Nanostructure Synthesis and Fabrication
Room Evergreen Ballroom & Foyer - Session NS-TuP

Nanostructures Synthesis and Fabrication Poster Session

NS-TuP-1 Molybdenum Disulfides and Diselenides by Atomic Layer Deposition*, **Raul Zazpe**, J Prikryl, M Krbal, J Charvot, F Dvorak, F Bures, J Macak,* University of Pardubice, Czech Republic

The discovery and success of graphene paved the way for developing two-dimensional materials with outstanding properties [1]. In particular, monolayers of two-dimensional transition metal dichalcogenides (2D TMDCs) possess a direct band gap [2] that is crucial for optoelectronic applications. Additionally, the direct band gap can be easily tuned by either chemical composition or external stimuli. In parallel to monolayer TMDCs structures, a high surface area layer of TMDCs flakes shows promising properties for hydrogen evolution [3], photodegradation of organic dyes [4] or as electrodes in Li ion batteries [5].

To date, various top-down (e.g. exfoliation) and bottom-up techniques, such as chemical vapor deposition (CVD) and atomic layer deposition (ALD) have been reported for the preparation of 2D-TMDCs [1]. However, ALD is the only technique enabling sub-nanometer thickness control, which is revealed as a crucial factor in the properties of 2D TMCDs materials. In the last years, it has been reported the possibility to employ ALD as a technique to grow MoS_2, which has been extensively studied for many different applications. In these works $(CH_3)_2S_2$ [6] or H_2S [7, 8] were used as the S precursor and $Mo(CO)_6$ [6], $MoCl_5$ [7] or $Mo(thd)_3$ [8] as the Mo precursors. Further, important efforts have also been devoted to attain the ALD fabrication of $MoSe_2$, since it possesses higher electrical conductivity than MoS_2 [9, 10]. Recently, we have shown that ALD deposition of $MoSe_2$ [11] or Mo-O-Se [12] is feasible using $(CH_3)_2S_2$ as the Se precursor and the $MoCl_5$ or $Mo(CO)_6$, respectively, as the Mo precursors.

The presentation will focus on the synthesis of MoS_2 and $MoSe_2$ by ALD, their characterization and applications in various fields. Experimental details and some recent photocatalytic, battery and hydrogen evolution results will be presented and discussed.

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NS-TuP-2 Wafer-scale MoS_2 Thin Film Deposition via H_2S Plasma Sulfurization of ALD-grown MoO_3 at Low Temperature*, J Ahn, **Jeong-Hun Choi**,* Korea Maritime and Ocean University, Republic of Korea

Molybdenum disulfide has attracted great interest due to its outstanding mechanical, electrical and optical properties. These unique properties make MoS_2 investigated as a promising candidate material for opto-electronic, sensing and catalysis applications. MoS_2 thin films have been achieved by a variety of methods such as sputtering and chemical vapor deposition. Nevertheless, these methods are limited to controlling the number of layer and uniformity over wafer scale. The most crucial problem of these methods is that they demand high growth temperature or additional heat treatment. High temperature process hinders the application of MoS_2 to a wide range such as flexible and transparent devices. In this work, MoS_2 thin films were deposited by H_2S plasma sulfurization of ALD-grown MoO_3 thin films. While ALD-grown MoO_3 provided precise thickness control and uniformity, H_2S plasma process effectively sulfurized MoO_3 into MoS_2 at low temperature. The sulfurization behavior and physical quality of MoS_2 thin films were investigated under various plasma conditions. The film thickness was measured by ellipsometry and Raman analysis. X-ray photoelectron spectroscopy was carried out to analyze the chemical composition of MoO_3 and MoS_2 thin films. The crystallization behavior of the films was characterized by X-ray diffraction. Furthermore, the potential of MoS_2 for electric device component was investigated.

NS-TuP-3 ALD-based Synthesis of Few-layer Transition Metal Disulfides with Wafer-scale Uniformity for Device Integration*, **Tao Chen**, Y Wang, H Zhu, L Chen, Q Sun, D Zhang,* Fudan University, China

Different transition metal disulfides (TMDs) ultra-thin films with wafer-scale uniformity have been successfully synthesized by ALD-based process. Two growth routes have been developed: sulfurizing transition metal oxides deposited by ALD, and annealing amorphous TMD films deposited by ALD. Molybdenum hexacarbonyl and ozone were used as precursors to deposit MoO_3 film by plasma enhanced ALD followed by sulfurization in a tube furnace to form MoS_2 TMD films. Tungsten hexachloride and hexamethyldisilathiane (HMDST) were used as ALD precursors to deposit WS_2 films which were further annealed at high temperature to improve crystallinity. Both approaches can produce high-quality and thickness-controllable TMD films with wafer-scale uniformity, which have been confirmed by AFM, XPS, Raman and TEM characterizations. Field-effect transistor (FET) device arrays have been further fabricated based on both films showing excellent homogeneous and reproducible electrical performance. The FET on/off ratio was about ~10^4 with decent mobility over 10 $cm^2V^{-1}s^{-1}$. These experimental results demonstrated attractive and promising potentials of the novel two-dimensional TMD films in future micro-/nanoelectronics device integrations and applications by using ALD-based techniques.

NS-TuP-4 Overcoming Agglomeration and Adhesion in Particle ALD*, **Benjamin Greenberg**, J Wollmershauser, B Feigelson,* U.S. Naval Research Laboratory

The fundamental challenge of particle ALD (pALD) is that small particles are sticky. Nanoparticles (NPs) in particular are highly susceptible to van der Waals, dipole-dipole, electrostatic, and chemical forces. When NPs are fluidized or agitated to expose their surfaces to ALD precursors, these forces can cause persistent agglomeration and adhesion to reactor surfaces, preventing conformal coating and reducing core-shell NP yield. To understand and overcome these obstacles, we examine NPs coated in a reactor with two agitation modes, rotation and vibration. We analyze high-speed videos of NP motion while varying agitation parameters (velocity, frequency, timing) as well as NP material and size. After pALD, we weigh the coated powders and study core-shell NP composition and morphology via TEM and N2 adsorption measurements.

NS-TuP-5 Density Function Theory for Nucleation of MoF_6 with Oxide Surfaces in Atomic Layer Deposition of MoS_2*, **Matthew Lawson**,* Boise State University

Several two-dimensional (2D) atomic-layered transition metal dichalcogenides (TMDs) are of great interest for electronic and optoelectronic applications due to their wide direct band gaps for few layer materials. Beyond mechanical or liquid exfoliation of bulk materials, high quality 2D TMDs have been grown via chemical vapor deposition (CVD) but growth is typically performed at high temperatures. Several studies have reported atomic layer deposition (ALD) of thin TMD films at lower temperatures, but as-deposited films are typically amorphous our nano-crystalline. Complementary to *in-situ* experimental studies of the growth and nucleation of nanoscale films, we have employed density functional theory (DFT) to understand the nuanced interactions during precursor nucleation. Hydroxyl groups are commonly found on metal oxide surfaces and play an important role during many ALD processes. To develop a deeper understanding of the ALD of MoS_2 from MoF_6 and H_2S, we studied the reactivity of MoF_6 with three substrates: Al_2O_3, MgO, and HfO_2 without hydroxyls and fully saturated with hydroxyls using DFT. We calculated the electronic distribution of the surfaces, how the electronic structures changed with single MoF_6 precursors, and calculated the valence electron transfer. Our calculations support the important role of hydroxyls in the nucleation of MoF6 with oxide surface and provide insight into the formation of precursor bonds at the surface.

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