Influence of chirality on the thermal conductivity of single-walled carbon nanotubes*

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The influence of chirality on the thermal conductivity of single-walled carbon nanotubes (SWNTs) is discussed in this paper, using a non-equilibrium molecular dynamics (NEMD) method. The tube lengths of the SWNTs studied here are 20, 50, and 100 nm, respectively, and at each length the relationship between chiral angle and thermal conductivity of a SWNT is revealed. We find that if the tube length is relatively short, the influence of chirality on the thermal conductivity of a SWNT is more obvious and that a SWNT with a larger chiral angle has a greater thermal conductivity. Moreover, the thermal conductivity of a zigzag SWNT is smaller than that of an armchair one. As the tube length becomes longer, the thermal conductivity increases while the influence of chirality on the thermal conductivity decreases.

Keywords: single-walled carbon nanotube, thermal conductivity, chiral angle, molecular dynamics simulation

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1. Introduction

Since the preparation of a carbon nanotube (CNT) was realized,[1] the unique mechanical, electrical, optical, and thermal properties of the quasi-one-dimensional CNT structure have manifested great potential in many applications, such as electrical devices, hydrogen storage medium, field emission displays, nanoscale electronic devices, sensors, and probes.[2] Especially driven by the miniaturization trend of electronic devices, the application of CNTs to effectively dissipating waste heat has attracted broad attention, on the microscale or nanoscale. With its high axial thermal conductivity and one-direction conductance, the CNT has been considered one of the best new materials to promote a new industrial revolution in the present century. Many studies have been carried out on the relationship between thermal conductivity of CNT and other influential factors like temperature, length, impurity, and diameter of CNTs, to try to find out the optimum conditions for industrial application. Research[3–8] indicated that the thermal conductivity first increases and then decreases with the rising temperature. So a peak appears at a certain temperature, but there is no unanimous view on at what temperature the peak occurs. That the increasing length of the SWNT would improve its thermal conductivity was a conclusion which gained broad acceptance[9–13] even though concrete results would be divergent because of the different methods adopted. The existence of impurity definitely worked as a weakening factor, but the extent of decline caused by the different impurities would not be the same.[14–16] For the effect of the diameter, Shiomi and Maruyama[17] have proposed that the diameter should present little influence on the thermal conductivity of a SWNT when its tube length was short, while the thermal conductivity would decrease with the increase of diameter when the tube length was long enough. Chirality is also a particular characteristic of SWNTs and it has been proved that the chiral angle is a very important parameter for SWNTs, which has a high influence on their physical properties, such as conductivity.[18] However, the influence of chirality on the thermal conductivity of SWNTs has not been investigated so widely. Limited researches have been done to evaluate the dependence of chirality on the thermal conductivity. In the literature,[19] it was argued that chirality had little influence on the thermal conductivity of CNTs when the diameters were the same. But Zhang *et al.*[20] concluded through their calculation results that the thermal conductivity of chiral SWNTs was lower than those of zigzag and armchair ones, and the thermal conductivity of a zigzag SWNT was the highest. Falat *et al.*[21] indicated that chirality greatly affected thermal conductivity even though the changing relationship between them was not so clear. Generally speaking, the existing investigations have not come to a unanimous conclusion about the effect of chirality on the thermal conductivity of SWNTs and so, more work needs to be done to understand this effect. Therefore, our simulations are concentrated on the effect of chirality on the thermal conductivity of SWNTs.

In the present work, we use a non-equilibrium molecular dynamics (NEMD) method to investigate the long-disputed influence of the chiral angle on the thermal conductivity of SWNTs, with the AIREBO[22] potential used to describe

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interatomic interactions. Given the conclusions mentioned in the literature,[23] to only investigate the effect of chirality on thermal conductivity, we not only use nearly the same diameters but also adopted shorter SWNTs, to further exclude the influence from the diameter in our simulation. Four groups of SWNTs are investigated by using the NEMD method in our simulations: SWNTs with a relatively small diameter, which leads to scarcely different chirality samples including a longer length and a shorter length, namely, a) smaller-diameter shorter SWNTs and b) smaller-diameter longer SWNTs; SWNTs with a larger diameter that leads to diversity of chirality are also used with a longer length and a shorter length, namely, c) larger-diameter shorter SWNTs and d) larger-diameter longer SWNTs.

The rest of this paper is organized as follows. Subsection 2.1 contains the details concerning the definition of chiral angle and relevant notions. A brief overview of the theoretical background regarding the computation of thermal conductivity and the setup of our simulations are given in Subsection 2.2. The main results obtained in the present work are given and analyzed in Section 3. The key conclusions drawn from the present work are found in Section 4.

2. Procedure

2.1. Chiral angle

The chirality and diameter of SWNTs are determined by the only vector $R = m \cdot a_1 + n \cdot a_2$. Here, m and n are integers; a_1 and a_2 are unit vectors of graphite; R is the lattice vector of two-dimensional graphene. The schematic diagram is shown in Fig. 1. Then the diameter of a SWNT is defined as $d = |R|/\pi = a \cdot \sqrt{m^2 + m \cdot n + n^2}/\pi$, $a = 1.42 \cdot \sqrt{3}$ is the lattice constant. When $m = n$, the SWNT is called an armchair SWNT; when $m = 0$ or $n = 0$, this kind of SWNT is named a zigzag SWNT. Chirality includes the cross angle from a zigzag SWNT to an armchair SWNT and the cross angle between the two is 30°. So the chiral angle is defined as the angle between the vector R and the orientation of a zigzag SWNT. It is formulated as $\theta = \tan^{-1}\left|-\sqrt{3} \cdot n/(2m+n)\right|$.

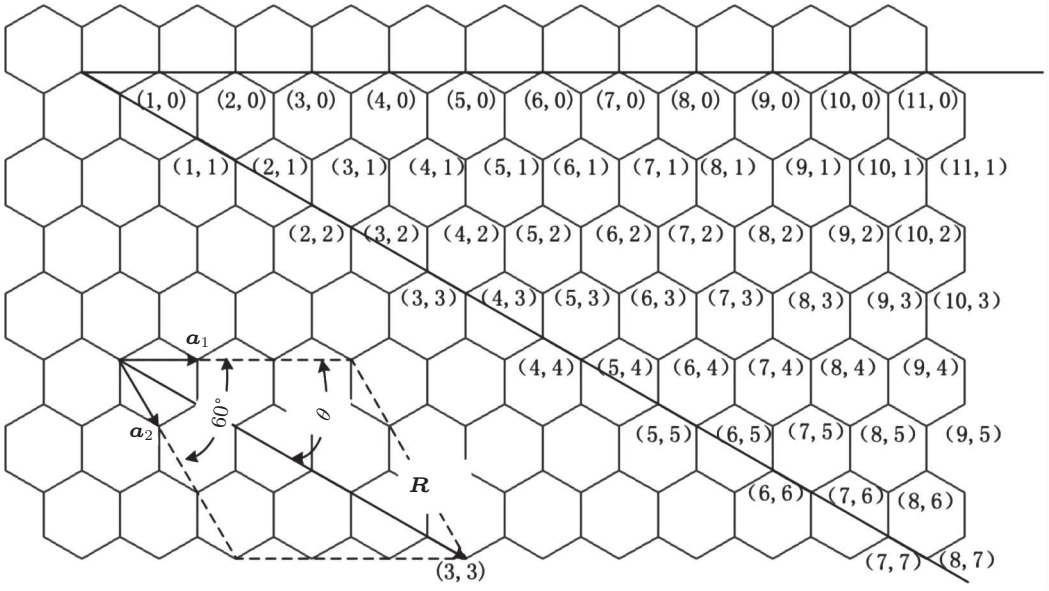


Fig. 1. Graphene hexagonal lattice with lattice vectors a_1 and a_2. Configuration of SWNTs with different chiralities.

2.2. NEMD approach

NEMD was employed in this paper to calculate the thermal conductivity of SWNTs. The simulation structure was demonstrated in Fig. 2: two ends of a SWNT were fixed as a frozen wall, of which the atoms were kept still to prevent sublimation during the whole simulation process. Beside the two walls, the area colored in red was a hot region and the area colored in blue was a cold region.

The non-equilibrium conductance is established through adding heat current to the system, thus producing a stable temperature gradient, and then thermal conductivity can be obtained via Fourier's law

$$\lambda = -\frac{J}{\partial T/\partial z}, \tag{1}$$

in which J is the heat flux, and $\partial T/\partial z$ is the temperature gradient along the z axial direction.

In a molecular dynamics (MD) simulation of this paper, an Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO)[22] potential is adopted to describe the carbon–carbon interatomic interactions. AIREBO has been

widely used to study the heat transfer problems of carbon materials.[19] It has the following form:

$$E = \frac{1}{2}\sum_{i}\sum_{j\neq i}\left[E_{ij}^{\mathrm{REBO}} + E_{ij}^{\mathrm{LJ}} + \sum_{k\neq i,j}\sum_{l\neq i,j,k} E_{kijl}^{\mathrm{TORSION}}\right]. \quad (2)$$

Here, E^{REBO} used to describe the interactions between covalent atoms has the same form as that of hydrocarbon REBO potential, which was established by Brenner,[24] and the coefficients are basically no different from the Brenner potential function, that is,

$$E_{ij}^{\mathrm{REBO}} = V_{ij}^{\mathrm{R}} + b_{ij}V_{ij}^{\mathrm{A}}, \quad (3)$$

where V_{ij}^{R} and V_{ij}^{A} are the repulsive and attractive interaction energies between atoms i and j; the b_{ij} term represents the many-body bonding parameter.

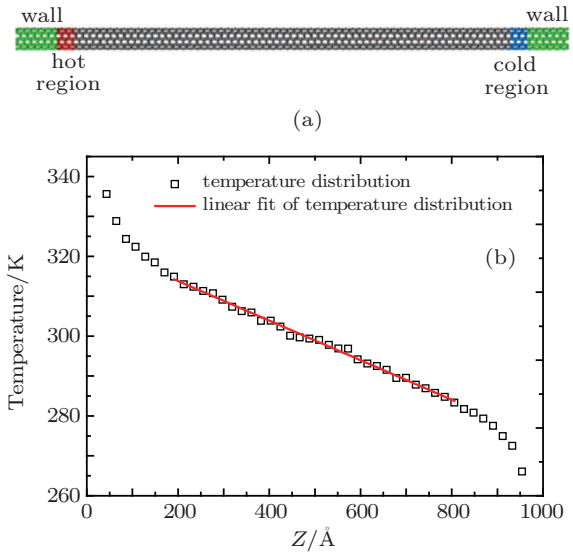


Fig. 2. (color online) (a) Schematic structure of SWNTs used in MD simulation and (b) a typical temperature distribution of SWNTs with chirality (12, 12).

The E^{LJ} term that is responsible for the long-range interaction between non-bonded atoms is based on the Lennard–Jones 12-6 potential and is defined as

$$E_{ij}^{\mathrm{LJ}} = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right], \quad (4)$$

The E^{TORSION} term is used to describe dihedral-angle inter-molecular interactions whose role is deemed to be not significant in the analysis of carbon nanotubes,[22] hence, it is not considered in the present work.

The bond length of carbon–carbon in simulations is 1.44 Å, and the cross-sectional area of a SWNT is the ring area $S = \pi \cdot D \cdot \delta$, in which, D is the diameter of a SWNT, δ is the wall thickness that uses a Van der Waals thickness of 3.4 Å.[17] In the NEMD simulation, a stable heat current is added into the system to establish a stable temperature gradient. A certain amount of kinetic energy is added into the hot region while at the same time, the same amount of kinetic energy is taken from the cold region. These processes are realized using a variant of the algorithm proposed by Jund and Jullien,[25] which conserves the total momentum of the system. Heat flux is added into (or taken from) the corresponding region by rescaling the velocity of atoms.

All MD simulations are accomplished with using the LAMMPS[26] packages, in time steps of $\Delta t = 0.1$ fs. Firstly, to make the whole system relaxed at a room temperature of 298 K, velocity and NVE (constant volume without thermostat) relaxation are rescaled for 100 ps. After equilibration, a constant heat current is applied to the system for another 400 ps, then a steady temperature gradient is achieved across the system. Carbon nanotubes are separated into slabs with the same thickness along the axial direction (heat flowing orientation). The local temperature of each slab can be obtained through kinetic energy of the in-slab atoms. The last 0.1 ns is averaged to obtain the smooth temperature profile. Figure 2(b) shows the temperature distribution of (12,12) SWNT along the tube length. It is $\sim$ 900 Å long between the hot region and the cold region. For the mismatching between internal phonons and phonons in the hot or cold regions, there are jumps in the temperature distribution. The middle section, however, is linear. So we calculate the thermal conductivity of SWNT through fitting the middle linear part of temperature configuration, which is shown in Fig. 2(b), the solid line is the temperature fitting line of the SWNT. Then the temperature gradient is easily obtained by calculating the slope of the temperature fitting line. In addition, the error of thermal conductivity can be computed through the linearity deviation.

3. Results and discussion

Our simulations are performed for four groups of SWNTs: a) Group A is smaller-diameter shorter SWNTs with a tube length of 20 nm; b) Group B is larger-diameter shorter SWNTs with a tube length of 20 nm; c) Group C is smaller-diameter longer SWNTs with a tube length of 50 nm; d) Group D is larger-diameter longer SWNTs with a tube length of 100 nm.

To more objectively reflect the influence of chirality on thermal conductivity, the tube lengths of all SWNTs that flowed by heat current in simulations are fixed at the same length in one group, excluding the effect resulting from the tube length. As can be seen from Table 1, diameters of all SWNTs are more or less the same, with a standard error of 0.14 Å for the smaller-diameter SWNTs and 0.12 Å for the larger-diameter SWNTs. So it is possible to ignore the effect of diameter. Moreover, since the tube length is short for simulations of the first two groups, where phonon transfer is

purely ballistic, thermal conductivity is almost independent of diameter according to the literature.[17] Consequently, chirality is the most important factor that affects thermal conductivity of SWNT in our simulation. Heat current is adjusted in accordance with the system size to establish a more reasonable temperature gradient. If the temperature gradient is too small, statistical temperature fluctuation will result in a larger error, while the reverse case will lead to nonlinear effects.[27] Due to the small diameter, the number of atoms is small in Group A and so it is in Group C, thus the heat currents allocated to the systems in Group B and Group D are 1.6×10^{-7} W and 3.2×10^{-7} W respectively.

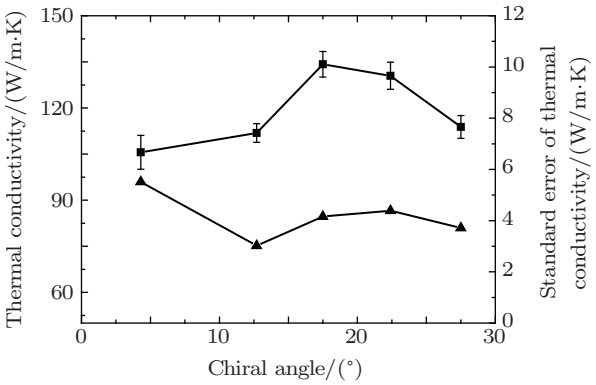


Fig. 3. Chiral-angle-dependent thermal conductivity and standard error of the thermal conductivity of smaller-diameter shorter SWNTs with a tube length of 20 nm (Group A), where the solid square represents the thermal conductivity and the solid triangle denotes the standard error of thermal conductivity.

Figure 3 shows that the thermal conductivity ranges from 105.56 W/m·K to 134.19 W/m·K in Group A. The thermal conductivity of chiral SWNTs first increases and then decreases as the chiral angle increases, and the lowest value happens at a chiral angle of 4.3° while the highest value appears at a chiral angle of 17.5°. The difference between the maximum and the minimum is 28.63 W/m·K, corresponding to a relative percentage difference of about 27.1%. The large discrepancy in the thermal conductivity of SWNTs between different chiral angles is shown in Fig. 3, which proves that chirality indeed exerts an influence on thermal conductivity. Since samples in this group do not include zigzag and armchair SWNTs, corresponding to chiral angles of 0° and 30°, respectively, the results reflect that the thermal conductivity of chiral SWNTs is dependent on their chiral angle. The thermal conductivity of SWNTs with a larger chiral angle is higher than that of SWNTs with a smaller chiral angle. In addition, figure 3 demonstrates the standard error of thermal conductivity that originates from linearity deviation. It lightly changes with the chiral angle, but is near 4 W/m·K and kept at 5%.

Group C, which is the longer version of Group A, shows a small difference from Group A. The thermal conductivity ranges from 122.16 W/m·K to 139.10 W/m·K, which narrows the gap between the maximum and the minimum down to 16.94 W/m·K, corresponding to a relative percentage reduction of about 13.8%, which are shown in Fig. 4. Moreover, that thermal conductivity of SWNTs with a larger chiral angle is higher than that of SWNTs with a smaller chiral angle is also clearly demonstrated in this group of simulations. But on the whole, we can conclude that the influence of chirality is less significant on these longer SWNTs. The standard error of thermal conductivity changes less with chiral angle. It keeps around 2 W/m· K, within 2%. Compared with the results from Group A, the distribution of thermal conductivity and its standard error in this group is much gentler. Consequently, increasing tube length leads to the increase of thermal conductivity[17,28] but weakens the influence of chirality. With the tube length getting longer, at the average temperature more atoms are included, which naturally brings about a smaller error range and smooth distribution. From the comparison between these two groups of simulations, the conclusions can be drawn that an effect of the chirality on the thermal conductivity of those smaller-diameter SWNTs is not so obvious, and becomes much more inconspicuous with increasing tube length, and so, tube length is a promoting factor for thermal conductivity.

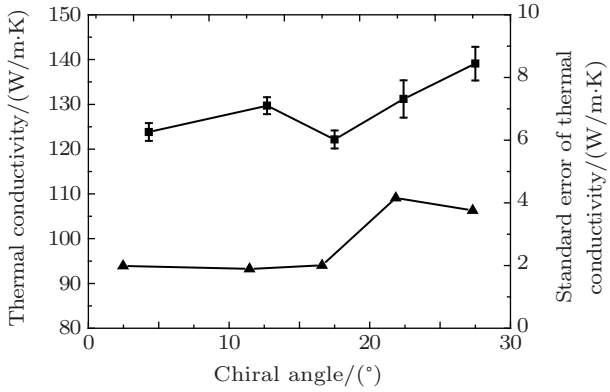


Fig. 4. Chiral-angle-dependent thermal conductivity and standard error of thermal conductivity of smaller-diameter longer SWNTs with a tube length of 50 nm (Group C) where the solid square represents the thermal conductivity and the solid triangle denotes the standard error of thermal conductivity.

The zigzag and armchair SWNTs are not included in the simulations of the above two groups and the samples lack, owing to the small diameter, which leads to scarce selective SWNTs with almost the same diameter, so it is necessary to conduct the simulations again with larger-diameter SWNTs.

Table 1 gives a view of the geometric parameters of larger-diameter SWNTs. The diameters are some 16.60 Å, which leads to the sample being twice as large as the smaller-diameter ones. Most importantly, the zigzag and the armchair SWNTs are included in these groups. In Fig. 5, the range of

thermal conductivity is from 98.15 W/m·K to 150.53 W/m·K for Group B in which the diameter of the sample increases but the tube length keeps constant compared with those in Group A. The difference between the maximum and the minimum is 52.4 W/m·K, corresponding to a percentage error of about 50%. This larger discrepancy demonstrates that chirality has an important influence on thermal conductivity, which is more significant than that in the smaller-diameter groups. That is to say, the effect of chirality becomes more obvious with the increase of SWNT diameter. The thermal conductivity of SWNT with a larger chiral angle is much higher than that of SWNT with a smaller chiral angle as a whole, *n* which is illustrated in Fig. 5, and the thermal conductivity of an armchair SWNT is higher than that of a zigzag SWNT. Compared with Group A, the increase of diameter does not improve the thermal conductivity, which accords well with the conclusion summarized in the literature.[23]

Table 1. Geometric parameters of SWNTs: the part above including five samples is for SWNTs with the smaller diameter and the part below including ten samples is for SWNTs with the larger diameter.

Properties	Smaller-diameter SWNTs									
Chirality	(11,1)		(10,3)		(9,4)		(8,5)		(7,6)	
Diameter/Å	9.16		9.36		9.16		9.02		8.95	
Chiral angle/(°)	4.3		12.7		17.5		22.4		27.5	
Properties	Larger-diameter SWNTs									
Chirality	(21,0)	(20,2)	(19,3)	(18,5)	(17,6)	(16,8)	(15,9)	(14,10)	(13,11)	(12,12)
Diameter/Å	16.67	16.73	16.41	16.63	16.41	16.80	16.67	16.58	16.52	16.50
Chiral angle/(°)	0	4.7	7.2	11.9	14.6	19.1	21.8	24.5	27.2	30

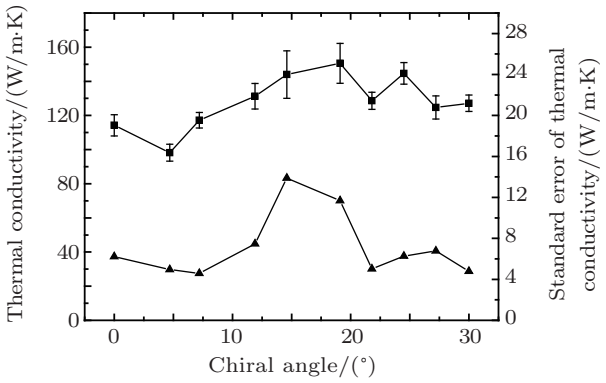


Fig. 5. Chiral-angle-dependent thermal conductivity and standard error of thermal conductivity of larger-diameter shorter SWNTs with tube length of 20 nm (Group B), where the solid square represents the thermal conductivity and the solid triangle represents the standard error of thermal conductivity.

When tube length augments to 100 nm, thermal conductivity increases two or three fold. The extent of the increase is much more obvious than in the previous simulations. The maximum is 380.45 W/m·K, while the minimum is 325.95 W/m·K, and their difference is 54.5 W/m·K, corresponding to a relative percentage difference of 16%. From the results shown in Fig.6, it can be seen that thermal conductivity of a zigzag SWNT is smaller than that of an armchair one, while the difference in thermal conductivity between different chiral SWNTs becomes smaller. The change tendency from Group B to Group D is similar to that from Group A to Group C, where the longer SWNT includes more phonon modes then reduces the influence of chirality. However, the results demonstrated in our simulations are different from what was suggested in the literature.[20] In the Zhang *et al.* work,[20] only three SWNTs, i.e., (20, 0), (11, 11), and (10, 13), which respectively represent a zigzag SWNT, an armchair SWNT, and a chiral SWNT, were investigated to discuss the relationship between their thermal conductivity and chirality. A homogenous non-equilibrium Green–Kubo method based on the Brenner potential[29] was employed. In their work, periodic conditions were used to model infinitely long systems and the SWNTs were less than 3 nm in length. This treatment could cause artifacts,[30] because phonons with a wavelength greater than twice that of the simulation-domain size would be cut off. Then we assume that the chirality dependence in their work is not so referential. In the Zhang and Li work,[31] using the same method as ours, they showed that the thermal conductivity of an armchair SWNT is larger than that of a zigzag one, which is consistent with our results, even though they concluded that thermal conductivity is not so sensitive to the chirality as electronic conductivity. In Fig. 6, we can see that the standard error of thermal conductivity for the longer system is around 4 W/m·K, within 1%. It is smaller than that of the shorter ones, which is due to the same reasons that the number of atoms incredibly increases in each slab as the tube length and diameter increase. As for chiral SWNTs, that the ones with a larger chiral angle are greater than the ones with a smaller chiral angle is fading compared with what is concluded in the previous simulations where the influence from chirality is still obvious. But this distribution tendency is close to what has been shown in the literature,[21] but it does not exclude the diameter effects, since the diameters of SWNTs were largely different in the literature. At the same time, when the tube length becomes longer, a thermal conductivity increase is much more signifi-

cant in Group D than in Group C, which is partially because of the larger-diameter dependence where nonlinear phonon collisions increase.[17]

We repeated the above simulations at least three times, and the results are within minor difference. From the analyses of the simulations on four groups, we find that the effect of chirality on thermal conductivity holds when the tube lengths of SWNTs are shorter and the diameters of SWNTs are larger, while its influence weakens when the tubes turn longer or the diameter decreases. The longer the SWNTs become, the higher the thermal conductivity is and the smaller the calculating error is. In addition, simulation results reflect that the chiral SWNT with a larger chiral angle has a higher thermal conductivity than the others, and thermal conductivity of an armchair SWNT is larger than that of a zigzag one.

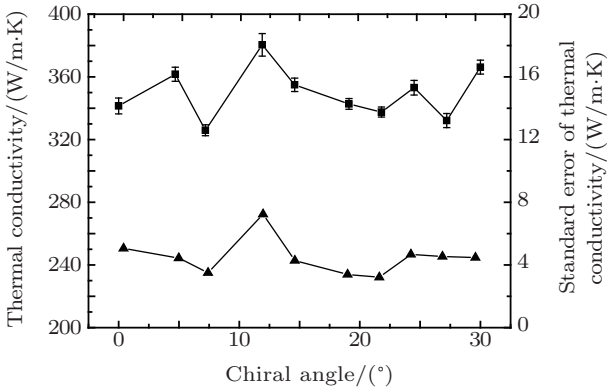


Fig. 6. Chiral-angle-dependent thermal conductivity and standard error of thermal conductivity of larger-diameter shorter SWNTs with a tube length of 100 nm (Group D), where the solid square represents the thermal conductivity and the solid triangle denotes the standard error of thermal conductivity.

To better understand the mechanism of the above phenomenon, we calculate vibrational density of states (VDOS) of SWNT in Group B by taking the Fourier transform of the atomic velocity autocorrelation function (VACF).[32] The results demonstrate that there is little divergence of VDOS in the ten different systems from the view of the full frequency range (shown in the inset of Fig. 7), which indicates that the middle and high frequency distributions of VDOS are identical. However, the low-frequency range shows differences, which is illustrated in Fig. 7. As can be seen, an armchair SWNT with a chiral angle of 30° has more vibration modes at low frequency than a zigzag SWNT with a chiral angle of 0°, which leads to a higher thermal conductivity. This is in accordance with our previous calculation results, which are demonstrated in Figs. 3–6. On the other hand, we notice that the difference is not so significant between the two samples, which means that the difference in thermal conductivity could not be large, either.

From Fig. 8, we can relate the thermal conductivity to the length–diameter ratio when chiral angles are 4.5° and 27.2°, respectively. As can be seen, the difference in thermal conductivity between the two chiral SWNTs becomes narrower as the length–diameter ratio increases. This indicates that the influence of chirality on the thermal conductivity of SWNTs is more significant when the length–diameter ratio is smaller. Besides, compared with length, diameter and chirality have a minor effect on the thermal conductivity of SWNTs.

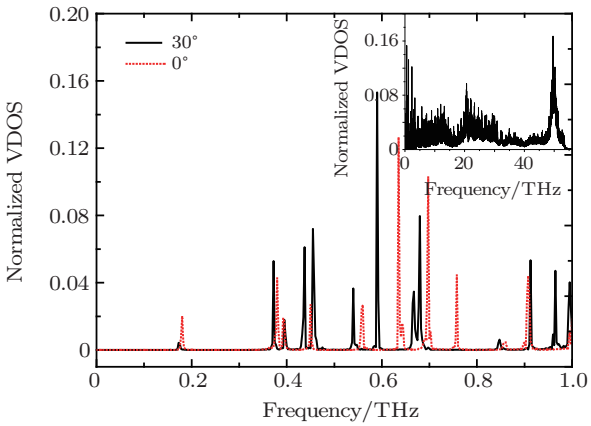


Fig. 7. (color online) Normalized vibrational densities of states of SWNTs (in Group B) with different chiralities, where the thick line represents the data of an armchair SWNT with a chiral angle of 30° and the dot line is for a zigzag SWNT with a chiral angle of 0°.

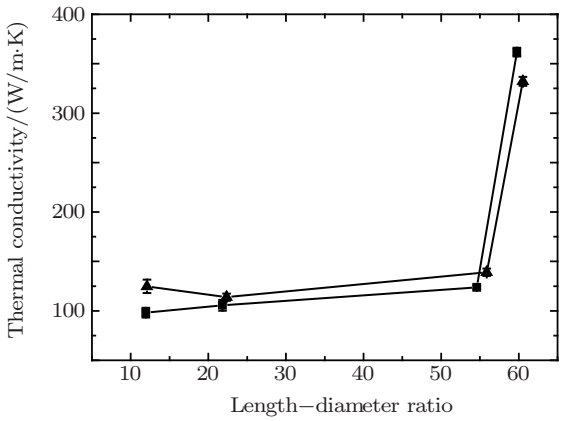


Fig. 8. Variations of thermal conductivity with length–diameter ratio, where the solid square represents a SWNT with a chiral angle of 4.5° and the solid triangle is for a SWNT with a chiral angle of 27.2°.

4. Conclusions

In this work, thermal conductivity values of SWNTs with different chiralities are calculated to investigate the influence of chiral angle on the thermal conductivity of SWNTs, using the NEMD approach. Four sets of SWNTs are examined. Results indicate that (i) when the tube length is relatively short, the influence of chirality on the thermal conductivity of SWNTs is more obvious than when the tube length is longer; (ii) the effect of chirality is more significantly shown in larger-diameter SWNTs, so when the tube length becomes longer, the thermal conductivity is improved while the influence of chirality on the thermal conductivity decreases, but when the diameter becomes larger, the thermal conductivity does not change

much while the influence of chirality on the thermal conductivity increases; (iii) with a larger chiral angle, the thermal conductivity is greater and that of zigzag SWNTs is smaller than that of armchair ones; (iv) the increase of tube length reduces the standard error of thermal conductivity. From the above discussion, we can safely draw a conclusion that the chirality has an important influence on shorter SWNTs while the diameter takes its place when the tubes become longer. Although from the simulation results of the four SWNT goups in this paper, we do not find an intensive dependence of chirality on the thermal conductivity, the analyses of the present work suggest that we should further investigate the influence of chirality with more divergent conditions, such as SWNTs with larger diameters or under higher or lower environment temperatures in future works.

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