Electron transport in disordered mirror twin grain boundaries of molybdenum disulfide

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The interest in semiconducting transition metal dichalcogenides (TMDs) has increased recently. Since a large-scale synthesis of these materials is significantly important for applications, large-area polycrystalline TMDs have been investigated in many growth techniques. It has been reported that some grain boundary geometries give rise to metallic quasi-1D states, resulting in a Tomonaga Luttinger liquid [1]. As a dominant defect, however, grain boundaries are expected to degrade the transport properties. Among various grain boundaries with different geometries, we focus on the rather common mirror twin boundary (MTB). Our simulations are performed based on an atomistic tight-binding model [2] recalibrated with DFT calculations, and in the framework of Landauer-Büttiker Green's function formalism. The band structure of a MoS_2 ribbon with a periodic MTB along its axis shows dispersive grain boundary states within the bulk gap, as also reported by DFT calculation [1] and scanning tunneling spectroscopy [3]. We study the conductivity robustness of these metallic states against various disorders. Short-range disorder is found to affect the transmission over the whole energy range, see Fig. 1(a), while long-range disorder is only effective close to edges of the transmission plateaus [4]. For the electron transport across the MTB, the conductance of 2D MoS_2 decreases for both electrons and holes, see Fig.1 (c). Notably, the transmission in the range of spin-orbit splitting of the valence band is totally suppressed due to spin-valley locking, see Fig. 1(b) [4].

References

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Figures

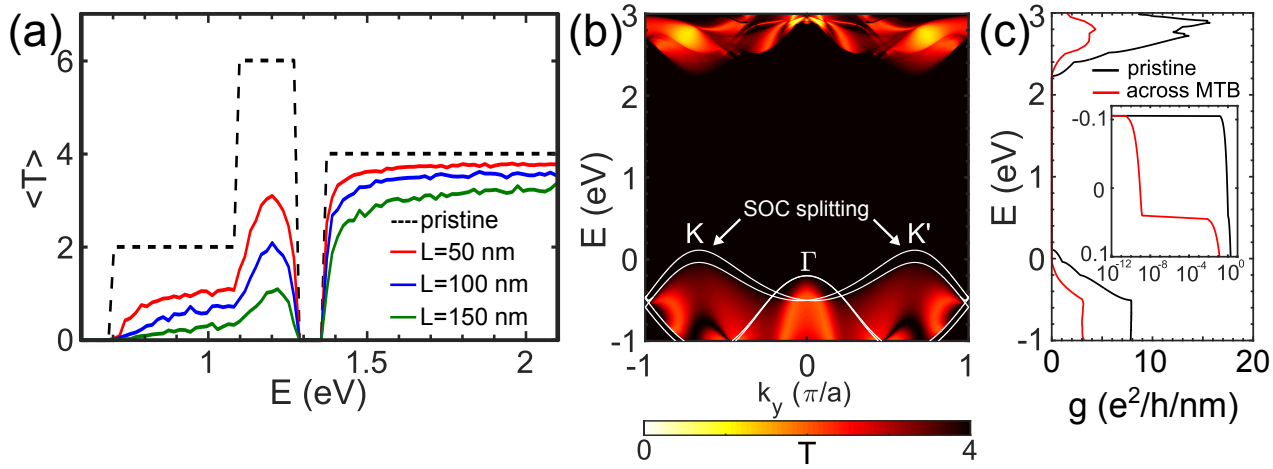

Figure 1: (a) Average transmission coefficient as a function of the electron energy E for the MTB system in the pristine case and in the presence of Anderson disorder with a strength 100 meV and L varying from 50 nm to 150 nm. (b) Transmission coefficient as a function of the wave number and the electron energy for 2D MoS2 with a transverse MTB. The white lines correspond to the band profile of 2D MoS2. (c) Zero-temperature conductance per unit of width as a function of the electron energy for pristine 2D MoS2 and in the presence of a transverse MTB. Inset: Conductance at the top of the valence band in logarithmic scale.