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Multiscale modeling and simulation of nanotube-based torsional oscillators

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Abstract In this paper, we propose the first numerical study of nanotube-based torsional oscillators via developing a new multiscale model. The edge-to-edge technique was employed in this multiscale method to couple the molecular model, i.e., nanotubes, and the continuum model, i.e., the metal paddle. Without losing accuracy, the metal paddle was treated as the rigid body in the continuum model. Torsional oscillators containing (10,0) nanotubes were mainly studied. We considered various initial angles of twist to depict linear/nonlinear characteristics of torsional oscillators. Furthermore, effects of vacancy defects and temperature on mechanisms of nanotube-based torsional oscillators were discussed.

Keywords Nanotube · Torsional oscillator · Multiscale · Vacancy defects · Temperature

Introduction

Since the discovery of carbon nanotubes (CNTs) [1] in 1991, these special cylindrical nanostructures have been intensively studied and discussed. Their extraordinary mechanical and electrical properties [2] ensure that CNTs will play an essential role in the design of nanoscale devices, such as nanotweezers [3], nanogears [4], nanotube motors [5], and axial nano-oscillators [6]. Recently, a nanoelectromechanical device [7–9] based on an individual CNT serving as a torsional spring and mechanical support has been successfully fabricated. Williams and co-workers [7, 8] 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. Papadakis et al. [9] used similar techniques to synthesize so-called torsional 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 0.1 MHz. Applications for this type of oscillator include being used as sensors and clocks for high-frequency electronics.

Although experimental observations have indicated the potential applications of nanotube-based torsional oscillators, the mechanisms have not been studied thoroughly. Numerical methods, especially molecular dynamics (MD) simulation, have become a powerful tool for revealing complex physical phenomena [6]. Unfortunately, no numerical analysis of nanotube-based torsional oscillators is reported so far due to the limitation of MD on length scales. A torsional oscillator may contain up to billions or trillions of atoms because of the large dimensions of the metal paddle. Therefore, intensive computation results in the infeasibility of MD models of torsional oscillators.

Recently developed multiscale modeling techniques, such as the bridging domain coupling method [10], have shown promise in treating phenomena at nano and larger scales. Based on the edge-to-edge coupling method [11], we develop a multiscale method to study the mechanical behavior of nanotube-based torsional oscillators. In the proposed multiscale model, the nanotube is modeled with molecular dynamics while

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the metal paddle is modeled as continua. To simplify the simulation, the metal paddle is further modeled as a rigid body. We will investigate mechanisms of torsional oscillators at various initial angles of twist. Effects of defects and temperature on mechanisms of nanotube-based torsional oscillators will also be considered.

Multiscale modeling

In a nanotube-based torsional oscillator, a part of the nanotube is embedded in the metal paddle. We believe this portion of the nanotube has an 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 paddle, as shown in Fig. 1, which illustrates the multiscale model of a carbon nanotube-based torsional oscillator.

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. This differs from previous research [10] in that there was an 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 this paper. In other words, there are some carbon atoms on the interface Γ_{int}. In Fig. 1, l is the length of the carbon nanotube at each side, and d represents the diameter of the tube. The metal paddle has the dimensions of length a, width b, and thickness c. In this paper, we assume that nanotubes attached with the metal paddle on each side have the same length.

In a torsional oscillator studied here, the axes of the nanotubes coincide with each other and are assumed to pass the centroid of the metal paddle. The axes of the nanotubes also coincide with the axis that the metal paddle rotates about, as shown in Fig. 1. 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. The equations of motion are

$$J\ddot{\theta} = T, \tag{1}$$

where J is the angular moment of inertia of the metal paddle to its centroid, θ is the rotation angle of the metal paddle, and T is the torque applied on the metal paddle. The torque results from forces of the atoms located on the interface Γ_{int} due to the torsion of nanotubes. It has been observed [9] that vertical deflections of nanotubes could be negligible compared to torsional deflections. Therefore, the torque T can be computed by:

$$T\mathbf{e}_z = \sum_I \mathbf{r}_I \times \mathbf{F}_I, \tag{2}$$

where $\mathbf{F}_I$ is the atomic force on atom I that is located at the interface between the nanotube and the metal paddle, and $\mathbf{r}_I$ is the position vector of atom I with respect to the tube axis. Both $\mathbf{F}_I$ and $\mathbf{r}_I$ are projected on the x–y plane, while the tube axis is denoted by $\mathbf{e}_z$.

In the molecular model, molecular dynamics is utilized. We employ the modified Morse potential function, proposed by Belytschko and Xiao [12], to describe the interaction between bonded carbon atoms. Since the modified Morse potential consists of the bond stretching energy and the bond angle-bending energy, simply gluing carbon atoms on the molecular/continuum interface will not account for the bond angle-bending energy between the nanotubes in the molecular model and the one in the continuum model, although the tube in the continuum model is ignored due to the assumption of no deformation. Here, we employ the molecular/continuum coupling similar to what proposed in the edge-to-edge coupling method [11], in which the bond angle-bending potential at the interface can be considered by introducing virtual atoms and bonds.

Figure 2 illustrates the molecular/continuum coupling technique utilized in this paper. Carbon atoms e, f, and g are in the molecular domain, while atom g is located at the interface. Corresponding to atom g, a "virtual atom" h is inside the continuum model. In addition, bond gh is the so-called "virtual bond." It should be noted that only zigzag nanotubes are considered in this paper. A similar strategy can be conducted for other nanotubes such as armchair tubes. Since the metal paddle is viewed as a rigid body, virtual

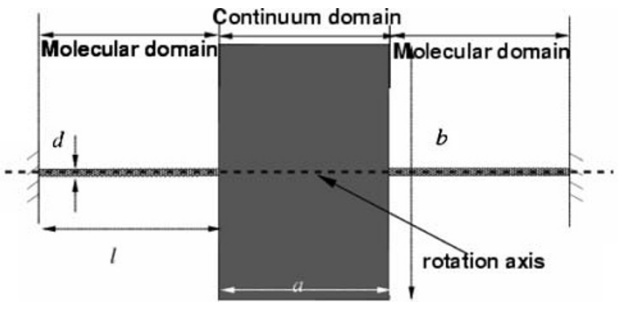

Fig. 1 Multiscale model of a CNT-based torsional oscillator

bonds have no change in their length, so there is no change in the bond-stretching energy of virtual bonds. However, the angles between the virtual bonds and their neighboring bonds in the molecular model, e.g., the ones between bonds *gh* and *ge*/*gf* shown in Fig. 2, may change during the rotation of the metal paddle and the torsion of the nanotube so that the bond angle-bending potential exists at the molecular/continuum interface. Such an angle-bending potential must be considered in molecular dynamics simulations because it affects the atomic forces of carbon atoms that are on or close to the molecular/continuum interfaces. In the example given in Fig. 2, those atoms include atoms *e*, *f*, and *g*. Consequently, the equations of motion in the molecular model are

$$m_I \mathbf{x}_I = \mathbf{f}_I^{\text{ext}} - \frac{\partial (E + E_{\text{virtual}})}{\partial \mathbf{x}_I}, \tag{3}$$

where $\mathbf{x}_I$ is the location of atom I and $\mathbf{f}_I^{\text{ext}}$ is the external force applied on the atoms. The external force can be due to the gravity of the metal paddle. E is the potential energy of the tubes in the molecular model; E_{virtual} is the potential due to angle change between the virtual bonds and other realistic bonds at the molecular/continuum interfaces.

One of the keys in this multiscale modeling is to identify the location of virtual atoms. We employ finite element approximation by treating the entire metal paddle as an eight-node block element. The kinetic variables of a virtual atom are evaluated from eight nodes located at vertices of the metal paddle.

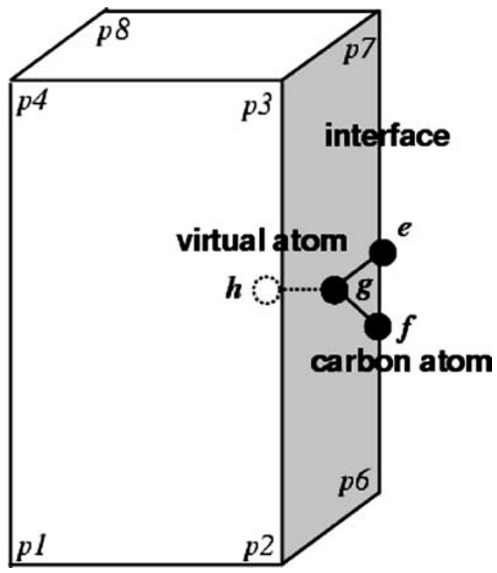

Fig. 2 The schematic diagram of virtual atoms/bonds at the interface

At the beginning of a multiscale simulation, the metal paddle is given an initial angle of twist. Therefore, the displacements of atoms at the continuum/molecular interfaces and virtual atoms can be determined through finite element approximation in the continuum model as boundary conditions in the molecular model. Molecular dynamics simulation in the molecular model is conducted through solving the equations of motion in Eq. 3. The Verlet velocity algorithm is employed. At each time step, we use Eq. 2 to calculate the torque acting on the metal paddle. This torque is due to the atomic forces of atoms on the continuum/molecular interfaces. Then, the rotation of the metal paddle can be determined by solving Eq. 1. The above procedure is iterative until the target time is reached.

Results and discussions

In this paper, we mainly consider torsional oscillators that contain (10,0) tubes. We first study the mechanical behaviors of torsional oscillators that are isolated systems at zero temperature initially. Nanotubes with the length of 4.12 nm connect and support the metal paddle. The material of the metal paddle is gold, which has a density of 19,300 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 m^2. The metal paddle is initially given a twist angle of 10°. With the multiscale simulation, we obtained the evolution of angle change for the metal paddle, as shown in Fig. 3. The resonant oscillation is stable, and the calculated frequency is 3.34 GHz.

Here, we consider (10,0) tubes with various lengths, including 8.38, 12.64, 16.90, and 21.16 nm. The calculated resonance frequencies are 2.35, 1.92, 1.67 and

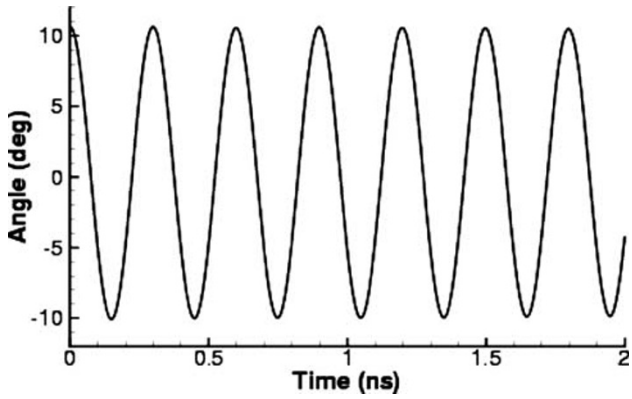

Fig. 3 Evolution of angle change of the metal paddle in a torsional oscillator containing (10,0) tubes

1.50 GHz, respectively. It can be seen that resonance frequencies are inversely proportional to the square root of the nanotube length. Furthermore, if the same (10,0) nanotubes are used, but the angular moment of inertia of the metal paddle is increased by 2, 4, and 8 times, the simulation outcomes indicate that resonance frequencies are reduced by $\sqrt{2}$, 2 and $2\sqrt{2}$ times, respectively. Based on the above data, the following relation of frequencies between any two nanotube-based torsional oscillators can be concluded:

$$\frac{f_1}{f_2} = \sqrt{\frac{J_2 l_2}{J_1 l_1}} \tag{4}$$

where f_1 and f_2 are the frequencies, J_1 and J_2 the angular moments of inertia of the metal paddles, and l_1 and l_2 the length of nanotubes in torsional oscillators 1 and 2, respectively. It should be noted that nanotubes in those two torsional oscillators have the same diameter.

It is known that the resonance frequency, f, of a linear torsional oscillation system can be theoretically predicted via the following equation:

$$f = \frac{1}{2\pi}\sqrt{\frac{k}{J}}, \tag{5}$$

where k is the torsional stiffness of the embedded linear torsional spring and J is the angular moment of inertia of the paddle. Indeed, Eq. 4 can be derived from Eq. 5 since nanotubes' torsional stiffness is inversely proportional to the length if nanotubes are taken as linear torsional springs. At this point, the proposed multiscale modeling is verified with theoretical prediction.

In previous research [W.Y. Hou and S.P. Xiao, submitted], a carbon nanotube was observed to have a constant torsional stiffness within small angles of twist. Therefore, nanotubes can be viewed as linear torsional elements, and frequencies of torsional oscillators can be predicted via Eq. 4 or 5. However, carbon nanotubes exhibit nonlinear characteristics when being employed as torsional springs under large angles of twist. If the angle of twist becomes larger, the nanotube's torsional stiffness becomes smaller until the torsional buckling occurs. In these cases, frequencies of torsional oscillators cannot be predicted by Eq. 4 or 5 anymore. The developed multiscale method is an alternative. For the torsional oscillator we studied above, the calculated resonance frequency is 3.34 GHz (see Fig. 3) when the initial angle of twist is 10°. If initial angles of twist become 30° and 60°, the resonance frequencies are dropped to 3.06 GHz and 2.49 GHz, respectively. It should be noted that we do not consider the occurrence of buckling in this paper.

Research has shown that vacancy defects can dramatically reduce the stiffness, strength, and torsional stiffness of nanotubes [W.Y. Hou and S.P. Xiao, submitted, 13]. Therefore, we believe that vacancy defects have significant effects on the resonance frequencies of nanotube-based torsional oscillators. Vacancy defects can be caused by ion irradiation, absorption of electrons, or nanotube fabrication processes. Such defects are modeled by taking out atoms, followed by bond reconstruction [13]. In this paper, we consider two uncertainties associated with vacancy defects on nanotubes. One is the number of missing atoms, and the other is the location of a vacancy defect. Due to the unique structures of single-walled carbon nanotubes, they can be mapped onto two-dimensional (2D) graphene planes with a thickness of 0.34 nm. Consequently, a 3D model can be simplified as a 2D surface problem when considering vacancy defects on nanotubes. On the other hand, since vacancy defects occur on carbon nanotubes in a completely random manner, we employ a homogeneous Poisson point process to determine the occurrence probability of a specified number of Poisson points, i.e., missing atoms in this paper, via

$$P(N(A) = k) = \frac{\mathrm{e}^{-\lambda A}(\lambda A)^k}{k!}, \quad k = 1, 2, 3 \ldots \tag{6}$$

where A is the plane area, $N(A)$ is the number of Poisson points (missing atoms) on this area A, and λ is the Poisson point density (missing atom density) per area.

For a given number of Poisson points, they are deposed on a two-dimensional graphene sheet, to which the considered nanotube can be mapped, at random positions. We mark the carbon atoms, which are the nearest ones to the Poisson points, as the missing atoms. After taking out the missing atoms, we perform bond reconstruction to generate one-atom, two-atom, and/or cluster-atom vacancy defects. Even for the same number of missing atoms, the numbers and locations of vacancy defects can vary from case to case. For example, a vacancy-defected (10,0) nanotube shown in Fig. 4 contains five one-atom vacancies, two two-atom vacancies, and one cluster-atom vacancy.

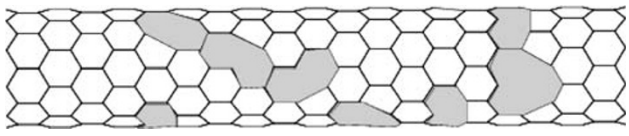

Fig. 4 A (10,0) nanotube with randomly located vacancy defects

In this study, we choose (10,0) tubes with the length of 4.12 nm as torsional springs for nanotube-based torsional oscillators. The surface area of the carbon nanotube is 20.24 nm^2. The metal paddle has an angular moment of inertia of 0.0237e–36 kg m^2. The following missing atom densities are considered: 0.1, 1, 2 and 3 nm^{-2}. For each given missing atom density, 100 simulations are conducted. The number of simulations for a specific number of missing atoms is based on its probability via Eq. 6. Figure 5 shows the relationship between the resonance frequency and the missing atom density on the carbon nanotube surface. Due to uncertainties of vacancy defects, the resonance frequencies follow the Gaussian distribution. We can see that on average a larger missing atom density results in a lower resonance frequency since the nanotube with more missing atoms generally has less torsional stiffness. However, due to the uncertainties of vacancy defects, it is possible that a torsional oscillator embedding a nanotube with more missing atoms has higher resonance frequency.

Previous research showed that temperature effects were significant on mechanisms of some nanoscale devices [6]. We first investigate temperature effects on the frequencies of nanotube-based torsional oscillators. (10,0) nanotubes with the length of 8.24 nm are selected as torsional springs in resonant oscillators. The metal paddle has a moment of inertia of 0.1261×10^{-36}kg m^2 with respect to the rotation axis, i.e., tube axis. The oscillator has a frequency of 1.45 GHz when it is an isolated system. Here, we conducted multiscale simulations at various temperatures. In the molecular model, the Hoover thermostat is employed [14] to maintain nanotubes at a constant temperature. The frequencies are calculated based on the oscillation of the metal paddle during the first several cycles. The calculated frequencies are 1.44, 1.42, 1.40, and 1.35 GHz at 100, 300, 600 and 800 K, respectively. It is evident that temperature has a slight effect on the resonance frequencies of nanotube-based torsional oscillators. However, we observed another phenomenon: energy dissipation of the torsional oscillators at a finite temperature.

Energy dissipation is always observed when nanoscale devices are at finite temperatures [6] due to the heat exchange between devices and their surroundings. Here, we study the energy dissipation of torsional oscillators with various frequencies, including 5.53, 10.99, 15.39, 30.30 and 38.46 GHz, at the room temperature of 300 K. It should be noted that the same (10,0) nanotubes with the length of 4.12 nm are employed in those oscillators. Various frequencies are due to different dimensions of the metal paddles. The evolutions of the maximum angular kinetic energies of those torsional oscillators are shown in Fig. 6. It is evident that high frequency results in large energy dissipation. For the torsional oscillator having the frequency of 38.46 GHz, the system energy dissipates 85% during 2 ns. It is known that temperature is one of the macroscopic parameters and is related to the kinetic energy of atoms. We believe that the high-speed rotation of the metal paddle drives large vibration of atoms during the torsion of the nanotube. Therefore, the temperature of the nanotube is higher in the torsional oscillator with a higher resonance frequency. Consequently, the loss of energy is faster due to the high temperature gradient between the torsional oscillator and its surrounding.

To validate the proposed multiscale modeling, we employ the experimental outcomes of Papadakis et al. [9] as the reference. They tested nine devices and

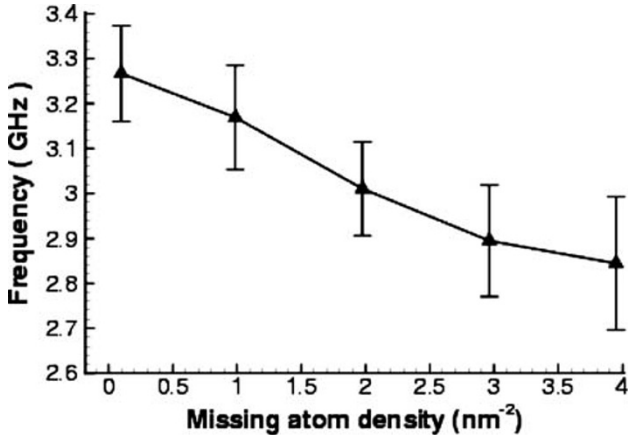

Fig. 5 Vacancy defect effects on the resonance frequency (solid line represents mean values of resonance frequencies that follow the Gaussian distribution; vertical lines represent + /– one standard deviation)

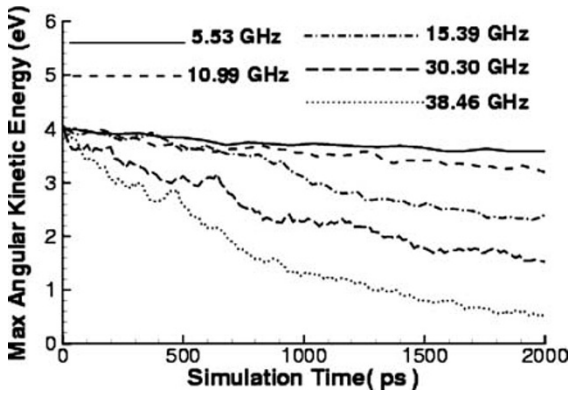

Fig. 6 Energy dissipation of nanotube-based torsional oscillators with various resonance frequencies at 300 K

Table 1 Comparison of numerical results with experimental outcomes

Devices	F_0 (MHz)	F_1 (MHz)	F_2 (MHz)
1	1.68	1.33	2.91
2	2.37	1.84	5.90
3	2.50	1.53	5.00
4	3.27	2.30	8.37
5	2.92	1.28	3.20
6	3.79	1.38	3.83
7	4.12	1.60	4.24
8	2.98	1.06	3.11
9	2.04	0.97	2.74

F_0 is the resonance frequency measured by Papadakis et al. [9], F_1 is the frequency calculated via the proposed multiscale method, and F_2 is the numerical result considering mechanical coupling

obtained resonance frequencies between 1.68 and 4.12 MHz. The comparison is illustrated in Table 1. It can be seen that multiscale simulations provide close values (F_1) to experimental observations (F_0) for Devices 1 and 2. However, all the calculated frequencies are lower than the experimental outcomes. This is because we only model the outermost tube of the multi-walled carbon nanotubes (MWNT) that were utilized in the experiments. With the consideration of fully mechanical coupling [9] between interlayer tubes, we predict the resonance frequencies (F_2), which are close to the experimental results for Devices 5, 6, 7, and 8. Furthermore, all the measured frequencies are in the ranges of numerical solutions. Variations may be due to vacancy defects on the nanotubes, as in the preceding discussion.

Although nanotube-based torsional oscillators were fabricated and observed through experimental techniques, numerical studies have not been reported yet. We propose a multiscale method in which the metal paddle was treated as the rigid body while nanotubes were modeled by molecular dynamics. The multiscale method has advantages for investigating the nonlinear characteristics of nanotube-based torsional oscillators, including the effects of vacancy defects and temperature. Such a multiscale method can be extended to model and study other nanodevices.

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