Thermal transport in strained, isotopically engineered and functionalized graphene

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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 $\approx$ 300 K. In order to build functional devices it is necessary to be able to manipulate and tailor these properties, which requires a deep understanding of the behavior of phonons in graphene. We perform extensive equilibrium molecular dynamics simulations to understand the mechanism of heat transport in suspended graphene in various conditions. 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. This behavior stems from strain-induced changes in the dispe rsion relations and population of low-frequency phonon modes. Divergence would lead to a strong size dependence of experimental measurements of thermal conductivity. Finally, in view of the recent fabrication of graphene with predefined concentrations of carbon isotopes and of functionalized graphene, we investigate the effect of isotopic mass disorder and functionalization on the thermal conductivity of unstrained and strained graphene.