



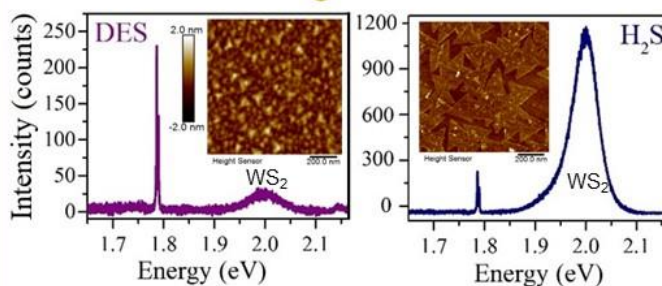
MIP: 2D Crystal Consortium
DMR-1539916, EFRI-1433378

Precursors for carbon-free transition metal dichalcogenide (TMD) films

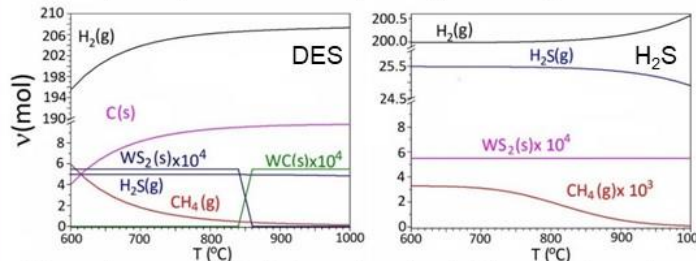
2018

Transition metal dichalcogenides (TMDs) such as WS_2 exhibit intriguing properties in monolayer form including direct bandgaps and large exciton binding energies. A major challenge in harnessing their potential is the uniform growth of high quality monolayers over large substrate areas. Metalorganic chemical vapor deposition (MOCVD) is a promising technique for TMD synthesis but the impact of precursor chemistry on TMD growth and properties is not well understood at present. In this work, the 2DCC-MIP team investigated the effect of the choice of chalcogen precursors in a cold-wall reactor geometry for the specific case of WS_2 . The investigation reveals that diethyl sulfide (DES) results in incorporation of carbon in the films, which can be correlated to a reduced lateral growth rate and quenching of photoluminescence from the WS_2 films compared to growth with hydrogen sulfide (H_2S). As a part of this investigation, thermodynamic modelling was also employed to understand the possible reaction outcomes. The calculations predict the formation of carbon when DES is used for growth consistent with the experimental observations. These results help in identifying promising precursors for the synthesis of high quality TMD films.

Diethyl sulfide (DES)  vs. Hydrogen sulfide (H_2S) 



DES leads to carbon incorporation which quenches the photoluminescence from WS_2 monolayers at ~ 1.98 eV compared to growth with H_2S .



The results are consistent with thermodynamic calculations predicting carbon formation with DES compared to H_2S .



What Has Been Achieved: The study investigated the growth of WS_2 films by MOCVD comparing the properties of monolayers grown with diethyl sulfide (DES) versus hydrogen sulfide. The results show considerable carbon incorporation in WS_2 when DES is used which prohibits lateral growth of domains and significantly reduces the photoluminescence intensity from the layers.

Importance of Achievement: Large scale growth of epitaxial TMDs is a major hurdle in the application of these novel materials. Large scale reliable growth by MOCVD requires understanding the effect of precursor chemistry on film properties. This work was directed at identifying the effect of using different sulfur-based precursors on the growth and properties of WS_2 .

Unique Features of the MIP That Enabled Project: The project utilized the chalcogenide MOCVD system in the 2DCC-MIP which is one of the few systems world-wide that is set up to use toxic hydride precursors such as H_2S .

Publications:

[T. H. Choudhury](#), [H. Simchi](#), [R. Boichot](#), [M. Chubarov](#), [S. E. Mohny](#), and [J. M. Redwing](#), "Chalcogen Precursor Effect on Cold-Wall Gas-Source Chemical Vapor Deposition Growth of WS_2 ", *Cryst. Growth Des.* 2018, 18, 8, 4357-4364