

PCSI

Room Ballroom - Session PCSI-ThM

Semiconductor Heterostructures & Epitaxy

Moderator: Joe Falson, Caltech

8:30am **PCSI-ThM-1 Epitaxial Growth, Materials Characterization, and Detector Assessments of Quinary GaInAsSbBi**, *Rigo Carrasco, Alexander Newell, Zinah Alsaad, Julie Logan, Christian Morath, Diana Maestas*, Air Force Research Laboratory, USA; *Christopher Hains*, Aerovironment Inc, USA; *Preston Webster*, Air Force Research Laboratory, USA

INVITED

Alloying Bi in group III-V material systems has been the subject of extensive study due to the large bandgap reduction behavior per percent of Bi incorporated, and the high degree of device optimization flexibility this property affords. When alloyed with infrared materials, such as InAsSb to create InAsSbBi, a wide design space is unlocked where lattice constant and bandgap may be tuned to desired wavelengths, while maintaining a lattice-matched condition to a commercially available substrate. However, achieving proper Bi compositions in this alloy to the desired wavelength extension while maintaining smooth surface morphologies, and device-ready optoelectronic quality proved to be difficult.

Adding Ga to the mix may offer a path to mitigate these difficulties. Here, quinary GaInAsSbBi alloys are grown lattice matched on GaSb by molecular beam epitaxy. Essential and rapid growth feedback by Normarski interference contrast imaging is used to determine the ideal Bi flux condition to attain smooth surface morphologies. Fortunately, with only 0.3% Bi, ~14% Ga and corresponding As and Sb compositions that allow for a lattice-matched condition, photoluminescence extending beyond 5 μm emission, and minority carrier lifetimes $> 1 \mu\text{s}$ were realized. This motivated *nBn* device structures to be grown and fabricated into variable area single pixel device arrays. Detector dark current, and quantum efficiency are determined as a function of bias, temperature and displacement damage due to 63 MeV proton irradiation. The *nBns* are also fabricated into small format 350x256 focal plane arrays and hybridized to an analog read-out integrated circuit. This allows for direct evaluations of sensitivity, noise spectra, uniformity, operability, and radiation tolerance. A discussion on the growth feedback strategy, materials characterization results and device performance will be provided, followed by current efforts and progress.

9:00am **PCSI-ThM-7 Pressure-Dependent Photoluminescence and Strain Response of a 1.7 μm Cutoff InGaAsSb/AlGaAsSb Multi-Quantum Well**, *Meghan Verano*, New Mexico State University

The photoluminescence response of a molecular beam epitaxy-grown InGaAsSb/AlGaAsSb multi-quantum well heterostructure is investigated as a function of hydrostatic pressure up to 1.35 GPa at 10 K. Pressure-dependent photoluminescence measurements were performed using a diamond anvil cell, with pressure calibrated by ruby fluorescence. The emission peak exhibits a systematic blue shift with increasing pressure, with a measured pressure coefficient of approximately 77 meV/GPa. At the same time, the integrated photoluminescence intensity decreases with pressure, consistent with enhanced non-radiative recombination through a defect level located above the conduction-band edge at ambient pressure that becomes electronically active under compression. The strain in the quantum well is quantified using the Murnaghan equation of state, and analysis of the transition energy as a function of strain yields a hydrostatic deformation potential of approximately -4.4 eV. These measurements demonstrate the use of hydrostatic pressure as a sensitive probe of band-structure evolution, strain response, and defect-mediated recombination in quaternary III-V quantum-well heterostructures, providing insight relevant to the optimization of infrared optoelectronic materials and devices.

9:05am **PCSI-ThM-8 Probing THz-Driven Excitons in Magnetic and Conventional Semiconductors**, *Meghan Verano*, New Mexico State University

When a terahertz field is driven into a material, it is theorized that excitons in conventional semiconductors, such as gallium arsenide, will first ionize and then stabilize with increasing field strength. This adiabatic stabilization is something we aim to observe using absorption spectroscopy techniques. We first predict to see the exciton peak broaden and suppress asymmetrically as a result of the THz coupling to and disrupting the exciton. Following this broadening, the peak should again narrow, indicating an increase in exciton lifetime. The ionization rate can be extracted from fitting the Fano resonance to the absorption line shapes. In preparation for this planned THz experiment, control data has been taken on bulk and quantum well gallium arsenide using absorption spectroscopy with near infrared LED in the range of 820 - 870 nm. Nickel phosphorus trisulphide is another

material of interest. As a Mott insulator, the excitons pair in different ways than a conventional semiconductor. NiPS₃ excitons rely on the antiferromagnetic ordering of the material to survive, and this ordering is only present below 150 K. These excitons are far more robust, with a binding energy of a few hundred meV, and do not arise out of conventional band theory. We hope to use THz pump along with spectroscopy as a probe to observe magnon-exciton coupling by observing how the exciton spectrum changes under resonant pumping of magnon mode at 300 GHz in the absorption data, and phonon-exciton coupling in photoluminescence data. NiPS₃ samples have been prepared using an exfoliation and stacking technique using tape and a polymer stamp, as this Van der Waals material can be stripped down to atomically thin layers. This work is supported by NSF DMR 2333941 and NSF PREM grant DMR-2423992.

9:10am **PCSI-ThM-9 Spin-Orbit-Coupled Electronic and Vibrational Properties of ZnO/ZnS Quantum-Dot Heterostructures**, *Wisdom Benson*, Howard University

ZnO/ZnS quantum-dot heterostructures combine a polar oxide core with a wide-bandgap sulfide shell. Quantum confinement, local strain, and chemical bonding at the interface can change band-edge states and lattice vibrations. We connect Raman spectroscopy with first-principles calculations to study these coupled electronic, vibrational, dielectric, and spin-dependent effects.

We construct an isolated 2,870-atom Zn₁₃₆₆O₃₁₀S₁₁₉₄ model from a MatterSim-relaxed geometry. PBEsol/SIESTA calculations test the large heterostructure. A 42-atom Zn₁₄O₂₈ reference uses our published Quantum ESPRESSO workflow [1]: PBE+U, fully relativistic norm-conserving pseudopotentials, noncollinear spin-orbit coupling, and density-functional perturbation theory. These calculations provide band-edge orbital character, phonon modes, Raman tensors, Born effective charges, and dielectric response. Room-temperature 532 nm Raman spectra provide the experimental mode reference.

The ZnO reference has a calculated 4.54 eV HOMO-LUMO gap. Its valence edge is mainly O 2p, its conduction edge is mainly Zn 4s, and Zn 3d states lie several electronvolts below the Fermi level. Spin-orbit coupling slightly narrows the gap and lifts valence-edge degeneracies by about 0.1 eV. In the ZnO/ZnS structure, O occupies the inner region, S forms the outer shell, and Zn spans both regions. This geometry provides a direct basis for testing how interface strain and local bonding reshape band-edge and Raman-active states. The combined workflow links measured phonons to atomic structure, dielectric screening, and spin-dependent electronic behavior. These links support rational interface design for ultraviolet optoelectronics, sensing, and quantum technologies.

9:15am **PCSI-ThM-10 Sapphire Nitridation for Highly Crystalline (0002) AlN Heteroepitaxy**, *Spencer Gellerup*, Oak Ridge National Laboratory; *Matthew Brahlek, Kyle Kelley*, Oak Ridge National Laboratory

Direct nitridation of sapphire and aluminum oxide substrates via nitrogen plasma treatments is well reported for improving heteroepitaxy of AlN. In this work, plasma treatments of c-plane sapphire were conducted in-situ in a sputtering chamber directly preceding AlN deposition. Plasma treatment parameters were varied to investigate variations in resulting aluminum oxynitride formation via x-ray reflection, where x-ray diffraction was used to determine AlN crystalline texture and mosaicity. AlN (0002) rocking curve full-width-half max of $\sim 0.1^\circ$ was measured for optimal sapphire plasma treatments. A narrow processing window is reported to maintain crystalline registry with the sapphire substrate, without growing too thick and rough leading to disordered AlN films. Transmission electron microscopy interrogated the thickness, crystallinity, and stoichiometry via electron energy loss spectroscopy (EELS) of the aluminum oxynitride buffer layer. Improving AlN quality through the use of nitriding sapphire with CMOS compatible fabrication will enhance device performance and templating with other materials.

9:20am **PCSI-ThM-11 TiZrN-based Coatings for Dry Machining Deposited by Dual-beam EB-PVD**, *Glenn Cassar, Andre Giordimaina, Kieran Axisa*, University of Malta

TiZrN-based hard coatings are attractive candidates for dry machining applications, but their deposition via electron-beam physical vapor deposition is typically limited by markedly different evaporation rates between Ti and Zr. In this study, TiZrN-based coatings were developed on AISI H13 (DIN 1.2344) steel substrates using a plasma-assisted dual-beam EB-PVD process. Such coatings were investigated for the long-term objective of enabling multifunctional Ti-Zr coating systems, such as TiZrCrN, but initial trials showed preferential Ti evaporation from the melt pool,

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generating a Ti-rich vapor flux and restricting Zr incorporation. To avoid Zr-depleted coatings, Ti-Zr targets with varied Ti:Zr ratios were investigated to compensate for the differential evaporation and to achieve compositionally controlled TiZrN-based coatings. The deposited coatings were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX) nanoindentation and pin-on-disk tribology, with emphasis on the correlation between composition, microstructure, mechanical properties, and wear behavior relevant to dry-machining conditions. By treating source chemistry as an active process-control variable, the study aims at providing an EB route towards compositionally controlled TiZrN-based coatings for lubricant-free machining.

11:00am **PCSI-ThM-31 Closing Remarks**

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