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# Atomic Structure of $W_{1-x}Mo_xS_2$ Alloys and Heterostructures

Danielle Reifsnyder Hickey[1], Saiphaneendra Bachu,[1] Mikhail Chubarov,[2] Joan M. Redwing,[1,2] and Nasim Alem[1,2]

[1.] Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA.
[2.] 2D Crystal Consortium, Materials Research Institute, The Pennsylvania State University, University Park, PA.

The introduction of dopants can offer a method to directly link the materials' properties at the atomic level to their macroscale electronic, thermal, and mechanical properties [1]. The resulting doped structures can be random or ordered, which can include the clustering of cations or the formation of ordered superstructures within a material, depending on the growth conditions [1,2]. Two-dimensional (2D) transition metal dichalcogenides (TMDs) are a particularly interesting system for the study of doped materials because the atomic positions can be directly imaged in projection by electron microscopy. Moreover, 2D TMDs are at the frontier of next-generation optoelectronics, which means that a thorough understanding of how to grow alloys and tune their properties can lead to exciting technological advances.

Previous observations of cation ordering in 2D $W_{1-x}Mo_xS_2$ [2] and the selective association of cations with specific anion defects within the crystal lattice [3] have motivated us to further explore the atomic structure of TMD alloy systems and how the precursor ratios and chalcogen fluctuations during growth can lead to dissimilar microstructures.

This work will present the resulting microstructures of $W_{1-x}Mo_xS_2$ grown under various conditions. $W_{1-x}Mo_xS_2$ growth was performed via metalorganic chemical vapor deposition (MOCVD) [4]. Films were transferred using a wet-chemical method [5] from a sapphire growth substrate onto TEM grids for analysis. High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) imaging was performed on an FEI Titan$^3$ G2 at an accelerating voltage of 80 kV. By varying the cation precursor ratios and creating sulfur concentration fluctuations during growth, we achieve new insights into the resulting microstructures and defects formed by this system. Using S/TEM imaging and spectroscopy, this work highlights (1) the effects of cation concentration on dopant distribution, (2) the changes in bond lengths and strain upon incorporation of various dopant concentrations, and (3) the observation of defects associated with various ternary structures. This investigation enables us to directly link the growth conditions to the resulting atomic structure and to further uncover the underlying physics and chemistry in the development of novel alloys with unprecedented macroscale electronic, thermal, and optoelectronic properties [6].

References:

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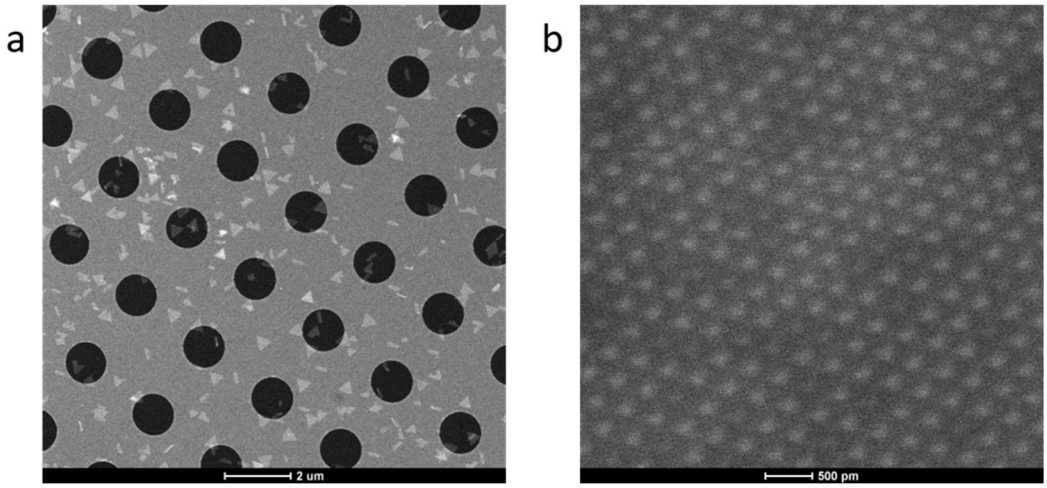


**Figure 1**. HAADF-STEM images of a multilayer $W_{1-x}Mo_xS_2$ alloy film on a Quantifoil TEM grid at (a) low and (b) high magnification.

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