A topologically-derived dislocation theory for twist and stretch moiré superlattices in bilayer graphene

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The elastic theory of dislocations allows modeling of materials at the meso and continuum scale by solving for the strain fields resulting from a line source of incompatibility in the displacement field due to the removal or addition of a half-plane of atoms. The theory of dislocations is integral to bridging the scale gap between the atomic and continuum scales by introducing atomic defects into otherwise continuous media. As 2D materials continue to advance from the laboratory to applications, a dislocation theory of 2D materials will be able to predict the mechanical response at the interface of 2D materials. Dislocations between two 2D materials have been analyzed with atomistic and hierarchical models, which provide critical information like core effects and structural relaxation to build and verify the dislocation theory for 2D materials. However, it is uncertain if the dislocation theory of continuous 3D materials holds in 2D materials that readily deform out of plane and have highly anisotropic bonds especially when dislocation theory often neglects core effects. Here we show that a continuum dislocation theory holds in 2D materials by extending a dislocation model developed by Daw that finds the minimum energy configuration of an array of dislocations. The in-plane directions are treated continuously, but the out-of-plane direction is treated discretely as a finite difference using Peierls-Nabarro like core interactions. In comparisons to atomistic simulations using classical potentials, the maximum structure deviation is 6%, while the maximum line energy deviation is 0.019 eV/Å. Several applications of our model are shown, including predicting the variation of structure with twist angle, and describing dislocation line tension and junction energies.

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