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Research Article

Mass Transport Induced by Heat Current in Carbon Nanotubes

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Transport of helium atoms in the carbon nanotubes is investigated in the presence of temperature gradients. The heat current flowing along the carbon nanotubes can induce a stable directed transport of helium; it is demonstrated that the heat current density rather than the temperature gradient performs as a fundamental physical factor to the mass transport. We provide an alternative route to control the mass transport by using heat. Our results reported here are also relevant for understanding the transition from thermal energy to mechanical energy.

1. Introduction

The study of transport is always a challenge issue with incalculable value to us. Thermal and mass transports are the two important transports and have attracted substantial concerns [1]. In thermal transport, thermal conduction is the transfer of heat energy by microscopic diffusion and collisions of particles or quasiparticles within a body due to a temperature gradient. The mass transport refers to the orientated flow of particles. Even if thermal transport is a deviation from mass transport in physical principle, researchers are always trying to find out their inherent relationship [2, 3].

Recently, an experimental result shows that thermal gradients can drive the subnanometer motion of cargoes along carbon nanotubes (CNTs) [4]. Another numerical result shows that the fullerene encapsulated in carbon nanotubes can also be driven by temperature gradients [5]. More and more studies focus on nanoparticle manipulation using heat [6–8]. A model of carbon nanotubes filled with fullerene (C60) reported that the temperature can pumping large particles [9]. The Langevin model of a thermally -driven double-walled nanotubes motor has described the dynamics of nanoelectromechanical device activated by heat [10]. It was also reported that the velocity of C60 induced by temperature gradients had a linear relationship with heat flux [6]. These few previous efforts suggest that the heat originated from temperature gradients can induce the motion of particles. However, the underline physics of mass transport driven by heat is still not so clear.

In this paper, we will study the carbon nanotubes filled with helium (He) atoms and investigate the transport of He atoms induced by the heat flowing through the CNTs. By constructing the relationship between the mass flux and the heat current, we try to reveal some fundamental physics about the energy transport and its transformation. The obtained results are of significance for understanding the thermally induced mass transport in quasi-one-dimensional materials and may be useful for controlling the mass transport.

Figure 1 shows the carbon nanotubes filled with He atoms. Here we use He atoms as the fillings just because of their stable chemical properties. Two heat baths (with temperature T_H and T_C, resp.) are connected to the two sides of the CNTs. The two ends of the CNTs are fixed to avoid their spurious global rotation. The fixed region and the heat baths occupy one layer and six layers of atoms, respectively. In order to keep a stable number of helium atoms, the periodic boundary is applied for He atoms along the axial direction of the CNTs. That means a helium atom will be inset in one end of the CNTs when another Helium atom goes out of another end of the CNTs. In our simulations, we have used classical molecular

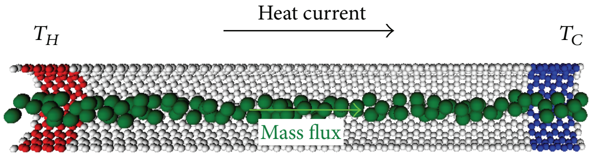

Figure 1: Diagram of the carbon nanotubes (filled with helium atoms, the green balls) coupling to two heat baths (the red and blue balls). The temperatures of the red part and blue part are T_H and T_C, respectively. As $T_H > T_C$, the heat current will flow from the left side to the right side. Accordingly, a mass flux induced by the temperature gradient will occur along the axial direction of the CNTs. The length of CNTs is 12 nm.

dynamics method based on the Tersoff-Brenner potential [11] of carbon-carbon (C–C) bonding interactions. The Lennard-Jones (LJ) potentials form [12, 13]

$$H_{\mathrm{LJ}}\left(r_{ij}\right) = -\frac{A}{r_{ij}^{6}} + \frac{B}{r_{ij}^{12}} \tag{1}$$

is used for van der Waals interactions of He–He and He–C couplings. The parameters of LJ are $A = 1.2553\ \mathrm{eV} \times \mathrm{Å}^6$ and $B = 418.3\ \mathrm{eV} \times \mathrm{Å}^{12}$ for He–He interaction and $A = 7.062\ \mathrm{eV} \times \mathrm{Å}^6$ and $B = 7455.6\ \mathrm{eV} \times \mathrm{Å}^{12}$ for He–C interaction, respectively. The equations of motion for atoms in either the left or right Nosé-Hoover thermostat are [14, 15]

$$\begin{gathered} \frac{d}{dt} p_i = F_i - \Gamma p_i, \\ \frac{d}{dt} \Gamma = \frac{1}{Q}\left[\sum_i \frac{p_i^2}{2m_i} - \frac{3N_C k_B T_0}{2}\right], \end{gathered} \tag{2}$$

where p_i is the momentum and F_i is the force applied on the ith atom; $Q = 3N_C k_B T_0 \tau^2/2$, where τ is the relaxation time, which is set to $1ps$. Γ is the dynamic parameter of the thermostat; $T(t)$ is the instant temperature of the heat baths at time t, which is defined as $(m_{Ci}/3k_B)(v_x(t)^2 + v_y(t)^2 + v_z(t)^2)$, where $v(t)$ is the time-dependent velocity; T_0 (T_H or T_C) is the set temperature of the heat baths. N_C is the number of the atoms in the heat baths, k_B is the Boltzmann constants and m_C is the mass of the carbon atom. The set temperatures of the heat baths, T_H and T_C, are placed in the two ends of the CNTs and the temperature gradient is denoted by $\nabla T = \Delta T/L = (T_H - T_C)/L$, where L is the length of the CNTs. For the convenience of comparison, we use the average temperature 300 K, which is near the room temperature. The atoms between the two thermostats follow Newton's law of motion:

$$\frac{d}{dt} r_j = \frac{p_j}{m}, \qquad \frac{d}{dt} p_j = F_j, \tag{3}$$

where j runs over all of the atoms between the two thermostats.

We integrate these equations of motion by Verlet method [16]. The time step is 0.55 fs. Generally, as shown in Figure 1, the heat current can stabilize around the set value when the temperature gradients are applied to the CNTs after 2 ns. At the same time, the mass flux driven by heat current occurs along the axial direction of CNTs. The heat bath acts on the particle with a force $-\Gamma p_i$; thus the power of heat bath is $-\Gamma p_i^2/m_C$, which can also be regarded as the heat flux that comes out of the high temperature heat bath and is injected into the low temperature heat bath. The total heat flux injected from the heat bath to the system can be obtained by $J_h = \sum_i [-\Gamma p_i^2/m_i] = -3\Gamma N_C k_B T(t)$, where the subscript i runs over all the particles in the thermostat [17]. The average velocity of He is obtained by $V_a = (1/N_H)\sum_i^{N_H} \langle V_i \rangle$, where V_i is the velocity of the ith helium atom, $\langle\,\rangle$ means a time average, and N_H is the total number of He atoms. The mass flux is defined as

$$J_m = \rho_H m_H V_a = \frac{N_C m_H V}{L}, \tag{4}$$

where m_H is the mass of single He atom and ρ_H is the mass density of He in CNTs.

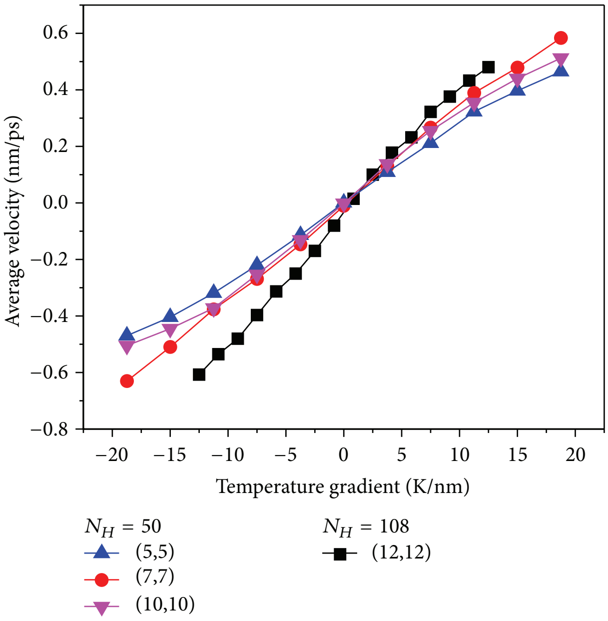

Figure 2: Temperature gradient dependence of average velocity of He atoms in armchair CNTs for different diameters of the CNTs. The mass densities of He in (5, 5), (7, 7), (10, 10), and (12, 12) are 66.39, 33.89, 16.6, and 16.6 amu/nm^3, respectively.

When applying the temperature gradients on the CNTs, a stable flowing of He atoms along CNTs will occur. Figure 2 shows the temperature gradient dependence of average velocity of He atoms for different diameters of CNTs. To consider the diameter dependence of CNTs on the mass transport, here we study armchair chirality of the CNTs (5, 5), (7, 7), (10, 10), and (12, 12). Obviously, the average velocity increases with temperature gradient. However, the average velocity of He atoms depends on the diameter of CNTs with slight irregularities.

From our model, when applying temperature gradient on CNTs, the motion of He atoms occurs with a heat current flow from the hot heat baths to the cold heat baths along

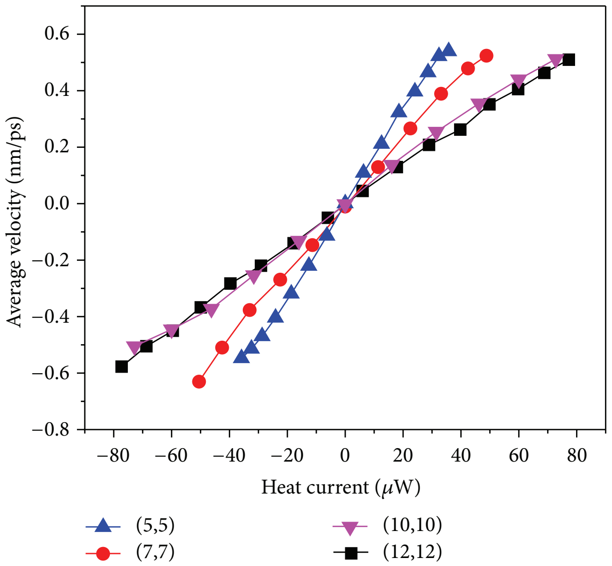

FIGURE 3: Heat current dependence of average velocity of He atoms in armchair CNTs for different diameters of CNTs. The CNTs are the same as in Figure 2.

the surface of CNTs. If one uses the heat current, which is corresponds to the temperature gradient, to plot the x-axis, one would find an organized result comparing to Figure 2. As shown in Figure 3, if the heat current flowing through the CNTs is the same, the CNTs with chirality of (5, 5) can drive higher average velocity of He atoms than that of (7, 7). When the diameter of armchair CNTs increases, the ability to drive the motion of He atom reduces. Then it is not difficult to find the conflicts between temperature gradients and heat current. In order to solve the conflicts, we plot the heat current density as the transverse axis and the average velocity as the longitudinal axis.

As illustrated in Figure 4, the curves for different diameters as shown in Figure 3 all run together and the average velocity in the CNTs is proportional to the heat current density via the CNTs. This relationship is independent of the diameter as well as the length of CNTs. In Figure 4, we also provide the results of two zigzag CNTs, (20, 0) and (16, 0). When the driving heat current density ranges from about −2 to 2 uW/nm^2, the linear relationship between average velocity and heat current density is still valid. This indicates that the heat current density determines the average velocity, which may be independent of the structure of the CNTs. Since the mass flux is obtained from (3), which means that the mass flux does not depend on the cross section area, then the mass flux is proportional to the average velocity as well as the heat current density.

In summary, we have studied the temperature gradient driven mass flux in the CNTs using nonequilibrium molecular dynamics. It is reported that relationship between mass flux and heat current density rather than average velocity versus temperature gradients can describe the fundamental physics of temperature gradient induced mass transport better. Our results try to connect energy transport and mass transport from a new point of view, which would help researchers understand the physical mechanism of transport. Although we demonstrate a universal relationship between heat and motion, more physical properties such as the transfer efficiency need to be addressed in detail. Even so, our results are an illumination to control mass flux by using heat conduction.

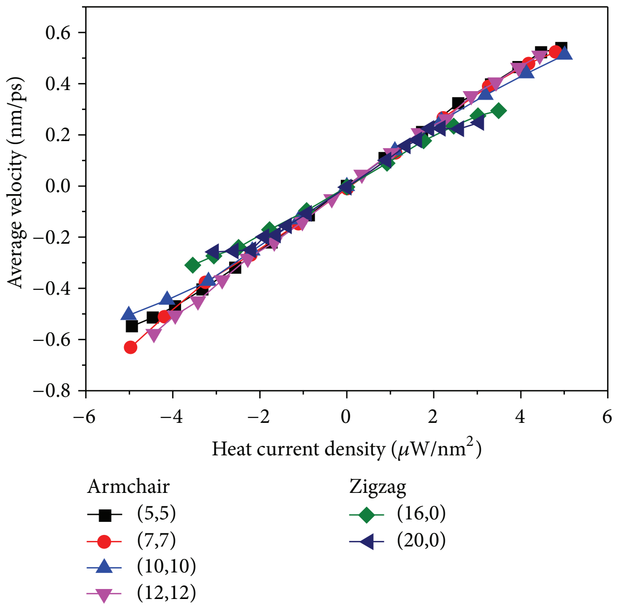

FIGURE 4: Average velocity versus heat current density for different chiralities, diameter, and lengths of CNTs. The heat current density is obtained by $J_d = J_h/S$, where J_h is the total heat flux injected from the heat bath to the system and S is the area of cross section of CNTs, respectively. The mass density of He in (16,0) and (20, 0) is 16.6 amu/nm^3.

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