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An anomalous wave-like kinetic energy transport in graphene nanoribbons at high heat flux

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ABSTRACT

Most investigations of thermal transport in graphene focused on low heat fluxes when the Fourier heat conduction law is valid. Here thermal transport in armchair graphene nanoribbons was investigated at high heat flux by non-equilibrium molecular dynamics simulations. Besides the energy transported through the Fourier heat conduction, an anomalous wave-like kinetic energy transport was observed. By comparing the two energy transportation paths, we find that the latter constitutes a considerable amount of the total energy and efficiently transports the energy at high heat flux. It means that the heat transfer efficiency in graphene would be greatly improved through wave kinetics. The frequency of the wave (low frequency phonon) would decrease and the amplitude of vibration would increase when the length of the graphene increases. This finding would be useful for thermal analysis when is graphene used as a heat dissipation material.

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1. Introduction

Graphene has attracted more and more attention in the past several years because of its excellent electronic and thermal properties [1–4]. Excellent electronic property results by its application in interconnection wires or channel material in integrated circuits [5,6]. And its good thermal property makes it applicable for heat dissipation [7,8]. For the latter application, one should know the exact value of the thermal conductivity. And the higher the thermal conductivity, the more effective the heat dissipation. Plenty of experimental and computational results have been obtained in the past several years. Among these, molecular dynamics simulation is widely used and accepted as a useful method to discover thermal property of pristine, isotope and vacancy defects of graphenes [9–12].

In the open literature, thermal conductivity of graphene was obtained with low heat fluxes and the Fourier heat conduction law was assumed to be valid. However, in this work, thermal transport was investigated under high heat flux. From the results, a new phenomenon was found where wave-like kinetic energy transport was observed under high heat fluxes and the heat transport efficiency or effective thermal conductivity was greatly improved.

2. Model

The unit cell of graphene used here was 4.26 Å × 2.4595 Å. The armchair graphene nanoribbons (AGNRs) were created through building a super-cell of the unit cell. There were 51 cells along the edge of armchair direction, and 11 cells along the edge of zigzag direction. Fig. 1 shows the unit cell and the super-cell of graphene simulated in this work. The size along the Z direction was set to 20 Å to avoid the effect of the periodic boundary conditions. This value should also increase when the length of GNRs increases. The thickness of graphene was considered as 3.35 Å here as used by many people in their MD simulations [3,4]. In some other simulations, 1.42 Å was considered as graphene's thickness. In our opinion, the Van der Waals radius (3.4 Å) of carbon atom should be close to the real thickness of graphene. According to the experimental measurements, the value was approximated to 3.35–3.4 Å, and a detailed discussion about this could be found in Ref. [13]. In all MD simulations performed herein, the reactive empirical bond order (REBO/Brenner) potential [14] was used to describe the C−C interactions in graphene. This potential has been widely used by other researchers to calculate thermal transport properties of carbon nano-materials [15–17].

3. Works

All MD calculations were performed using the LAMMPS [18] package. Periodic boundary condition was adopted. In the first

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stage of MD simulations, the system was relaxed at constant atmospheric pressure and $T=300$ K for 160 ps with time step 0.4 fs, using the Nose–Hoover thermostat and barostat [19,20] method. After NPT (constant pressure and temperature) relaxation, the system was relaxed as an NVT (constant volume and temperature) ensemble for 200 ps. Then the system was controlled as an NVE ensemble for another 40 ps and the system average temperature was monitored. The system was assumed to reach an equilibrium state if the temperature was kept at the value we set at the beginning. At this juncture, the non-equilibrium molecular dynamics simulation (NEMD) method was used to impose heat flux. The NEMD method has been widely used to research the thermal properties of crystalline, amorphous, bulk, and nanoscale materials. We applied a constant heat flux to the system by the Muller-Plathe method [21–23] (the NEMD method). In this method, the simulation box was divided into 100 slabs along the heat transfer direction, where the 1st slab was assigned to be the cold region while the 51th slab was assigned as the hot one. The hottest atom (with the highest kinetic energy) in the cold region and the coldest atom (with the lowest kinetic energy) in the hot region were selected. The two sets of atoms were paired up and their velocities were exchanged. Over time, this induced a temperature gradient in the system. The heat flux J can be defined from the exchanged kinetic energy between the two selected layers according to the following equations:

$$J=\frac{\sum N_{swap}(1/2)(mv_h{}^2-mv_c{}^2)}{N_{swap}t_{swap}} \tag{1}$$

t_{swap} and N_{swap} are the swap interval and number of swap, respectively, and m is atomic mass; v_h and v_c are the velocities of hottest and coldest atoms, respectively.

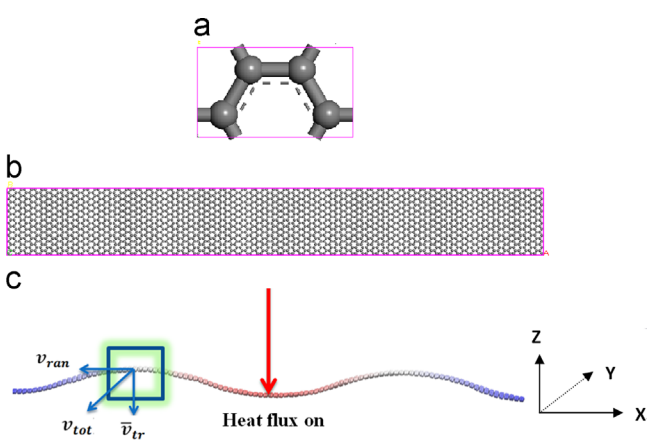

Fig. 1. (a) Unit cell of graphene. (b) The super-cell of armchair graphene nanoribbons. (c) A typical deformation when a high heat flux is imposed on the graphene nanoribbons.

Then the thermal conductivity was computed by the Fourier law;

$$\kappa=\frac{J}{2A\ \partial T/\partial x} \tag{2}$$

The vibrational density of states function $G(\omega)$ was calculated from the Fourier transform of the velocity auto-correlation function [24–26];

$$G(\omega)=\frac{1}{\sqrt{2\pi}}\int e^{i\omega t}\left(\sum_{j=1}^{N} v_j(t)v_j(0)dt\right) \tag{3}$$

$v_j(t)$ denotes its velocity at time t and ω is the vibration wave number. Here ensemble average was substituted with time averaging. In this MD simulation, time step was 0.4 fs. The averaging was performed over 400,000 steps after the system reached equilibrium for 160 ps in the NVT ensemble. The coordinates and velocities were recorded every 20 steps.

4. Analysis

Different heat fluxes can be added to the system by changing the swap interval t_{swap} in Eq. (1). The thermal conductivities obtained under different heat fluxes are shown in Fig. 2. It can be seen that these values are much lower than the experimental thermal conductivity of graphene, which is 3000–5000 W/m K [27]. The smaller calculation result is caused by the intrinsic size effect of MD simulations. Although MD simulation has obvious limitations, it can be used to evaluate the isotope [9,28], substrate coupling [29], and other influences of thermal conductivity of graphene successfully. We believe that it is reasonable to use MD simulation to obtain the heat flux effect on thermal conductivity of graphene. We will show more evidences of this in the following text.

From the data shown in Fig. 2, it could also be found that thermal conductivities of graphene nanoribbons increased with increasing heat flux density. We assumed that thermal conductivity is an intrinsic property under the Fourier heat conduction framework and does not vary with the added heat flux. Therefore, the increased thermal conductivity can be explained only by another path which can take heat from the hot region to the cold region.

How do we explain the effective thermal conductivity or efficient heat transport increased with increasing heat flux? We tried to find the internal mechanism by analyzing the atoms' movement. When a heat flux density of 1258 GW/m^2 was imposed, the vibrations of the graphene nanoribbons became regular, as shown in Fig. 3(a). The coordinates of the atoms were registered every 20 steps to record the atomic vibration information. It was a surprise that the positions of atoms in the Z direction varied with time and looked like a wave as shown in Fig. 3(b).

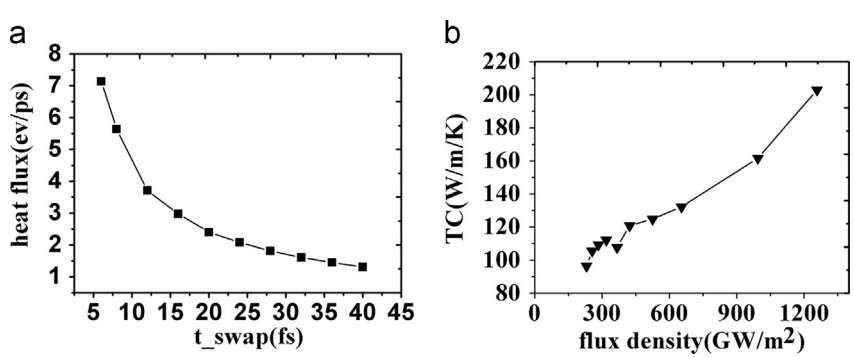

Fig. 2. (a) Heat flux changed with the exchanging rate. (b) The relationship between thermal conductivity and heat flux density.

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