Study of diameter and chirality dependence of thermal conductivity of carbon nanotubes using Green Kubo relations

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ABSTRACT

Molecular dynamics has been proven to be a well-established tool for calculating transport coefficients like thermal, electrical conductivity and shear and bulk viscosity of condensed matter. Green Kubo relations provide a formalism wherein transport properties of systems can be calculated via an equilibrium molecular dynamics simulation. The aim of this report is to successfully develop a formalism for calculating thermal transport properties of Single Walled Carbon Nanotubes (SWNTs) using Green Kubo relations.

Solid state Argon and Iron were chosen for a benchmark study of thermal conductivity due to their ease of being accurately represented in the form of existing potentials and readily available experimental data to corroborate. The theoretically calculated values were then compared with the experimental data to ascertain the predicting power of Green Kubo relation.

Single Walled Carbon Nanotubes were modelled using Tersoff potential for estimation of thermal conductivities using Green Kubo formalism. Dependence of thermal conductivity on structural parameters like length, diameter, temperature and chirality of nanotubes was studied and also compared with the available experimental data.