# 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, 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 Burkhart, 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 ~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 $As_4$ or $As_2$, and with arsenic beam equivalent pressures in the range $5x10^{-7}$ to $1x10^{-5}$ 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 Baksi,*** *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.

[1] Denis R. Candido, Michael E. Flatt ́e, and J. Carlos Egues. Blurring the boundaries between topological and nontopological phenomena in dots. Phys. Rev. Lett., 121:256804, Dec 2018.

[2] S. Schmid, M. Meyer, F. Jabeen, G. Bastard, F. Hartmann, and S. H ̈ofling. Exploring the phase diagram of InAs/GaSb/InAs trilayer quantum wells. Phys. Rev. B, 105:155304, Apr 2022.

[3] M. Marcinkiewicz, S. Ruffenach, S. S. Krishtopenko, A. M. Kadykov, C. Consejo, D. B. But, W. Desrat, W. Knap, J. Torres, A. V. Ikonnikov, K. E. Spirin, S. V. Morozov, V. I. Gavrilenko, N. N. Mikhailov, S. A. Dvoretskii, and F. Teppe. Temperature-driven single-valley Dirac fermions in HgTe quantum wells. Phys. Rev. B, 96:035405, Jul 2017.

[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.

9:15am **NAMBE1-TuM-6 Group IV Superconductor-Semiconductor Epitaxy for Integrated Quantum Electronics**, 
***Patrick Strohbeen,*** New York University*; Julian Steele, Carla Verdi, Ardeshir 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 $\lambda_d$, exhibit significant hybridization between one another when $\lambda_d << a_0$. 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 shevrons angle, it follows that the facets planes are {112} family, rather than the lowest surface energy and highest atomic packing density {111} planes.

[1] W.F. Schiela et al., PRX Quantum 5(3), 030102 (2024).

[2] A. Elbaroudy et al., J. Vac. Sci. Technol. A 42(3), 031304 (2024).

[3] S. Telkamp et al., Adv. Electron. Mater. 2400687 (2025).

9:45am **NAMBE1-TuM-8 Synthesis and Temperature-Dependent Momentum Microscopy of Type-II Dirac Semimetal $NiTe_2$**, 
***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 ($NiTe_2$) 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 $NiTe_2$ 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 $NiTe_2$ films (thickness ~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 $NiTe_2$. 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 $NiTe_2$, 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, $NiTe_2$, molecular beam epitaxy, Momentum Microscopy, XPS, Raman spectroscopy, electronic properties, quantum materials

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