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Role of Interatomic Potentials in Simulation of Thermal Transport in Carbon Nanotubes

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ABSTRACT

Interatomic potentials, which describe interactions between elements of nanosystems, are crucial in theoretical study of their physical properties. We focus on two well known empirical potentials, i.e. Tersoff's and Brenner's potentials, and compare their performance in calculation of thermal transport in carbon nanotubes. In this way, we study the temperature and diameter dependence of thermal conductivity of single walled armchair carbon nanotube by using the mentioned interatomic potentials. We take advantage of direct non-equilibrium molecular dynamics simulation, which well resembles the experimental set up for thermal conductivity measurement. The results show that increasing the temperature increases the conductivity in contrast with diameter growth which decreases the thermal conductivity. It is important to note that both interatomic potentials describe the system behavior very well, however they lead to different conductivity values. It is found that the difference between the performance of studied potentials can be seen more obviously in longer tubes. We also observe a peak in thermal conductivity by increasing system temperature. System is deformed at T≈1000 K, when Tersoff's potential is employed for description of interactions. While its instability occurs at higher temperature (T≈1600 K), when we try to simulate system by Brenner's potential.

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NOMENCLATURE

A	Cross section area (m^2)	NEMD	Non-equilibrium molecular dynamics
b_{ij}	Bond order	Q	Heat (J)
CNT	Carbon nanotube	r	Radius (nm)
D	Diameter (nm)	r_{ij}	Distance between atoms i and j (m)
dT/dz	Temperature gradient (K/m)	SWCNT	Single walled carbon nanotube
E	Energy (J)	t	Time (s)
EMD	Equlibrium molecular dynamics	T	Temperature (K)
$f_c(r_{ij})$	Cutoff function	U	Potential energy (J)
HNEMD	Homogeneous non-equlibrium molecular dynamics	$V(r_{ij})$	Interaction between atoms i and j (J)
J_{heat}	Heat flux ($J/s.m^2$)	$V^A(r_{ij})$	Attractive pair potential (J)
L	Length (nm)	$V^R(r_{ij})$	Repulsive pair potential (J)
MD	Molecular dynamics	λ	Thermal conductivity (W/m.K)

1. INTRODUCTION

By reducing the size of electrical and mechanical systems to nanometer scales, transferring the generated heat to the environment seems crucially essential for their proper functionality and longer life expectancy. Thus, materials with high thermal conductivity that can quickly remove the heat from the device have attracted the attention of many researchers. Simple atomic structure of carbon nanotubes (CNTs) and their excellent mechanical, electrical and thermal characteristics have made them good candidates for use in nanoelectronics [1-4]. For example, they can be used in integrated circuits as transistors and interconnectors, or tools for heat transfer management [5-7].

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Theoretical studies and experimental measurements have reported high thermal conductivity in the axial direction of CNTs [8-10]. Factors such as temperature, temperature gradient, length, diameter, defects and impurities have impact on the heat transport [11, 12]. Due to the differences in the theoretical methods employed in the study of thermal conductivity, significant discrepancy has been observed in results. So far, no analytical theory of heat transport could properly represent the thermal transport of CNTs [13]. Also different methods and conditions prevailing in the measuring process of thermal conductivity have comprised various values of thermal conductivity ranging from 290 to 25000 W/m.K [14, 15]. Molecular dynamics (MD) is one of the most conventional methods to investigate the heat transport in carbon nanostructures. In this method, Newton's equations are used to find the position and velocity of particles in each time step. Therefore, we just need to know the interatomic potentials in this procedure. Due to the availability of forces field for a wide range of materials, obtaining precise empirical potentials from ab initio calculations for simple models is almost (may be an almost) an easy task [2]. Molecular dynamics simulations can be classified into three groups: equilibrium MD (EMD) based on Green-Kubo relation, non-equilibrium MD (NEMD) based on Fourier's law, and homogeneous non-equilibrium MD (HNEMD) [7]. The simulation accuracy extremely depends on the precision of employed potential for describing the interactions between components in the system under consideration [16]. Tersoff [17], Brenner I [18], Brenner II [19] and intermolecular reactive bond order (AIREBO) [20] are the most common potentials used for investigation of structures including covalent bonds.

High crystalline order, long phonon mean free path and high speed phonons positively affect thermal transport mechanism [21]. Hence, phonons play a major role in heat transport in nanotubes. Phonons contribute to the heat capacity of CNTs a hundred times more than the electrons. Consequently, share of electrons can be ignored in thermal transport process [22]. Various phonon modes such as acoustic modes (transverse, longitudinal, torsional and radial breathing) and optical modes participate in the transport of thermal energy in CNTs. Thermal phonon mean free path of the nanotubes is estimated in the order of micrometers. Phonon mean free path reduces due to the dispersion of phonon-phonon, phonon-boundary and phonon-defect interactions [23].

The thermal conductivity of CNTs was studied by many authors applying different interatomic potentials [1]. Understanding how interatomic potentials describe phonon transport in a CNT is important, since the behavior of CNT-based devices in heat transfer applications are resulted from their atomic interactions. Molecular dynamics studies are considered as classical approaches. However, the quantum effects have been included in interatomic potentials [24]. Due to various MD methods and different boundary conditions of performed simulations, comparing the effect of different potentials on the thermal transport gives no significant results. Various studies confirm the reliability of both Tersoff's and Brenner's potentials in description of heat transfer in nanosystems [25]. There has been no precise comparison between the performance of these potentials in explanation of thermal properties of nanostructures thus far. Moreover, physical limits of the studied systems, e.g. temperaure, for their appropriate performance are not checked in detail. Hence, our main goal is the investigation of different interatomic potentials' influence on the thermal transport mechanism. We focus on different (and identical) terms of the mentioned well-known many body potentials, which play crucial roles in the investigation of thermal transport in nanotubes. We also determine thermal limits, in which these potentials can properly describe atomic interactions.

In this way, we calculate thermal conductivity of armchair single walled CNTs (SWCNTs) by NEMD method using a direct application of Fourier's law. It should be noted that the choice of axial boundary condition influences the thermal transport. The phonon mean free path in SWCNT is several microns [26], and for nanotubes shorter than this length phonon scattering from the ends will be important. When nanotubes are modeled with periodic boundary conditions, boundary scattering is eliminated. This elimination leads to an abnormal increase of the thermal conductivity by leaving phonon-phonon interactions as the only scattering mechanism [27, 28]. Furthermore, applying free boundary conditions causes the system displacement. So, in our simulations the ends of the tubes along the axial direction are kept fixed rigidly during the simulation to avoid being displaced by the pseudo transfer of momentum, and the parts between fixed and temperature controlled slabs are in an attempt to reduce reflecting of heat from the edge [29-34]. The dependence of thermal conductivity on the diameter and temperature is also considered in the present paper.

The organization of the remainder of the article is as follows. In the next section, we briefly go over the theoretical background for thermal conductivity calculation. Then, in section 3, Brenner and Tersoff potentials are introduced. The thermal conductivity of armchair carbon nanotubes is calculated for both types of potentials in section 4. Finally, in section 5, we present a brief discussion and summary of the work.

2. NON-EQUILIBRIUM MOLECULAR DYNAMICS

The nonequilibrium MD method resembles experimental measurement setup to obtain thermal

conductivity. In direct NEMD, a temperature gradient is exerted on the system to establish heat flux along a particular direction, taken here as the tube axis. According to Fourier's law for small temperature gradient, the thermal conductivity, λ, has linear relation with heat flux produced by the temperature gradient.

$$J_{heat}=\frac{1}{A}\frac{dQ}{dt}=-\lambda\frac{dT}{dz}, \quad (1)$$

where J_{heat} denotes steady state heat flux, which is defined as the amount of energy Q transferred through the cross sectional area A at time interval dt. dT/dz refers to temperature gradient along z direction in the system.

Firstly, the whole system has been brought to equilibrium at temperature T, using Nose-Hoover thermostat for about 5ps. Then, to simulate heat flow from hot to cold region, tube length is split into N slabs with equal widths. The outermost layer at each end of the CNT is fixed rigidly. Second slabs after the fixed ends act as buffers to reduce heat reflection from the tube ends. To generate a thermal current through the nanotube, energy is transferred continuously from one region, denoted as the 'heat sink' with the temperature $T_{cold}=T-\Delta T/2$, to another one, the 'heat source' with the assigned temperature $T_{hot}=T+\Delta T/2$. They are placed at the third layer from each end of tube with temperature difference equal to ΔT=20K. The hot/cold region is created by rescaling particle velocities in the source/sink region at each timestep [12]. We solve Newton's classical equations of motion for atoms in the intermediate regions.

After reaching the dynamic steady state, the resulting heat flux can be calculated exactly by taking time average of the net energy added to the system at every time step:

$$J_{heat}=\frac{\sum_{t=1}^{N_t}\left|\Delta E_{hot,t}-\Delta E_{cold,t}\right|}{2A\sum_{t=1}^{N_t}\Delta t}, \quad (2)$$

where $\Delta t=0.35$ fs is the simulation time step and N_t refers to the total number of simulation steps served for data gathering. $\Delta E_{hot,t}$ and $E_{cold,t}$ denote additional kinetic energy which are added to hot slab and removed from cold slab to maintain their temperature constant. Here, $A=2\pi rdr$ is the cross sectional area of an annular ring with thickness $dr=3.35$Å and radius of tube. The instantaneous temperature in each slab is defined by the energy equipartition theorem. The temperature gradient can be obtained by applying a linear least-squares fitting to the temperatures profile of intermediate region (Figure 1).

Once the temperature gradient and heat flux is obtained, we can calculate thermal conductivity using Fourier's law.

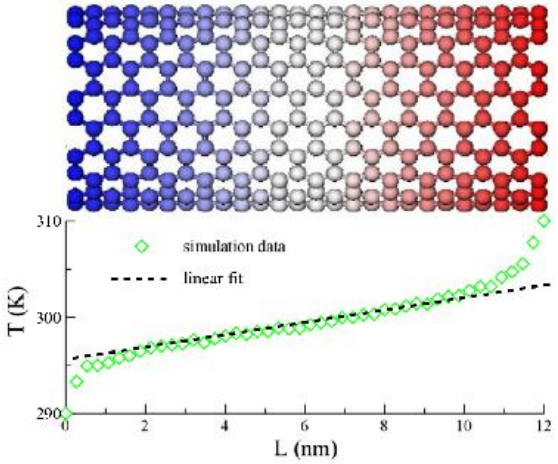

Figure 1. Temperature profile for a SWCNT of length $L=12.47$ nm, obtained from NEMD simulation. Green diamonds show data points for temperature of tube slabs by imposing temperature differences $\Delta T=20K$ to tube ends at $T=300K$. The best linear fit to simulation data is plotted by dashed line

3. INTERATOMIC POTENTIAL

The carbon-carbon interactions are described using the bond-order potentials presented by Tersoff [17] and Brenner [18] in a simplified form [35]. Both potentials are three body potentials which are written in the two body formalism as below:

$$U=\sum_i\sum_{j(>i)}V(r_{ij}),$$
$$V(r_{ij})=f_c(r_{ij})[V^R(r_{ij})+b_{ij}V^R(r_{ij})], \quad (3)$$

where r_{ij} is the distance between pairs of nearest-neighbour atoms i and j. $V(r_{ij})$ denotes the interaction energy between atom i and j, the nearest neighbors. The function $f_c(r_{ij})$ defines cut off value for pair potential, which restricts the interactions to the nearest neighbors. Here, $V^R(r_{ij})$ denotes the repulsive pair potential and $V^A(r_{ij})$ refers to the attractive force between conduction electrons, respectively.

The bond order, b_{ij}, includes many body interactions between atoms i and j, regarding the atomic environment. It is a function of number and strength of bonds and the cosine of the angle of the bonds between atoms i and k and atoms i and j which reduces monotonically [36]. It should be noted that $b_{ij}\neq b_{ji}$, which means that the energy associated to a bond is not equally divided between two atoms. In the Brenner potential, the bond order term is substituted with $\bar{b}_{ij}=b_{ij}+b_{ji}$. The general form of bond order is the same for both Tersoff and Brenner potentials, since it includes similar physical concepts. The parameters are obtained by fitting to experimental data.

4. THERMAL CONDUCTIVITY

To clarify the role of potential type used in the study of heat transport, the effects of temperature and diameter on thermal conductivity of armchair carbon nanotubes are investigated by utilizing the Tersoff and the Brenner potentials.

In the first part of this study, we calculate thermal conductivity of (5,5) nanotube against the temperature for 12 nm and 20 nm nanotube lengths. As temperature rises, two things happen. On the one hand, more phonons will be excited, which play a positive role in heat transport. On the other hand, umklapp scattering of phonons which leads to a decrease in the phonon mean free path increases. At low temperatures, umklapp scattering can not significantly disturb the positive effects of increased energy carriers. Hence, as expected from theoretical and experimental studies [12, 37], one can clearly see that thermal conductivity curve grows with increasing temperature for both types of used potentials. The obtained results show a power law behavior for thermal conductivity against the temperature.

Thermal conductivity values obtained by both potentials are closer together at low temperatures. But, as temperature rises simulations done by Brenner potential result in higher values of thermal conductivity than Tersoff one.

Increasing the lattice vibrations along the length of nanotube, which are responsible for heat transfer, causes an increase of atom's interacting energy as the temperature grows. Since, unlike the Tersoff potential, the Brenner potential takes into account the contibution of energy of both interacting atoms, it estimates higher values for thermal conductivity. The temperature growth leads to higher lattice vibration, which reveals discrepancy of energy contribution associated to an atomic interaction between Tersoff and Brenner potentials.

It is obviously seen from the lower panel of Figure 2 that, longer carbon nanotubes result in higher values of thermal conductivity for both applied potentials. As we mentioned earlier, phonon mean free path of nanotubes have been reported to be in the order of micrometer. But scatterings from boundaries limit their phonon mean free path to the size of system. Hence, increasing the length of nanotubes rises their phonon mean free path [38]. Also, the number of atoms which participate in the lattice vibration increases. Since the Brenner potential considers contribution of both interacting atoms, it gains more higher values for thermal conductivity, as the length grows. According to the above-mentioned facts, the curves of Brenner and Tersoff go farther apart for larger nanotubes.

We also check the diameter dependence of thermal conductivity for two different lengths at the room temperature.

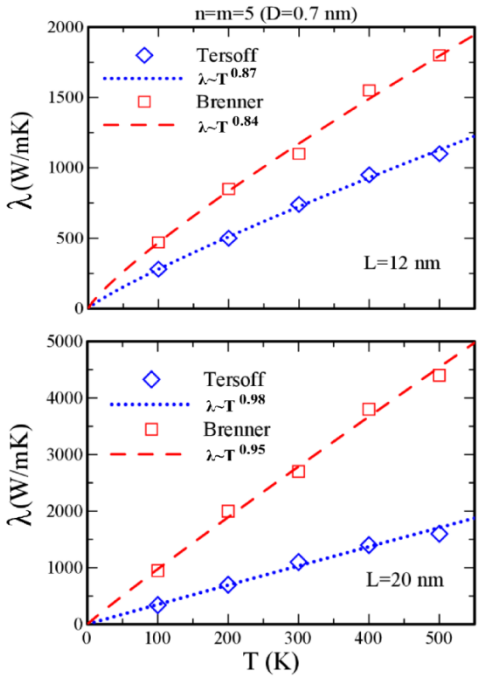

Figure 2. Thermal conductivity of (5,5) carbon nanotube versus the temperature, for lengths equal to 12 nm (upper panel) and 20 nm (lower panel). The blue diamonds and red squares represent data points obtained by utilizing Brenner and Tersoff potential, respectively. The dashed and dotted lines show fitting results with power-law functions

According to Figure 3, one can clearly see that by increasing the diameter at the fixed length and temperature, thermal conductivity decreases with a power-law manner for both types of potentials. Increasing the diameter results in excitation of more transverse phonon modes. Coupling between these transverse phonon modes with longitudinal modes which are responsible for the transport of heat along the axial direction in the nanotubes, leads to a significant power-law reduction of thermal conductivity. The obtained results from both investigated potentials are in good agreement with the experimental and theoretical studies [7, 39, 40].

As we have seen earlier, the Brenner potential estimates higher values for thermal conductivity. For short nanotubes, distance between two plots is constant as the diameter increases, and it does not change significantly in the case of longer nanotubes. It is due to the fact that, transverse phonon modes, which do not have influential impact on interactions participating in heat transfer process, will be more excited as the diameter increases. Therefore, increasing the diameter does not make a significant change in the interval of Brenner and Tersoff curves.

The thermal conductivity of armchair SWCNTs with 12 nm length is also calculated for temperatures from 500 to1500 K (Figure 4).

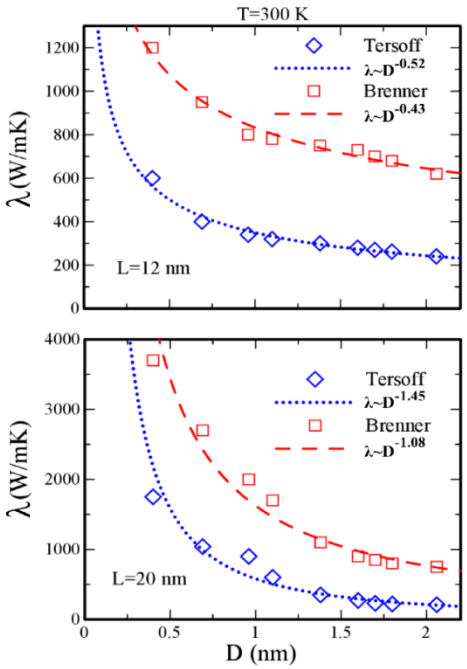

Figure 3. Diameter dependence of thermal conductivity in an armchair SWCNT for two different values of length at room temperature. Thermal conductivity decreases for both type of potentials as the diameter increases

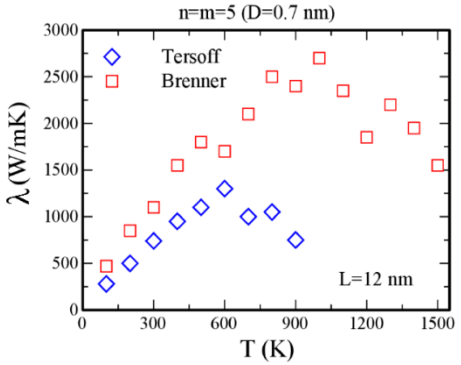

Figure 4. Thermal conductivity against temperature over 100-1500 K for two different interatomic potentials; Tersoff and Brenner. A peaking behavior can be observed for both types of potential. But the peak of thermal conductivity occurs at lower temperature when we use the Tersoff interatomic potential

A peaking behavior is observed in thermal conductivity graph as a function of temperature for both employed potentials. The rising and falling in the thermal conductivity can be generally attributed to the competition between positive excitation of phonon modes and resistive umklapp processes at different temperatures. At low temperatures, positive effects come over on destructive phonon phonon interactions. In contrast, umklapp process becomes stronger as the temperature grows. It is in good agreement with the reported results from theoretical and experimental works [38, 41]. It has been stated that the peak position moves to the higher temperatures as the length of the nanotube decreases.

It is worth noting that, in our study the peak position and its value shifts to higher temperatures and higher conductivity for CNTs studied by Brenner potential. It is also important to mention that the Tersoff potential is not able to model carbon-carbon interactions at very high temperatures. So, carbon-carbon bonds break at 1000 K in structures investigated by Tersoff potential.

Experimental studies of the thermal transport in CNTs with a diameter of 1 to 3 nm have reported thermal conductivity in the range of 2000-8000 W/m.K [42]. According to the results obtained in this work, it seems that applying the Brenner potential gives better estimation of thermal conductivity than using Tersoff potential.

5. CONCLUSION

A precise investigation of thermal conductivity in carbon nanotubes can be useful in designing thermal transport management devices for nanoelectronic applications. In this study we have compared Tersoff's and Brenner's interatomic potentials performance in description of carbon-carbon interactions, which leads to different results for thermal transport in nanosystems. We have discussed their detailed differences that affect out-coming results. In this procedure, using a direct NEMD simulation approach, the thermal conductivity of armchair SWCNT at several temperatures and diameters has been calculated. By imposing fixed boundary conditions, we have tried to avoid undesirable displacements and unrealistic scattering.

For both types of potential, our results show a power-law increase in the thermal conductivity as a function of temperature at low temperatures, which follows a decrease as the temperature reaches higher values. The peaking behavior is due to the competition between positive influence of increasing excited phonon modes and destructive effect of umklapp scattering. The thermal conductivity begins to decrease sooner in the case of Tersoff potential.

Strong diameter dependence has been observed in thermal conductivity of armchair carbon nanotube for both Tersoff and Brenner interatomic potentials. By increasing the tube diameter, more transverse phonon modes are excited, and their destructive interplay disturbs conduction process. As the length of nanotube confines the phonon mean free path, thermal conductivity obviously increases by nanotube elongation. It is worth noting that, we have found greater discrepancies between the results obtained by using the mentioned potentials, in the case of longer nanotubes.

Both Tersoff and Brenner potentials are able to reveal the general trends and physical mechanisms that control the heat transfer in nanotubes. However, Tersoff potential underestimates the value of thermal conductivity and can not describe very well the interatomic bonds at very high temperatures. On the other hand, the Brenner potential takes into account the contribution of energy of both interacting atoms, which leads to more realistic results.

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Molecular Dynamics

چکیده

پتانسیل‌های میان‌ذره‌ای توصیف‌کننده‌ی ساختار نانوسامانه‌ها در مطالعه‌ی ویژگی‌های فیزیکی آن‌ها نقش مهمی دارند. ما در این پژوهش روی پتانسیل‌های ترسف و برنر تمرکز کرده، عملکرد آن‌ها را در محاسبه‌ی ترابرد گرما در نانولوله‌ها با هم مقایسه نموده‌ایم. در این راستا، ما بستگی رسانش گرمایی نانونوله کربنی تک‌دیواره‌ی آرمچیر را به دما و قطر نانولوله با بهره‌گیری از دو پتانسیل اشاره شده مورد بررسی قرار داده‌ایم. در بررسی سامانه مورد نظر روش دینامیک مولکولی ناتعادلی سرراست برای محاسبه ترابرد گرمایی به کار گرفته شده است. این روش به خوبی شرایط آزمایشگاهی برای اندازه‌گیری رسانش گرمایی شبیه‌سازی می‌نماید. بررسی‌های ما نشان دادند که با افزایش دما رسانش افزایش یافته اما با افزایش قطر کاهش می‌یابد. نکته حائز اهمیت این است که هر دو پتانسیل بین ذره‌ای به خوبی رفتار رسانش را توصیف می‌کنند، هرچند مقدارهای متفاوتی به دست می‌دهند. با افزایش طول نانولوله تمایز میان نتایج حاصل از دو پتانسیل مورد نظر بیشتر آشکار می‌شود. با افزایش تدریجی دمای سامانه یک قله در رفتار رسانش گرمایی بر حسب دما مشاهده می‌شود. زمانی که از پتانسیل ترسف برای توصیف برهم‌کنش‌ها استفاده می‌کنیم، سامانه در دمای $T\approx1000$ K از هم می‌پاشد. ولی ناپایداری نانولوله هنگام به‌کارگیری پتانسیل برنر در دمای بالاتری ($T\approx1600$ K) اتفاق می‌افتد.

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