Thermal Transport in Graphene with Defect and Doping: Phonon Modes Analysis

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Abstract

The effects of defect and isotopic doping with different ratios on the thermal conductivity of graphene are investigated by using non-equilibrium molecular dynamics simulations and normal mode analysis method. In contrast to the persisted size dependent thermal conductivity in the pristine graphene, thermal conductivity of defected graphene quickly saturates when the size is greater than 100 nm. Similar to the pristine graphene, we find the thermal conductivity of defected and doped graphene follows $\sim T^{-\alpha}$ behavior, and the power exponent α is sensitive to the defect and doping ratio. The spectral phonon relaxation time and normalized accumulation thermal conductivity with respect to the phonon mean free path (MFP) reveal that the long-MFP phonon modes are strongly suppressed in the defected and doped graphene, resulting in the suppressed size dependence and the weaker temperature dependence of the thermal conductivity compared to the pristine graphene. The phonon modal analysis in our work establishes a deep understanding of the defect and doping effects on the thermal transport in graphene, which would provide effective guidance to the graphene-based phonon engineering applications.