Equilibrium limit of boundary scattering in carbon nanostructures: molecular dynamics calculations of thermal transport

Justin Haskins, Alper Kinaci, Cem Sevik, Tahir Cagin

It is widely known that graphene and many of its derivative nanostructures have exceedingly high reported thermal conductivities (up to 4000 W/mK at 300 K). Such attractive thermal properties beg the use of these structures in practical devices; however, to implement these materials while preserving transport quality, the influence of structure on thermal conductivity should be thoroughly understood. For graphene nanostructures, having average phonon mean free paths on the order of one micron, a primary concern is how size influences the potential for heat conduction. To investigate this, we employ a novel technique to evaluate the lattice thermal conductivity from the Green-Kubo relations and equilibrium molecular dynamics in systems where phonon-boundary scattering dominates heat flow. Specifically, the thermal conductivities of graphene nanoribbons and carbon nanotubes are calculated in sizes up to 3 microns, and the relative influence of boundary scattering on thermal transport is determined to be dominant at sizes < 1 micron, after which the thermal transport largely depends on the quality of the nanostructure interface. The method is also extended to carbon nanostructures (fullerenes) where phonon confinement, as opposed to boundary scattering, dominates, and general trends related to the influence of curvature on thermal transport in these materials are discussed.