Electron transport along and through MoS$_2$ grain boundaries

Jejune PARK$^{1,2}$
Mireille Mouis$^1$, François Triozon$^2$, Kanhao Xue$^{1,3}$, Alessandro Cresti$^1$

$^1$ Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, IMEP-LAHC, 38000 Grenoble, France
$^2$ CEA, LETI, Minatec Campus and Univ. Grenoble Alpes, 38054 Grenoble, France
$^3$ School of Optical and Electronic Information, Huazhong University of Science and Technology, Wuhan 430074, China

jejune.park@grenoble-inp.fr

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 microscopy [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

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.