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A search for the dominant heat conducting phonon modes in graphene: An atomistic simulation study HENGJI ZHANG, Department of Physics, University of Texas at Dallas, KYEONGJAE CHO, Department of Physics and Department Materials Science and Engineering, University of Texas at Dallas
— We have performed an equilibrium molecular dynamic (MD) simulation study to investigate phonon thermal transport in graphene at 300K with Green-Kubo method. Using a newly optimized reactive empirical bond order carbon potential (Lindsay, et al. Physical Review B 81, 205441, 2010), our calculated thermal conductivity (TC) of defect free graphene is about 3000 W/mK in good agreement with experiments(∼3000-5000 W/mK). A maximum of ∼1000 fold reduction in TC is possible to achieve for graphene with defects and surrounding viscous medium. As we decompose the in-plane and out-plane phonon vibration modes of graphene in MD simulations, the out of plane vibration modes (ZA phonon) contribute to about 50% of the overall TC. This large contribution from ZA modes is explained with density of states analysis. We have clarified a recent controversy on which polarization mode in graphene is the main heat carrier.

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