Multiscale Model for Interlayer Dislocations in Bilayer Graphene

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We present a model to describe the interlayer dislocations in bilayer materials. The bilayer material is divided into two sheets; the in-plane deformation and out-of-plane buckling of each sheet can be described by classical linear elastic theory. The interaction between two sheets is described by 3-dimensional generalized stacking-fault energy (GSFE) which obtained from first principle calculations. The force balance between these two contributions determines the structure of the bilayer materials. We apply this approach to determine the structure and energetics of four interlayer dislocations and twist grain boundaries in bilayer graphene. A pronounced buckling is formed at the position of partial dislocation. The results from our model are in excellent quantitative match to the atomistic results.