Divergence of the Thermal Conductivity in Uniaxially Strained Graphene

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Abstract

Unique heat transport properties make graphene a strong candidate to applications in future thermal management devices. At room temperature its thermal conductivity is dominated by phonons and values as large as 5000 W/m-K have been measured for suspended graphene at ≈ 300 K [1]. Graphene is also a very interesting candidate for phononics and a graphene-based thermal diode has been proposed [2]. However, in order to build functional devices it is necessary to manipulate and tailor phonon transport properties, which requires a deep understanding of the behavior of phonons in graphene. We perform extensive equilibrium molecular dynamics simulations, based on the Tersoff interatomic potential, to understanding the mechanism of heat transport in suspended graphene under various conditions. We show that the thermal conductivity of unstrained graphene, calculated from the fluctuations of the heat current at equilibrium, is finite and converges with size at finite temperature. Studying size convergence we demonstrate that low-frequency out-of-plane vibrational modes act as scatterers and limit the thermal conductivity to a large but finite value. We then show that the thermal conductivity of an extended periodic graphene model under uniaxial tensile strain diverges logarithmically with the size of the model, when strain exceeds a threshold value of 2%. Tensile strain changes the dispersion relations of phonons in graphene, including a linearization of the originally quadratic dispersion of out-of-plane modes. An analysis of phonon populations and lifetimes shows that the divergent behavior is caused by changes in the occupation of low-frequency out-of-plane phonons and an increase in their lifetimes due to strain. Furthermore, the divergence observed in our simulations would lead to a strong size dependence in experimental measurements of thermal conductivity, which allows for a direct verification. In view of the recent fabrication of graphene with predefined concentrations of carbon isotopes [3], we also investigate the effect of isotopic mass disorder on the thermal conductivity of unstrained and strained graphene. Our simulation results show that even for the highest concentration of ^{13}C isotopes (50%), the divergence of the thermal conductivity remains. Finally, we investigate the thermal conductivity of unstrained and strained functionalized graphene.

References

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