Domain wall network model for control of interfacial ferroelectricity in twisted bilayers of transition metal dichalcogenides

Vladimir Enaldiev[1,2]
V.I. Fal'ko[1,2,3]
[1]*University of Manchester, School of Physics and Astronomy, Oxford Road, Manchester, M13 9PL, United Kingdom*
[2]*National Graphene Institute, University of Manchester, Booth St. E., M13 9PL, United Kingdom*
[3]*Henry Royce Institute, University of Manchester, Booth St. E., M13 9PL, United Kingdom*
vladimir.enaldiev@manchester.ac.uk

Twistronic heterostructures are van der Waals materials for which mesoscale moiré periodicity considerably modifies electron and structural properties. Recently, a new phenomenon, interfacial ferroelectricity [1,2], has been discovered in slightly twisted homobilayers of semiconducting transition metal dichalcogenides (TMD) with parallel orientation of unit cells in constituent layers. Origin of the effect is related with interlayer charge transfer in domains formed by relaxation of moiré pattern. Thanks to out-of-plane direction of spontaneous polarisations in shape of domains can be modified applying external electric field in field effect transistor geometry. In my talk I formulate an analytical domain wall network model [3], which allows one to efficiently follow evolution of domain structure under external electric field. In particular, I show that for perfect (C_3-symmetric) relaxed moiré superlattice our model admits two regimes set by threshold electric field, determined by the model parameters. For electric field below the threshold, each domain wall in the network behaves like spring with clamped ends at the network nodes and bends to increase area of domains with favourable direction of polarisation. At the threshold field, the bending finishes by touching conditions for each pair of domain wall coming to the same node of the network. For post-threshold electric fields evolution of domain wall network represents a universal scaling of threshold structure with scaling parameter given by ratio of applied field to the threshold one. Finally, I demonstrate extension of the model on the case of irregular domains emerging in real twistronic heterostructures because of transfer-induced inhomogeneous strain [4].

References

[1] A. Weston, et al, Nature Nanotechnology, 17 (2022) 390
[2] X. Wang, et al, Nature Nanotechnology, 17 (2022) 367
[3] V.V. Enaldiev et al, Nano Letters, 22 (2022) 1534
[4] L. Molino, et al, arXiv:2210.03074

Figures

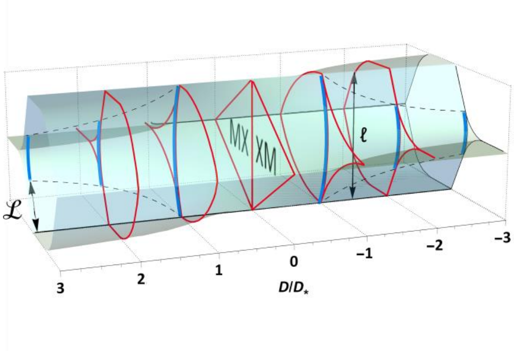

Figure 1: Variation of reconstructed moiré supercell in marginally twisted TMD homobilayers under out-of-plane displacement field D in units of threshold field D_*.