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Defect, temperature, and strain effects on lattice heat conductivity of egg-tray graphene

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Abstract

Micro and nano devices generally have the characteristics of high performance and compact size, so their own heat transfer and heat dissipation problems are becoming more and more serious. Therefore, it is necessary to clarify the heat transport mechanism in the micro-nano structure by analyzing the heat transport properties of nanomaterials, and then control the thermal conductivity of nanodevices. We have investigated the lattice heat transfer of egg-tray graphene using non-equilibrium molecular dynamics simulations. Three structures (I, II and III) are studied according to the number of hexagons as 10, 16, and 56 respectively. The increases of lattice thermal conductivity with an increase of length in sub-microns implies the large mean free path of phonons in egg-tray graphene, similar as that of graphene. The large-size-limit thermal conductivity is 43, 45, and 60 W/m·K for I, II, and III respectively, much smaller than that of graphene (393 W/m·K) in our model. The thermal conductivity decreases with an increase of strain, as well as temperature. The heat transfer performance of Structure-II is sensitive to both phonon modes and phonon quantities in compression, while in tension it is determined only by the phonon modes. Our results may be useful in thermal conductivity engineering and heat transfer management in egg-tray graphene.

Keywords: egg-tray graphene; molecular dynamics; thermal conductivity; phonon density of states
1. Introduction

Since its discovery, graphene has been extensively studied and used for its outstanding properties [1], such as excellent optical [2], electrical [3] and mechanical properties [4], and high thermal conductivity [5]. Structural defects are inevitable during the material manufacturing process. Many defects have been observed in graphene, such as vacancies [6], Stone-Wales(SW) defects [7], pentagon–octagon–pentagon (5-8-5) defects [8], etc. On one hand, these structural defects in graphene can adversely impair the mechanical properties [9] and heat transfer properties [10, 11]. On the other hand, the graphene’s adsorption characteristics and ion transport properties can be improved [12-14]. In addition, the zero electronic band gap of pristine graphene greatly limits its application in electronics. Therefore, many methods are applied to open the band gap of graphene. Among these efforts, the introduction of defects is proved to be an efficient approach adjusting the electronic characteristics of graphene. [15].

Egg-tray graphene is a class of graphene derivatives with egg-tray shape. Studies have found that its electronic properties show great changes, ranging from semi-metallic to semi-conducting. And the ability to adsorb lithium atoms is stronger than that of perfect graphene. Therefore, it is of great significance to study this new type of graphene derivative, which can broaden the application field of graphene. In addition, the problem of heat dissipation in micro-nano devices is a very serious problem. The research on the thermal conductivity of the egg-tray graphene will provide a theoretical basis for the selection of micro-nano devices.
Micro-nano-scale heat transfer is an emerging research field. Micro-nano devices have the two major characteristics of high performance and compact size, which determines that the micro-nano devices have higher consumption, and the energy is limited in a small volume space, and part of the energy conversion will be converted into heat energy. Therefore, there are serious heat dissipation problems in micro-nano devices. The heat transfer at the micro-nano scale is different from the macro heat transfer. On the macro scale, the heat transport performance of a material is an essential attribute of the material, and generally does not change with the change of the material structure. In the micro-nano scale, the size of the structure, the external environment, and the change of the structure can significantly change the thermal conductivity of the model. In this regard, one of the key parameters is the thermal conductivity. Scholars have discovered that graphene has a high thermal conductivity [17-19]. Teng et al. [20] found that the thermal conductivity of graphene increases with increasing length. The heat transfer of graphene was analyzed by phonon density of states. In addition, the results show that it decreases as the defect density increases [21]. Graphene's thermal conductivity is sensitive to tensile strain. Ning et al. [22] studied the thermal conductivity of graphene under various strains, and analyzed the relationship between phonon frequency, strain and thermal conductivity.

In this work, non-equilibrium molecular dynamics methods were used to study the heat transfer of three egg-tray graphene structures and compared with graphene.
The factors affecting heat transfer were also discussed. In addition, the transport mechanisms in Structure-II were further investigated by phonon density of states (PDOS). We found that the Structure-II exhibits different heat transfer mechanisms under tensile strains and compressive strains.

2. Materials and Methods

Three egg-tray graphene structures were selected as research objects, and their heat transfer properties were analyzed. They differ in the number of hexagons surrounded the pentagons and heptagons, which results in different lattice constants and depths. The atomic structures of egg-tray graphene are shown in Fig. 1. Table 1 shows the unit cell sizes of different egg-tray graphenes. These egg-tray graphene structures are constructed by combining the pentagon and heptagon defects in graphene, and each unit cell of egg-tray graphene contains two pentagons and two heptagons.

**Table 1.** The unit cell sizes of three egg-tray graphenes [16].

<table>
<thead>
<tr>
<th>Type</th>
<th>No. of C atoms</th>
<th>5 ring</th>
<th>6 ring</th>
<th>7 ring</th>
<th>a(Å)</th>
<th>b(Å)</th>
<th>γ(°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>28</td>
<td>2</td>
<td>10</td>
<td>2</td>
<td>7.99</td>
<td>8.92</td>
<td>90.00</td>
</tr>
<tr>
<td>II</td>
<td>40</td>
<td>2</td>
<td>16</td>
<td>2</td>
<td>7.64</td>
<td>12.86</td>
<td>90.00</td>
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<tr>
<td>III</td>
<td>120</td>
<td>2</td>
<td>56</td>
<td>2</td>
<td>16.12</td>
<td>16.59</td>
<td>90.00</td>
</tr>
</tbody>
</table>
Fig. 1. The structures of egg-tray graphenes. (a) The structure of egg-tray graphene I; (b) The unit cell of Structure I; (c) The structure of egg-tray graphene II; (d) The unit cell of Structure II; (e) The structure of egg-tray graphene III; (f) The unit cell of Structure III.
Based on the egg-tray graphene model, the thermal conductivity has been studied by MD simulations, which is a well-established and suitable approach for atomistic modeling [23]. Here, a large-scale atomic/molecular massively parallel simulator (LAMMPS) has been used for simulation [24]. Structural analysis of egg-tray graphene was conducted using the visualization software OVITO [25], and data processing of egg-tray graphene was performed using Python. The Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential [26] was used to describe C-C atom interactions and the AIREBO force field parameters are selected according to Reference [26]. The AIREBO potential is developed on the basis of REBO and is widely used in modeling graphene [27-30] and the calculation of thermal conductivity of hydrocarbon systems [31-33]. Periodic boundary conditions were applied in all three directions.

At present, there are three methods for calculating thermal conductivity using molecular dynamics: equilibrium molecular dynamics simulation method (EMD) [34], non-equilibrium molecular dynamics simulation method (NEMD) [35], and reverse nonequilibrium molecular dynamics methods (RNEMD) [36]. The EMD method is difficult to deal with substances other than elemental substances, and the simulation is usually performed under the micro-canonical or canonical ensemble. The time-dependent convergence process of micro-regular to heat flow is an exponential curve, so the simulation time and step size are usually very long and the error is large [34]. Since the RNEMD method only exchanges the speed of the atoms, if the atomic masses of the exchanged atoms are different, the energy will not be
conserved during the exchange, which will make the system energy lower and lower. This article is based on the NEMD method to analyze the thermal conductivity of graphene nanostructures. By adding or decreasing the same amount of heat to the hot and cold slabs at the same time, the temperature gradient of the system is formed in the direction of heat flow, and Fourier law is used to calculate the thermal conductivity. First, the egg-tray graphene structures were relaxed in the isothermal-isobaric (NPT) set for 100 ps at a temperature of 10 K. The time-step was set to be 0.001 ps. The velocities of the atoms were controlled by using the Nosé-Hoover temperature thermostat [37], and the velocity Verlet algorithm was used to integrate the Hamiltonian equations of the determined motion. Next, the equilibrium system was gradually heated from 10 K to $T$ for 100 ps. $T$ was the temperature at which the thermal conductivity was calculated. Then, the system was relaxed at a temperature of $T$ for 200 ps under NPT set to obtain an equilibrium state. Finally, the system was relaxed for 300 ps under NVE set to achieve a nonequilibrium steady state. After relaxation, the thermal conductivity of the relaxed model was analyzed. As shown in Fig. 2, a heat flux was simulated by adding heat at 1/4 of the model (hot slab) and reducing the same amount of heat at 3/4 of the model (cold slab). Then the thermal conductivity of the model was calculated. During this process, the rate of heat addition was chosen to be 0.2586 eV/ps. And the thickness of the three kinds of egg-tray graphenes (Structure-I, Structure-II and Structure-III) was selected to be 3.3 Å, which is the same as the thickness of graphene [38]. The calculation of the thermal conductivity is shown in the Supplementary documents.
Thermal conductivity is closely related to phonon transport. Therefore, the PDOS has been studied to understand the mechanism of heat transfer. The PDOS calculation and data results are shown in the Supplementary Information.

Fig. 2. The simulation model of the NEMD calculations and temperature gradients of various models. (a) The simulation model of the NEMD calculations, the hot slab and cold slab are shown in red; (b) Temperature gradients of various models.

3. Results and discussion
3.1 Thermal conductivity of pristine egg-tray graphene nanoribbons at room temperature

The thermal conductivity of three egg-tray graphene models at a length of 30 nm was calculated at room temperature (300 K) and compared with the graphene model. Fig. 2 (b) shows the temperature gradients of the four models. And thermal error-bars are also marked in the figure. During calculating the thermal conductivity, the same energy is added and reduced to the hot slab and the cold slab, respectively, thereby forming a temperature gradient.

After fitting the curves in the Fig. 2 (b), the temperature gradients of the three egg-tray graphene structures and graphene were 0.47452, 0.46126, 0.43926 and 0.10105 K/nm, respectively. The thermal conductivities of Structure-I, Structure-II, Structure-III and graphene were calculated to be 23, 28, 35, and 102 W/m·K, respectively. Thermal conductivity decreases with increasing temperature gradient.

Thermal conductivity of graphene is much higher than that of egg-tray graphene. This difference could be reflected by two factors. On the one hand, due to the small temperature gradient of graphene during heat transfer, which indicates good thermal conductivity. On the other hand, there are pentagonal and heptagonal defects in egg-tray graphene, which will undoubtedly reduce the thermal conductivity of the material. In this work, in order to better study the thermal conductivity of egg-tray graphene, the relationships between length, temperature and strain and thermal conductivity were discussed.
3.2 Length dependence of thermal conductivity of egg-tray graphene

The thermal conductivity of graphene has a strong length dependence [39]. We expect the similar behaviors of egg-tray graphene. Therefore, the thermal conductivities of egg-tray graphene structures were studied for various lengths, in the range of 30-150 nm. All the thicknesses are kept the same as that of graphene for ease of comparison.

As length increases, the difference in thermal conductivity between graphene and egg-tray graphene structures is enlarged (Fig. 3). In the testing range of 30-150 nm, the thermal conductivity of the egg-tray graphene is length-dependent. With the length longer than 110 nm, the growth trend of each egg-tray graphene gradually set to slow. The length effect, however, is smaller than that of egg-tray graphene structures.
The three kinds of egg-tray graphene in 150 nm ribbons also have different temperature gradients. Those curve fitting parameters are summarized in Table S1 in Supplementary Information. The temperature gradient in the three structures is in increase order as Structure-III < Structure-II < Structure-I, indicating that Structure-III has the highest thermal conductivity. This result is consistent with the results of Fig. 3.

The difference in thermal conductivity of the three egg-tray graphene structures reflects the difference of their atomistic structures. It has been found that Structure-III is the most stable structure of all egg-tray graphene structures [16], and therefore has the highest thermal conductivity. The difference between Structure-I and Structure-II is the difference in the number of hexagons between pentagons and heptagons. Each unit cell of Structure-I contains 10 hexagons, while each unit cell of
Structure-II contains 16 hexagons, which results in different lattice constants and depths. The thermal conductivity increases with the increase of the number of hexagons in the egg-tray graphene.

3.3 Ideal phonon thermal conductivity of egg-tray graphene in infinite length

For non-equilibrium molecular dynamics simulations, the thermal conductivity is limited by the size of the model. The thermal conductivity of the model at infinite length can be roughly estimated with

\[ \frac{1}{\kappa} = \frac{1}{\kappa_\infty} \left( \frac{l}{L} + 1 \right) [37], \]

where \( \kappa \) is the model thermal conductivity, \( \kappa_\infty \) is the thermal conductivity at infinite length, \( l \) is the effective phonon mean free path, and \( L \) is the model length. The curves of reciprocal of thermal conductivity and reciprocal of length of graphene and egg-tray graphene structures are plotted in Fig. 4(a). Those curve fitting parameters are summarized in Table S2 in Supplementary Information. The intercept of the fitted curve is the inverse of the thermal conductivity of the egg-tray graphene at infinite length. The calculated thermal conductivity of Structure-I, Structure-II, Structure-III and graphene are 43, 45, 60, and 393 W/m·K, respectively, at infinite length, as shown in Fig. 4(b). The thermal conductivity of egg-tray graphene is much smaller than that of graphene, suggesting the high sensitivity of pentagonal and heptagonal defects on the thermal conductivity of graphene.
3.4 Strain effects

Thermal conductivity of graphene and carbon nanotubes is sensitive to strain [22, 43]. It is expected that the strain might have influence on the lattice heat conductivity. To quantify the strain effect, tensile and compressive strains of 0-0.1 were applied to the x-direction of the three egg-tray graphene structures to analyze the relationship between tensile and compressive strains and thermal conductivity and compared it with graphene. We apply a fixed strain rate of $10^{-9}\text{s}^{-1}$ to the system.
Fig. 5. Effects of tensile and compressive strains on thermal conductivity of egg-tray graphene. (a) The models of Structure-II under strain; (b) The curves of thermal conductivity versus strain of various models; (c) The stress distribution of Structure-II under strain.

The morphologies of Structure-II under strain are shown in Fig. 5 (a). The stress distribution of Structure-II under strain are displayed in Fig. 5 (c). Under tensile and compressive strains, the thermal conductivity decreases with increasing strain (Fig. 5 (b)). Our results agree with previous analysis of graphene thermal conductivity [22, 43]. The thermal conductivity of graphene is about 3 times that of egg-tray graphene.
The strain effect can be understood as follows. When tensile strain is applied to egg-tray graphene, the stress in the egg-tray graphene became larger with increasing strain (see Fig. 5 (c)), and the bonding ability between the atoms weakens. According to the phonon scattering theory, weak bonding ability relatively strengthens the atomic vibration, thereby increasing the number of phonons emitted by the atomic vibration. This will result in an increase in phonon scattering and a decrease in average free path of phonons. In turn, applied tensile strains reduce thermal conductivity. When compressive strain is applied to egg-tray graphene, its structure will bend, which will lead to enhanced phonon scattering and reduce thermal conductivity [43].

![Fig. 6.](image)

**Fig. 6.** (a) The stress-strain curve of egg-tray graphene and (b) the change curve of elastic modulus and tensile strength.

Fig. 6 shows the stress-strain curves of egg-tray graphene structures, as well as their elastic modulus and tensile strength. It could be found that graphene is significantly different from egg-tray graphene structures, and the tensile strength and elastic modulus of graphene are both greater than that of egg-tray graphene. For the
elastic modulus of egg-tray graphene structures, Structure-I, Structure-II, and Structure-III gradually increase; and compared of tensile strength, Structure-II is the largest, structure-III is second, and Structure-I is the smallest. The elastic modulus and strength limit values of the three structures differ little.

3.5 Phonon density of states

To have more atomistic insights on the mechanism of thermal conductivity, we further analyzed the transport mechanisms of Structure-II using the phonon density of states (PDOS)[44, 45], as shown in Fig. 7. The PDOS calculation and data results are shown in the Supplementary Information.

![Fig. 7. The PDOS of Structure-II under strains. (a) The PDOS of Structure-II under tensile strains; (b) The PDOS of Structure-II under compressive strains.](image)

The PDOS of graphene and Structure-II are quite different. With strains, high-frequency phonons play a more important role in graphene [22]. The peak
value of the high-frequency phonons of graphene is near 52-53 THz (inset of Fig. 7 (a)). The peak value of the high-frequency phonons of egg-tray graphene is near 50-52 THz, which is slightly smaller than the value of graphene. The egg-tray graphene structure has larger phonon vibrations, and the number of low-frequency phonons and high-frequency phonons is equivalent, which will lead to a decrease in the average speed of the system. This phenomenon is also reflected in Fig.7 (b).

From the point of view of phonon scattering, a large number of phonons will aggravate the collision between phonons. When phonon scattering increases, the average free path is reduced, leading to a reduction in thermal conductivity.

As can be seen from Fig.7 that the PDOS of Structure-II is different under tensile and compressive strains, indicating that the factors affecting the thermal conductivity of Structure-II are different under both tensile and compression strains. The PDOS under tensile strains is displayed in Fig. 7 (a). In the low frequency band, the difference in PDOS of Structure-II under different tensile strains is not obvious. As the strain increases, the high-frequency phonon peak shifted to the left, which indicates that the number of high-frequency phonons decreases when tensile strain is applied. Some high-frequency phonons are converted to low-frequency phonons. This means that the reduction of average frequency of the phonon results in a reduction in system energy. Since the phonons are the main carrier in the heat transfer process, a decrease in the total energy of the system means a reduction in the average velocity of the phonons. As a consequence, the thermal conductivity of the system decreases. When tensile strain is applied to graphene, the high-frequency
phonon peak shifted to the left. Therefore, thermal conductivity decreases. Our
result agree with literature [33].

The PDOS under compressive strains is illustrated in Fig 7 (b). There is no
obvious left-shift phenomenon of high-frequency phonons under compressive strains.
The PDOS of egg-tray graphene is larger and the number of excited phonons is
larger without strain, leading to a large thermal conductivity. Under compressive
strain, the phonon mode and the number of phonons affect the thermal conductivity
of egg-tray graphene. In the low frequency band, the difference in PDOS of
graphene under different compressive strains is not obvious. When the strain
increases, the high-frequency phonon peak shifted to the left (see illustration in Fig.
7 (b)).

In general, under the effects of both tensile and compressive strains, the thermal
conductivity decreases with increasing strains, but the mechanism is different. Under
tensile strains, the change in phonon mode leads to the change in heat transfer
performance of egg-tray graphene; under compressive strains, the combination of
phonon mode and phonon quantity causes a change in its heat transfer performance
of egg-tray graphene. By applying different strains to the egg-tray graphene
structures, the thermal conductivity of the structures can be adjusted, which suggests
a feasible approach to engineering the thermal conductivity of new materials.

3.6 Temperature effect

The temperature has profound impact on the thermal conductivity of the
material. The curves of the thermal conductivity graphene and three egg-tray graphene structures as a function of temperature are displayed in Fig. 8. It was found that the thermal conductivity of graphene increases first and then decreases with increasing temperature, while the thermal conductivity of the three egg-tray graphene structures decreases with increasing temperature. Our results of graphene agree with previous studies. [41, 42], validated our model and method.

![Graph showing thermal conductivity vs temperature]

**Fig. 8.** Effects of temperature on thermal conductivity of various models.

Despite the difference in thermal conductivity, the three egg-tray graphene structures show the same temperature dependence of thermal conductivity at 100-800 K. The thermal conductivity of the three egg-tray graphene structures decreases with increasing temperature. Such a trend can be understood as follows. In solid state physics, $\kappa = \frac{1}{3}clv$ can be used to represent the thermal conductivity of the model, where $K$ is the model thermal conductivity, $c$ is the specific heat, $l$ is the
effective phonon mean free path, and \( v \) is the phonon velocity. In the heat transfer process of nanostructures, when the temperature of the system is high, the vibration of the atoms is more intense, and the number of phonons scattered is also greater. In general, the more phonons scatter, the smaller the mean free path of the phonons are, which in turn results to a decrease in thermal conductivity.

4. Conclusions

The thermal conductivities of three egg-tray graphene structures have been studied by non-equilibrium molecular dynamics simulations. The effect of length, temperature and strain on thermal conductivity have been analyzed. Structure-III has the highest thermal conductivity, followed by Structure-II, and the Structure-I. An increase in the number of hexagons leads to an increase in thermal conductivity. The thermal conductivity decreases with increasing strain and temperature but increases with increasing length. The calculated thermal conductivity of Structure-I, Structure-II, and Structure-III are 43, 45, and 60 W/m·K, respectively, at infinite length, much smaller than that of graphene. Under tensile strain, the bonding ability between atoms weakens, resulting in an increase in phonon scattering and a decrease in thermal conductivity. However, under compressive strain, its structure bends, which will lead to enhanced phonon scattering and reduce thermal conductivity. The heat transfer performance of Structure-II is determined by both phonon modes and phonon quantities in compression, while in tension it is determined only by the phonon modes. Our results suggest a feasible approach to tailor the thermal conductivity by changing the length, temperature, and strain of egg-tray graphene,
which might benefit the material design of graphene-based electronics. In addition, our computational result of the thermal conductivity is a novel contribution in micro-nano-scale heat transfer.

Compliance with Ethical Standards

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