

2D Materials

Room A215 - Session 2D-FrM

2D Late News Session

Moderators: Daniel Gunlycke, U.S. Naval Research Laboratory, Ivan Oleynik, University of South Florida

10:40am **2D-FrM8 Mechanistic Insights into a Modified ALD Process to Achieve Crystalline MoS₂ Thin Films**, *Nathaniel Richey, L. Zeng, M. Yasheng, J. Shi, I. Oh, S.F. Bent*, Stanford University

Stimulated by the discovery of two-dimensional (2D) graphene, 2D transition metal chalcogenides (TMDs) are attracting much attention owing to their similar layered structure and graphene-analogous properties. Numerous research efforts are under way to explore their potential applications, such as optoelectronics, electrochemical cells, and energy harvesting devices. However, challenges remain in the development of controllable growth methods for TMDs with large-scale conformality at moderate growth temperatures. There has been an increasing trend toward resolving these issues by employing atomic layer deposition (ALD) due to its promise of layer-by-layer growth.

Despite the promise brought by ALD, further effort is needed as the TMD films grown using low temperature ALD often show non-ideal stoichiometry and require high-temperature post-annealing to improve the film quality. As an example, the known ALD processes that use Mo(CO)₆ and H₂S as the precursors have shown an ALD window of 150 ~ 175 °C. However, results from both literature and our laboratory show that the S-to-Mo ratio is close to 1.5:1, relatively far from the ideal value of 2:1, with the presence of undesired MoO_x species. We performed an investigation into the mechanisms of this ALD process. Based on understanding that ligand loss is a rate limiting step in the ALD process, a new methodology was developed that produces higher-quality MoS₂ films from these same precursors. These results were achieved by using a slightly elevated growth temperature and enhancing the chemical vapor deposition component of Mo(CO)₆ for better CO removal. A series of MoS₂ films were synthesized on Si substrates by this modified process, resulting in controllable linear growth behavior, a S-to-Mo ratio of 2:1, and strong characteristic MoS₂ Raman peaks. Additional characterization tools, including grazing incident X-ray diffraction (GIXRD), X-ray reflectivity (XRR) and atomic force microscopy (AFM), were also used to examine the film crystallinity, density, and surface morphology. By characterizing the material as a function of process conditions, we are able to elucidate fundamental mechanisms and key kinetic factors behind the MoS₂ growth process using Mo(CO)₆ and H₂S. This study may help shed some light on future design of ALD processes for 2D TMDs.

11:00am **2D-FrM9 The Electronic Properties of Quasi-One-Dimensional TiS₃ and ZrS₃**, *Simeon Gilbert*, University of Nebraska-Lincoln; *H. Yi*, Synchrotron SOLEIL; *A. Lipatov, T. Komesu*, University of Nebraska-Lincoln; *A.J. Yost*, Oklahoma State University; *A. Sinitskii*, University of Nebraska-Lincoln; *J. Avila*, Synchrotron SOLEIL, France; *M.C. Asensio*, Madrid Institute of Materials Science; *P.A. Dowben*, University of Nebraska-Lincoln

The transition metal trichalcogenides (TMTs) are an emerging class of 2D materials in which 2D sheets are formed by the van der Waals-like bonding of quasi-1D chains. Here we present our work on the electronic properties of two TMTs, TiS₃ and ZrS₃, including the experimental band structure from nanospot angle resolved photoemission spectroscopy (nanoARPES). The band structures of both TMTs exhibit strong in-plane anisotropy due to their quasi-1D structure. The extracted effective hole mass for both materials is doubled along the chain direction, giving rise to a preferential charge transport direction. Additionally, high resolution nanoARPES measurements show a spin-orbit coupling splitting at the top of the valence band in TiS₃. This spin-orbit coupling splitting is expected to increase for heavier TMTs such as ZrS₃. We also show that metals such as Au and Pt can form Ohmic contacts with TMTs rather than Schottky barriers using X-ray photoemission spectroscopy at the metal-semiconductor interface. Other advantages of TMTs include clean edge termination, band gaps of ~1eV and high predicted electron mobilities. Combined with their anisotropic electron transport, strong spin-orbit coupling and Ohmic contacts, these advantages make the TMTs strong candidates for use in nanoscale electronics, optoelectronics and spintronics.

11:40am **2D-FrM11 Definition of CVD Graphene Micro Ribbons with Lithography and Oxygen Plasma Ashing**, *Fernando Cesar Rufino, A.M. Pascon*, UNICAMP, Brazil; *D.R.G. Larrudé*, Mackenzie Presbyterian University, Brazil; *L. Espindola, F.H. Cioldin, J.A. Diniz*, UNICAMP, Brazil

The excellent physical properties of graphene [1], such as transport (high electron mobility 250000 cm²/Vs), elasticity (in the order of TPa) and mechanical strength (in the order of GPa), make this 2D material a strong candidate in electronic devices development, especially in the area of radiofrequency and applications in sensors. In researches related to electronic devices, graphene can be a great ally in the development and miniaturization of Field Effect Transistors, FET. Concerns related to the miniaturization process are the equipment and the materials necessary to achieve this objective, since the repeatability and the cost of the manufacturing process are two essential variables to ensure the viability of the proposed project.

In this work, we present the union of conventional techniques in the fabrication of microdevices and the application of graphene obtained by chemical vapor deposition (CVD), in the development of Field Effect Transistors based on Graphene, GFET [2]. In the fabricated GFETs, the conduction channel is formed by parallel micro ribbons of graphene, with the smallest dimension of 250 nm of width. This dimension was obtained by Photolithography and oxygen plasma ashing. Through these two techniques we can ensure the repeatability of the fabrication process and these are low cost techniques when compared to what is commonly found in the literature, which is the definition of graphene patterns by Electron Beam Lithography (high cost and low repeatability technique). In addition, the characteristics of good quality graphene remain at the end of the fabrication process, as proven by Raman spectroscopy.

The GFETs were fabricated on two different substrates. One on Si/SiO₂ and another on glass. In both materials, the same structures with the same parameters were fabricated and were able to reach dimensions in the order of 360 nm, for comparisons we used Atomic Force Microscope (AFM) to verify the roughness and Scanning Electronics Microscope (SEM) for detection and measurement of the structures. The graphene used in the fabrication of the devices was the last material to be transferred to the sample by fishing and using PMMA [3], ensuring the least possible handling of the material and therefore possible contaminations.

References:

- [1] K. S. Novoselov et al, *Science* **306**, 666 (2004).
- [2] F. C. Rufino et al, *SBMicro* 2018.
- [3] L. Jiao et al., *Am. Chem. Soc.*, 12612 (2008).

12:00pm **2D-FrM12 Reactivity of Metal Contacts with Monolayer Tungsten Disulfide**, *Ama Agyapong, K.A. Cooley, S.E. Mohny*, The Pennsylvania State University

Using two-dimensional transition metal dichalcogenides (TMD) for electronics, optoelectronics, and catalysis often requires integration with a metal, motivating fundamental studies of metal-TMD interactions. We previously published predictions on the reactivity of metals with tungsten disulfide based on thermodynamics. [1] Our current work employs an easy approach to test these predictions on reactivity of metal contacts with monolayer (1L) WS₂ using Raman spectroscopy performed through the backside of the contact. Au, Cu, Pd, Al, and Ti were deposited by electron beam evaporation onto 1L WS₂ grown on a sapphire substrate and capped with a thin film of silica to avoid agglomeration of the metal during annealing. Samples were annealed at 100, 200, and 300 °C under Ar for 1 hour. The results from Raman spectroscopy are in excellent agreement with the predictions from thermodynamics. Au, Cu, and Pd did not react with 1L WS₂ upon deposition or annealing. Reaction of Al with 1L WS₂ occurred upon annealing, while Ti reacted upon deposition, as indicated by loss of the characteristic peaks in the Raman spectrum for WS₂. We will also describe interesting changes in the Raman spectrum for WS₂ from Au/WS₂ samples and present transmission electron microscopy of these samples.

[1] Yitian Zeng, Anna C. Domask, Suzanne E. Mohny, Condensed phase diagrams for the metal-W-S systems and their relevance for contacts to WS₂, *Materials Science and Engineering: B*, Volume 212, October 2016, Pages 78- 88: <http://dx.doi.org/10.1016/j.mseb.2016.07.005>.

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