Charge Transport across Angle Mismatched-Grain Boundaries (GBs) in 2D Materials

Commercial applications of 2D materials require wafer-scale production. Currently, chemical vapor deposition (CVD) is the most popular and cheapest technique to grow such large-area 2D films. CVD-grown films are inherently polycrystalline, consisting of many single crystalline grains each with random crystal orientation and separated by GBs. To study the impact of GB mismatch angles on electrical transport, I developed a numerical model which uses electronic bandstructure calculated from first-principles and computes electron transmission coefficients from simultaneous conservation of energy and transverse momentum to essentially evaluate the GB resistivity in a Landauer formalism [J5]. We found that the GB resistivity strongly depends on the magnitude of mismatch angle and the orientation of individual grains with respect to the physical boundary itself. The dependence is found to be stronger in graphene than MoS_2 GBs which was attributed to the steep bandstructure of graphene as compared to the flatter parabolic bands in MoS_2. In an ongoing work, I found out that deviations from straight line GBs could result in leaky (low resistive) segments which reduce the overall resistance of such GBs.