The Disparate Thermal Conductivity Of Carbon Nanotube And Diamond Nanowires Studied By Atomistic Simulation

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Background

Faced with the well publicized limits of present-day micro-electronics fabrication technology, manufacturers will likely turn to nanostructures, such as carbon nanotubes or nanowires, in order to continue to increase circuit density and performance. However, the thermal properties of these structures must be quantified before they can be used efficiently in designs. In this work we use atomistic simulation to study thermal transport by phonons in carbon nanotubes and diamond nanowires, focusing on the effective thermal conductivity of these structures.

The longitudinal thermal conductivities of nanotubes have recently been measured. At $T = 300K$, Shi[1] found $\lambda = 3000$W/m K for a multi-walled nanotube and $\lambda = 1200$W/m K for a 150nm diameter multi-walled nanotube bundle. Hone *et al.*[2,3] estimated the thermal conductivity of single-walled nanotubes, based on the measured thermal conductivity of crystaline rope of single-walled nanotubes, to be in the range $\lambda = 1750$ to 5800 W/m K.

Atomistic simulations are an attractive complement to these difficult experiments because of the details they can provide. Unfortunately, they are limited to relatively small systems and short simulation times. Structure size is particularly important because the phonon mean free paths in nanotubes are thought to be long. Recent measurements suggest a mean-free path of 500nm for a multi-walled nanotube.[1] Simulating a multiwalled tube of this length seems prohibitively expensive. An even longer mean free path is expected for a single-walled nanotube since there is no mechanism for phonon scattering between the wall layers. Periodic boundary conditions are often employed in simulations so that phonons can travel several periods before they scatter, thus simulating a much larger structure. Using quasi-equilibrim and equilibrium approaches, respectively, Berber *et al.*[4] and Che *et al.*[5] have computed the longitudinal thermal conductivity of periodic single-walled nanotubes using perioidic boundary conditions finding high values comparable to those deduced experimentally.

However, in most anticipated applications nanotubes lengths will be comparable to the phonon mean free path. In this study we compute the effective thermal conductivies for nanotubes of several lengths and subject to different model boundary conditions. Results are compared to diamond wires of comparable dimensions. Unlike nanotubes, whose "clean" structure is thought to reduce phonon scattering, the irregular stuctures of diamond nanowires are expected to scatter phonon substantially, as observed in atomistic simulations of silicon nanowires.[6]

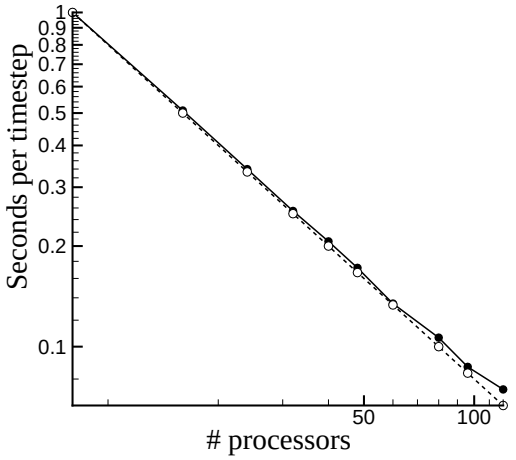

Figure 1: Run time scaling on IBM SP: —— code, - - - - theretical maximum.

Methods

We use the Brenner[7] potential to simulate the carbon atoms. This same potential has been used previously to study thermal conductivity[4,5] and various other properties of carbon nanotubes. Because it is a strictly classical potential, it will fail at low temperatures where quantum effects become significant, but it has been shown to be adequate at moderate termpatures and above.[8]

We have implemented our algorithm in parallel to permit simulations with $\sim 10^5$ atoms and $\sim 10^6$ timesteps. The atoms in the nanotube or diamond nanowire are distributed among the processors based on their axial position. MPI is used for interprocessor communications. Although communication must occur each timestep, run times scale well with numbers of processors (figure 1). We have used up to 120 processors.

In our nonequilibrium approach, atomic velocities were rescaled in local regions to maintain a temperature gradient. Each hot and cold region was one-tenth of the total length of the structure. The heat flux, cross-sectional area, and temperature gradient give the thermal conductivity.

Results

Here we present results for a nanotube and a diamond rod. Both have a diameter of 1.1nm. The thermostats were set at $T_{\text{hot}} = 300\text{K}$ and $T_{\text{cold}} = 280\text{K}$ in both cases.

The temperature profile for a 0.5μm long nanotube is shown in figure 2. Statistics were accumulated over 10^6 timesteps. Using the constant temperature gradient clearly seen in figure 2 and the heat flux required to maintain it, we found a high λ for the 0.5μm long tube comparable to experiments. However, it was suppressed by nearly a factor of 4 in a 90nm long tube.

The comparison simulation of a 90nm long diamond rod predicted λ to be one-sixth that for the nanotube of the same length, as expected due to increased phonon scattering.

References

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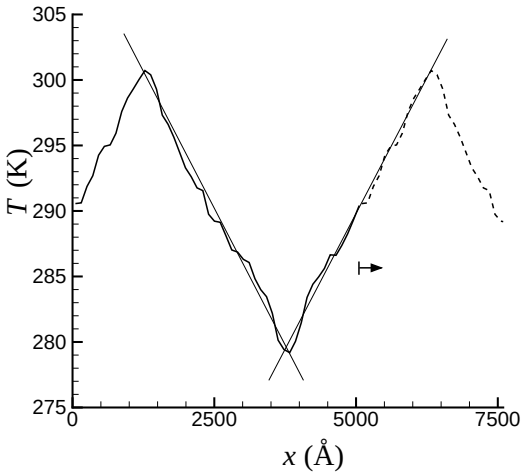

Figure 2: Temperature profile in temperature controled perioidic single-walled nanotube. The ---- is the periodic continuation.

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