Studies of Nanotube-based Co-axial and Resonant Oscillators

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ABSTRACT

In this paper, we first investigate mechanisms of nanotube-based co-axial oscillators based on molecular dynamics simulation. If an oscillator is an isolated system, stable oscillations of the inner tube inside of the outer tube can be observed with high oscillatory frequencies. We also study the interlayer friction between the outer tube and the inner tube when nano-oscillators are at finite temperatures. Based on the above studies, we propose to design a nanoelectromechanical oscillator system, which can provide stable oscillation. In addition, we propose the first numerical study of nanotube-based resonant oscillators via a new multiscale method.

Keywords: carbon nanotubes, oscillators, molecular dynamics, multiscale, energy dissipation

1 INTRODUCTION

Since being discovered by Ijimma [1] in 1990, carbon nanotubes (CNTs) hold promise in designing novel nanoscale materials and devices. CNTs can be designed as scanning probe tips, field emission sources or used as other nanoelectronics components, such as molecular wires and diodes. In addition, their extraordinary mechanical and electrical properties ensure CNTs to play an essential role in design of nanoscale devices, including nanotweezers [2] and nanogears [3].

Cumings and Zettl [4] realized the ultra-low friction between nanotube walls in nanoscale linear bearings and constant-force nanosprings when demonstrating the controlled and reversible telescopic extension of multi-walled carbon nanotubes (MWNTs). Consequently, MWNTs have been used to design novel nanoscale devices based on the relative motion of nanotube walls. Nanotube-based co-axial oscillators have been of interest to scientists and engineers since Zheng et al. [5] designed multi-walled carbon nanotubes as gigahertz oscillators in 2002. Unlike other nanotube-based machines, energy dissipation plays a key role and needs to be considered when designing a stable nano-oscillator.

Recently, a nanoelectromechanical device [6,7] based on an individual CNT serving as a torsional spring and mechanical support has been successfully fabricated. P. A. Williams and co-workers [6] reported fabrication of nanoscale mechanical devices, which consist of a suspended lever, i.e., the "paddle", connected by CNTs as torsion beams to stationary leads. S. J. Papadakis et al. [7] used similar techniques to synthesis so-called resonant oscillators. The metal paddles in their experiments were on CNTs so that the tubes were strained primarily in torsion. In addition, they predicted that one of their oscillators could have the resonance frequency of 0.1MHz. Regarding to the applications of such kind of oscillators, they could be used as sensors and clocks for high frequency electronics.

In this paper, we employ molecular dynamics to study nanotube-based co-axial oscillators. Temperature effects on mechanisms of co-axial oscillators are mainly investigated. A new nanoelectromechanical device containing a nanotube-based co-axial oscillator is designed to provide stable oscillations. Next, we propose the first numerical modeling and simulation of nanotube-based resonant oscillators via a multiscale method.

2 OSCILLATION MECHANISM OF NANOTUBE-BASED CO-AXIAL OSCILLATORS

We mainly study double-walled carbon nanotube-based co-axial oscillators in this section. A schematic representation of a (10,10)/(5,5) carbon nanotube-based co-axial oscillator is illustrated in Figure 1(a). A middle segment of the outer tube is fixed in this nanomechanical system. The length of the (10,10) outer tube is $L_{outer} = 3.7nm$ while the length of the (5,5) inner tube is $L_{inner} = 2.5nm$. The initial extrusion length is half of the inner tube length. Once the inner tube is released without any initial velocity, the interlayer force, due to the van der Waals energy between the inner tube and the outer tube, will drive the inner tube to move towards the center of the outer tube.

We first investigate the oscillation mechanism of an isolated oscillator, i.e. no heat exchange between the oscillator and its surrounding. The profile of separation distance between the inner tube and the outer tube is shown in Figure 1(b) during the oscillation of the inner tube inside of the outer tube. We can see that the amplitude of the separation distance keeps constant, and it is equal to the

initial extrusion length. As a conclusion, the oscillation of this nanomechanical oscillator is stable and the calculated oscillatory frequency is 55.55 GHz, which is referred to as the reference oscillatory frequency of this nano-oscillator.

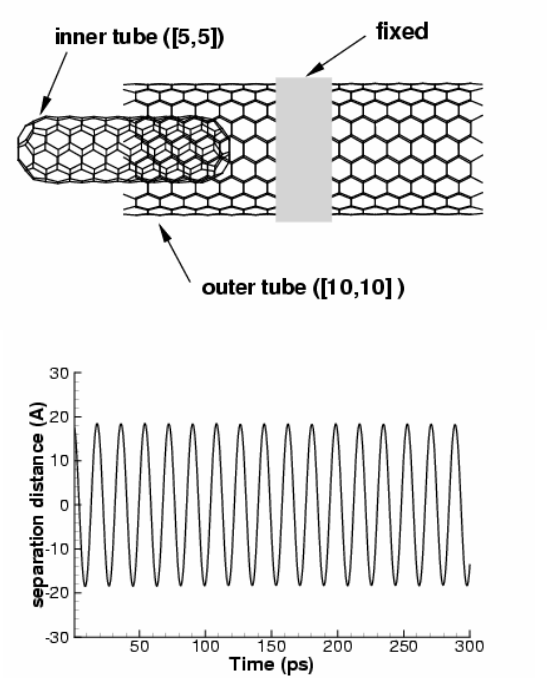

Figure 1. A (10,10)/(5,5) carbon nanotube-based co-axial oscillator. Top: schematic representation Bottom: profile of center-of-distance separation

Based on the above study, we found that an isolated nano-oscillator would be stable if the initial temperature equals zero. However, this is a very rare situation. In this paper, we also investigate the temperature effects on oscillation mechanisms of the (10,10)/(5,5) carbon nanotube-based co-axial oscillator. We first study the oscillation mechanism of the nano-oscillator at 300K. As shown in Figure 2(a), we find that a stable oscillatory frequency and amplitude cannot be obtained. The oscillatory amplitude decays until the nano-oscillator eventually stops. This phenomenon is caused by interlayer friction, which mainly dissipates the interlayer energy of the oscillator. Such dissipated energy was transferred to kinetic energy of the outer tube, and the artificial thermostat thereafter dissipates the energy of the outer tube. Consequently, the whole energy of the system is dissipated.

To study the temperature-related interlayer friction, three different temperatures are considered: 100K, 300K, and 1000K. Figure 2(b) shows the evolutions of the maximum interlayer energy of the nano-oscillator when the outer tube is at various temperatures. It can be seen that a nano-oscillator dissipates energy faster at a higher temperature. We calculate the effective interlayer friction at 0.05 ns based on the following equation:

$$F_{eff} = \frac{1}{4\xi_{\max} f}\frac{dE_{LJ}}{dt} \quad (1)$$

where ξ_{max} is the oscillatory amplitude of the nanotube-based oscillator, f the oscillatory frequency, and dE_{LJ}/dt the interlayer energy dissipation rate. Here, we think the interlayer friction results in the energy dissipation, mainly the interlayer energy dissipation. The calculated effective frictions are 0.0021, 0.0053, and 0.0133 pN per atom for the oscillator at temperatures of 100K, 300K, and 1000K, respectively. The interlayer friction is in the same order of what Cumming and Zettles [4] predicted, i.e. 0.015 pN per atom. Our studies show that the interlayer friction will be larger under a higher temperature. We can see that the oscillator will stop in a very short time, i.e. 0.1 ns, at a temperature of 1000K.

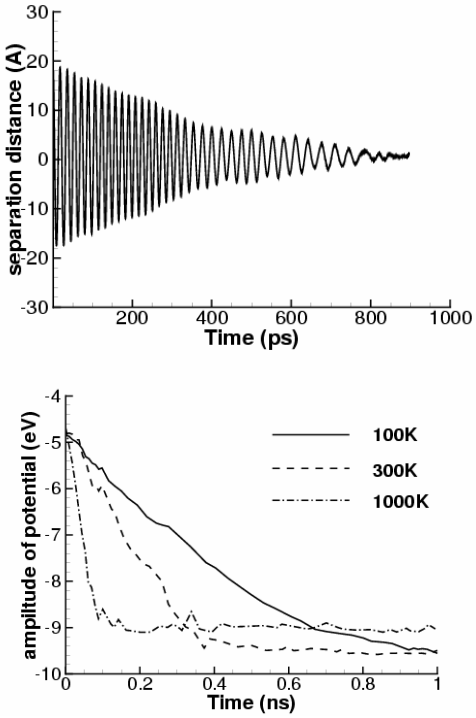

Figure 2. Top: Oscillating of the oscillator at 300K. Bottom: Interlayer energy dissipation at different temperatures

The above simulations result in a conclusion that a stable nanotube-based oscillator should be isolated with an initial zero temperature. This requirement would limit the applications of nano-oscillators since a stable nano-oscillator at specific temperatures, especially high temperatures, is attractive to engineers. Here, we propose to design a stable nanoelectromechanical oscillator as shown in Figure 3. In the proposed design, the two-walled carbon nanotube is positioned on the top of a conducting groundplane. Atomic materials for the conducting electrodes 1 and 2 are deposited on the top of the outer nanotube. In this nanoelectromechanical oscillator, the

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inner tube may be induced to move by applying a high voltage to the electrode opposite the position of the inner nanotube while another electrode is applied with a low voltage. If the electromagnetic force due to the applied high voltage is sufficiently strong, the static friction acting upon the inner nanotube may be overcome and lateral motion will be induced as a result. For example, when a high voltage is applied to electrode 1 and a low voltage is applied to electrode 2, the inner tube will move to lie underneath electrode 1 due to the force induced by the inhomogeneous electromagnetic field inside the outer tube. A signal was generated at sensor 1 when it was pressured by the inner tube. This signal can be read as logical 1. Then, if a high voltage is applied on electrode 2 and a low voltage is applied on electrode 1, the inner tube will move from left to right due to the induced electromagnetic forces. Consequently, the inner tube can move to reach sensor 2, which will generate a logical 0 signal.

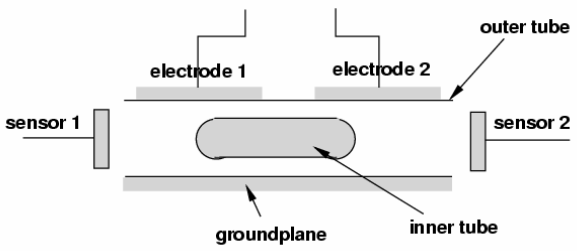

Figure 3. A nanoelectromechanical oscillator

3 OSCILLATION MECHANISM OF NANOTUBE-BASED RESONANT OSCILLATORS

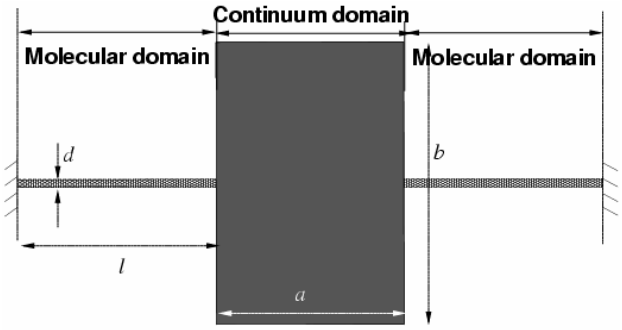

Figure 4. Multiscale model of CNT based resonant oscillator

In a nanotube-based resonant oscillator, a part of the nanotube is embedded in the metal paddle. We think such potion of the nanotube has insignificant effect on the momentum of inertia of the metal paddle. Therefore, the nanotube in this oscillator can be viewed as two individual tubes connecting with the metal padddle as shown in Figure 4, which illustrates the multiscale model of a carbon nanotube-based resonant oscillator.

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In such a multiscale model, the total domain, Ω_0, is divided into three sub-domains: two molecular domains (carbon nanotubes), Ω_M, and one continuum domain (the metal paddle), Ω_C. There is no overlapping subdomain between the continuum and molecular domains. Indeed, the molecular and continuum domains are attached with each other via the interfaces Γ_{int}. In the resonant oscillator studied here, the axis the nanotubes are assumed to pass the centroid of the metal paddle. Therefore, the metal paddle mainly has the motion of torsion. We believe that the metal paddle has no large deformation during its rotation. Therefore, the metal paddle can be simplified as a rigid body. Here, we employ the molecular/continuum coupling that is the same as the one proposed in the edge-to-edge coupling method [8], in which the bond angle-bending potential at the interface is considered by introducing virtual atoms and bonds.

In this paper, we mainly consider resonant oscillators that contain (10,0) tubes. We first study mechanical behaviors of resonant oscillators that are isolated systems at zero temperature initially. Nanotubes have the length of 4.12 nm connecting the metal paddle. The material of the metal paddle is gold, whose density is 19300 kg/m^3. The dimensions of the metal paddle are: length of 4.18 nm, width of 10.0 nm and thickness of 3.2 nm. Consequently, the angular moment of inertia of the metal paddle is 0.0237e-36 $kg \cdot m^2$. The metal paddle is initially given a twist of angle of 10 ^{o}. With the multiscale simulation, we obtained the evolution of angle change for the metal paddle as shown in Figure 5. It can be see that the resonant oscillation is stable and the calculated frequency is 3.34 GHz.

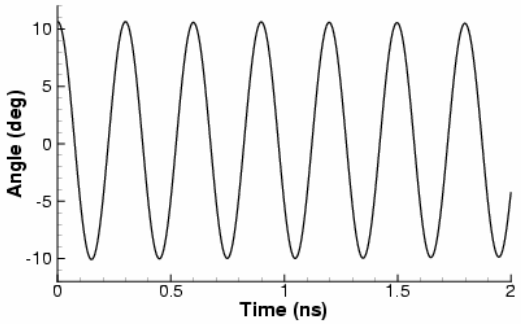

Figure 5. Evolution of angle change of the metal paddle in a resonant oscillator containing (10,0) tubes

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