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Oscillators based on double-walled armchair@zigzag carbon nanotubes containing inner tubes with different helical rises

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Abstract

A novel approach is presented to improve the oscillatory behavior of oscillators based on double-walled carbon nanotubes containing rotating inner tubes applied with different helical rises. The influence of the helical rise on the oscillatory amplitude, frequency, and stability of inner tubes with different helical rises in armchair@zigzag bitubes is investigated using the molecular dynamics method. Our simulated results show that the oscillatory behavior is very sensitive to the applied helical rise. The inner tube with $h = 10 \text{ \AA}$ has the most ideal hexagon after the energy minimization and NVT process in the armchair@zigzag bitubes, superior even to the inner tube without a helical rise, and thus it exhibits better oscillatory behavior compared with other modes. Therefore, we can apply an appropriate helical rise on the inner tube to produce a stable and smooth oscillator based on double-walled carbon nanotubes.

Keywords: double-walled carbon nanotube, oscillator, helical rise, stability, molecular dynamics

(Some figures may appear in colour only in the online journal)

1. Introduction

Since their discovery by Iijima [1] in the early 1990s, carbon nanotubes (CNTs) have shown broad prospects as components for micrometer and nanometer scale electromechanical systems (M/NEMS) [2–6] due to their unique mechanical, electrical, and semiconductor properties. These unique properties have been engaged for building several types of nanosized devices such as nanobearings [7], nanomotors [8], nanoswitches [9], resonators [10], gigahertz oscillators [11, 12], strain sensors [13–15], and other NEMS components [16, 17]. Cumings and Zettl [18] pulled a core tube out from outer shells and found the core tube retracting into the outer shells and ultra-low friction between the tube walls. Zheng and colleagues [19] reported that the sliding of the inner shell inside the outer shell of multiwalled carbon nanotubes (MWCNTs) could generate oscillatory frequencies in the

gigahertz range. Legoas *et al* [20] investigated the oscillatory behavior of CNT oscillators by molecular dynamics (MD) simulation, finding that MWCNT oscillators are dynamically stable when the radius difference between the inner and outer tubes is around $3.4 \text{ \AA}$. Román Pérez and Soler [21] reported that the van der Waals interactions between the inner and outer nanotubes are prominent in driving the oscillations of nanotube oscillators and they are central to oscillatory stability. Recently, Cai *et al* [22] used an MD simulation approach to investigate rotational double-walled carbon nanotube (DWCNT) systems in which the inner tube has a rotational motion. They found that the armchair@zigzag incommensurate model with a gap larger than 0.335 nm could act as a high-amplitude oscillator. From the above review of the oscillatory behavior of MWCNT oscillators, it is noted that oscillation instability and high energy dissipation are still problems to be solved. In order to enhance these oscillatory

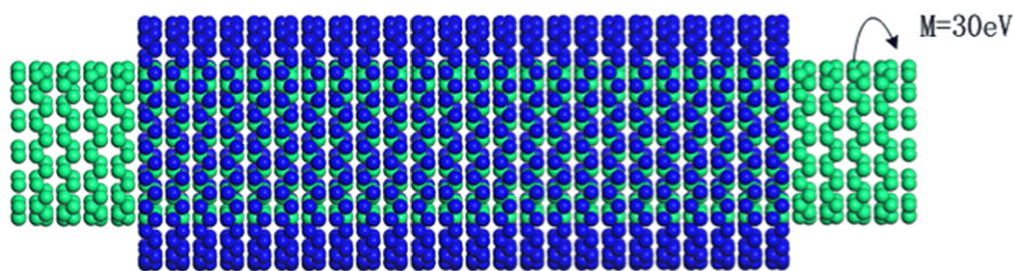


Figure 1. Oscillator based on double-walled carbon nanotubes.

behaviors, we propose a novel method in which a different length of helical rise is applied on the inner tubes in DWCNT-based oscillators. The influence of the helical rise on the oscillation amplitude, frequency, and stability of inner tubes is especially examined. In this paper, only oscillators based on double-walled armchair@zigzag carbon nanotubes are considered.

2. Molecular dynamics model

The oscillator mode based on DWCNTs is shown in figure 1. Both the outer and inner tubes have opened ends, and the outer tube is fixed throughout the simulation. The two tubes in each mode have a symmetrical layout along the axis. On the basis of the theory of low-friction oscillation [20], the gap between the inner and outer walls is nearly 3.4 Å. The detailed geometric parameters of the inner and outer tube are given in table 1. The internal configuration of each tube in the DWCNT system is characterized by the chiral indices (n, m). We elect that the outer tube is of the (24, 0) zigzag-type configuration and the inner tube is of the (9, 9) armchair-type configuration. Figure 2(a) shows the schematics of a (9, 9) tube applied with a helical rise h . Here we define the stagger length of tube ends as the length h of the helical rise. In all our simulations, we cut off parts of the length h of helical rise (see the blue dashed boxes of figure 2(a)). The four inner tubes with different h (0, 5, 10, and 15 Å), are plotted in figures 2(b)–(e), respectively. We find that the regular hexagon (as shown in figure 2(b)) of the armchair-type tube changes to an irregular hexagon when the tube is respectively applied with a helical rise of 5 (figure 2(c)), 10 (figure 2(d)), and 15 Å (figure 2(e)).

In this work, we use an MD simulation method to investigate the oscillatory behavior of rotational DWCNT bearing systems. Considering the degree of difficulty in rotating the inner tube in a practical operation, we apply a torque on the core tube rather than directly rotating the core tube as described by Cai *et al* [22]. In order to achieve a smooth and stable oscillation, a number of simulations are conducted to search for an appropriate torque. The torque of 30 eV is finally chosen from our simulations, which will result in an approximate 300 GHz initial rotational frequency of the inner tube. A too high initial rotational frequency will induce a larger energy loss, whereas a too low rotational frequency cannot trigger a valid oscillation. For the model of

Table 1. Geometric parameters of the carbon nanotube-based oscillator in figure 1.

Tube (n, m)	Length (Å)	Radius (Å)	Gap between walls (Å)	Helical rise (Å)	Atoms in walls
(24, 0)	49.730	9.53		0	1152
(9, 9)	69.531	6.19		0	1026
(9, 9)	69.336	6.19	3.34	5	1024
(9, 9)	69.436	6.19		10	1024
(9, 9)	69.478	6.19		15	1023

DWCNTs, the adaptive intermolecular reactive empirical bond order (AIREBO) [23, 24] potential is used, which can describe both the covalent bond between carbon atoms and the long-range van der Waals interactions for the force field. At the beginning of the simulation, the whole system is put in a heat bath with the temperature around 300 K for 60 ps, to gently increase the whole system's temperature to around 300 K after the energy minimization. The total number of particles, the system's volume, and the absolute temperature are constant for 60 ps (called the canonical *NVT* ensemble). Then we apply a torque $\mathbf{M}$ of 30 eV on the inner tube under the constant temperature for 40 ps, where the torque direction is the same as the direction of helical rise, as shown in figure 1. Thereafter, we remove the torque of inner tube and vary the whole system under a constant energy condition (the microcanonical *NVE* ensemble, where *NV* is the same as given above and *E* is the total energy in the system). The time step for all simulations is chosen to be 1 fs. The total time for the simulation is 3000 ps.

3. Results and discussion

Figure 3 gives the history of the positions of the mass center of (9, 9) inner tubes (MCITs) with different h before the *NVE*. As shown in the inset of figure 3(a), we can see that the four modes of the MCITs are identical to their initial position during the energy minimization. However, as shown in figure 3(b), the curves of the four MCITs fluctuate with time during the *NVT* because the thermal motion of atoms breaks the equilibrium status, and then the four MCITs tend to be stable after torque $\mathbf{M}$ is applied to the inner tube. We can see

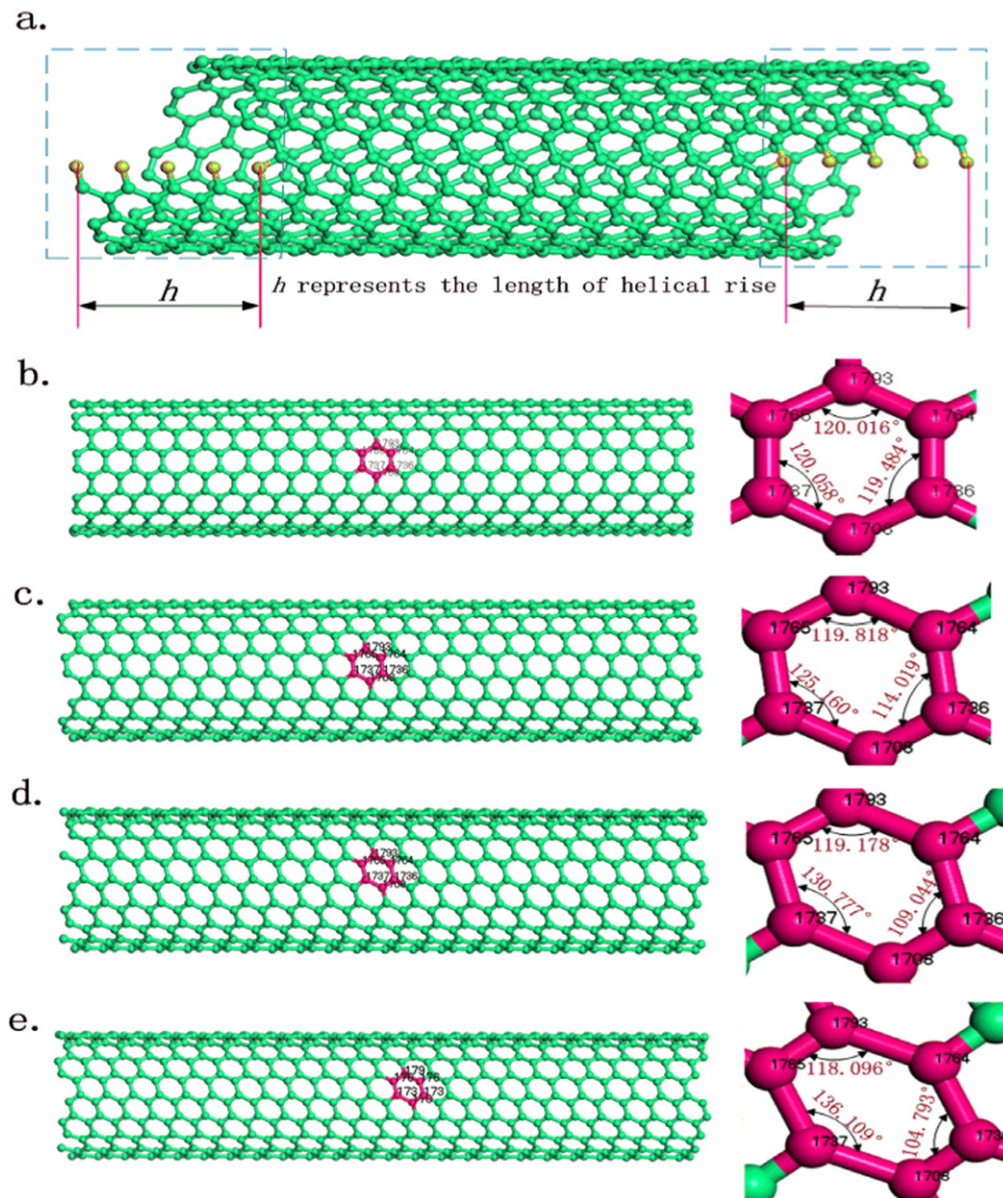


Figure 2. Schematic diagrams of (9, 9) tubes with different lengths of helical rise h . (a) Diagrammatic sketch of helical rise h , (b) without helical rise, i.e. $h = 0$ Å, (c) $h = 5$ Å, (d) $h = 10$ Å, and (e) $h = 15$ Å.

from figure 3 that the MCITs are almost unchanged during the time for which the torque is applied, while the inner tube is just rotating due to the torque applied. In other words, the axial oscillation of the inner tube is restricted by the applied torque at that time, which is dissimilar to the work of Cai *et al* [22]. When the systems enter *NVE*, all four MCITs are at the lower side of their initial positions. Figure 4 shows the MCITs of all four models with respect to time during the *NVE*. For the inner tube without a helical rise, the oscillation is still stable after 800 ps, but the equilibrium position of the inner tube is not identical to its initial position. It should be noted that the oscillation amplitude of the inner tube without any helical rise is very small. Because during the *NVE*, except for the van der Waals forces, the DWCNT with no helical rise does not have additional energy input for breaking the equilibrium status, this triggers a bigger

oscillation of the inner tube. For the inner tube with $h = 10$ Å, the oscillation tends to be metastable and the initial and equilibrium positions of the inner tube match well after 800 ps. In the remaining two cases, the oscillations tend to be unstable, and the equilibrium positions of the inner tubes are not identical to their initial positions. The amplitudes and frequencies of the inner tubes are listed in table 2. Considering the amplitudes and frequencies of the inner tubes, we find that the amplitude of the inner tubes without a helical rise mode is the lowest (0.2 Å in table 2) but the frequency can reach gigahertz (25 GHz). For the inner tube with $h = 10$ Å, the amplitude (5.5 Å in table 2) is higher than that of the inner tube with $h = 0$ Å, but the frequency (5 GHz) is lower than that of inner tube with $h = 0$ Å. The oscillatory amplitudes and frequencies of the remaining two modes are uncertain because of their unstable oscillations.

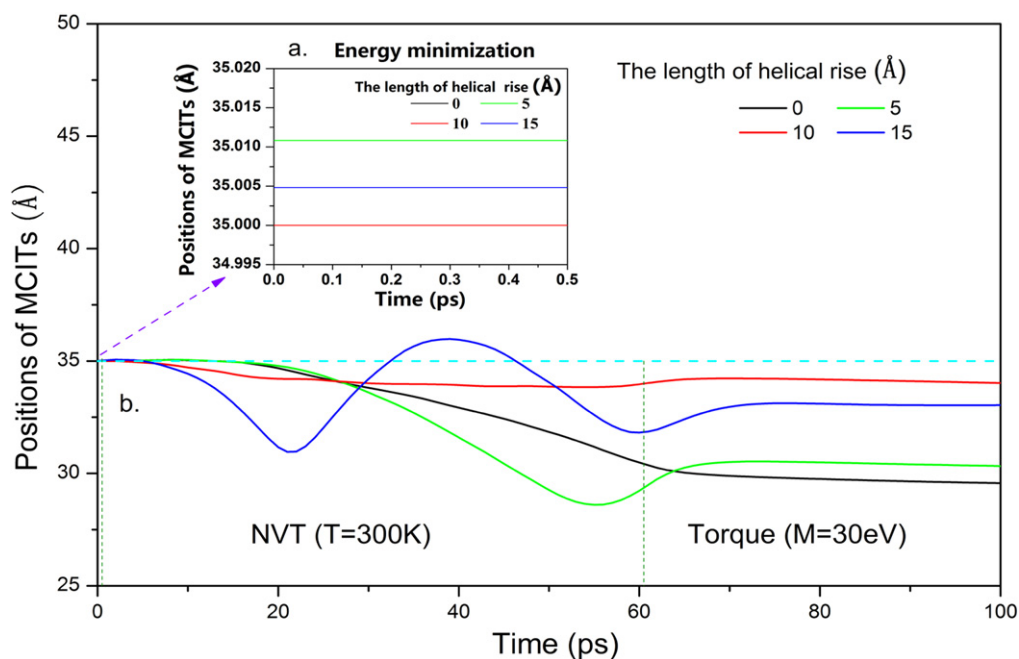


Figure 3. Histories of positions of MCITs with different h in the (9, 9)@(24, 0) carbon nanotube-based oscillators before 100 ps. (a) During energy minimization, and (b) during *NVT* and torque. (The broken line represents the initial position of the MCITs.)

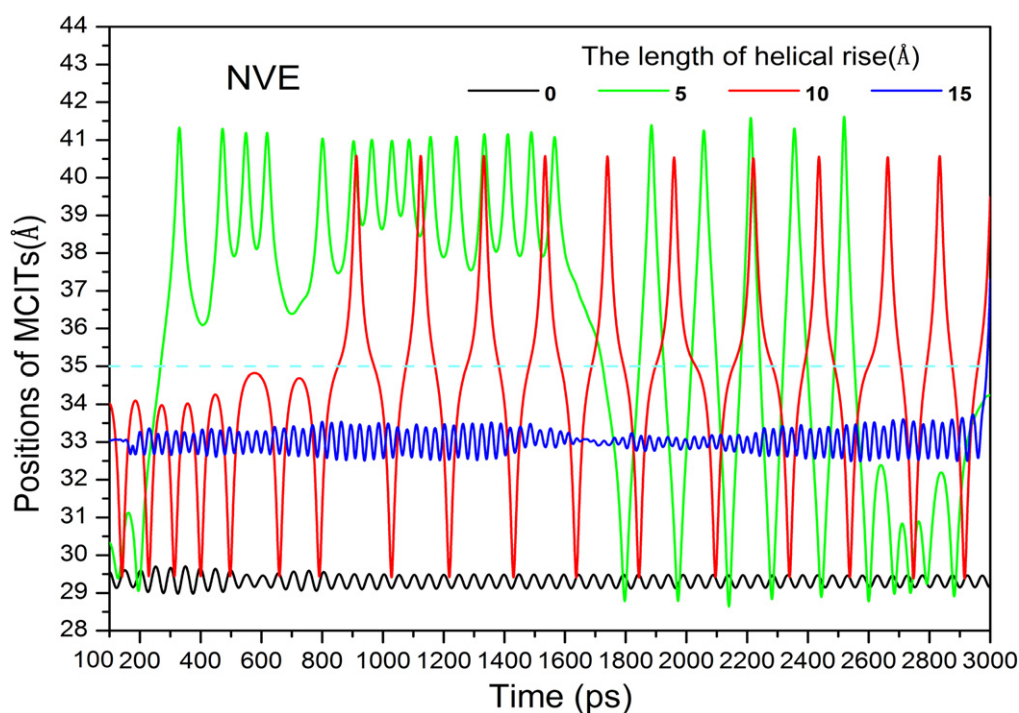


Figure 4. Positions of MCITs with different h during *NVE* (the broken line represents the initial position of MCITs).

Table 2. Oscillation amplitude and frequency of MCITs in bitube (9, 9)@(24, 0) after 800 ps.

Helical rise (Å)	Oscillation amplitude (Å)	Oscillation frequency (GHz)
0	0.2	25
5	—	—
10	5.5	5
15	—	—

The oscillation restoring forces (i.e. the total van der Waals forces of the inner tube along the axial direction) of all four inner tubes are shown in figure 5. The restoring forces of inner tubes with $h = 0$ and 10 Å exhibit metastable periodic variation. The peak restoring force of the inner tube with $h = 0$ Å is the lowest (around 0.015 nN) of the four modes after 800 ps, approximately one-tenth of those with a helical rise. For the $h = 5$ and 15 Å modes, the restoring forces of the inner tubes exhibit unstable variation, resulting in

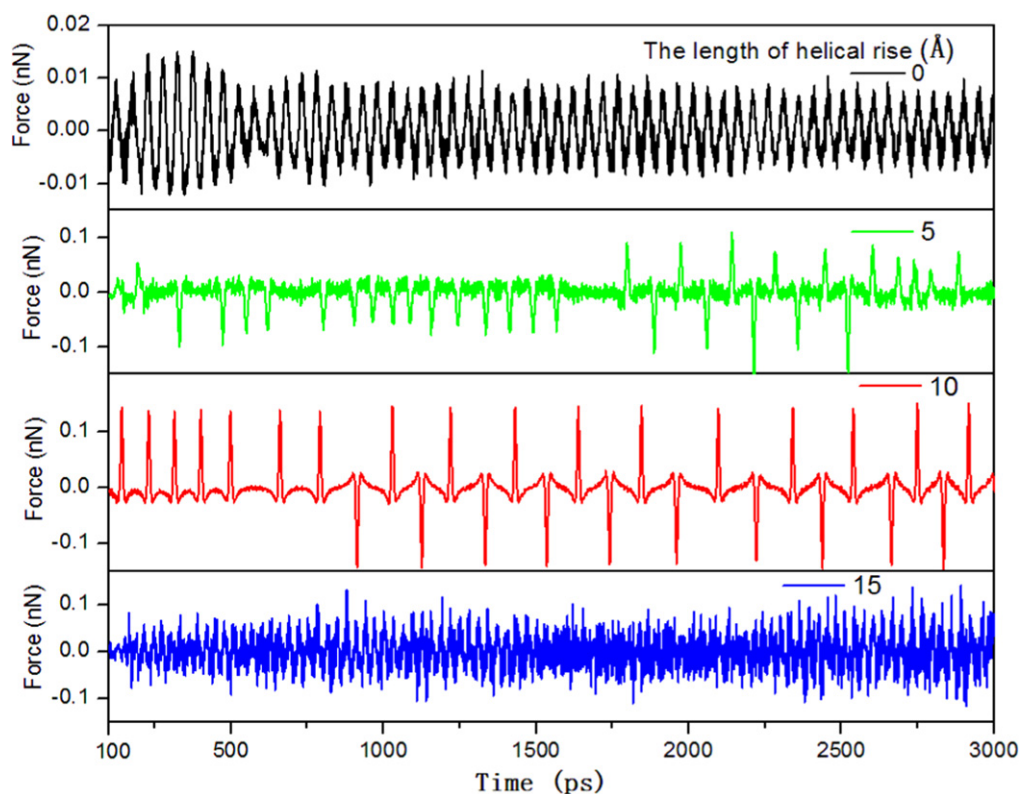


Figure 5. Restoring force of inner tubes with different h with respect to time.

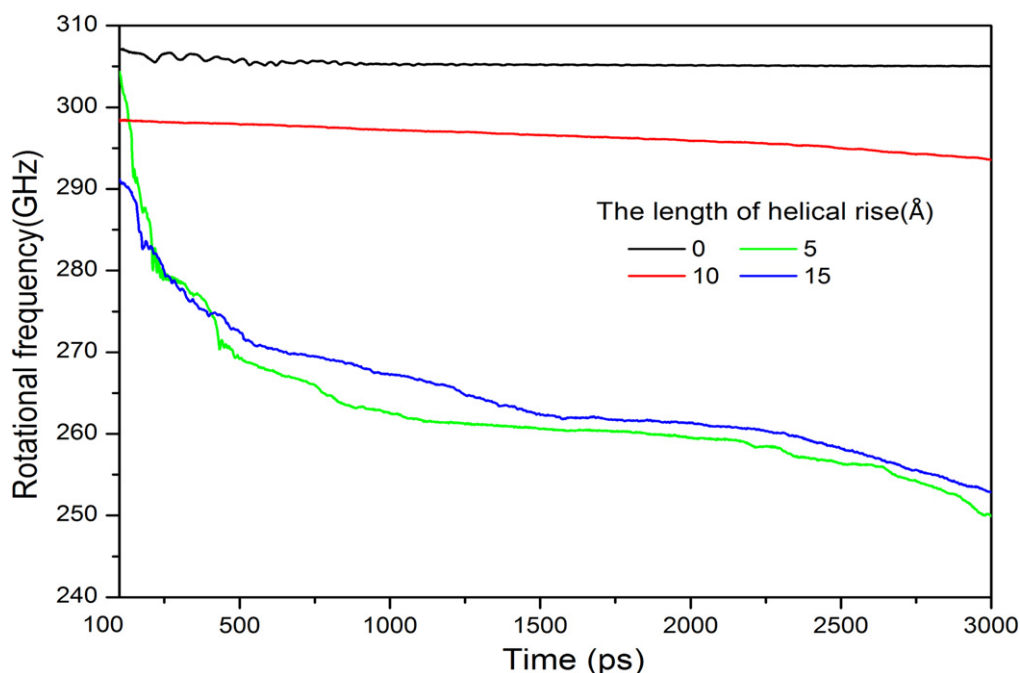


Figure 6. Histories of rotational frequency of inner tubes with different h in the (9, 9)@(24, 0) carbon nanotube-based oscillator.

unstable oscillation of their MCITs (see figure 4) because the van der Waals interactions between the inner and outer nanotubes are central to oscillatory stability, as previously illustrated by Román Pérez and Soler [21].

Figure 6 shows the histories of the rotational frequencies of the inner tubes with different h . The rotational frequencies

of the inner tubes with $h = 0$ and $10 \text{ \AA}$ are reduced slightly with respect to time, whereas the rotational frequencies decline significantly for the inner tubes with $h = 5$ and $15 \text{ \AA}$. It also can be seen from figures 4 and 6 that the inner tube oscillation is more stable when there is less decrease in rotational frequency.

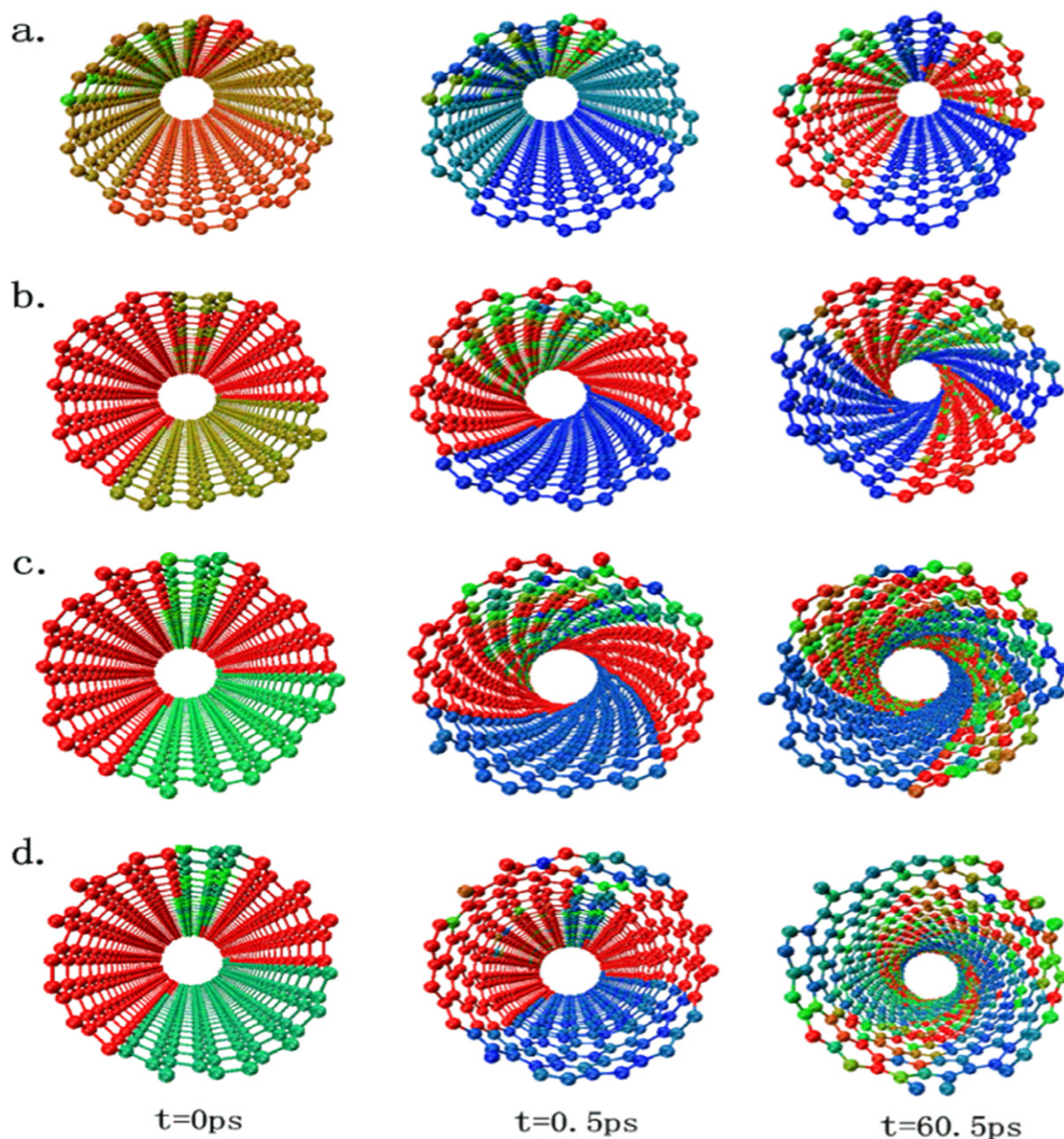


Figure 7. Equivalent stress distribution of four inner tubes (a) with $h = 0$ Å, (b) $h = 5$ Å, (c) $h = 10$ Å, and (d) $h = 15$ Å (red represents the maximum equivalent stress; blue represents the minimum equivalent stress).

Cauchy stresses are also calculated to compare the stress relaxation during energy minimization and *NVT*. Figures 7(a)–(d) show the equivalent stress distributions of four inner tubes, colored according to the equivalent stress. In figure 7, red and blue represent the maximum and minimum of equivalent stresses, respectively. The equivalent stresses of the inner tubes with a helical rise are much greater than those of the inner tube without helical rise in the initial configuration ($t = 0$ ps) because they suffer from self-torque due to distortion of the hexagon structure after the helical rise is applied. The equivalent stresses in the four inner tubes relax significantly after energy minimization and then relax further compared with their corresponding initial states after the canonical *NVT* ensemble at around 300 K for 60 ps, due to the thermal motion of the atoms gradually dispelling the twisted

state of the inner tubes. The relaxation of the inner tube self-torque leads to the variation of the tube structure.

Figures 8(a)–(d) list the evolution of a specified labeled bond (also shown in figure 2) in the inner tubes with different h , where $t = 0.5$ ps and 60.5 ps represent the end times of energy minimization and *NVT*, respectively. To represent the extent of distortion of the tube's hexagon, the difference between the maximum and minimum bond angles of the labeled hexagons, shown in figures 2 and 8, is introduced here and listed in table 3. We find that for the armchair@zigzag bitube systems the extent of distortion of the inner tube's hexagon in the inner tube without a helical rise (i.e., $h = 0$) tends to be more extreme than the initial configuration after the energy minimization and *NVT* processes because of interaction with the outer zigzag nanotube. For inner tubes

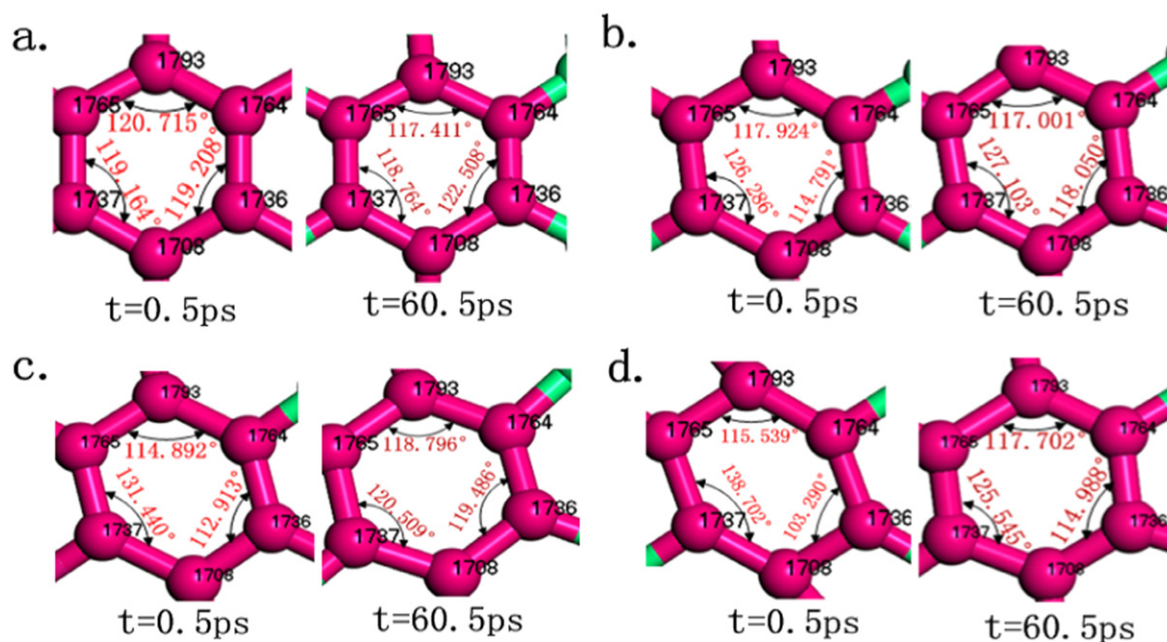


Figure 8. Variation of labeled bond angles of four inner tube hexagons with time. (a) Tube with $h = 0\text{ Å}$. (b) Tube with $h = 5\text{ Å}$. (c) Tube with $h = 10\text{ Å}$. (d) Tube with $h = 15\text{ Å}$.

with helical rise $h \neq 0$, however, the extent of distortion can be reduced to different degrees, especially for the inner tube with $h = 10\text{ Å}$, where the difference between the maximum and minimum bond angles in the labeled hexagon changes from 21.733° in the initial state to 1.713° after the NVT, an outcome that is superior even to that of the inner tube without a helical rise. We consider, therefore, that the inner tube with $h = 10\text{ Å}$ exhibits the most desirable oscillatory behavior compared with other modes because it has the most ideal hexagon after the energy minimization and NVT processes in the armchair@zigzag bitubes.

4. Conclusions

We have proposed a novel method in which different lengths of helical rise are applied to the inner tubes in the DWCNTs-based oscillators to improve their oscillatory behaviors. The influence of the helical rise on the oscillation amplitude, frequency, and stability of the inner tubes with different helical rises in double-walled armchair@zigzag nanotubes are examined using a molecular dynamics method. It is found that helical rise plays an important part in the oscillatory behavior of the inner tubes. The oscillation of the inner tube with $h = 10\text{ Å}$ is stable and the initial and equilibrium positions match well after 800 ps, and the decrease in rotational frequency is small during the 3 ns simulation. We also examined the labeled bond angle and equivalent stress distribution of four inner tubes and found that the initial irregular hexagon of the tube with a helical rise could gradually be restored due to dissipation of the tube's self-torque with time. The inner tube with $h = 10\text{ Å}$ had the most ideal hexagon after the energy minimization and NVT process in the armchair@zigzag bitubes and it therefore exhibited superior oscillatory behavior

Table 3. Difference values between maximum and minimum bond angles.

Helical rise (Å)	The difference value between maximum and minimum bond angle		
	Initial	0.5 ps	60.5 ps
0	0.564°	1.551°	5.097°
5	11.141°	11.495°	10.102°
10	21.733°	18.231°	1.713°
15	31.316°	35.412°	10.557°

compared with other modes. The simulation results presented here indicate that a stable and smooth oscillator can be obtained by choosing an appropriate value of helical rise in oscillators based on double-walled nanotubes.

Acknowledgments

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References

- [1] Iijima S 1991 Helical microtubules of graphitic carbon *Nature* **354** 56–8
- [2] Chan Y *et al* 2015 Carbon nanotubes as a nonlinear buckled beam for nanoelectromechanical systems *Adv. Mater. Res.* **1082** 535–8
- [3] Lee S W and Campbell E E B 2013 Nanoelectromechanical devices with carbon nanotubes *Curr. Appl. Phys.* **13** 1844–59

- [4] Rasekh M *et al* 2014 NEMS thermal switch operating based on thermal expansion of carbon nanotubes *Physica E* **59** 210–7
- [5] Zang X N *et al* 2015 Graphene and carbon nanotube (CNT) in MEMS/NEMS applications *Microelectron. Eng.* **132** 192–206
- [6] Rosalba J M *et al* 2014 Electromechanical properties of carbon nanotubes *Phys. Chem. C* **118** 13936–44
- [7] Huang Z X 2008 Coaxial stability of nano-bearings constructed by double-walled carbon nanotubes *Nanotechnology* **19** 045701
- [8] Bailey S W D *et al* 2008 Carbon nanotube electron windmills: a novel design for nanomotors *Phys. Rev. Lett.* **100** 256802
- [9] Yang W D *et al* 2015 Pull-in instability of carbon nanotube-reinforced nano-switches considering scale, surface and thermal effects *Composites B* **82** 143–51
- [10] Chiu H Y *et al* 2008 Atomic-scale mass sensing using carbon nanotube resonators *Nano Lett.* **8** 4342–6
- [11] Qin Z *et al* 2008 Influence of water on the frequency of carbon nanotube oscillators *J. Comput. Theor. Nanosci.* **5** 1403–7
- [12] Legoas S B *et al* 2004 Gigahertz nanomechanical oscillators based on carbon nanotubes *Nanotechnology* **15** S184
- [13] Qiu W *et al* 2009 A new theoretical model of a carbon nanotube strain sensor *Chin. Phys. Lett.* **26** 080701
- [14] Qiu W *et al* 2010 Experimental study of the Raman strain rosette based on the carbon nanotube strain sensor *J. Raman Spectrosc.* **41** 1216–20
- [15] Qiu W *et al* 2013 The use of a carbon nanotube sensor for measuring strain by micro-Raman spectroscopy *Carbon* **53** 161–8
- [16] Zou J *et al* 2006 Self-assembly of single-walled carbon nanotubes into multiwalled carbon nanotubes in water: molecular dynamics simulations *Nano Lett.* **6** 430–4
- [17] Zou J *et al* 2006 Molecular dynamic studies of carbon water carbon composite nanotubes *Small* **2** 1348–55
- [18] Cumings J and Zettl A 2000 Low-friction nanoscale linear bearing realized from multiwall carbon nanotubes *Science* **289** 602–4
- [19] Zheng Q S and Jiang Q 2002 Multiwalled carbon nanotubes as gigahertz oscillators *Phys. Rev. Lett.* **88** 045503
- [20] Legoas S B *et al* 2003 Molecular-dynamics simulations of carbon nanotubes as gigahertz oscillators *Phys. Rev. Lett.* **90** 055504
- [21] Román Pérez G and Soler J M 2009 Efficient implementation of a van der Waals density functional: application to double-wall carbon nanotubes *Phys. Rev. Lett.* **103** 096102
- [22] Cai K *et al* 2014 Self-excited oscillation of rotating double-walled carbon nanotubes *Nano Lett.* **14** 2558–62
- [23] Brenner D W 1992 Erratum: empirical potential for hydrocarbons for use in simulating the chemical vapor deposition of diamond films *Phys. Rev. B* **46** 1948
- [24] Brenner D W *et al* 2002 A second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons *J. Phys.: Condens. Matter* **14** 783