Nanoscale Science and Technology
Room 206 A W - Session NS2-MoM

Advanced Nanomaterial for Quantum and Energy Applications

Moderators: Alex Belianinov, Sandia National Laboratory, **Wonhee Ko**, University of Tennessee, Knoxville

10:30am **NS2-MoM-10 Fabricating Color Centers using Liquid Metal Alloy Ion Source Focused Ion Beams*, Michael Titze,*** Sandia National Laboratories **INVITED**

Color centers are interesting candidates for transmitting quantum information. However, experiments using color centers are hindered by the difficulty of fabricating color centers deterministically. Liquid metal alloy ion source based focused ion beams (FIBs) hold the potential to deterministically fabricate color centers at scale. Often the challenge lies in having a source material that contains the ion of interest to form the color center of relevance. Example challenges include lack of wetting the filament material, evaporation of the element of interest, formation of hard to break oxides, and too little or too high viscosity of the source material, leading to a lack of formation of an emitting Taylor cone. In this talk we will discuss our current efforts in realizing a Na and Pb source. We will discuss the use of a AuSi eutectic where Na is added as an impurity that shows Na is outgassing during source fabrication. We will also present current results using a eutectic NaPb alloy, including the observation of evaporation of the source material when using standard source fabrication recipes, highlighting the need for in-situ thermometry. We will also present our work on fabricating quantum devices utilizing FIB created tin-vacancy centers in diamond and silicon vacancies in SiC showing how FIB enables the required targeting resolution for integration of color centers with quantum devices once a suitable source is fabricated.

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.

11:00am **NS2-MoM-12 Atomic-scale Vibrational Excitations at Amorphous/Crystalline Interfaces*, Kory Burns*[1]**, University of Virginia, USA*; Nooreen Qureshi,* University of Virginia*; Tymofil Pieshkov, Pulickel Ajayan,* Rice University*; Jordan Hachtel,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Isotopically pure amorphous Boron Nitride has an extremely low nuclear cross-section (inhibiting the absorption of thermal neutrons), high thermal stability, good measurement precision, and robustness to external perturbations; making it an ideal candidate for next-generation quantum sensors. Some of the most prominent issues in understanding thermal transport in candidate materials is the difficulty in fabricating dissimilar interfaces at scale and accurately characterizing their properties. In this presentation, amorphous BN is deposited on 3 different substrates by pulsed laser deposition. Next, an aberration-corrected scanning transmission electron microscope (STEM) with a monochromator on the electron energy loss spectrometer (EELS) is used to measure phonon modes at atomic resolution at the interface between the BN film and the substrate. The epitaxial strain between BN and the substrate is measured using off axis EELS, where the bright field disc is displaced in q-space relative to the EELS aperture to collect electrons that scatter at high angles. This ensure that electrons that scatter off the nucleus are interpreted in the EEL spectrum, and not ones that scatter of the material's electron cloud. This approach ensures that we can measure a localized response from individual atoms by suppressing long-range excitations from the dielectric environment. Accordingly, we reimagine the process used to calculate the localized phonon transport at interfaces and enhance the selection criteria of thin films and substrates for quantum sensing applications. Ultimately, this work reinforces the need to study the structure-property relationship of amorphous solids and discusses their implication in novel applications, including quantum sensors and radiation-hard electronics.

11:15am **NS2-MoM-13 Revealing Quantum Functionality of Topological Thin Films by *in situ* Characterization with Materials Cluster System*, Wonhee Ko,*** University of Tennessee, Knoxville

Achieving unique quantum functionality from the nanostructures is a key to realizing novel electronic and quantum devices. Thin films of quantum materials are a promising candidate, but the quantum states in these films are highly fragile to the ambient condition and require *in situ* growth and characterization techniques. We build materials cluster system that combines *in situ* epitaxial film growth and characterization instruments, such as molecular beam epitaxy (MBE), pulsed laser deposition (PLD), angle-resolved photoemission spectroscopy (ARPES), and scanning tunneling microscopy (STM). With the materials cluster system, we grew thin films of topological insulators and observed lattice and electronic structures in atomic scale. Interestingly, we found that the step edges possess Rashba edge states with unique spin texture, which interacts with topological surface states depending on the film thickness. Moreover, the strength of Rashba interaction was tunable by functionalizing step edges with selenium atoms. The results demonstrate that the unique quantum functionality can be exhibited by materials cluster system, which will become a foundational system to realize quantum devices with these films.

11:30am **NS2-MoM-14 Atomically Precise vertical Tunnel Field Effect Transistor (vTFET) for 10X Microelectronics Energy Efficiency in a General Purpose Transistor***, Desiree Salazar,* Energetics Inc.*; **Shashank Misra,*** Sandia National Laboratories, USA

Atomically Precise vertical Tunnel Field Effect Transistor (vTFET) for 10X Microelectronics Energy Efficiency in a General Purpose Transistor.Desiree Salazar, S. Misra, Emilie Lozier and T. Kaarsberg

The United States Department of Energy (DOE) Advanced Materials and Manufacturing Technology Office (AMMTO) is leading a multi-organization effort to counter alarming trends in U.S. computing energy use (e.g. **LBNL 2024 [https://usdoe-my.sharepoint.com/personal/tina_kaarsberg_ee_doe_gov/Documents/lbnl-2024-united-states-data-center-energy-usage-report.pdf]** forecasts that data centers will account for 26% of US electricity use by 2028 when cryptocoin mining is included) with its initiative in energy efficiency scaling for two decades (EES2) for microelectronics. Under this initiative, DOE/AMMTO has funded a portfolio of EES2 device technology R&D projects that promise >10X energy efficiency increase by 2030. This paper will highlight the first of these projects with Sandia National Laboratories to build on atomically precise manufacturing techniques to create a vertical tunnel field effect transistor (vTFET). Updates will be provided on the successful integration of front end of line (FEOL), back end of line (BEOL) and mid-! (MEOL) manufacturing processes (especially thermal budget) to fabricate this vTFET in a CMOS compatible process. One important discovery of the research in this area is "ultradoping" which makes the abrupt doping profiles needed for efficient vTFETs far more manufacturable. This talk also will present how these Sandia results integrate with version 1.0b of the EES2 roadmap that will be issued in Summer 2025. Version 1.0a of the Roadmap is available at EES2 Roadmap Version 1.0 [https://eere-exchange.energy.gov/FileContent.aspx?FileID=f4234e29-cc0c-4a56-a510-86b616ab5535] .

11:45am **NS2-MoM-15 Microwave-Assisted Direct Upcycling of Lithium Ion Battery Cathodes*, Clare Davis-Wheeler Chin,*** Sandia National Laboratories*; Kirsten Jones,* University of New Orleans*; Boyoung Song, Bryan Wygant, Anastasia Ilgen,* Sandia National Laboratories*; Candace Chan,* Arizona State University*; C.J. Pearce,* Sandia National Laboratories*; Winson Kuo, John Watt,* Los Alamos National Laboratory*; John B. Wiley,* University of New Orleans*; Kevin Leung,* Sandia National Laboratories

Rapid market growth of lithium ion-batteries (LIB) for electric vehicles has generated critical materials and sustainability challenges. LIB cathodes require cobalt, which is costly and primarily mined in conflict regions. In response, recent efforts focus on developing efficient, scalable methods for recycling spent LIB cathode materials. Here we report a direct-upcycling approach that exploits microwave (MW) heating for exfoliating layered cathode oxides $LiCoO_2$ (LCO) and $LiNi_xMn_yCo_zO_2$ (NMC) into nanosheets (NSs), which facilitates manipulation of Co:Ni:Mn stoichiometry and reassembly into functioning cathode materials. MW irradiation interacts directly with reaction species to promote heterogeneous heat distribution and instantaneous localized superheating, accelerating exfoliation rates and increasing conversion from bulk oxides to NSs. Our "one-pot" MW method decreases exfoliation time from 2 days (leading-edge electrochemical method) to 2 hours and is easily scaled to generate multi-gram yields. High-

[1] **JVST Highlighted Talk**

resolution transmission electron microscopy (HR-TEM) of MW-exfoliated LCO and NMC indicates conversion into mono- and bilayer NSs with yields >99%. LCO NSs also show increased catalytic activity over starting materials, indicating expanded use cases for recycled materials. The results of this work help establish a fundamental science foundation for sustainable scale-up and securing the LIB supply chain, which is a DOE priority.

Funding Statement

This work is funded by the Laboratory Directed Research and Development Program, project number 229371, at Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under Contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the document do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

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Author Index

Bold page numbers indicate presenter