging. In this presentation we will review the recent results on mid-IR interband lasers grown on (001) Si substrates and compare their performance with those grown on their native substrate. For the 2-3 μm wavelength range, the properties of GaInAsSb/AlGaAsSb type-I quantum well (QW) lasers will be presented [1, 2], while for the 3-5 μm wavelength range, the properties of type-II interband cascade lasers with high threading dislocation density will be discussed [3, 4].

These two approaches will allow to cover the whole wavelength range between 2 and 5 μm and will show that Sb-based lasers pave the way for the future epitaxial integration of III-Vs on Si.

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This work was partially funded by France 2030 program (EquipEx EXTRA and HYBAT, ANR-11-EQPX-0016, ANR-21-ESRE-0026), the French Occitanie Region (LASIDO project), the French Agency for Defense and Innovation (AID-DGA) and the Banque Publique d'Investissement (Hyquality Project DOS0188007/00).

2:00pm WME1-SaA-3 Molecular Beam Epitaxy of III-V Infrared Emitters on Silicon, *Stephanie Tomasulo*, U.S. Naval Research Laboratory

INVITED

Combining high-performance III-V emitters with Si substrates enables their incorporation into photonic integrated circuits, as well as novel device architectures that can improve cost effectiveness and thermal management. However, the InAs/GaSb/AlSb family of materials that is suitable for emission in the midwave infrared has a typical lattice constant (a) near 6.1 \AA , resulting in a 12% lattice mismatch with silicon at a=5.43 \AA . Additional differences, such as thermal and polar/non-polar mismatches, also occur when the two material systems are epitaxially combined. While these introduce significant challenges, our successful growth of interband cascade light emitting diodes on Si has produced CW output powers comparable to those of control devices grown on GaSb. This presentation will cover the challenges of III V growth on silicon, as well as the current status of mitigation techniques that enable high performance to be observed nonetheless.

2:30pm WME1-SaA-5 High-Quality Epitaxy of SiSn, GeSn, and SiGeSn Alloys Using MBE for Si-Based Optoelectronic Applications, *Shui-Qing Yu, Diandian Zhang, Nirosh Eldose, Dinesh Baral, Hryhorii Stanchuk, Fernando Oliveira, Wei Du, Gregory Salamo, University of Arkansas*

INVITED

Group IV semiconductor alloys GeSn, SiSn, and SiGeSn, are promising for next-generation electronic and optoelectronic applications due to their tunable band structures and CMOS compatibility. While significant progress has been made in SiGeSn/GeSn-based lasers and photodetectors via chemical vapor deposition (CVD), achieving high-quality epitaxial growth via molecular beam epitaxy (MBE) remains challenging due to phase separation, strain relaxation, and defect formation, which limit optoelectronic performance.

In this workshop, we discuss the MBE growth of GeSn, SiSn, and SiGeSn alloys, focusing on overcoming key challenges such as Sn incorporation, surface segregation, and defect suppression. We systematically investigated

growth temperatures from 100°C to 200°C, optimizing crystalline quality confirmed by high-resolution X-ray diffraction (HR-XRD) and atomic force microscopy (AFM). A major breakthrough includes the first reported direct bandgap photoluminescence (PL) emission from MBE-grown GeSn on Si (100) substrates without post-annealing, marking a critical step toward Si-based GeSn optoelectronic integration.

For SiSn, we achieved the growth of SiSn alloys with Sn content up to 5.5% on Si substrates. XRD and reciprocal space mapping (RSM) confirm successful epitaxial growth of pseudomorphic SiSn layers (3.2%-5.5% Sn) on Si (100), with full strain retention preventing defect-induced relaxation. This stability is crucial for bandgap engineering, advancing Si-compatible infrared photonic and electronic applications. Additionally, the study enables further exploration of short-range ordering phenomena in group-IV semiconductor alloys.

Further discussions cover lattice-matched Si0.42GeSn0.10 bulk materials and Si0.25GeSn0.09/Ge superlattices (SLs). XRD confirms strain-free growth on Ge substrates, while secondary ion mass spectrometry (SIMS) verifies high Si and Sn compositions. PL measurements reveal a strong emission peak at ~1850 nm in Ge/SiGeSn SLs, demonstrating potential as a mid-infrared group-IV light source.

In conclusion we will have discussed the ways in which this study lays a strong foundation for the high-quality epitaxial growth of SiSn, SiGeSn, and GeSn alloys, confirming their potential for future Si-compatible electronic and photonic applications. These findings offer valuable insights into group-IV semiconductor alloy growth, addressing key challenges in material stability and performance. Furthermore, this work paves the way for the development of advanced photonic and quantum devices, expanding the possibilities for next-generation semiconductor technologies.

3:00pm WME1-SaA-7 Quantum Dot Lasers – Old Dog, New Trick, Niche Production to High-Volume Manufacturing, *Andrew Clark, Kathryn E. Sautter, Amy Liu, IQE Inc.*

INVITED

As the amount of AI-driven data continues to surge, data centers have to deal with ever increasing power consumption, creating a financial and an environmental burden. One solution is to run the entire data center at a higher ambient temperature which will improve both operational and cost efficiencies. Operating temperature is a key metric for compound semiconductor photonic devices as it impacts device performance and reliability. The incumbent laser for many of today's data centers is an InP-based O-band laser mounted on a cooler to maintain the operating temperature at <60°C. End-users now request laser modules that can tolerate >85°C, and eventually >100°C. GaAs-based quantum dot lasers (QDL) have demonstrated that they can meet these demanding specifications.

Other QDL attributes include the obviation of optical isolator and thermoelectric coolers, leading to a simpler bill of materials and improved wall-plug efficiency. Its largest attribute is perhaps its ability to support mode-locked or comb laser fabrication which could lead to significant performance efficiency when it comes to massive data transfer. A QDL comb on a single chip can have a wide range of output wavelength lines, each capable of carrying many GB of data.

Discrete transceivers incorporating QDLs have been around for 15+ years, but the current re-emergence is fueled by the interplay of QDLs with silicon photonics (SiPh) including heterogeneous III-V epitaxy directly on a photonic integrated circuit (PIC) wafer. To deliver on all these opportunities and provide a path to high-volume manufacturing of QDL epiwafers requires a comprehensive foundry approach for epitaxy which must focus on the consolidation of QD performance, wafer scaling, and end-user device fabrication needs such as the integration with silicon photonics.

While epitaxial growth of QDL structures on GaAs substrates is not new, shifting from niche production to a high-volume manufacturing platform requires that epiwafer foundries adapt and develop existing and new production processes. In this work, we will review IQE's QDL epiwafer production process. Our benchmark process is based on multi-150mm growths on GaAs substrates, but the process is scalable from 75 mm to 200 mm with comparable results. For CMOS fabs interested in the SiPh market space where the use of native GaAs substrates is not feasible, our epi foundry solution is to offer QDL structures grown on Ge and Si substrates which can be scalable up to 300 mm. We will discuss the MBE challenges of growing on non-native substrates and will present material characterization and device performance of QDL structures grown directly on 300mm PIC wafers.

Saturday Afternoon, August 23, 2025

3:30pm WME1-SaA-9 Panel Discussion,

Workshop on MBE for Emerging Emitter Technologies

Room Tamaya ABC - Session WME2-SaA

AI/ML Techniques for MBE

Moderator: Kurt Eyink, Air Force Research Labs

4:15pm **WME2-SaA-12 Basic Machine Learning Techniques for Analyzing Materials Characterization Data**, *Alex Belianinov*, Sandia National Laboratory **INVITED**

Basic Machine Learning techniques may play a crucial role in materials characterization data by extracting meaningful patterns and insights from complex datasets. As science increasingly relies on high-throughput experimentation, and advanced characterization methods, the volume and the veracity of the produced data can be overwhelming. Machine learning algorithms like Principal Component Analysis, Non-negative Matrix Factorization, and clustering techniques are beginner friendly approaches that can quickly and efficiently analyze these data, identifying correlations and trends that may not be immediately apparent. Furthermore, machine learning can enhance the automation of data processing, leading to faster and more accurate interpretations of experimental results. In this presentation a few examples of materials data analyzed by out of the box unsupervised machine learning techniques will be shown with the intent of highlighting the power and ease of use of these methods.

4:45pm **WME2-SaA-14 Machine Learning Methods for MBE Growth Optimization**, *Mingyu Yu*, University of Delaware; *Isaiah Moses*, Pennsylvania State University, United States Minor Outlying Islands (the); *Ryan Trice*, *Wesley Reinhart*, *Stephanie Law*, Pennsylvania State University **INVITED**

Machine learning models hold the potential to explore parameter space autonomously, quickly establish process-performance relationships, and diagnose material synthesis in real time. This reduces reliance on manual intervention in parameter space exploration, enabling more precise and efficient mechanistic control. For molecular beam epitaxy (MBE), despite its breakthroughs in materials synthesis, its stringent growth conditions and complex epitaxial mechanisms make the process of optimizing growth process time-consuming and expensive. Therefore, leveraging machine learning to develop autonomous MBE growth platforms presents a highly promising prospect. In this talk, I will discuss efforts to synthesize two material systems using machine learning and Bayesian optimization. We begin with a comprehensive high-quality dataset of GaSe thin films grown on GaAs (111)B substrates. GaSe is an emerging two-dimensional semiconductor material with intriguing properties, including thickness-tunable bandgaps, nonlinear optical behaviors, and intrinsic p-type conductivity. We were interested in leveraging machine learning to analyze the relationships between growth conditions (Ga flux, Se:Ga flux ratio, and substrate temperature) and the resulting sample quality, as well as the correlations among various characterization results including in situ RHEED patterns and ex situ x-ray diffraction rocking curve full-width at half maximum (FWHM) and atomic force microscopy (AFM) root mean square (RMS) roughness. In this talk, I will discuss how unsupervised learning, mutual information analysis, and supervised learning can be used to understand the influence of different growth parameters on GaSe film quality. I will then move on to discussing our efforts to use Bayesian optimization along with machine learning to quickly find optimal growth parameters for the various polytypes of In₂Se₃. The techniques and code can be easily adapted to other materials and other MBE systems, making this approach broadly applicable to a wide range of problems.

5:15pm **WME2-SaA-16 Panel Discussion**,

Sunday Morning, August 24, 2025

Workshop on MBE for Emerging Emitter Technologies

Room Tamaya ABC - Session WME1-SuM

Quantum-Dot based Single Photon Emitters I

Moderator: Richard Mirin, National Institute of Standards and Technology

8:00am WME1-SuM-1 Welcome & Opening Remarks,

8:30am WME1-SuM-3 Growth and Characterization of Epitaxial InAs Quantum Dots for Efficient and Pure Single Photon Sources, *Kevin Silverman*, NIST - Boulder INVITED

Epitaxial quantum dots (QDs) grown by molecular beam epitaxy (MBE) currently serve as the backbone of the world's best performing single photon sources. Therefore, they are poised to play an important role in emerging quantum information systems, and in particular, quantum networking applications. To meet metrics of photon purity, indistinguishability, and efficiency excellent crystal quality, careful design, and precise control of QD density and shape is necessary. In this presentation, we will discuss the optical and electrical characterization needed to prove that an epitaxial QD device can meet these demands. In contrast to conventional optoelectronic devices, photoluminescence characterization (even at cryogenic temperatures) is insufficient for this purpose. We will explain the need for precision, cryogenic, resonant measurements and how results can directly feedback to improvements in growth conditions and device design. Depending on the intended application, charge noise and/or spin noise could be the major factor effecting performance. These two concerns can be separated with different spectroscopic methods and have different physical mechanisms. We will then discuss some of our latest research into improving InAs epitaxial single photon sources including the addition of Phosphorus based materials and monolithic microcavities for enhancing collection efficiency into a single mode fiber.

9:00am WME1-SuM-5 Low Noise Epitaxial Quantum Dots for Photonic Quantum Technologies, *Alisa Javadi*, University of Oklahoma INVITED

Efficient generation and detection of coherent single photons are key to advances in photonic quantum technologies such as quantum computation, quantum simulation, and quantum communication. Among many quantum emitters, semiconductor quantum dots are promising due to their deterministic and high-rate single-photon emission and the possibility of integration into nanostructures. However, poor quantum coherence between single photons created by independent emitters poses a major roadblock. I will discuss our recent work on achieving near-unity two-photon interference visibilities from two separate GaAs quantum dots [1,2]. This high visibility (~93%) is achieved under rigorous conditions: there is no Purcell enhancement, no temporal post-selection, no narrow spectral-filtering, nor frequency stabilization. One key component is the heterostructure, an n-i-p diode using material of excellent quality. The quantum dot charge is locked via Coulomb blockade; within a charging plateau, the exact emission frequency can be tuned via the bias applied to the gate; the charge noise is very low. A second key component is the quantum dot itself: the relatively large size confers multiple benefits such as larger oscillator strength and lower susceptibility to spin noise. This level of interference visibility from independent GaAs QDs is a first of its kind and matches the performance achieved in trapped ions and cold atoms, the seemingly most identical emitters. These results highlight the advantage of high-quality epitaxial quantum dots as a versatile choice for generating identical photons from multiple emitters.

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Workshop on MBE for Emerging Emitter Technologies

Room Tamaya ABC - Session WME2-SuM

Quantum-Dot based Single Photon Emitters II

Moderator: Richard Mirin, National Institute of Standards and Technology

10:00am WME2-SuM-9 Quantum Dots Obtained by Droplet Etching Epitaxy for Quantum Science and Technology, *Armando Rastelli*, Institute of Semiconductor and Solid State Physics, Johannes Kepler University (JKU) Linz, Austria INVITED

Entanglement is one of the most peculiar phenomena in quantum science and a key resource for quantum technologies. More than two decades after the initial proposal [1], semiconductor quantum dots (QDs) are now

Sunday Morning, August 24, 2025

beginning to outperform other light sources for the generation of entangled photon pairs.

Among different material systems, QDs in the (Al)GaAs material platform have demonstrated the highest degree of polarization entanglement to date together with other appealing features for quantum science and technology [2-4]. These QDs are obtained by GaAs overgrowth of an AlGaAs surface with nanoholes and are characterized by small inhomogeneous broadening, high oscillator strengths, shape with high in-plane symmetry, and high optical quality, especially when embedded in charge-tunable diode structures. In this talk, we will discuss the properties of GaAs QDs obtained by the droplet etching method [5] and present recent results relevant to their application in quantum communication, such as entanglement-based quantum key distribution [6], as well as open challenges [7].

[1] O. Benson, C. Santori, M. Pelton and Y. Yamamoto, *Phys. Rev. Lett.* **84**, 2513–2516 (2000).

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10:30am WME2-SuM-11 Toward a Scalable Single Photon Platform, *Chen Shang*, University of California Santa Barbara; *Sahil Patel*, *Zihang Wang*, *Sean Doan*, *Dirk Bouwmeester*, *Galan Moody*, *John Bowers*, University California Santa Barbara INVITED

The lack of scalable photon sources has been a major roadblock for quantum photonics to realize their full potential. Self-assembled InAs QDs currently hold the best all-around single photon emitter performance as a solid-state source, offering advantages of CMOS-compatible fabrication, highly tunable optical properties, and deterministic emission. The key challenge for deploying the InAs QD single photon source at large scale is the spatial and spectral randomness of each dot due to the self-assembling process on planar substrates. The prevalent method to combat this involves manipulating substrates to create preferential nucleation sites, either grooves or mesas. However, these “site-controlled” QDs typically exhibit inferior optical qualities and less repeatable charge tunability compared to their randomly situated counterparts on planar substrates. Such substrate alternations also limit the integrability with other devices. In this work, we utilize the intrinsic material properties, especially the coefficient of thermal expansion (CTE) mismatch between the GaAs substrate and the oxide layers and the asymmetric surface diffusion of indium adatoms, to develop site-controlled InAs QD single photon emitters nucleated on compartmentalized finite surfaces that will solve both issues simultaneously at wafer scale.

The growth template was fabricated first by oxide deposition on (001) GaAs. To ensure the “epi-ready” surface quality, the hexagonal pockets in two different orientations with respect to the III-V crystal were finished HF wet etching to remove the remaining post-dry etching oxide. The InAs QD material was then deposited in a Veeco Gen II molecular beam epitaxy chamber at elevated temperatures. Due to the CTE mismatch between the GaAs substrate and the oxide layers, the substrate was under a global biaxial compression at the QD deposition temperature of 500 °C. The oxide patterns introduce local non-uniform profile with higher strain at the vertices of the hexagon and the strain level lowers toward the center of the pocket. The slow diffusion axis in the [1 1 0] orientation shows as “ridges” on the calculated potential energy profile. As the vertices are being filled, the energy penalty for adding more atoms increases and would generate new local and central potential energy minimums on either side of the slow diffusion axis. Thus, additional indium atoms are funneled toward the newly defined energy minimums. Hyperspectral images were taken under cryogenic temperatures of the as-grown InAs QDs embedded in

Sunday Morning, August 24, 2025

GaAs. Emission from a single QD within one of the central minima was observed in the pocket in the preferred orientation.

11:00am **WME2-SuM-13 Automated High-Throughput Single Quantum Dot Photoluminescence Spectroscopy, *Edward B. Flagg*, West Virginia University** **INVITED**

To fully leverage single quantum dots for quantum photonics requires spatial and spectral alignment of photonic nanostructures to individual quantum dots. Limited control of both spatial location and spectral properties of individual quantum dots during growth significantly hampers scalability and even initial development of single quantum dot devices. We have developed a cryogenic micro-photoluminescence setup for automatic position finding and spectroscopy of individual quantum dots on a massive scale. Our system employs two-color, wide-field illumination photoluminescence imaging to obtain positions of individual quantum dots relative to fiducial markers over 50-micron square fields of view with high throughput and nanometer scale uncertainties. The system then automatically performs confocal illumination and fluorescence collection sequentially over single quantum dots, repeating over a number of fields covering millimeter scale areas. Thousands of quantum dots can be located and spectrally characterized in tens of hours. Images of a calibration array of fiducial markers covering the field of view provide information about image distortion aberrations to correct quantum dot locations. The estimated RMS position accuracy is 29 nm after correction. We applied our system to the characterization of wafers containing GaAs liquid droplet etching and epitaxy quantum dots, obtaining photoluminescence spectra of thousands of individual quantum dots separated into three 10-nm spectral ranges, including excitation power-dependent spectra and polarization dependence. Spectra exhibiting sharp emission lines are almost exclusively found at the short-wavelength end of the quantum dot distribution. Efforts to fabricate spectrally tailored photonic nanostructures around targeted quantum dots are ongoing.

11:30am **WME2-SuM-15 Panel Discussion,**

12:00pm **WME2-SuM-17 Closing Remarks,**

Monday Morning, August 25, 2025

NAMBE

Room Tamaya ABC - Session NAMBE1-MoM

Remote and van der Waals Epitaxy

Moderator: Justine Koepke, Sandia National Laboratories

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

8:15am NAMBE1-MoM-2 Art Gossard MBE Innovator Awardee Talk: 6.1 Å to 6.5 Å Families: from Type-II superlattice IR lasers and Detectors to Remote-Junction Solar Cells, **Yong-Hang Zhang**, Arizona State University

INVITED

8:45am NAMBE1-MoM-4 Epitaxy and Magnetotransport of GdAuGe on Gallium-Intercalated Graphene/SiC (0001), **Zachary LaDuka**, University of Wisconsin - Madison; **Chengye Dong**, Pennsylvania State University; **Nicholas Hagopian**, **Paul Voyles**, University of Wisconsin - Madison; **Joshua Robinson**, Pennsylvania State University; **Jason Kawasaki**, University of Wisconsin - Madison

Superconducting proximity effects in topological materials and magnetic materials are potential routes to artificially construct topological superconductors and spin-triplet superconductors, respectively. Motivated by recent demonstrations of proximity induced superconductivity in $(\text{Bi},\text{Sb})_2\text{Te}_3$ on gallium-intercalated graphene/SiC (*Nat. Mater.* **22**, 570-575 (2023)), here we demonstrate the molecular beam epitaxy growth of the antiferromagnetic topological nodal-line semimetal GdAuGe on gallium-intercalated graphene/SiC(0001), where the intercalated gallium layer is superconducting. This heterostructure provides a platform for investigating proximity-induced superconductivity in GdAuGe.

We compare the growth characteristics of GdAuGe on gallium-intercalated graphene/SiC to those on conventional graphene/SiC. While the in-plane epitaxial relationship remains unchanged—GdAuGe [2 -1 -1 0] || graphene [1 -1 0 0] || SiC [2 -1 -1 0]—the intercalated gallium layer modifies the potential energy landscape beneath the graphene without altering the graphene lattice. This system provides a platform to explore how remote interactions influence film growth in a van der Waals epitaxial system. Ongoing efforts focus on characterizing the structural and electronic properties of the films via x-ray diffraction, atomic force microscopy, and cross-sectional scanning transmission electron microscopy to assess crystallinity and interface quality, while low-temperature magnetotransport measurements will probe superconducting proximity effects from the gallium layer.

9:00am NAMBE1-MoM-5 Challenges of Remote Epitaxy in Ultra-High Vacuum: Clean Semiconductor-2D Material Stacks, **Manny de Jesus Lopez**, **Sadhvikas Addamane**, **Justine Koepke**, Sandia National Laboratories, USA; **Kevin Jones**, University of Florida, Gainesville; **Scott Schmucker**, Sandia National Laboratories, USA

The growth of high-quality heteroepitaxial films is often constrained by lattice mismatch and the availability of suitable substrate materials. Remote epitaxy (RE) offers the potential to overcome these limitations by incorporating a two-dimensional (2D) material, such as graphene, between the substrate and the epitaxial layer. This work explores RE techniques and addresses the challenges associated with traditional remote epitaxy processes. Conventional epitaxy relies on the formation of covalent or ionic bonds between incoming adatoms and the substrate lattice. In contrast, RE leverages a monolayer of graphene to mediate the interaction between the adatoms and the underlying substrate without direct bond formation. This lack of covalent bonding allows the epitaxial layer to relax, reducing the nucleation of dislocation defects and enabling the growth of relaxed epilayers on lattice-mismatched substrates. Despite the straightforward concept of RE, the growth mechanisms differ from conventional models due to the absence of covalent bonds, making it challenging to distinguish RE from processes such as van der Waals epitaxy or pinhole-seeded epitaxy. Additionally, the graphene transfer process can introduce structural defects that promote film nucleation and potentially obscure the RE mechanisms facilitated by weak interfacial forces. Advancing RE requires addressing the cleanliness of the graphene-substrate interface. This work discusses our efforts to improve the fabrication of III-V material stacks via MBE and to understand the competing influences of the remote substrate and graphene defects on through-graphene epitaxial growth. By performing the entire process within an ultra-high vacuum environment and exploring the use of alternative 2D materials, we aim to mitigate contamination and structural defects, providing a clearer understanding of the fundamental

growth mechanisms in remote epitaxy. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

9:15am NAMBE1-MoM-6 Impact of Graphene-induced Surface Reconstructions on the Mechanisms for Remote and van der Waals Epitaxy of GdAuGe on Graphene/SiC (0001), **Tae-hwan Jung**, **Nicholas Hagopian**, University of Wisconsin - Madison; **Quinn Campbell**, Sandia National Laboratories; **Anshu Sirohi**, University of Wisconsin - Madison; **Chengye Dong**, The Pennsylvania State University; **Sadhvikas Addamane**, **Justine Koepke**, Sandia National Laboratories; **Joshua Robinson**, The Pennsylvania State University; **Paul Voyles**, **Jason Kawasaki**, University of Wisconsin - Madison

Remote epitaxy has emerged as a promising technique for synthesizing single-crystalline membranes, enabling flexible electronics and the exploration of novel properties under extreme strain. This method relies on the premise that a film can grow on a graphene-covered substrate through remote interactions that penetrate the graphene, allowing the film to grow as if the graphene were semi-transparent. However, in several cases, epitaxial graphene is known to induce long-range reconstructions in the underlying substrate, which implies strong graphene-substrate interactions. Prime examples include the (6x2) reconstruction of graphene/Ge (110) and the $(6/3 \times 6\sqrt{3})R30^\circ$ reconstruction of Buffer-graphene on SiC (0001). The impact of these surface reconstructions on the mechanisms for remote and van der Waals epitaxy is typically overlooked. In this study, we investigate the transparency of graphene using two types on a 6H-SiC (0001) substrate: Epitaxial-graphene, which is more decoupled from the substrate, and Buffer-graphene, which remains partially covalently bonded to the underlying SiC. We find that GdAuGe films exhibit a distinct in-plane rotation of 30 degrees when grown on Buffer-graphene/SiC compared to Epitaxial-graphene/SiC. Additionally, scanning transmission electron microscopy (STEM) reveals interfacial reconstructions and semi-disordered layers in the GdAuGe at the graphene/GdAuGe interface. To elucidate the origin of these findings, Density Functional Theory (DFT) calculations show that Buffer-graphene induces stronger substrate potential fluctuations than Epitaxial-graphene, while X-ray Photoelectron Spectroscopy (XPS) is expected to reveal differences in bond strength between GdAuGe and the two graphene types, further supporting our results. These findings provide new insights into the role of graphene-substrate interactions in remote epitaxy and suggest possible strategies for controlling film orientation and interface structure.

*SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

9:30am NAMBE1-MoM-7 Selective Area Epitaxy of van der Waals Materials, **Ryan Trice**, **Stephanie Law**, Penn State University

Two-dimensional (2D) van der Waals (vdW) materials are interesting for a variety of applications ranging from optoelectronics and photocatalysis to energy storage and topological devices. However, vdW materials synthesized using common techniques like chemical or physical vapor deposition often have a high density of growth-related defects ranging from grain boundaries and twin defects to pyramidal growth and spiral defects. While pyramidal growth can be minimized through higher growth temperatures, grain boundaries, twin defects, and spiral defects are much harder to overcome. For many applications, especially in electronics and optics, these defects lead to non-radiative recombination, electron scattering, and other undesirable effects. Furthermore, the fabrication of 2D materials into quantum dots (QDs) through bottom-up methods faces problems with precise location placement and polydispersity in the QDs diameters. This makes the QDs difficult to characterize and is not ideal for most quantum computing and optical setups. Top-down nanofabrication approaches fix this issue but often cause significant damage to the surfaces or edges of the materials. To address these issues, we used selective area epitaxy (SAE) to grow Bi_2Se_3 thin films. SAE is a technique in which thin films nucleate and grow in defined areas on a wafer. This is done through use of a patterned mask where growth conditions are selected such that the film will only nucleate on the substrate.

In this talk, we will describe SAE growth of Bi_2Se_3 on Al_2O_3 (001) and Si (111) substrates using a SiO_2 mask. The mask was deposited onto a 10x10mm substrate by atomic layer deposition. Etching of the SiO_2 mask was done with standard photolithography techniques and a direct write laser beam lithography system, and the SiO_2 was removed from selected areas using a wet chemical etch, resulting in micron-scale holes of various shapes and sizes. The processed substrates were then loaded into a molecular beam epitaxy chamber for growth of the Bi_2Se_3 film. First, we will discuss the effects of different substrate temperatures on the selective growth of the

Monday Morning, August 25, 2025

Bi_2Se_3 thin films. Second, we will discuss the geometric influence of variously shaped patterns on the crystal quality of the selectively grown films. Third, we look at the effect and viability of nano-scale patterns for selective growth of vdW materials. Further studies will focus on using different materials for the substrate and mask. This approach could allow us to grow wafer-scale, defect-free 2D vdW QDs at specified areas on the wafer, thereby increasing the scalability and applicability of these materials to real-world challenges.

9:45am **NAMBE1-MoM-8 Impact of Point and Extended Defects on the Mechanism for Remote Epitaxy of GaAs on Graphene/Ge, Anshu Sirohi, Patrick Strohbeen, Sebastian Manzo, Katherine Su, Vivek Saraswat, Nicholas Hagopian, Paul Voyles, Michael Arnold, Jason Kawasaki, University of Wisconsin - Madison**

Remote epitaxy is an advanced approach that enables the growth of single crystalline thin films on graphene-terminated substrates without direct chemical bonding between the films and the substrates^{1,2}. In the simplest picture, the grown films imitate the crystallographic structure of the underlying substrate as if the graphene layer were transparent. This approach facilitates lattice-matched epitaxy while empowering film exfoliation, wafer recycling and flexible device integration³. However, the microscopic mechanisms for remote epitaxy remain unclear, in particular, the role of point and extended defects as nucleation sites. The potential fluctuation through graphene on atomically flat GaAs is calculated by DFT to be ~ 15 meV, which is small compared to kT at growth temperatures. This opens the question of whether 15 meV is enough to serve as a template for epitaxial alignment. On the other hand, the potential fluctuation at a graphene covered atomic step edge should be much larger compared to flat regions, potentially enhancing remote interaction. Therefore, investigating early-stage nucleation on graphene-terminated substrates and the effect of the density of atomic steps are crucial to comprehend the possible intrinsic mechanism of epitaxy.

Here, we focus on most commonly used system i.e. III-V semiconductor GaAs. The films of GaAs were synthesized on graphene terminated germanium substrates using molecular beam epitaxy. The structural and chemical properties were characterized using RHEED, XRD, and XPS, evidencing the formation of crystalline GaAs films. Detailed surface morphological information before and after film growth were analyzed using AFM and in-situ STM. Preliminary results indicate that the nucleation of the GaAs film is influenced by the atomic steps on Ge111. Additionally, on Ge110, the nucleation appears to be strongly affected by the surface reconstructions of Gr/Ge110.

All these insights will allow me to shed light on the early stage nucleation in the monolayer regime in GaAs/Gr/Ge system.

References:

- [1] Kim Y et al. *Nature* 544 340 (2017).
- [2] Lee M L. *Nature* 544 301–2 (2017).
- [3] Guo, Y. et al. *Nano Lett.* 20, 33–42 (2019).

NAMBE

Room Tamaya ABC - Session NAMBE2-MoM

Bismuth-containing Alloys

Moderator: Corey White, University of Illinois at Urbana-Champaign

10:30am **NAMBE2-MoM-11 Molecular Beam Epitaxy Growth and Optoelectronic Properties of Droplet-Free Lattice-Matched GaInAsSbBi on GaSb with Photoluminescence Wavelength Exceeding 5 μm , Preston T. Webster, Air Force Research Laboratory, Space Vehicles Directorate; Rigo A. Carrasco, Alexander T. Newell, Alexander W. Duchane, Air force Research Laboratory, Space Vehicles Directorate; Aaron J. Muhowski, Victor J. Patel, Samuel D. Hawkins, Sandia National Laboratories; Marko S. Milosavljevic, Shane R. Johnson, Arizona State University; Julie V. Logan, Christian P. Morath, Diana Maestas, Air force Research Laboratory, Space Vehicles Directorate**

While the performance of mid-wave infrared HgCdTe focal plane arrays are unparalleled, their relatively poor yield of manufacturing has motivated research into a multitude of III-V semiconductor alternatives. However, unlike HgCdTe which is tunable across the entire infrared spectrum with a lattice-matched (albeit *bespoke*) substrate, the III-V material and substrate options available present an MBE growth challenge. Type-II superlattice and metamorphic growth strategies have been the subject of a great deal of research to overcome the problem that, at present, there are no III-V

random alloy solutions that can cover the full mid- to long-wave infrared spectral range on a commercially-available lattice-matched substrate. III-V alloys containing the heaviest group-V element Bi have long been known to offer the design freedom to achieve this degree of cutoff tunability with a lattice-matched substrate, however, they have historically proven to be very challenging to grow with smooth surface morphologies and high optoelectronic quality.

In this work, Ga is found to be the key to improving the incorporation quality of Bi in alloys of GaInAsSbBi . GaInAsSbBi alloys are grown lattice-matched on GaSb by molecular beam epitaxy demonstrating smooth surface morphologies, >5 μm wavelength photoluminescence emission, and minority carrier lifetimes > 1 μs [1]. At a growth temperature of 400 $^{\circ}\text{C}$, the Ga flux is systematically increased, while the Bi flux is systematically decreased to identify GaInAsSbBi growth conditions that yield smooth droplet-free surface morphologies. The minority carrier lifetime is evaluated using time-resolved photoluminescence, where it is observed that GaInAsSbBi samples exhibit minority carrier lifetimes comparable to their Bi-free GaInAsSb counterparts, on the order of 1.5 - 2 μs . The bandgap and Urbach energy are evaluated from steady-state photoluminescence to gain insight into the impact of the incorporated Bi. Coupled with Rutherford backscattering spectrometry measurements of the Bi mole fraction, bandgap reduction rates of 97 meV/% Bi in InAsSbBi and 150 meV/% Bi in GaInAsSbBi are observed, significantly higher than previous experimental evaluations in InAsSbBi (35-55 meV/% Bi). The inclusion of Ga in the quinary alloy is effective in suppressing Bi's tendency to incorporate in clusters (which contribute to tail states that increase the Urbach energy slope) for Ga mole fractions $> 9\%$, maximizing the bandgap reduction per unit Bi and overall optoelectronic quality.

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

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

10:45am **NAMBE2-MoM-12 Growth of InGaBiAs for Extended Short Wave Infrared Photodetectors, Mrudul Parasnis, Md Toriquil Islam, Nuha Ahmed-Babikir, James Bork, Abhilasha Kamboj, Alimir Razi, Jamie Phillips, Joshua 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 demonstrated that $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ photodetectors have a wavelength of 1.7 μm . Incorporation of bismuth into $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ reduces the bandgap by 56 meV per %Bi, thereby extending the detection wavelength. In this work, we show that InGaBiAs can be used as a promising material for short wave infrared (SWIR) photodetectors and extend the operational wavelength beyond 1.7 μm . The structure of SWIR photodetectors consist of Be doped InGaAs as a p-type capping layer and Si doped InGaAs as n-type region, both grown at 490 $^{\circ}\text{C}$ and lattice matched to InP substrate. InGaBiAs acts as an active region and is grown at low temperatures of 265 $^{\circ}\text{C}$ (Band edge thermometry). Diodes with this p-i-n structure are fabricated into mesa devices using standard photolithography, chemical etching, and metallization processes. Our findings show that incorporating 1.5% Bi into InGaBiAs successfully extends the wavelength up to 2 μm .

The device properties have a strong dependency on the Bi/As flux ratio. We have observed that the dark current density, capacitance and spectral response are influenced by the growth conditions and flux ratios. A 5% increase in arsenic shows an increase in carrier lifetime by two orders of magnitude. The devices grown with about 7% higher arsenic flux showcased reduced dark current density ($1.55 \times 10^{-3} \text{ A/cm}^2$ at -0.1V) and enhanced spectral response compared to stoichiometric conditions. We identified two distinct activation energies for each growth condition, in order to analyze factors limiting dark current in stoichiometric, low As and high As flux growth conditions.

[1] *Crystals* **17**, 7, 63 (2017) [2] *J. Vac. Sci. Technol. A* **40**, 042702 (2022) [3] *Appl. Phys. Lett.* **99**, 031110 (2011) [4] *Appl. Phys. Lett.* **100**, 112110 (2012)

Monday Morning, August 25, 2025

11:00am **NAMBE2-MoM-13 Performance of Mid-Wave Infrared GaInAsSbBi nBn Photodetectors Before and as a Function of High Energy Proton Exposure, Julie Logan, Alex Newell, Rigo Carrasco, Christopher Hains, Gamini Ariyawansa, Joshua Duran, Diana Maestas, Christian Morath, Preston Webster, Air Force Research Lab**

There are presently no III-V random alloy detector solutions that can cover the full mid- to long-wave infrared spectral range on a commercially-available lattice-matched substrate. This technology gap forces compromise through either the management of defects introduced in metamorphic growth, use of strain-balanced InAs/InAsSb type-II superlattice which has reduced absorption and transport performance, or use of InSb which lacks design flexibility at this single cutoff wavelength of 5.5 μm . To overcome these limitations, the bulk random alloy GaInAsSbBi material system is being developed which can simultaneously be grown lattice-matched on GaSb substrates while obtaining cutoff tunability due to the bandgap reduction rate of 150 meV/% Bi in GaInAsSbBi. The incorporation of Ga into the random alloy suppresses Bi's tendency to cluster and allows full exploitation of Bi's strong influence on bandgap to provide future tunability throughout the infrared spectral range.

Molecular beam epitaxy grown GaInAsSbBi *nBn* photodetectors are produced which exhibit a 4.8 μm cutoff wavelength at 130 K (0.3 μm longer than its Bi-free GaInAsSb counterpart *nBn* detectors), and these variable-area detector arrays are radiometrically characterized before and as a function of proton irradiation to evaluate anticipated operation in the space radiation environment. These photodetectors are produced with varied composition of the AlGaAsSb barrier to optimize the valence band alignment to the absorber material. It is shown that group-V composition in the barrier is more impactful than group-III composition in determining the photo-current turn-on and quantum efficiency (thus controlling the valence band alignment). The shot-noise limited noise equivalent irradiance for the most optimized structure characterized is 14 \times above the expectation for a hypothetical detector with unity quantum efficiency and Rule 07 dark current. Upon exposure to 63 MeV protons, defects generated in the crystal structure of the photodetector result in an increase in dark-current and reduction in quantum efficiency. These both result in an increase in noise equivalent irradiance, with a damage factor of 3.6 \times 10 $^{-2}$ photons/p $^{+}$, which is notably lower than the 10 $^{-1}$ photons/p $^{+}$ reported for MWIR SL-based *nBn* detectors. Most of the improved radiation hardness is attributable to a lower rate of degradation in the dark current and minority carrier lifetime with irradiation. This could indicate that the incorporation of heavy Bi atoms enhances the radiation hardness of the material in a way analogous to Hg in HgCdTe, making them more suitable for space applications than other III-V detector solutions.

11:15am **NAMBE2-MoM-14 Improving Bi Incorporation in InSbBi and AlInSbBi, Amberly Ricks, University of Texas at Austin; Corey White, University of Illinois at Urbana Champaign; Seth Bank, University of Texas at Austin**

InSb-based alloys are a promising alternative to HgCdTe for long-wave infrared (LWIR) operation.^{1,2} Adding small amounts of Bi into InSb leads to large bandgap reductions extending the infrared response,³ where most of the bandgap change occurs in the valence band.^{4,5} The integration of Bi into wide-bandgap alloys like AlInSb can decouple the lattice parameter from band alignments, offering a novel solution to dark currents in InSbBi-based devices (e.g. as barriers). A challenge associated with growing Bi-containing III-V alloys is Bi forming droplets on the film surface instead of integrating into the alloy, requiring specific growth conditions.^{6,7} Thus, it is essential to investigate the growth space for InSbBi and AlInSbBi due to their combined potential as active and barrier layers for LWIR devices.

To explore Bi incorporation kinetics, InSbBi films were grown with a modulated Bi flux by solid-source MBE on n-InSb. Growth parameters promoting Bi incorporation³ were used: a 300°C substrate temperature, a 0.975x V/III flux ratio, and a \sim 1 $\mu\text{m}/\text{hr}$ growth rate. Bi dose was modulated from 4 ML (for a 7.5 ML period) to 25 ML (for a 45 ML period). ω -20 X-ray diffraction (XRD) measurements suggested similar Bi concentrations for all films, but atomic force microscopy (AFM) showed smooth surfaces (RMS roughness of \sim 1 nm) for the two shortest period samples. This indicates that Bi can be incorporated without droplets by utilizing the kinetics of Bi atoms and perhaps suppressing the formation of Bi nuclei. Experiments are underway to study higher Bi fluxes and other duty cycles.

To explore the solubility limits of Al, AlInSbBi films were grown by MBE at Al concentrations from 1-5%. The same growth parameters used for InSbBi were applied to enhance Bi incorporation, but with a continuous supply of Bi. ω -20 XRD measurements showed a 0.5% Bi limit was reached for all

AlInSbBi films, and AFM showed there were no droplets. Growths are underway with higher Bi fluxes to verify if the upper limit was reached, and future experiments will further investigate the interplay between Al and Bi. Understanding the growth space for both InSbBi and AlInSbBi will provide opportunities to create enhanced *nBn* devices lattice matched to InSb substrates that access the LWIR.

This work was supported by the NSF (DMR-2119302).

- 1 S. Svensson et al., *Appl. Opt.*, 56, 2017
- 2 P. Martyniuk, M. Kopytko, and A. Rogalski, *Opto-Electron. Rev.*, 22, 2014
- 3 R. White et al., *Appl. Phys. Lett.*, 121, 2022
- 4 R. Kudrawiec et al., *Semicond. Sci. Technol.*, 30, 2015
- 5 S. Francoeur et al., *Appl. Phys. Lett.*, 82, 2003
- 6 M. Rajpalke et al., *Appl. Phys. Lett.*, 105, 2014
- 7 A. Ptak et al., *J. Cryst. Growth*, 338, 2012

11:30am **NAMBE2-MoM-15 Impact of Hydrogenation on the Minority Carrier Lifetime of InAsSbBi and the Sensitivity of InAsSbBi nBn Photodetectors, Mach Michaels, Georgia Institute of Technology; Mangal Dhoubhadel, Khalid Hossain, JP Analytical, LLC; Alexander Duchane, Rigo Carrasco, Luke Helms, Air Force Research Laboratory; Christopher Hains, A-Tech, LLC, a BlueHalo Company (ATA BlueHalo); Julie Logan, Christian Morath, Diana Maestas, Preston Webster, Air Force Research Laboratory**

As decreasing rocket launch costs continually reduce the barrier to access space, space-based surveillance missions previously performed using a small quantity of exquisite sensing assets are being re-envisioned as larger constellations of satellites, necessitating the production of more sensors. The current state-of-the-art for mid- to long-wave infrared detection is HgCdTe-based, however, there has been a growing interest in more manufacturable III-V alloys to support these larger sensing constellations of tomorrow. III-V alloys incorporating the heaviest group-V element Bi, such as InAsSbBi, can be tuned to span the entire infrared spectral range with a lattice-matched commercially available substrate, however, the growth of these alloys is challenging. Relatively low growth temperatures conducive to incorporating higher mole fractions of Bi necessary to reach long-wave infrared cutoffs results in relatively higher defect content that degrades the minority carrier lifetime, a critical parameter governing the overall photodetector sensitivity. It has recently been shown that post-growth hydrogenation is effective in passivating these defects and improving the minority carrier lifetime in InAsSbBi [1], motivating the study of its effects on InAsSbBi *nBn* photodetectors.

In this work, molecular beam epitaxy grown InAsSb/InAsSbBi/InAsSb photoluminescence test structures and 4.32 μm cutoff InAsSbBi *nBn* photodetectors are examined before and after hydrogenation treatments using deuterium. In the photoluminescence test structures, the hydrogenation process yields a 4 \times improvement in the minority carrier lifetime, up to 1.2 μs . However, the lifetime of the *nBn* photodetectors remains unchanged following hydrogenation, as does the shot noise equivalent irradiance evaluation of their overall sensitivity. Instead, the hydrogenated *nBn* photodetectors exhibit a significantly higher reverse bias turn-on, suggesting that the hydrogenation process has modified the valence band alignment across the barrier/absorber interface. Secondary ion mass spectrometry measurements confirm that the deuterium delivered by the hydrogenation process is trapped in the overlying AlGaAsSb barrier layer in these structures and as such, cannot passivate the InAsSbBi absorber volume below. This result motivates future work to prioritize the so-called inverted *nBn* structure wherein the InAsSbBi active region is grown on the AlGaAsSb barrier.

[1] *Appl. Phys. Lett.* **124**, 021104 (2024).

11:45am **NAMBE2-MoM-16 Synthesis of Epitaxial Bi_{1-x}Sb_x Nanomembranes, Saad Mohammad Bhuiya, University of New Mexico, Bangladesh**

Bismuth-antimony (Bi_{1-x}Sb_x) alloys with x = 0.07–0.22 are known to host topologically protected states, making them promising candidates for quantum information processing. Establishing robust processes for synthesizing single-crystalline Bi_{1-x}Sb_x compounds compatible with widely used substrates is crucial for materials and device characterization. In this work, we demonstrate the synthesis of Bi_{1-x}Sb_x nanomembranes (NMs), structural elements that can be epitaxially grown on semiconductor substrates and transferred onto different hosts. These NMs present exciting opportunities for integrating topological states with additional functionalities. Furthermore, due to their elastic deformability, they offer a

Monday Morning, August 25, 2025

unique platform for investigating the effects of strain on $\text{Bi}_{1-x}\text{Sb}_x$ topological insulators.

Our synthesis approach involved epitaxial growth via molecular beam epitaxy (MBE), selective substrate removal, and NM transfer. We grew $\text{Bi}_{1-x}\text{Sb}_x$ layers with a target Sb composition of 8% on GaAs (111)A substrates (AXT Inc.). The substrates were degassed at 500 °C and deoxidized at 620 °C under As overpressure before deposition. The epitaxial films, designed to be ~100 nm thick, were grown at temperatures between 150–200 °C across different runs, with a deposition rate of ~4 nm/min. In situ reflection high-energy electron diffraction (RHEED) provided real-time monitoring, while ex situ characterization was conducted via x-ray diffraction (XRD), Raman spectroscopy, and electron microscopy. XRD revealed sharp diffraction peaks corresponding to $\text{Bi}_{1-x}\text{Sb}_x$, and Raman spectroscopy confirmed the presence of characteristic vibrational modes. Scanning electron microscopy (SEM) showed a relatively smooth film surface with some randomly distributed regions of increased thickness, whose structural properties remain under investigation.

We isolated the $\text{Bi}_{1-x}\text{Sb}_x$ NMs by selectively etching the GaAs (111)A substrate in an $\text{NH}_4\text{OH}:\text{H}_2\text{O}_2$ solution. To preserve NM integrity, the films were capped with a photoresist and mounted onto a glass substrate using crystal bond adhesive, with the GaAs surface facing upward. A customized jet etcher facilitated precise substrate removal. Following etching, the NM was released by dissolving the crystal bond and photoresist in acetone. The freestanding NM was then transferred onto an oxidized silicon substrate, although this method allows for versatile host selection. Optical imaging, SEM, and Raman spectroscopy confirmed the NM's structural integrity and the complete removal of GaAs. Profilometry measurements indicated a final NM thickness of ~98 nm, closely matching the intended epitaxial layer thickness.

Monday Afternoon, August 25, 2025

NAMBE

Room Tamaya ABC - Session NAMBE1-MoA

Photonic Devices

Moderator: John McLearnay, Tufts University

1:30pm NAMBE1-MoA-1 ErAs/Semiconductor Nanocomposites for 1.55 μm -Pumped and Hybrid Terahertz Photoconductive Switches, *Angelique Gordon, Wilder Acuna, Weipeng Wu, James Bork, Matthew Doty, Xi Wang, M. Benjamin Jungfleisch, Lars Gundlach, Joshua Zide, University of Delaware*

We present our latest results on the growth of ErAs/III-V semiconductor materials designed for photoconductive devices operating at 1.55 μm telecom-wavelength and for hybrid emitters. Terahertz (THz) technology holds significant promise across various fields, including biomedical imaging, communications, astronomy, and spectroscopy. Bridging the "Terahertz Gap" requires new materials engineered for high-performance and reliable technology. Photoconductive switches (PCS), key components for THz pulse generation and detection, face challenges under 1.55 μm excitation. ErAs:InGaAs and other nanocomposites have been explored for this purpose, but their high electron concentration, due to the Fermi level residing in the conduction band, limits dark resistivity. To address this, we propose ErAs:[(InGaBiAs)_x(InAlBiAs)_{1-x}], a digital alloy with incorporated nanoparticles, as suitable PCS material for telecom-wavelength usage¹. ErAs nanoparticles ensure sub-picosecond carrier lifetimes ensuring high temporal resolution while simultaneously pinning the Fermi level within the bandgap. The freedom offered by the InGaAlBiAs short-period superlattice enables tunable bandgap engineering—aluminum raises the conduction band edge while bismuth, incorporated through low-temperature, stoichiometric growth, maintains a bandgap suitable for 1.55 μm excitation. This approach achieves both low carrier concentration and high dark resistivity, enhancing the performance of THz photoconductive devices at telecom wavelengths. We also demonstrate a Hybrid THz emitter that integrates a sputtered Ta/CoFeB/Pt spintronic emitter and an MBE grown ErAs:GaAs photoconductive antenna (PCA) into a single device². This device enables independent and tunable excitation of two THz emitters, facilitating control over emerging THz functionalities such as elliptical polarization and pulse shaping.

[1] W. Acuna, et al., *Adv. Funct. Mater.* **34**, 2041853, (2024).

[2] W. Wu, et al., *Adv. Opt. Mater.* **2402374**, (2024).

1:45pm NAMBE1-MoA-2 Regrowth of GaSb Photonic Crystal Surface-Emitting Lasers by Molecular Beam Epitaxy, *Bradley J. Thompson, Air Force Research Laboratory, Sensors Directorate; Samuel M. Linser, KBR & Air Force Research Laboratory, Sensors Directorate; Sadhvikhas Addamane, Sandia National Laboratories; Thomas Rotter, Ganesh Balakrishnan, University of New Mexico; Ricky Gibson, Air Force Research Laboratory, Sensors Directorate*

The photonic crystal surface-emitting laser (PCSEL) is promising device for scaling power and brightness of semiconductor lasers [1]. Embedding a 2D photonic crystal near the active region of semiconductor laser defines the cavity and enables surface-emission. Not unlike distributed feedback (DFB) lasers this requires an epitaxial regrowth step, though for the PCSEL the feature sizes are smaller than those of the DFB laser and the lithographic features are closer to the active region. To operate a PCSEL in single-mode at the Γ -point a high-index contrast and appropriate symmetry of the photonic crystal are necessary. This requires control of the regrowth profile of the 2D photonic crystal. Output powers of 50W continuous-wave have been reported in GaAs-based devices operating around a wavelength of 1 μm [2] utilizing metal-organic chemical vapor deposition (MOCVD). While these devices can be extended to longer wavelengths the necessary regrowth becomes challenging [3], particularly in antimonide-based devices due to the higher adatom mobility and the larger lattice constant required for the extend-short-wave infrared (e-SWIR) wavelengths. To date a maximum of 30mW from a 250 μm aperture device have been reported [4]. Performance gains are expected with improved regrowth and the ability to optimize device based on high-fill factor air-void photonic crystals. Here we report on initial regrowth samples and devices exploring the molecular beam epitaxy (MBE) parameter space for devices emitting nominally at a wavelength of 2 μm . Initial samples show higher uniformity and regularity in the embedded 2D photonic crystal, based on scanning electron microscope (SEM) images, than what have previously been reported. Limitations to optimization of GaSb-based devices based on the material and growth decisions will also be discussed.

[1] S. Noda, et al., "High-power and high-beam-quality photonic-crystal surface-emitting lasers: a tutorial" *Advances in Optics and Photonics*, **15**(4), 977-1032 (2023).

[2] M. Yoshida, et al., "High-brightness scalable continuous-wave single-mode photonic-crystal laser" *Nature*, **618**(7966), 727-732 (2023).

[3] W. Lee, et al., "Comparison of Thermal and Atomic-Hydrogen-Assisted Oxide Desorption Methods for Regrowth of GaSb-Based Cascade Diode Lasers" *J. Electron. Mater.* **50**, 5522-5528 (2021).

[4] L. Shterengas, et al., "Photonic Crystal Surface Emitting GaSb-based Type-I Quantum Well Diode Lasers" *IEEE Journal of Selected Topics in Quantum Electronics*, **31**(2), 1-7 (2025).

2:00pm NAMBE1-MoA-3 Growth and Optimization of Opto-electronic performance of InGaAsSb Photodetectors using Molecular Beam Epitaxy, *Neha Noaman, Nathan Gajowski, Punam Murkute, Vinita Rogers, Sanjay Krishna, The Ohio State University*

The quaternary alloy, $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$, grown lattice-matched to GaSb substrates, is a promising alternative to extended InGaAs for Short-Wave Infrared (SWIR) detection due to its tunable wavelength range from 1.7 μm to 3 μm . This flexibility is essential for advanced imaging and sensing applications, positioning InGaAsSb as a key material for next-generation infrared devices. Yet, GaSb-based devices face challenges like high background doping and surface leakage, which hinder performance. Various growth techniques and architectures, including unipolar barrier designs, have been explored in the literature to mitigate these issues. Developing an optimal InGaAsSb-based structure requires a comprehensive understanding of the material's properties and key device performance metrics¹. This work presents the molecular beam epitaxial (MBE) growth and characterization of the nominal composition $\text{In}_{0.29}\text{Ga}_{0.71}\text{As}_{0.25}\text{Sb}_{0.75}$ on a GaSb substrate. The growth temperature was estimated to be in the range of 450°C–460°C. Reflection High-Energy Electron Diffraction (RHEED) patterns confirmed that the InGaAsSb layer grows with a (4×2) surface reconstruction. Following MBE growth, the surface and structural properties of the alloy were characterized using High-Resolution X-Ray Diffraction (HR-XRD), Atomic Force Microscopy (AFM), Nomarski imaging, and photoluminescence (PL). Two structures were fabricated: a bulk structure with a 500 nm thick InGaAsSb layer and a homojunction p-i-n structure with a 1 μm thick intrinsic layer. The bulk InGaAsSb exhibited a lattice mismatch of 0.164% and a surface roughness of 1.02 Å, indicating good crystalline quality. The PL peak was observed at approximately 2.33 μm . However, HR-XRD scans of the p-i-n structure revealed evidence of spontaneous superlattice formation in the active region, which is currently under investigation. This behavior may be attributed to growth near the miscibility gap ($x \approx 0.3$). PL measurements showed no detectable peak shift despite the presence of the superlattice. Ongoing studies focus on optoelectronic properties like minority carrier lifetime and background doping to assess the superlattice's impact on performance.

1. K. Mamić, L. A. Hanks, J. E. Fletcher, A. P. Craig and A. R. J. Marshall, *Semiconductor Science and Technology* **39** (11), 115002 (2024).
2. I. P. Ipatova, V. A. Shchukin, V. G. Malyshkin, A. Y. Maslov and E. Anastassakis, *Solid State Communications* **78** (1), 19-24 (1991).

2:15pm NAMBE1-MoA-4 Growth-Temperature Effect on Group-V Compositions in 'W' Structured GaAsSb/InGaAs/GaAsP Quantum Wells, *Zon Ma, National Chung Hsing University, Taiwan; Chao-Chia Cheng, Chun-Nien Liu, Jenn-Inn Chyi, Charles W. Tu, National Tsing Hua University, Taiwan*

The display cutout area, "notch" or "Dynamic Island", of an iPhone is located at the top of the display and houses the front-facing camera, vertical-cavity surface-emitting lasers (VCSELs), and detectors for Face ID. These VCSELs use top and bottom AlAs/GaAs Distributed Bragg Reflectors (DBRs) as the vertical cavity, and the emission wavelength is limited to 980 nm, which cannot penetrate the display, and hence the "notch". It is desirable, however, to utilize the whole display, edge to edge, if the wavelength can be 1380 nm. Furthermore, the minimum permissible exposure for eye safety is about 500 times higher at 1380 nm than at 980 nm. Therefore, many groups are pursuing long wavelength emission on GaAs substrates for these two reasons. There have been several approaches. One is wafer bonding of InP-based lasers and GaAs-based DBRs, which is a more complicated process than simpler epitaxy. Other approaches are dilute nitrides and self-assembled InAs quantum dots, but they suffer from low output power due to material defects and small active volumes, respectively. This paper studies another approach: type-II InGaAs/GaAsSb 'W'-quantum wells (QWs) with GaAsP strain compensating

Monday Afternoon, August 25, 2025

layers grown on GaAs (001) substrates by MBE. The schematic band diagrams are shown in Fig. 1. The control of group-V compositions in ternary and quaternary compounds, such as GaAsP, InAsP, GaAsSb, InAsSb, InGaAsP, and InGaAsSb, is a significant challenge. The growth temperature was varied from 450 to 540°C while other growth parameters were kept the same. The designed QW thicknesses and material compositions (Sb, In, and P%) are 15 nm-GaAs0.9Sb0.1, 3 nm-In0.3Ga0.7As, and 15 nm-GaAs0.75P0.25, respectively. Fig. 2 shows the x-ray rocking curves (XRCs) and simulations of 'W'-QWs grown at five different growth temperatures. The extracted results from XRC analysis prove that the group-V compositions (As, Sb) and (As, P) are varied as a function of growth temperature. The phosphorus composition in GaAsP increases at growth temperature >500°C. At higher temperatures, the group-V materials desorb readily and compete with each other during the growth. The desorption affects the growth rate and, consequently, QW thickness. Unlike the P incorporation behavior, the Sb composition in GaAsSb decreases with higher growth temperature. This can be attributed to the lower sticking coefficient of Sb at higher temperatures. The different incorporation behaviors of P and Sb were numerically extracted as shown in Fig. 3. Photoluminescence (PL) emissions are observed from shorter to longer wavelengths by increasing Sb incorporation. The very low Sb composition creates type I GaAsSb/InGaAs QWs, resulting in stronger PL at shorter wavelengths, as shown in Fig. 4. In summary, the different incorporation behaviors of group-V materials in GaAsSb/InGaAs/ GaAsP 'W'-QW affected by the growth temperature are experimentally investigated. XRC determines the material compositions, QW thicknesses, and crystalline quality. The emitted PL characteristics are in good agreement with XRC. The optimum growth temperature range of 450-500°C for 'W'-QW is revealed to achieve better Sb incorporation and extend the PL emission wavelength.

2:30pm NAMBE1-MoA-5 III-V Quantum Dot Lasers and Photodetectors Monolithically Integrated with Silicon Photonics by Two-Step Growth, Alec Skipper, Rosalyn Koscica, UC Santa Barbara; Bei Shi, Aeluma Inc.; Gerald Leake, Joshua Herman, AIM Photonics; Michael Zylstra, Analog Photonics; Kaiyin Feng, Chen Shang, UC Santa Barbara; David Haram, AIM Photonics; Jonathan Klamkin, Aeluma Inc.; John Bowers, UC Santa Barbara

The integration of lasers with silicon photonics is required to produce highly-efficient low-footprint photonic integrated circuits (PICs) for applications in data communication, LIDAR, and biosensing. Monolithic integration through the direct growth of III-V semiconductor materials on patterned silicon photonics wafers would enable large-scale production of PICs by utilizing 300 mm silicon wafers and eliminating costly III-V substrates from the process. However, growth on patterned silicon photonics wafers introduces new challenges in material quality, coupling efficiency, and growth uniformity. In this work, we report a two-step growth approach using metal-organic chemical vapor deposition (MOCVD) and molecular beam epitaxy (MBE) to create InAs quantum dot lasers and photodetectors coupled to silicon nitride waveguides on foundry-processed silicon photonics wafers.

By combining MOCVD's high-quality selective III-V buffers on silicon with MBE's precise control of growth parameters for quantum dots, we can mitigate many of the difficulties associated with III-V growth on patterned silicon photonics wafers. Photonic integrated circuits with silicon nitride couplers, silicon nitride waveguides, silicon ring resonators, and silicon nitride distributed Bragg reflectors all embedded in silicon dioxide were fabricated at AIM Photonics on 300 mm silicon-on-insulator wafers. Pockets were etched through the silicon dioxide leaving the silicon nitride couplers exposed on the silicon dioxide sidewalls. Anti-phase domain-free GaP, a GaAs buffer, and InGaAs strained layer superlattices were grown by MOCVD to reduce the defect density. Selective MOCVD growth was used in the exposed silicon pockets to prevent the deposition of polycrystalline III-V on the sidewalls containing the nitride couplers. A separate confinement heterostructure laser stack was then grown by MBE on diced 3.2 x 2.6 cm coupons with an InAs quantum dot active region aligned to the nitride couplers. This material was then fabricated into 4 mm long and 4 um wide ridge waveguide devices with contacts for electrical bias.

Using this method, we demonstrate waveguide-coupled lasers and photodetectors monolithically integrated with foundry-processed silicon photonics wafers. Lasers operate in the O-band for data communication applications and show mW-scale output powers measured in-fiber when coupled out of the chip. Photodetectors were characterized as a function of bias voltage when excited by 1.3 um input laser light coupled from off-chip. The photodetectors show a highly linear response with sub-nA dark current. Together with the integrated laser results, this represents a major step forward in creating scalable PICs with on-chip III-V devices.

This material is based on research sponsored by Defense Advanced Research Projects Agency (No. HR0011-20-C-0142) and Air Force Research Laboratory under AIM Photonics (agreement number FA8650-21-2-1000). The U.S. Government is authorized to reproduce and distribute reprints for Governmental purposes notwithstanding any copyright notation thereon. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the United States Air Force, the Air Force Research Laboratory, or the U.S. Government.

2:45pm NAMBE1-MoA-6 Optical Enhancement of GaAsP Solar Cells on GaP/Si with Distributed Bragg Reflectors, Bora Kim, Adrian Birge, Brian Li, Corey White, Devon Lee, Minjoo Larry Lee, University of Illinois Urbana-Champaign

Epitaxial III-V/Si tandem solar cells offer a path to high efficiency at lower cost¹. 1.7 eV GaAs_{1-y}P_y (GaAsP) is an optimal top cell for Si-based tandems, leveraging a GaP nucleation and a GaAsP graded buffer. Despite advances in dislocation control in GaAsP subcells on Si with two-step growth, strained layer superlattices, tailored doping profiles, and compositional grading², high threading dislocation density (TDD) still limits minority carrier diffusion lengths. Thinner GaAsP absorbers can mitigate challenges with low diffusion lengths but incur optical losses due to incomplete absorption. A distributed Bragg reflector (DBR) resolves this limitation by reflecting transmitted photons back into the absorber, enhancing effective optical path length and carrier collection while enabling thinner GaAsP. Here, we demonstrate the first GaAsP single-junction (1J) cell on Si with a 1.46% efficiency boost from a 20-period Al_{0.20}Ga_{0.80}AsP/Al_{0.80}Ga_{0.20}AsP DBR, highlighting photon management for high-performance GaAsP/Si tandem solar cells.

We grew GaAsP solar cells via MBE on GaP/Si (001) templates with a 500 nm p-GaP buffer, a 1.8 μ m p-GaAsP graded buffer and a 750 nm GaAsP absorber. Compared to our previous best GaAsP 1J devices³, we reduced the cell thickness by 2.2 μ m, allowing >2 μ m for the DBR without exceeding the thermal expansion cracking threshold of ~6 mm.

The 20-period AlGaAsP DBR calibration shows a 95.7% peak reflectance with a 55 nm bandwidth, closely matching calculations (97.2%, 60 nm). Electron channeling contrast imaging reveals similar TDD (\sim 7-8 \times 10⁶ cm⁻²) in cells with or without a DBR, indicating negligible impact from DBR growth. External quantum efficiency (EQE) measurements show enhanced carrier collection at 660-730 nm due to DBR reflection, increasing EQE-calculated short-circuit current density (EQE-J_{SC}) by 1.42 mA/cm². EQE at 450-550 nm was lower than expected, likely due to elevated window/emitter interface recombination loss. Nevertheless, the DBR cell exhibits a 1.46% absolute efficiency gain due to increased J_{SC} and a 12 mV open-circuit voltage (V_{OC}) boost. Additionally, V_{OC} and fill factors closely match our previous best n+/i/p cells³.

This work demonstrates 15%-efficient GaAsP solar cells on Si with an AlGaAsP rear DBR, where DBR reflection improves near-bandedge EQE and J_{SC}. Our results show the promise of DBRs for high-efficiency, low-cost GaAsP/Si tandems, with potential for enhanced radiation hardness in space applications with a thin absorber.

[1] J. F. Geisz et. al., *Semicond. Sci. Technol.*, **17** (2018). [2] J. T. Boyer et. al., *Cryst. Growth Des.*, **20** (2020). [3] S. Fan et. al., *Cell Rep. Phys. Sci.*, **1** (2020).

3:00pm NAMBE1-MoA-7 Interface Fermi-Level Engineering for Selective Hole Extraction Without P-Type Doping in CdTe Solar Cells to Reach High Open Circuit Voltage (>1 V), Zheng Ju, Xin Qi, Xiaoyang Liu, Arizona State University; Jiarui Gong, Texas A&M University; Razine Hossain, Nathan Rosenblatt, Tyler McCarthy, Allison McMinn, Martha McCartney, David Smith, Arizona State University; Zhenqiang Ma, University of Wisconsin - Madison; Yong-Hang Zhang, Arizona State University

Solar cells, along with other optoelectronic devices such as photodiodes, light-emitting diodes (LEDs), and lasers, rely on p-n junctions to either collect photogenerated carriers in absorber regions or inject carriers into the active region. The use of p-n junctions in solar cells is advantageous because the electric field within the device yields the efficient extraction of photogenerated carriers for high power conversion. The doping levels in the p- and n-regions set the built-in voltage (V_b) across the device, which in turn limits the maximum achievable open circuit voltage (V_{oc}). A higher V_b is preferred as it creates a stronger electric field in the absorber region, reducing the transit time for photogenerated carriers, enhancing their collection at the contacts, and improving overall conversion efficiency.

Solar cells with a V_{oc} exceeding 1 V have been developed using an n-type CdTe/MgCdTe double-heterostructure (DH) absorber with an n-type indium

Monday Afternoon, August 25, 2025

tin oxide (ITO) transparent layer forming a hole-selective contact. No p-type doping is used in the devices. The ITO layer is directly deposited atop the MgCdTe barrier layer. Charge transfer from the ITO and the n-type absorber to the interface states between the ITO and the top MgCdTe barrier results in a Fermi level near the valence band edge of the CdTe layer. This charged interface functions effectively as a "p-region," achieving a V_{bi} of up to 1.01 V. A straightforward model is proposed to explain the relationship between Mg composition in the barrier layer and the corresponding V_{bi} . The modeling results are in good agreement with experimental results obtained from capacitance-voltage (C-V) measurements. X-ray photoelectron spectroscopy (XPS) measurements on samples having a MgCdTe top barrier layer with different Mg compositions confirm the correlation between the interface Fermi-level position and the observed V_{bi} . The devices, tested by the National Renewable Energy Laboratory (NREL), show a V_{oc} over 1 V (1.0164 ± 0.0026 V), consistent with the V_{bi} derived from C-V measurements, thereby confirming that V_{bi} limits V_{oc} in these devices. The integrated J_{sc} from EQE is 24.88 mA/cm², attributed to the absence of an absorptive hole-selective contact layer, such as a-Si:H. The efficiency of this device reaches 17.3%.

This innovative approach to addressing the challenge of low p-type doping in CdTe solar cells can potentially be applied to other interfaces involving semiconductors, transparent conductive oxides (TCOs), and certain metals, offering broad applications not only in photovoltaics but also in photodetectors, LEDs, and lasers.

NAMBE

Room Tamaya ABC - Session NAMBE2-MoA

Infrared Materials

Moderator: Aaron J. Muhowski, Sandia National Laboratories

3:30pm NAMBE2-MoA-9 James S. Harris MBE Scientific Discovery Awardee Talk: Breaking the Rules: Perturbing Oxides to Unleash Novel Properties, *Darrell Schlom*, Cornell University **INVITED**

When it comes to perturbing oxides to unleash the novel phenomena they possess, oxide MBE rocks! In this talk I will highlight a few examples from the past >35 years of oxide MBE demonstrating how the atomic-layer control made possible by this technique can be used to break synthesis rules and create metastable compounds and heterostructures with exciting properties. Examples include the use of strain engineering, interface engineering, epitaxial stabilization, or dimensional confinement to transmute materials from ground states that are "vegetables" into ground states that are ferroelectric, ferromagnetic, both at the same time (multiferroic), or superconducting. A key element of this modern alchemy is the availability of underlying substrates with appropriate structural motifs to strain these complex oxide thin films to percent levels—far beyond where they would crack or plastically deform in bulk—or to stabilize metastable polymorphs. I will also describe the recent discovery of conducting α -(Al_xGa_{1-x})₂O₃ films with a bandgap exceeding 7 eV. This makes α -(Al_xGa_{1-x})₂O₃ the highest bandgap semiconductor known.

* The work reported was performed in collaboration with superb students, postdocs, colleagues, and collaborators from around the world. Although it is only possible to acknowledge a small fraction, I am deeply grateful for the exploratory fever instilled by my Ph.D. advisor—James S. Harris—for whom this award is dedicated, together with the achievements and advice from leading collaborators: Long-Qing Chen, Chang-Beom Eom, Craig J. Fennie, Venkat Gopalan, Christo Guguschev, Debdeep Jena, Stanislav Kamba, Lena F. Kourkoutis, Jeremy Levy, Zi-Kui Liu, Jochen Mannhart, David A. Muller, Nate Orloff, Xiaoqing Pan, Karin M. Rabe, Ramamoorthy Ramesh, Peter Schiffer, Kyle M. Shen, Dmitri A. Tenne, Reinhart Uecker, and Huili Grace Xing.

4:00pm NAMBE2-MoA-11 Deep Level Transient Spectroscopy and Time-Resolved Photoluminescence as a Function of Room Temperature 63 MeV Proton Irradiation of InAs Nbn Detectors Grown by Molecular Beam Epitaxy, *Rigo Carrasco*, Air Force Research Laboratory, USA; *Christopher Hains*, *Alexander Newell*, *Christian Morath*, *Preston Webster*, Air Force Research Laboratory; *Evan Anderson*, Sandia National Laboratory

A semiconductor material's technology readiness for space-based sensing applications is largely dictated by its detection capability, where a holistic examination of the material's detector dark current and quantum efficiency determines its sensitivity. One of the most significant detriments to a detector's performance are crystalline defects that introduce deep levels within the band gap that act as recombination centers. These defects can

naturally arise during semiconductor growth, and over the course of a detector's space-based mission life from exposure to cosmic rays, high energy ions in the Van Allen belts and magnetosphere, and solar events. These defects lead to a decrease in the minority carrier lifetime which yields a corresponding increase in dark current and decrease in quantum efficiency. As a result, there is motivation to investigate candidate materials' minority carrier lifetimes and corresponding defect character both before and after high energy proton irradiation to characterize the materials-level factor that inhibits detector performance throughout its mission life.

Here, we report the defect characteristics of an InAs n Bn detector structure grown by molecular beam epitaxy. The detector structure's minority carrier lifetime is examined by time resolved photoluminescence and the defect character is assessed by deep level transient spectroscopy. Deep level transient spectroscopy is carried out using a medium-frequency impedance analyzer to collect the time-resolved capacitance transients over temperatures ranging from 10-300 K. Analysis of the transient data indicates the presence of one defect level with an activation energy greater than the InAs bandgap energy (~650 meV) which is shown to be due to a defect in the AlGaAsSb barrier, and another level with a ~30 meV activation energy in the InAs. The concentration of the latter defect is then shown to increase monotonically with each step dose of room temperature 63 MeV proton irradiation. The minority carrier lifetime is also measured as a function of step-wise proton fluence to evaluate the lifetime damage factor, to compare with the 30 meV irradiation-dependent defect level identified in the deep-level transient spectroscopy analysis. The results are analyzed alongside dark current and capacitance-voltage measurements of the InAs n Bn to tie the results of both techniques to typical device benchmark measurements. A discussion on synthesizing the results from these two techniques will be provided, giving a characterization suite that can provide a materials-level connection to device performance. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

4:15pm NAMBE2-MoA-12 Evaluation of the Optical Absorption Properties of MBE Grown InAs/InAsSb and InGaAs/InAsSb Superlattices for Infrared Photodetector Applications, *Marko Milosavljevic*, Arizona State University; *Rigo Carrasco*, *Alexander Newell*, Air Force Research Laboratory, USA; *Jaden Love*, *Stefan Zollner*, New Mexico State University; *Christian Morath*, *Diana Maestas*, *Preston Webster*, Air Force Research Laboratory, USA; *Shane Johnson*, Arizona State University

Several midwave (3 - 5 μ m) and longwave (8 - 12 μ m) type-II InAs/InAsSb and InGaAs/InAsSb superlattices are grown by molecular beam epitaxy and investigated using spectroscopic ellipsometry. The work evaluates the absorption edge and the refractive index of these superlattice materials for photodetector design and performance. In particular, the absorption edge position, width, and absorption intensity determine the photodetection wavelength range and the photodetector material thickness required to achieve optimal detectivity.

A Kramers-Kronig consistent model for the refractive index and absorption coefficient in the vicinity of the fundamental bandgap of the superlattice miniband structure is developed. A fit of this model to the raw ellipsometric data establishes the bandgap energy, the magnitude of the absorption coefficient at the bandgap, the characteristic energy width of Urbach tail below the bandgap, and the impact of the Coulomb interaction, all of which determine the shape of the absorption edge. The absorption coefficient is modeled using an Urbach-tail absorption edge coupled to the observed power law behavior of absorption above the bandgap. The refractive index is modeled using a long wavelength pole oscillator and a Cauchy integral over the absorption coefficient model, which as well mirrors the shape of the absorption edge and provides the energy position of the transverse optical phonon absorption peak that typically occurs at energies below the measurement range. Measuring the optical constants of superlattices is challenging since they contain a large number of interfaces and must be grown thick to ensure enough periods to determine the optical properties of the miniband structure. For the samples measured, this results in the presence of spurious periodic interference peaks in the optical constants extracted using a point-by-point fit. Multi-sample fits to the same midwave superlattice structures grown at various thicknesses significantly reduces the presence of the interference peaks and in general improves the fit to the model and the extraction of the key absorption edge parameters.

In comparing the superlattice results, the shorter period InGaAs/InAsSb superlattices exhibit stronger absorption with a broader absorption tail compared to the InAs/InAsSb superlattices. The shorter period superlattices have larger electron-hole wavefunction overlap, but with a greater number of frozen-in tail states that result from alloy and interface disorder at the

Monday Afternoon, August 25, 2025

superlattice interfaces. These results are compared and evaluated with additional measurements of thick bulk layers of the superlattice binary and ternary constituents.

4:30pm NAMBE2-MoA-13 Tunable Low-Loss Plasmonic Resonances in Heavily-Doped InAs for Infrared Optoelectronic Devices, Thomas Shearer, Ethan Caudill, Kiernan Arledge, Tetsuya Mishima, University of Oklahoma; Chadwick Canedy, John Murphy, Jill Nolde, Chase Ellis, US Naval Research Laboratory; Priyantha Weerasinghe, Amethyst Research Inc.; Michael Lloyd, NIST-Gaithersburg; Terry Golding, Amethyst Research Inc.; Igor Vurgaftman, Jerry Meyer, US Naval Research Laboratory; Michael Santos, Joseph Tischler, University of Oklahoma

Metals like gold, silver, and aluminum, which have a plasma frequency in the ultraviolet, have traditionally been used for plasmonic enhancement of optoelectronic devices such as emitters and detectors of visible light. However, these metals are of limited use for infrared plasmonic enhancement due to losses that become increasingly high at frequencies far below the plasma frequency. We have explored the use of heavily-doped InAs as a low-loss conductor for plasmonic enhancement of infrared devices. The infrared plasma frequency of InAs can be tuned by *n*-type doping and this plasmonic material can be monolithically integrated with III-V infrared optoelectronic devices during growth by molecular beam epitaxy (MBE).

Heavily-doped InAs layers were grown in three separate MBE systems using either Te or Si as the *n*-type dopant. The surface morphology was assessed by optical microscopy and atomic force microscopy. The plasma frequency and optical scattering rate were determined by fitting ellipsometry measurements as a function of infrared wavelength. A plasma frequency corresponding to an infrared wavelength of 4.5 to 10.5 μm in air was obtained for an electron concentration between 6.0 and $0.9 \times 10^{19} \text{ cm}^{-3}$. A trend of decreasing optical scattering rate (1500 to 500 cm^{-1}) was observed as the plasma frequency was increased, or equivalently as the plasma wavelength was decreased (10.5 to 4.5 μm).

The doped InAs materials were photolithographically patterned and dry etched to form one-dimensional gratings with several pitches and linewidths up to 5 μm . Reflectivity measurements were performed using a Fourier transform infrared spectrometer equipped with an infrared microscope. Several plasmonic resonances were observed with up to 95% absorption and quality factors around 7. Modeling by finite-element electromagnetic calculations (COMSOL) confirmed that the experimental results demonstrated tunable low-loss plasma resonances at infrared frequencies.

This material is based upon work supported by the Office of the Undersecretary of Defense for Research and Engineering Basic Research Office STTR under Contract No. W911NF-21-P-0024. Disclaimer: The content of the information does not necessarily reflect the position or the policy of the Government, and no official endorsement should be inferred.

4:45pm NAMBE2-MoA-14 Impact of Uncracked Group V Species on Unintentional Doping in AlInAsSb, Ellie Wang, J. Andrew McArthur, University of Texas at Austin; Hannaneh Karimi, Joe Campbell, University of Virginia; Seth Bank, University of Texas at Austin

$\text{Al}_x\text{In}_{1-x}\text{As}_y\text{Sb}_{1-y}$ (referred to as AlInAsSb) grown as a digital alloy by molecular beam epitaxy (MBE) has been shown to have characteristics useful for avalanche photodetectors (APD) operating in the near- to mid-IR. In addition to a broadly tunable bandgap over a wide compositional range, the material system has favorable band offsets and exhibits low excess noise due to low impact ionization coefficient ratios ¹. However, another consideration is the unintentional doping (UID) concentration, which depends on factors in the system, such as the source material and growth temperature, and is susceptible in the digital alloy due to the complex layers and interfaces. This important factor influences characteristics such as the electric field profile, depletion, and mobility ². We have previously shown UID reduction in AlInAsSb by outgassing the MBE source material ³. Another potential avenue is through the group-V sources, such as by using As_4 instead As_2 . Not only does As_2 contain contaminants such as sulfur that can contribute to impurity concentrations, but lowering the cracker temperature in the cell could also reduce the outgassing of impurities during growth ^{4,5}.

Here, we compare the effects of As_4 and As_2 on the UID concentration of InAlAs on InP. InAlAs PIN diodes containing each arsenic species were grown by MBE on semi-insulating InP substrates. The transition from As_2 to As_4 was achieved by reducing the cracker temperature in the two-zone effusion cell. High-resolution X-ray diffraction ω -2 θ scans indicated nominal strain-balancing to the substrate. Devices were fabricated, and capacitance-

voltage characteristics were measured at room temperature to calculate carrier concentration versus depletion depth. A ~2-fold reduction in UID was observed, with a carrier concentration of $\sim 1 \times 10^{17} \text{ cm}^{-3}$ in the As_4 device versus $\sim 4 \times 10^{16} \text{ cm}^{-3}$ in the As_2 device. Dark and light current-voltage characteristics were also collected. While both devices showed comparable photoresponse, the onset of tunneling in the As_4 device was increased by >20%; importantly, just prior to breakdown of the As_2 device (-16 V), the dark current was an order of magnitude lower for the As_4 device. These results suggest that using As_4 is a feasible path to enhance APD sensitivity by decreasing the UID. Further reduction is anticipated through the antimony species, and additional investigation of the effects on digital alloys are in progress. This work was supported by DARPA and ARO.

¹S. R. Bank, et al. *JSTQE*, 2018. ²D. Chen, et al. *APL*, 2021. ³J. A. McArthur, et al. *ACS Crys. Gr. and Des.* (submitted). ⁴B. J. Skromme, et al. *J. Appl. Phys.*, 1985. ⁵R. Chow, et al. *JVSTB*, 1990.

Monday Evening, August 25, 2025

NAMBE

Room Tamaya DE - Session NAMBE-MoP

NAMBE Poster Session

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Monday Evening, August 25, 2025

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

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

NAMBE-MoP-5 Optical and Electrical Properties Study of Transferred Ge0.82Sn0.18 Flakes Based on Layer Transfer Process, *Haochen Zhao, Suhoo Park, Shedrack Dafe, Tuofu Zhama, Chandan Samanta, Zijun Chen, Yuping Zeng*, University of Delaware

GeSn alloys with high Sn content have garnered significant interest in optoelectronic and semiconductor applications due to their tunable direct bandgap and improved carrier transport properties. In this study, we investigate the optical and electrical properties of Ge0.82Sn0.18 flakes using a layer transfer process. GeSn was epitaxially grown on an InP substrate and subsequently released. The exfoliated Ge0.82Sn0.18 flakes were first transferred onto a KBr substrate to facilitate small-area transmission and reflection measurements, enabling the extraction of optical properties such as absorption and bandgap characteristics. The optical analysis confirms strong absorption, reinforcing the potential of GeSn for infrared photonic applications. To evaluate the electrical properties, the GeSn layers were transferred onto SiO_2/Si substrates, where transmission line method (TLM) and Hall bar structures can be fabricated. Electrical characterization reveals enhanced carrier mobility, highlighting the suitability of GeSn for high-performance electronic devices. This study demonstrates a scalable and effective approach for integrating GeSn onto insulator substrates, providing valuable insights into its fundamental optical and electronic behavior. These findings pave the way for future advancements in CMOS-compatible optoelectronics and high-speed transistor technologies.

NAMBE-MoP-8 Examining Magnetic Depth Profiles of Oxide MBE Grown PdCoO_2 Delafossite Thin Films with Post-Growth Helium Implantation, *Sangsoo Kim*, Oak Ridge National Laboratory

The delafossite PdCoO_2 consists of alternating layers of highly conductive palladium and Mott insulating octahedral cobalt oxides. While PdCoO_2 is diamagnetic in bulk crystals, both Co and Pd layers exhibit magnetic metastability. We have recently demonstrated [1] that small perturbations, such as strain, can induce itinerant magnetism in helium-implanted thin films. This positions PdCoO_2 as a promising material for future spintronics, serving as a platform for itinerant and emergent magnetism through helium microscope patterning [2] of the surface. A key question remains regarding the locality of the emergent magnetization relative to the helium implantation sites, in thin films of finite depth: after helium is implanted, are there other extrinsic effects that may affect the magnetism, such as vacancies or micro-strain distortions [3]? In this talk, we examine data from muon spectroscopy measurements alongside simulated depth profiles from TRIM [4] calculations, correlating the helium implantation depth profile with the muon magnetic volume fraction. Our analysis reveals extraneous magnetic sites located 10 to 30 nm from the surface that cannot be accounted for by helium implantation alone. This suggests that helium implantation does not fully explain the induced magnetization in PdCoO_2 , necessitating additional surface-sensitive measurements to characterize the remaining magnetization.

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

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

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

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

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

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

Non-ambient stages for measuring epitaxial films with x-ray diffraction enable temperature-dependent characterization of epitaxial films not otherwise available in bulk form or as powders. To demonstrate the strain evolution and thermal properties of epitaxial films at different temperatures, we use an Anton-Paar DCS 350 stage on a PAN'alytical Empyrean diffractometer to measure antimonide-based strained-layer

Monday Evening, August 25, 2025

superlattices (SLS) and epitaxially stabilized α -Sn_{1-x}Ge_x films.

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

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

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

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

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

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

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

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

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

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This work was supported by NSF QLCI HQAN and ARL

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

AlN is a wide bandgap material commonly used as a buffer but also as part of the active layer of heterostructure for the UVC applications. However, the absence of native substrates limits the crystalline quality of AlN films and, consequently, the overall performance of heterostructure that relays on its optical properties. Since III/V flux ratio and the substrate temperature are the two key growth parameters that significantly affect film properties even with small variations, identifying optimal conditions is challenging. In this work, we investigated the influence of these parameters on the structural, morphological, and optical properties of AlN/Si(111) thin films deposited by plasma assisted molecular beam epitaxy. Growth temperature varied from 790°C to 850°C, and the aluminum cell flux was adjusted between 1.91×10^{-7} and 2.4×10^{-7} Torr. Optical characterization was performed using a thermal modulation spectroscopy technique. Unlike more traditional methods, such as photoreflectance, which employ lock-in amplifiers to measure $\Delta R/R$ our approach determined $\Delta R/R$ by simply subtracting reflectance signals, using a perturbation light at 785 nm. The 785 nm laser is not absorbed by the film but by the substrate, as the substrate heats up, changes the refractive index of AlN and leads to changes in the reflectance spectrum that allows the bandgap identification. Our measurements indicate a bandgap of approximately 6eV at room temperature, which is consistent with literature values. X-ray diffraction (XRD) diffractograms confirm the formation of the wurtzite phase, with an average FWHM of 820 arcseconds for the main (002) peak. AFM and SEM analyses reveal a uniformly planar morphology with a root-mean-square (rms) roughness of 1nm. Optimal growth was achieved at 850 °C with an aluminum cell flux of 1.91×10^{-7} Torr having the best structural and optical quality of the film.

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

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

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

Monday Evening, August 25, 2025

layer forms and investigate the role of defects in emission properties after passivation in these materials. We will be looking at the interplay between the inherent defects in the grown monolayer and external processes.

NAMBE-MoP-20 Influence of the Growth Temperature and Surface Reconstruction on the Performance of Intermediate-Band Solar Cells Based on InAs Submonolayer Quantum Dots, Ahmad Alzeidan, Lucas. A. T de Souza, Alain A. Quivy, Institute of Physics, University of São Paulo, Brazil
The submonolayer technique is an alternative method for growing quantum dots (QDs) in a flexible manner, achieving high surface density without the presence of a wetting layer, which is typical of conventional quantum dots obtained in the Stranski-Krastanov (SK) growth mode. InAs/GaAs submonolayer quantum dots (SMLQDs) are formed through the cyclic deposition of a fractional monolayer of InAs (typically 30–70%), followed by the growth of a few monolayers (MLs) of GaAs. The small two-dimensional (2D) InAs islands that nucleate in successive InAs submonolayers tend to vertically stack due to the local strain field caused by lattice mismatch, eventually forming individual QDs, the height of which depends on the number of cycle repetitions. Our recent studies [1, 2] indicate that growing InAs/GaAs SMLQDs in the presence of a (2x4) surface reconstruction at a higher temperature than usually (525 °C instead of 480–510 °C) enhances the performance of infrared photodetectors, when compared to the common c(4x4) reconstruction obtained at lower temperature.

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

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

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

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

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

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

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

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

GaN promises significant application in high power RF devices. It is critical to reduce dislocation density in GaN epilayers for reliable HEMT device operation. This study investigates the epitaxial growth of GaN on AlN buffer layers by MBE. The growth started with a 100-nm thick AlN buffer layer on SiC substrate. For sample 240812B(S1), only an AlN buffer layer was grown. Two methods were utilized for the subsequent growth of GaN at 780°C. For Sample 240815A (S2), 640nm GaN was grown under a Ga/N flux ratio of 1.8, while for Sample 240822A(S3), 70nm GaN buffer layer was first grown at Ga/N flux ratio of 0.9 prior to the growth of 540nm GaN at Ga/N flux ratio of 1.8. For both samples, an AlGaN barrier layer and a GaN cap layer were grown on top.

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

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

Monday Evening, August 25, 2025

carrier mobility is related to the reduction of dislocation density and surface pits. This work provides crucial insights into interfacial engineering for GaN RF device applications.

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

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

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

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

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

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

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

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

Topological states are predicted to exist in Ge-Sn digital alloys composed of atomically-controlled, monolayer-digitized structures of α -Sn and Ge grown on Ge (111). However, realizing these structures is nontrivial. The Ge-Sn system is metastable at Sn compositions above 1.1 % due to the difference in the two constituent elements' lattice constants of 14.7 %. Additionally, α -Sn, the diamond crystal lattice phase of Sn, is unstable at temperatures above 13.2 $^{\circ}\text{C}$. Here, we demonstrate the monolayer-by-monolayer growth of Ge-Sn digital alloys using low-temperature molecular beam epitaxy, which enables growth of the metastable α -Sn phase near the critical temperature for the crystal-amorphous transition and allows atomically precise control of layering within the structure. We investigate the progression of the surface morphology of these structures via scanning tunneling microscopy, from which we find that Sn forms quasi-2D island structures at thicknesses beyond a wetting layer. We quantify the extent of interdiffusion of the atomic layers through cross-sectional transmission electron microscopy and atom probe tomography. As the structure grows, we provide insight into the breakdown of epitaxial growth, driven by both the metastability of the Ge-Sn system and slow growth kinetics at the low growth temperatures. Finally, we measure the band structure of select digital alloy materials through angle-resolved photoelectron emission spectroscopy. This work exhibits the feasibility of digital alloy growth in the Ge-Sn system, emphasizing the growth kinetics and morphology of metastable Ge-Sn digital alloys.

This work was performed in part at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. This article has been authored by an employee of National Technology & Engineering Solutions of Sandia, LLC under Contract No. DE-NA0003525 with the U.S. Department of Energy (DOE). The employee owns all right, title and interest in and to the article and is solely responsible for its contents. The United States Government retains and the publisher, by accepting the article for publication, acknowledges that the United States Government retains a non-exclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this article or allow others to do so, for United States Government purposes. The DOE will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan <https://www.energy.gov/downloads/doe-public-access-plan>. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

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

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

We propose a purely continuum model based on extending the Cahn-Hilliard equations, which have been successfully applied in modeling a variety of phase separation problems, for multilayer epitaxial growth. Here, the presence and absence of adatoms are considered the two phases, replicating the effects of interatomic interactions. By introducing an

Monday Evening, August 25, 2025

interlayer stepping term into the simulation model, we are able to replicate the effects of an ES potential and produce step meandering and step bunching structures. Finally, we show that our simulation matches empirical growths where the ES potential is present, such as Bismuth surfactancy studies on GaSb grown via MBE [6].

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

Bottom-up synthesized carbon nanostructures, particularly graphene nanoribbons (GNRs), possess atomically precise architectures and tunable electronic properties, making them promising candidates for next-generation electronic devices and advanced technologies. On-surface synthesis of atomically precise GNRs has been demonstrated using molecular beam epitaxy (MBE), which involves the deposition of monomer precursors and subsequent polymerization on the surface. However, their synthesis typically relies on metal substrates (e.g., Au, Cu, and Ag), which must be transferred to insulating substrates to enable device integration. Conventional transfer methods, such as chemical etching and hydrogen bubble delamination, face significant challenges in maintaining the structural and functional integrity of the materials. Chemical etching often introduces irreversible chemical damage, degrading material quality, while hydrogen bubble delamination is problematic for metal thin films due to weak adhesion and mechanical fragility. These limitations restrict the scalability and reliability of current transfer techniques. Here, we present a wafer-scale, etch-free transfer method using low-melting-point metals (LMPMs), Field's metal (51% In, 32.5% Bi, 16.5% Sn), to address these challenges. This method provides robust mechanical support for metal thin films during hydrogen bubble delamination, enabling the transfer of carbon nanostructures without the use of harsh etchants while preserving their structural integrity. As a demonstration, 7-armchair graphene nanoribbons (7-AGNRs) were synthesized on Au(111)/mica substrates and successfully transferred onto SiO₂/Si substrates using this method. Raman spectroscopy confirmed the preservation of structural uniformity and minimal defect density after transfer. The scalability of this method was further validated through wafer-scale transfer of Au thin films from 100-mm sapphire substrates. Additionally, field-effect transistors (FETs) fabricated using transferred GNRs exhibited stable electronic performance. This work establishes LMPM-assisted transfer as a versatile and scalable platform for integrating carbon nanostructures into various technological applications.

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

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

consideration is Nb that superconducts at 9K and can possibly be used in a structure at a higher temperature of 1K.

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

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

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

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

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

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

Monday Evening, August 25, 2025

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

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

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

Here we present our recent results on the controlled synthesis of screw dislocations (SDs) in epitaxially grown (001) GaAs nanomembranes (NMs) or ultra-thin sheets where the lateral size-to-thickness ratio exceeds 10^2 . Our approach to SDs' synthesis involves stacking GaAs NMs at a non-zero twist angle to form twisted bicrystals (TBiCs). This configuration generates an array of twist boundaries at the interface, which act as seeds for the growth of SDs along the thickness direction in the bonded crystals. The propagation of SDs from the interfacial twist boundary is driven by thermal energy during annealing.

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

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

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

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

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

quantum technology applications. Authors acknowledge support from the Massachusetts Technology Collaborative (award number 22032), and the National Science Foundation (award number OSI 2329067).

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

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

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

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

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

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

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

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

The infrared wavelength range is relevant to several technology areas, including biosensing, trace gas sensing, environmental monitoring, defense,

Monday Evening, August 25, 2025

security, and wireless communication. A wide range of molecular species have rotational and vibrational absorbance in the infrared, allowing for infrared emitters to enable the identification and monitoring of these species for industrial applications and environmental monitoring. In order to enable these technologies to be realized, there is a need for compact, high efficiency emitters.

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

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

The AlInN alloys hold significant potential for various device applications such as high electron mobility transistors, vertical-cavity surface-emitting lasers, and deep-UV LEDs. However, challenges arise due to the substantial difference in surface mobility between Al and In atoms, leading to distinct optimal growth temperatures for AlN and InN. Moreover, the presence of a large lattice mismatch and In segregation further complicates the growth process of AlInN alloys. In this work, we report the first successful demonstration of growing InAlN/AlN quantum well structures on Si(111) substrates, a particularly challenging platform due to thermal and lattice constraints. To address the difficulties associated with In incorporation and segregation, we employed the metal-modulated epitaxy (MME) technique to grow AlInN alloys by MBE. The MME approach, involving the alternate supply of Al and In while maintaining a steady N flux, proved essential in minimizing indium segregation and enabling the formation of more defined quantum wells. AlInN quantum wells (QWs) with AlN barriers were grown on Si(111) substrates using a Riber C21 MBE system. Active nitrogen species were generated via an RF-plasma source at 190 W with a N flux of 0.2 sccm, while beam equivalent pressures for In and Al were 1.4×10^{-7} and 2.8×10^{-7} Torr, respectively. Three distinct QWs (QW1, QW2, QW3) with varying In concentrations were grown on Si (Fig. 1). RHEED patterns remained streaky throughout, though 3D spots appeared during QW3 growth, indicating increasing surface roughness (Fig. 2). AFM confirmed this with an RMS roughness of 8 nm (Fig. 3). SIMS profiles revealed three In peaks, consistent with QWs of different composition, and a surface-leaning In shoulder in QW3, likely linked to In segregation at higher In content (Fig. 4). HRXRD curves exhibited satellite peaks near the AlN(0002) reflection (Fig. 5), evidencing the presence of AlInN layers and interference effects. Finally, room-temperature CL spectra showed a strong emission centered at 3.27 eV, presumably from the superposition of emissions from all three QWs (Fig. 6).

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

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

that the various species have on the growth and processing of thin film material samples and devices.

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

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

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

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

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

In this work, synthesis records detailing several hundred individual plasma-assisted molecular beam epitaxy (PAMBE) thin film crystal growth experiments of transition metal as well as group-III nitride compounds have been organized into distinct, material composition-specific data sets. For each growth record, the complete set of experiment parameters (substrate temperature, growth duration, element source conditions, etc.) are associated with material properties of interest, including binary measures

Monday Evening, August 25, 2025

of crystallinity (1 for monocrystalline, 0 for polycrystalline) as well as surface morphology (1 for atomically-flat, 0 for three-dimensional growth) as determined by *in-situ* reflection high-energy electron diffraction (RHEED) patterns. A Bragg-Williams derived measure of lattice ordering ($0 \leq S^2 \leq 1$) is also investigated as a continuous, structural figure of merit for investigation.

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

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

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

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

NAMBE-MoP-43 Low Temperature Growth of Ultra-Thin CdSe/ZnSe Quantum Wells, *Yang A. Vázquez-Soto, Jorge Pérez-Saavedra, Frantisek Sutara, Isaac Hernández-Calderón, CINVESTAV, Mexico; Masakazu Kobayashi*, Waseda University, Japan

CdSe has demonstrated great capabilities for the elaboration of light emitting nanostructures such as quantum dots and ultra-thin quantum wells (UTQWs). In fully strained CdSe/ZnSe ultra-thin quantum wells grown on GaAs (001) substrates CdSe is under large biaxial compressive stress resulting in a critical thickness of around 3.5 monolayers (MLs). We grow the CdSe by means of atomic layer epitaxy (ALE). During each Cd-Se ALE cycle a nominal coverage of 0.5 ML is obtained due to the surface reconstruction properties of Cd. We have observed that in the 260 – 290 °C range higher substrate temperatures (T_s) produce a lower Cd content of the UTQWs, as indicated by the blue-shifted UTQW excitonic emission [1]. This is attributed to the thermally activated substitution of Cd atoms by Zn during the first stages of ZnSe growth on top of the CdSe layer due to the chemical interaction of Zn atoms with underlaying Cd atoms which are removed from the UTQW layer and reevaporated or mixed with the Zn atoms of the growing ZnSe barrier. Then, the resulting Cd content of the UTQW is slightly lower than 100%. One could expect that lowering T_s below 260 °C will allow us to reach 100% Cd content quantum well layers, which would be evident by the red shift of the excitonic emission as the Cd content increases. With the purpose of investigating the structural and excitonic properties of CdSe UTQWs grown at lower temperatures we elaborated heterostructures containing nominally 1 and 3 ML CdSe UTQWs at $T_s = 230$ and 250 °C. Deoxidized GaAs(001) semi-insulating substrates covered by a 500 nm thick buffer layer of ZnSe grown by molecular beam epitaxy at 275 °C were employed for the growth. After the ZnSe buffer layer was finished, a careful procedure was used to set the desired T_s . We obtained photoluminescence spectra using a typical setup with an HeCd laser as excitation. The low and room temperature excitonic spectra of the heterostructures showed larger than expected red shifts and broadening of the peaks and reduced excitonic emissions. These results strongly suggest that, besides the Cd content increase, the low T_s produce significant roughness of the CdSe layers due to reduced surface diffusion and the characteristics of the growth mode. The observed exciton emission energies are compared with theoretical calculations considering several configurations of the QW roughness.

1. I. Hernández-Calderón, J.C. Salcedo Reyes, A. Alfaro-Martínez, M. García Rocha, *Microelectronics J.* 36, 985 (2005).

NAMBE-MoP-44 Caltech Thermal Laser Evaporation System: Design and Capabilities, *David Catherall*, Caltech

Current state-of-the-art thin film deposition methods based on thermal evaporation are difficult to apply to films containing refractory elements including W, Ta, Mo, and Re. Thermal laser epitaxy (TLE) is a new deposition method that relies on laser heating rather than resistive heaters or electron beams to heat source material, enabling thermal evaporation of essentially all elements, most without crucibles. However, the method remains relatively unexplored: initial attempts contemporary with the development of MBE were technologically limited, and only one group in recent years has reported thin film deposition using TLE. Here, we present the design of the TLE system at Caltech, the only TLE system in the US at present, and discuss a number of issues that were solved during the initial operation.

Tuesday Morning, August 26, 2025

NAMBE

Room Tamaya ABC - Session NAMBE1-TuM

Quantum Materials

Moderator: Matthew Brahlek, Oak Ridge National Laboratory

8:00am **NAMBE1-TuM-1 NAMBE Young Investigator Awardee Talk: Problem? Add an Element! The Series of Events that brought us to GaInAsSbBi, Preston Webster**, Air Force Research Laboratory **INVITED**

8:30am **NAMBE1-TuM-3 Exploring MBE Deposited Superconductor Bilayers to Control Qubit Base Material Properties, Kevin Grossklaus, Felipe Contipelli, Kunal Tiwari, Duncan Miller, MIT Lincoln Laboratory; Serra Erdamar, Washington University, St. Louis; Luke Burkhardt, Michael Gingras, Bethany Niedzielski, Christopher O'Connell, Hannah Stickler, Dan Calawa, David Kim, MIT Lincoln Laboratory; Aranya Goswami, William Oliver, Massachusetts Institute of Technology; Mollie Schwartz, Kyle Serniak, MIT Lincoln Laboratory**

In order to improve superconducting qubit performance, new materials and processing approaches are actively being sought which will enable devices low in sources of material loss or resilient to them. Interfaces, surfaces, and interior microstructure may all be expected to play a role in final material performance. The superconducting base metallization makes up the majority of the device structures in each qubit, including signal carrying lines, capacitors, and resonators. The capability to control the properties of this material offers an opportunity to affect device performance directly. Molecular beam epitaxy (MBE) deposition enables engineering of base material structure and interfaces through careful control of deposition conditions, layer thicknesses, and vacuum-growth interface conditions.

In this work we will present new results from the near room temperature MBE deposition of metallic superconducting bilayers on silicon substrates, focusing on the Ta and Al system. The effects of varying relative layer thicknesses on film structure and superconducting properties have been systematically examined. Materials characterization by AFM, XRD, RHEED, SEM, and TEM of Ta deposited on epitaxial Al layers of varying thickness will be shown and the effects of varying Al underlayer thickness on Ta film structure will be discussed. The effects of combining different relative thicknesses of Ta and Al on the superconducting critical transition temperature (T_c) of the combined multilayer stack have been examined by electrical testing at cryogenic temperatures. Changes to multilayer T_c relative to stand-alone layers of either Ta or Al will be discussed in terms of possible applications. Design of different bilayer base metals may offer new device processing routes and opportunities for controlling superconducting gap and loss in quantum devices.

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8:45am **NAMBE1-TuM-4 Exploring Arsenic Flux-Induced Surface Morphology Control in InAs/GaInSb Quantum Wells for Spintronic and Quantum Applications, Jimmy Rushing**, Tufts University

The InAs/GaSb heterostructure was first conceived and investigated in the 1980s for IR detection applications [1]. Recent advancements have shown that InAs/Ga(In)Sb quantum wells (QWs) can present as a topologically protected quantum spin hall insulator (QSHI) with an insulating bulk and conducting helical edge states [2-3]. These properties mean that QSHIs could be a key component in spintronic and topological quantum computing applications [3-5]. Producing a topological phase transition in InAs/GaSb QWs requires precise QW thickness, composition and quality control, particularly at the interface between disparate materials. Additionally, our computations show that surface orientation could also play an important role, where growing these QWs on the (111)A surface could provide benefits over the (001) due to its higher symmetry and out of plane polarization effects.

Ga(In)Sb(111)A frequently grows with a rough morphology characterized by pyramidal peaks covering the surface. However, exposing these surfaces to an arsenic over-pressure results in a dramatic smoothing effect. Our results show that III-Sb surfaces with macroscopically resolvable features \sim 70nm in height, with rms roughness $>$ 10nm, can be smoothed (etched) to an atomically flat surface ($<$ 3nm max features and $<$ 0.5nm rms roughness) in a matter of seconds. This phenomenon first surfaced in results (presented at

NAMBE 2024) where a rough GaInSb(111)A surface was found to smooth after capping with a thin 8nm-thick layer of InAs. After reducing the InAs thickness to 1ML and still observing smoothing of the rough GaSb(111)A surface, we next found that we could achieve almost identical results by simply exposing the GaSb(111)A surface to an arsenic flux. This suggests that arsenic is the primary mover in these profound morphological changes. Finally, preliminary results show that the smoothing can be accomplished with As₄ or As₂, and with arsenic beam equivalent pressures in the range 5×10^{-7} to 1×10^{-5} Torr.

We will describe our efforts to gain control and understanding of this phenomenon through the modulation of arsenic bath time, arsenic bath flux, and terminating material. We intend to deploy this powerful new MBE growth/etch technique as follows: (1) to smooth heterointerfaces for QW and QD deposition, (2) to control local strain while growing metamorphic buffers, and (3) as a processing tool for patterning nanocavities for future quantum devices. We believe this approach will open the door to implementing this technique to create a widening array of novel III-Sb-based nanostructures on (111)A surfaces.

References in SI.

9:00am **NAMBE1-TuM-5 Molecular Beam Epitaxy Growth of InAs_{1-x}Bi_x on GaSb for Topological Insulating States, Merve Baksı, James Rushing, Xikae Xie, Avery Hanna, Larry Qui, Ekow Williams, Paul J. Simmonds**, Tufts University

Incorporation of bismuth (Bi) into III-V semiconductors has attracted significant interest not only for its ability to extend infrared optoelectronic applications across a wide spectral range but also for its potential to induce topologically protected surface states, which could form the foundation for certain quantum computing technologies [1].

Motivated by the small inverted band gap that can be induced in InAs/GaSb quantum wells (QWs) [2], we propose engineering the band structure and inducing the edge states through Bi incorporation into InAs layers. This enhancement is expected to improve robustness against thermal fluctuations, making the material viable for room temperature applications as opposed to the topological HgTe/CdTe QW system with a temperature dependent band gap [3].

Theoretical studies predict that InAs_{1-x}Bi_x quantum wells exhibit a topological insulating state when the Bi composition reaches $x\approx 0.15$, with an estimated inverted gap of approximately 30 meV [1]. Given these predictions, InAsBi emerges as a promising candidate for realizing two-dimensional topological insulators (2D TIs). However, achieving such high Bi incorporation remains challenging due to the significant miscibility gap and the limited solubility of Bi in III-V materials [4].

In this work, we investigate the molecular beam epitaxy (MBE) growth of InAsBi on GaSb substrates, focusing on optimizing Bi incorporation and structural quality. By leveraging MBE growth techniques, we aim to systematically control Bi incorporation and assess its impact on electronic and structural properties of InAsBi in reduced dimensions. Our findings will contribute to the advancement of III-V-based topological materials and their potential integration into future quantum devices.

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[4] K. Y. Ma, Z. M. Fang, R. M. Cohen, and G. B. Stringfellow. Organometallic vapor-phase epitaxy growth and characterization of Bi-containing III/V alloys. *Journal of Applied Physics*, 68(9):4586–4591, 11 1990.

Tuesday Morning, August 26, 2025

9:15am **NAMBE1-TuM-6 Group IV Superconductor-Semiconductor Epitaxy for Integrated Quantum Electronics**, *Jacob Issokson, Patrick Strohbeen, New York University; Julian Steele, Carla Verdi, Ardesir Baktash, University of Queensland, Australia; Alisa Danilenko, New York University; Yi-Hsun Chen, University of Queensland, Australia; Jechiel van Dijk, New York University; Lianzhou Wang, University of Queensland, Australia; Eugene Demler, ETH Zurich, Switzerland; Salva Salmani-Rezaie, Ohio State University; Peter Jacobson, University of Queensland, Australia; Javad Shabani, New York University*

Inducing superconductivity in group IV systems (C, Si, Ge) has been an active area of research for the past couple decades since the first discovery of a superconducting state in a heavily boron-doped diamond single crystal in 2004. Utilizing a concept initially proposed by Cohen in the early 1960's, this state was created through non-equilibrium doping wherein significant hybridization between dopants and the parent band insulator (semiconductor) causes significant density of states (DOS) at the Fermi level. This is thought to then give rise to a Bardeen-Cooper-Schreiffer (BCS)-like coupling between conduction electrons (holes) in the system. Figure 1a shows a schematic of such large doping concentrations in comparison to more typical dilute doping levels. Where the dopants (orange circles) with Bohr radius a_0 at a separation of λ_d , exhibit significant hybridization between one another when $\lambda_d \ll a_0$. In the case of acceptor dopants, this transforms the discrete acceptor levels normally present into a new band at the Fermi level. The nature of this band, whether it is dispersive with heavy carriers or a non-dispersive defect band, and its implications towards the observed superconducting state remains elusive within these hyperdoped semiconductor systems.

Here, I will discuss the progress made at NYU in the epitaxial growth of thin films of superconducting Ge thin films grown via molecular beam epitaxy to address these open questions. We show superconductivity at 3 K in both single layers (Fig. 1b) and double layer (Fig. 1c) structures demonstrating good control over superconductivity during growth. The underlying atomic structure is illuminated through a combination of cross-sectional scanning transmission electron microscopy and synchrotron x-ray scattering measurements conducted at ANSTO in Australia. The experimental crystal structure obtained from these measurements is used to calculate the electronic behavior of this material that demonstrates this hyperdoped germanium material to be a candidate narrow-band superconductor. I will conclude with a discussion on device implications and future directions of this work in relation to quantum technologies.

9:30am **NAMBE1-TuM-7 Characterization and Thermal Behavior of Epitaxial Aluminum Films on InGaAs for Topological Qubits**, *Ahmed Elbaroudy, Francois Sfigakis, Sandra Gibson, Peyton Shi, Jonathan Baugh, Zbigniew Wasilewski, University of Waterloo, Canada*

Topological superconductivity is a major research focus in condensed matter physics, often explored through superconductor-semiconductor (SP-SE) hybrid structures. When a superconductor is brought into proximity with a one-dimensional channel in semiconductors exhibiting strong spin-orbit coupling, a large g-factor, and high mobility, a topological phase can emerge. Ideally, this phase features doubly degenerate ground states with Majorana bound states (MBSs) at zero energy[1]. Aluminum is well-suited for inducing such proximity effects due to its self-limiting oxide, hard induced gap, stable charge parity, and long coherence length[1].

In our approach, InGaAs serves as a surface barrier to an InAs quantum well. This barrier plays a critical role in controlling the strength of proximity coupling between the superconductor and the two-dimensional electron gas (2DEG) while also shielding the 2DEG from surface imperfections. Achieving a high-quality SP-SE interface is essential for realizing MBSs. Recently, we reported on studies of how in-situ epitaxial Al growth conditions—specifically the growth rate and substrate temperature—affect interface quality [2]. We showed that at lower deposition rates (0.1–0.5 Å/s), Al forms disconnected islands, whereas rates above 1.5 Å/s induce an abrupt transition from 3D to 2D growth, resulting in a continuous film.

In the present work, we demonstrate that if the substrate temperature during Al deposition rises above ~ 100 °C, as occurs at a slow growth rate of 0.1 Å/s, indium from the InGaAs barrier diffuses into Al. In contrast, no indium diffusion is detected when the maximum substrate temperature stays below ~ 40 °C, as is the case for a high growth rate of 3 Å/s. This suggests that interlayers between the barrier and aluminum, such as GaAs [3], which are typically added to prevent diffusion, may be unnecessary if the thermal budget during Al deposition is sufficiently low.

In a separate experiment, we deposited 10 nm of Al at 3 Å/s and then intentionally raised the substrate temperature to 150 °C. RHEED patterns

transitioned from 2D streaks to 3D spots with chevrons, indicating that Al dewets to form faceted islands. This was confirmed with ex situ AFM measurements. From the angles between the facet slopes as well as the RHEED chevrons angle, it follows that the facets planes are {112} family, rather than the lowest surface energy and highest atomic packing density {111} planes.

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9:45am **NAMBE1-TuM-8 Synthesis and Temperature-Dependent Momentum Microscopy of Type-II Dirac Semimetal NiTe₂**, *Nurul Azam, Syed Mohammad Shahed, Northeastern University, Quantum Materials and Sensing Institute; Imrankhan Mulani, Howard University, Quantum Materials and Sensing Institute; Sugata Chowdhury, Howard University; Alberto De la Torre, Arun Bansil, Swastik Kar, Northeastern University, Quantum Materials and Sensing Institute*

Nickel ditelluride (NiTe₂) has recently gained significant attention due to the presence of Type-II Dirac fermions near the Fermi energy. The tilted Dirac cones provide a platform for electronic and magnetic properties with dissipationless carrier transport, facilitating ultrahigh carrier mobility and large non-saturating magnetoresistance. Here, we demonstrate the molecular beam epitaxy (MBE) synthesis of thin films of NiTe₂ on the GaAs (111) surface. We utilized a state-of-the-art ultrahigh vacuum system where synthesis is monitored with RHEED, enabling the growth of high-quality NiTe₂ films (thickness \sim 25 nm). Our MBE system is directly connected with a multimode photoemission microscope that allows us to perform photoemission electron microscopy (PEEM), X-ray photoelectron spectroscopy (XPS), and a direct imaging of momentum states (momentum microscopy) with an energy resolution of <25 meV – all from the same micron-scale region of the samples over 15 K $<$ T $<$ 300 K. Our UHV-connected system preserves the pristine surface of the as-grown material without requiring capping, enabling the investigation of surface morphology, spatial variations of chemical bonding, and band structures over a wide range of temperatures. Unlike angle-resolved photoemission spectroscopy (ARPES), our energy-resolved momentum microscopy allows the direct measurement of the full 3D band structure (E, k_x, k_y) without the need for angle-by-angle measurements. We will present a comparison of band structures measured between room and cryogenic temperatures. Additionally, detailed results from ex-situ crystallographic investigations, including transmission electron microscopy (TEM) and X-ray diffraction (XRD) reveal the high structural integrity of the grown crystals. We will also present results from temperature-dependent Raman spectroscopy that reveal the evolution of Raman modes of NiTe₂. The experimental observations will be interpreted using first principles density functional theory and other modeling. Our study provides an in-depth understanding of the electronic and optical properties of NiTe₂, highlighting its potential for electronic, optoelectronic, and quantum technology applications. Authors acknowledge support from the Massachusetts Technology Collaborative (award number 22032), and the National Science Foundation (award number OSI 2329067).

Keywords: Type-II Dirac semimetal, NiTe₂, molecular beam epitaxy, Momentum Microscopy, XPS, Raman spectroscopy, electronic properties, quantum materials

NAMBE

Room Tamaya ABC - Session NAMBE2-TuM

III-Nitrides

Moderator: Brelon May, Idaho National Laboratory

10:30am **NAMBE2-TuM-11 Kilo-Volt Class Lateral NiO_x/GaN Super-Heterojunction Diode via Ammonia Molecular Beam Epitaxy (NH₃-MBE)**, *Yizheng Liu, University of California at Santa Barbara; Zachary Biegler, University of California Santa Barbara; Ashley Wissel-Garcia, James Speck, Sriram Krishnamoorthy, University of California at Santa Barbara*

This work reports the fabrication and characterization of the lateral kilo-volt class NiO_x/GaN super-heterojunction (SHJ) diodes via ammonia molecular beam epitaxy (NH₃-MBE), accomplishing \sim 2.8 kV breakdown voltage, and maximum critical electric field > 1 MV/cm. The Si-doped GaN (\sim 250 nm) was grown at 790 °C with a 200 sccm NH₃ flow on a semi-insulating Fe-doped GaN-on-sapphire template after an unintentionally doped (UID) buffer layer with two-dimensional sheet charge density ($gn \sim 1.1 \times 10^{13}$ cm⁻²)

Tuesday Morning, August 26, 2025

and electron mobility ($\mu_n \sim 462 \text{ cm}^2/\text{V}\cdot\text{s}$) confirmed by high-voltage capacitance-voltage (C-V) and room temperature Hall effect measurements.

The MBE grown GaN epilayer underwent a blanket plasma-etch by using BCl_3/Cl_2 reactive ion etching (RIE) to reduce the two-dimensional sheet charge density down to $7.32 \times 10^{12} \text{ cm}^{-2}$ to mitigate built-in junction electric field. After optical lithography, the etched GaN was mesa-isolated using RIE, then an e-beam evaporated Ti/Al/Ni/Au (30/120/30/50 nm) metal stack was annealed at 820 °C in nitrogen (N_2) environment to form high quality Ohmic contact on the mesa, which was confirmed via rectangular transmission line measurements (RTLM). After cathode formation, an 86-nm p^- NiO_x was deposited via reactive magnetron sputtering to form a charge-balanced extension region. The acceptor concentration (N_a) in sputtered p^- NiO_x was extracted to be $8.19 \times 10^{17} \text{ cm}^{-3}$ via heterojunction diode capacitance-voltage (C-V) method at 10 kHz, and the N_a concentration was stabilized by a 5-minute N_2 anneal. Following the p^- NiO_x deposition, a ~ 15 -nm p^{++} NiO_x contact layer was sputtered on the sidewall, covering a planar extension portion of the p^- NiO_x , then a Ni/Au (50/100 nm) anode Ohmic stack was deposited via e-beam evaporation on p^{++} NiO_x . Finally, a 2- μm epoxy-based polymer photoresist (SU-8) was applied to the SHJ diodes as a passivation layer to conclude device fabrication.

The NiO_x/GaN SHJ diode exhibits a 2-7.5 mA/mm linear forward current density at 5 V, and a reverse leakage of $\sim 10^{-7}$ - 10^{-5} mA/mm under low reverse bias (-5 V) with a rectifying ratio (J_{on}/J_{off}) of 10^5 - 10^7 for devices with 16, 25, and 50- μm anode-to-cathode distances (L_{AC}). The 50- μm L_{AC} SHJ diodes exhibited the highest breakdown voltage at ~ 2.8 kV with SU-8 passivation, showing a 5X improvement of breakdown voltage at reverse leakage of 10^{-5} A/mm compared to its reference counterparts that were not charge-balanced. The maximum breakdown field of SHJ diode was extracted to be > 1 MV/cm on a 16- μm L_{AC} device.

Acknowledgement: We acknowledge the funding from U.S. Department of Energy (DOE) ARPA-E OPEN 2021 program (DE-AR0001591).

10:45am NAMBE2-TuM-12 Limitations and Effects of Heavy Metal Doping in GaN, *J. Pierce Fix, Montana State University; Kevin Vallejo, Idaho National Laboratory; Nicholas Borys, Montana State University; Brelon May, Idaho National Laboratory*

The doping of third-party elements is the backbone of the microelectronics industry, as it allows delicate control of electron/hole concentration, but it can also be used to imbue a host matrix with unique magnetic or optical properties. Wurtzite gallium nitride is a widely studied large bandgap semiconductor. There are reports of doping GaN with numerous elements, with some being extensively employed in commercial applications. However, there are still a few elements which remain completely unexplored. This work investigates the doping limits and effects of select transition metals, lanthanoids, and actinoids in GaN. The structural, electronic, and optical properties of these first-of-a-kind combinations are presented. Embedding single crystal wide bandgap materials with additional functionality will provide building blocks for new multifunctional hybrid systems for novel sensors, quantum science, or meta-multiferroics. Leveraging the non-centrosymmetric piezoelectric host matrix and atomic-level control of dopant species could allow for active tuning of proximity and correlated phenomena, potentially opening the door for applications of actinide elements beyond nuclear fuels.

11:00am NAMBE2-TuM-13 Investigation of Composition Fluctuations and Band Tail States in Plasma Assisted MBE-Grown High Al-Fraction AlGaN, *David Storm, Yuanping Chen, LeighAnn Larkin, Mihee Ji, Gregory Garrett, Anand Sampath, Michael Wraback, Army Research Laboratory; Jonathan Pratt, Agnes Xavier, Siddharth Rajan, Ohio State University*

Ultrawide bandgap materials such as AlN and high Al-fraction AlGaN are attractive materials for high power electronic devices. However, while electron mobility in AlGaN grown by MOCVD is well described by transport models incorporating scattering from alloy disorder, dislocations, and phonons, electron mobility in plasma assisted MBE (PAMBE) grown high Al-fraction AlGaN exhibits anomalously low electron mobility, suggesting an additional scattering mechanism is operative. We have grown a series of 500 nm-thick $\text{Al}_{0.85}\text{Ga}_{0.15}\text{N}$ layers at various temperatures between 700 °C and 875 °C by PAMBE. These layers were doped with Si at a nominal concentration of $3 \times 10^{19} \text{ cm}^{-3}$. We observe that both the Hall mobility and carrier density decrease by ~50% as growth temperature increases over the range investigated. In addition, we have observed sub-bandgap emission by photoluminescence spectroscopy and note that the intensity of this sub-bandgap emission increases as the growth temperature of the layers increases. We hypothesize that the density of localized states responsible for the sub-bandgap emission arise from compositional fluctuations in

PAMBE-grown AlGaN, and that this density of states increases with growth temperature, leading to more effective filling of the deep localized states by electrons associated with n-type doping, which may open more availability of unoccupied shallow traps in band tail states. The interaction of the doping electrons with these shallow localized states via a “capture and release” mechanism may contribute to the observed reduced electron mobility. We will discuss the effect of growth parameters on compositional fluctuations and optical and transport properties.

11:15am NAMBE2-TuM-14 Sc-Rich Monocrystalline ScGaN Grown by MBE Exhibits Attractive Ferroelectric Properties, *Samuel Yang, Shubham Mondal, Jae Hun Kim, Zetian Mi, University of Michigan, Ann Arbor*

Solid solutions of wurtzite III-nitrides and rare-earth nitrides form a flourishing class of ferroelectric (FE) nitrides, including ScAlN, ScGaN, YAIN, and quaternary alloys. However, many desirable properties of FE nitrides, including exceptional piezoelectric response, optical non-linearity, and lower coercive fields, only manifest at high Sc compositions. Theoretical studies predict for ScAlN, 56% Sc is possible before transitioning to a nonpolar cubic structure. Nevertheless, growing ScAlN beyond 40% Sc has proven challenging. Alternatively, the solubility of ScN in GaN is predicted to be greater than in AlN. Furthermore, initial studies on ScGaN have recognised the potential for lower coercive fields while maintaining many desirable properties of ScAlN.

To this end, we investigate the MBE growth and FE properties of ScGaN with Sc compositions up to over 50%. 45 nm-thick ScGaN films are grown on GaN-on-sapphire templates under moderately nitrogen rich conditions. EDS confirms Sc compositions of 35%, 47%, and 56% in a series of samples. AFM shows sub-1 nm roughness over 25 μm^2 scan areas, even for $\text{Sc}_{0.56}\text{Ga}_{0.44}\text{N}$. (002) plane XRD rocking curves reveal FWHMs ranging from 650 arcsec to 1550 arcsec for $\text{Sc}_{0.35}\text{Ga}_{0.65}\text{N}$ and $\text{Sc}_{0.56}\text{Ga}_{0.44}\text{N}$, respectively. Furthermore, a (102) plane ϕ scan demonstrates excellent epitaxial registry between $\text{Sc}_{0.56}\text{Ga}_{0.44}\text{N}$ and GaN. Despite large lattice mismatch and distortion, phase-pure single-crystal growth can still be achieved. Electrical characterisation illustrates unambiguous FE switching with decreasing coercive field and remanent polarisation with increasing Sc, matching expectations that greater Sc content flattens the wurtzite structure towards a nonpolar state. Most notably, the coercive field decreases from 2.5 MV cm^{-1} at $\text{Sc}_{0.35}\text{Ga}_{0.65}\text{N}$ to 1.2 MV cm^{-1} at $\text{Sc}_{0.56}\text{Ga}_{0.44}\text{N}$, comparable to members in the HZO family. Moreover, the fatiguing characteristics of $\text{Sc}_{0.56}\text{Ga}_{0.44}\text{N}$ show non-zero polarisation remaining after 10^9 cycles, significant improvement over 10^6 - 10^7 cycles in MBE-grown $\text{Sc}_{0.2}\text{Al}_{0.8}\text{N}$. These results serve as a first glance into the realm of Sc-rich FE nitrides to harness outstanding FE, piezoelectric, and optical properties in a nitride platform. Further study is anticipated to continue developing the advanced epitaxy to grow ScGaN towards the predicted phase transition content of 66% Sc and beyond.

11:30am NAMBE2-TuM-15 Towards High Wall-Plug Efficiency Nanowire-based Red Micro-LEDs, *Yifu Guo, Ayush Pandey, Reddeppa Maddaka, Yixin Xiao, Yakshita Malhotra, Jiangnan Liu, Yuanpeng Wu, Kai Sun, Zetian Mi, University of Michigan, Ann Arbor*

Displays for future technologies such as augmented and virtual reality require ultra-high resolution and efficient power consumption, for which III-nitride LEDs at the (sub)micron scale (micro-LEDs) have been under intense investigation. Conventional top-down processing of micro-LEDs, however, requires a plasma etch to define mesas for individual devices on a wafer. As the mesa size shrink down to the micrometer regime, device efficiency loss due to plasma-induced non-radiative centers on the sidewall surfaces is further exacerbated with increasing surface-to-volume ratio. In addition, while the III-nitride family has shown immense promise for micro-LED applications due to a host of desirable properties (such as tunable bandgap across the entire visible spectrum and low surface recombination velocity), it also presents a host of material challenges, such as the large lattice mismatch and lack of intermiscibility between InN and GaN and spectral variation under different operating conditions due to quantum-confined Stark effect, that must be overcome for the device's eventual commercialization.

Here, we show that by utilizing a combination of strategies for relieving strain and enhancing the carrier injection efficiencies, including the bottom-up approach, nitrogen polarity, Mg-doped AlGaN electron-blocking layer, and a p-GaN layer with gradient doping, unprecedentedly high wall-plug efficiency for a sub-micron red LED has been achieved. The bottom-up approach, achieved via selective area epitaxy, eliminates the need for a plasma etch step through the device stack during device fabrication,

Tuesday Morning, August 26, 2025

thereby protecting the active region from the deleterious surface damage mentioned above. In addition, the bottom-up nanowires form a strain-relaxed and nearly defect-free template that allows for high quality InGaN active region with the very high levels of indium incorporation needed for red emission. To reduce electron overflow and achieve high wall-plug efficiency with these N-polar red-emitting nanowires, we have also incorporated an AlGaN EBL, as well as a p-GaN layer with graded Mg-doping.

The resultant nanowire-based InGaN micro-LED exhibited an emission wavelength of \sim 650 nm at a peak external quantum efficiency of \sim 12.8% and a wall-plug efficiency of \sim 12.2%, corresponding to a peak electrical efficiency of \sim 95%. Through this work, we demonstrate that the hitherto low electrical efficiency of nanowire-based devices can be overcome through careful design of the device heterostructure and that such devices can form the foundation of future micro-LED displays.

11:45am NAMBE2-TuM-16 High Permittivity Epitaxial BaTiO_3 Thin Films on AlGaN/GaN Heterostructures for RF Electronics, *Eric Jin, Vikrant Gokhale, James Champlain, US Naval Research Laboratory; James Hart, NOVA Research, Inc.; Andrew Lang, Matthew Hardy, Neeraj Nepal, D. Scott Katzer, Brian Downey, Virginia Wheeler, US Naval Research Laboratory*

Development of AlGaN/GaN high electron mobility transistors (HEMTs) has resulted in a myriad of applications, including high output RF power amplifiers, owing to the high breakdown field strength and excellent transport characteristics observed in III-nitride semiconductors. However, despite their wide bandgap, breakdown voltage in lateral HEMTs is ultimately limited due to the high peak electric fields leading to premature breakdown when compared to theoretical limits. Field management strategies leveraging high permittivity gate dielectrics including BaTiO_3 (BTO) have recently been shown to improve electric field distribution, thereby increasing breakdown voltage. These heterostructures typically utilize BTO dielectric layers deposited by RF sputtering, which are susceptible to low crystal quality or polycrystalline films, having lower dielectric constants (κ) than bulk or single crystalline BTO. Enhancing the crystal quality of the BTO film can both improve the quality of the oxide/nitride interface and increase κ , leading to further improvements in device voltage handling.

In this work, we demonstrate the growth of epitaxial (111)-oriented BTO thin films onto AlGaN/GaN HEMT heterostructures by RF-plasma assisted oxide molecular beam epitaxy. An epitaxial 2 nm SrTiO_3 (STO) / 1 nm TiO_2 bilayer stack is first deposited on the AlGaN surface to reduce the lattice mismatch and to provide a seed layer to facilitate crystalline and well-oriented BTO growth. The addition of the STO layer is necessary to achieve highly crystalline BTO due to its tetragonal structure and slightly larger unit cell volume compared to STO. Transmission electron microscopy imaging confirms the epitaxial orientation of the BTO film. Van der Pauw Hall effect measurements show no significant change in the sheet resistance, electron mobility, or electron density of the GaN channel due to the presence of the epitaxial BTO layers.

We investigate the effect of BTO growth temperature on structural and electrical properties by depositing the BTO layers at substrate temperatures ranging from 550-850 °C and find that the BTO crystallinity improves as growth temperature is increased. I - V and C - V measurements on test capacitor structures fabricated on the BTO on AlGaN/GaN heterostructures demonstrate trends of increasing κ values of the oxide layers and reduced leakage with increasing BTO growth temperature. A BTO κ of 340 is measured on a sample grown at 850 °C. Finally, loss tangent measurements indicate $\tan \delta$ values as low as $\sim 2 \times 10^{-3}$. These results indicate a promising approach to building high quality HEMTs with improved interfaces and enhanced RF and power performance.

Tuesday Afternoon, August 26, 2025

NAMBE

Room Tamaya ABC - Session NAMBE1-TuA

Oxides and Group IV Materials

Moderators: Ezra Bussman, Sandia National Laboratories, Sriram Krishnamoorthy, University of California at Santa Barbara

1:30pm NAMBE1-TuA-1 Development of Erbium Doped Epitaxial Scheelite Thin Films for Quantum Communication Applications, Ignas Masiulionis, University of Chicago; **Bonnie Lin,** Massachusetts Institute of Technology; **Gregory D. Grant,** University of Chicago; **Junghwa Kim,** Massachusetts Institute of Technology; **Jiefei Zhang,** Argonne National Laboratory; **James M. LeBeau,** Massachusetts Institute of Technology; **David D. Awschalom,** Supratik Guha, University of Chicago

The Er³⁺ ion, when embedded in a solid-state dielectric host, is an excellent candidate qubit for quantum communication and networking applications due to its well-shielded 4f-4f telecom c-band transition. CaWO₄ has emerged as an intriguing host material for Er, with promising optical and spin properties demonstrated in bulk crystals [1,2]. CaMoO₄ is another compound, similar to CaWO₄, that is yet to be explored as a host material. Both compounds have a tetragonal (scheelite) structure, with low lattice mismatch (~3.1%) with silicon, presenting a unique opportunity for epitaxial growth on silicon and future on-chip integration for devices.

Precise stoichiometric control is essential for realizing high quality host materials for such applications. This control is best ensured via selection of self-limiting growth regimes in addition to pre-calibrated control of the flux delivery, with pre-growth flux control lacking adequate precision. In this work, we present our results of obtaining epitaxial scheelite thin film growth on oxide substrates under self limiting growth conditions, a first step towards epitaxial growth of these complex oxides on silicon. We utilize Ca, MoO₃, WO₃, and oxygen (atomic or molecular) for the growths of these scheelites using molecular beam deposition, followed by post-growth anneals in oxidizing environments. We have carried out structural characterization using X-ray diffraction (XRD) and scanning transmission electron microscope (STEM) to confirm epitaxial scheelite growth. These scheelite were doped with natural abundance Er³⁺ (1 - 100 ppm range). Er³⁺ 4f-4f emission have been examined via various optical characterization methods, including transient spectral hole burning (TSHB) and time-resolved photoluminescence excitation (PLE). In the annealed Er:CaMoO₄ films, we observe TSHB linewidths of 500 MHz, inhomogeneous linewidths of 18 GHz, and T1 optical lifetimes up to 5 ms.

This material is based upon work supported by the Department of Defense/Air Force Office of Scientific Research through the University of Maryland.

[1] Marianne Le Dantec et al., Twenty-three-millisecond electron spin coherence of erbium ions in a natural-abundance crystal. *Sci. Adv.* 7, eabj9786 (2021). DOI: 10.1126/sciadv.abj9786

[2] Mahmet T. Uysal et al., Spin-photon entanglement of a single Er³⁺ ion in the telecom band. *arXiv:2406.06515v2*

1:45pm NAMBE1-TuA-2 Rapid Exploration of Oxide Growth Space through *in situ* Growth and Etching, Stephen Schaefer, Davi Febba, National Renewable Energy Laboratory; Michelle Smeaton, Kingsley Egbo, Glenn Teeter, Syed Hasan, William Callahan, Andriy Zakutayev, national renewable Energy Laboratory; M. Brooks Tellekamp, National Renewable Energy Laboratory

Beta phase gallium oxide (β -Ga₂O₃) is an emerging ultra-wide bandgap semiconductor that has attracted attention for its potential to outperform existing materials operating at high breakdown voltages and high temperature. Alloying of In and Al in β -Ga₂O₃ provides the ability to individually engineer the bandgap and lattice parameters of the material, providing a useful toolbox for heterostructure engineering. However, the tendency of (Al_xIn_yGa_{1-x-y})₂O₃ alloys to form competing phases, along with the complex suboxide chemistry of Ga and In, results in a growth window that is difficult to map and an alloy which is difficult to control.

We describe a “high-throughput” molecular beam epitaxy (MBE) technique to screen the growth conditions for complex oxide growth space where suboxide desorption plays a key role. As a model system, we apply the method to the Ga₂O₃-In₂O₃ alloy system to determine appropriate synthesis conditions for monoclinic (Al_xGa_{1-x-y}In_y)₂O₃ alloys. By leveraging the sub-oxide chemistry of Ga₂O₃ and *in-situ* monitoring by reflection high-energy electron diffraction (RHEED), a cyclical growth and etch-back method is developed to rapidly characterize the (In_yGa_{1-y})₂O₃ growth space. This cyclical method provides approximately 10x increase in experimental

throughput and 46x improvement in Ga₂O₃ substrate utilization. Growth conditions for monoclinic (In_yGa_{1-y})₂O₃ are identified and targeted growths are characterized *ex-situ* to confirm improved In incorporation. These conditions are then used to grow quaternary (Al_xGa_{1-x-y}In_y)₂O₃ with Al cation composition x ranging from 1% – 24% and In cation composition y ranging from 3% to 16%. The structural, chemical and optical properties of the alloys are investigated. An (Al_{0.17}Ga_{0.76}In_{0.07})₂O₃ alloy lattice-matched to Ga₂O₃ is examined by high resolution microscopy, highlighting the correlation between surface facets and composition. Such lattice-matched material can be grown arbitrarily thick without elastic strain and relaxation, making it suitable for high voltage diodes, transistor barriers, and epitaxial dielectrics.

2:00pm NAMBE1-TuA-3 Metastable Iron-Oxide Phases by Epitaxial Matching to 4H-SiC (0001), Alexandra Fonseca Montenegro, Faisal Kimbugwe Kimbugwe, Marzieh Baan, Sevim Polat Genlik, Maryam Ghazisaeidi, Tyler Grassman, Roberto Myers, The Ohio State University
Wustite Fe₁-xO is the non-stoichiometric cubic rock salt phase of iron oxide which is stable at ambient pressure above 500C, but decomposes into Fe and Fe₃O₄ at room temperature. We aim to use epitaxial lattice matching to stabilize stoichiometric FeO. Lattice matching of iron oxide to miscut (4-deg) 4H-SiC (0001) substrates is explored via gas source molecular beam epitaxy (GSMBE) using an Fe-effusion cell and either O-plasma or molecular O₂. Si-face 4H-SiC provides close lattice matching to stoichiometric FeO, however the heterovalent interface poses strong challenges, e.g. careful control of the interface bond ordering to avoid formation of SiO_x silicate ring structures at the interface. Density functional theory (DFT) calculations predict the most energetically favorable interface structure. HRXRD simulation and measurement is used to identify the present phases, such as Fe₁-xO, Fe, Fe₃O₄, and Fe₂O₃. We will discuss observations in RHEED, AFM, and XPS. Additionally, defect characterization is extensively explored via transmission electron microscopy (TEM) and electron channeling contrast imaging (ECCI), enabling a statistical quantification of misfit dislocations along the interface. Superconducting quantum interference device (SQUID) magnetometry, with its high sensitivity to weak magnetic fields, is employed to measure the magnetic responses of films with varying misfit dislocation densities. The relationship between dislocation density, phase stability, and magnetic response provides valuable insight into the fundamental properties of Fe-O thin films and their potential for spintronic and magnetoelectric applications.

This work was supported by the AFOSR under MURI grant FA9550-23-1-0330

2:15pm NAMBE1-TuA-4 SiGe/SnGe Superlattices Grown Using Molecular Beam Epitaxy, Allison McMinn, Tyler McCarthy, Arizona State University; Yicheng Wang, Dartmouth; Xiaoyang Liu, Razine Hossain, Xin Qi, Zheng Ju, Arizona State University; David Jaeger, University of North Texas; Jifeng Liu, Dartmouth; David Smith, Yong-Hang Zhang, Arizona State University

The Group-IV material system, including Si, Ge, and their alloys, has been one of the semiconductor industry's most utilized and researched material families for over half a century. The expansion of this material family by the addition of α -Sn, the diamond cubic semiconducting form of Sn, in the last couple of decades has fostered new research into low-cost IR materials, novel IR detector concepts based on momentum(k)-space charge separation (k -SCS) effect, and short-range ordering (SRO) effects in semiconductors. SRO is referred to as the preferential local arrangements of constituent atoms over a short distance deviating from a completely random distribution. Superlattices (SLs) made of these Group-IV elements and alloys offer a platform with additional degrees of freedom regarding band structure design, alloy composition profile control, and strain balancing for these device applications and materials physics studies.

Structures such as Si_xGe_{1-x}/Sn_yGe_{1-y}SL were designed and grown via MBE at substrate temperatures between 200 to 250°C to study these effects. To the best of our knowledge, this is the first report on SiGe/SnGe SLs. The targeted compositions chosen were x=15% and y=17.5% with period thicknesses of 2.38 and 2.35 nm, respectively, for a SL of 50 periods. HRXRD shows multiple satellite peaks and Pendellösung fringes; some features are due to shutter operation deviating from the designed SL.

APT measurements confirm expected interdiffusion at the interfaces in the SL, creating an equivalent tertiary Si_xGe_{1-x-y}Sn_y/Si_xGe_{1-x-y}Sn_y SL instead of the designed binary Si_{0.15}Ge_{0.85}/Sn_{0.175}Ge_{0.825} SL. The layers exhibit periodical composition variations between average values of a~2% and b~9% and c~4% and d~6%. The actual Si and Sn compositions in the corresponding layers were lower than the designed 15% and 17.5% values, respectively, with maximum incorporation values being ~6% Si in a SiGe and ~11% Sn in

Tuesday Afternoon, August 26, 2025

a SnGe layer. Dark and bright field TEM images reveal structure features introduced by the actual shutter operations, which have some irregularities. The individual SL period thicknesses estimated from TEM are 4.5 nm for the $\text{Si}_{0.02}\text{Ge}_{0.89}\text{Sn}_{0.09}$ layers and 3.2 nm for the $\text{Si}_{0.04}\text{Ge}_{0.9}\text{Sn}_{0.06}$ layers. Higher magnifications verify the interdiffusion seen in APT between adjacent SL layers, and the interfaces are not perfectly abrupt. Additionally, the chemical SRO in the SL was characterized as showing a significant difference compared to CVD-grown SiGeSn alloys. The study of SRO may lead toward new band engineering techniques beyond composition and strain, as well as the emergence of novel phase-change materials for Si electronics/photonics.

2:30pm NAMBE1-TuA-5 Intervalance Band Transitions of α -Sn Films on InSb Substrates with Different Surface Reconstructions, *Jaden Love, Jan Hrabovsky, Carlos A. Armenta*, New Mexico State University; *Aaron N. Engel, Chris Palmstrom*, University of California at Santa Barbara; *Stefan Zollner*, New Mexico State University

Gray-tin, α -Sn, is a single crystalline phase of tin that crystallizes in the FCC diamond-like cubic structure with a known lattice constant of 6.4892 Å at room temperature. The unit cell belongs to space group O_{h}^{7} ($\text{Fd}3m$) and contains 8 atoms located at the Wyckoff positions (0,0,0) and (1/4, 1/4, 1/4) [5]. α -Sn is a gapless semiconductor that has an inverted $\Gamma_{\bar{\gamma}}$ band positioned between the $\Gamma_{\bar{g}}^{+v}$ (heavy hole) and the $\Gamma_{\bar{g}}^{+s}$ (split off) bands [1]. The $\bar{\Gamma}_0$ peak of α -Sn is attributed to allowed interband transitions from the $\Gamma_{\bar{\gamma}}$ band to $\Gamma_{\bar{g}}^{+v}$ band or $\Gamma_{\bar{g}}^{+c}$ (light hole) band [1]. The interest in α -Sn stems from the ability to tune its band structure by changing the amount of doping, strain, and film thickness causing the material to behave like a topological insulator or semi-metal [3,4,6].

MBE was used to grow two 30 nm α -Sn layers on InSb (100) with c(8x2) and c(4x4) surface reconstructions. The c(8x2) substrate surface was prepared using an atomic hydrogen clean and light annealing to smooth the surface. The c(4x4) substrate surface was prepared using an atomic hydrogen clean and an anneal at higher temperatures under Sb₄ flux. These differences in MBE surface preparations lead to an Sb-terminated c(4x4) substrate surface and an In rich c(8x2) substrate surface [2]. Termination of the substrate surface with Sb reduces unintentional hole doping by In therefore limiting the allowed transitions from the $\Gamma_{\bar{\gamma}}$ band to the $\Gamma_{\bar{g}}^{+v}$ band, especially at low temperatures.

Here we discuss the presence of a strong $\bar{\Gamma}_0$ peak appearing in the extinction coefficient at 0.45 eV in room temperature infrared spectroscopic ellipsometry measurements. Temperature-dependent IR ellipsometry spectra were taken from 300 K - 10 K and show that the $\bar{\Gamma}_0$ peak amplitude is larger at higher temperatures for α -Sn films grown on InSb (100) c(4x4) substrates. Using the integrated $\bar{\Gamma}_0$ peak intensity of the dielectric function, we will calculate the carrier concentration as a function of temperature. Additionally high-resolution x-ray diffraction will be used to determine the strain of the α -Sn films.

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- [5] Landolt and R. Bornstein, *Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik*, 4 (1955).
- [6] H. Song, et al., *Adv. Eng. Mater.* 21, 1900410, (2019).

2:45pm NAMBE1-TuA-6 Epitaxial Growth and Optical Properties of GeSn Alloys on Ge (100) and Si (100) via Molecular Beam Epitaxy, *Nirosh Meckamalil Eldose, Diandian Zhang, Dinesh Baral, Hryhorii Stanchuk, Fernando Maia de Oliveira, Sudip Acharya, Wei Du, Fisher Yu, Gregory J. Salamo*, University of Arkansas

Group IV alloys of Ge and Sn have attracted significant interest for electronic and optoelectronic applications on a Si platform. [1] The incorporation of α -Sn into Ge with concentrations as low as 6% induces an indirect-to-direct bandgap transition, offering enhanced optical properties compared to pure Ge. Higher Sn content enables mid- and long-wavelength infrared emission and detection, making GeSn a promising material for photonic integration. [2,3] However, the low (~1%) solid solubility of Sn in Ge and the substantial (~14%) lattice mismatch between α -Sn and Ge present major challenges in achieving Sn-rich $\text{Ge}_{1-x}\text{Sn}_x$ structures.

We report on the synthesis of high-quality strained and relaxed GeSn layers with significant Sn content grown on Ge (100) and Si (100) substrates via molecular beam epitaxy (MBE). A critical challenge in MBE growth is incorporating high Sn concentrations while suppressing Sn surface

segregation. Growth temperatures ranging from 100°C to 200°C were investigated to optimize the crystalline quality of GeSn. High crystalline quality was demonstrated using high-resolution X-ray diffraction (HRXRD), while atomic force microscopy (AFM) provided insights into the surface morphology of the films. In this study, we report on the roles of strain relaxation and defect density on the GeSn optical properties. To accomplish this, we use photoluminescence (PL) from the defect transitions to measure the change in defect density with changes in GeSn film thickness and relaxation.

In addition, we report the first observation of direct bandgap PL emission from MBE-grown GeSn on Si (100) substrates without post annealing as shown in supplementary section Fig.1 (e). Secondary ion mass spectrometry (SIMS) depth profile of GeSn, confirming a Sn content of 11.4%, consistent with XRD-RSM measurements shown in supplementary section Fig. 1 (b and d). The GeSn layer, approximately 500 nm thick, exhibits a uniform Sn distribution, indicating homogeneous incorporation and ensuring compositional consistency and structural integrity, marking a significant step toward using MBE for integrating GeSn-based optoelectronic devices with Si technology.

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

NAMBE

Room Tamaya ABC - Session NAMBE2-TuA

Low Dimensional Nanostructures

Moderator: **Thaddeus Asel**, Air Force Research Laboratory

3:30pm NAMBE2-TuA-9 Optical and Structural Investigations of Antimonide-Exposed InAs/GaAs Quantum Dots in an InGaAs Quantum Well Matrix for 1380 nm Photoluminescent Emission, *Bhavya Kondapavuluri, Kai-Yang Hsu, Pin-Chih Liu, Yuan Ze University, Taiwan; Wei-Sheng Liu, Yuan Ye University, Taiwan; Ba Laji, Yuan Ze University, Taiwan; Jen-Inn Chyi, National Central University, Taiwan*

The increasing demand for high-speed optical communication has driven research beyond the conventional C (1530–1565 nm) and L (1565–1625 nm) bands, focusing on photon sources that emit in the O (1260–1360 nm), E (1360–1460 nm), and S (1460–1530 nm) bands, which remain compatible with existing optical infrastructure. Concurrently, advancements in facial recognition technology necessitate cost-effective and efficient photon sources operating at wavelengths of 1380 nm and beyond, ensuring enhanced safety for human-eye interactions. To address these technological needs, we investigate the extension of quantum dot (QD) emission wavelengths on GaAs substrates, which offer superior structural robustness and a more cost-effective alternative to InP-based vertical cavity surface-emitting lasers (VCSELs). In this study, high-quality InAs/InGaAs quantum dot-in-a-well (DWELL) heterostructures were fabricated using molecular beam epitaxy (MBE), achieving room-temperature photoluminescence (PL) emission at 1380 nm. The incorporation of an $\text{In}_x\text{Ga}_{1-x}\text{As}$ matrix ($x = 14\%$) facilitated strain relaxation, enhancing In adatom surface diffusion and leading to the formation of QDs with an average diameter of 50 nm and a height of 7.6 nm. These uniform QDs exhibited a strong PL emission at 1310 nm with a narrow full width at half maximum (FWHM) of 29 meV.

To further redshift the emission wavelength, a 15-second antimony (Sb) exposure was applied immediately after QD deposition, leveraging its surfactant effect. This treatment promoted QD ripening, increasing the average QD diameter to 70 nm and the height to 8.2 nm, while reducing dot density. The structural enlargement is attributed to the alleviation of elastic strain, supported by the InGaAs strain-balancing layer, which facilitated Sb incorporation into the QD top layer. As a result, the emission wavelength was successfully extended to 1380 nm. However, the Sb surfactant effect also introduced inhomogeneous broadening, increasing the FWHM to 33 meV.

Temperature-dependent PL analysis revealed that Sb exposure induced bandgap shrinkage and enhanced hole confinement, as evidenced by an

Tuesday Afternoon, August 26, 2025

increase in activation energy from 254 meV (untreated QDs) to 294 meV. Power-dependent PL measurements further confirmed the retention of type-I band alignment following Sb exposure. However, excessive Sb soaking (25 seconds) led to degraded optical properties and reduced QD uniformity.

These findings provide crucial insights into optimizing Sb exposure for InAs DWELL heterostructures grown on GaAs, advancing the development of long-wavelength photon sources for next-generation optoelectronic applications.

3:45pm NAMBE2-TuA-10 Photonic Crystal Surface Emitting Lasers (PCSELs) based on InAs Quantum Dots-in-a-Well, Thomas Rotter, Subhashree Seth, Mega Frost, Andrei Sharma, Carter Heinrich, Samiha Nuzhat, Center for High Technology Materials, UNM; Chhabindra Gautam, University of Texas at Arlington; Sadhvikas Addamane, Center for Integrated Nanotechnologies, Sandia National Laboratories; Weidong Zhou, University of Texas at Arlington; Ganesh Balakrishnan, Center for High Technology Materials, UNM

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

Photonics 2018, 5(3), 27

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

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

4:00pm NAMBE2-TuA-11 Spatial and Spectral Control Over MBE Grown InAs/GaAs Quantum Dots for Device Platforms, Nazifa Tasnim Arony, University of Delaware; Lauren N. McCabe, University of Delaware (Now working at Yale University); Joshya Rajagopal, Lan Mai, Lottie Murray, Prashant Ramesh, Matthew Doty, Joshua Zide, University of Delaware

Over the past few decades, InAs quantum dots (QDs) grown epitaxially on GaAs substrates have attracted significant attention due to their promising applications as single-photon emitters and as potential qubits. Additionally, the compatibility of GaAs platform with existing semiconductor manufacturing techniques offers a path toward building practical, large-scale quantum devices with applications in quantum sensing, computing and information processing. To create fully functional epitaxial quantum devices, it is essential to achieve uniformity in spatial, spectral, and structural properties, along with ensuring scalability. Recent work from our group has shown a method for site-controlled QD growth, where InAs/GaAs QDs are grown on nanofabricated substrates containing site-templated arrays of nano-pits. [1] Despite these advancements, one of the major challenges is maintaining high-quality optical emission from these QDs, as impurities introduced during the fabrication processes can affect their performance. In this work, we investigate the use of quantum dot columns (QDCs) as a buffer layer for the topmost QD arrays. This approach helps

"bury" defects beneath the QDCs, effectively improving the optical quality of the QDs. Additionally, we present initial photoluminescence (PL) data demonstrating the spectral control of InAs/GaAs QDs using the 'cap and flush' technique, which further explores the possibility of tuning the emission properties of these quantum dots.

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

4:15pm NAMBE2-TuA-12 2D-Assisted Nanoscale Nucleation for Selective III-V on Silicon Heteroepitaxy, Corey White, University of Illinois Urbana-Champaign; Yiteng Wang, University of Illinois at Urbana-Champaign; Archishman Saha, Soo Ho Choi, University of Illinois Urbana-Champaign; Kuangye Lu, Ne Myo Han, Massachusetts Institute of Technology; Ze-Wei Chen, University of Illinois Urbana-Champaign; Doa Kwon, Jeehwan Kim, Massachusetts Institute of Technology; Hyunseok Kim, University of Illinois at Urbana-Champaign; Minjoo Larry Lee, University of Illinois Urbana-Champaign

Selective area growth (SAG) presents an opportunity to monolithically integrate dissimilar materials during growth. Historically, SAG has relied only on conventional dielectric mask materials,^{1,2} ultimately limiting the potential of the technique. Recently, two-dimensional (2D) masks, which are ultra-thin, flexible, and possess "slippery" sp² bonds, have been employed in SAG by both MOCVD³ and MBE.⁴ Such masks have the potential to enable long adatom diffusion lengths and reduced dislocations in lattice mismatched III-V heteroepitaxy. By applying this growth technique to III-V on Si heteroepitaxy, we predict the formation of dislocations and anti-phase boundaries can be mitigated due to the strain-accommodating nature of graphene. Here, we present the first selective MBE-nucleation of templated GaAs and GaP grown in nanoscale openings in an amorphous graphene (a-Gr) mask on Si.

A selective growth regime was identified on a-Gr at a slow growth rate of 0.15 Å/s, a relatively high V/III flux ratio, and a substrate temperature of 605 °C. Under these conditions, growth of GaAs and GaP was performed in nanoholes (diameters ≤ 100 nm) etched in an a-Gr mask on Si. Structural characterization was performed by atomic force microscopy, scanning electron microscopy (SEM), and high-resolution transmission electron microscopy (HR-TEM).

GaAs nanoseeds grown in ~100 nm diameter holes were ~30 nm tall and ~100 nm in diameter with most of the nuclei showing clear faceting in planview SEM. Unsurprisingly, HR-TEM revealed that the majority of the nuclei were relaxed and single-crystalline with misfit dislocations visible along the GaAs/Si interface. Furthermore, energy dispersive X-ray spectroscopy showed no signs of oxide present at the interface indicating successful deoxidation. Recently, fabrication optimization has enabled nanoholes as small as 20 nm in diameter with templated growth of both GaAs and GaP resulting in nanoseeds as small as ~25 nm in diameter or less and ~10 nm tall, on the order of a conventional self-assembled quantum dot. HR-TEM investigations of these smaller nuclei are underway and the effects of nuclei size and lattice mismatch on dislocation formation and strain accumulation will be presented at the conference.

Here, we have demonstrated the first 2D-assisted SAG of GaAs and GaP on Si via a nanopatterned a-Gr mask. Such templated growth has the potential to unlock new III-V on silicon templates for (opto)electronics applications.

¹S. Lee et. al., *J. Appl. Phys.* **92** (2002).

²D. Ironside et. al., *Prog. Quantum Electron.* **77** (2021).

³H. Kim et. al., *Nature Nanotechnology*, **17** (2022).

⁴S. Manzo et. al., *ACS Appl. Mater. Interfaces*, **15** (2023).

4:30pm NAMBE2-TuA-13 Production Processing of 300mm BTO Films on Silicon, for Photonic Applications, Sabina Hatch, DCA Instruments, Finland

Molecular Beam Epitaxy (MBE) growth on 300 mm/12" silicon wafers has, until now, been hindered by plastic deformation during thermal processing. This is primarily due to the thermal and gravitational stresses that generate slip lines and can severely degrade the electrical properties.[1] Here, DCA Instruments presents the first instance of slip-free high-temperature MBE processing of 300 mm silicon wafers through the development of novel MBE technology.

The 300mm/12" production MBE system capability was thoroughly tested by growing a Barium Titanate (BTO) film on 12" Si wafers and examining the material properties (i.e. film thickness, lattice parameter, refractive index, and rocking curve). The low 3-sigma variation (for > 100 wafers) over the 12" wafer demonstrates the system's suitability for production processing. Further verification is provided by the excellent device performance (and

Tuesday Afternoon, August 26, 2025

sigma) across the 12" wafer, i.e. optical losses $< 5 \text{ dB.cm}^{-1}$, leakage current $< 10 \mu\text{A}$, and $V.\pi < 2.5 \text{ V}$.

More importantly, for MBE to be a viable technology for SEMI-FAB production environments, it requires an ultra-low particle count and cross-compatibility with the SEMI-FAB infrastructure.

To achieve these exceptional results and achieve SEMI-FAB compatibility, fundamental changes were made to MBE production system. These include (but are not limited to):

1. The integration of a Brooks® equipment front entry module (EFEM) with FOUP cassettes for wafer loading and unloading was required for ultra-low particle generation.
2. Modification of the automated wafer transfer system to handle bare Si wafers.
3. Upgrading the control software to allow automated processing using feedback control from analytical tools (e.g. RHEED, flux monitoring) to improve throughput and reliability.

The ongoing limitations for BTO growth on 300 mm wafers and expected advancements to address these issues for MBE production technology will also be discussed.

[1] Thin Solid Films. Volume 315, Issues 1–2, 2 March 1998, Pages 286–293

4:45pm NAMBE2-TuA-14 MBE of Epitaxial Al/Ge Quantum Wells for Quantum Computing. *Jason Dong, Joshua Thompson, Bernardo Langa Jr, Chomani Gaspe, Riis Card, Laboratory for Physical Sciences; Brycelynn Bailey, Shiva Davari Dolatabadi, Hugh Churchill, University of Arkansas; Thomas Hazard, Kyle Serniak, MIT Lincoln Laboratory; Kasra Sardashti, Christopher Richardson, Laboratory for Physical Sciences*

High mobility strained Ge quantum wells (QWs) have been of interest as a material host for hole spin qubits [1] and superconducting-semiconducting Josephson junctions (JJs) [2]. To date, these Ge QWs have been grown using Chemical Vapor Deposition (CVD) grown material with JJs created with *ex-situ* superconducting contacts. Epitaxial superconducting contacts are often desired in superconductor/semiconductor JJs due to their high transparency. The difficulty of integrating epitaxial superconductor deposition on Ge QWs grown by CVD motivates the investigation of the growth of Ge QWs with MBE.

In this work, we investigate the growth of Ge QWs on float zone silicon substrates with epitaxial Al by MBE. Using two electron guns, the unintentionally doped Ge QWs are grown strained on $\text{Si}_{0.2}\text{Ge}_{0.8}$ virtual substrates, which are grown with a reverse graded buffer layer (RGBL) sitting on an abrupt metamorphic Ge buffer. The effect of different growth conditions and different layer thickness of the Ge QWs are investigated with XRD, AFM, defect selective etching, and low temperature magnetotransport measurements. An optimal RGBL thickness that maximizes relaxation of the metamorphic buffer and minimizes the defect density is identified. Low temperature mobilities of shallow QWs exceeding $44,000 \text{ cm}^2/\text{Vs}$ are obtained. The mobility of the shallow MBE-grown Ge QWs is comparable to those grown using CVD. Modeling the mobility of samples with varying depths from the surface indicate that bulk 3D impurities do not limit that low-temperature transport in these samples. Rather, surface scattering is the limiting scattering mechanism in shallow QWs, while interface roughness scattering is identified to be the limiting mechanism in deeper quantum wells. The spatial length scale of the interface roughness strongly influences the interface roughness scattering, and evidence of this length scale is observed with AFM. The impact of different growth conditions on the interface roughness and how the mobility can be further improved will be discussed. Finally, we have recently demonstrated gate tunable superconductivity with JJs fabricated from our material [3]. These findings demonstrate Ge QWs grown by MBE as an emerging platform for quantum computing.

[1] Watzinger et al. "A germanium hole spin qubit" *Nat. Commun.* 9, 3902 (2018).

[2] Vigneau et al. "Germanium Quantum-Well Josephson Field-Effect Transistors and Interferometers" *Nano Letters* 19(2), 1023–1027 (2019).

[3] Thompson et al. "Characterization of MBE-grown Ge/SiGe Josephson junctions for voltage tunable qubits" in APS March Meeting 2025

5:00pm NAMBE2-TuA-15 Reducing Contact Resistance of Ultra-thin High Al-content AlGaN PolFETs Grown by NH₃-MBE. *Ashley Wissel-Garcia, University of California at Santa Barbara; Yinxuan Zhu, Siddharth Rajan, The Ohio State University; James Speck, University of California at Santa Barbara* Ultrawide bandgap (UWBG) AlGaN is a promising material for future RF devices due to its predicted high critical electric field; however, the

difficulty in making low resistance contact to high Al-content AlGaN field effect transistors degrades on-resistance and high-frequency performance. In this work, we show how careful optimization of growth and device design leads to successful operation of UWBG AlGaN polarization-doped field effect transistor (PolFET) channels and reverse-graded AlGaN contacts. The total thickness of the AlGaN devices was limited to avoid relaxation due to the large in-plane lattice mismatches between AlN and AlGaN. Devices were epitaxially grown by NH₃-MBE using a Veeco Gen930 system. Before growth, the AlN template substrate surface was cleaned in-situ with Ga polishing. A 300 nm homoepitaxial AlN buffer layer followed by Si δ-doping and 4 nm Al_{0.5}Ga_{0.5}N spacer served as the back barrier. The 40 nm thick Al_xGa_{1-x}N channels were grown by linearly grading from $x = 0.5$ to 0.75 while maintaining a constant V/III ratio and doping with $2 \times 10^{18} \text{ cm}^{-3}$ Si donors. For the channel-only device, ohmic source and drain contacts were made to Al_{0.75}Ga_{0.25}N with annealed Vanadium-based contact stacks with a contact resistance of $5 \Omega\text{-mm}$. The highly scaled channel-only device had $\mu_n = 80 \text{ cm}^2/\text{V}\cdot\text{s}$, achieved a maximum I_{ds} of 850 mA/mm, and f_T/f_{max} of 26/27.8 GHz. Reverse graded Al_xGa_{1-x}N contacts were grown on the same channel structure by linearly grading the composition from $x = 0.75$ to 0.15. Si dopant concentrations in the reverse graded contacts were varied to determine the most effective concentration to counteract the 3D hole gas formed from the compositional grade. The highest Si dopant concentration, $5 \times 10^{19} \text{ cm}^{-3}$, created an insulating layer and depleted the channel charge. Contacts doped with $2 \times 10^{19} \text{ cm}^{-3}$ and $1 \times 10^{19} \text{ cm}^{-3}$ Si donors remained conductive, but μ_n and n_s were degraded by a factor of 2 in the higher doped layers, possibly due to DX center formation. Ohmic source and drain contacts were made to the device doped with $1 \times 10^{19} \text{ cm}^{-3}$ Si with Ti-based contacts to Al_{0.15}Ga_{0.85}N, and the gate recess etch did not degrade the channel mobility. The contact resistance of the graded contact device was $0.6 \Omega\text{-mm}$ – an order of magnitude better than the channel-only device. The unscaled graded contact device achieved a maximum I_{ds} of 800 mA/mm, which is double that of the unscaled channel-only PolFET. This work shows that state of the art UWBG AlGaN RF devices can be grown by NH₃-MBE and that careful understanding of material properties is needed to produce high quality devices. This work was funded by the Army Research Office (Award # W911NF2220163).

5:15pm NAMBE2-TuA-16 Molecular Beam Epitaxy Growth and X-Ray Analysis of α and γ MnTe. *Candice R. Forrester, Sina Mohammadi, Aran Barton, Jisoo Moon, The City University of New York; Rei Miyazawa, Masakazu Kobayashi, Waseda University, Japan; Maria C. Tamargo, The City University of New York*

MnTe is the subject of renewed attention due to its promising magnetic properties. MnTe has two prominent phases: α -MnTe and γ -MnTe, each having distinct crystalline and magnetic properties. In particular, α -MnTe has recently been shown to exhibit a novel class of magnetism known as altermagnetism, which may significantly broaden the frontiers for unconventional d-wave superconductivity and for new and better spintronic devices.^{1,2} However, the growth of pure single phase MnTe could be challenging. In this study we report the growth of MnTe using molecular beam epitaxy (MBE). Several growth parameters were varied to optimize the MnTe properties including Te:Mn ratio and growth temperature (T_g), as well as different substrates and buffer layers. High resolution X-ray diffraction 2θ-ω scans and pole figure analysis were done to characterize the layers.

MnTe layers grown on InP(111)B, in which the Te:Mn beam equivalent pressure (BEP) ratio was varied between 180:1 to 5:1 resulted in predominantly γ -MnTe phase. While the higher Te:Mn BEP ratios exhibited only γ -MnTe phase, the very low ratios exhibited mixed α -MnTe and γ -MnTe phases. Variation of the T_g also had an important effect on the crystalline phase. For example, with Te:Mn BEP ratio of 1:5, higher growth temperatures (350 – 400°C) yielded a significant increase in the presence of the α -MnTe phase. Growth of the MnTe on InP(111)A substrates using optimized flux ratios and T_g resulted in predominantly α -MnTe, although some evidence of the γ -phase was seen in 2θ-ω scans. Furthermore, the intensity of the γ -MnTe peaks in the 2θ-ω scans remains the same while intensity of the α -MnTe signal increases as a function of thickness, suggesting that the mixed phases are formed near the interface, and that use of the appropriate substrate-layer interface or buffer layers may lead to fully single phase materials.

Evidence of the mixed phases, even for residual quantities, was particularly clear in the pole figure analysis. For example, pole figures indicated that for high BEP ratio samples grown on InP(111)B, two cubic phases could be distinguished; one cubic phase is aligned to the substrate and another one is rotated by 60°. A hexagonal phase, which may originate from the buffer

Tuesday Afternoon, August 26, 2025

layer, was also observed. A single hexagonal phase was identified when the layer was grown on InP(111)A. In both cases, the relationship between the substrate symmetry and that of the layer provides key evidence to understand the details of the epitaxial relationship of the structure.

1. *Phys. Rev. X* **12**, 031042 (2022)
2. *Phys. Rev. X* **12**, 040501 (2022)

Wednesday Morning, August 27, 2025

NAMBE

Room Tamaya ABC - Session NAMBE1-WeM

Heteroepitaxy

Moderator: Seth Bank, University of Texas at Austin

8:00am NAMBE1-WeM-1 Heteroepitaxial Growth of Highly Anisotropic Sb₂Se₃ Films on GaAs, *Kelly Xiao*, Stanford University; *Virat Tara*, University of Washington; *Pooja Reddy, Jarod Meyer*, Stanford University; *Alec Skipper*, University of California Santa Barbara; *Rui Chen*, University of Washington; *Leland Nordin*, University of Central Florida; *Arka Majumdar*, University of Washington; *Kunal Mukherjee*, Stanford University

Antimony selenide (Sb₂Se₃) is a versatile semiconductor with applications in photovoltaics, optoelectronics, and most recently as a phase change material (PCM) for reconfigurable photonic integrated circuits. Sb₂Se₃ is one of few binary PCMs that simultaneously exhibits both large amorphous-crystalline refractive index contrast and low loss in the near-infrared.¹ Notably, crystalline Sb₂Se₃ has a highly anisotropic “quasi-1D” orthorhombic structure due to covalent bonding along one axis and van der Waals bonding along the other two axes. Harnessing this unique anisotropy has the potential to mitigate inconsistent performance in current polycrystalline PCM films associated with individual randomly oriented grains exhibiting different optical responses,² as well as to unlock light polarization control or detection functionalities in birefringent and dichroic single crystalline films. Heteroepitaxial integration and solid-phase epitaxy of Sb₂Se₃ on single crystal substrates are therefore important avenues to exploit anisotropic waveguide-integrated Sb₂Se₃ for photonics.

The quasi-1D structure has prominent consequences on growth. In this work, we demonstrate a synthesis route towards textured-epitaxial Sb₂Se₃ films directly on arsenic-capped GaAs(001) substrates via molecular beam epitaxy (MBE). We use a large relative Se/Sb flux ratio of 20 to achieve coalesced films, in contrast with previous MBE work showing sparse Sb₂Se₃ nanostripe formation on GaAs.³ Not only do we find a ribbon-like surface morphology, the 1D axis unexpectedly remains aligned to the (2x1) reconstructed GaAs template to largely suppress 90° rotational domains, which otherwise commonly form on cubic substrates. X-ray diffraction indicates that for growth temperatures of 230–265°C, neighboring in-plane aligned domains deviate slightly in their out-of-plane orientations to constitute an in-plane “rotated” fiber texture. More importantly, we identify a narrow epitaxial growth window at a lower range of 180–200 °C. We show remarkable optical anisotropy along all three primary directions in epitaxial films, with giant out-of-plane birefringence ($\Delta n > 1$) at telecom bands.

Furthermore, we find that below 150 °C, MBE conditions can produce amorphous Sb₂Se₃ films, opening opportunities for heteroepitaxy. We will present initial results on laser-crystallized Sb₂Se₃, using the as-grown crystalline Sb₂Se₃ model system to inform our understanding of activating anisotropic crystallization in initially disordered phases.

¹M. Delaney et al., *Adv. Func. Mat.* **30**(36), 2002447 (2020).

²C. Laprais et al., *Adv. Opt. Mat.* **12**(28), 2401214 (2024).

³P. Wojnar et al., *Nanoscale* **16**(41), 19477 (2024).

8:15am NAMBE1-WeM-2 Evaluating Dopant Candidates for N-Type SnTe Films Grown by Molecular Beam Epitaxy, *Qihua Zhang, Mary Kathleen Caucci, Maria Hilde, Susan Sinnot, Stephanie Law*, The Pennsylvania State University

SnTe is a desirable narrow bandgap semiconductor owing to its mid-infrared plasmonic capabilities, in-plane ferroelectricity, and topologically non-trivial band structure. However, due to the negative formation energy of Sn vacancies, the synthesized SnTe thin films are predominantly *p*-type even without extrinsic dopants, which limits their potential in thermoelectric and spintronic applications. While attempts have been made to develop *n*-type SnTe bulk crystals, these efforts have not extended to thin films.

In this work, we investigate on the effect of incorporating electron dopants in SnTe thin films by molecular beam epitaxy. We first demonstrate the molecular beam epitaxy (MBE) growths of SnTe layers on InP substrate, which has a 7.8% lattice mismatch to SnTe. Using interfacial misfit array, high quality SnTe layers with a full-width-at-half-maximum (FWHM) of 0.09° in XRD rocking curves and root-mean-square (RMS) roughness of 0.2 nm has been obtained. We next study the effects of group V elements, Sb and Bi, as dopants in SnTe films. We found that Sb is an unsuitable electron

dopant and has a detrimental effect on the SnTe surface morphology. However, by doping Bi into SnTe films, a 2.5 times reduction in free hole concentrations is observed while the smooth surface can be retained. However, the addition of Bi dopants also induces twin domains in the films. Using first-principles calculations with density functional theory, we show that the preferred substitutional site of the Sb and Bi dopants depends on growth conditions: positively charged Sb_{Sn}⁺¹ impurity is only found in heavily Sn-poor conditions while the Bi_{Sn}⁺¹ is favored in all but the Sn-rich growth conditions. Moreover, for both Sb and Bi dopants, the substitutional sites form complexes with Sn vacancies which act as shallow acceptors and limit the reduction of free hole concentrations. We further evaluate alloying SnTe with In and Pb. Surprisingly, by alloying SnTe with up to 30% In content, up to $1.7 \times 10^{16} \text{ cm}^{-2}$ in electron sheet concentrations is obtained, while alloyed InSnTe film retained the rock-salt cubic structure and excellent crystal quality with a FWHM of 0.11° in the InSnTe (222) diffraction peak. The surface band structure of both SnTe and In-doped SnTe samples are studied using angle-resolved photoemission spectroscopy. DFT results regarding to the In substitutional sites in SnTe will also be discussed. This study presents a rare demonstration of *n*-type SnTe films grown by MBE, and serves as a critical milestone towards realizing *n*-type SnTe epitaxial layers.

8:30am NAMBE1-WeM-3 Tunable Electrical Conductivity in Ferromagnetic Semiconductor Samarium Nitride, *Kevin Vallejo*, Idaho National Laboratory

Rare-earth nitrides (RENs) are an exciting family of materials with a wide variety of properties desirable in the field of spintronics, infrared detectors, intrinsically ferromagnetic-based tunnel junctions, and as strongly correlated electron materials. The electronic configuration of elements containing 4f orbitals is a source of interesting new physics: as an example, samarium nitride (SmN) has been reported to support the coexistence of semiconductor behavior, ferromagnetic states, and superconductivity. Motivated by these properties and exciting opportunities, there has been an increased interest in the synthesis and study of high-quality rare-earth nitride materials. In this study we present an analysis of the synthesis of SmN thin films on MgO(001) using molecular beam epitaxy with varying growth conditions to create different levels of N vacancies. We report on the structure of different samples grown under different regimes of N availability and substrate temperature (T_{sub}), and measure their transport properties as a function of carrier concentration. We find that T_{sub} impacts the availability of carriers by a factor of 13x, compared to N availability that only increases carriers by a factor of 2x.

Structural characterization of these films indicate a uniform rocksalt crystal structure, with no appreciable difference in lattice constant or crystal quality beyond the difference in full width half-maximum of the SmN(200) peak of >0.14°. These promising results indicate a path forward in the epitaxy of versatile materials able to provide monolithic integration of different electronic behaviors without the associated strain brought about by heteroepitaxial integration of dissimilar materials.

8:45am NAMBE1-WeM-4 Formation of [111]-Ge Domains in Layered α -FeGe₂ by MBE and Solid Phase Epitaxy, *Moritz Hansemann, Michael Hanke, Achim Trampert, Jens Herfort*, Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungszverbund Berlin, Germany

α -FeGe₂ is a promising new candidate in the emerging field of magnetic 2D-materials [1]. The α -phase of FeGe₂ fits neatly into this category with a predicted ferromagnetic to antiferromagnetic phase transition [2][3] and its self-organized layered structure [4]. This makes it also an interesting candidate for spintronics applications and the study of 2D-magnetism. We grow α -FeGe₂ on GaAs (001) by MBE utilizing solid phase epitaxy. In a two step process we first grow a layer of Fe₃Si that is subsequently overgrown by amorphous Germanium. This approach limits interdiffusion of Fe into the GaAs and allows for a sharp interface. The solid phase epitaxy is subsequently fulfilled by *in situ* annealing and forming the α -FeGe₂. This method allows us to grow α -FeGe₂ with high crystalline quality and long range order with thicknesses ranging between 4 nm and 25 nm. We present comprehensive analysis by XRR, XRD, AFM and TEM. From AFM we report very smooth surfaces with RMS= 0.5 nm, reproducing the GaAs surface. Additionally we find agglomerates on the surface, that we can link to the Germanium content in the layer. In the TEM micrographs we see layers with very few crystalline defects and homogeneity over long distances. The layers are occasionally interrupted by small Germanium domains, in which the [111] crystal direction is aligned with the [001] growth direction. These grow in a competing manor to the α -FeGe₂ in the solid phase epitaxy and are a known problem of the solid phase epitaxy process [5]. Further we

Wednesday Morning, August 27, 2025

present GID measurements performed at the synchrotron PETRA III at DESY, that confirm the presence of the [111]-domains. These domains are also likely nucleation sites for the previously mentioned Ge-agglomerates visible in AFM.

References

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9:00am NAMBE1-WeM-5 Twin-free $(\text{MnSb}_2\text{Te}_4)_x(\text{Sb}_2\text{Te}_3)_{1-x}$ Growth on $\text{In}_2\text{Se}_3/\text{InP}(111):B$ Substrates by Molecular Beam Epitaxy, Jisoo Moon, Candice R. Forrester, City College of New York; Sina Mohammadi, City College of New York, City University of New York; Lia Krusin-Elbaum, Maria C. Tamargo, City College of New York

MnSb_2Te_4 (MST) is a magnetic topological material in which Mn-Sb antisite defects play a critical role in determining the magnetic ground state. Due to the similar ionic radii of Mn and Sb, site-mixing is energetically preferred, driving the system easily to the ferromagnetic state. Antiferromagnetic MST crystals have been achieved by tuning growth parameters, such as the amount of Mn during synthesis, and through a post-growth treatment that introduces H^+ ions into the system. However, the effects of other types of crystalline defects on the site-mixing and, consequently, on the magnetic properties of this material system have not been considered. Here, we utilize our recent twin-free $\text{In}_2\text{Se}_3/\text{InP}(111):B$ substrate for molecular beam epitaxy growth of $(\text{MnSb}_2\text{Te}_4)_x(\text{Sb}_2\text{Te}_3)_{1-x}$, aimed at suppressing interfacial defects between the substrate and MST layers, thus towards twin-free MST. Un-twinned thin In_2Se_3 layers are formed via a selenium passivation technique during the oxide desorption of $\text{InP}(111):B$ substrates. To prevent MST intermixing with In_2Se_3 , thin topological insulator (TI) insertion layers are employed to separate the MST from In_2Se_3 . ϕ -scan result of X-ray diffraction (XRD) shows the MST grown on the un-twinned In_2Se_3 is indeed twin-free, too. Low-temperature magnetic susceptibility measurements indicate a weakened ferromagnetic ground state, which is also consistent with electronic transport results. The concentration of the magnetic septuple layer (SL), van der Waals unit layer of MST, is investigated using high-resolution XRD, energy-dispersive X-ray spectroscopy, and transmission electron microscopy, which exhibit significantly lower concentrations of the SLs than in the ones grown on sapphire substrates. Considering the latter is expected to be twinned and, therefore, more defective, the SL concentration and Mn distribution under similar growth conditions appear to be closely related to crystalline defects. We will present more findings from XRD and atomic force microscopy for different growth parameters. The successful growth of twin-defect-suppressed MST will provide a new opportunity to better understand the relationship between material properties and defect types and levels in this material system.

9:15am NAMBE1-WeM-6 Epitaxial Growth of SnGeSe Ternary Alloys on GaAs Substrates, Kira Martin, Pooja D. Reddy, Jarod E. Meyer, Kelly Xiao, Tri Nguyen, Kunal Mukherjee, Stanford University

The heteroepitaxy of low-symmetry, non-cubic semiconductors on cubic substrates is a key challenge for integrating anisotropic electronic and optical properties on to technologically relevant device platforms. Tin selenide (SnSe) and Germanium selenide (GeSe) are layered orthorhombic ($a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$) IV-VI semiconductors with bandgaps in the near-infrared and useful electrical, optical, and thermoelectric properties.^{1,2} SnSe and GeSe comprise of bilayer structures with strong in-plane covalent bonding and weak van der Waals (vdW) bonding out-of-plane.³ Alloying across the completely miscible SnSe-GeSe system helps tune the anisotropy, as the structure of GeSe is more anisotropic than SnSe. Developing heteroepitaxial growth of SnGeSe alloys on cubic III-V and Si/Ge substrates is a critical step towards utilizing the tunable anisotropic optical and electronic properties of orthorhombic structures for applications such as polarization sensitive detectors.

Despite the structural similarities between SnSe and GeSe, we find that thin film alloy synthesis is complicated by the low sticking coefficient and glass-forming character of GeSe. We deposit IV-VI alloys on arsenic-capped GaAs(001) substrates using molecular beam epitaxy (MBE). The substrate was prepared by thermally desorbing the arsenic cap and then dosing the substrate surface with a PbSe flux at 420°C . A 50 nm buffer layer of SnSe was then grown at 300°C before growing the SnGeSe alloy film at 160°C , based on seeing minimal Ge sticking in related IV-VI materials above 230°C .⁴ The relative beam equivalent pressures (BEP) of SnSe and GeSe compound effusion cells were changed to systematically sweep composition from crystalline SnSe to amorphous GeSe. Reflection high energy electron diffraction indicates Sn-rich growths are crystalline, but increasing GeSe BEP ratio eventually results in amorphous growth.

Alloy composition and structural information for the crystalline phases was determined using high resolution X-ray diffraction. The vdW-bonded 'a-axis' is in the out-of-plane direction, and reciprocal space maps show an in-plane epitaxial relationship with two 90° rotated domains—the 'b' and 'c' axes of the IV-VI alloys aligned to the in-plane $\langle 110 \rangle$ axes of GaAs. We will explore how the structural quality and optical properties of SnGeSe change as a function of Ge composition and study the potential for post-growth annealing to crystallize Ge-rich amorphous SnGeSe alloys into the orthorhombic phase.

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²Y. Kim et al., *J. Korean Phys. Soc.* **72**(2), 238 (2018).

³S. Yang et al., *Nano Res.* **11**(1), 554 (2018).

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9:30am NAMBE1-WeM-7 Controlling Antiphase Twins in Bi_2Se_3 via Step-Terminated Al_2O_3 Substrates, Matthew Brahlek, Jane Chen, Oak Ridge National Laboratory; Rob Moore, Oak Ridge Nation; Alessandro R. Mazza, Oak Ridge National Laboratory

The epitaxial synthesis of high-quality 2D layered materials is an essential driver of both fundamental physics studies as well as being central to bridge to technological applications. Bi_2Se_3 , a prototypical 2D layered topological insulator, suffers from myriad defects imparted during the growth, either thermodynamically or due to the interaction with substrates. In this study, we demonstrate that step-terminated Al_2O_3 substrates with a high miscut angle (3°) can effectively suppress a particular hard-to-mitigate defect, the antiphase twin. Systematic investigations across a range of growth temperatures and substrate miscut angles confirm that atomic step edges act as preferential nucleation sites, stabilizing a single twin domain. First-principles calculations suggest a significant energy barrier for twin boundary formation at step edges, supporting the experimental observations. Detailed structural characterization indicates that this twin-selectivity is lost through the mechanism of the 2D layers overgrowing the step edges, leading to higher twin density as the thickness increases. These findings highlight the complex energetic landscape unique to 2D materials that is driven by interplay between substrate topology, nucleation dynamics, and defect formation, which is critical to optimizing growth strategies to improve material quality for quantum and electronic applications.

9:45am NAMBE1-WeM-8 "Kinetic Roughening" in Low-temperature MBE Growth of III-As Heterostructures on $\text{InP}(111)\text{B}$, Esperanza Luna, Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin, Germany; Seyed Ali Hosseini Farahabadi, Milad Entezami, Man Chun Alan Tam, Zbigniew Wasilewski, University of Waterloo, Canada

MBE growth of III-V semiconductors on (111)-oriented substrates has gained renewed interest in recent years. For example, the use of $\text{InGaAs}/\text{InAlAs}$ short-period superlattices SL grown on $\text{InP}(111)\text{B}$ substrates have been proposed as an alternative antenna material for time-domain spectroscopy (TDS) systems using $1.55 \mu\text{m}$ femtosecond laser pumps. Furthermore, low temperature (LT) growth leading to the incorporation of excess As via arsenic antisites should enable more efficient TDS systems due to a faster recombination of photocarriers through As antisites in the structure. The first prerequisite however is the growth of high-quality LT $\text{InGaAs}/\text{InAlAs}$ SPSL on $\text{InP}(111)\text{B}$, an effort which combines the challenges of $\text{InGaAs}/\text{InAlAs}$ growth on $\text{InP}(111)\text{B}$ with those of LT MBE.

To explore the impact of the LT substrate temperature (T_s) on the SL structure, 50 periods of lattice-matched $\text{InGaAs}/\text{InAlAs}$ on $\text{InP}(111)\text{B}$ were grown changing T_s every 10 periods of SL from 450°C to 250°C while maintaining other parameters unchanged. The sample microstructure was investigated using a combination of scanning transmission electron

Wednesday Morning, August 27, 2025

microscopy (S)TEM techniques.

We find that whereas the first 10 periods of InGaAs/InAlAs SL ($T_s = 450^\circ\text{C}$) grow in a regular fashion, the structure progressively deteriorates as T_s is reduced, with a dramatic degradation for the SL grown at the lowest T_s of 250°C (Fig. 1). We observe a noticeable change in the microstructure after reducing T_s from 450°C to 400°C , the resulting periods are characterized by a high density of in-plane microtwins and staking-faults (Fig. 2). The situation rapidly evolves towards even more defective layers as T_s is further reduced (Fig. 1). In fact, the SL grown at $T_s = 250^\circ\text{C}$ is highly defective, its microstructure resembles the initial stages of breakdown of epitaxy.

We note that the observed microstructure and its dependence on T_s can be explained in terms of the critical role of step-flow growth and of Ehrlich-Schwoebel (ES) barriers when growing on the (111)B-oriented substrate. Despite the use of InP(111)B substrates with a 2° miscut to promote step-flow growth, it is obvious that reduction of T_s below 400°C without further change of i.e. the V/III ratio, is not enough to maintain the regular step-flow regime, leading to a "kinetic roughening". We suggest that a readjustment of the growth conditions for each individual T_s might help to preserve the step-flow growth mode and to overcome the impact of ES barriers, leading to higher quality layers. We believe that these results are of general validity to other material systems and contribute to the understanding of the always challenging growth on (111)-oriented substrates.

NAMBE

Room Tamaya ABC - Session NAMBE2-WeM

Advanced MBE Techniques

Moderator: Stephanie Law, Penn State University

10:30am NAMBE2-WeM-11 Artificial Intelligence for on-the-Fly Analysis and Control During Oxide Molecular Beam Epitaxy, Tiffany Kaspar, Emily Saldanha, Henry Sprueill, Jenna Pope, Sarah Akers, Derek Hopkins, Ethan King, Pacific Northwest National Laboratory

Thin film deposition is a fundamental technology for the discovery, optimization, and manufacturing of functional materials. Deposition by molecular beam epitaxy (MBE) typically employs reflection high energy electron diffraction (RHEED) as a real-time in situ probe of the growing film. However, the state of the art for RHEED analysis during deposition requires meticulous human observation and often fails to avoid negative film outcomes. We are working to employ artificial intelligence (AI)-accelerated analysis of in situ data streams for on-the-fly feedback control of the MBE deposition process that will enable successful synthesis of novel materials with desired structure and functional properties. This in situ feedback control is a critical component of autonomous experimentation (AE), which promises orders-of-magnitude acceleration of materials discovery, optimization, and adoption in advanced technologies. Here we present a machine-learning-enabled framework for the analysis of RHEED pattern images in real time (one image per second). We demonstrate this framework using RHEED images collected from the deposition of epitaxial oxide thin films such as anatase TiO_2 on $\text{SrTiO}_3(001)$. On-the-fly feedback control of the deposition process is shown to improve film outcomes. Both recipe-based interventions and sophisticated AI-enhanced real-time parameter control will be discussed.

10:45am NAMBE2-WeM-12 A Novel Approach for P-Type Doping in Semiconductor Heterostructures: Interface Fermi-Level Position Engineering, Xiaoyang Liu, Xin Qi, Zheng Ju, Nathan Rosenblatt, Razine Hossain, Yong-Hang Zhang, Arizona State University

Many semiconductors and oxides are difficult to dope p-type. This can be understood by using the hydrogen model, which gives the dopant ionization energy as a function of effective mass and dielectric constant. In most semiconductors, an increase in bandgap leads to a larger effective mass and a smaller dielectric constant. Therefore, many materials like some II-VI and wide-bandgap III-V semiconductors and oxides exhibit high dopant binding energies, limiting the achievable doping concentration. For example, at 300K , CdTe and GaN have high acceptor binding energies of ~ 73 meV and ~ 250 meV, respectively. As a result, the hole concentration remains below 8×10^{16} and $4 \times 10^{15} \text{ cm}^{-3}$, respectively, even when the p-type atomic doping concentration reaches 10^{19} cm^{-3} , due to very low acceptor activation.

Here we demonstrate a novel approach to circumvent this fundamental doping limitation by utilizing the interface states of ITO on a lattice-mismatched heterostructure to achieve "p-type" doping without the use of

any dopants. These interfacial states spread across the forbidden gap and have a substantially lower density than states in the bulk, allowing easier manipulation of the interface Fermi level. We refer to this method as *interface Fermi-level position engineering*.

A model for this approach is developed based on the following assumptions: 1. the interface states arise from dangling bonds at the lattice-mismatched interface; 2. these states are uniformly distributed in the bandgap; 3. Anderson's rule determines the initial band offset; and 4. equilibrium is reached as electrons from ITO and the n-type layer fill the interface states. According to the model, varying the Mg content in the MgCdTe barrier layer modifies the lattice mismatch and the interface density of states so that the Fermi level position at the interface can be tailored.

A series of n-type CdTe/MgCdTe double-heterostructures (DH) with different Mg compositions in the top MgCdTe barrier layers were grown and "p-n junctions" were formed by simply depositing an n-type ITO layer onto the top MgCdTe barrier layers. The ITO/MgCdTe interface then acts as an effective "p-region" induced by charge transfer. C-V measurements of the samples with different Mg compositions match the theoretical predictions. The sample with 40% Mg shows a V_{bi} over 1 V , much higher than that (0.2 V) determined by the work function difference between bulk ITO ($\sim 4.6\text{ eV}$) and n-type CdTe ($\sim 4.4\text{ eV}$), confirming the critical role of the interface states in modifying V_{bi} . This method provides a new approach to overcoming p-type doping limitations in wide-bandgap semiconductors and oxides.

11:00am NAMBE2-WeM-13 GaP Planar Coalescence Over Embedded Dielectric Gratings by Molecular Beam Epitaxy, Ashlee Garcia, Will Doyle, University of Texas at Austin; Yiteng Wang, Corey White, University of Illinois at Urbana-Champaign; Byron Aguilar, University of Texas at Austin; Minjoo Lee, University of Illinois at Urbana-Champaign; Daniel Wasserman, Seth Bank, University of Texas at Austin

Selective area growth (SAG) of III-V semiconductors by molecular beam epitaxy (MBE) enables the seamless integration of dielectrics, metals and high-quality crystalline semiconductors, which presents exciting pathways for the advancement of GaP-based applications such as nonlinear integrated photonics,¹ interfacing with cold atoms,² metasurfaces,³ high-contrast photonics,⁴ and site-controlled quantum-confined structures.⁵⁻⁷

While GaP has long been a valuable material in photonics, there has been a recent growing interest in realizing it as a nanophotonic platform due to its high transparency, high refractive index, large $\chi^{(2)}$ nonlinearity and lattice constant near that of silicon.¹ However, etch-induced roughness and growth quality due to substrate requirements currently limit the performance of GaP nanophotonics.⁸ Leveraging all-MBE regrowth of GaP could enable deterministic growth of quantum-confined structures and patterned thin films boasting epitaxially smooth surfaces,⁵⁻⁸ and realize advanced photonic design capabilities via the incorporation of amorphous materials into single-crystalline GaP. Here we demonstrate all-MBE regrowth of (100) GaP over SiO_2 gratings using a two-stage approach pioneered by Ironside,⁹ which combines periodic supply epitaxy (PSE) for lateral epitaxial overgrowth with planar coalescence.

Selective GaP PSE was performed over SiO_2 gratings, aligned to [0-11], [010] and [011], on a GaP wafer. Enhanced lateral growth was observed for [010]-aligned gratings forming {101} facets. By then continuously growing at $0.35 \mu\text{m/hr}$, restoration of the planar (100) surface was achieved above [010]- and [011]-aligned gratings. Atomic force microscopy showed high quality restored surfaces with root-mean-square (RMS) roughness values ranging from 0.9 to 3 nm, lower than that of optimized GaAs regrowth⁵. Cross-sectional scanning electron microscopy showed that, like GaAs, the [010]-aligned gratings were completely encapsulated by GaP, whereas, gratings along [011], saw the formation of high aspect ratio voids due to limited {0-11} growth, demonstrating a wide range of embedded GaP geometries achievable under a restored planar surface. This work was supported by NASA via the Quantum Pathways Institute (Award 80NSSC22K0287).

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Wednesday Morning, August 27, 2025

11:15am **NAMBE2-WeM-14 High-Efficiency Entangled Photon Sources Using (111)-Oriented Quantum Optical Metasurfaces**, *Trevor Blaikie, University of Waterloo, Canada; Simon Stich, Walter Schottky Institut, Technische Universität München, Germany; Vitaliy Sultanov, Max-Planck Institute for the Science of Light, Germany; Maria Chekhova, Max Planck Institute for the Science of Light, Germany; Mikhail Belkin, Walter Schottky Institut, Technische Universität München, Germany; Zbigniew Wasilewski, University of Waterloo, Canada*

High-efficiency, sub-wavelength-thickness sources of entangled photons for quantum optical applications enable the miniaturization of photonic quantum processing units and advancements in nanoscale photonic quantum state engineering, with promising applications in quantum imaging, computing, sensing, metrology, and communication.

Spontaneous parametric downconversion (SPDC), a second-order nonlinear optical process, is widely used for generating entangled photon pairs. The SPDC conversion rate increases with the second-order electrical susceptibility ($\chi^{(2)}$) of the nonlinear medium.

GaAs has one of the highest $\chi^{(2)}$ values (400–500 pm/V) among traditional materials, but its use is limited by SPDC momentum conservation requirements. These constraints relax at sub-wavelength thicknesses of the medium, allowing SPDC over a broader wavelength range. However, GaAs's $\chi^{(2)}$ tensor symmetry requires electric field components in all three crystal basis dimensions for SPDC to occur. With the pump beam incident normally on a (001) surface, achieving the necessary vertical electric field component is challenging, leading to low conversion efficiency.

To address this, we switch the optical axis to the [111] direction, where photons traveling normally to the surface naturally have electric field components in all three crystal basis dimensions. This approach enables SPDC without the need for additional layer patterning.

Towards this goal, we have grown GaAs/AlGaAs layers on GaAs (111)B substrates. Initial measurements show that unpatterned AlGaAs (111)B layers generate photon pairs at rates two orders of magnitude higher than thin films of GaP, a commonly used nonlinear material. Additional patterning of these layers enabled still further efficiency improvement.

Epitaxial growth on GaAs (111) substrates has been largely abandoned since the late 90s due to significant difficulties in growing defect-free homoepitaxial and heteroepitaxial layers with smooth surfaces and interfaces. We will discuss the latest SPDC results and present the strategies developed to optimize the growth of smooth GaAs/AlGaAs layers on GaAs (111)B substrates.

11:30am **NAMBE2-WeM-15 Crystalline Direction and Shadowing Effect on Overgrowth of Patterned Features on GaAs (001)**, *Xizheng Fang, Yiteng Wang, Adrian Birge, Minjoo Lee, University of Illinois Urbana-Champaign*
Epitaxial regrowth on patterned substrates has been widely explored for photonics applications¹, including embedded voids for photonic crystal surface emitting lasers² and Bragg mirror on patterned lasers³. Regrowth on etched heterostructures also enables the formation of quantum-confined wires with novel charge transport properties⁴. Regrowth morphology depends on many factors, including mass redistribution during deoxidation, shadowing, adatom diffusion, and different incorporation rates on different facets. In this work, we show that growth on etched trenches can be switched from planar to faceted based on trench orientation and that growing without substrate rotation can lead to nonconformal growth and the formation of lateral heterostructures.

The starting materials in this study were either epi-ready GaAs or 125 nm GaAs/125 nm AlAs templates, both with (001) surface orientation. 3 μ m-wide trenches were dry etched to a depth of 0.25–0.70 μ m over a wide range of in-plane directions. GaAs/AlAs superlattices (SLs) with periods of 60–100 nm were grown at 0.5–1.0 μ m/hr with V/III ratios of 15–30. Substrate temperatures (T_{sub}) of 400–610°C were used to analyze the effects of adatom diffusion on regrowth.

The morphology of GaAs/AlAs SLs grown on trenches depends strongly on their in-plane direction. On [010]-oriented trenches, SL growth is highly conformal and became increasingly planar with time, even at $T_{\text{sub}}=400^{\circ}\text{C}$. In contrast, overgrowth on [110]-oriented trenches led to the formation of prominent {111}B and {113}B facets at the end of SL growth with decreased conformality and thickness uniformity; layers grown on the {111}B facet were ~40% as thick as those grown on the (001) surface.

We next investigated shadowing effects by performing SL growth over trenches without substrate rotation. Thermal oxide desorption at 650°C without rotation causes GaAs etching near sidewalls where the As₂ flux is shadowed; ~60% of the Ga evaporates, and the rest redeposits epitaxially

against the opposite sidewall with line-of-sight to the As₂ cell. SL growth at 610°C without rotation on trenches etched into 125 nm GaAs/125 nm AlAs templates enables novel vertical+lateral heterostructures (e.g., nanosheets) where thin GaAs layers are surrounded by AlAs barriers on three sides. In summary, crystallographic direction and shadowing effects strongly influences the conformality of MBE regrowth over trenches, enabling the formation of lateral heterostructures with potential (opto)electronics applications.

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[4] Chinni, et. al., *IEEE J-EDS* 5, (2017).

11:45am **NAMBE2-WeM-16 Thermal Laser Epitaxy System for Synthesis of Thin Films Containing Refractory Elements**, *David Catherall, Yifei Yan, Fin Donachie, Austin Minnich, California Institute of Technology*

Molecular beam epitaxy (MBE) has well-known challenges in producing flux from highly-refractory elements such as W owing to high temperatures ~3000 °C required to achieve adequate vapor pressure. Thermal laser epitaxy (TLE) has been proposed as a new technique to overcome this challenge by relying on laser heating of elemental sources. Here, we introduce a custom TLE system at Caltech which employs laser substrate heating and fiber laser heating of source materials. Our system is comprised of a UHV chamber with 1070 nm fiber lasers for source material heating, 10.6 μ m CO₂ laser for substrate heating, various in-situ diagnostics, and connection with a transfer line into a nitrogen glovebox. In this talk, we will describe the design and preliminary results from this system.

12:00pm **NAMBE2-WeM-17 Rolled-Up Metamaterials (RUMMS) for Infrared Imaging**, *Gokul Nanda Gopakumar, Stephanie Law, Pennsylvania State University*

Subwavelength information about an object is carried by waves with large wavevectors. The diffraction limit is caused by the rapid evanescent decay of these large wavevector modes at the surface of a material. Hyperbolic materials allow light with large wave vectors to propagate within the material without decaying exponentially close to the surface. These materials have a negative real part of the permittivity tensor along at least one direction and a positive permittivity along at least one other direction, leading to an open isofrequency surface, in contrast to the closed isofrequency surface of normal materials. In a flat hyperbolic material, the sub-diffractive information will still exponentially decay once it leaves the hyperbolic medium. However, in a rolled-up hyperbolic material, the wavevector of the light decreases as it propagates radially, and the image is magnified, enabling propagation beyond the surface.

In this work, we present rolled up semiconductor-based infrared hyperbolic metamaterials. We fabricate these structures by using a strained bilayer that can be released from the substrate. The strained bilayer is grown using molecular beam epitaxy and comprises of a compressively strained Ga_{1-x}In_xSb bottom layer and tensile strained GaSb top layer grown on top of an AlSb sacrificial layer. A layer of Si:InAs layer is grown on top of the bilayer because heavily doped III-V semiconductors can act as an optical metal in the IR. Fabrication of rectangular mesas is done using standard lithographic and wet etching techniques. Finally, a wet etch that selectively removes the sacrificial layer is used to gradually release the strained bilayer, causing it to roll up. By changing the alloy composition, we tune the stress in the bilayers to change the diameter of the rolled-up tube. The number of turns in the rolled-up tube can also be increased by increasing the etching time. The result is a RUMM that has alternating layers of dielectric (Ga_{1-x}In_xSb and GaSb) and metal (Si:InAs) in the radial direction.

The growth of the strained bilayer and determination of the strain are evaluated using High resolution X-ray diffraction. Scanning electron microscopy is used to image the rolled-up tubes and correlate their diameter to the bilayer strain. Finally, infrared spectroscopy will be used to measure the optical properties of the RUMMs. This is the first step in creating a fully semiconductor-based curved hyperbolic metamaterial that can be used in subdiffractive imaging in the IR wavelength range.

12:15pm **NAMBE2-WeM-18 Spectroscopic Ellipsometry as an in Situ Technique to Control MBE Growth**, *Jackson Niedel, Owen Peterson, Hatim Saeed, Kenyon College; Qihua Zhang, Stephanie Law, Maria Hilse, Penn State University; Frank Peiris, Kenyon College*

It is imperative to develop *in-situ* tools that will yield instant feedback in growing novel and challenging structures, such as topological insulators and transition metal dichalcogenides. Using several examples, we will show that

Wednesday Morning, August 27, 2025

by incorporating a spectroscopic ellipsometer into a molecular-beam epitaxy growth chamber, the growth parameters of binary and ternary films can be obtained layer-by-layer, during their entire growth cycle. Obtaining continuous ellipsometry spectra during the growth of a ~25 nm thick PtSe₂ film, we determined the thickness dependent dielectric functions of PtSe₂. In addition, we map how the sample composition (i.e., PtSe₂ and void) changes during the growth of the film. We have also explored (Bi_xIr_{1-x})₂Se₃ and have obtained the composition-dependent dielectric functions of this ternary system. By using the calibrated dielectric functions, the composition and thickness of any (Bi_xIr_{1-x})₂Se₃ film can be obtained immediately at any stage of the growth cycle. We tested the model for universality among MBE growth systems and found that the model was transferable between systems. Furthermore, the generalized model allowed us to monitor sticking and desorption coefficients as well as temperature-induced composition changes in the (Bi_xIr_{1-x})₂Se₃ thin films.

12:30pm NAMBE2-WeM-19 Closing Remarks & Thank You,

Author Index

Bold page numbers indicate presenter

— A —

A. Carrasco, Rigo: NAMBE-MoP-4, 15
A. Quivy, Alain: NAMBE-MoP-20, 18
Acharya, Sudip: NAMBE1-TuA-6, 29
Acuna, Wilder: NAMBE1-MoA-1, 11
Addamane, Sadhvikas: NAMBE1-MoM-5, 7; NAMBE1-MoM-6, 7; NAMBE2-TuA-10, 30
Addamane, Sadhvikas: NAMBE1-MoA-2, 11
Addame, Sadhivakas J.: NAMBE-MoP-33, 21
Aguilar, Byron: NAMBE2-WeM-13, 35
Ahmed-Babikir, Nuha: NAMBE2-MoM-12, 8
Aidoo-Mensah, Clifford: NAMBE-MoP-39, 22
Akers, Sarah: NAMBE2-WeM-11, 35
Alsaad, Zinah: NAMBE-MoP-12, **16**
Alzeidan, Ahmad: NAMBE-MoP-20, **18**
Anderson, Evan: NAMBE2-MoA-11, 13
Ariyawansa, Gamini: NAMBE2-MoM-13, 9
Arledge, Kiernan: NAMBE2-MoA-13, 14
Armenta, Carlos A.: NAMBE1-TuA-5, 29
Arnold, Michael: NAMBE1-MoM-8, 8
Arony, Nazifa Tasnim: NAMBE2-TuA-11, **30**
Awschalom, David D.: NAMBE1-TuA-1, 28
Azam, Nurul: NAMBE1-TuM-8, **25**; NAMBE-MoP-34, **21**

— B —

Baan, Marzieh: NAMBE1-TuA-3, 28
Bailey, Brycelynn: NAMBE2-TuA-14, 31
Baker, Lukas: NAMBE-MoP-30, 20
Baksi, Merve: NAMBE1-TuM-5, **24**
Baktash, Ardeshir: NAMBE1-TuM-6, 25
Balakrishnan, Ganesh: NAMBE1-MoA-2, 11; NAMBE2-TuA-10, 30; NAMBE-MoP-24, 19; WME1-SaM-1, **1**; WME1-SaM-2, 1
Bank, Seth: NAMBE2-MoA-14, 14; NAMBE2-MoM-14, 9; NAMBE2-WeM-13, 35
Bansil, Arun: NAMBE1-TuM-8, 25
Baral, Dinesh: NAMBE1-TuA-6, 29; NAMBE-MoP-31, **20**; NAMBE-MoP-32, 20; WME1-SaA-5, 3
Barton, Aran: NAMBE2-TuA-16, 31
Baruah, Rashmita: NAMBE-MoP-42, 23
Baskin, Maria: NAMBE-MoP-1, **15**
Batchuluun, Oyut: NAMBE-MoP-35, 21
Battaglia, Julian: NAMBE-MoP-29, 20
Baugh, Jonathan: NAMBE1-TuM-7, 25
Belianinov, Alex: WME2-SaA-12, **4**
Belkin, Mikhail: NAMBE2-WeM-14, 36
Bhuiya, Saad Mohammad: NAMBE2-MoM-16, **9**
Biasiol, Giorgio: NAMBE-MoP-35, **21**
Biegler, Zachary: NAMBE2-TuM-11, 25
Birge, Adrian: NAMBE1-MoA-6, 12; NAMBE2-WeM-15, 36
Blaikie, Trevor: NAMBE2-WeM-14, 36
Bork, James: NAMBE1-MoA-1, 11; NAMBE2-MoM-12, 8
Borys, Nicholas: NAMBE2-TuM-12, 26
Boulares, Ibrahim: NAMBE-MoP-16, 17
Bouwmeester, Dirk: WME2-SuM-11, 5
Bowers, John: NAMBE1-MoA-5, 12; WME2-SuM-11, 5
Bradich, Adelaide: NAMBE-MoP-27, **19**
Brahlek, Matthew: NAMBE1-WeM-7, **34**
Burkhart, Luke: NAMBE1-TuM-3, 24
Bussmann, Ezra: NAMBE-MoP-27, 19

— C —

C. Tamargo, Maria: NAMBE1-WeM-5, 34
Calawa, Dan: NAMBE1-TuM-3, 24
Callahan, William: NAMBE1-TuA-2, 28
Campbell, Joe: NAMBE2-MoA-14, 14
Campbell, Quinn: NAMBE1-MoM-6, 7
Canedy, Chadwick: NAMBE2-MoA-13, 14
Card, Riis: NAMBE2-TuA-14, 31

Carrasco, Rigo: NAMBE2-MoA-11, **13**; NAMBE2-MoA-12, 13; NAMBE2-MoM-13, 9; NAMBE2-MoM-15, 9; NAMBE-MoP-24, 19
Carrasco, Rigo A.: NAMBE2-MoM-11, 8
Casallas Moreno, Yenny Lucero: NAMBE-MoP-38, 22
Casallas-Moreno, Yenny Lucero: NAMBE-MoP-17, 17
Catherall, David: NAMBE2-WeM-16, **36**; NAMBE-MoP-44, **23**
Caucci, Mary Kathleen: NAMBE1-WeM-2, 33
Caudill, Ethan: NAMBE2-MoA-13, 14
Cavallo, Francesca: NAMBE-MoP-33, 21
Cerutti, Laurent: WME1-SaA-1, **3**
Champlain, James: NAMBE2-TuM-16, 27
Chekhova, Maria: NAMBE2-WeM-14, 36
Chen, Jane: NAMBE1-WeM-7, 34
Chen, Rui: NAMBE1-WeM-1, 33
Chen, Yi-Hsun: NAMBE1-TuM-6, 25
Chen, Yuanping: NAMBE2-TuM-13, 26
Chen, Ze-Wei: NAMBE2-TuA-12, 30
Chen, Zijun: NAMBE-MoP-5, 16
Cheng, Chao-Chia: NAMBE1-MoA-4, 11
Choi, Soo Ho: NAMBE2-TuA-12, 30
Chowdhury, Ruhin: NAMBE-MoP-33, **21**
Chowdhury, Sugata: NAMBE1-TuM-8, 25; NAMBE-MoP-34, 21
Churchill, Hugh: NAMBE2-TuA-14, 31
Chyi, Jen-Inn: NAMBE2-TuA-9, 29
Chyi, Jenn-Inn: NAMBE1-MoA-4, 11
Clark, Andrew: WME1-SaA-7, **3**
Cohen-Elias, Doron: NAMBE-MoP-1, 15
Contipelli, Felipe: NAMBE1-TuM-3, 24
Contreras, Edgar Agustin: NAMBE-MoP-17, **17**; NAMBE-MoP-38, **22**
Cowan, Tyler: NAMBE-MoP-30, 20
Cresswell, Zach: NAMBE-MoP-15, 17
Csonka, Szabolcs: NAMBE-MoP-35, 21
Curcio, Davide: NAMBE-MoP-35, 21

— D —

Dafe, Shedrack: NAMBE-MoP-5, 16
Daluizio, Franco: NAMBE-MoP-29, 20
Danilenko, Alisa: NAMBE1-TuM-6, 25
Davari Dolatabadi, Shiva: NAMBE2-TuA-14, 31
de Jesus Lopez, Manny: NAMBE1-MoM-5, **7**
De la Torre, Alberto: NAMBE-MoP-34, 21
de Souza, Lucas. A. T: NAMBE-MoP-20, 18
Demler, Eugene: NAMBE1-TuM-6, 25
Deshmukh, Yugwini: NAMBE-MoP-42, **23**
Dhoubadel, Mangal: NAMBE2-MoM-15, 9
Díaz-Thomas, Daniel: WME1-SaA-1, 3
Dindial, Krishna: NAMBE-MoP-30, 20
Doan, Sean: WME2-SuM-11, 5
Donachie, Fin: NAMBE2-WeM-16, 36
Dong, Chengye: NAMBE1-MoM-4, 7; NAMBE1-MoM-6, 7
Dong, Jason: NAMBE2-TuA-14, **31**
Doty, Matthew: NAMBE1-MoA-1, 11; NAMBE2-TuA-11, 30
Downey, Brian: NAMBE2-TuM-16, 27
Doyle, Will: NAMBE2-WeM-13, 35
Du, Wei: NAMBE1-TuA-6, 29; NAMBE-MoP-31, 20; NAMBE-MoP-32, 20; WME1-SaA-5, 3
Duchane, Alexander: NAMBE2-MoM-15, 9
Duchane, Alexander W.: NAMBE2-MoM-11, 8
Duran, Joshua: NAMBE2-MoM-13, 9
Durbin, Steven: NAMBE-MoP-39, 22; NAMBE-MoP-40, 22

— E —

Egbo, Kingsley: NAMBE1-TuA-2, 28

Eickhoff, Joshua: NAMBE-MoP-16, **17**
Elbaroudy, Ahmed: NAMBE1-TuM-7, 25
Eldose, Nirosh: WME1-SaA-5, 3
ELDOSE, NIROSH: NAMBE-MoP-32, 20
Eldose, Nirosh M.: NAMBE-MoP-31, 20
Ellis, Chase: NAMBE2-MoA-13, 14
Engel, Aaron N.: NAMBE1-TuA-5, 29
Engel-Herbert, Roman: NAMBE-MoP-2, 15
Entezami, Milad: NAMBE1-WeM-8, 34
Erdamar, Serra: NAMBE1-TuM-3, 24

— F —

Faeth, Brendan: WME2-SaM-15, **2**
Fagot, Maëva: WME1-SaA-1, 3
Falson, Joseph: WME2-SaM-11, **1**
Fan, Shanhai: WME1-SaM-2, 1
Fan, Shizhao: NAMBE-MoP-22, **18**; NAMBE-MoP-23, 18
Fang, Xizheng: NAMBE2-WeM-15, **36**
Fazlioglu, Benazir: NAMBE-MoP-2, 15
Febba, Davi: NAMBE1-TuA-2, 28
Feng, Kaiyin: NAMBE1-MoA-5, 12
Fix, J. Pierce: NAMBE2-TuM-12, 26
Flagg, Edward B.: WME2-SuM-13, **6**
Fonseca Montenegro, Alexandra: NAMBE1-TuA-3, **28**
Forrester, Candice R.: NAMBE2-TuA-16, **31**
Frost, Mega: NAMBE2-TuA-10, 30

— G —

Gajowski, Nathan: NAMBE1-MoA-3, 11
Gallardo Hernández, Salvador: NAMBE-MoP-38, 22
Gallardo-Hernandez, Salvador: NAMBE-MoP-17, 17
Garcia, Ashlee: NAMBE2-WeM-13, **35**
Garrett, Gregory: NAMBE2-TuM-13, 26
Gaspe, Chomani: NAMBE2-TuA-14, 31
Gautam, Chhabindra: NAMBE2-TuA-10, 30; WME1-SaM-2, 1
Ghazisaeidi, Maryam: NAMBE1-TuA-3, 28
Gibson, Ricky: NAMBE1-MoA-2, **11**
Gibson, Sandra: NAMBE1-TuM-7, 25
Gilbert, Audrey: WME1-SaA-1, 3
Gingras, Michael: NAMBE1-TuM-3, 24
Gofryk, Krzystof: NAMBE-MoP-15, 17
Gokhale, Vikrant: NAMBE2-TuM-16, 27
Golding, Terry: NAMBE2-MoA-13, 14
Gong, Jiarui: NAMBE1-MoA-7, 12
Gopakumar, Gokul Nanda: NAMBE2-WeM-17, **36**
Gordon, Angelique: NAMBE1-MoA-1, **11**
Goswami, Aranya: NAMBE1-TuM-3, 24
Grant, Gregory D.: NAMBE1-TuA-1, 28
Grassman, Tyler: NAMBE1-TuA-3, 28
Grossklaus, Kevin: NAMBE1-TuM-3, **24**
Guha, Supratik: NAMBE1-TuA-1, 28
Gundlach, Lars: NAMBE1-MoA-1, 11
Guo, Yifu: NAMBE2-TuM-15, **26**

— H —

Hagopian, Nicholas: NAMBE1-MoM-4, 7; NAMBE1-MoM-6, 7; NAMBE1-MoM-8, 8
Hains, Chris: NAMBE-MoP-24, 19
Hains, Christopher: NAMBE2-MoA-11, 13; NAMBE2-MoM-13, 9; NAMBE2-MoM-15, 9
Han, Ne Myo: NAMBE2-TuA-12, 30
Hanke, Michael: NAMBE1-WeM-4, 33
Hanna, Avery: NAMBE1-TuM-5, 24
Hansemann, Moritz: NAMBE1-WeM-4, **33**
Harame, David: NAMBE1-MoA-5, 12
Hardy, Matthew: NAMBE2-TuM-16, 27
Hart, James: NAMBE2-TuM-16, 27
Hasan, Syed: NAMBE1-TuA-2, 28
Hatch, Sabina: NAMBE2-TuA-13, **30**
Hawkins, Samuel D.: NAMBE2-MoM-11, 8
Hazard, Thomas: NAMBE2-TuA-14, 31

Author Index

Heinrich, Carter: NAMBE2-TuA-10, 30
Helms, Luke: NAMBE2-MoM-15, 9
Herfort, Jens: NAMBE1-WeM-4, 33
Herman, Joshua: NAMBE1-MoA-5, 12
Hernández Martínez, Jorge Ivan: NAMBE-MoP-38, 22
Hernández-Calderón, Isaac: NAMBE-MoP-43, 23
Hilse, Maria: NAMBE1-WeM-2, 33; NAMBE2-WeM-18, 36
Holloway, Richard: NAMBE-MoP-29, 20
Hopkins, Derek: NAMBE2-WeM-11, 35
Hossain, Khalid: NAMBE2-MoM-15, 9
Hossain, Razine: NAMBE1-MoA-7, 12; NAMBE1-TuA-4, 28; NAMBE2-WeM-12, 35
Hosseini Farahabadi, Seyed Ali: NAMBE1-WeM-8, 34
Hrabovsky, Jan: NAMBE1-TuA-5, 29; NAMBE-MoP-4, 15
Hsu, Kai-Yang: NAMBE2-TuA-9, 29
Hurley, David: NAMBE-MoP-15, 17
—I—
Islam, Md Toriquel: NAMBE2-MoM-12, 8
Issokson, Jacob: NAMBE1-TuM-6, 25; NAMBE-MoP-30, 20
Iyer, Shanthi: NAMBE-MoP-42, 23
—J—
J Salamo, Gregory: NAMBE1-TuA-6, 29
Jacobson, Peter: NAMBE1-TuM-6, 25
Jaeger, David: NAMBE1-TuA-4, 28
Janssen, Shelby: NAMBE-MoP-29, 20
Javadi, Alisa: WME1-SuM-5, 5
Ji, Mihee: NAMBE2-TuM-13, 26
Jin, Eric: NAMBE2-TuM-16, 27
Johnson, Shane: NAMBE2-MoA-12, 13
Johnson, Shane R.: NAMBE2-MoM-11, 8
Johnson, Trent: NAMBE-MoP-21, 18
Jones, Kevin: NAMBE1-MoM-5, 7
Joshi, Ram: NAMBE-MoP-27, 19; NAMBE-MoP-31, 20
Ju, Zheng: NAMBE1-MoA-7, 12; NAMBE1-TuA-4, 28; NAMBE2-WeM-12, 35
Jung, Taehwan: NAMBE1-MoM-6, 7
Jungfleisch, M. Benjamin: NAMBE1-MoA-1, 11
—K—
Kamboj, Abhilasha: NAMBE2-MoM-12, 8
Kang, Taein: NAMBE-MoP-9, 16
Kar, Swastik: NAMBE1-TuM-8, 25
Karimi, Hannaneh: NAMBE2-MoA-14, 14
Kaspar, Tiffany: NAMBE2-WeM-11, 35
Katzer, D. Scott: NAMBE2-TuM-16, 27
Kawasaki, Jason: NAMBE1-MoM-4, 7; NAMBE1-MoM-6, 7; NAMBE1-MoM-8, 8; NAMBE-MoP-16, 17
Kiefer, Arnold: NAMBE-MoP-13, 16
Kim, Bora: NAMBE1-MoA-6, 12
Kim, David: NAMBE1-TuM-3, 24
Kim, Hyunseok: NAMBE2-TuA-12, 30
Kim, Jae Hun: NAMBE2-TuM-14, 26
Kim, Jeehwan: NAMBE2-TuA-12, 30
Kim, Jong Su: NAMBE-MoP-9, 16
Kim, Junghwa: NAMBE1-TuA-1, 28
Kim, Sangsoo: NAMBE-MoP-8, 16
Kimbugwe, Faisal Kimbugwe: NAMBE1-TuA-3, 28
King, Ethan: NAMBE2-WeM-11, 35
Kirshtein, Arkadz: NAMBE-MoP-28, 19
Kirti, Magdhi: NAMBE-MoP-35, 21
Klamkin, Jonathan: NAMBE1-MoA-5, 12
Kobayashi, Masakazu: NAMBE2-TuA-16, 31; NAMBE-MoP-43, 23
Kodigala, Ashok: WME1-SaM-6, 1
Koepke, Justine: NAMBE1-MoM-5, 7; NAMBE1-MoM-6, 7
Kondapavuluri, Bhavya: NAMBE2-TuA-9, 29
Kornblum, Lior: NAMBE-MoP-1, 15
Koscica, Rosalyn: NAMBE1-MoA-5, 12
Krishna, Sanjay: NAMBE1-MoA-3, 11
Krishnamoorthy, Sriram: NAMBE2-TuM-11, 25
Krusin-Elbaum, Lia: NAMBE1-WeM-5, 34
Kuchoor, Hirandeep Reddy: NAMBE-MoP-42, 23
Kwon, Doa: NAMBE2-TuA-12, 30
—L—
LaDuka, Zachary: NAMBE1-MoM-4, 7
Laji, Ba: NAMBE2-TuA-9, 29
Lang, Andrew: NAMBE2-TuM-16, 27
Langa Jr., Bernardo: NAMBE2-TuA-14, 31
Larkin, LeighAnn: NAMBE2-TuM-13, 26
Law, Stephanie: NAMBE1-MoM-7, 7; NAMBE1-WeM-2, 33; NAMBE2-WeM-17, 36; NAMBE2-WeM-18, 36; NAMBE-MoP-37, 21; WME2-SaA-14, 4
Leake, Gerald: NAMBE1-MoA-5, 12
LeBeau, James M.: NAMBE1-TuA-1, 28
Lee, Devon: NAMBE1-MoA-6, 12
Lee, Minjoo: NAMBE2-WeM-13, 35; NAMBE2-WeM-15, 36
Lee, Minjoo Larry: NAMBE1-MoA-6, 12; NAMBE2-TuA-12, 30; WME2-SaM-13, 1
Lee, Sang Jun: NAMBE-MoP-9, 16
Levy, Ido: NAMBE-MoP-30, 20
Li, Brian: NAMBE1-MoA-6, 12
Li, Jia: NAMBE-MoP-42, 23
Liang, Yunfan: NAMBE-MoP-27, 19
Lin, Bonnie: NAMBE1-TuA-1, 28
Linser, Samuel M.: NAMBE1-MoA-2, 11
Liu, Amy: WME1-SaA-7, 3
Liu, Chun-Nien: NAMBE1-MoA-4, 11
Liu, Jiangnan: NAMBE2-TuM-15, 26
Liu, Jifeng: NAMBE1-TuA-4, 28; NAMBE-MoP-27, 19; NAMBE-MoP-3, 15
Liu, Pin-Chih: NAMBE2-TuA-9, 29
Liu, Wei-Sheng: NAMBE2-TuA-9, 29
Liu, Xiaoyang: NAMBE1-MoA-7, 12; NAMBE1-TuA-4, 28; NAMBE2-WeM-12, 35
Liu, Yizheng: NAMBE2-TuM-11, 25
Lloyd, Michael: NAMBE2-MoA-13, 14
Logan, Julie: NAMBE2-MoM-13, 9; NAMBE2-MoM-15, 9; NAMBE-MoP-12, 16; NAMBE-MoP-24, 19
Logan, Julie V.: NAMBE2-MoM-11, 8
López López, Máximo: NAMBE-MoP-38, 22
López-López, Máximo: NAMBE-MoP-17, 17
Love, Jaden: NAMBE1-TuA-5, 29; NAMBE2-MoA-12, 13
Lu, Kuangye: NAMBE2-TuA-12, 30
Luna, Esperanza: NAMBE1-WeM-8, 34
—M—
Ma, Zhenqiang: NAMBE1-MoA-7, 12
Ma, Zon: NAMBE1-MoA-4, 11
Maddaka, Reddeppa: NAMBE2-TuM-15, 26
Maestas, Diana: NAMBE2-MoA-12, 13; NAMBE2-MoM-11, 8; NAMBE2-MoM-13, 9; NAMBE2-MoM-15, 9; NAMBE-MoP-12, 16; NAMBE-MoP-24, 19
Mai, Lan: NAMBE2-TuA-11, 30
Maia de Oliveira, Fernando: NAMBE1-TuA-6, 29
Majumdar, Arka: NAMBE1-WeM-1, 33
Makin, Robert: NAMBE-MoP-39, 22; NAMBE-MoP-40, 22
Makk, Peter: NAMBE-MoP-35, 21
Malhotra, Yakshita: NAMBE2-TuM-15, 26
Mantooth, H. Alan: NAMBE-MoP-14, 17
Manzo, Sebastian: NAMBE1-MoM-8, 8
Markowitz, Matthew Markowitz: NAMBE-MoP-25, 19
Martin, Kira: NAMBE1-WeM-6, 34
Masiilionis, Ignas: NAMBE1-TuA-1, 28
Maurtua, Collin: NAMBE-MoP-18, 17
May, Breton: NAMBE2-TuM-12, 26; NAMBE-MoP-15, 17; NAMBE-MoP-40, 22
Mazur, Yuriy I.: NAMBE-MoP-14, 17
Mazza, Alessandro R.: NAMBE1-WeM-7, 34
McArthur, J. Andrew: NAMBE2-MoA-14, 14
McCabe, Lauren N.: NAMBE2-TuA-11, 30
McCarthy, Tyler: NAMBE1-MoA-7, 12; NAMBE1-TuA-4, 28
McCartney, Martha: NAMBE1-MoA-7, 12
McDonough, Molly: NAMBE-MoP-37, 21
McMinn, Allison: NAMBE1-MoA-7, 12; NAMBE1-TuA-4, 28
Meckamalil Eldose, Nirosh: NAMBE1-TuA-6, 29
Menasuta, T. Pan: NAMBE-MoP-28, 19
Messelcar, Andrew: NAMBE-MoP-39, 22; NAMBE-MoP-40, 22
Meyer, Jarod: NAMBE1-WeM-1, 33
Meyer, Jarod E.: NAMBE1-WeM-6, 34
Meyer, Jerry: NAMBE2-MoA-13, 14
Mi, Zetian: NAMBE2-TuM-14, 26; NAMBE2-TuM-15, 26
Michaels, Mach: NAMBE2-MoM-15, 9
Mikalsen, Melissa: NAMBE-MoP-30, 20
Millan-Almaraz, Jesus Roberto: NAMBE-MoP-17, 17
Miller, Duncan: NAMBE1-TuM-3, 24
Milosavljevic, Marko: NAMBE2-MoA-12, 13
Milosavljevic, Marko S.: NAMBE2-MoM-11, 8
Minnich, Austin: NAMBE2-WeM-16, 36
Miri, Mohammad Ali: NAMBE-MoP-25, 19
Mishima, Tetsuya: NAMBE2-MoA-13, 14
Miyazawa, Rei: NAMBE2-TuA-16, 31
Mohammadi, Sina: NAMBE1-WeM-5, 34; NAMBE2-TuA-16, 31; NAMBE-MoP-25, 19
Mondal, Shubham: NAMBE2-TuM-14, 26
Monticone, Francesco: NAMBE-MoP-25, 19
Moody, Galan: WME2-SuM-11, 5
Moon, Jisoo: NAMBE1-WeM-5, 34; NAMBE1-TuA-16, 31
Moore, Rob: NAMBE1-WeM-7, 34
Morath, Christian: NAMBE2-MoA-11, 13; NAMBE2-MoA-12, 13; NAMBE2-MoM-13, 9; NAMBE2-MoM-15, 9; NAMBE-MoP-12, 16; NAMBE-MoP-24, 19
Morath, Christian P.: NAMBE2-MoM-11, 8
Moses, Isaiah: WME2-SaA-14, 4
Muhowski, Aaron J.: NAMBE2-MoM-11, 8
Mukherjee, Kunal: NAMBE1-WeM-1, 33; NAMBE1-WeM-6, 34
Mulani, Imrankhan: NAMBE1-TuM-8, 25
Murkute, Punam: NAMBE1-MoA-3, 11
Murphy, John: NAMBE2-MoA-13, 14
Murray, Lottie: NAMBE2-TuA-11, 30
Mustakim, Ahmed: NAMBE-MoP-15, 17
Mutlu, Zafer: NAMBE-MoP-29, 20; NAMBE-MoP-36, 21
Myers, Roberto: NAMBE1-TuA-3, 28
—N—
Najmaei, Sina: NAMBE-MoP-16, 17
Nakamura, Hiro: NAMBE-MoP-27, 19
Nakamura, Hiroyuki: NAMBE-MoP-31, 20
Nayir, Nadire: NAMBE-MoP-2, 15
Neely, Jordan P.: NAMBE-MoP-33, 21
Nepal, Neeraj: NAMBE2-TuM-16, 27
Newell, Alex: NAMBE2-MoM-13, 9
Newell, Alexander: NAMBE2-MoA-11, 13; NAMBE2-MoA-12, 13; NAMBE-MoP-24, 19
Newell, Alexander T.: NAMBE2-MoM-11, 8
Nguyen, Tri: NAMBE1-WeM-6, 34
Niedel, Jackson: NAMBE2-WeM-18, 36
Niedzielski, Bethany: NAMBE1-TuM-3, 24

Author Index

Nolde, Jill: NAMBE2-MoA-13, 14
Nooman, Neha: NAMBE1-MoA-3, **11**
Nordin, Leland: NAMBE1-WeM-1, 33
Nuzhat, Samiha: NAMBE2-TuA-10, 30
—O—
O'Connell, Christopher: NAMBE1-TuM-3, 24
Oliveira, Fernando: NAMBE-MoP-32, 20;
WME1-SaA-5, 3
Oliveira, Fernando Maia de: NAMBE-MoP-31, 20
Oliver, William: NAMBE1-TuM-3, 24
—P—
Palmstrom, Chris: NAMBE1-TuA-5, 29
Pan, Mingsen: WME1-SaM-2, 1
Pandey, Ayush: NAMBE2-TuM-15, 26
Parasnis, Mrudul: NAMBE2-MoM-12, **8**
Park, Suho: NAMBE-MoP-3, 15; NAMBE-MoP-5, 16
Patel, Sahil: WME2-SuM-11, 5
Patel, Victor J.: NAMBE2-MoM-11, 8
Peiris, Frank: NAMBE2-WeM-18, **36**
Pérez-Saavedra, Jorge: NAMBE-MoP-43, 23
Peterson, Owen: NAMBE2-WeM-18, 36
Phillips, Jamie: NAMBE2-MoM-12, 8
Polat Genlik, Sevim: NAMBE1-TuA-3, 28
Pope, Jenna: NAMBE2-WeM-11, 35
Prakash, Divya J.: NAMBE-MoP-33, 21
Pratt, Jonathan: NAMBE2-TuM-13, **26**
Prok, Tamas: NAMBE-MoP-35, 21
—Q—
Qi, Xin: NAMBE1-MoA-7, 12; NAMBE1-TuA-4, 28; NAMBE2-WeM-12, 35
Qiu, Lawrence: NAMBE-MoP-28, **19**
Qui, Larry: NAMBE1-TuM-5, 24
—R—
R. Forrester, Candice: NAMBE1-WeM-5, 34
Rable, Jeff: NAMBE-MoP-34, 21
Rajagopal, Joshya: NAMBE2-TuA-11, 30
Rajan, Siddharth: NAMBE2-TuA-15, 31; NAMBE2-TuM-13, 26
Ramesh, Prashant: NAMBE2-TuA-11, 30
Rastelli, Armando: WME2-SuM-9, **5**
Razi, Alimir: NAMBE2-MoM-12, 8
Reddy, Pooja: NAMBE1-WeM-1, 33
Reddy, Pooja D.: NAMBE1-WeM-6, 34
Reinhart, Wesley: WME2-SaA-14, 4
Remis, Andres: WME1-SaA-1, 3
Renteria, Emma J.: NAMBE-MoP-33, 21
Reyner, Charles: NAMBE-MoP-13, 16
Rhodes, Daniel: NAMBE-MoP-16, 17
Richardson, Christopher: NAMBE2-TuA-14, 31
Ricks, Amberly: NAMBE2-MoM-14, **9**
Robinson, Joshua: NAMBE1-MoM-4, 7; NAMBE1-MoM-6, 7
Rodriguez, Jean-Baptiste: WME1-SaA-1, 3
Rogers, Vinita: NAMBE1-MoA-3, 11
Rosenblatt, Nathan: NAMBE1-MoA-7, 12; NAMBE2-WeM-12, 35
Rotter, Thomas: NAMBE1-MoA-2, 11; NAMBE2-TuA-10, **30**; WME1-SaM-2, 1
Rouillard, Yves: WME1-SaA-1, 3
Rushing, James: NAMBE1-TuM-5, 24
Rushing, Jimmy: NAMBE1-TuM-4, **24**
—S—
Saeed, Hatim: NAMBE2-WeM-18, 36
Saha, Archishman: NAMBE2-TuA-12, 30
Salamo, Gregory: NAMBE-MoP-32, 20; WME1-SaA-5, 3
Salamo, Gregory J.: NAMBE-MoP-14, 17; NAMBE-MoP-31, 20
Saldanha, Emily: NAMBE2-WeM-11, 35
Salmani-Rezaie, Salva: NAMBE1-TuM-6, 25; NAMBE-MoP-30, 20

Samanta, Chandan: NAMBE-MoP-3, 15; NAMBE-MoP-5, 16
Sampath, Anand: NAMBE2-TuM-13, 26
Sanga, Cem: NAMBE-MoP-2, 15
Santos, Michael: NAMBE2-MoA-13, 14
Saraswat, Vivek: NAMBE1-MoM-8, 8
Sardashti, Kasra: NAMBE2-TuA-14, 31
Sarker, Mamun: NAMBE-MoP-29, 20
Sarney, Wendy: NAMBE-MoP-16, 17
Sautter, Kathryn E.: WME1-SaA-7, 3
Sbuelz, Luca: NAMBE-MoP-35, 21
Schaefer, Stephen: NAMBE1-TuA-2, 28
Schlom, Darrell: NAMBE2-MoA-9, **13**
Schmucker, Scott: NAMBE1-MoM-5, 7
Schwartz, Mollie: NAMBE1-TuM-3, 24
Serniak, Kyle: NAMBE1-TuM-3, 24; NAMBE2-TuA-14, 31
Seth, Subhashree: NAMBE2-TuA-10, 30
Sfigakis, Francois: NAMBE1-TuM-7, 25
Shabani, Javad: NAMBE1-TuM-6, 25; NAMBE-MoP-30, 20
Shahed, Syed M.: NAMBE-MoP-34, 21
Shahed, Syed Mohammad: NAMBE1-TuM-8, 25
Shang, Chen: NAMBE1-MoA-5, 12; WME2-SuM-11, **5**
Sharma, Andrei: NAMBE2-TuA-10, 30
Shearer, Thomas: NAMBE2-MoA-13, 14
Shetty, Satish: NAMBE-MoP-14, **17**
Shi, Bei: NAMBE1-MoA-5, 12
Shi, Peyton: NAMBE1-TuM-7, 25
Shima, Darryl: NAMBE-MoP-24, 19
Shima, Darryl M.: NAMBE-MoP-33, 21
Shusterman, Sergey Shay: NAMBE-MoP-1, 15
Sicron, Noam: NAMBE-MoP-1, 15
Silverman, Kevin: WME1-SuM-3, **5**
Simmonds, Paul J.: NAMBE1-TuM-5, 24
Sinitskii, Alexander: NAMBE-MoP-29, 20
Sinnott, Susan: NAMBE1-WeM-2, 33
Sirohi, Anshu: NAMBE1-MoM-6, 7; NAMBE1-MoM-8, 8
Skipper, Alec: NAMBE1-MoA-5, **12**; NAMBE1-WeM-1, 33
Smeaton, Michelle: NAMBE1-TuA-2, 28
Smith, David: NAMBE1-MoA-7, 12; NAMBE1-TuA-4, 28
Song, Jin Dong: NAMBE-MoP-9, 16
Speck, James: NAMBE2-TuA-15, 31; NAMBE2-TuM-11, 25
Spruell, Henry: NAMBE2-WeM-11, 35
Stanchu, Hryhorii: NAMBE1-TuA-6, 29; NAMBE-MoP-31, 20; NAMBE-MoP-32, 20; WME1-SaA-5, 3
Steele, Julian: NAMBE1-TuM-6, 25
Stich, Simon: NAMBE2-WeM-14, 36
Stickler, Hannah: NAMBE1-TuM-3, 24
Storm, David: NAMBE2-TuM-13, 26
Strickland, William: NAMBE-MoP-30, 20
Strohbeen, Patrick: NAMBE1-MoM-8, 8; NAMBE1-TuM-6, 25; NAMBE-MoP-30, 20
Su, Katherine: NAMBE1-MoM-8, 8
Sultanov, Vitaliy: NAMBE2-WeM-14, 36
Sun, Kai: NAMBE2-TuM-15, 26
Sutara, Frantisek: NAMBE-MoP-43, 23
Suto, Mate: NAMBE-MoP-35, 21
Sweepe, Thomas: NAMBE-MoP-29, 20
—T—
T. Webster, Preston: NAMBE-MoP-4, 15
Tam, Man Chun Alan: NAMBE1-WeM-8, 34
Tamargo, Maria: NAMBE-MoP-25, 19
Tamargo, Maria C.: NAMBE2-TuA-16, 31
Tara, Virat: NAMBE1-WeM-1, 33
Teeter, Glenn: NAMBE1-TuA-2, 28
Tellekamp, M. Brooks: NAMBE1-TuA-2, **28**

Thompson, Bradley J.: NAMBE1-MoA-2, 11; WME1-SaM-4, **1**
Thompson, Joshua: NAMBE2-TuA-14, 31
Tischler, Joseph: NAMBE2-MoA-13, 14
Tiwari, Kunal: NAMBE1-TuM-3, 24
Tomasulo, Stephanie: WME1-SaA-3, **3**
Torre, Alberto De la: NAMBE1-TuM-8, 25
Tournié, Eric: WME1-SaA-1, 3
Tóvári, Endre: NAMBE-MoP-35, 21
Trampert, Achim: NAMBE1-WeM-4, 33
Trejo-Hernández, Raul: NAMBE-MoP-17, 17
Trice, Ryan: NAMBE1-MoM-7, **7**; WME2-SaA-14, 4
Tu, Charles W.: NAMBE1-MoA-4, **11**
Tubthong, Chanita: NAMBE-MoP-28, 19
—V—
Vallejo, Kevin: NAMBE1-WeM-3, **33**; NAMBE2-TuM-12, 26; NAMBE-MoP-15, 17; NAMBE-MoP-40, **22**
van Dijk, Jechiel: NAMBE1-TuM-6, 25
van Duin, Adri: NAMBE-MoP-2, 15
Vandervelde, Thomas E.: NAMBE-MoP-28, 19
Vargas Hernández, Luis: NAMBE-MoP-38, 22
Vázquez-Soto, Yang A.: NAMBE-MoP-43, 23
Verdi, Carla: NAMBE1-TuM-6, 25
Voyles, Paul: NAMBE1-MoM-4, 7; NAMBE1-MoM-6, 7; NAMBE1-MoM-8, 8
Vurgaftman, Igor: NAMBE2-MoA-13, 14
—W—
Wang, Ellie: NAMBE2-MoA-14, **14**
Wang, Lianzhou: NAMBE1-TuM-6, 25
Wang, Xi: NAMBE1-MoA-1, 11
Wang, Yicheng: NAMBE1-TuA-4, 28
Wang, Yiteng: NAMBE2-TuA-12, 30; NAMBE2-WeM-13, 35; NAMBE2-WeM-15, 36
Wang, Zhichao: NAMBE-MoP-23, 18
Wang, Zihang: WME2-SuM-11, 5
Wasilewski, Zbigniew: NAMBE1-TuM-7, **25**; NAMBE1-WeM-8, 34; NAMBE2-WeM-14, 36
Wasserman, Daniel: NAMBE2-WeM-13, 35
Webster, Preston: NAMBE1-TuM-1, **24**; NAMBE2-MoA-11, 13; NAMBE2-MoA-12, 13; NAMBE2-MoM-13, 9; NAMBE2-MoM-15, 9; NAMBE-MoP-12, 16; NAMBE-MoP-24, 19
Webster, Preston T.: NAMBE2-MoM-11, **8**
Weerasinghe, Priyantha: NAMBE2-MoA-13, 14
Welch, Alex: NAMBE-MoP-29, 20
Welp, Eric: NAMBE-MoP-37, 21
West, Damien: NAMBE-MoP-27, 19
Wheeler, Virginia: NAMBE2-TuM-16, 27
White, Corey: NAMBE1-MoA-6, 12; NAMBE2-MoM-14, 9; NAMBE2-TuA-12, **30**; NAMBE2-WeM-13, 35
White, Joshua: NAMBE-MoP-42, 23
Williams, Ekow: NAMBE1-TuM-5, 24
Wissel-Garcia, Ashley: NAMBE2-TuA-15, **31**; NAMBE2-TuM-11, 25
Wraback, Michael: NAMBE2-TuM-13, 26
Wu, Weipeng: NAMBE1-MoA-1, 11
Wu, Yuanpeng: NAMBE2-TuM-15, 26
—X—
Xavier, Agnes: NAMBE2-TuM-13, 26
Xiao, Kelly: NAMBE1-WeM-1, **33**; NAMBE1-WeM-6, 34
Xiao, Yixin: NAMBE2-TuM-15, 26
Xie, Xikae: NAMBE1-TuM-5, 24
—Y—
Yadav, Sonam: NAMBE-MoP-4, **15**
Yan, Yifei: NAMBE2-WeM-11, 36
Yang, Samuel: NAMBE2-TuM-14, **26**

Author Index

Yawit, Howard: NAMBE-MoP-29, 20
Yee-Rendón, Cristo Manuel: NAMBE-MoP-17, 17
Yin, Yihao: NAMBE-MoP-23, 18
Yu, Fisher: NAMBE1-TuA-6, 29
Yu, Mingyu: WME2-SaA-14, 4
Yu, Shui-Qing: NAMBE-MoP-27, 19; NAMBE-MoP-3, 15; NAMBE-MoP-31, 20; NAMBE-MoP-32, 20; WME1-SaA-5, **3**
Yumigeta, Kentaro: NAMBE-MoP-29, **20**
Yusufoglu, Muhammed: NAMBE-MoP-29, 20; NAMBE-MoP-36, **21**
— Z —
Zakutayev, Andriy: NAMBE1-TuA-2, 28

Zambrano Serrano, Mario Alberto: NAMBE-MoP-38, 22
Zarkesh-Ha, Payman: NAMBE-MoP-12, 16
Zeng, Yuping: NAMBE-MoP-3, **15**; NAMBE-MoP-5, **16**
Zhama, Tuofu: NAMBE-MoP-3, 15; NAMBE-MoP-5, 16
Zhang, Diandian: NAMBE1-TuA-6, 29; NAMBE-MoP-31, 20; NAMBE-MoP-32, **20**; WME1-SaA-5, 3
Zhang, Jiefei: NAMBE1-TuA-1, 28
Zhang, Qihua: NAMBE1-WeM-2, **33**; NAMBE2-WeM-18, 36; NAMBE-MoP-37, 21
Zhang, Shengbai: NAMBE-MoP-27, 19

Zhang, Yong-Hang: NAMBE1-MoA-7, 12; NAMBE1-MoM-2, **7**; NAMBE1-TuA-4, 28; NAMBE2-WeM-12, 35
Zhao, Haiyang: NAMBE-MoP-23, **18**
Zhao, Haochen: NAMBE-MoP-3, 15; NAMBE-MoP-5, 16
Zhou, Weidong: NAMBE2-TuA-10, 30; WME1-SaM-2, **1**
Zhu, Yinxuan: NAMBE2-TuA-15, 31
Zide, Joshua: NAMBE1-MoA-1, 11; NAMBE2-MoM-12, 8; NAMBE2-TuA-11, 30
Zollner, Stefan: NAMBE1-TuA-5, 29; NAMBE2-MoA-12, 13; NAMBE-MoP-4, 15
Zylstra, Michael: NAMBE1-MoA-5, 12