Thermal transport engineering in polycrystalline graphene: Nonequilibrium molecular dynamics study

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Abstract
Synthesized graphene sheets usually have several types of defects that could influence their thermal properties. During chemical vapor deposition technique for producing industry-scale graphene sheets, it usually leads to the formation of polycrystalline graphene structures instead of single crystal structure. In this research, using non-equilibrium molecular dynamics (NEMD) simulations and optimized Tersoff potential function, the thermal conductivity of ultra-fine polycrystalline graphene with various grain sizes is calculated. It is found that the thermal conductivity of polycrystalline graphene significantly decreases when the grain size decreases. Extrapolating NEMD results based on a 1D thermal resistance model, the thermal conductivity for larger grain sizes is also estimated. The effects of Nitrogen doping and mechanical strain on the thermal conductivity of polycrystalline graphene are also calculated. We finally discuss the underlying mechanism in thermal conductivity suppression by calculating the phonon power spectra.