# Thursday Evening, September 25, 2025

## Nanoscale Science and Technology Room Ballroom BC - Session NS-ThP

### Nanoscale Science and Technology Poster Session

### NS-ThP-1 Single and Dual Sintering Techniques on Flexible Metal Nanoparticle Patterns, *Md. Mahfujur Rahman*, *Rajib Chowdhury, Seonhee Jang*, University of Louisiana

The application of metallic nanoparticle (NP) inks has become the center of developing flexible printed electronic devices such as solar cells, displays, wearables, and sensors. The approach of defining the mechanical, electrical, and material properties of printed patterns depends on the type of metallic NPs. The most utilized NPs are silver (Ag), gold (Au), and copper (Cu). Ag NPs are highly considered for their excellent electrical conductivity and resistance to oxidation. On the other hand, Cu NPs are highly preferred because of their affordability to Ag NPs, yet they are highly prone to oxidation. During printing of metallic NP inks for conductive patterns, a lack of electrical conductivity in the patterns is observed because of induced organic additives and stabilizing agents. Consequently, sintering is essential for removing these organic residues and enhancing the conductivity of the printed patterns.

This study focuses on utilizing two metallic inks of Ag NP ink (PSI-211, NovaCentrix) and Cu NP ink (CP-008, NovaCentrix) to fabricate the conductive patterns on flexible polyimide (PI) sheets. Either single or dual sintering processes were conducted to optimize the electrical conductivity. For the single sintering process, the printed metal NP patterns were subjected to either laser irradiation (LO) or thermal treatment (TO). During the LO sintering process, the Ag and Cu NPs underwent Nd:YAG laser irradiation at 600 and 800 mJ for 15 and 30 s, respectively. For the TO sintering process, Ag and Cu NPs were introduced in a formic acid (FA) vapor environment at 140 and 260 °C for 1.5 and 15 min, respectively. The dual sintering method involved thermal treatment followed by laser irradiation (TL) and laser irradiation followed by thermal treatment (LT).

After sintering, a microstructural analysis was conducted using scanning electron microscopy. The analysis confirmed that the LT condition for sintering of the Ag NP pattern showed improved particle agglomeration and necking. Atomic force microscopy (AFM) analysis revealed the highest roughness of 48 nm, indicating superior grain growth. With a resistance ratio ( $R/R_0$ ) of 1.75 during the folding test, the Ag NP pattern sintered using the LT condition showed the lowest electrical sheet resistance. Through agglomeration and coalescence during sintering, the Cu NP pattern sintered with the TO condition displayed the most uniform grain growth. The Cu NP pattern sintered under the TO condition had the highest mechanical Vickers hardness of 55.36 N/mm<sup>2</sup> because of the improved connection between the NPs. Additionally, the Cu NP pattern showed the highest roughness value of 51.36 nm.

### NS-ThP-2 Impacts of Hydrogen Adsorption on Carbon Nanotube–Metal Schottky Contacts, Chuntian Huang, Nini Ye, Haijun Luo, Hezhu Shao, Changkun Dong, Wenzhou University, China

Carbon nanotube (CNT)-metal Schottky contacts are widely employed in different types of electronic devices, including field effect transistors (FET) and gas sensors. CNTs are normally considered stable on electronic properties with gas adsorptions. In this work, performance changes of the multi-walled carbon nanotube (MWCNT)-metal junctions related to hydrogen adsorptions were illustrated. MWCNT/Pd and MWCNT/Au Schottky junctions based resistive sensors were constructed to investigate the low-pressure gas sensing performances for hydrogen in the range of 1e–7 to 1e–3 Pa. Two types of sensors presented opposite behaviors with hydrogen adsorptions, i.e., the sensor resistance rose for the MWCNT/Pd sensor but dropped for the MWCNT/Au sensor with increasing hydrogen pressure. The work function reductions of Pd and CNT are considered the key cause, which could change the Schottky barrier properties dramatically.

Such effects were investigated by the first-principles calculations. The work functions of Pd and MWCNT tend to decrease with the dissociated hydrogen adsorptions, while the electronic properties of Au remain constant. The work function of the Pd-CNT Schottky junction drops with hydrogen adsorptions on either CNT or Pd according to the analysis of the density of states (DOS) and charge density difference. It is expected that electrons transfer from Pd of lower work function to CNT after the H adsorption, leading to the resistance increase of the Schottky junction for the p-type MWCNTs. On the other side, the resistance of the Au-CNT Schottky junction would decrease for the electron transformation from CNT

to Au. The results are consistent with the experimental investigation and provide important reference significance for applications of metal-CNT junctions.

NS-ThP-3 The Nanoscale Materials Characterization Facility (NMCF) at the University of Virginia, *Catherine Dukes*, Diane Dickie, Graham Frazier, Helge Heinrich, Art Lichtenberger, Joe Thompson, Richard White, University of Virginia

The Nanoscale Materials Characterization Facility and Innovations in Fabrication clean-room microfabrication/biomanufacturing facility are advanced user facilities within UVa's School of Engineering and Applied Science. Our instruments are available for researchers from academic and industrial institutions on a pay-for-time basis. We provide comprehensive services in materials preparation and processing, as well as a suite of advanced analytical techniques. Researchers are welcome to (1) visit the NMCF for collaborative sample science or (2) send specimens for remote analyses by one of five expert instrument scientists, ensuring personalized guidance and optimized results.

We operate two transmission electron microscopes: a 200kV Talos system and a 300 kV Themis with probe correction for sub-Å resolution and monochromated EELS. Both offer EDS for compositional analysis and mapping, as well as sample holders for in-situ cooling, heating, biasing, liquid-cell and gas-cell experiments. A Helios dual-beam FIB-SEM is used for surface, cross-sectional, and 3D imaging, EDS analysis, orientation mapping with electron-backscatter diffraction and TEM sample preparation. Additionally, two standalone scanning electron microscopes are available: a Quanta 650 FE-SEM with EDS and EBSD, and a Phenom XLG2 environmental SEM for electron imaging and EDS.

Four X-ray powder diffraction systems are available for analyzing bulk composition and phase orientation, with specialized stages for in situ heating and X-ray reflectivity. An X-ray fluorescence spectrometer provides highly sensitive elemental analysis for Z > 10. The facility also features an integrated Renishaw Raman spectrometer/Bruker AFM system for molecular identification, surface chemistry, and nano-scale topography, along with a Invenio-S FTIR for chemical fingerprinting and organic material identification.

For quantitative surface composition and chemistry, two X-ray photoelectron spectrometers are available: a Versaprobe III small-spot instrument with ion gun for depth profiling, hot-cold stage, and processing chamber; and a HiPP-Lab ambient-pressure XPS with *in-situ* high-temp liquid cell, plasma processing, glove box, sample prep chamber and gas reaction cell. Optical instrumentation includes a white-light profilometer for surface metrology, and a digital light microscope for 2D/3D imaging and videography.

A complete suite of metallurgical equipment for cutting, mounting, polishing, sputter coating, etching, and plasma cleaning, as well as Rockwell and Vickers hardness testing, is also available.

Contact: https://engineering.virginia.edu/NMCF

#### NS-ThP-4 Exciton-Polariton Devices from Two-Dimensional Chalcogenide Semiconductors, Deep Jariwala, University of Pennsylvania

The isolation of stable atomically thin two-dimensional (2D) materials on arbitrary substrates has led to a revolution in solid state physics and semiconductor device research over the past decade. A variety of other 2D materials (including semiconductors) with varying properties have been isolated raising the prospects for devices assembled by van der Waals forces. Particularly, these van der Waals bonded semiconductors exhibit strong excitonic resonances and large optical dielectric constants as compared to bulk 3D semiconductors..

First, I will focus on the subject of strong light-matter coupling in excitonic 2D semiconductors, namely chalcogenides of Mo and W. Visible spectrum band-gaps with strong excitonic absorption makes transition metal dichalcogenides (TMDCs) of molybdenum and tungsten as attractive candidates for investigating strong light-matter interaction formation of hybrid states. We will present our recent work on the light trapping in multi-layer TMDCs when coupled to reflective substrates. Next, I will show the extension of these results to superlattices of excitonic chalcogenides, multilayer halide perovskites as well as metal organic chalcogenides. These hybrid multilayers and materials offer a unique opportunity to tailor the light-dispersion in the strong to ultra-strong coupling regime. Finally, if time permits, I will discuss the physics of strong light-matter coupling and it's applications in phase modulator devices, photovoltaic devices as well as control of light in magnetic semiconductors.

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NS-ThP-5 Scalable Photonics with Low-Dimensional Superlattices, Jason Lynch, Deep Jariwala, University of Pennsylvania

Superlattices of III-V semiconductors have long been used in state-of-theart photodetectors, light emitting diodes, and lasers while plasmonic superlattices promise to surpass the diffraction limit of light and confine light on the nanometer scale. However, both cases typically use threedimensional media which do not leverage the advantages of improved electro-optical properties, flexibility, and stability found in low-dimensional media. Recent research has demonstrated superlattices with monolayer semiconductors, but they normally use exfoliated flakes which limit their lateral areas to several square microns. As the growth of large-area, lowdimensional materials becomes more common, integrating lowdimensional media into superlattices promises to improve the performance of commercially available photonic devices. In this poster, we highlight two of our recent works that use 2D layers to improve the tunability and stability of centimeter-scale superlattices. First, we stack monolayer transition metal dichalcogenides (TMDCs) into a superlattice to increase the light-matter interaction strength without sacrificing their ideal monolayer properties. By electrostatically doping the TMDC layers, the system is actively modulated between the strong and weak coupling regime of exciton-polaritons which drastically alters reflected light. Using spectroscopic ellipsometry, the TMDC superlattice is observed to produce a full  $2\pi$  phase shift in the reflected light. Second, we improve the thermal stability in a TiN-dielectric hyperbolic superlattice by replacing the threedimensional  $AI_2O_3$  with two-dimensional hBN. The new mixed-dimensional interface prevents atoms from diffusing across the TiN-hBN interface. This results in the superlattice maintaining its stratified geometry upon annealing at high temperatures (800 °C) for at least 10 hours. Both works study centimeter-scale superlattices whose fabrication techniques (wettransfer and sputtering) can be implemented commercially. Therefore, our work promises to bring the improved qualities of low-dimensional media to practical, large-area photonic systems.

### NS-ThP-6 Optical Readout Approaches for Photonic Thermometry, Kevin Douglass, Michal Chojnacky, Thinh Bui, CH S S PAVAN Kumar, Nikolai Klimov, National Institute of Standards & Technology

NIST is developing a fully packaged photonic-based temperature sensor with the aim of replacing resistance-based thermometry.One of the major deliverables of our photonic thermometry project is creating readout methodologies tailored to the measurement need from highest accuracy metrology applications to real world temperature sensing with fit-forpurpose accuracy in a robust deployable system.Over the past year we have developed and tested various photonic readout strategies to achieve these various goals. These approaches will be described in detail with supporting data to compare their respective advantages and disadvantages.

### NS-ThP-7 A Comprehensive Investigation of Raman Laser-Induced Structural Modification in CVD-Grown Monolayer MoS<sub>2</sub>, Sieun Jang, Seonha Park, Songkil Kim, Pusan National University, Republic of Korea

Molybdenum disulfide (MoS<sub>2</sub>) has been extensively explored to be utilized as an electronic material in a variety of device applications. In particular, the tunability of MoS<sub>2</sub> enhances its electrical properties making it an intriguing candidate for field-effect transistors (FETs), while also extending beyond electrical properties to structural phase engineering. Raman laser irradiation offers a straightforward method to induce modifications via thermal processes without the intervention of other chemical substances. However, most studies on the modification of MoS<sub>2</sub> have focused on multilayered structures or have been conducted under low-power laser conditions, leaving the feasibility of phase transition in monolayer MoS<sub>2</sub> elusive. In this study, we fundamentally elucidated the effects of highpower Raman laser irradiation on the surface of chemical vapor deposition (CVD)-grown monolayer MoS<sub>2</sub> under ambient conditions and uncovered the underlying mechanisms of laser-induced modifications by applying intense photon energy with highly interactive reactions. Our results revealed both etching and deposition phenomena in two discernible regions, and it can be demonstrated by intensity threshold based on the spatial distribution of laser irradiance within the laser spot. Furthermore, phase transition was found to be inhibited due to the promoted oxidation and the deposition of hydrogenated amorphous carbon, and p-type doping was observed, likely occurring in the region beneath the hydrogenated amorphous carbon deposition as substitutional doping on the 2H phase of MoS<sub>2</sub>. To compare the thermal effects, MoS<sub>2</sub> modifications were further analyzed using simplified heat transfer estimations. These findings deepen our understanding of how Raman laser irradiation modifies MoS<sub>2</sub> under ambient conditions, providing guidelines for optimizing its modification processes.

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