Electron transport along and through MoS_2 grain boundaries

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Depending on the growth technique, transition metal dichalcogenides can show a polycrystalline nature. The presence of grain boundaries is expected to significantly affect electron transport. In this contribution, we focus on the common mirror twin boundary (MTB) with a 60° angle between adjacent grains in MoS_2, see fig. 1(a). Our simulations are based on an atomistic tight-binding model [1] recalibrated on DFT calculations, and on the Landauer-Büttiker Green's function approach. The band structure of a zigzag MoS_2 ribbon (z-MoS_2) with a periodic MTB along its axis, see fig. 1(b), shows the appearance of dispersive grain boundary states within the bulk gap, as also reported by scanning tunneling spectroscopy [2]. We investigate the conductivity robustness of these states against short-range (sulfur vacancies) and long-range (Gaussian potential) disorders. We consider rough ribbons in order to completely suppress the edge contribution to transmission [3]. Long-range disorder is effective only close to the van Hove singularities, see fig. 2(a), where new conductive channels are activated. Conversely, short-range disorder strongly suppresses the transmission over the whole energy range, see fig. 2(b). A quantitative scaling analysis will be presented. When the MTB is orthogonal to the transport direction, the conductance of 2D MoS_2 decreases for both electrons and holes, see fig. 3(a). This is due to the lower density of states of the MTB compared to the bulk. The angle-resolved transmission is found to be reversed in the two (K/K') valleys as a consequence of the trigonal warping effect, see fig. 3(b).

References

[1] H. Rostami et al., J. Phys. Condens. Matter, 28 (2016) 495001
[2] Y. Ma et al., ACS Nano, 11 (2017) 5130
[3] J. Park et al., J. Appl. Phys., 124 (2018) 224302

Figures

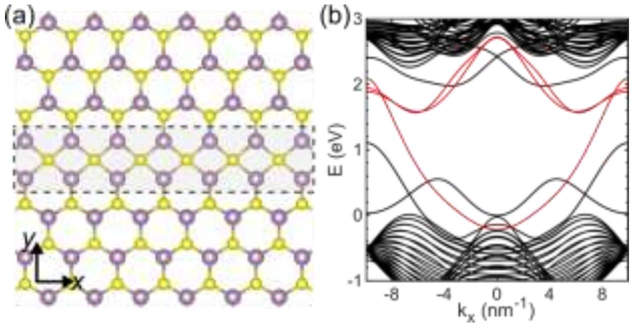

Figure 1: (a) Sketch of a MTB, highlighted in a grey box, in MoS_2. Mo and S atoms are in purple and yellow, respectively. (b) Band structure of a 10 nm-wide z-MoS_2 with a periodic MTB along its axis. MTB states are in red.

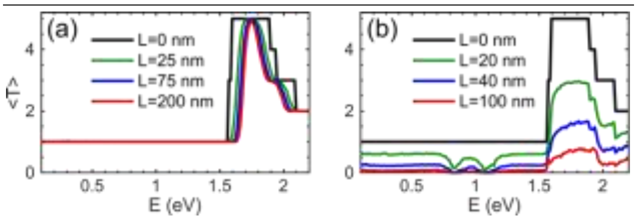

Figure 2: Average transmission coefficient vs. energy for the z-MoS_2 of fig. 1 with (a) short-range and (b) long-range disorders over a whole ribbon section with length *L*. The averaging is performed over 100 disorder realizations.

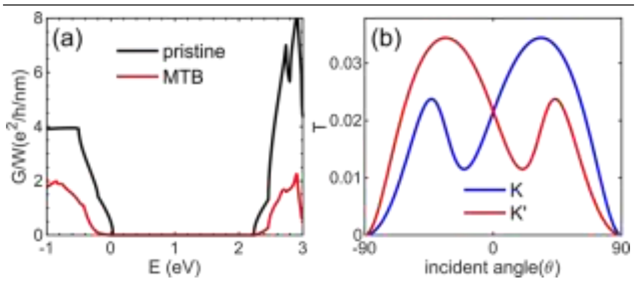

Figure 3: (a) Conductance per unit of width vs. energy for pristine 2D MoS_2 (black line) and in the presence of a transverse MTB (red line). (b) Angle- and valley-resolved transmission coefficients at energy *E* = -70 meV.