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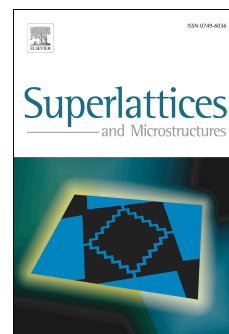
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A study of thermal conductivity in graphene diodes and transistors with intrinsic defects and subjected to metal impurities

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Abstract

In this paper, the effect of the presence of cavities resulting from the fabrication process and the effect of common metal impurities added during the synthesis process on the thermal conductivity of single-layer graphene sheets, diodes and transistors have been investigated by using the Reverse Non Equilibrium Molecular Dynamics (RNEMD) method. The obtained results show that thermal conductivity generally diminishes by increasing the concentration of nanoparticles and increases when porosities and impurities are at the edges of sheets. Regarding a better thermal management in graphene with the addition of nanoparticles, and considering its existing porosity, a lower thermal conductivity is achieved by adding more nanoparticles. By increasing the diameter of pores from 0.5 *nm* to 4.4 *nm* in a specific single-layer graphene sheet, thermal conductivity diminishes from 67 W/mk to 1.43 W/mk; while it diminishes from 45 to 1.0 W/mk for the same structure containing both the defects and nanoparticles over the defects. In evaluating the influences of cavities and metallic nanoparticles on thermal conductivity, it was observed that changing the share of cavities or nanoparticles

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