Birth and growth of point defects in graphene

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ABSTRACT

In the field of electronics, due to its excellent mechanical and electrical properties, graphene has become the most promising material for the production of next generation thin and flexible electronic components. However, these properties depend on the presence of topological defects in the graphene lattice. In order to provide a model of graphene behavior allowing to study the birth and evolution of some of these defects, we present an atomic force-constants model based on the LCBOPII potential (Long-range Carbon Bond-Order Potential II), by Jan H. Los et al. [1], that accounts for interatomic interactions up to fourth neighbors. We have obtained explicit expressions of the potential derivatives as well as the force-constant values, from which we have computed the phonon dispersion curves by applying dynamics of crystal lattices, which are used to verify the model when they are compared with experimentally curves.

In addition, we have applied discrete dislocations to the graphene lattice, following the discrete dislocations theory developed by Ariza and Ortiz [2], and we have calculated the atomic displacements and the energy associated with the evolution of dipoles and quadrupoles in graphene.

REFERENCES

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