

High Resolution S/TEM Study of Defects in MOCVD Grown Mono to Few Layer WS₂

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Two-dimensional (2D) Transition metal dichalcogenides (TMDCs) are interesting material systems for optoelectronic device applications due to their semiconducting behavior and their electronic structure transition from indirect to direct band gap upon thinning to a monolayer due to quantum confinement [1, 2]. While these materials systems have a strong potential to be incorporated in electronics and optoelectronics, the electronic properties of TMDs and thus their device performance strongly depends on the atomic structure of their defects (vacancies, dislocations and grain boundaries) [3].

To integrate the 2D TMDs into devices, it is also essential to synthesize them on large scale with uniform thickness. To date, majority of the devices made of 2D materials use exfoliated flakes rather than continuous films grown using controlled methods. Recently, monolayer WSe₂ films have been grown using metalorganic chemical vapor deposition (MOCVD) with both metal and chalcogen precursors outside the reaction chamber to allow accurate control of their ratios and flow rates [4]. In this paper, we extend that work to MOCVD grown WS₂ films and use high-resolution Scanning/Transmission Electron Microscopy (HR-S/TEM) to study the epitaxial nature and the resulting defect structure of the films. Figure 1a shows an optical image of the WS₂ film, removed from the sapphire growth substrate, covering the holey carbon quantifoil grid over a large area. The grown WS₂ is a coalesced monolayer film with triangles of few layer regions. A higher magnification TEM image and the corresponding diffraction pattern (DP) are presented in Figure 1b and 1c. The diffraction spots indicate the single orientation and thus the epitaxy of the grown film. Figure 1d is an Annular Dark Field STEM (ADF-STEM) image showing a grain boundary and the variation of number of layers on the top of one of those triangles. This presentation will further show the observed defect structures not only in single phase TMDs but also in the alloy TMD structures [5].

References:

- [1] Jariwala, Deep *et al*, ACS nano **8.2** (2014), p. 1102.
- [2] Zhao, Weijie *et al*, ACS nano **7.1** (2012), p. 791.
- [3] Zhou, Wu *et al*, Nano letters **13.6** (2013), p. 2615.
- [4] Zhang, Xiaotian *et al*, Nano letters (2018).
- [5] This work was supported by National Science Foundation CAREER AWARD (NSF CAREER grant #424-36 61X4).

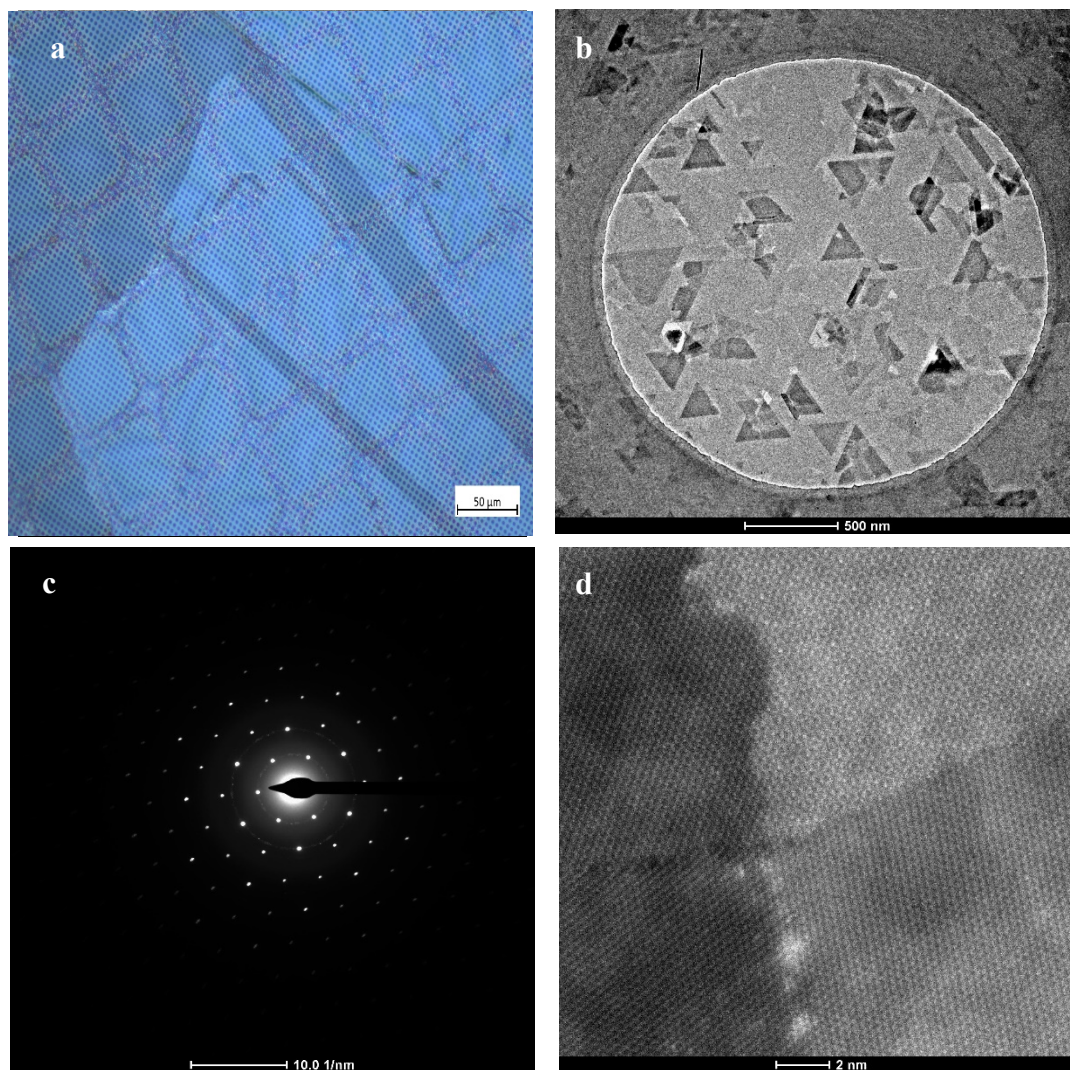


Figure 1 (a) Optical image of WS₂ film covering the holey carbon grid, (b) and (c) HR-TEM image and the corresponding diffraction pattern and (d) an ADF-STEM image of a grain boundary going through regions of film with varying thickness