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Thermal rectification of a single-wall carbon nanotube: A molecular dynamics study

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ABSTRACT

We have investigated the thermal rectification phenomenon in a single-wall mass graded carbon nanotube by molecular dynamics simulation. Second generation Brenner potential has been used to model the inter atomic carbon interaction. Fixed boundary condition has been taken into account. We compare our findings to a previous study by Alaghemandi et al. [18] which has been done with a different potential and boundary condition. The dependence of the rectification factor R on temperature, nanotube diameter and length as well as mass gradient is obtained. It is shown that by increasing the temperature, the rectification decreases whereas by increasing the other parameters namely the mass gradient, diameter and the tube length it increases.

1. Introduction

Rectification is a transport process that takes place faster in one direction than in the opposite one. This phenomenon has attracted much attention in recent years [1]. In electronics this phenomenon has been used extensively in ubiquitous devices such as diodes and electric rectifiers [2,3]. The phenomenon of rectification is not restricted to electronic flow. In 1970 it was experimentally shown that rectification can occur in thermal current. For detailed review on thermal rectification in solid state physics see [4]. Recently the process of thermal rectification of heat flow has been detected in nano-sized materials. It has been empirically shown that externally mass-loaded carbon and boron nitride nanotubes are capable of exhibiting thermal rectification [5]. The empirical findings of Chang et al. have stimulated the interest of theoreticians on the issue of thermal rectification [5]. Thermal property of nanoscale materials is also important both for fundamental physical theory and for applications [6]. In recent years, different carbon nanotubes (CNTs) [5,7–10] and Graphene Nano Ribbon (GNR) [11–13] structures have been proposed as candidates for thermal rectifiers [14]. These nano-sized carbon-based materials would have deep implications in thermal energy control such as on-chip cooling, high efficiency energy conversion and other phononics applications. Li and co-workers could theoretically show that thermal rectification appears in a one-dimensional (1D) chain with non-linear interaction among the masses [14] and also in a mass-graded monoatomic chain interacting through the Fermi–Pasta–Ulam (FPU) potential [15,16]. The anharmonicity is the key feature which leads the thermal rectification in these one-dimensional model systems. In fact the overlap of the vibrational spectra at the two ends of the chain is the reason for the existence of the thermal rectification. Recently Alaghemandi et al. have executed extensive simulation and have shown that mass graded single-walled carbon nanotubes (SWCNTs) exhibit thermal rectification [17–19]. They have studied the dependence of rectification on the tube diameter, length, mass gradient and temperature. According to their results, rectification magnitude increases with increasing the CNT diameter as well as the mass gradient. Moreover, they showed that the rectification magnitude decreases when the temperature is enhanced. They have used reverse non-equilibrium molecular dynamics [20]. The interaction potential between carbon atoms is adopted from a mechanical viewpoint and includes radial harmonic, angular and torsion terms [21]. In this paper we study the thermal rectification of a SWCNT with the reactive empirical bond order (REBO) interaction potential [22] between carbon atoms and find the differences/similarities of our results with those found by Alaghemandi et al.

2. Methodology

We have used classical non-equilibrium molecular dynamics (NEMD) simulation to calculate the thermal conductivity of an

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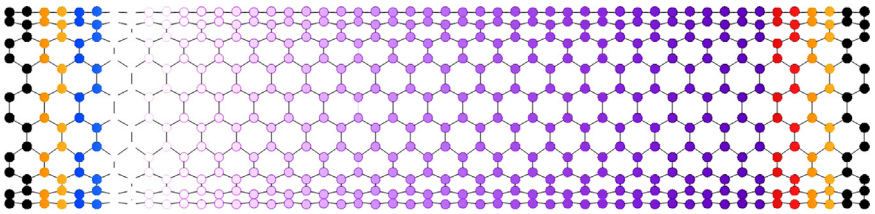

Fig. 1. (Color online) Single-walled carbon nanotube under fixed boundary condition. Two layers (black atoms) from each side are kept fixed during the simulation. Blue (red) atoms are connected to the low (high) temperature thermostat. All the other atoms are simulated in the NVE ensemble. Dark purple indicates high mass region.

armchair single-wall carbon nanotube (SWCNT). The interaction between two carbon atoms C–C is modelled by the second-generation reactive empirical bond order (REBO) potential [22]. Simulations were performed using the LAMMPS package [23]. The velocity Verlet method was employed to integrate the equations of motion with a time step of 1 fs. First, the entire nanotube is coupled to a Nosé–Hoover thermostat at temperature T and MD is performed to equilibrate and relax the system for 1 ns. After equilibrium, we fix the atoms of one unit cell (two rings) of carbon atoms from each end of the CNT. The third unit cell from each end is coupled to a Nose–Hoover thermostat. The second unit cell is not connected to a thermostat in order to suppress the phonon reflection from edges. The hot (cold) reservoir temperature is set to $T+\Delta T$ ($T-\Delta T$) respectively. In our simulations we have taken $\Delta T = 10$ K. See Fig. 1 for illustration.

We then perform a run for 10 ns. As a result of coupling the system ends to thermostats with different temperatures, a temperature gradient emerges and a heat flux is established along the CNT axis. After the system reaches steady state, the thermal conductivity K of the CNT along its axis is evaluated according to the Fourier law $Q = -KdT/dz$ as follows:

$$K = -\frac{\langle Q(t)\rangle}{dT/dz} \tag{1}$$

where dT/dz is the temperature gradient along the CNT axis and the brackets denote time average of thermal flux. We remark that the instantaneous heat flux $\mathbf{Q}(t)$ is found from the following relation:

$$\mathbf{Q}(t) = \frac{d}{dt}\sum_i \mathbf{r}_i(t)\varepsilon_i(t) \tag{2}$$

where $\varepsilon_i(t) = p_i^2/2m + \frac{1}{2}\sum_{j\neq i} V(\mathbf{r}_i, \mathbf{r}_j)$ is the instant total energy of particle i. In computation, people normally do not directly proceed with (2). Instead, they compute the heat flux in a different manner. The heat flux is taken as the work done by the thermostat on the system. In the Nośe–Hoover thermostat [24] the equation of motion for particle i becomes

$$\dot{\mathbf{p}}_i = -\xi\mathbf{p}_i + \mathbf{F}_i \tag{3}$$

where $\mathbf{F}_i$ is the systematic force exerted on particle i. The heat bath acts on the particle with a force $-\xi\mathbf{p}_i$ thus the input power of the heat bath to the system is $-\xi\mathbf{p}_i \cdot \mathbf{p}_i/m$ which can also be regarded as the thermal current associated to particle i. Summation over i gives

$$\mathbf{Q}(t) = -\sum_i \xi\frac{\mathbf{p}_i \cdot \mathbf{p}_i}{m} \tag{4}$$

Coming back to (1) the temperature gradient is found by applying a linear fit to the temperature of the intermediate slabs. The ratio in Eq. (1) produces a reasonable value provided that the system is fully equilibrated and the simulation is sampled over a sufficiently long time. It has been theoretically shown that implementation of a non-uniform mass distribution with a mass gradient α along the axis of CNT renders possible thermal rectification [17,18]. The mass of carbon atoms is assumed to increase with a gradient $\alpha = dm/dz$ along the CNT axis. This increase mimics the effect of mass grading by deposition of heavy molecules such as $C_9H_{16}Pt$ on the CNT [5]. The left end of the CNT is set at $z=0$. We have performed extensive MD simulations to see the differences/similarities with the results of Alaghemandi et al. [18]. The main differences between our model and reference [17] are as follows: the interatomic potential in Ref. [18] is adopted from a continuum mechanics whereas we have used REBO. Second, they used periodic boundary condition but we have used fixed boundary condition. We remark that in experiments performed to measure the thermal conductivity of CNTs, both ends of the CNT are quite kept fixed (suspended actually over a trench) on a substrate [25–29] therefore the fixed boundary condition is more compatible with experiment. Third, they used reverse NEMD for establishing a thermal current but in our model two thermostats do the task. The thermal rectification factor R is defined as

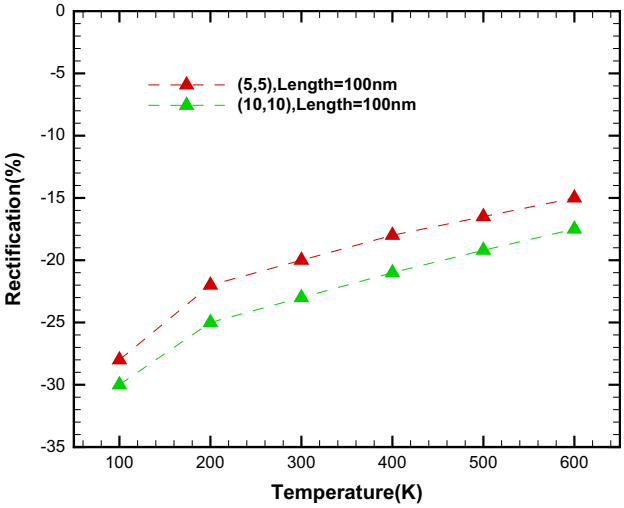

Fig. 2. (Color online) Rectification factor versus temperature for armchair (5, 5) and (10, 10) CNTs having various diameters. Tube length has been $L=100$ nm. Fixed boundary condition has been implemented and $\alpha = 5.76$ gr/mol nm.

$$R = \frac{K_{H\to L} - K_{L\to H}}{K_{L\to H}} \times 100 \tag{5}$$

Note $K_{H\to L}$ stands for the thermal conductivity of the system when heat flows from the high-mass region to the low-mass region. Visa versa applies to $K_{L\to H}$.

3. Results

In this section we present our simulation results. Fig. 2 shows the rectification factor R versus temperature for a CNT of length $L=100$ nm for two values of chiral indices (n,m), i.e. (5, 5) and (10, 10) which correspond to diameters $d=0.677$ nm and $d=1.354$ nm respectively. By increasing the temperature, the modulus of R decreases towards zero. For low temperatures,