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Characterisation of Planar Defects in Ternary Layered Chalcogenides for Electronic Devices

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The ongoing trend of device miniaturisation, along with emergence of novel scalable processing methods such as liquid phase exfoliation [1], has stirred an interest in the use of 2-D layered semiconductors in electronic devices. One such candidate systems are the ternary chalcogenides (e.g. $TlGaSe_2$ and $TlGaS_2$), which possess exotic properties such as low band gaps [2-3] and low thermal conductivity [4]. However, these materials are prone to atomic-scale structural defects, either from growth or from processing, which in turn can influence their electronic properties, resulting in significant changes of device characteristics. Therefore, structural studies of these materials at atomic-scale followed by their electronic structure simulation can establish structure-property correlations.
In this work, $TlGaSe_2$ and $TlGaS_2$ are characterised via transmission electron microscopy (TEM), with results being correlated to density functional theory (DFT) calculations. Selected area electron diffraction (SAD) patterns of the dispersed materials display streaking [Figure 1], which when correlated to electron diffraction simulations, indicate the presence of stacking faults in random ordering. This is further proven via scanning TEM (STEM) [Figure 2] and multislice simulations. Stacking fault energies calculated via DFT show a preference for the system to include such faults. Furthermore, band gap calculations of both the bulk and faulted structures show that the introduction of these planar defects alters the band gap, which can have implications for future device applications.

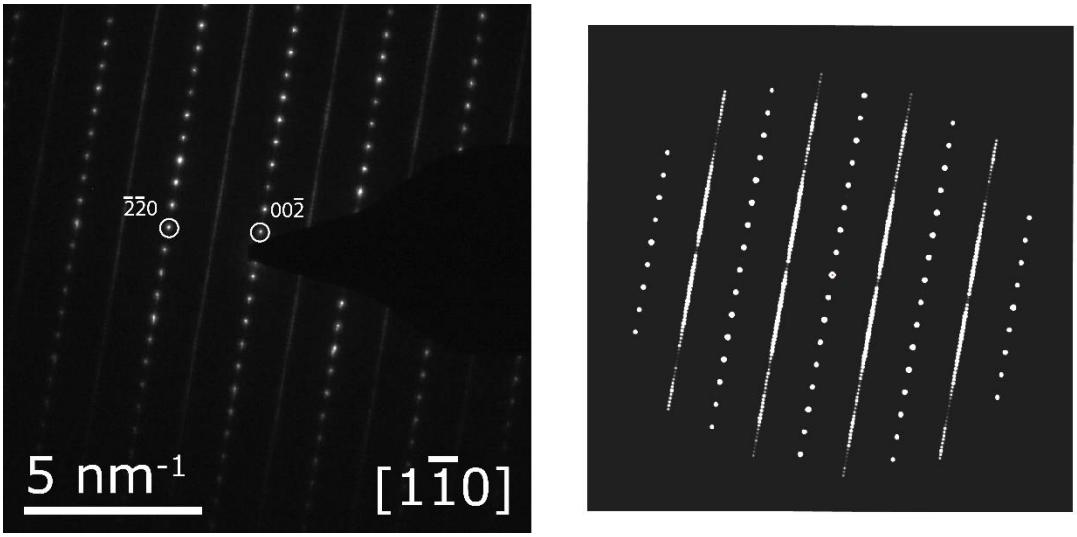

Figure 1: Selected Area Diffraction Pattern (SADP) (left) of $TlGaSe_2$ along [1-10] showing streaking along *hhl*, where *l* is odd. Simulated electron diffraction pattern (right) of an AAAAB stacking of $TlGaSe_2$ layers replicates what is observed in the SADP

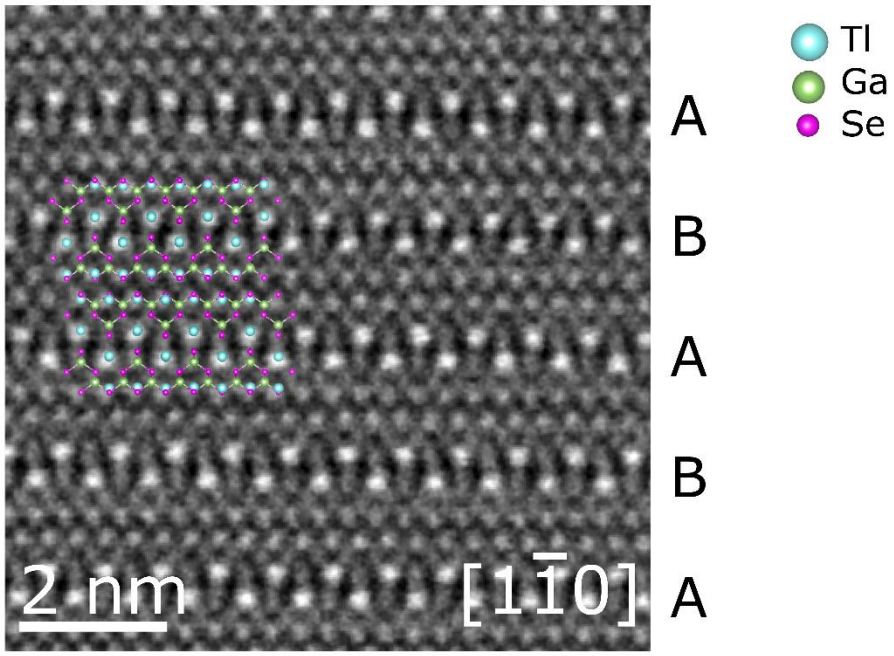

Figure 2: Scanning Transmission Electron Microscopy (STEM) of $TlGaSe_2$ along [1-10], showing ABABA stacking of the layers. Overlayed, BA stacked structure of $TlGaSe_2$

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