Misorientation Angle-Dependent Electrical Transport across MoS_2 Grain Boundaries

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Abstract: Grain boundaries (GBs) in monolayer transition metal dichalcogenides have atomic de fect structures and band dispersion relation that depends on misorientation angle (α) of the merging flakes. Here, we explore the resulting dependences between α, defect structure, and electrical transport across monolayer MoS_2 GBs by correlating field effect device measurements, transmission electron microscopy (TEM) analysis of devices and control samples, and first principles calculations of the TEM-observed structures. It is observed that the inter-domain mobility is minimized for $\alpha \sim 9°$ and increases nonlinearly by two orders of magnitude before saturating at ~16 $cm^2V^{-1}s^{-1}$ around $\alpha \approx 20°$. This trend is explained via density function theory and experimental tunnelling barrier estimates, both of which indicate GB electrostatic barriers that peak around 0.5 eV at low angle decrease rapidly to ~0.15 eV as α increases. Additionally, by employing inert-environment fabrication, we observe mobilities up to 115 $cm^2V^{-1}s^{-1}$. Generally, our observed mobilities are more than double previously reported values for monolayer MoS_2 single-crystal samples at 300K.

References:

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