

## Atomic Structure of Thin MoSe<sub>2</sub> Films Grown by Molecular Beam Epitaxy

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Two-dimensional (2D) layered materials such as transition metal dichalcogenides (TMDs) hold great promise for novel semiconductor device [1]. Due to the existence of energy gap, no out of plane dangling bonds and possibility of abrupt heterostructures at atomic scales, these materials are of interest for steep “turn on - turn off” tunneling transistors, using interband Zener-tunneling of electrons to beat the Boltzmann thermal limit of switching of 60 mV/decade. TMD materials are shown to exhibit novel properties such as indirect to direct bandgap transition when their thickness is about a monolayer, valley polarization, strain dependent bandgap variation, etc. These properties make TMD materials as a favorable choice for a wide range of micro- and optoelectronics applications. However, epitaxial growth of a few layer TMD materials with a high quality is a challenging technological task. Here we report the electron microscopy analysis of thin MoSe<sub>2</sub> films grown by Molecular Beam Epitaxy (MBE).

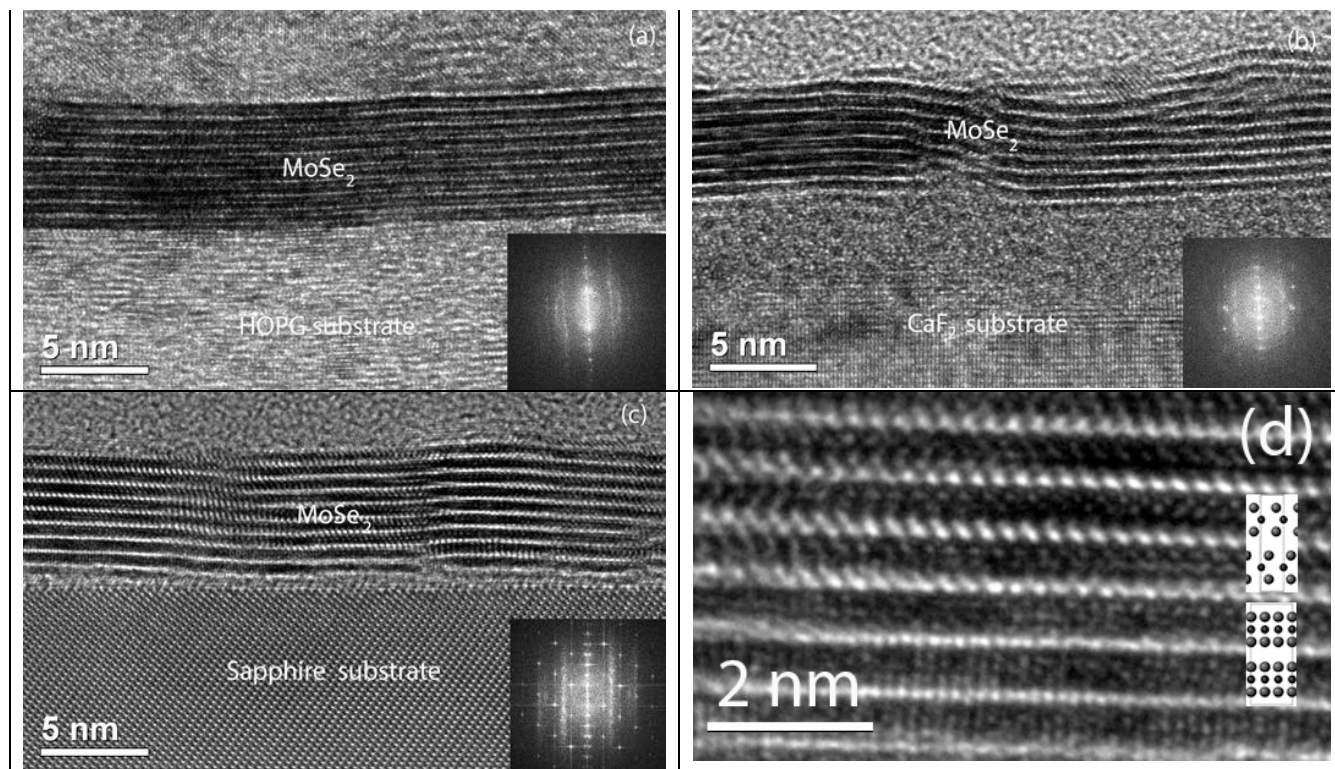
The MoSe<sub>2</sub> films have been grown by MBE on three different substrates, HOPG, CaF<sub>2</sub> and sapphire. The atomic structure has been characterized by Transmission Electron Microscopy (TEM) in two projections: in the cross-sectional (Fig. 1) and plan view (Fig. 2) directions. FEI-Titan 80-300 kV microscope has been employed with 0.2 nm (point-to point) and 0.134 nm resolution, in TEM and STEM modes, respectively. The compositional analysis was performed by Energy Dispersive X-ray Spectroscopy (Oxford Inca EDS, 133 kV spectral resolution) and Electron Energy Loss Spectroscopy (Gatan Tridem EELS system, 0.8 eV spectral resolution).

As one can see from the cross sectional TEM images of Figure 1, the MoSe<sub>2</sub> growth on all three substrates results in a smooth MoSe<sub>2</sub> films with abrupt interfaces. MoSe<sub>2</sub> is primarily of hexagonal 2H structure (space group: P6<sub>3</sub>/mmc). The MoSe<sub>2</sub> films are poly-crystalline with 5-20 nm crystallites (Fig. 2) that are well aligned in growth direction (z-direction), but may have some in plane mis-orientations (x-y directions). In spite of the fact that the MoSe<sub>2</sub> layers are attached to substrate by weak van der Waals forces, the MoSe<sub>2</sub> films are conformal to the substrate so the substrates have a clear effect on the film orientation. The MoSe<sub>2</sub> films grown on CaF<sub>2</sub> and sapphire seem to have smaller grain sizes (~ 5 nm) and to be more disordered in x-y directions as compared to HOPG substrate (10-20 nm). Some areas exhibit turbostratic disorder. All three samples contain crystal defects such as grain boundaries. Cross-sectional TEM image of MoSe<sub>2</sub> film grown on sapphire evidences an amorphous-like interfacial passivation layer on top of Al<sub>2</sub>O<sub>3</sub>. Triangular grains that have been observed in plan view images (Fig. 2) are also typical for CVD grown TMD materials.

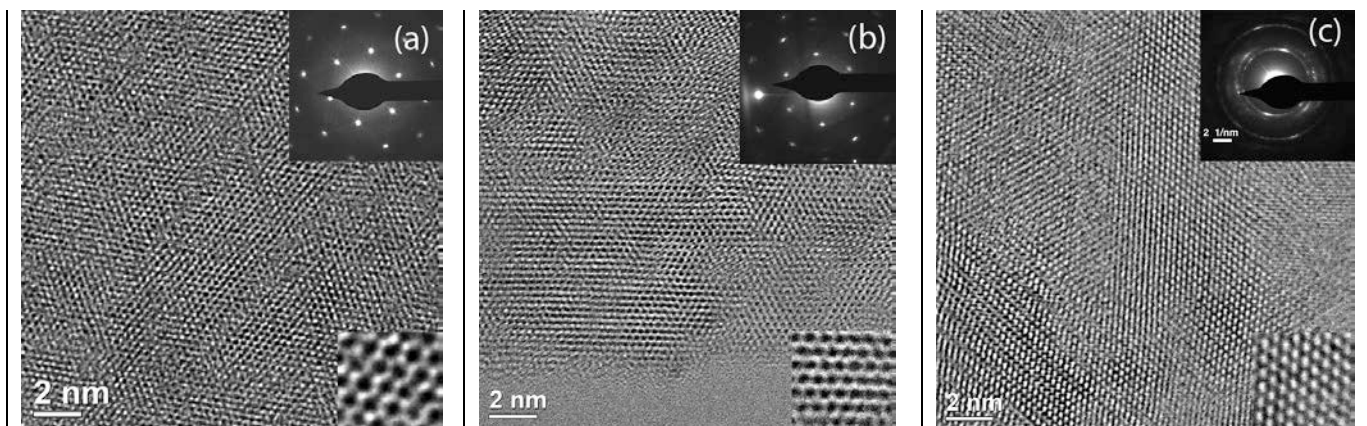
This observation agrees well with theory that in compound 2D material systems it is energetically favorable for one of the elements to terminate the edge over the other. The small grain size is most likely due to the small mobility of the Mo atoms on the growth surface. The larger grain size of MoSe<sub>2</sub> films grown on HOPG may indicate on higher mobility of the Mo atoms. Increasing mobility of Mo atoms by using different substrate or some interfacial layers may lead to higher grain size, and further improved quality of MBE grown MoSe<sub>2</sub> films.

## References:

[1] Yang Su et.al., APL, 103 , 263104 (2013)



**Figure 1.** Typical cross-sectional HRTEM images of MoSe<sub>2</sub> on HOPG (a), CaF<sub>2</sub> (b) and Sapphire (c) substrates. Inserted are Fourier Transformations from the MoSe<sub>2</sub> layers and substrates. (d) is enlarged fragment of (c) to demonstrate turbo static disorder.



**Figure 2.** Plan view HRTEM images of MoSe<sub>2</sub> on HOPG (a), CaF<sub>2</sub> (b) and Sapphire (c). Inserted are corresponding electron diffraction patterns (top right corners) and enlarged fragments of the images (bottom right corners).