

# Unravelling Grain Orientation and Stacking Order in Bilayer MoS<sub>2</sub> Using Electron Diffraction

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## Abstract

MoS<sub>2</sub> is an n-type 2D semiconductor which has shown great promise for application in next-generation nanoelectronics [1]. In bilayer MoS<sub>2</sub>, interactions between individual MoS<sub>2</sub> layers and changes in stacking order can strongly modify the electrical [2] and optical [2,3] properties, thereby providing an additional degree of freedom compared to a monolayer. Consequently, it is critical to efficiently characterize the orientation and stacking differences over a large area in synthetic MoS<sub>2</sub> to not only understand the influence on electrical properties, but also potentially allow for better control during material growth.

In this work, we use an electron diffraction method based on dynamical scattering to efficiently map stacking order from a large area. This method relies on the changes in symmetry from 6-fold (bilayer MoS<sub>2</sub> with AA' stacking) to 3-fold (in bilayer with AB stacking or monolayer) which result in an intensity asymmetry between the {1-100} spots as shown in Fig. 1. This asymmetry is reflected onto the corresponding dark-field TEM images as shown in Fig 2.

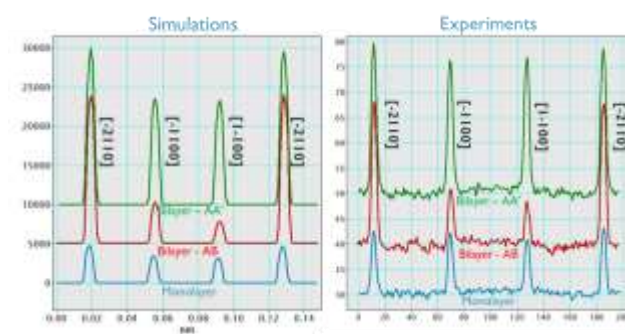
Similar information can be obtained with a very high SNR using a direct electron camera to acquire a diffraction pattern at each probe position leading to much richer data. Results from both these methods will be presented, compared and discussed in more detail.

## References

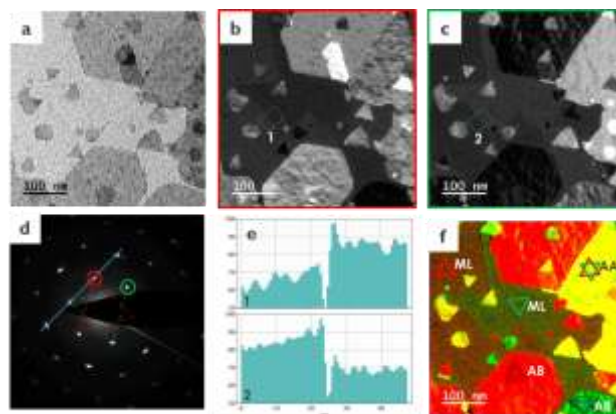
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## Figures



**Figure 1:** Line profiles from multislice electron diffraction simulations and experimental nano-beam electron diffraction patterns (NBED)



**Figure 2:** (a) Bright-field and (b,c) dark-field TEM images acquired with spots marked by the red and green circle respectively in (d) electron diffraction pattern. (e) line profiles from b & c. (f) artificially coloured composite of images b & c, triangles indicate the orientation of Mo sublattice