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SPIN IN CARBON NANOTUBE-BASED OSCILLATORS

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In this paper, molecular dynamics simulations are performed on a [10, 10]/[5, 5] carbon nanotube-based oscillator. In our work, we observed a spin phenomenon of the inner tube when it oscillated in an isolated oscillator system. If there exist a rocking motion when the inner tube started to oscillate, an axial torque would be observed, and it would drive the inner tube to spin. When the oscillation became stable, the torque almost vanished, and the spin was stabilized with a constant frequency of 21.78 GHz. Such a spin phenomenon was also observed when the oscillator system was at a room temperature of 300 K. However, both magnitude and direction of the spin angular velocity varied from time to time, even after the oscillation of the inner tube stopped due to the energy dissipation.

Keywords: Nanotube; nano-scillator; spin.

1. Introduction

Based on their unique mechanical and electronic properties,[1] carbon nanotubes, especially multi-walled nanotubes (MWNTs), are expected to play a key role in some nanodevice and machine designs.[2–6] This prediction was based on the relative motion of nanotube walls. After considering that the relative motion of nanotube walls was controlled by the potential relief of interlayer interaction energy, Lozovik and his co-workers[2] proposed to use double-walled nanotubes as nut and bolt pairs. Then, a set of new Nanoelectromechanical Systems (NEMS), such as a nanodrill and a nanoresistor,[3] was designed. Furthermore, when the cases in which the corrugation of interlayer energy had little or no effect

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on relative motion of nanotube walls were considered, nanobearings,[4] nanogears,[5] and a mechanical nanoswitch[6] were designed. Cumings and Zettl[4] found that there was ultra-low friction due to interlayer interaction in MWNTs. By analyzing this occurrence, a nanoscale linear bearing was realized. Srivastava[5] proposed a phenomenological model for the laser-powered gear motor. This model was tested through molecular dynamics simulations. Based on Cumings and Zettl's idea, Forro[6] pointed out the possibility of designing a nanoswitch operated by electrostatic forces.

Recently, carbon nanotube-based oscillators have been of interest to engineers since Zheng *et al.*[7,8] predicted that multi-walled carbon nanotubes can be used as gigahertz oscillators. Some molecular dynamics simulations have been performed to simulate the mechanical behavior of double-walled carbon nanotube-based oscillators. Legoas *et al.*[9] performed the first molecular dynamics simulation for nanotube-based oscillators. They used a standard molecular force field and observed frequencies as large as 38 GHz. Legoas and his coworkers[10] also pointed out that stable oscillators were only possible when the interlayer distances between the outer and inner tubes were of ~ 0.34 nm. Zhao *et al.*[11] studied energy dissipation mechanisms in carbon nanotube-based oscillators. They observed a rocking motion of oscillators with short lengths (less than 3.0 nm). In other research work,[12,13] mechanical energy dissipation in nanotube-based oscillators was also studied. In addition, a gigahertz actuator, based on multi-walled carbon nanotube encapsulating metallic ions, was demonstrated by Kang and Hwang.[14]

2. Methodology

In this paper, we use molecular dynamics to study the oscillating mechanism of a [10, 10]/[5, 5] double-walled carbon nanotube-based oscillator. The interlayer distance between the outer and inner tubes is 0.34 nm. We do not consider incommensurate effects in this paper. The schematic representation of this nanomechanical system is illustrated in Fig. 1, which is similar to the one proposed by Zheng and his collaborators.[7] The length of the outer tube is 3.57 nm, and the length of the inner tube is 2.5 nm. A middle segment of the outer tube is fixed in this nanomechanical system. The potential function we use for carbon–carbon bonds is the second-generation reactive empirical bond order (REBO) potential function.[15] This potential includes chemical reactions and remote effects, caused

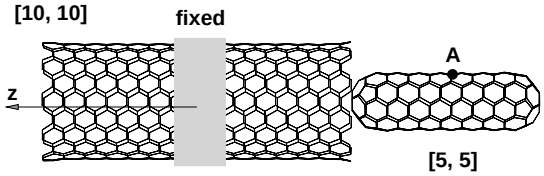


Fig. 1. A [10, 10]/[5, 5] carbon nanotube-based oscillator.

by conjugated bonding. The potential function can be written as follows:

$$E = \sum_i \sum_{j,j>i} [V^R(r_{ij}) - b_{ij} V^A(r_{ij})], \tag{1}$$

where r_{ij} is the bond length between atom i and atom j; $V^R(r_{ij})$ and $V^A(r_{ij})$ are pair-additive interactions that represent all the interatomic repulsions and attractions from valence electrons, respectively; b_{ij} contains the functions that depend on the local coordinates and bond angles for atoms i and j.

In addition, we use a Lennard–Jones 6–12 potential[16] as van der Waals energy for nonbonded interactions between interval layers:

$$E_{LJ}(r) = \frac{A}{\sigma^6}\left[\frac{1}{2} y_0^6 \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right], \tag{2}$$

where $A = 24.3 \times 10^{-25}$ Jnm^6, $\sigma = 1.42$ nm and $y_0 = 2.7$. The interlayer equilibrium distance is 0.34 nm, which produces the minimum van der Waals energy. This distance matches the thickness of a graphite sheet, and it also satisfies the criterion proposed by Legoas *et al.*[10] for stable nanotube-based oscillators. In molecular dynamics simulations, the following equations of motion need to be solved:

$$m_i \ddot{r}_i = -\frac{\partial E}{\partial r_i} - \frac{\partial E_{LJ}}{\partial r_i}, \tag{3}$$

where r_i is the position of atom i.

Before performing molecular dynamics simulations, we conduct the energy minimization to this double-walled carbon nanotube-based system. As a result, the inner tube is inside the outer tube, and they have a common axis. Then, the inner tube is pulled out of the outer tube with an initial extrusion length L. The initial extrusion length is set to equal the length of the inner tube for all the simulations in this paper. The simulation starts once the inner tube is released without initial velocity. During the simulations, we investigate the motion of atom A, which is shown in Fig. 1, to study the inner tube oscillating mechanism. Since atom A is in the middle of the inner tube, its z coordinate represents the center-of-distance separation between the inner tube and the outer tube.

3. Results and Discussion

We first assume that the simulated oscillator is an isolated system, i.e., no heat transfer between the oscillator and its surroundings, and its initial temperature is 0 K. Figure 2 shows the z-coordinate profile of atom A, which implies the relative motion between the inner tube and the outer tube. It can be seen that the oscillating amplitude of the inner tube decays during the first several oscillations. This observation implies that the interlay energy dissipates. We believe that this interlayer energy dissipation is due to the interlayer friction resulting from the rocking motion, which was mentioned by Zhao *et al.*[11] The rocking motion is the transverse vibration of the inner tube, and it is also observed in

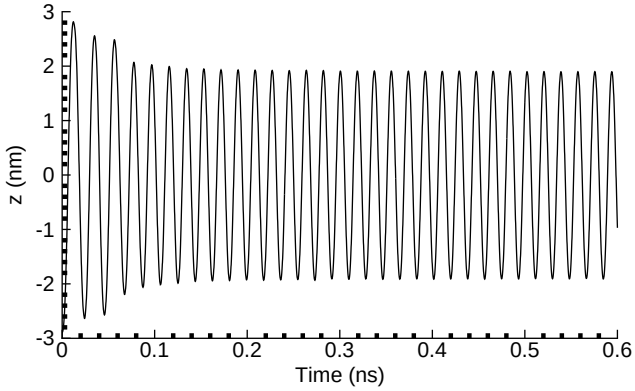


Fig. 2. The *z*-coordinate profile of atom *A* illustrates oscillation of the inner tube inside the outer tube.

our simulations. Such interlayer energy dissipation can be also illustrated in the evolution of the amplitude of the interlayer energy, shown in Fig. 3. The interlayer energy reaches a peak when the inner tube has a zero center-of-mass velocity. In the mean time, the center-of-distance separation between the outer tube and the inner tube reaches a peak. Since the amplitude of the center-of-distance separation does not decrease from the second to third oscillations, shown in Fig. 2, the amplitude of the interlayer energy keeps the same at the period between 0.022 ns to 0.055 ns. When the rocking motion vanishes at the time of 0.15 ns, the amplitudes of both the center-of-distance separation and the interlayer energy become constant, i.e., the oscillation becomes stable. The calculated frequency is 54.64 GHz, which is different from what Legoas *et al.* obtained.[9,10] It might be due to different potential functions that were used to describe carbon–carbon bonds and interlayer interactions in Refs. 9 and 10. The other reason can be that the whole outer tube was fixed in their simulations.

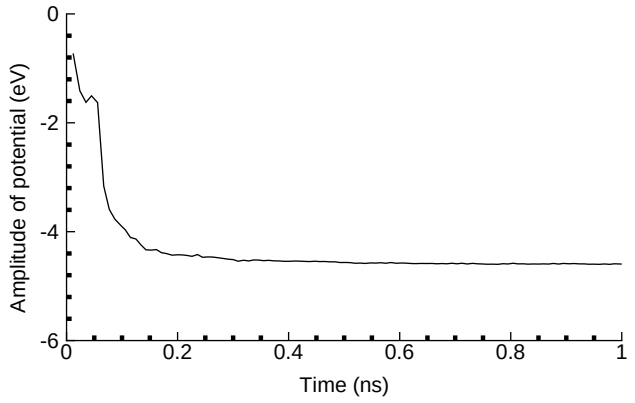


Fig. 3. The evolution of the amplitude of the interlayer energy shows that the motion of the oscillator becomes stable after 0.15 ns.

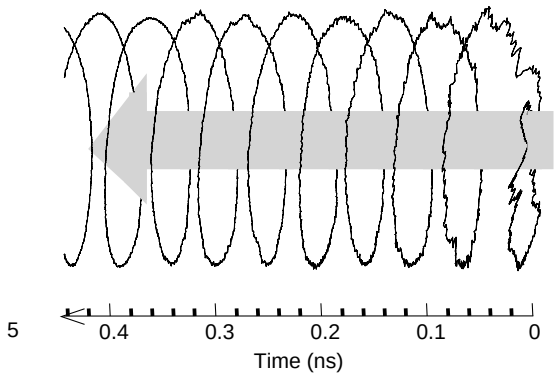


Fig. 4. Evolution of the position of atom *A* on the *X*–*Y* plane with time demonstrates a spin phenomenon of the inner tube in a double-walled carbon nanotube-based oscillator.

An interesting phenomenon observed in our simulation is that the inner tube spins (self-rotation of the inner tube about its axis) during its oscillation. Figure 4 shows the motion of atom *A* on the *X*–*Y* plane with time, and one can see that the inner tube spins counterclockwise when viewed from the right end of the outer tube. The interlayer friction resulting from the rocking motion not only reduces the amplitude of center-of-distance separation but also produces axial torque on the inner tube. The evolution of the time-averaged axial torque, which is produced on the inner tube, is shown in Fig. 5. We can see that there is a finite value of torque, –0.00013 nN nm, on each atom at the beginning of the oscillation. This negative torque drives the inner tube to spin counterclockwise. When the rocking motion vanishes, the magnitude of torque becomes much small (< 0.00003 nN nm per atom) without much influence on the spin motion. As a result, the spin becomes steady, and the calculated spin frequency is 21.78 GHz. The work of the initial torque applied on the inner tube is computed to be 3.06 eV, which is also the rotational kinetic energy of the inner tube when it spins. Such energy comes from part of the dissipated interlayer energy, which is 3.6 eV calculated from Fig. 3. The rest

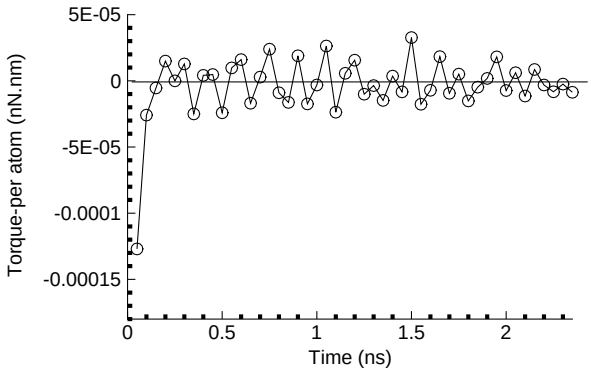


Fig. 5. Evolution of axial torque produced on the inner tube. The torque are averaged on each atom for every 50 picoseconds.

of dissipated interlayer energy results in increasing the temperature of the oscillator from 0 K to 5 K and the potential energy of nanotubes as well. We should note that if the initial extrusion of the inner tube is less than a threshold length, e.g., half of the inner tube length in our studies, no rocking motion occurs.[11] The initial torque will become a near zero value. Therefore, there is no spin phenomenon observed.

There were some studies of temperature effects on energy dissipation[13] in gigahertz nanotube-based oscillators. If an initial temperature was given,[13] energy of the nanooscillator would be dissipated even without the rocking motion of the inner tube. In this paper, we also study the mechanism of carbon nanotube-based oscillators at a room temperature of 300 K. With difference from Ref. 13, we implement the Hoover thermostat[17] into the molecular dynamics simulation to maintain a constant temperature of the outer tube. In this case, as shown in Fig. 6, the amplitude of the center-of-distance separation decays to a close-to-zero value, and the oscillation eventually stops. In the meantime, we find that the calculated torque does not vanish with time, and its magnitude

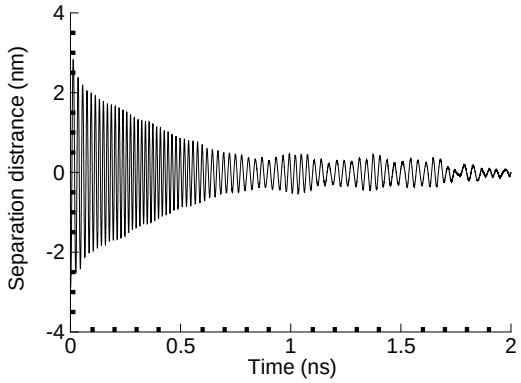


Fig. 6. Evolution of center-of-distance separation when the outer tube is at a room temperature of 300 K.

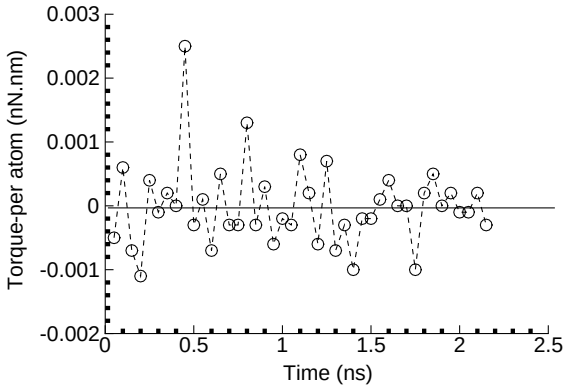
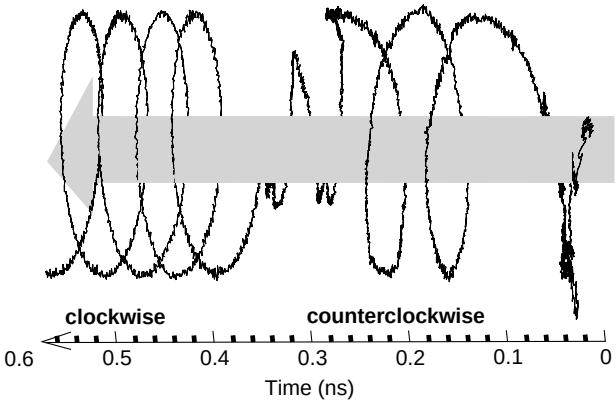
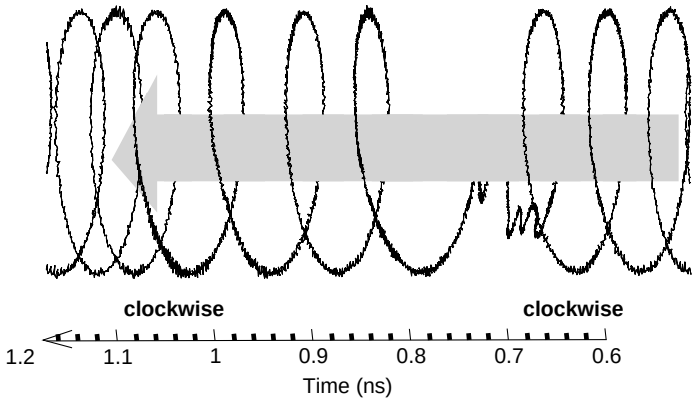


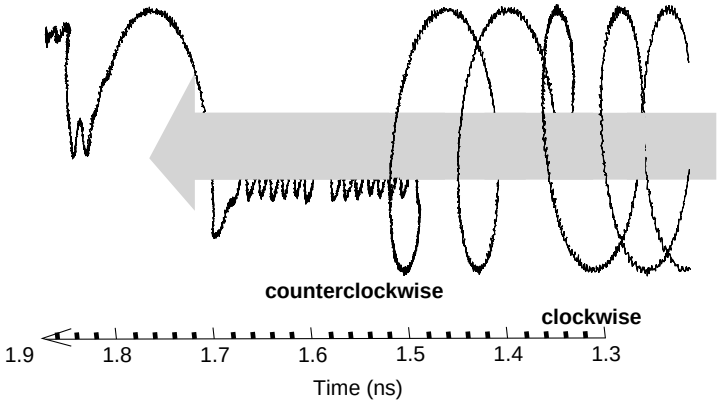
Fig. 7. Time-averaged axial torque produced on each atom of the inner tube when the outer tube is at a room temperature of 300 K.



(a)



(b)



(c)

Fig. 8. Spin of the inner tube when the outer tube is at a room temperature of 300 K.

can be as high as 0.0025 nN nm per atom, shown in Fig. 7. Consequently, the spin angular velocity, including its magnitude and direction, is various from time to time.

The following discussion is based on what can be observed in Figs. 7 and 8. There is a negative torque produced on the inner tube at the beginning of the oscillation when the outer tube is at room temperature. This negative torque drives the inner tube to spin counterclockwise when viewed from the right end of the outer tube. The spin angular velocity is 104.7 rad/ns at the time of 0.2 ns. During the period between the time of 0.25 ns and 0.4 ns, the torque are almost non-negative so that the counterclockwise spin of the inner tube stops, and the clockwise spin starts. A large torque of 0.0025 nN nm per atom at the time of 0.450 ns accelerates the angular velocity to 158.9 rad/ns. Then, since the positive torque are dominant until the time of 1.3 ns, the inner tube keeps spinning clockwise although the spin stops for a moment around the time of 0.7 ns. However, the angular velocities are various because the positive torque accelerate the spin while the negative torque decelerate it. The angular velocities are 89.8 rad/ns at 0.65 ns, 93.6 rad/ns at 1.05 ns, 176.5 rad/ns at 1.15 ns, and 121.2 rad/ns at 1.2 ns. The negative torque between 1.3 ns and 1.5 ns makes the inner tube change its spin direction from clockwise to counterclockwise. We can see that no regular spin can be found for the inner tube during its oscillation if the outer tube is at room temperature. Even after the oscillation stops, the inner tube keeps spinning but with various spin angular velocities and directions from time to time.

4. Conclusions

We studied a double-walled carbon nanotube-based oscillator. When the oscillator was an isolated system with an initial temperature of 0 K, the oscillating became sustainable and the frequency could be 54.64 GHz. We observed a spin phenomenon of the inner tube due to the axial torque caused by the rocking motion. The spin could also become sustainable and the spin frequency was 21.78 GHz. If the oscillator was at room temperature, its oscillation would stop eventually. In addition, the spin was irregular because of finite-valued torque, which could accelerate/decelerate the spin and even change its clockwise/counterclockwise direction. Such spin phenomenon has not been observed in previous researchers' work. We think the spin of the inner tube may be important in contributing to the overall stability of nano-oscillators with the gigahertz speed of the lateral vibration. Further experimental investigations need to be done in the future. We believe that the observation of spin phenomenon will help us fully understand mechanisms of carbon nanotube-based oscillators. Such observation will also benefit the applications of nanotube-based oscillators in memory cell design.

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