VIBRATION CHARACTERISTICS OF EMBEDDED DOUBLE WALLED CARBON NANOTUBES SUBJECTED TO AN AXIAL PRESSURE

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1. General Introduction

The study of vibration in carbon nanotubes (CNTs) is currently a major topic of interest [1-3] that increases understanding of their dynamic mechanical behavior. The radial breathing mode (RBM) is the lowest but the strongest feature observed from Raman spectroscopy, where all the carbon atoms in a CNT move in the radial direction synchronously, as if the tubes are “breathing” [4]. This is unique to CNTs, and cannot be found in other carbon systems [5]. RBM in CNTs is a standard, straightforward method for precisely determining the diameter of a CNT, distinguishing the CNTs chiral-index assignments, or characterizing CNTs conglomerates [6-10]. For CNTs, pressure studies are motivated by the need to investigate mechanical stability, pressure-induced phase transitions (such as vibrational characteristics), and the effects of intertube interactions. In addition, the influence of the CNTs based composite [11] such as matrix surrounding CNTs is also important for the study of vibrational property of CNTs.

In this study, the frequency of the RBM of embedded double walled carbon nanotubes (DWCNTs) subjected to an axial pressure is studied by using an elastic continuum mechanics model. The theoretical approach is in terms of a simplified model of DWCNTs with the van der Waals (vdW) interaction between the inner and outer nanotubes, and a Winkler spring model for the surrounding elastic medium. The influences of the axial half-wave number \( m \), circumference wave number \( n \) of nanotubes and the matrix surrounding tubes on the RBM frequency of the DWCNTs under varying axial pressure are considered. Compared to previous results obtained from experimental and simulation investigations, the continuum shell model can be used to predict the frequency of the RBM of CNTs under pressure reasonably. This investigation will be helpful in nanodevice technologies such as nanoprobes and nanosensors.

2. Theoretical Approach

2.1 Governing Equations of DWCNTs

A continuum elastic shell model (Fig. 1) is used to analyze the characteristics of the RBM frequency of DWCNTs subjected to an axial pressure. The cylindrical shell is used to designate a coordinate system \((x, \theta, z)\). The coordinates \( x \), \( \theta \), and \( z \) refer to the axial, circumferential and radial directions, respectively. The displacements for the CNTs are \( u \), \( v \), and \( w \) corresponding to the \( x \), \( \theta \), and \( z \) directions, respectively. The dimensions of the nanotubes are defined as the thickness \( h \), radius \( R \), length \( L \), Poisson’s ratio \( \nu \) and density \( \rho \).

Based on our previous work [6] and Love’s first approximation shell theory, the equation of motion for simply supported CNTs is given by:

\[
\begin{align*}
\frac{\partial^2 u}{\partial x^2} + (1 - \nu) \frac{\partial^2 u}{\partial y^2} + (1 + \nu) \frac{\partial^2 v}{\partial x^2} - v \frac{\partial w}{\partial x} + 2R \frac{\partial^2 \theta}{\partial x \partial y} - \frac{R}{\theta} \frac{\partial^2 \theta}{\partial x^2} + 2R \frac{\partial^2 \theta}{\partial y^2} + \frac{1}{\theta} \frac{\partial \theta}{\partial x} = 0 \quad (1)
\end{align*}
\]

For \( \nu \), \( \theta \), and \( \beta \) respectively, the equation of motion for the DWCNTs is:

\[
\begin{align*}
2R \frac{\partial^2 \theta}{\partial x \partial y} - \frac{R^2 \theta}{\partial x^2} + \beta \times \\
[1 - \nu] \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^3 w}{\partial x^3} + \frac{\partial^3 \theta}{\partial x^3} = 0 \quad (2)
\end{align*}
\]

\[
\frac{\nu \partial^2 w}{\partial t^2} + \frac{\partial^2 w}{\partial x^2} - \frac{w}{R^2} + 2\Phi \frac{\partial \theta}{\partial x} + \beta \times
\]

\[
\begin{align*}
\frac{\partial^2 \theta}{\partial t^2} + \frac{\partial^2 \theta}{\partial x^2} = 0
\end{align*}
\]
where $w = \frac{1 - v^2}{Eh}$, $\beta = h^2/12R$, $p_x$ is the axial pressure acting on the both ends of the DWCNTs and $p_e$ is the transverse external pressures (including pressures from matrix effect and vdWs interaction forces) on the tubes.

### 2.2 The Matrix Model

The Winkler spring model has been widely used to study the vibration and axially compressed buckling of embedded DWCNTs [12]. Fig. 2 (a) shows the Winkler spring model of a DWCNT embedded in an elastic matrix. The pressure $p_0$, acting on the outer tube of the DWCNTs due to the surrounding elastic medium, can be given by

$$p_0 = -c_0w_2$$  \hspace{1cm} (4)

where the negative sign indicates that the pressure $p_0$ is opposite to the deflection of the nanotube. $c_0$ is a spring constant relative to the elastic matrix, the diameter of the nanotube, and the wavelength of vibrational modes [12]. The surrounding material is assumed to be a rigid matrix with elasticity. Although the parameter $c_0$ seems insufficient to describe the elasticity of this material, the assumption was used commonly to fibers embedded in elastic matrix.

### 2.3 The Van Der Waals (vdW) Interaction Forces

To study the vibrational behavior of DWCNTs, a double-elastic shell model was developed that assumes each of the nested tubes in a CNT is an individual elastic shell, and the adjacent tubes are coupled to each other by normal vdW interactions. The pressures from vdW forces exerted on the inner and outer nanotubes through vdW interaction pressures (Fig. 2 (b)) are given as

$$p_1 = c_{12}(w_2 - w_1)$$  \hspace{1cm} (5)

$$p_2 = c_{21}(w_1 - w_2)$$  \hspace{1cm} (6)

where $w_k (k = 1, 2)$ are the radial displacements of the inner and outer nanotubes, and $c_{ij}$ ($i, j = 1, 2$) is the vdW interaction coefficient between nanotubes, which can be estimated using the Lennard-Jones potential [13]:

$$c_{ij} = \frac{\pi \varepsilon R_j \sigma^6}{3a^4} \left[ 1120 - 1001a^6H_{ij}^3 \right]$$  \hspace{1cm} (7)

where $H_{ij} = \Phi - \frac{R_i R_j}{(R_i + R_j)^2}$

$$K_{ij} = \frac{4R_i R_j}{(R_i + R_j)^2}$$  \hspace{1cm} (9)

where $a$ is the carbon-carbon bond length (0.142 nm), $R_i$ and $R_j$ are the inner and outer radii of the DWCNTs, and $\sigma$ and $\varepsilon$ are the vdW radius and the well depth of the Lennard-Jones potential, respectively. The vdW parameters in the Lennard-Jones potential are $\varepsilon = 2.967$ meV and $\sigma = 0.34$ nm as reported by Saito et al. [13].

### 2.4 RBM Frequency of DWCNTs

Considering the effect of matrix and vdW force, we get the transverse external pressures for inner and outer tubes, respectively.

$$p_{in}^m = c_{12}(w_2 - w_1)$$  \hspace{1cm} (10)

$$p_{out}^m = c_{21}w_1 - (c_{21} + c_0)w_2$$  \hspace{1cm} (11)

We substitute Eqs. (10) and (11) into Eqs. (1)–(3). The governing equations for the RBM frequency of inner and outer tubes of DWCNTs subjected to an axial pressure can be expressed as:

For inner tube:

$$\frac{\partial^2 u_1}{\partial x^2} + \frac{(1 - v) \partial^2 u_1}{\partial \theta^2} + \frac{(1 + v) \partial^2 v_1}{\partial x^2 \partial \theta} - \frac{v \partial w_1}{r \partial x} \frac{\partial^2 w_1}{\partial x^2} + 2 \frac{\partial^2 w_1}{\partial x^2 \partial \theta} + \frac{\partial^2 v_1}{\partial \theta^2} = 0$$

For outer tube:

$$\frac{\partial^2 u_2}{\partial x^2} + \frac{(1 - v) \partial^2 u_2}{\partial \theta^2} + \frac{(1 + v) \partial^2 v_2}{\partial x^2 \partial \theta} - \frac{v \partial w_2}{r \partial x} \frac{\partial^2 w_2}{\partial x^2} + 2 \frac{\partial^2 w_2}{\partial x^2 \partial \theta} + \frac{\partial^2 v_2}{\partial \theta^2} = 0$$
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\[
\begin{align*}
(1 + v) \frac{\partial^2 u_2}{\partial x^2} + \frac{\partial^2 v_2}{\partial x^2} + (1 - v) \frac{\partial^2 v_2}{\partial x^2} + \frac{2}{R^2} \frac{\partial^2 w_2}{\partial \theta^2} &+ 2 \Phi \frac{\partial v_2}{\partial x} \frac{\partial w_2}{\partial x} - \frac{\partial w_2}{\partial \theta} + \beta \times \\
(1 - v) \frac{\partial^2 v_2}{\partial x^2} + \frac{\partial^2 v_2}{\partial x^2} + \frac{\partial^3 w_2}{\partial x^2 \partial \theta} + \frac{\partial^3 w_2}{\partial x^2 \partial \theta} &+ \frac{\partial^2 w_2}{\partial \theta^2} \\
&= 0 \\
2 \Phi c_{21} w_1 + v \frac{\partial u_2}{\partial x} + \frac{\partial v_2}{\partial x} + 2 \Phi \frac{\partial^2 w_2}{\partial x^2} - \frac{w_2}{R^2} &- \frac{\partial^2 w_2}{\partial \theta^2} - 2 \Phi \omega (c_{21} + c_0) \\
+ \beta \left[ (u - 2) \frac{\partial^3 v_2}{\partial x^2 \partial \theta^2} - \frac{R^2}{\partial \theta^2} \frac{\partial^3 w_2}{\partial \theta^2} - \frac{2}{\partial x^2} \frac{\partial^3 w_2}{\partial \theta^2} \\
- \frac{4}{\partial R^2} \frac{\partial^3 w_2}{\partial \theta^2} \right] &= 0
\end{align*}
\]

where \( r \) and \( R \) are the radius of inner tube and outer tube of the DWCNT, respectively. To simplify the calculation, Eqs. (11) \( - \) (15) can be rewritten as:

\[
\begin{align*}
L_{11} & = \frac{\partial^2}{\partial x^2} + (1 - v) \frac{\partial^2}{\partial \theta^2} \\
L_{12} & = \frac{2r}{\partial x} \frac{\partial^2}{\partial x \partial \theta} \\
L_{13} & = -\frac{2r}{\partial x} \frac{\partial}{\partial \theta} \\
L_{22} & = \frac{2r}{\partial x} \frac{\partial^2}{\partial x^2} + (1 - v) \frac{\partial^2}{\partial x^2} + 2 \Phi \frac{\partial}{\partial x} \frac{\partial^2}{\partial \theta^2} \\
L_{23} & = -\frac{\partial}{\partial x} \frac{\partial^2}{\partial \theta^2} + \beta \left[ \frac{\partial^3}{\partial x^2 \partial \theta} + \frac{\partial^3}{\partial \theta^2} \right] \\
L_{31} & = \frac{\partial}{\partial x} \frac{\partial}{\partial \theta} \\
L_{32} & = \frac{\partial}{\partial x} \frac{\partial}{\partial \theta} + \beta \left[ (u - 2) \frac{\partial^3}{\partial x^2 \partial \theta} - \frac{\partial^3}{\partial \theta^2} \right]
\end{align*}
\]

The general solution for the displacements \( u, v \) and \( w \) in the inner and outer tubes of DWCNTs can be given by:

\[
\begin{align*}
u & = A_k \sin (n \theta) \cos \frac{mlx}{L} e^{i \omega t} \\
v & = B_k \cos (n \theta) \sin \frac{mlx}{L} e^{i \omega t} \\
W & = C_k \sin (n \theta) \sin \frac{mlx}{L} e^{i \omega t} (k = 1, 2)
\end{align*}
\]

where \( A_k, B_k \) and \( C_k \) are the longitudinal, circumferential and radial amplitudes of displacement in the inner tube \( (k = 1) \) and the outer tube \( (k = 2) \), respectively. \( \omega \) is the circular frequency of RBM and \( t \) is time. The wave numbers \( m \) and \( n \) are the axial half-wave and circumferential numbers, respectively.
3. Results and Discussion

The influence of different nanotube parameters on the frequency of the RBM was investigated by using the proposed method. For DWCNTs, the elastic modulus is 1.0 TPa, Poisson’s ratio is 0.27, and the mass density is 2.3 g/cm$^3$. We consider DWCNTs with an inner diameter of 2.2 nm and an outer diameter of 3.0 nm [12].

Based on the present theoretical approach, we firstly calculate the frequency of the RBM of isolated SWCNTs under no pressure as a function of radius. After comparison [6], it is found that the calculated frequencies of the RBM of SWCNTs with varying radius under no pressure agree closely with the values reported in the literatures using Raman scattering technique [14], first-principles calculations [15] and molecular dynamics method (MD) and finite element method (FEM) [16], which verifies that the continuum elastic shell model can accurately describes the frequency of the RBM of CNTs.

The frequencies of the RBM of DWCNTs with different circumferential wave numbers ($n = 1 – 4$), axial half-wave numbers ($m = 1 – 4$) and different matrix surrounding DWCNTs subjected to pressure were investigated and the results are shown in Figs. 3 – 5. The RBM frequency variation ratio $\eta$ of DWCNTs is defined as:

$$\eta = \frac{f_p - f_0}{f_0}$$

(23)

where $f_p$ is the RBM frequency of the DWCNTs exposed to an axial pressure, and $f_0$ is the RBM frequency of DWCNTs without any axial pressure.

The variation ratios of the RBM frequency have a positive logarithmic relationship with increasing pressure in these figures. The curves of RBM frequency variation ratio in each figure start from different positions, and are parallel to each other without cross point. Each tube exhibits the frequency variation ratio of DWCNTs below 0.1. The axial half-waves of $m$, circumference wave number $n$ and the effect of matrix all play important roles as the pressure increases. From the comparison of Fig. 3 – 5, we can see that with the increasing axial pressure on both ends of DWCNTs, the RBM frequency variation ratios present different trends and different ranges. Fig. 3 shows the RBM frequency variation ratio of DWCNTs as a function of axial pressure with axial half-wave numbers $m$ varying from 1 to 4. The DWCNTs have the same circumference wave numbers, $n = 2$ and matrix effect $c_0 = 0.1c_{12}$. The frequency variation ratio DWCNTs increase with the increasing axial half-wave number. The lowest frequency variation ratio happens when axial half-wave numbers $m = 1$, which means the growth rate of RBM frequency is the lowest one in that condition. Fig. 4 shows RBM frequency variation ratio of DWCNTs as a function of axial pressure with circumference wave numbers $n$ varying from 1 to 4. The DWCNTs have the same axial half-wave numbers, $m = 1$ and matrix effect $c_0 = 0.1c_{12}$. All of the frequency variation ratios of DWCNTs decrease with the increasing circumference wave number and the lowest frequency variation ratio happens when circumference wave number $n = 1$. From the figure, we can see that the variation ranges of the four curves have changed obviously, which means the circumference wave number $n$ shows the most strongly influence on RBM frequency variation ratio. Fig. 5 shows RBM frequency variation ratio of DWCNTs surrounded by different elastic matrices as a function of axial pressure. The DWCNTs have the same axial half-wave numbers, $m = 1$ and circumference wave number, $n = 2$. All of the frequency variation ratio decrease with the enhancement of elastic matrix, which explains that the matrix surrounding the tubes can reinforce the vibrational property of DWCNTs.

4. Conclusions

The RBM of embedded DWCNTs subjected to an axial pressure was investigated. The analysis was based on a continuum mechanics model where each tube of a DWCNT was described as an individual elastic shell and coupled to each other by vdW interactions. Compared with experimental and simulation investigations on the frequency of the RBM of isolated SWCNTs with increasing radius, the continuum shell model can be used to reasonably predict the RBM frequency of CNTs subjected to pressure. It is found that RBM frequency variation ratio in DWCNTs under increasing axial pressure depends on circumferential wave numbers, axial half-wave numbers and matrix elastic modulus. With increasing axial pressure on the both ends of DWCNTs, the frequency variation ratio increase
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with increasing axial half-wave number, decrease with increasing circumference wave number and the RBM frequency of DWCNTs can be reinforced by the surrounding matrix. This investigation will be helpful in the application of CNTs in future.

Figures

Fig.1. Schematic showing the cylindrical coordinates of the CNT model used for analysis.

Fig.2. Schematic diagram describing analysis model of CNTs subjected to pressure. (a) displays the longitudinal cross-section, which shows the surrounding matrix and axial pressure acting on both ends of the DWCNT. (b) displays the latitudinal cross-section, which shows the vdW force between the inner and outer tubes.

Fig.3. RBM frequency variation ratio of DWCNTs as a function of axial pressure. The DWCNTs have the same circumference wave numbers, $n = 2$ and matrix effect $c_0 = 0.1c_{12}$. However, they have axial half-wave number $m$ that varies from 1 to 4.

Fig.4. RBM frequency variation ratio of DWCNTs as a function of axial pressure. The DWCNTs have the same axial half-wave numbers, $m = 1$ and matrix effect $c_0 = 0.1c_{12}$. However, they have circumference wave number $n$ that varies from 1 to 4.
Fig.5. RBM frequency variation ratio of DWCNTs as a function of axial pressure. The DWCNTs have the same axial half-wave number, $m = 1$ and circumference wave number, $n = 2$. However, different matrix surrounding the DWCNTs.

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