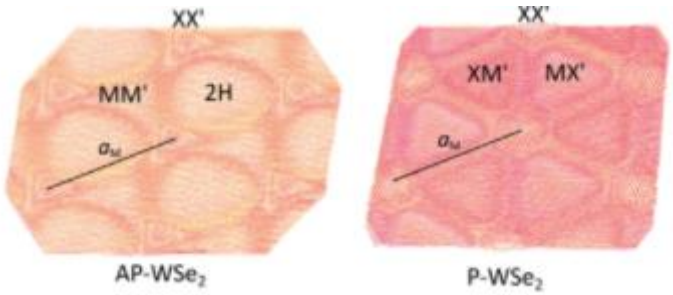
Electronic properties of marginally twisted bilayers of transition metal dichalcogenides

Vladimir Fal'ko

National Graphene Institute, University of Manchester, Manchester M13 9PL, UK



Abstract

We discuss lattice structure and physical properties of twisted bilayers of transition-metal dichalcogenide. We show that for 'marginally' (small-angle) lattice recbnstruction results in the neworks of domains with the energertically preferential stacking and domain walls, which are similar to dislocations in bulk crystals. In some cases, such domains feature weak interfacial ferroelectric polarisation, which gives rise to the tunability of domain wall networks by an out-of-plane electric field. Also, inhomogeneous strain near domain walls gives rise to substantial pieelectric charges, producing -- together with stacking-dependent interlayer hybridization of band-edge states – arrays of dot-like features for electrons and holes in thetwisted bilayers. All tehse effects are fully quantified for semiconducting MX_2/MX_2 bilayers (M=Mo,W; X=S,Se).