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Atomic scale mass delivery driven by bend kink in single walled carbon nanotube

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ABSTRACT

The possibility of atomic scale mass delivery by bend kink in single walled carbon nanotube was investigated with the aid of molecular dynamics simulation. By keeping the bending angle while moving the tube end, the encapsulated atomic scale mass such as atom, molecule and atom group were successfully delivered through the nanotube. The van der Waals interaction between the encapsulated mass and the tube wall provided the driving force for the delivery. There were no dramatic changes in the van der Waals interaction, and a smooth and steady delivery was achieved when constant loading rate was applied. The influence of temperature on the atom group delivery was also analyzed. It is found raising temperature is harmful to the smooth movement of the atom group. However, the delivery rate can be promoted under higher temperature when the atom group is situated before the kink during the delivery.

1. Introduction

Carbon nanotubes (CNTs) have been attracted considerable interest since they were discovered in 1991. With their excellent properties being revealed, CNTs become hot candidates in many application fields. One of the interesting applications is the mass delivery in atomic scale. Indeed, they have many advantages for mass delivery. For example, they are mechanically robust and can endure large strain and structural deformation [1–4]. Their semi-one dimension structures provide precise directions for mass conveying. In addition, their tubular shapes allow the atoms or particles to travel either inside or outside of the tube walls [5–7].

Many research groups have shown that atomic scale mass can be delivered along the nanotubes by various driving force. Barreiro et al. demonstrated that masses attached to an ablated outer wall of a multiwalled CNT can be actuated by imposing a thermal gradient along the nanotube [8]. Also by imposing a thermal gradient, Zambrano et al. showed that water nanodroplets can be driven through single- and double-walled CNTs [9]. Dong et al. realized mass flow in nanotube junction by electric current driven heating, diffusion, and electromigration under low bias voltages [10]. Regan et al. accomplished controllable and reversible indium transport along the outside wall of nanotube by applying a voltage gradient on the nanotube [5]. Insepov et al. predicted that an axial gas flow inside a CNT can be pumped out by producing Rayleigh traveling waves on the nanotube surface [11]. Recently, studies based on molecular dynamics (MD) simulation showed that buckled single walled carbon nanotubes (SWCNTs) can be used for atomic scale mass delivery. Chang [12] found that once a section of a SWCNT with an appropriate diameter is collapsed, molecules inside can be accelerated by a domino wave, which is generated by the successive collapse of the neighboring portions of the SWCNT. Wang [13,14] demonstrated that a complete atomic transportation in a SWCNT can be achieved when torsion loading with a high rate is applied to the SWCNT. In addition, molecular simulations from Wang [15] showed that if proper torsion load is applied, it is possible to squeeze certain type of atoms out of the SWCNT while leaving other atoms inside, thereby realizing atom separation.

It is considered that the nonequivalent van der Waals force between the tube wall and the encapsulated masses plays an important role in the atomic scale mass delivery in buckled SWCNTs. When the wall of nanotube buckles, the nonequivalent van der Waals force can be increased dramatically, thus it can serve as a driving force for atoms, molecules and possibly larger masses. Moreover, there are advantages by using buckled nanotube to delivery mass. One advantage is that the mass delivery system can be performed for thousands of times without break down because

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of the well flexibility of nanotubes [16,17]. Another advantage is that such method is suitable for many types of materials because the van der Waals interaction exits for all materials.

Here we explore the possibility of atomic scale mass delivery in SWCNT. Comparing with the buckling modes in transverse compression and twist load, bend-induced buckling usually occurs in local area of a nanotube [18,19]. It seems an obstacle to drive the masses in the nanotube by means of continuous collapse of the tube wall. However with the aid of molecular dynamics method, we will show if the proper loading condition is applied to the nanotube, atomic scale mass delivery can also be realized in bended SWCNT with a kink. Furthermore, we will investigate the influences of particle mass and temperature on the delivery efficiency.

2. Simulation methods

A buckled (10,0) SWCNT with only one kink is obtained by bending it (170 Å in length) for 35° (Fig. 1). The two ends of the nanotube are saturated with H atoms. In order to produce a continuous driving force in the nanotube, the left end of the nanotube is fixed, while the quasistatic displacement load is applied on the right end. Four carbon atom layers and the hydrogen atoms on either end of the SWCNT (highlighted in Fig. 1) are clamped in the simulation except for when the load is applied. It has been reported that the additional kinks will be induced in SWCNT by over bending [20,21]. To avoid this phenomenon, we keep the bending angle as constant by confining the load direction along the BC line (upward or downward), as shown in Fig. 1.

The force field for the simulation is COMPASS force field, which is a general all-atom force field for atomistic simulation of common organic molecules, inorganic small molecules and polymers [22]. It is the first ab initio force field that has been parameterized and validated using condensed-phase properties, in addition to various ab initio and empirical data for molecules in isolation. The time step in MD simulation is 1 fs. The Andersen method [23] is employed to control the thermodynamic temperature.

3. Results and discussion

Before the load is applied, an Ar atom is put into the pre-buckled nanotube, on the left side of the kink. Then an initial relaxation is carried out to achieve the minimum energy state. Fig. 2(a) and (b) shows the Ar atom and the SWCNT after the relaxation. The Ar atom is in the middle of the tube, about 12 Å away from the center of the kink (Fig. 2). The top view of the atomic system (Fig. 2(b)) shows that the Ar atom is located near the side wall of the nanotube. Fig. 3 shows the change of potential energy if the Ar atom moves transversely in the tube from its initial position. The moving path is indicated in Fig. 2(b) by the dashed line. From Fig. 3, there are two potential wells in the transverse direction, corresponding to two paths of low potential energy along the tube axis in the buckling area. The potential barrier between the two wells is formed by the inward collapse of the tube wall.

To active the Ar atom, the right tube end is moved at a constant loading rate of 16.67 m/s. When the load is upward, the kink moves right. Meanwhile, the Ar atom gradually leaves the left tube end. After 60 ps, the distance between the Ar atom and the left tube end increases for 16.7 Å (Fig. 4(a)). When the load is downward, the kink moves left, and the Ar atom moves toward the left end for 17.6 Å after 60 ps (Fig. 4(b)). No more kinks are generated during the process. In addition, the displacement in the transverse direction can be neglected, because it is less than 1 Å during the whole delivery. It is evident that they did not cross the potential barrier to the other side wall because the width of the buckled tube is more than 16 Å (Fig. 3).

Linear relationship is found between the displacement of the encapsulated Ar atom and the displacement of the right tube end. From Fig. 5, the rate of the Ar atom becomes constant as soon as a constant loading rate is applied on the right tube end. When the loading rate is 16.67 m/s downward, the Ar atom can achieve a constant rate 35.0 m/s. When the load is upward, the Ar atom can ultimately reach a larger rate, which is about 46.7 m/s. The smooth

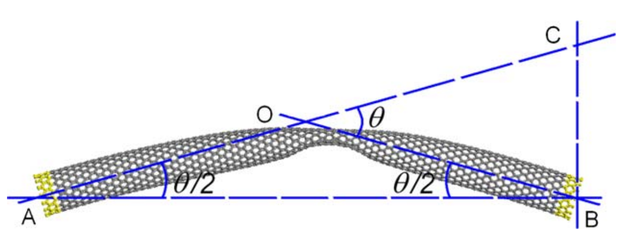

Fig. 1. Buckled (10,0) SWCNT with the bending angle θ = 35°. The atoms highlighted in yellow are clamped. Load is applied on the right end of the tube by moving the clamped atoms on the right end along the BC line. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

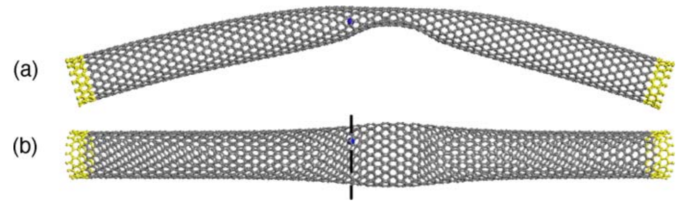

Fig. 2. The buckled (10,0) SWCNT with an encapsulated Ar atom when no load is applied. (a) Side view; (b) top view. The Ar atom is located in the middle of the tube, and it finds the lowest potential energy near the side tube.

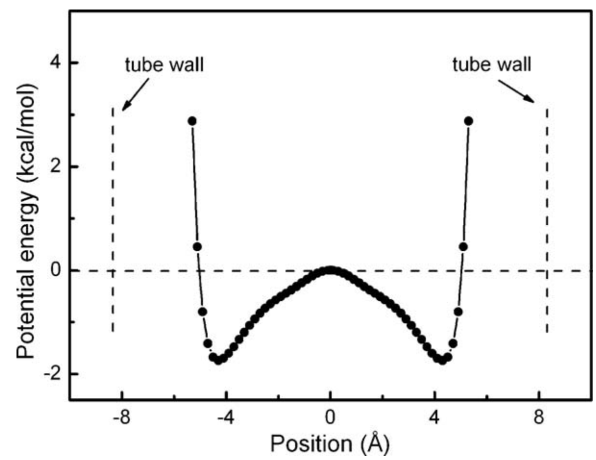

Fig. 3. Potential energy along the path indicated in Fig. 2.

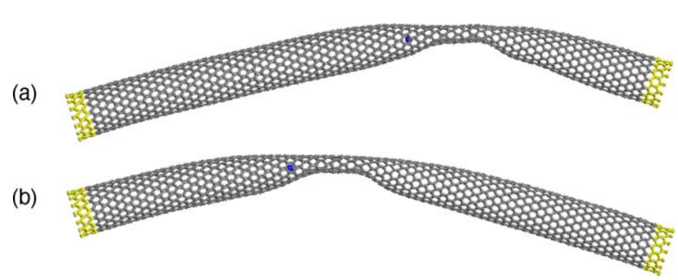

Fig. 4. Final positions of the Ar atom when the right end of the tube is moved (a) upward and (b) downward for 10 Å. The delivery distance is 16.7 Å rightward and 17.6 Å leftward in figure (a) and (b), respectively.