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(Research Article)
Investigation of defects in the thermal conductivity and phonon spectra of graphene

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Abstract

Graphene is one of the carbon nanostructures that has been considered in many industries today due to its high thermal properties. In this work, due to the high thermal conductivity and the presence of various defects during the synthesis of graphene, the simultaneous investigation of the effects of the vacancy defects and Stone-Wales to high-density defects on the thermal conductivity of graphene has been studied. This work has been used to simulate a reverse non-equilibrium molecular dynamics simulation with using Airebo potential was used to model the interactions between all atoms, which is an empirical potential. This describes the potential of non-binding interactions by matching the behavior of inter-molecular interactions, which is here for carbon-carbon interactions, graphene is used. It also studies the phonon spectra and overlaps on the thermal conductivity of graphene nanoribbons. The results show that the thermal conductivity of graphene nanoribbons reduces both defects by a maximum of 46% for low deficit density and a minimum of 25% for maximum density, that is, decreasing the density of the defect in the thermal conductivity reduction relative to the defective nano-tubes.

Keywords: Graphene nanoribbons, Dynamic molecular simulation, Vacancy defect, Stone-Wales defect, Thermal conductivity.

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