

Vibration and Buckling of In-Plane Loaded Double-Walled Carbon Nano-Tubes

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Abstract

The paper studies vibration and buckling of in-plane loaded double-walled carbon nanotubes. Timoshenko beam theory was used to investigate the vibration and buckling behavior of double-walled and simply supported carbon nanotubes. The influence of in-plane loads on the natural frequencies was determined. The results show that while the natural frequencies decrease with increasing compressive in-plane loads an increase in frequencies is observed for tension type of in-plane loads. The effects of in-plane loads are more pronounced for lower modes and some mode changes are observed at critical in-plane loads.

Key words: Nanostructures, Vibration, Multiwalled carbon nanotubes.

Introduction

After the invention of carbon nanotubes (CNTs) by Iijima (1991), several studies (Dai et al., 1996; Bachtold et al., 2001; Dharap, 2004) showed that they have good electrical properties and high mechanical strength so they can be used for nanoelectronics, nanodevices, and nanocomposites. Since molecular dynamic simulations are difficult for large scale systems, continuum mechanics models were used to study the elastic behavior of CNTs (Ru, 2000a, 2000b; Yoon et al., 2002, 2003a, 2003b, 2004, 2005; Wang and Varadan, 2005). The classical beam theory of Euler has been used to study the dynamic and static behavior of multi-walled nanotubes (MWNTs) to show that the classical theory is adequate for large aspect (length-to-diameter) ratios.

Non-coaxial interlayer radial displacements in transverse vibration in MWNTs using multiple Euler beam model were studied by Yoon et al. (2002, 2003a). Since the characteristic wavelength of transverse waves in MWNTs would be just a few times larger than the outermost diameter of MWNTs (Yoon et al., 2002), Timoshenko-beam theory was used to study vibration and wave propagation in

CNTs (Yoon et al., 2004, 2005), and it was concluded that both the Timoshenko-beam and the double-beam effects are significant when the wavelength of transverse waves of DWNTs is just a few times larger than the outer diameter of DWNTs. It is the case encountered when the higher-order frequencies (within the terahertz range) of short DWNT (of smaller aspect ratio around or below 20) are considered.

Extensive research has been devoted to the application of CNTs as chemical and mechanical sensors (Kong, 2000; Dhrap, 2004). As stated by Zhang et al. (2005), the basic principle of sensing is based on the natural (resonant) frequency shift of CNT resonator when it is subjected to an axial strain due to an external load. Zhang et al. (2005) applied a double elastic beam model to study transverse vibrations of double-walled carbon nanotubes under compressive axial load.

In the present study, a double elastic Timoshenko model was used to study transverse vibration and buckling of in-plane loaded DWNTs by taking into account the non-coaxial displacements. DWNTs were assumed as simply supported at both ends. The object of the study is to examine the effect of external load on vibration and to determine the variations

of the natural frequencies with the external load and the wave number.

Double Timoshenko-Beam Theory

The present paper studies transverse vibration of in-plane loaded DWNTs, as shown in Figure 1, based on Timoshenko-beam model. The inner and outer walls of the tube have diameters of d_1 and d_2 , respectively, and the tube length is L . As stated by Yoon et al. (2002), unlike the single-beam model which assumes that all originally concentric tubes of a MWNT remain coaxial during vibration in the MWNT, a multi-beam model considers interlayer radial displacements and individual deflection curves of nested tubes within the MWNT. Thus each of the inner and outer tubes of DWNTs is modeled as a Timoshenko-elastic beam. The transverse deflection $w(x,t)$ and the slope $\varphi(x,t)$ of a Timoshenko-beam due to bending deformation alone are determined by the following 2 coupled equations (Timoshenko, 1974):

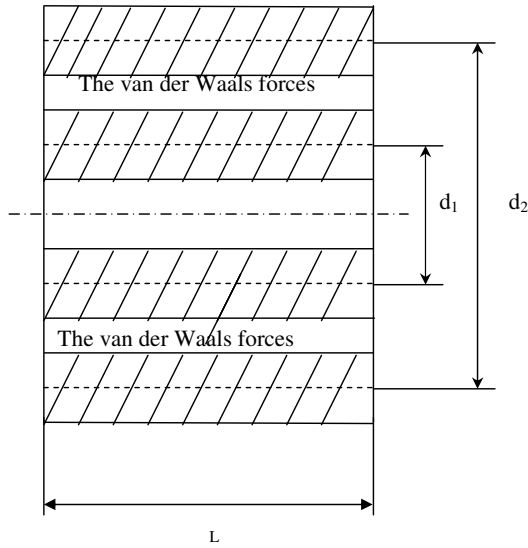


Figure 1. Geometry of double-wall carbon nanotubes.

$$\begin{aligned}
 -GAk \left(\frac{\partial \varphi}{\partial x} - \frac{\partial^2 w}{\partial x^2} \right) + \sigma_x \frac{\partial^2 w}{\partial x^2} &= \rho A \frac{\partial^2 w}{\partial t^2}, \\
 EI \frac{\partial^2 \varphi}{\partial x^2} - GAk \left(\varphi - \frac{\partial w}{\partial x} \right) &= \rho I \frac{\partial^2 \varphi}{\partial t^2}
 \end{aligned} \quad (1)$$

where x is the axial coordinate, t is time, I and A are the moment of inertia and the cross-section area of the beam, respectively, σ_x is the distributed pressure

per unit axial length, E and G are the Young modulus and shear modulus, respectively, ρ is the mass density per unit volume, and k is the shear correction coefficient, which is about 0.6-0.7 for thin walled circular cross sections and 0.9 for solid circular cross sections (Timoshenko, 1974).

Application of Eq. (1) to each of the inner and outer tubes of DWNT gives the following equations for transverse vibration of a DWNT:

$$\begin{aligned}
 -GA_1 k \left(\frac{\partial \varphi_1}{\partial x} - \frac{\partial^2 w_1}{\partial x^2} \right) + \sigma_x \frac{\partial^2 w_1}{\partial x^2} + p &= \rho A_1 \frac{\partial^2 w_1}{\partial t^2}, \\
 EI_1 \frac{\partial^2 \varphi_1}{\partial x^2} - GA_1 k \left(\varphi_1 - \frac{\partial w_1}{\partial x} \right) &= \rho I_1 \frac{\partial^2 \varphi_1}{\partial t^2}, \\
 -GA_2 k \left(\frac{\partial \varphi_2}{\partial x} - \frac{\partial^2 w_2}{\partial x^2} \right) + \sigma_x \frac{\partial^2 w_2}{\partial x^2} + p &= \rho A_2 \frac{\partial^2 w_2}{\partial t^2}, \\
 EI_2 \frac{\partial^2 \varphi_2}{\partial x^2} - GA_2 k \left(\varphi_2 - \frac{\partial w_2}{\partial x} \right) &= \rho I_2 \frac{\partial^2 \varphi_2}{\partial t^2}
 \end{aligned} \quad (2)$$

where σ_x is the axial external load, p is the van der Waals interaction pressure between the 2 tubes per unit axial length and the subscripts 1 and 2 are used to denote the quantities of the inner and outer tubes, respectively. Each tube is assumed to have the same Young's modulus of 1 TPa, shear modulus of 0.4 TPa, Poisson ratio of 0.25, shear coefficient of 0.8, and mass density of 2.3 g/cm³ with the effective thickness of 0.35 nm (Wang and Varadan, 2005).

The deflections of the 2 tubes are coupled through the van der Waals intertube interaction pressure. Since the inner and outer tubes of a DWNT are originally concentric and the van der Waals interaction is determined by the interlayer spacing, the net van der Waals interaction pressure remains zero for each tube provided they deform coaxially. Therefore, for small-amplitude linear transverse vibrations, the interaction pressure at any point between these 2 tubes depends linearly on the difference of their deflection curves at that point.

$$p = c(w_2 - w_1) \quad (3)$$

Here, the van der Waals interaction coefficient c for interaction pressure per unit axial length can be estimated in erg/cm² as (Yoon et al., 2003):

$$c = \frac{400 r_1}{0.16 D^2}, \quad (4)$$

where r_1 is the inner radius of DWNTs and $D = 0.142$ nm. Substitution of Eq. (3) into Eq. (2) leads to 4 coupled equations for 4 unknowns $w_i(x,t)$ and $\varphi_i(x,t)$ ($i = 1, 2$).

Transverse vibration of DWNTs

Since finding an analytical solution is possible for simply supported boundary conditions for the present problem, the inner and outer tubes of the DWNT are assumed simply supported. As a result, the boundary conditions have the following form:

$$\left. \begin{aligned} w_i(0, t) = w_i(L, t) = 0 \\ \frac{\partial \varphi_i(0, t)}{\partial x} = \frac{\partial \varphi_i(L, t)}{\partial x} = 0 \end{aligned} \right\}, \quad i = 1, 2, \quad (5)$$

To satisfy boundary conditions given by Eq. (5), the displacement field for DWNT is written in the following form:

$$\left. \begin{aligned} w_i = W_i \sin \frac{n\pi x}{L} \sin \omega t \\ \varphi_i = \Phi_i \cos \frac{n\pi x}{L} \sin \omega t \end{aligned} \right\}, \quad i = 1, 2, \quad (6)$$

where W_1 and W_2 represent the modal amplitudes of deflections of the inner and the outer tubes, and Φ_1 and Φ_2 represent, respectively, the modal amplitudes of the slopes of the inner and the outer tubes due to bending deformation alone. Integer n is the half wave number and ω is the circular frequency. Substitution of Eqs. (6) and (3) into Eq. (2) yields the following non-dimensional eigen-value equation:

$$\begin{bmatrix} (\Omega^2 - \lambda^2 \alpha - \beta - \lambda^2 N_x) & (\lambda \alpha) \\ (\lambda \alpha) & (\gamma \Omega^2 - \lambda^2 - \alpha) \\ (\beta) & 0 \\ 0 & 0 \\ \beta & 0 \\ 0 & 0 \\ (\varepsilon \Omega^2 - \varepsilon \lambda^2 \alpha - \beta - \varepsilon \lambda^2 N_x) & (\varepsilon \lambda \alpha) \\ (\varepsilon \lambda \alpha) & (\delta \gamma \Omega^2 - \delta \lambda^2 - \varepsilon \alpha) \end{bmatrix} \begin{Bmatrix} W_1 \\ \Phi_1 \\ W_2 \\ \Phi_2 \end{Bmatrix} = 0 \quad (7)$$

The non-dimensional variables in Eq. (5) are defined as follows:

$$\Omega^2 = \frac{\rho A_1 \omega^2 L^4}{EI_1}, \quad N_x = \frac{\sigma_x A_1 L^2}{EI_1}, \quad (8)$$

$$\lambda = n\pi \quad \varepsilon = \frac{A_2}{A_1}, \quad \delta = \frac{I_2}{I_1}, \quad (9)$$

$$\alpha = \frac{k A_1 G L^2}{EI_1}, \quad \beta = \frac{c L^4}{EI_1}, \quad \gamma = \frac{I_1}{A_1 L^2}, \quad (10)$$

$$I_1 = \frac{1}{2} \left[\left(R_1 + \frac{0.35}{2} \right)^4 - \left(R_1 - \frac{0.35}{2} \right)^4 \right], \quad (11)$$

$$I_2 = \frac{1}{2} \left[\left(R_2 + \frac{0.35}{2} \right)^4 - \left(R_2 - \frac{0.35}{2} \right)^4 \right],$$

$$A_1 = \pi \left[\left(R_1 + \frac{0.35}{2} \right)^2 - \left(R_1 - \frac{0.35}{2} \right)^2 \right], \quad (12)$$

$$A_2 = \pi \left[\left(R_2 + \frac{0.35}{2} \right)^2 - \left(R_2 - \frac{0.35}{2} \right)^2 \right]$$

As stated by Yoon et al. (2005), this eigen-value equation gives 4 n-order frequencies, Ω_{n1} , Ω_{n2} , Ω_{n3} , and Ω_{n4} . For given n , nanotubes vibrate in similar mode shapes with different amplitudes. These frequencies and mode shapes are important for the design process to understand the dynamic behavior of nanotubes. The transverse vibration equation obtained for the n th mode by substituting $\sigma_x = 0$ is consistent with that given by Yoon et al. (2005). The non-dimensional critical buckling loads of DWNT can be determined by setting $\Omega = 0$ in Eq. (7) and solving it for N_x .

Determination of the eigen-values of Eq. (7) requires the dimensions of the nanotube to be specified. Diameters of the inner and the outer walls of the tube were taken as $d_1 = 0.7$ nm and $d_2 = 1.4$ nm, respectively. The effective thickness of single-walled carbon nanotubes was taken to be 0.35 nm. The length of the tube was selected such that $L/d_2 = 10$, 20, and 50. The eigen-value equation given in Eq. (7) was solved by the Newton-Rapson method and the iterations were stopped when the absolute value of the difference between the frequencies calculated at 2 successive iterations was less than 10^{-6} .

Free vibration frequencies predicted by the present model were compared with the results reported by He et al. (2006) in Table 1. They used the Donell shell model to study the vibration of CNT.

The difference between these 2 results is within the acceptable range for engineering applications. They also compared their results with the experimental results. This shows the validity of the present beam model.

Table 1. Comparison of frequency (Hz) of DWCTs with shell model of He et al.

Theory	$R_i = 0.5 \text{ nm}$	$R_i = 1 \text{ nm}$
Present	4.7404	3.0308
Ref.	4.4590	2.8960
%difference	6.31	4.65

Variations in non-dimensional frequencies are given in Figures 2-4. In these figures, taking in-plane load value as zero ($N_x = 0$) leads to non-dimensional free vibration frequencies.

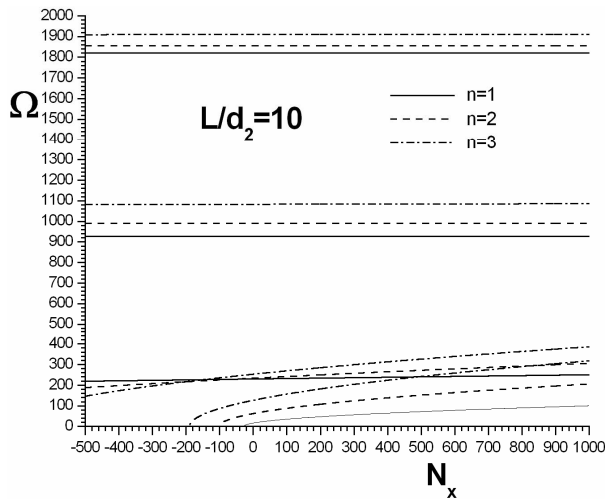


Figure 2. Variation of dimensionless frequency parameter with in-plane load for $L/d_2 = 10$.

Positive N_x corresponds to tension type in-plane loads, whereas negative N_x stands for compression type loading. Increasing in-plane compression loads decreases non-dimensional frequencies to zero (the lowest of these loads is called critical buckling load). On the other hand, positive tension type loading causes an increase in frequencies. Non-dimensional frequency results were given for the first 3 modes ($n = 1, 2, \text{ and } 3$). As stated before, there are 4 frequencies ($\Omega_{n1}, \Omega_{n2}, \Omega_{n3}, \text{ and } \Omega_{n4}$) for each mode for Timoshenko beam theory. As can be seen from the figures, the effect of in-plane loads is more pronounced for lower modes for all L/d_2 ratios. It is

also possible to find buckling loads for higher modes. However, for the present range of external compressive loads, higher buckling loads were not observed because they are not important for physical applications since any value over the critical value load will buckle the nanotube. It is interesting to note that some mode changes were observed due to in-plane loads (crossing of frequency curves for some values of in-plane loads e.g., $N_x = -140$ for $L/d_2 = 10$).

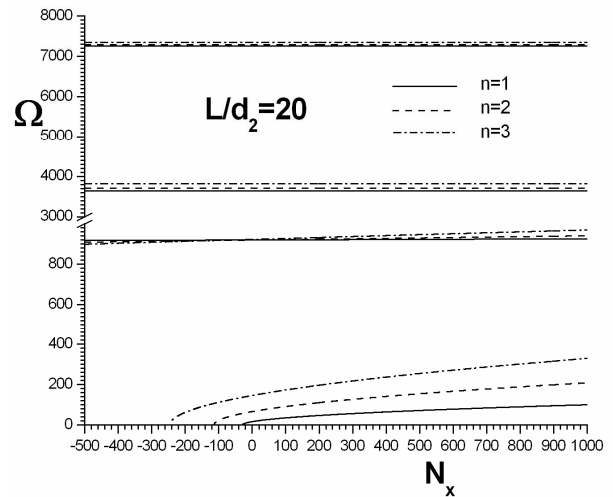


Figure 3. Variation of dimensionless frequency parameter with in-plane load for $L/d_2 = 20$.

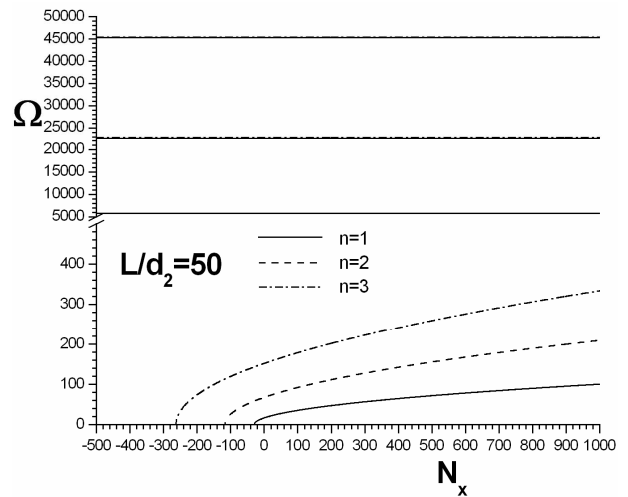


Figure 4. Variation of dimensionless frequency parameter with in-plane load for $L/d_2 = 50$.

Dimensionless critical load parameters are given in Table 2. Dimensionless critical buckling loads increase with both increasing L/d_2 ratios and n mode numbers, and dimensionless critical buckling loads are more affected by smaller L/d_2 ratios.

Table 2. Dimensionless buckling load parameter for DWNT for different modes and for different L/d_2 ratios.

L/d	n	N_x
10	1	28.567368
	2	102.227914
	3	189.705035
20	1	29.347445
	2	114.269471
	3	245.592806
50	1	29.566963
	2	117.765922
	3	263.093526

Conclusions

Based on Timoshenko beam theory, a double-elastic beam model was presented for transverse vibrations of double-walled carbon nanotubes under axial loads. The interaction of van der Waals pressure between the inner and outer tubes and the effect of compressive and tension type axial loads were incorporated in the formulation. The vibration behavior of simply supported double-walled carbon nanotubes was studied. It is concluded that the effects of axial load on

the natural frequencies of double-walled carbon nanotubes were sensitive to the vibration modes. Frequencies were found to decrease with increasing compressive in-plane loads where an increase in natural frequencies was observed for increasing tension type in-plane loads. Critical axial buckling loads were also given in the study. The present study can be extended to other classic boundary conditions.

Nomenclature

E	elastic modulus for a nanotube
G	shear modulus for nanotube
ν	Poisson's ratio
r	radius of tube
σ_x	in-plane stress
w	displacements in z-direction
φ	slope due to bending
A	cross sectional area of nanotube
I	moment of inertia
t	time
ρ	density of carbon nanotube
Ω	non-dimensional frequency parameter
p	van der Waals interaction pressure
c	interaction coefficient
n	half wave number
ω	radial frequency

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