Journal of
Computational and Theoretical Nanoscience
Vol. 5, 655–658, 2008

Energy Dissipation in the Double-Walled Carbon Nanotube Based Mechanical Oscillators

Zhiping Xu

Department of Engineering Mechanics, Tsinghua University, Beijing 100084, China

We have performed atomic simulations of double-walled carbon nanotube with the inner shell oscillating inside the outer one at frequencies in the GHz range. It's found that energy exchanging with phonon bath results in a short lifetime of few nanoseconds and low *Q*-factor about one thousand. Phonon power spectrum analysis confirmed the coupling as the intrinsic source of energy dissipation and its enhancement at higher temperature. The importance of angular symmetry and the instabilities introduced by the atoms in tube ends are discussed, which have been found to contribute remarkably to the energy dissipation and should be treated attentively in practice.

Keywords: Carbon Nanotube, Energy Dissipation, GHz Oscillator, Molecular Dynamics.

1. INTRODUCTION

Carbon nanotube based devices have shown great promises in the nano-electromechanical systems (NEMs) because of their intriguing physical and chemical properties. Theoretical and experimental studies have shown that carbon nanotube has high Young's modulus on the order of 1 TPa and tensile strength of 63 GPa.[1] However, the intershell shear strength of the multi-walled carbon nanotube has been observed with an ultra-low value of 0.08∼0.3 MPa.[2, 3] This extremely high anisotropy suggests the possibilities of building nanoscale machines through the relative motion of cylindrical graphene shells. For instance, the multi-walled carbon nanotube based axial oscillator model[4] has been shown to possess ultrahigh frequency up to GHz, which was confirmed later by the subsequent numerical studies.[5–8] The high frequency and quasi-one dimensional nature make this kind of device good candidates of building blocks of NEMs. However the amplitude of the oscillation observed during the simulation was found to decay to zero within few nanoseconds. The short lifetime greatly limits its practical application because it brings difficulties for the energy supplement and signal detection. Thus where the dissipation arises and how to reduce it become critical issues and should receive wide attention.

It is necessary to understand the intrinsic mechanism of the dynamical process if we want to reduce the damping. Previous molecular dynamics simulation works proposed several dissipation mechanisms, such as the ends effects,[5] intertube commensurabilities[6, 7] and energy exchanging with instabilities (rocking, waving motion, etc.).[8, 9] Based on the atomistic simulation carried out by ourselves and analysis on the previously reported results, we will give a general discussion of the energy dissipation process with consideration on the effects of temperature, size and structure of the system. Especially, the role of angular symmetry and structural imperfection at tube ends are investigated here.

2. METHODS

In our work, we have investigated the double-walled carbon nanotubes with equal length as shown in Figure 1. As the inner tube is pulled out at a distance x, the surface traction resulting from the intershell van der Waals forces will attract it back into the outshell. The potential profile of the intershell interaction in a typical 10 nm long double-walled carbon nanotube (5, 5)@(10, 10) has been calculated using the Lennard-Jones formula

$$V_{ij} = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right] \tag{1}$$

and plotted in Figure 1. In the expression, r_{ij} represents the interatomic distance and parameters $\varepsilon = 0.00313$ eV, $\sigma = 3.234$ Å (Ref. [10]) have been used.

As seen from the energy surface in Figure 1, when the intertube displacement is small, the energy corrugation is dominated by the shear strength of contacted graphite surface. However as the displacement increases, the left ends of inner tube and right ends of the outer one move close. The resulting repulsive interaction between the ends leads to a sharp arising of potential energy. Furthermore, since the carbon atoms at the tube ends have at least one dangling σ bonds, instabilities are expected to occur and introduce large damping on the axial oscillation.

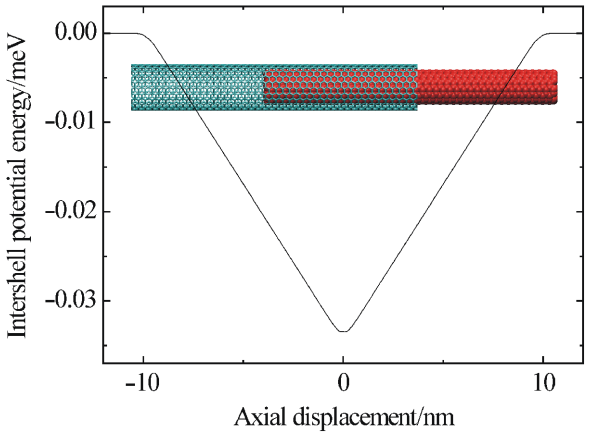

Fig. 1. The atomic configuration of the double-walled carbon nanotube (5, 5)@(10, 10) based mechanical oscillator and the potential profile along the axial displacement between the centers of the mass in the inner (red) and outer tube (gray) respectively.

To investigate the effects of these factors, we have carried out molecular dynamics simulation using the modified Dreiding force field, which was successfully applied to predict the equilibrium structure of fullerene structures.[11] Before performing the NVE dynamic simulation, we have firstly equilibrated the system using a Nosé-Hoover thermostat for 200 ps, where the coupling time constant is set to 0.1 ps. After that the inner tube is pulled out with an initial extrusion of 2 nm and equations of motion are solved subsequently using the verlocity-Verlet algorithm without any constraints. The time step of 1.0 fs is used and confirmed to conserve the total energy of the system well.[12]

3. RESULTS

Firstly we have examined the double-walled carbon nanotubes (5, 5)@(10, 10) with the length of 10 nm and the environmental temperature of 300 K. The oscillatory and dissipative behavior is plotted in Figure 2(a) through the evolution of amplitude. The axial oscillation decays quickly and the amplitude shrinks to zero in five nanoseconds. Corresponding frequency statistics (see Fig. 2(b)) yields $f = 45$ GHz which is consistent with the theoretical estimation

$$f = \frac{\alpha}{4}\sqrt{\frac{\Pi}{\Delta L}} \tag{2}$$

given by Zheng and Jiang,[4] where L is the length of nanotube, Δ is the initial extrusion, Π represents an average value of van der Waals interaction and α is a variable depends on the number of graphene shells. Moreover as expected from the expression (2), the frequency is observed to rise up as the amplitude of oscillation shrinks down.

To characterize the damping behavior of the mechanical oscillators, a well-defined quality factor is helpful. Following Jiang et al.'s work[13] we define $Q = 2\pi E_{\text{pot}}/\Delta E_{\text{pot}}$, where E_{pot} and ΔE_{pot} are the maximum potential energy and its loss in single oscillatory period. After n cycles

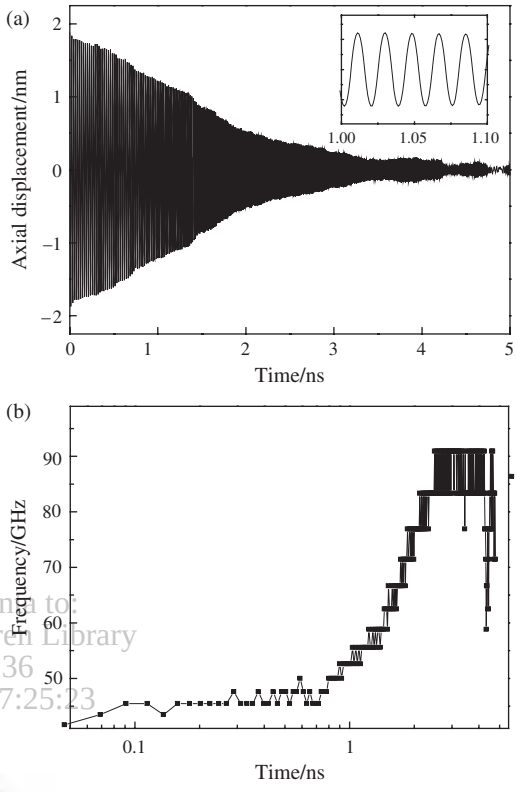

Fig. 2. Intershell oscillatory motion of the 10 nm long (5, 5)@(10, 10) nanotubes at 300 K. (a) The evolution of axial amplitude, the periodic pattern is plotted as inset; (b) the frequency calculated with time dependence.

of the oscillation, the extrusion energy of the nanotube decreases to E_n, and Q gives a quantitative measurement of the energy loss. By fitting the results presented in Figure 2(a) with the expression $E_n = E_{\text{pot}}(1 - 2\pi/Q)^n$, we obtain a rough estimation of $Q = 880$ for the (5, 5)@(10, 10) oscillator, which is a little lower in comparison with $Q \sim 1500$ observed in the cantilevered carbon nanotube beam oscillators at the same temperature, i.e., $T = 300$ K.[13]

As pointed out previously,[9] the energy dissipation of axial oscillation is caused by the energy transferring from sliding into the lattice vibration modes, through a resonant or non-resonant manner. As indicated by the Boltzmann distribution $\rho(E) = \exp(-E/k_{\text{B}}T)$, the low frequency phonons will contribute less at lower temperature. Moreover the amplitude of intrashell elastic distortion which obstructs the sliding motion will be weaken as temperature decreases. Thus the coupling with lower temperature is expected to reduce the energy dissipation. To make this purpose, the (5, 5)@(10, 10) system with the environmental temperature at 0 K has been studied in comparison with 300 K. The results are presented in Figure 3.

To investigate the occupation of lattice vibration modes, we have calculated the phonon spectrum density $I(\omega)$ as the Fourier transformation of velocity autocorrelation function

$$C_v(\tau) = \langle v_i(\tau) \cdot v_i(0) \rangle, \quad i = 1, 2, \ldots, 3N \tag{3}$$

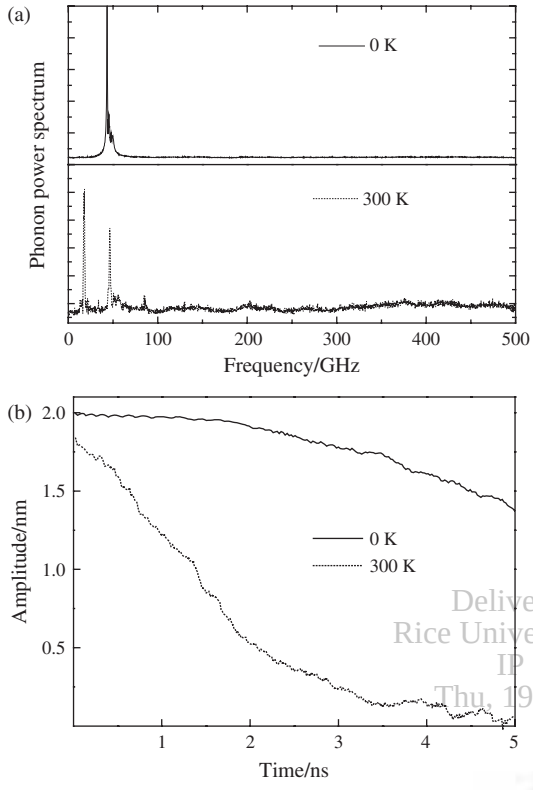

Fig. 3. The effect of environmental temperature on the energy dissipation in the 10 nm long (5, 5)@(10, 10) nanotubes. (a) Phonon power spectrum through Fourier transformation of the velocity autocorrelation function, (b) amplitude decaying with initial temperature at 0 K (solid line) and 300 K (dot) are shown.

where v_i is the velocity of carbon atom and $3N$ is the degree of freedom in the system. From the results depicted in Figure 3(a) we can see that, as expected, less phonon modes within GHz frequencies are activated and participate in the energy sharing at 0 K. As a result, the amplitude loss have been reduced by a factor 75%, as shown in Figure 3(b).

Another important factor on the dissipation process is the symmetry of the nanotube. It is found that the potential surface of intershell sliding and rotation in double-walled carbon nanotube systems can be tuned through changing the chiralities of nanotubes.[14] The axially commensurate nanotubes have much larger size-dependent shear strength than the incommensurate systems, and molecular dynamics simulation studies[6, 7] have revealed the enhancement of damping in the axially commensurate systems.

Besides of the axial commensurability, the angular symmetry can also affect the sliding dynamics strongly as addressed below, yet which has not been studied up to now. We have noticed the double-walled carbon nanotubes (5, 5) @(10, 10) studied possess here angular five-fold symmetry and thus have a periodic barrier $U_\theta = 0.0216$ meV/atom while rotating, which is even larger than the axial corrugation $U_z = 0.00745$ meV/atom.[14] Natually as the sliding tube deviates from the minimum of angular potential surface, it will bear considerable angular force and can be driven to rotate. Significant intershell rotation has been observed in our simulation and the angular velocity ω is found to be on the order of 0.1 rad/ps, which corresponds to the height of angular potential barrier. While in double-walled carbon nanotubes without this angular symmetry, (7, 7)@(12, 12) for example, the potential barrier decreases to the order of 10^{-12} meV/atom. Our calculation shows that the angular velocity excited in this system is one order lower than (5, 5)@(10, 10) system. This negligibly small rotational energy contributes little to the damping of sliding. To investigate this effect, we have examined both these two kinds of nanotubes at 0 K for comparison. The results (Fig. 4) show a 30% reduction of amplitude attenuation in the 5 ns simulation. We have also simulated incommensurate double-walled carbon nanotubes such as (11, 2)@(12, 12) and (5, 0)@(8, 8) and found the angular speed is also limited on the order of 0.01 rad/ps.

Now let we turn to another major factor arising from the imperfective atomic structure of double-walled carbon nanotubes shown in Figure 1. The atoms saturated by hydrogen at the tube ends have different chemical circumstance in comparison with the atoms in the central region. The hydrogen terminated dangling bonds presented at the ends can introduce instabilities when they cross each other. This peculiar "edge effects" has been argued to be able to contribute remarkably to the energy dissipation.[5]

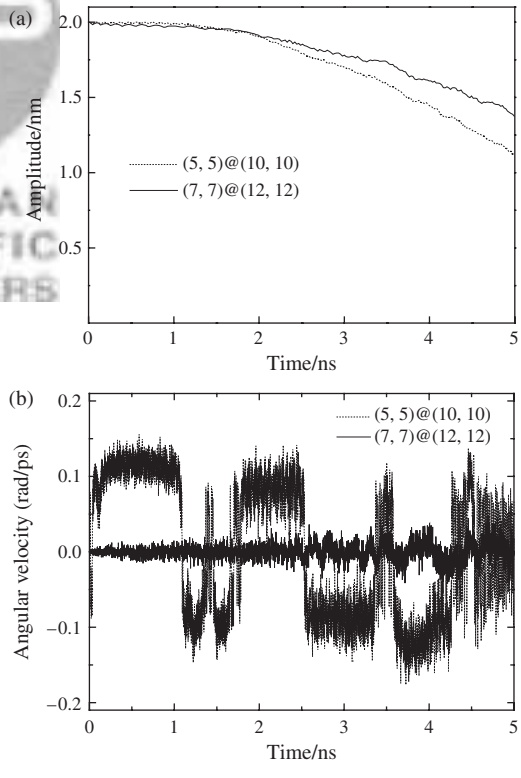

Fig. 4. Effects of the angular potential barriers on the energy dissipation of sliding. (a) Oscillatory amplitude damping of (5, 5)@(10, 10) (dot) and (7, 7)@(12, 12) (solid line) nanotubes, (b) corresponding angular velocities excited during the axial sliding.

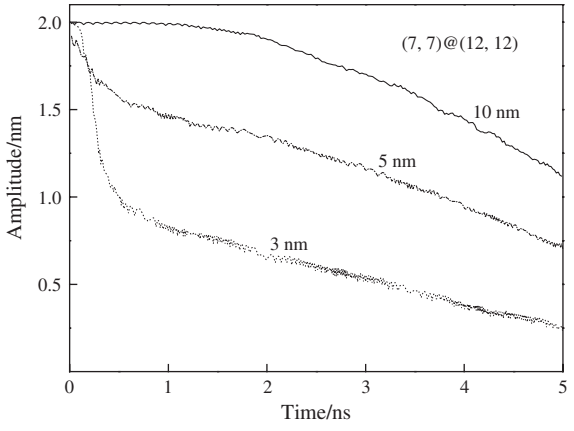

Fig. 5. Decaying of the axial oscillatory amplitude in the double-walled carbon nanotube (7, 7)@(12, 12), with different length of 3 (dot), 5 (dash-dot) and 10 nm (solid line) respectively.

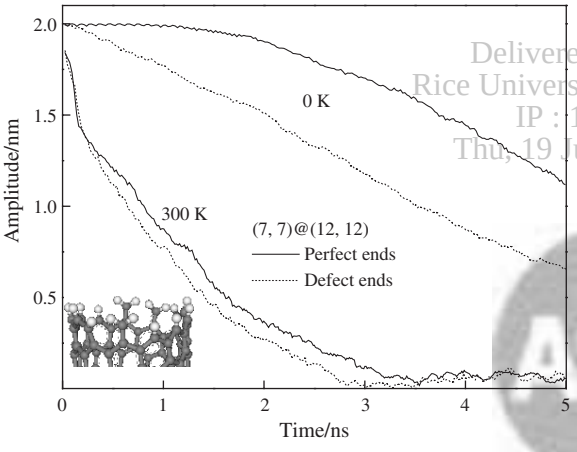

Fig. 6. Effects of end imperfection on the damping. The damping oscillatory amplitudes for (7, 7)@(12, 12) with perfect ends (solid line) and defective ends (dot) are depicted. The defective ends have been illustrated as inset, with both carbon atoms (gray) and hydrogen (white) atoms.

This feature is general and could not be avoided within our current oscillator model setup, however it will be weaken at a larger length scale as in experiment where $L =$ 330 nm[3]. To investigate the contribution of edge atoms, we have studied systems of different axial lengths firstly. As shown in Figure 5, we have found that longer double-walled carbon nanotubes have lower damping against oscillation. This can be explained that the ratio between the number of end atoms and sp^2 bonded lattice atoms has been reduced in long nanotube. By supposing the contribution from the hexagonal lattice to the damping is the same for these three systems, this result distinctly shows the contribution of the ends atoms.

To get more insight into the edge effects, we have further introduced imperfection into the tube ends. This is the typical situation in experiment, because of the limitation of the end opening technique[3] and contamination from the environment. We introduce defects in the tube ends by removing some atoms as shown in the inset of Figure 6. Comparing with the "perfect" ends which contain hydrogen terminated armchair edge only, the atoms in the "defective" ends may have one or two dangling σ bonds. From the simulation results shown in Figure 6, we have found that end defects can significantly enhance the damping, especially at low temperature, because other routes of energy dissipation such as the phonon coupling has not been activated too much.

4. CONCLUSION

In conclusion, we have performed atomistic simulation on the double-walled carbon nanotube based mechanical oscillators. The oscillatory behavior has been shown to possess ultrahigh frequency in the GHz range but decay quickly within nanoseconds with the quality factor around one thousand. The kinetic energy of sliding is dissipated through transferring energy to other lattice vibration modes. The damping rate has been found to be related to the environmental temperature, symmetry, size and atomic structure of the system. Especially we have addressed the importance of the low frequency phonon occupation, angular symmetry of the intershell energy surface and instabilities introduced at atoms in tube ends. From the engineering point of view, our results suggest that low damping in the oscillatory devices can be achieved through using low-symmetry but perfect structures and operating at low temperature.

References

1. M. F. Yu, B. I. Yakobson, and R. S. Ruoff, *J. Phys. Chem. B* 104, 8764 **(2000)**.
2. M. F. Yu, O. Lourie, M. J. Dyer, K. Moloni, T. F. Kelly, and R. S. Ruoff, *Science* 287, 637 **(2000)**.
3. J. Cumings and A. Zettl, *Science* 289, 602 **(2000)**.
4. Q. Zheng and Q. Jiang, *Phys. Rev. Lett.* 88, 045503 **(2002)**.
5. P. Tangney, S. G. Louie, and M. L. Cohen, *Phys. Rev. Lett.* 93, 065503 **(2004)**.
6. W. Guo, Y. Guo, H. Gao, Q. Zheng, and W. Zhong, *Phys. Rev. Lett.* 91, 125501 **(2003)**.
7. J. L. Rivera, C. McCabe, and P. T. Cummings, *Nano Lett.* 3, 1001 **(2003)**.
8. Y. Zhao, C. Ma, G. Chen, and Q. Jiang, *Phys. Rev. Lett.* 91, 175504 **(2003)**.
9. Y. Zhao, C. Ma, L. Wong, G. Chen, Z. Xu, Q. Zheng, Q. Jiang, and A. T. Chwang, *Nanotechnology* 17, 1032 **(2006)**.
10. F. F. Abraham and I. P. Batra, *Surface Sci.* 209, L125 **(1989)**.
11. Y. Guo, N. Karasawa, and W. A. Goddard, *Nature* 351, 464 **(1990)**.
12. E. Lindahl, B. Hess, and D. Van der Spoel, *J. Mol. Mol.* 7, 306 **(2001)**.
13. H. Jiang, M. F. Yu, B. Liu, and Y. Huang, *Phys. Rev. Lett.* 93, 185501 **(2004)**.
14. A. V. Belikov, Y. E. Lozovik, A. G. Nikolaev, and A. M. Popov, *Chem. Phys. Lett.* 385, 72 **(2004)**.

Received: 20 March 2007. Accepted: 18 April 2007.