Vibration of Double-walled Carbon Nanotubes Predicted by Timoshenko Beam Models and Molecular Dynamics

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Abstract

Vibration of double-walled carbon nanotubes (DWCNTs) are studied by using different beam models of continuum mechanics and the molecular dynamics (MD) simulations. The models of the double Euler beam (DEB) and the double Timoshenko beam (DTB), with the energy of van der Waals interaction between layers taken into consideration are applied to predict the natural frequencies of DWCNTs with one ends fixed. For the relatively long DWCNTs, the results obtained by the DEB model and the DTB model are very close, and the MD simulations show that these two models can predict the natural frequencies well. However, for the vibration of the relatively short DWCNTs, the difference between the DEB model and the DTB model becomes obvious, and the DTB model offers much better predictions than the DEB model.

Keywords: double-walled carbon nanotubes, double-Timoshenko beam, molecular dynamics simulation, van der Waals, natural frequency

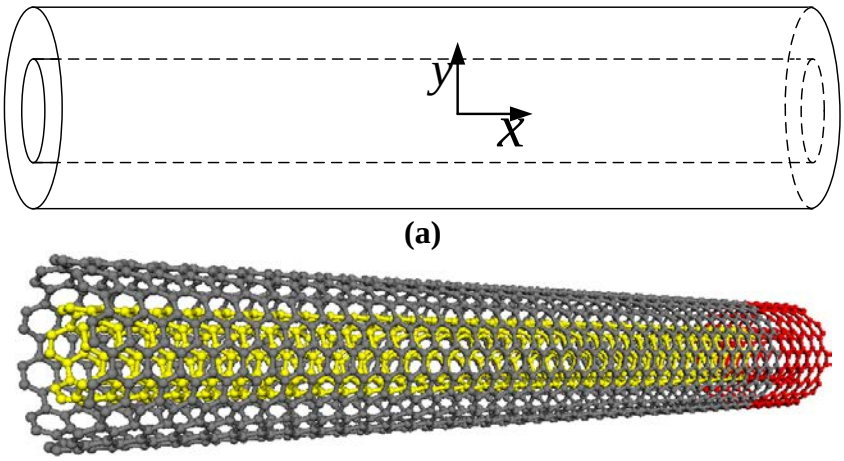
1. Introduction

Carbon nanotubes (CNTs) have attracted lots of researches for their novel electronic properties and superior mechanical strength (Ahlskog et al. 2001; Cumings & Zettl 2000; Postma et al. 2001; Roschier et al. 2001; Rueckes et al. 2000). Experiments and MD simulations have been effectively used to study mechanical behavior, including vibrational behavior, of CNTs. Treacy et al. (1996) estimated Young's modulus of isolated CNTs by measuring, in the transmission electron microscope, the amplitude of their intrinsic thermal vibration. Hsiesh et al. (2006) investigated the intrinsic thermal vibration of a CNT using MD simulations. There are some difficulties encountered in experiments study on the mechanical behavior of CNTs, and MD simulations remain expensive for large scale systems. Continuum mechanics models, including the Euler beam model are widely used in vibration and buckling analyses and in sound wave propagation problems (Yoon et al. 2003a; Yoon et al. 2003b). Besides, the Timosheko beam model with the rotary inertia and the shear deformation taken into account has been used to analyze the vibration and wave propagation of short CNTs which may be used widely as nanoelectronic materials (Ahlskog et al. 2001; Roschier et al. 2001) and AFM tip (Ishikawa et al. 2002; Snow et al. 2002). Yoon et al. (2005) studied vibration of short DWCNTs with supported-supported boundary condition and they found that the Timoshenko-beam model, rather than the Euler-beam model, is relevant for terahertz vibration of short DWCNTs. For more boundary conditions, Wang et al. (2006) solved the governing Timoshenko equations for DWCNTs by using the differential quadrature method. They show that the frequencies are significantly over predicted by the Euler beam theory when the

length-to-diameter ratios are small. Wang et al. (2010) studied the thermal vibration of single-walled CNTs based on the model of Timoshenko beam, together with the law of energy equipartition and MD simulations. Wang & Hu (2012) analyzed the difference in natural frequencies predicted by using the DEB model and the MD simulation, they found that the difference is obvious for high-order frequencies and more accurate models, such as Timoshenko beam model, are needed to predict the natural frequencies of a DWCNT.

The primary objective of this study is to derive theoretical solutions of DTB model and check the validity of it, in studying the vibration, simulated via the MD simulations, of a DWCNT with one end fixed and the other end free. For this purpose, Section 2 presents the natural frequency of a model of DTB to be used to model the vibration of a DWCNT. Section 3 gives the MD simulation for the free vibration of DWCNTs based on the Brenner potential and Lennard-Jones pair potential. Section 4 outlines a comparison, which is verified by using results of MD simulations in Section 3, between the DTB model and DEB model. Finally, the paper ends with Section 5 with some conclusions.

2. Double-Timoshenko-beams model



(a)

(b)

Figure 1. Models for DWCNT (a) Continuum mechanics model (b) Molecular structure model

This section starts with the dynamic equation of a DTB of infinite length and uniform cross section placed along direction x in the frame of coordinates (x, y, z), the dynamic equations of the inner and outer tubes for a DWCNT are (Huang 1961; Ru 2000)

$$\rho A_1 \frac{\partial^2 w_1}{\partial t^2} + \beta A_1 G \left(\frac{\partial \varphi_1}{\partial x} - \frac{\partial^2 w_1}{\partial x^2} \right) = C_{12} \left(w_2 - w_1 \right), \tag{1a}$$

$$\rho I_1 \frac{\partial^2 \varphi_1}{\partial t^2} + \beta A_1 G_1 \left(\varphi_1 - \frac{\partial w_1}{\partial x} \right) - E_1 I_1 \frac{\partial^2 \varphi_1}{\partial x^2} = 0, \tag{1b}$$

$$\rho A_2 \frac{\partial^2 w_2}{\partial t^2} + \beta A_2 G_2 \left(\frac{\partial \varphi_2}{\partial x} - \frac{\partial^2 w_2}{\partial x^2} \right) = C_{12} \left(w_1 - w_2 \right), \tag{1c}$$

$$\rho I_2 \frac{\partial^2 \varphi_2}{\partial t^2} + \beta A_2 G_2 \left(\varphi_2 - \frac{\partial w_2}{\partial x} \right) - E_2 I_2 \frac{\partial^2 \varphi_2}{\partial x^2} = 0, \tag{1d}$$

where $w_k(x,t)$ (k=1, 2) is the displacement of section x of the kth tube in direction y at the moment t, φ_k is the slope of the deflection curve of the kth tube when the shearing force is neglected, A_k is the cross section area of the kth tube, $I_k = \int y^2 \mathrm{d}A_k$ is the moment of inertia for the cross section of the kth tube, β is the form factor of shear depending on the shape of the cross section, and β =0.5 holds for the circular tube of the thin wall (Timoshenko et al. 1972). C_{jk} is the coefficient of the van der Waals (vdW) interaction for the interaction pressure per unit axial length and estimated based on an effective interaction width (He et al. 2005). E_k, ρ_k, G_k are Young's modulus, mass density and shear modulus of the kth tube respectively. The boundary conditions of a cantilever beam are

$$w_k(0,t)=0, \quad \varphi_k(0,t)=0, \quad \frac{\partial^2 w_k(L,t)}{\partial x^2}=0, \quad \frac{\partial^2 \varphi_k(L,t)}{\partial x^2}=0. \tag{2}$$

Both nested tubes with the same boundary conditions have the same vibrational modes, $\hat{w}(x)$, $\hat{\varphi}(x)$. The dynamic deflection and slope can be given by

$$w_k = a_k \hat{w}_n(x) e^{j\omega t}, \quad \varphi_k = a_k \hat{\varphi}_n(x) e^{j\omega t}, \tag{3}$$

where $\hat{w}$ represents the deflection amplitude of the beam, $\hat{\varphi}$ the slope amplitude of the beam due to bending deformation alone, and $j \equiv \sqrt{-1}$. Let

$$\xi = x / L. \tag{4}$$

Substituting Equation (3), (4) into Equation (1), one obtains

$$a_1 \frac{\partial^2 \hat{w}_n}{\partial \xi^2} - a_1 L \frac{\partial \hat{\varphi}_n}{\partial \xi} + a_1 b_1^2 s_1^2 \hat{w}_n = \frac{C_{12} L^2}{\beta A_1 G_1}(a_1 \hat{w}_n - a_2 \hat{w}_n), \tag{5a}$$

$$s_1^2 \frac{\partial^2 \hat{\varphi}_n}{\partial \xi^2} + \frac{1}{L}\frac{\partial \hat{w}_n}{\partial \xi} - (1 - b_1^2 r_1^2 s_1^2)\hat{\varphi}_n = 0, \tag{5b}$$

$$a_2 \frac{\partial^2 \hat{w}_n}{\partial \xi^2} - a_2 L \frac{\partial \hat{\varphi}_n}{\partial \xi} + a_2 b_2^2 s_2^2 \hat{w}_n = \frac{C_{12} L^2}{\beta A_2 G_2}(a_2 \hat{w}_n - a_1 \hat{w}_n), \tag{5c}$$

$$s_2^2 \frac{\partial^2 \hat{\varphi}_n}{\partial \xi^2} + \frac{1}{L}\frac{\partial \hat{w}_n}{\partial \xi} - (1 - b_2^2 r_2^2 s_2^2)\hat{\varphi}_n = 0, \tag{5d}$$

where

$$b_k^2 = \frac{\rho A_k L^4 \omega^2}{E_k I_k}, \quad r_k^2 = \frac{I_k}{A_k L^2}, \quad s_k^2 = \frac{E_k I_k}{\beta A_k G_k L^2}. \tag{6}$$

So

$$\frac{\partial^4 \hat{w}_n}{\partial \xi^4} + B\frac{\partial^2 \hat{w}_n}{\partial \xi^2} - C\hat{w}_n = 0, \tag{7}$$

where $B = b_1^2 s_1^2 + b_1^2 r_1^2 - \frac{C_{12} L^2}{\beta A_1 G_1}(1 - \frac{a_2}{a_1})$, $C = \frac{(1 - b_1^2 r_1^2 s_1^2)\left[b_1^2 s_1^2 - \frac{C_{12} L^2}{\beta A_1 G_1}(1 - \frac{a_2}{a_1}) \right]}{s_1^2}$.

The solutions $\hat{w}_n, \hat{\varphi}_n$ of Equation(7) reads

$$\hat{w}_n = C_1 \cosh \alpha_1 \xi + C_2 \sinh \alpha_1 \xi + C_3 \cos \alpha_2 \xi + C_4 \sin \alpha_2 \xi, \tag{8a}$$

$$\hat{\varphi}_n = C_1' \sinh \alpha_1 \xi + C_2' \cosh \alpha_1 \xi + C_3' \sin \alpha_2 \xi + C_4' \cos \alpha_2 \xi, \tag{8b}$$

where

$$\begin{matrix}\alpha_1\\ \alpha_2\end{matrix}=\left(\frac{\mp B+\sqrt{B^2+4C}}{2}\right)^{1/2}. \tag{9}$$

And $\sqrt{B^2+4C}>B$ is assumed.

In the case of $\sqrt{B^2+4C}<B$, then Equation (7) should be replaced by (Huang 1961)

$$\hat{w}_n = C_1\cos\alpha_1'\xi + jC_2\sin\alpha_1'\xi + C_3\cos\alpha_2\xi + C_4\sin\alpha_2\xi, \tag{10a}$$

$$\hat{\varphi}_n = jC_1'\sin\alpha_1'\xi + C_2'\cos\alpha_1'\xi + C_3'\sin\alpha_2\xi + C_4'\cos\alpha_2\xi, \tag{10b}$$

where $\alpha_1 = j\alpha_1'$.

In Equations (8) and (10), only one half of the constants are independent since they are related by Equations (5) as following

$$C_1 = \frac{L}{b_1\alpha_1}\left[1-b_1^2s_1^2(\alpha_1^2+r_1^2)\right]C_1' = \Lambda_1C_1', \tag{11a}$$

$$C_2 = \frac{L}{b_1\alpha_1}\left[1-b_1^2s_1^2(\alpha_1^2+r_1^2)\right]C_2' = \Lambda_2C_2', \tag{11b}$$

$$C_3 = -\frac{L}{b_1\alpha_2}\left[1+b_1^2s_1^2(\alpha_2^2-r_1^2)\right]C_3' = \Lambda_3C_3', \tag{11c}$$

$$C_4 = \frac{L}{b_1\alpha_2}\left[1+b_1^2s_1^2(\alpha_2^2-r_1^2)\right]C_4' = \Lambda_4C_4'. \tag{11d}$$

The natural frequency ω of the cantilever Timoshenko beam can be determined from the determinant of the follow matrix

$$\begin{vmatrix} \Lambda_1 & 0 & \Lambda_3 & 0 \\ 0 & 1 & 0 & 1 \\ \Lambda_1\alpha_1^2\cosh\alpha_1 & \Lambda_2\alpha_1^2\sinh\alpha_1 & -\Lambda_3\alpha_2^2\cos\alpha_2 & -\Lambda_4\alpha_2^2\sin\alpha_2 \\ \alpha_1^2\sinh\alpha_1 & \alpha_1^2\cosh\alpha_1 & -\alpha_2^2\sin\alpha_2 & -\alpha_2^2\cos\alpha_2 \end{vmatrix} = 0. \tag{12}$$

$$\begin{vmatrix} \Lambda_1 & 0 & \Lambda_3 & 0 \\ 0 & 1 & 0 & 1 \\ -\Lambda_1\alpha_1'^2\cos\alpha_1' & -\Lambda_2 j\alpha_1'^2\sin\alpha_1' & -\Lambda_3\alpha_2^2\cos\alpha_2 & -\Lambda_4\alpha_2^2\sin\alpha_2 \\ -j\alpha_1'^2\sin\alpha_1' & -\alpha_1'^2\cos\alpha_1' & -\alpha_2^2\sin\alpha_2 & -\alpha_2^2\cos\alpha_2 \end{vmatrix} = 0. \tag{13}$$

Solving Equation (12) and (13), one can obtain the natural frequency of the double Timoshenko beam with one end fixed.

3. Molecular dynamics model

The MD simulations are carried out using Brenner's second generation reactive empirical bond order (REBO) potential (Brenner et al. 2002) which has been widely used in a great number of studies on the mechanical behavior of carbon materials. In the REBO potential, the chemical binding energy E_b can be simply written as a sum over nearest neighbors in the form

$$E_b = \sum_i \sum_{j(>i)} [V^R(r_{ij}) - b_{ij}V^A(r_{ij})], \tag{14}$$

where r_{ij} is the distance between pairs of nearest-neighbour atoms *i* and *j*, b_{ij} is a many-body empirical bond-order function. The functions $V^R(r_{ij})$ and $V^A(r_{ij})$ are interatomic repulsion and attraction terms, which represent bonding from valence

electrons, respectively.

The long range vdW interaction is calculated by Lennard-Jones 12-6 potential, given by

$$E = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \tag{15}$$

with well-depth energy of ε=4.7483×10^{-22} J and equilibrium distance of σ=0.34nm.

The atoms in the red region shown in Figure 1(b) are fixed in order to simulate the cantilever boundary condition. The DWCNT is allowed vibrating freely for 2×10^{6} steps with time step 1fs at a room temperature (300K) using Nose-Hoover thermostat (Hoover 1985; Nose 1984a; Nose 1984b; Nose 1991) after the system is fully relaxed for 2ns. The coordinates histories in *y* direction of one random of the free atoms are recorded for certain duration, and the natural frequencies are computed by using the fast Fourier transform (FFT) method. The frequencies of a (9, 0)/(18, 0) zigzag DWCNT with 7.614nm length are shown in Figure 2, in which every peak represents one natural frequency of the DWCNT. It shows that although the diameters of the inner and outer tubes are different, the atoms oscillate in the same frequencies due to the effect of vdW force between these two tubes.

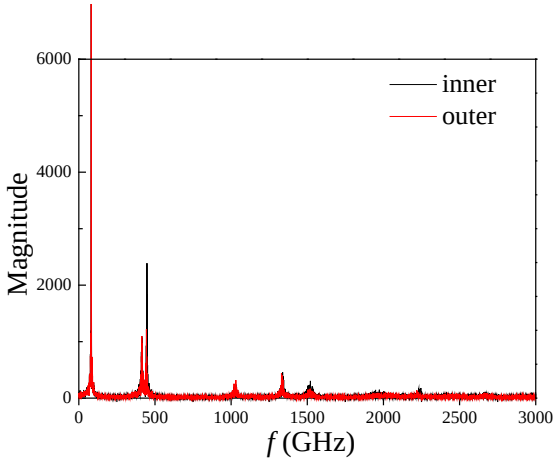


Figure 2. Magnitude-frequency curves of atoms on inner tube and outer tube with the same 7.614nm length

4. Results and Discussions

To predict the free vibration of a DWCNT, it is necessary to know Young's modulus *E* and the shear modulus *G* or Poisson's ratio μ. The previous studies based on the REBO potential gave a great variety of Young's modulus and Poisson's ratio of single-walled CNTs. For our calculations, the inner and outer tubes of DWCNT is assumed to have the same geometrical and material parameters where *E*=0.87TPa and μ=0.41 are given by MD tensile method introduced in (Liu & Wang 2012) when the thickness of the wall was chosen as 0.34nm.

Vibration of (5, 5)/(10, 10) DWCNTs and (9, 0)/(18, 0) DWCNTs with one end fixed are simulated by MD method. Figure 3 and Figure 4 show the first-order natural frequencies of these two kinds of DWCNTs with different lengths calculated by MD

and beam models. From Figure 3 and Figure 4, it can be found that the DTB model and DEB model which is introduced by Yoon et al.(2003b) give very similar frequencies if the aspect ratio L/d is about bigger than 8. However, the difference between these two beam models becomes obvious along with the aspect ratio getting small, and the DEB model gives the higher frequencies. From the comparison with results of MD simulations, the DTB beam model offers much better predictions than the DEB beam model. It suggests rotary inertia and shear deformation are significant for the vibration of short DWCNTs. And the DTB model is relevant for vibration of short DWCNTs.

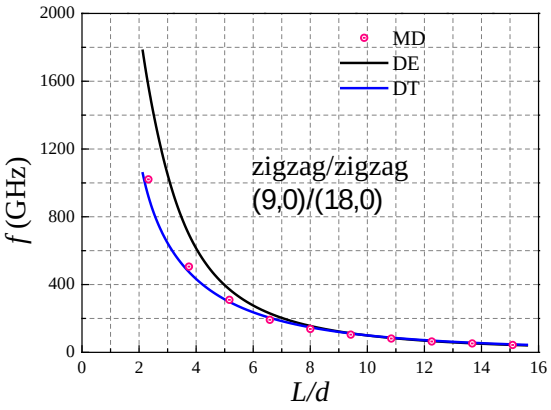


Figure 3. (9, 0)/(18, 0) DWCNT frequencies calculated by beam models and MD

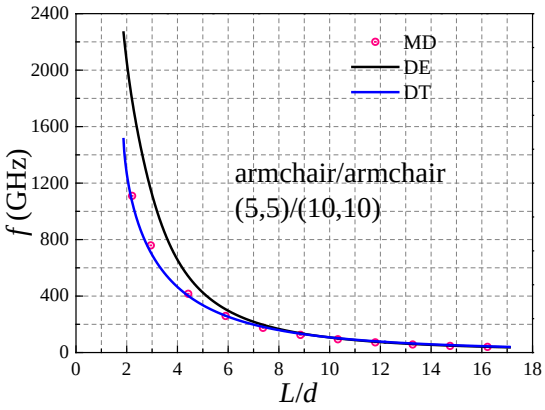


Figure 4. (5, 5)/(10, 10) DWCNT frequencies calculated by beam models and MD

High-order frequencies can be obtained according to the magnitude-frequency curves as shown in Figure 2. Note that some peaks response frequencies of the longitudinal vibration not the transverse vibration of the DWCNT. And frequencies responded by these peaks should be ignored in the statistical process. Figure 5 shows the first ten frequencies of (5, 5)/(10, 10) DWCNTs in different lengths. One can see that the natural frequencies predicted by the DTB model are better than those based on the DEB model, especially when the DWCNT getting very short. That's because the shorter of the DWCNT, the greater the impacts of rotary inertia and shear deformation on the free vibration of DWCNT. However, the differences in natural frequencies, mainly high-order frequencies, predicted by DTB model and the MD simulation still looks obvious. More accurate models, such as shell model, may give a better prediction for the natural frequencies of such a DWCNT.

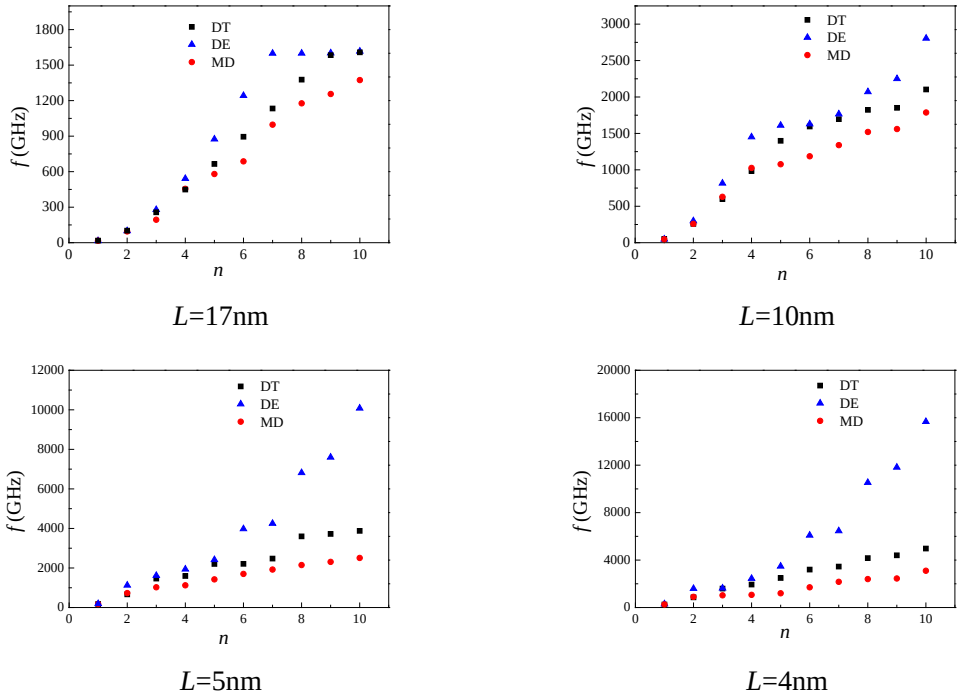


Figure 5. The first ten natural frequencies of (5, 5)/(10, 10) DWCNTs in different lengths

5. Conclusions

Free vibration of cantilever DWCNTs is studied using MD simulation and a DTB model which considers vdW force between the inner and outer tubes and treats the inner and outer tubes as two individual Timoshenko beams. A theoretical solution of cantilever DTB model has been obtained to predict the resonant frequency of DWCNTs with one end fixed. A comparison for the first-order frequencies between DTB model and DEB model shows that for the relatively long DWCNTs, the results obtained by the DTB model and the DEB model are very close, and the MD simulations show that both of these two models can predict the natural frequencies well. However, for the vibration of the relatively short DWCNTs, the difference between the DTB model and the DEB model becomes obvious, and the DTB model offers much better predictions than the DEB model. For high-order frequencies of DWCNTs, DTB model gives much better predictions than DEB model, especially when the length of DWCNTs is very short.

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