

Predicting and observing topological defects in 2D materials

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Grain boundaries and dislocations are intrinsic topological defects of polycrystalline materials that inevitably affect their physical properties. In my talk, I will first discuss the structure of topological defects in two-dimensional (2D) materials such as graphene and monolayer transition metal dichalcogenides [1,2] as well as their electronic transport properties predicted by theory [3,4]. Our most recent efforts involved joint experiment-theory studies of well-ordered topological defects in graphene. In particular, a line defect with valley-filtering properties has been produced in a controlled way at the transmission electron microscopy (TEM) conditions [5]. Periodic grain boundary defects have been investigated in polycrystalline samples of epitaxial graphene grown on SiC substrates using scanning tunneling microscopy (STM) [6]. The latter study allowed observing the buckling transition of grain boundaries predicted to occur in 2D polycrystals. Unlike graphene, monolayer transition metal dichalcogenides (MoS₂ and alike) combine a two-valley electronic band structure with strong spin-orbit effects. The latter can be employed for creating spin-polarized currents and adds yet another conservation law of the electronic transport across regular defects [7], such as the inversion domain boundaries frequently observed in dichalcogenide materials [8].

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