A Molecular Dynamics Modeling on Cantilevered Triple-Walled Carbon Nanotube Resonators

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ABSTRACT

We introduce intertube interactions of a cantilevered triple-walled carbon-nanotube (TWCNT) resonators via classical molecular dynamics simulations. The fundamental frequencies of TWCNT resonators were less than those of single- and double-walled carbon nanotubes of a given diameter because of the increasing intertube disturbance. Our results imply that for a nanotube with a given diameter, the frequency of a multi-walled carbon nanotube resonator can be controlled by inserting or extracting small-diameter single-walled carbon nanotubes.

Keywords: nanotube, molecular dynamics, resonance, mechanical properties

1 INTRODUCTION

Since the discovery of carbon nanotubes (CNTs) in 1991, extensive studies have shown that CNTs have exceptional mechanical and electronic properties [1]. The mechanical behaviors of single-walled carbon nanotubes (SWCNTs) or multi-walled carbon nanotubes (MWCNTs) have been the subject of numerous recent studies. CNTs hold substantial promise as structural elements in nanoscale devices, nanoelectronics, and nanocomposite materials [1–3]. Computer simulations have advanced the field and have helped reveal the potential of CNT devices in future technologies. Molecular dynamics (MD) has often been used to study and predict the performance of nanoscale machine components. Because of the impracticality of controlled experiments on the nanoscale, as well as the cost and impracticality of MD simulations, especially for large-scale systems, continuum mechanical models have been effectively used to study the mechanical behaviors of CNTs [4, 5]. However, classical continuum mechanics cannot easily predict resonant frequencies of single-walled CNTs because of the size of a single-walled CNT and the ambiguities in the definition of its wall thickness.

Resonators are widely used as key components in signal processing systems [6]. Reducing the size of a resonator enhances its resonant frequency and reduces its energy consumption [7]. A higher resonant frequency generally implies that a sensor can achieve a higher sensitivity [8]. The mechanical quality factor also strongly influences the sensitivity of nanoelectromechanical system-based devices. For wireless communications, higher frequency resonators enable production of higher frequency filters, oscillators, and mixers [6]. The advancement of high-frequency nanoelectromechanical systems is resulting in a variety of new applications, including mechanical mass or charge detectors [9,10] and nanodevices for high-frequency signal processing [11] and biological imaging [12].

Recently, some researchers have considered potential applications of CNTs as resonators [13] and oscillators [14]. For example, the vibrational properties of nanotubes have been studied, and the amplitude of thermal vibrations of cantilevered nanotubes has been used to predict the Young's modulus [15-17]. CNTs exhibit appealing properties, such as an extremely high in-plane elastic modulus and thermal conductivity. Properties such as these, as well as the perfect atomic structure on the nanometer-scale, imply that CNTs have potential applications in nanoelectromechanical systems as components of high-frequency oscillators for sensing and signal processing applications [7-9]. For example, Poncharal et al. [9] demonstrated how to exploit the resonance of a cantilevered CNT to estimate the mass of an attached carbonaceous particle as light as 30 fg inside a transmission electron microscope. Recently, Jensen et al. [8] demonstrated a room-temperature, CNT-based nanomechanical resonator with atomic mass resolution, which is based on a nanotube radio receiver design [18]. Chiu et al. [19] addressed atomic-scale mass sensors by using suspended CNT resonators.

In this paper, we use an atomistic modeling technique to explore the properties of double-walled (DW) and triple-walled (TW) CNTs as nanoresonators. Jiang et al. [20]

studied the energy dissipation of cantilevered single-walled CNT oscillators via classical MD simulations. Recently, the vibrational characteristics of DWCNT resonators were investigated via continuum models [21-23]. However, TWCNT resonators have never been investigated, so, in this report we investigate cantilevered TWCNT resonators via classical MD simulations. In general, DWCNTs are stronger than SWCNTs, and TWCNTs are stronger than DWCNTs. Therefore, according to conventional wisdom, DWCNT resonators should have higher frequencies than SWCNT resonators, and TWCNT resonators should have higher frequencies than DWCNT resonators. However, we suggest that the fundamental frequencies of TWCNT resonators are less than those of DWCNT and/or SWCNT resonators with a given diameter.

2 METHODS AND STRUCTURE

We used classical MD methods to model the oscillation behaviors of SW-, DW-, and TWCNT resonators. Interactions between carbon atoms that form covalent bonds on a CNT were modeled using the Tersoff-Brenner potential [24, 25], which has been extensively applied to carbon systems [26] and is responsible for the experimental effectiveness of the simulation results [27]. The long-range interactions of carbon were characterized using the Lennard-Jones 12–6 (LJ12–6) potential based on the parameters obtained by Ulbricht *et al.* [28]. In this work, the respective parameters of the LJ12–6 potential were $\varepsilon_{carbon} = 2.4038\times10^{-3}$ eV and $\sigma_{carbon} = 3.37$ Å, and the cutoff distance of the LJ12-6 potential was 10 Å. The MD methods utilized in our previous works [29-33] were implemented using the velocity Verlet algorithm, a Gunsteren–Berendsen thermostat to control the temperature, and neighbor lists to improve the computing performance. The MD time step was 5×10^{-4} ps. The initial atomic velocities were determined according to the Maxwell distribution, and the magnitudes were adjusted in order to fit the temperature of the system. In all the MD simulations, the temperature was set to 1 K.

Precision experiments have proven that the interwall spacing of DWCNTs can vary from 3.0 – 5.4 Å [34]. However, high stability configurations have occurred when the interwall spacing was approximately 3.3 Å or 3.5 Å, and an armchair tube was in the outer position [35]. In this work, in order to investigate TWCNT resonators, we selected the (3,3)(8,8)(13,13) TWCNT with an interwall spacing of 3.4 Å, which is considered to be one of the most stable TWCNTs. The left ends of all the walls were fixed during the classical MD simulations. The lengths were changed in 10-Å steps from 10 – 100 Å. In order to obtain the resonant frequencies, we performed MD simulations under an external force of 0.001 eV/Å per atom applied along the transverse direction for an initial time of 2.5 ps. After removal of the bending force, the CNT resonators were allowed to oscillate freely. The fundamental

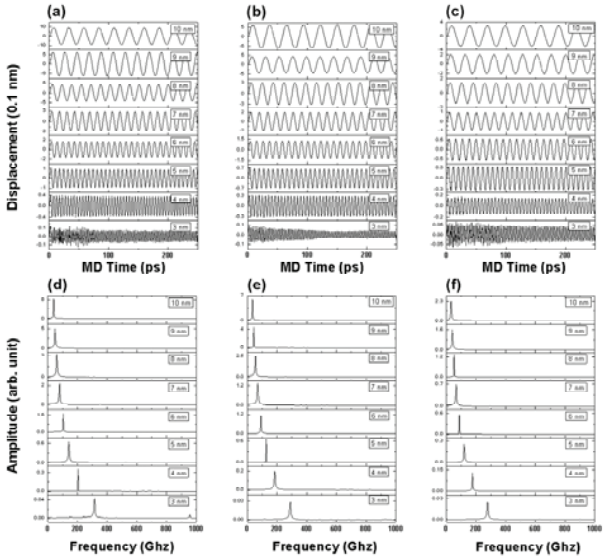

Figure 1: Displacements of tips of (a) SW13, (b) DW8@13 and (c) TW3@8@13 as functions of the MD time with respect to the nanotube length, which ranges from 3 – 10 nm. Spectra of (d) SW13, (e) DW8@13 and (f) TW3@8@13 as functions of frequency.

resonance frequencies (f) were analyzed via the fast Fourier transform (FFT) based on data sampled at 0.05 ps.

3 RESTULS AND DISCUSSION

We performed MD simulations of six cases: (3,3), (8,8), and (13,13) SWCNTs, (3,3)(8,8) and (8,8)(13,13) DWCNTs, and (3,3)(8,8)(13,13) TWCNT, which are denoted by SW3, SW8, SW13, DW3@8, DW8@13, and TW3@8@13, respectively. Figures 1(a)-(c) show the respective displacements of the tips of SW13 and DW8@13 and TW3@8@13 as functions of MD time with respect to nanotube length, which ranged from 3-10 nm. Figures 1(d)-(f) show the spectra as functions of frequency based on FFT calculation for Figs. 1(a)-(c), respectively. In all cases, the fundamental frequency rapidly decreases as the nanotube length increases.

Figures 2(a)-(c) show the respective atomic structures of the TW3@8@13, DW8@13, and SW13 resonators for all the MD simulation times. Although the same force was applied in all three cases, the displacements of the tips differed because the bending strength was increased as the number of walls increased. As discussed above, as the number of walls increases, CNTs generally become increasingly stronger. Therefore, according to conventional wisdom, TWCNT resonators should have higher frequencies than SWCNT or DWCNT resonators. The strengthened beam structure TW3@8@13 might have a higher resonance frequency than the hollow beam structure

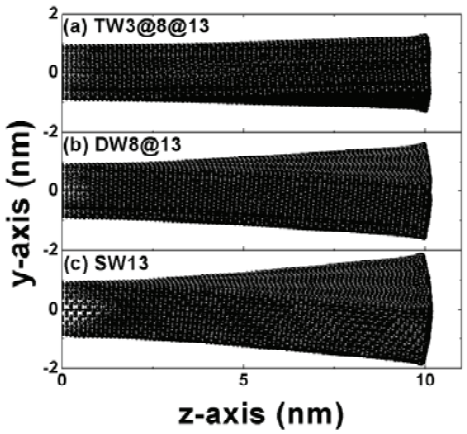

Figure 2: Atomic structures of (a) TW3@8@13, (b) DW8@13, and (c) SW13 resonators for all the MD simulation times.

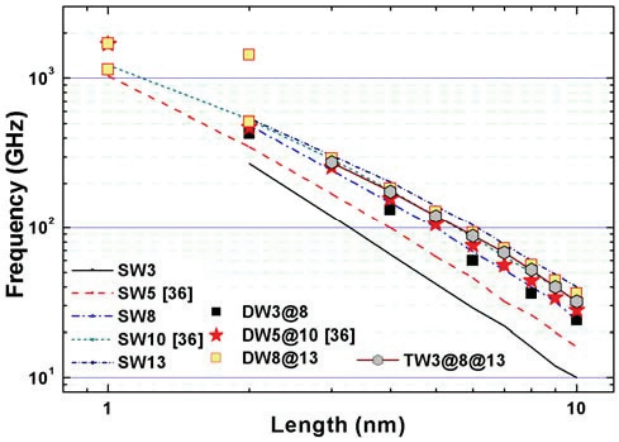

Figure 3: Frequency as a function of length.

SW13 and DW8@13. However, in Fig. 1, for a given length, the difference between the fundamental frequencies is negligible with respect to the number of the walls because the vibrational properties in the cases of DWCNTs are greatly affected by the interwall interactions due to the vibrational deflections of the inner and the outer nanotubes. Natsuki et al. [22], who studied the vibration characteristics of both-side-clamped DWCNTs, found that SWCNTs had larger vibrational frequencies than DWCNTs at least 30%. The vibrational frequencies of DWCNTs were between those of the inner and the outer nanotubes. They discussed the fact that the characteristic frequencies in the cases of DWCNT are greatly affected by the vibrational deflection of the inner and the outer nanotubes. Their results for bridge-type DWCNT resonators provide important information relevant to our results for cantilevered-type DWCNT resonators. In this work, the vibrational frequencies of DW8@13 were about 10% less than those of SW13 with a given diameter. The figure of 10% in this work is less than that of the 30% found in the previous work [22]. However, the difference does not imply that the two works are inconsistent; in this work, we considered one-side-clamped DWCNT resonators whereas Natsuki et al. [22] considered both-side-clamped DWCNT resonators.

Figure 3 shows the frequency *vs*. length plots for five SWCNTs, three DWCNTs, and one TWCNT. The data for the (5,5) SWCNT (SW5), (10,10) SWCNT (SW10), and (5,5)(10,10) DWCNT (DW5@10) were obtained from a previous work [36]. The frequencies are almost linear in the log-log plot. For very short DWCNTs, below a length of 2 nm, the intertube disturbance results in a very high frequency. When the outer and the inner wall lengths are equal, the vibrational frequencies of the former are higher than those of the latter. Therefore, a slowly deflective inner wall can affect the deflective vibration of the outer wall, so such noncoaxial intertube vibration phenomena ensure that the vibrational frequencies of DWCNTs are less than those of SWCNTs with a given length and diameter. We can exploit such noncoaxial intertube vibration phenomena to explain the vibrational frequencies of TWCNT resonators. The interactions of the inner-middle, inner-outer, and middle-outer nanotubes of TWCNTs are considered to be coupled via van der Waals forces. The frequencies of SW13, DW8@13, and TW3@8@13 are 40, 36, and 32 GHz, respectively. Therefore, the frequency of an MWCNT resonator can be decreased by inserting a small-diameter SWCNT because of the increasing intertube disturbance. Many previous works [21-23] have considered an MWCNT as a single rigid beam. However, this study shows that intertube interactions should be considered in order to analyze the vibrations of MWCNT resonators.

Our finding that the cantilevered TWCNT resonator has a slightly lower fundamental frequency than the corresponding DW- and SWCNT resonators is very important. In this work, we used the (3,3)(8,8)(13,13) TWCNT a the interwall space of 3.4 Å. However, the interwall spacing of MWCNTs ranges from 3.0 – 5.4 Å in experiments [34] and from 3.3 – 3.5 Å in ab-initio calculations with four different combinations of armchair/zigzag tubes [35]. Therefore, in order to help determine whether such phenomena are primarily due to intertube interactions, further work should include various MD simulations of different intertube spacings; the MD simulations should be carried out in temperature ranges substantially higher than the 1 K in the present work. Thermal dissipation should be considered because experiments will most likely be conducted at far higher temperatures than 1 K. The Q-factor is expected to be greatly decreased as the temperature is increased, such as in the study on a cantilevered CNT beam oscillator in the previous work by Jiang et al. [20]. We anticipate that these phenomena will be empirically confirmed.

4 SUMMARY

In summary, this report introduced the intertube interactions of cantilevered TWCNT resonators via classical MD simulations of the (3,3)(8,8)(13,13) TWCNT. Our results showed that the fundamental frequencies of TWCNT resonators are less than those of DWCNT and/or

SWCNT resonators with a given diameter because of the increasing intertube disturbance. For a nanotube with a given diameter, the frequency of an MWCNT resonator can be decreased by inserting small-diameter SWCNTs because of the increasing intertube disturbance.

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