Study of topological defects in graphene

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Abstract

We present an assessment of the stability of defects at finite temperature and how the transport properties can be modified by the inclusion of defects in graphene. Additionally, we also exhibit the power of the discrete dislocation theory (DD) developed by Ariza&Ortiz [1,2] to predict easily and reliably harmonic displacement field of defects. In particular, we study the stability of different defects, such as dislocation quadropole and dipole arrangements [3], stacking faults [4], partial dislocations [4] and grain boundaries against annihilation. Most of these defects have been observed stable [5,6] in graphene. In order to carry out this study, we first use the theory of discrete dislocation to compute the harmonic atomic structure of defects, employing for this, either linearized empirical potentials such as Airebo [7] and Aizawa [8] or linearized semi-empirical potential such as tight binding [9]. The benefit of the latter is that we can predict electronic properties due to defects and also requires less computational time than *ab initio* simulations. Tight binding potentials represent a compromise between *ab initio* and empirical potentials. Straight afterwards, using LAMMPS code (Sandia National Laboratories Large-scale Atomic/molecular Massively Parallel Simulator) and the defective configuration predicted by discrete dislocation theory as initial condition, we study the stability of defects at finite temperature. As a result, on one hand, we predict high stability of dislocation dipole and quadropole configurations against annihilation, unlikely dissociation of perfect dislocations into partial dislocations in graphene and change of electronic properties due to defects. On the other hand, we demonstrate the ability of the discrete dislocation theory to predict defective configurations.

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