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Oscillatory Behavior of Rare-gas Atoms in SWCNT

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Received: March 14, 2006; In Final Form: July 1, 2006

In this paper, we have investigated both the process of rare-gas atoms (He, Ne, Ar, Kr, Xe) injected into single-wall carbon nanotube (SWNT) and the mechanical oscillatory behavior of rare-gas atoms sliding in a SWCNT by using molecular dynamics simulations. The minimal diameters of SWCNT to encapsulate rare-gas atoms are obtained, which are from 6.246 to 7.828 Å. The threshold energies to encapsulate rare-gas atoms in SWCNT are also presented, which are less than 0.15 eV/atom. The oscillatory frequencies of the encapsulated atoms in zigzag SWCNT have been studied. The oscillatory frequencies are insensitive to the initial kinetic energy, but they are sensitive to the lengths and the radius of the tube, and they decrease as the length and the radius of the tube increases.

1. Introduction

Since Cummings and Zettl[1] reported the experimental observation of oscillatory properties of concentric multiwalled carbon nanotubes (MWCNTs), it shows that it is possible to fabricate micromechanical oscillators or resonators with frequency of gigahertz using the micromachining technique. At the same time Kolmogorov and Crespi[2] reported the tribological properties of MWCNT and showed that incommensurate tubes have extremely small shear strength. In 2002, Zheng and his collaborators[3] proposed that the nano-oscillators with the range of several gigahertz may be made by using multishell nanotubes. Subsequently, Legoas et al.[4] carried out some simulations and concluded that the sustained oscillations are possible when the radii difference between inner and outer DWCNTs is ∼3.4 Å, and the stable nano-oscillator's frequencies are as large as 38 GHz. Rivera and their collaborators[5] studied the behavior of the damping via MD simulations of DWCNTs at constant temperatures using the Dreiding model and found that the damping of the oscillation inversely depends on the length of the DWCNTs, which is in good agreement with the theoretical prediction of Zheng et al. Their following work,[6] for the incommensurate DWCNTs forming (7,0) and (9,9) structure at 298.15 K with axial lengths from 122.1 to 982.4 Å, also showed that the frequencies in the range of gigahertz decrease as the length of the system increases. Zhao et al.[7] studied the oscillations of DWCNTs on the energy dissipation mechanism using MD simulations and found that the energy dissipation mechanism depends on the overlap length of the DWCNTs, By comparing simulation of the outer tube, they also found that the deformation of the outer tube plays an important role in the damping of the oscillation.

Similar to the studies of DWCNTs, the mechanical oscillatory behaviors of a C_{60} molecule tunneling through a SWCNT were carried out by Liu et al.[8] They found that C_{60} performs a decaying oscillation with gradual decrease of the oscillatory amplitude and a gradual decrease of the oscillatory frequency, and this decay is sensitive to the change in the diameter and the degree of the helicity of the tube. They found the friction is smallest when the wall gap between C_{60} and SWCNT is around 4.0 Å (larger than ∼3.4 Å for DWCNTs).

On the other hand, the experimental investigation of the nano-oscillator is limited by the available techniques, as it is too small to directly measure the assembled nanodevices. Therefore, many numerical simulation tools at nanoscale have been proposed, i.e., computational nanoscience, including molecular dynamics simulation method,[9] Monte Carlo simulation method,[10] and ab initio molecular dynamics simulation methods and their extensions.[11] In this paper, as a straightforward method, a classical molecular dynamics method is used to study the behaviors of the rare-gas atoms encapsulated into the SWCNT; we have obtained the minimal radii of SWCNT absorbing rare-gas atoms which change from 3.12 to 4.306 Å, and the threshold energies to encapsulate different rare-gas atoms in different diameters of SWCNT, which are less than 0.15 eV/atom. From systematical studies, some relations of the oscillatory behaviors with the diameter and length of SWCNT have been attained for different rare-gas atoms, the oscillatory period is insensitive to the initial kinetic energy for the zigzag SWCNT, as the oscillatory amplitude increases with the increasing of the injection energy of the rare-gas atom. Finally, the oscillatory behaviors with the diameter and the length are calculated, it shows that the frequencies decrease as the length of the system increases, which is in good agreement with the other reports,[7] and an oscillation decaying with diameter is not observed in our system, which disagrees with Liu's report.[8] Our calculation also shows that the frequency is sensitive to the radius of the tube, and the frequencies decrease when the radius of the tube increases.

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10.1021/jp061567q CCC: $33.50
Published on Web 08/11/2006

TABLE 1: The Parameters of the TLHT Potential

two-body	three-body
$q_1 = 10.149804$	$Z = 20.0eV$
$q_2 = 7.936986$ Å^{-1}	$H = 0.205$
$q_3 = 261.527033eV$	$P = 1.340$
$q_4 = 0.527263$ Å^{-1}	$B = 0.588$ Å^{-1}
$q_5 = 3.071221$ Å	

2. Formulations

For a large number of atoms or molecules, the efficient method to model the structure and dynamics of nano-structures is the use of phenomenological interatomic and intermolecular potentials. As Rafii-Tabar summarized in ref 12, both the Tersoff potential and the Brenner−Tersoff-type potential are used to study the interatomic interaction of carbon nanotubes, where the Tersoff potential has 11 adjustable parameters and can accurately calculate the energy- and structure-related properties of the diamond crystal structure, and the Brenner−Tersoff-type potential, in which different parameters are evaluated for carbon species and successful calculations of various properties of diamond crystal and the individual graphite planes. The TLHT potential given by T. Takai et al.[13] is based on a two-body and an angle-dependent three-body interaction and has nine parameters that are evaluated from fits to various properties of C_2, graphite, and diamond crystal, it is used to describe interactions of carbon−carbon. Compared with the Tersoff potential and the Brenner−Tersoff-type potential, the TLHT potential has a simple form and is barely used to study the interatomic interaction of carbon nanotubes. Through our test, we found that a good dynamical stability can be easily obtained by using TLHT potential to describe an interatomic interaction of Carbon nanotubes. In this paper, the TLHT potential is used to describe the carbon−carbon interaction of the SWCNT, which has the following expressions:

$$E = \frac{1}{2}\sum_i\sum_{j\neq i} U_{ij} + \frac{1}{6}\sum_i\sum_{j\neq i}\sum_{k\neq j\neq i} U_{ijk} \tag{1}$$

Here a two-body interaction potential U_{ij} is given by

$$U_{ij} = e^{(q_1 - q_2 r_{ij})} - q_3\left[\frac{1}{2} - \frac{\arctan(q_4(r_{ij} - q_5))}{\pi}\right]^{12} \tag{2}$$

where r_{ij} refers to the distance between the particle i and j, and the parameters denoted by q_1 through q_5 are given in Table 1. The three-body part is described by an angle-dependent function:

$$U_{ijk} = Z\{P + (\cos\theta_i + H)(\cos\theta_j + H) \times (\cos\theta_k + H)\}\, e^{-B^2\left(r_{ij}^2 + r_{ik}^2 + r_{jk}^2\right)} \tag{3}$$

where, θ_i, θ_j, θ_k and r_{ij}, r_{ik}, r_{jk} represent the angles and the sides of the triangle formed by the three particles. The parameters Z, H, P, B are shown in Table 1.

Two-body Lennard-Jones potentials are used to model the interaction of rare-gas atoms with nanotube in this paper. As the short-range Lennard-Jones potential is unfit to the calculations of quantum mechanics, a screened-coulomb potential in the form of the Kr−C potential at short range is used as a modification[14], so the interatomic potential E between rare-gas atom and carbon atom is defined as follows:

$$E = \begin{cases} V_{Kr-C}(r_{ij})(r_{ij} < r_0) \\ V_{LJ}(r_{ij})(r_{ij} \geq r_0) \end{cases} \tag{4}$$

TABLE 2: Parameters *A*, *B* in Lennard-Jones Potential for Different Rare-gas Atoms

	A (eV. Å^6)	B (eV. Å^{12})
He	4.43408	3023.0054
Ne	10.17352	15716.0986
Ar	33.2556	89560.7617
Kr	48.0704	156546.04968
Xe	73.1416	313324.7727

where r_{ij} is the distance between the rare-gas atom and the carbon atom, and r_0 is determined by the relation of $V_{Kr-C}(r_0) = V_{LJ}(r_0)$. The Lennard-Jones potential is expressed as the following:

$$V_{LJ}(r_{ij}) = -\frac{A}{r_{ij}^{\,6}} + \frac{B}{r_{ij}^{\,12}} \tag{5}$$

where the parameters A, B for different rare-gas atoms are listed in Table 2. The Kr−C potential is given as follows:

$$V_{Kr-C}(r_{ij}) = \frac{V}{r_{ij}}(Ae^{aR} + Be^{bR} + Ce^{cR} + De^{dR}) \tag{6}$$

where Z_1 and Z_2 are the atomic number for rare-gas and carbon atoms, and their relations with V and R satisfy the following equations:

$$V = 14.40 \times Z_1 \times Z_2,\ R = \frac{r_{ij}}{au}, au = \frac{0.4685}{Z_1^{\,0.23} + Z_2^{\,0.23}} \tag{7}$$

The parameters A, B, C, D, a, b, c, d in eq 6 are set as 0.1818, 0.5099, 0.2802, 0.02817, −3.2, −0.9423, −0.4028, and −0.2016, respectively.

3. Results and Discussions

3.1. Process of Rare-Gas Atoms Injected into SWCNT. Adsorption of gases in the single-wall carbon nanotube has been studied by many people, most studied are the hydrogen storage because of its potential applications.[15] A significant amount of research[16] on the adsorption of atoms or molecules in a SWCNT bundle is also concentrated on the relations of adsorption with the sites, as the interstitial channel, the internal surface, and the groove (or external) surface can adsorb atoms. Here, our focus is to obtain the conditions of rare-gas atoms injected into SWCNT and then oscillate them in the tube. To systematically study the behavior of the atom in the nanotube, we choose two kinds of SWCNT, armchair and zigzag nanotubes; the corresponding coordinates of carbon nanotubes were generated by using the schemes in the literature. For some nanotubes, the lengths and radii are listed in Table 3. In our investigations, an isolated system A/SWCNT (A stands for He, Ne, Ar, Kr, or Xe) is considered. We do not consider the heat effect, and there is no energy exchange between A/SWCNT and the surrounding elements. Initially, a rare-gas atom with kinetic energy is placed at 0, 0, −1, with a symmetrical position to the nanotube, where the axial direction is along z-axis, the coordinate $O(0,0,0)$ is chosen at the center of one end of the tube.

Through a large number of calculational experiments, we found that the rare-gas atom can be absorbed in the nanotube, and it will stay in the nanotube all the time under appropriate radii and injection energies. First, given a relatively small injection energy, the relations of the radius of the nanotube to encapsulate rare-gas atoms are studied, and the minimal nanotubes encapsulating atoms He, Ne, Ar, Kr, and Xe, are presented as (8,0), (9,0), (11,0), (11,0), and (11,0) nanotubes;

TABLE 3: Lengths and Radii for Various SWCNT

	(7,0)	(8,0)	(5,5)	(9,0)	(10,0)	(11,0)	(12,0)	(7,7)	(13,0)
diameter (Å)	5.48	6.264	6.78	7.046	7.828	8.612	9.394	8.492	10.178
radius (Å)	2.74	3.12	3.39	3.523	3.914	4.306	4.697	4.746	5.089
length (Å)	19.2	19.2	23.3	19.2	19.2	19.2	19.9	23.3	19.2

TABLE 4: Threshold Energy E_{k0} of Rare-gas Atoms for Different Tubes

atoms	nanotubes	threshold energies $E_{k0}(eV)$
He	(8,0)	0.03
	(5,5)	0.02
	(9,0)	0.03
Ne	(9,0)	0.04
	(10,0)	0.04
Ar	(11,0)	0.09
Kr	(11,0)	0.13
Xe	(11,0)	0.15

their corresponding radii are 3.12, 3.523, 4.306, 4.306, and 4.306 Å; the wall gaps between He, Ne, Ar, Kr, Xe, and SWCNT are 2.64, 3.01, 3.43, 3.2, 3.43, and 3.1 Å, respectively. Except for the He atom, the minimal gaps are ~3.0 Å.

Here, we define a quantity E_{k0}-threshold energy. Below this threshold energy, the atom will oscillate in the nanotube, while above this energy, the atom's translational energy is larger than the barrier energy of the open-end of SWCNT, and the atom will go out from the other end of tube. In the calculation, we randomly chose an incident energy for a given rare-gas atom to study the dynamical processes of the atom in the SWCNT, if the atom could not be encapsulated in the tube, we chose a smaller energy until the atom could be encapsulated in the tube; otherwise we chose an energy with 10% of the encapsulated energy as an increment until the atom goes out of the tube, in this way, the largest energy to encapsulate rare-gas atom is the threshold energy. If using 1% as an interval, the final threshold energy will be more precise, but it needs more CPU time.

The threshold energies are presented in Table 4 for the rare-gas atoms He, Ne, Ar, Kr, and Xe moving in (8,0), (5,5), (9,0), (10,0), and (11,0) nanotubes. It shows that the threshold energy is insensitive to a tube radius for the same kind of rare-gas atom and same kind of tube, in comparison with (8,0) and (9,0) nanotubes for He atom, and (9,0) and (10,0) nanotubes for Ne atom, one can find the conclusion. For the same atom He, comparing (5,5) armchair and (8,0) zigzag nanotubes, the former threshold energy is smaller than the latter, which indicates the sliding resistance is related to the tube type, i.e., the sliding resistance of armchair conformation is larger than that of zigzag one. In ref 5, they suggested that sliding resistance for commensurate surfaces is greater than that for incommensurate surfaces, that also means the surface of different tube type will result in different friction. From Table 4, one can find that the threshold energy is related to the mass of the atom, especially for much larger atoms, the threshold energy increases with the atom mass. This is reasonable when the heavy atom has more friction, and it needs much more kinetic energy to overcome the barrier of the tube. The maximal threshold energy for rare-gas atoms is 0.15*eV*. In ref 17, they used temperature as an adjustable parameter, and it shows that at high temperatures, the CNT oscillator escaped from the outer nanotube, in analogy with the temperature, the effect of the injection energy is the same. All indicate that our calculations are consistent with others.

B. Oscillation of Rare-Gas Atoms in SWCNT. The concept of gigahertz oscillators based on the sliding of MWCNTs proposed by Cumings and Zettle has attracted a lot of attention. They found that, for the MWCNTs, the core shell with a certain amount of kinetic energy will oscillate since the friction of the core shell is very small. From the above discussions, given an appropriate kinetic energy for the atom and an appropriate diameter of the tube, the rare-gas atom can be encapsulated in the tube, and then oscillate in the tube. As shown in Figure 1, we have plotted the separation, the force, and the kinetic energy of atom Xe as a function of time in the tube (11,0). First, Xe, with the initial kinetic energy of 10^{-5}eV, is placed 1 Å away from the tube nozzle. Figure 1a shows the oscillation of Xe at (11,0) oscillator with time *T*. With the interaction potential, the restoring force $F_{res} = -dU/dx$ is calculated as shown in Figure 1b, and kinetic energy versus time is plotted in Figure 1c.

The oscillation process can be described as follows: Xe, with energy of 10^{-5}eV, moves in the direction of the axis tube. It accelerates entering into the tube due to the attractive interaction, and the force is positive. When the distance in *z*-direction increases, the van der Waals interaction reduced, and the atoms' force is 0 at 1.7 ps, then Xe atom moves uniformly in the tube until 4.4 ps. At this time, it approaches the other end of the tube, the excess van der Waals interaction energy creates a restoring force that opposes the Xe atom's moving direction. Due to the existence of repulsive force, it decelerates to a complete stop, then the atom accelerates in a reversed direction, and the situation is repeated on the opposite side until the whole oscillatory cycle is completed. The oscillatory process here is similar to the situation in ref 3−6, but the time at the force equal to 0 in the *z*-direction is very long, i.e., from 1.7−4.4 ps, during that time, the force is 0, and the atom moves uniformly and kinetic energy is constant, as shown in Figure 1b and c.

The same oscillatory motion can be observed for other rare-gas atoms when their initial kinetic energies are lower than E_{k0}. From Figure 1a, the stable oscillation is observed, indicating that the friction between Xe and the nanotube (11,0) is very small; the wall gap between Xe and the (11,0) tube is around 3.066 Å, which is very close to the radii difference between inner and outer DWCNTs given by Legaos at al., but smaller than the wall gap between C_{60} and SWCNT obtained by Liu et al. In general, the oscillator of rare-gas atoms in SWCNT is more stable than that of DWCNT and that of C_{60} in SWCNT. This can be explained by the fact that a single atom has a smaller contact area with SWCNT, both the friction and dissipation are very small, and a more sustained oscillator can be observed. That is consistent with the assumption that the nanoscale friction between surfaces is proportional to the contact area.[18]

At the same time, the relation period with the initial kinetic energy are studied, the results are listed in Table 5, here, an asterisk means there is no oscillatory motion occurring. When the initial kinetic energy is larger than the threshold energy E_{k0}, the atom goes out of the tube. Here, we only present the results for the atoms moving in the zigzag carbon nanotube. From Table 5, one can find that the radius of the tube has a significant impact on the oscillating period for the same atom; with the radius increasing, the period becomes longer. The reason is that the separation distance in the *X* and *Y* directions increases, and the velocity of the atom decreases. For the encapsulated rare gas atoms, the frequency is insensitive to the initial kinetic energy;

TABLE 5: The Relations of Period T (ps) with Initial Kinetic Energy (Ev) for Different Rare-Gas Atoms

atoms	nanotubes	gap	1 E−5 eV	1 E−4 eV	0.5 E−3 eV	1 E−3 eV	0.5 E−2 eV	1 E−2 eV	0.5 E−1 eV
He	(8,0)	2.04	4.5	4.5	4.5	4.3	4.6	4.5	*
	(9,0)	3.033	4.6	4.6	4.6	4.6	4.5	4.4	*
Ne	(10,0)	3.404	8.8	8.8	8.8	8.8	8.8	8.6	*
	(11,0)	3.796	10.2	10.1	10.2	10.1	10.2	10.2	*
Ar	(11,0)	3.426	8.6	8.6	8.5	8.6	8.6	8.5	8.6
Kr	(11,0)	3.276	10.8	10.8	10.8	10.8	10.8	10.7	10.8
Xe	(11,0)	3.066	12.2	12.2	12.3	12.3	12.3	12.5	12.2
	(12,0)	3.457	12.5	12.5	12.5	12.5	12.5	12.4	12.5

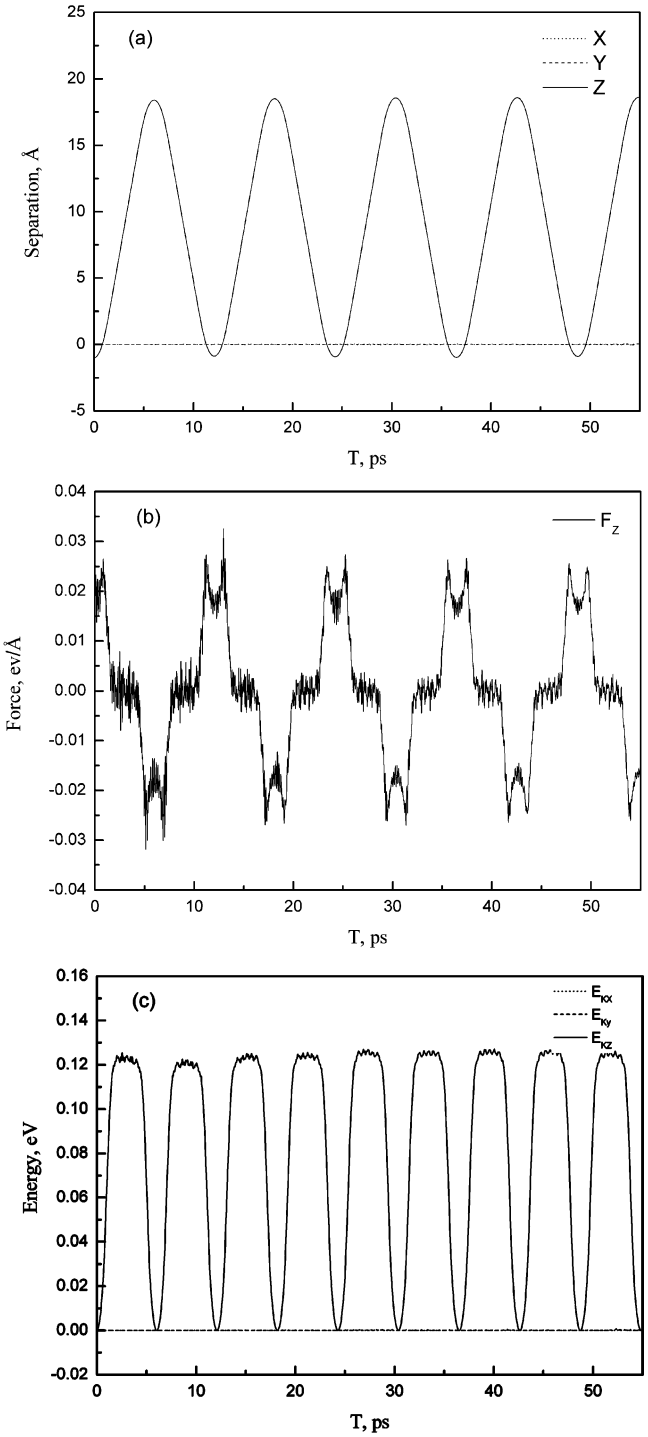

Figure 1. The dynamic process of Xe moving in the SWCNTs for at $E_{k0} = 10^{-5}$eV along axis of tube (11,0). (a) The changes in Xe atom position with time. (b) The changes of the restoring force with time in the axis direction. (c) The changes of the kinetic energy with time.

from the calculations of the oscillatory amplitude, we found the oscillatory amplitude increases with the initial energy. Both the amplitude and the velocity increase, so the period is unchanged.

The oscillation behaviors of the rare-gas atom in the tube are studied for the different initial positions where the atom enters the nanotube. Here Ar atom is initially placed at the positions of (0,1,−1), (0,2,−1), (0,3,−1), (0,4,−1). For (0,1,−1) and (0,2, − 1) cases, the Ar atom can be encapsulated and then oscillates in the tube, but for the former case, the Ar atom is encapsulated in the tube with much smaller injection energy than the latter one (0.2 eV), and the deviations in the *X* and *Y* directions are much smaller, so the oscillation is more stable, as shown in Figure 2. While for cases (0,3, − 1) and (0,4, −

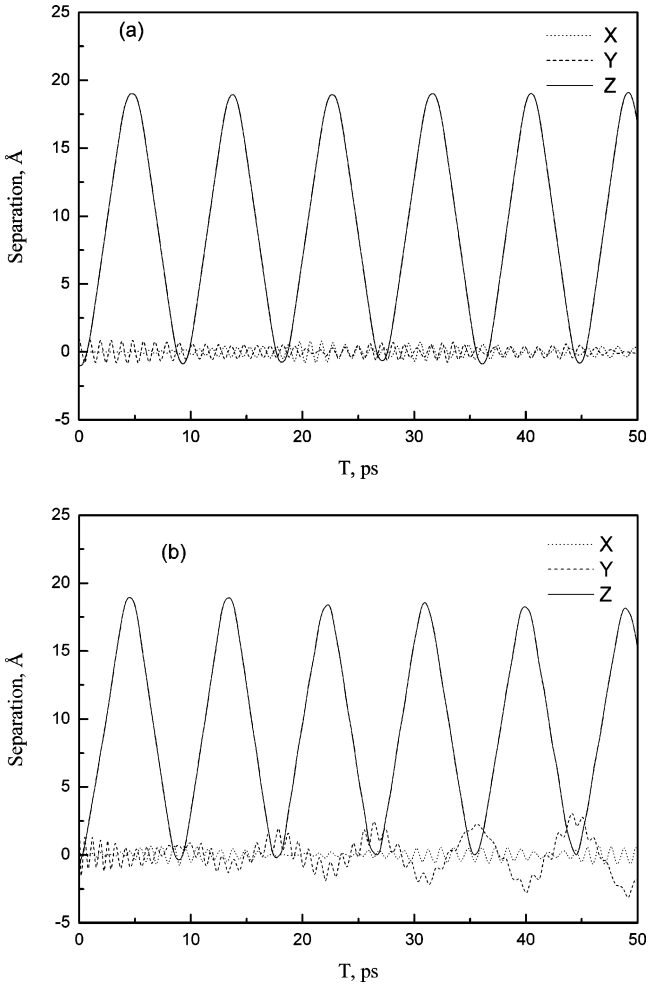

Figure 2. The oscillatory behavior of Ar at (11,0) oscillators: Here curves *x*1, *y*1, and *z*1 correspond to the results at the initial position (1,1,−1) and initial kinetic energy equal to 1 E − 5 eV; curves *x*2, *y*2, and *z*2 correspond to the results at the initial position (1,2,−1) and initial kinetic energy equal to 0.2 eV.

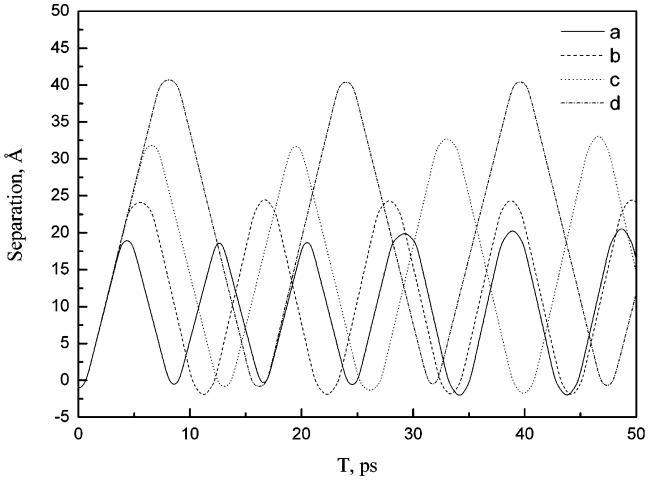

Figure 3. Oscillations of Ar at (9,0) oscillator at the initial kinetic energy equal to 10^{-5}eV for different lengths. The lengths of the tube are equal to 19.2 Å (curve a), 23.4 Å (curve b), 31.2 Å (curve c), and 39.0 Å (curve d), respectively.

1), the Ar atom cannot be encapsulated in the tube, so there is no oscillation.

Furthermore, simulations for varying lengths of the tube have been performed. For the (9,0) nanotube with length equal to 19.2 Å, 23.4 Å, 31.2 Å, and 39.0 Å, respectively, the separations are calculated, as shown in Figure 3, the Ar atom with injection energy equal to 1 E − 5 eV is placed initially at the position of (0,0,−1). It shows that the oscillatory frequency is inverse to the tube length, which is consistent with other reported work.[3,5]

4. Conclusion

Both the insertion of rare gas atoms into single-wall carbon nanotube and the oscillatory motion of the encapsulated rare-gas atoms in the SWCNT have been systematically studied. From our studies, we have found that under appropriate conditions any kind of atom can be encapsulated in the SWCNT, and the encapsulated atom with a relatively small kinetic energy will oscillate periodically in the tube. For the different atoms, there are corresponding threshold energies E_{k0}, below this energy, the atom will oscillate in the nanotube, while above this energy, the atom will transverse to the other end of the tube and go off. For the same kind of rare-gas atom, tube radius has no effect on the threshold energy, on the contrary, the nanotube type is related to the encapsulation of the atom, and the threshold energy of armchair tube is much smaller than that of zigzag one, which means the sliding resistance of armchair conformation is larger than that of zigzag one. And the threshold energy of heavy atom is larger than that of a light one. On the other hand, for the zigzag single carbon nanotube, the period of the encapsulated atom is insensitive to the initial kinetic energy, but sensitive to the tube length, that is, a longer tube corresponds to a longer period.

By controlling the length and selecting an aptitude atom, one can obtain an appointed gigahertz frequency. From our discussions, the advantage to obtaining gigahertz by using encapsulated atom in SWCNT is that the friction and dissipation of rare-gas atoms in the nanotube is smaller than that of DWCNTs and C_{60} at SWCNT, and realization of a more sustained oscillator is possible. For a larger wall gap between rare-gas atom and a SWCNT, or for higher incident energy of the rare-gas atom, the interaction strengths of a rare-gas atom with different carbons of the tube are different, the nanotube will deform. Therefore, it is necessary to select the suitable incident energy and wall gap between rare-gas atom and SWCNT to get a sustained oscillation.

Acknowledgment. This work was supported by a grant from NFS of the Education Commission of Jiangsu Province of China.

Supporting Information Available: Further details regarding the parameters and definitions used in our experiment. This material is available free of charge via the Internet at http://pubs.acs.org.

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