Phonon transport in finite length single-walled carbon nanotubes using a non-equilibrium molecular dynamics method

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SWNTs are expected to possess high thermal conductivity due to the quasi-one-dimensional structure and strong carbon bonds. An important feature of the SWNT thermal conductivity in terms of both physics and engineering is its length dependence [1], which occurs because the length-scale of phonon quasi-ballistic transport is usually longer than the tube-length in practical situations. In this study, we calculate the length dependence of the thermal conductivity of SWNTs for a range of nanotube-length up to 3.2 micrometers using a non-equilibrium molecular dynamics method. The simulation gives us access to detail pictures of phonon transport such as the dispersion and relaxation [2]. The results indicate two length-regimes with different trend of thermal conductivity; (1) the shorter tube-length regime (<200 nm) with contribution of diffusive-ballistic phonon transports from a wide range of phonon branches including optical phonons, and (2) the longer tube-length regime (>200 nm) with dominant contribution from the key low frequency phonons with mean free path well longer than the tube-length. In the latter regime, the thermal conductivity exhibits exponential divergence on the length with the exponent somewhat smaller than the available one-dimensional models. The phenomena will be discussed in terms of detailed pictures of phonon transport.

References:

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