Single-walled carbon nanotubes as ultrahigh frequency nanomechanical resonators

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The high stiffness and strength, low density, and large aspect ratio of single-walled carbon nanotubes make them good candidates as nanoresonators. Employing an atomistic modeling technique, molecular structural mechanics, this work predicts that the fundamental frequencies of cantilevered or bridged single-walled carbon nanotubes as nanomechanical resonators could reach the level of 10 GHz–1.5 THz. The effects of tube diameter, length and end constraints on the fundamental frequency have been discerned.

Resonators are key components in signal processing systems.[1] Reduction in the size of a resonator enhances its resonant frequency and reduces its energy consumption. For sensors, higher resonant frequency means higher sensitivity. For wireless communications, higher frequency resonators enable the production of higher frequency filters, oscillators, and mixers.[1] The advancement in high-frequency nanoelectromechanical systems brings about new applications ranging from mechanical mass or charge detectors[2,3] and nanodevices for high-frequency signal processing[4] to biological imaging.[5]

It has been predicted that, with advanced nanolithography, SiC resonators with fundamental frequencies above 10 GHz is attainable at the 10 nm scale.[6] The highest frequency nanomechanical resonator (1.029 GHz) so far, based on SiC, was recently fabricated from SiC using optical and electron-beam lithography.[7]

Meanwhile, some researchers turned their attention to carbon nanotubes (CNT) as resonators[8] and oscillators.[9] For example, the vibrational properties of nanotubes have been studied and the amplitude of thermal vibrations of cantilevered nanotubes has been used for predicting their Young's modulus.[10–12] But the potential of nanotubes as resonators has not been explored. Owing to their unique properties, such as high stiffness and strength, low density and large aspect ratio, carbon nanotubes, especially single-walled carbon nanotubes, seem to be well suited for the use as nanoresonators. However, because of the size of a single-walled carbon nanotube and the uncertainty in defining its wall thickness,[13] the classical continuum mechanics cannot be readily applied for predicting the resonant frequencies of single-walled carbon nanotubes. In this research, we explore the potential of single-walled carbon nanotubes as nanoresonators using an atomistic modeling technique.[14,15]

For the analysis of nanotube resonator, we adopt the molecular structural mechanics method.[14,15] The concept of this method originated from the observation of geometric similarities between nanoscopic fullerenes and macroscopic space frame structures. In a carbon nanotube, each atom is bonded covalently with three nearest neighbors. When a nanotube is subjected to external forces, the displacements of atomic nuclei are constrained by the covalent bonds. If a nanotube is viewed as a space frame with "beams" connecting the carbon atoms, its deformation can be modeled by the technique of structural mechanics. In essence, the covalent bond between two neighboring carbon atoms can be simulated as an equivalent structural beam with a circular cross section. Then, following the theory of structural mechanics, only three stiffness parameters, i.e., the tensile resistance EA, the flexural rigidity EI, and the torsional stiffness GJ, need to be determined for deformation analysis. Here, E and G are, respectively, the Young's modulus and shear modulus of the beam, A and J are, respectively, the cross-sectional area and polar inertia of the beam. Based on the energy equivalence between local potential energies in computational chemistry and elemental strain energies in structural mechanics, the tensile resistance, the flexural rigidity and the torsional stiffness for an equivalent beam can be determined.

From the viewpoint of molecular mechanics, the general expression of total steric potential energy is a sum of energies due to valence or bonded interactions and nonbonded interactions[16]

$$U = \sum U_r + \sum U_\theta + \sum (U_\phi + U_\omega) + \sum U_{\text{VDW}}, \quad (1)$$

where U_r, U_θ, U_ϕ, U_ω, and U_{VDW} are attributed to bond stretching, bond angle bending, dihedral angle torsion, out-of-plane torsion, and van der Waals interaction, respectively. From a structural mechanics viewpoint, the deformation of a space frame results in the change of strain energy. The strain energy for a beam element is given by[17]

$$U = \sum U_A + \sum U_M + \sum U_T + \sum U_V, \quad (2)$$

where U_A, U_M, U_T, and U_V are strain energies for axial tension, bending, torsion, and shear force, respectively. By considering the energy equivalence between Eqs. (1) and (2), a direct relationship between the structural mechanics parameters and the molecular mechanics force field constants can be established,[14] i.e.,

$$\frac{EA}{L} = k_r, \frac{EI}{L} = k_\theta, \frac{GJ}{L} = k_\tau, \quad (3)$$

where k_r, k_θ, and k_τ are the force field constants in molecular mechanics and L is the length of the equivalent beam. Then, following the procedure of the structural mechanics technique, the static or dynamic problems of carbon nanotubes can be readily solved.
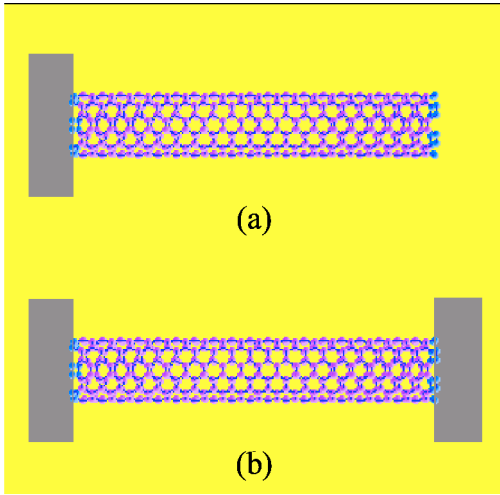
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FIG. 1. (Color online) Cantilevered (a) and bridged (b) single-walled carbon nanotube resonators.

The capability and efficiency of this molecular structural mechanics method have been verified in the modeling of single walled carbon nanotubes under tension or torsion. The calculated results of Young's modulus and shear modulus are in good agreement with the theoretical predictions and experimental results available in the literature.[14] Also, this method has been used for modeling of the buckling behavior of single-walled carbon nanotubes under hydrostatic pressure and the results are in reasonably good agreement with the prediction of *ab initio* calculations and existing experimental results.[18]

For determining the natural frequencies of a single-walled carbon nanotube, we consider its equivalent space framelike structure under the condition of free vibration. For the problem of free vibration of an undamped structure, the equation of motion is

$$[M]\{\ddot{y}\}+[K]\{y\}=\{0\}, \qquad (4)$$

where $[M]$ and $[K]$ are, respectively, the global mass and stiffness matrices, and $\{y\}$ and $\{\ddot{y}\}$ are, respectively, the nodal displacement vector and acceleration vector.

The global stiffness matrix $[K]$ of the frame structure can be assembled from the elemental stiffness matrix $[K]^e$, i.e., $[K]=\Sigma_{e=1}^{n}[K]^e$, where n is the number of beam elements. The assembling procedure follows the node-related technique in the finite element method.[19] The elemental stiffness matrix $[K]^e$ is identical to that used in modeling the elastic moduli of a carbon nanotube,[14] and assumes the following general form:

$$[K]^e=\begin{bmatrix}[k_{ii}]&[k_{ij}]\\ [k_{ji}]&[k_{jj}]\end{bmatrix}, \qquad (5)$$

where the submatrices $[k_{ii}]$, $[k_{ij}]$, $[k_{ji}]$, and $[k_{jj}]$ are designated stiffness coefficients related to the cross-sectional parameters of the beam element $i-j$.

The global mass matrix $[M]$ can be assembled from the elemental mass matrix. By considering the atomistic feature of a carbon nanotube, the masses of electrons are neglected
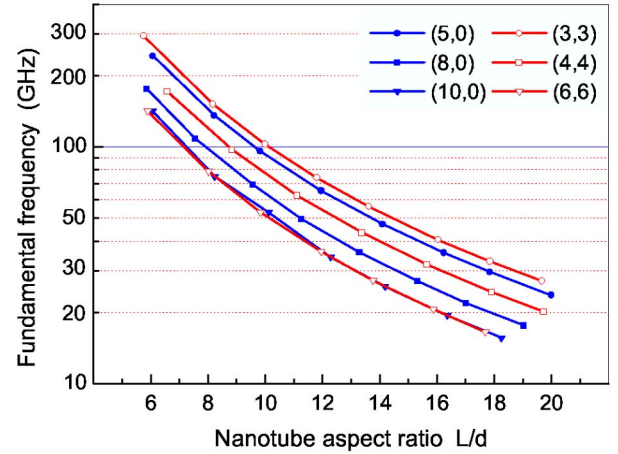
(a) Cantilevered nanotubes
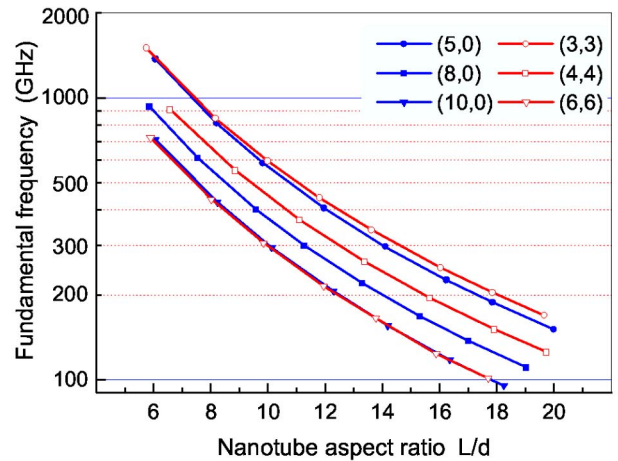
(b) Bridged nanotubes

FIG. 2. (Color online) Fundamental frequency of nanotube resonators, (m,n) denotes the chirality of an SWCNT.

and the masses of carbon nuclei ($m_c=1.9943\times10^{-26}$ kg) are assumed to be concentrated at the centers of atoms, i.e., the joints of beam members. Due to the extremely small radius ($r_c=2.75\times10^{-5}$ Å) of the carbon atomic nucleus,[20] the coefficients in the mass matrix corresponding to flexural rotation and torsional rotation[21] $\frac{2}{3}m_c r_c^2$, are assumed to be zero. Only the coefficients corresponding to translatory displacements are kept. Thus, the elemental mass matrix $[M]^e$ is given by

$$[M]^e=\text{diag}\left[\frac{m_c}{3}\ \frac{m_c}{3}\ \frac{m_c}{3}\ 0\ 0\ 0\right]. \qquad (6)$$

The factor 1/3 in the elements of the elemental mass matrix is introduced because of the three bonds of a carbon atom connecting with the three nearest neighboring atoms and it ensures that the nodal mass has the value of a single atom after matrix assembling.

The orders of the global stiffness matrix and mass matrix are reduced by the static condensation method[22] for more efficient computations. Then, the natural frequencies f and mode shapes are obtained from the solution of the eigenproblem

$$([K]_s - \omega^2 [M]_s)\{y_p\} = 0, \tag{7}$$

$[K]_s$, $[M]_s$ are the condensed stiffness matrix and condensed mass matrix, respectively, $\{y_p\}$ is the displacement vector corresponding to the primary coordinates, i.e., the translatory displacements of carbon atoms, and $\omega = 2\pi f$ is the angular frequency.

The resonant frequencies of nanotubes-based resonators depend on the tube diameter and length, as well as constraints on the nanotube ends. In this work, we analyze two forms of nanotube resonators, i.e., cantilevered and bridged (Fig. 1). The computational results of fundamental natural frequencies of single-walled carbon nanotube resonators are displayed in Fig. 2.

It is obvious from Fig. 2 that nanotube resonators can achieve very high resonant frequencies. For nanotubes with diameters of 0.4–0.8 nm and length/diameter ratios of 6–20, the fundamental frequencies are in the ranges of 10–300 GHz and 100–1500 GHz, respectively, for cantilevered and bridged nanotubes. For both nanotube boundary conditions, the fundamental frequency increases with the reduction in nanotube length. For the same aspect ratio, nanotubes with a smaller diameter have a higher fundamental frequency. Nanotube chirality does not have a significant effect on the fundamental frequency.

In summary, ultrahigh frequency nanomechanical resonators can be achieved using single-walled carbon nanotubes. With the smallest nanotubes [~0.4 nm (Ref. 23)], nanoresonators with terahertz frequencies can be accomplished. Such high frequency mechanical nanodevices will facilitate the development of the fastest scanning probe microscopes, magnetic resonant force microscope, and even mechanical supercomputers. In this paper, the ultrahigh frequencies of carbon nanotubes are demonstrated using the molecular structural mechanics method. Further theoretical studies and experimental measurements are needed to confirm these results.

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