Vibration Characteristics of Multiwalled Carbon Nanotubes Embedded in Elastic Media by a Nonlocal Elastic Shell Model

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In this paper, the vibrational behavior of the multiwalled carbon nanotubes (MWCNTs) embedded in elastic media is investigated by a nonlocal shell model. The nonlocal shell model is formulated by considering the small length scales effects, the interaction of van der Waals forces between two adjacent tubes and the reaction from the surrounding media, and a set of governing equations of motion for the MWCNTs are accordingly derived. In contrast to the beam models in the literature, which would only predict the resonant frequencies of bending vibrational modes by taking the MWCNT as a whole beam, the current shell model can find the resonant frequencies of three modes being classified as radial, axial, and circumferential for each nanotube of a MWCNT. Big influences from the small length scales and the van der Waals' forces are observed. Among these, noteworthy is the reduction in the radial frequencies due to the van der Waals' force interaction between two adjacent nanotubes. The numerical results also show that when the spring constant k_0 of the surrounding elastic medium reaches a certain value, the lowest resonant frequency of the double walled carbon nanotube drops dramatically. [DOI: 10.1115/1.2722305]

Keywords: vibration, multiwalled, carbon nanotubes, nonlocal shell, small length scale, van der Waals, resonant frequencies

1 Introduction

Carbon nanotubes [1], cylindrical-shaped tubes of seamless graphite with extraordinary electrical and mechanical properties [2–8] potentially have remarkable applications for novel materials or structures such as carbon-nanotube-reinforced composites [9,10] or as individual elements of nanometer-scale devices and sensors [11–13], and have attracted considerable attention worldwide [14–22]. Usually, the properties of carbon nanotubes are evaluated via experiments [2,8] or atomistic and molecular dynamics simulations [14,15]. As has been pointed out in the literature, these experiments are extremely difficult to conduct and control and the molecular dynamics simulations are very time-consuming for large systems [16,17] because of the involvement of internal nanolength scales. Therefore, many authors have made great efforts to extend the classical continuum mechanics to large-sized atomistic systems. Such kind of models can yield reasonable results when the nanotubes are large enough to be viewed as a homogenized material system [17,18]. However, the size of a nanotube is usually very small, maybe a few atoms in diameter, hence it may not be viewed as a continuum medium. Therefore, the small-scale may call the direct application of the classical continuum mechanics model into question [17]. Having realized the limitations of classical continuum models in the study of nanotechnology, some researchers started to use a nonlocal elastic model in their studies [17,18,21,22]. This nonlocal elastic model cannot only include the merits of the classical continuum model but also take the internal small-length scale into account.

In the classical (local) theory of elasticity, the stress at a reference point $x=(x_1,x_2,x_3)$ can be uniquely determined by the strains at that point. However, the nonlocal elasticity [23–25] postulates that the stress at a reference point x in a body not only depends on the strains at x but also depends on the strains of all other points x within the body considered. The stress-strain relations can be written as $\sigma_{ij}(x)=\int_v \alpha(|x'-x|,\tau)c_{ijkl}\epsilon_{kl}(x')dv(x')$, where $\alpha(|x'-x|,\tau)$ is the nonlocal moduli; $\tau=e_0a/l$ with a an internal characteristic length (e.g., lattice parameter, granular distance), l is an external characteristic length (e.g., crack length, wavelength), and e_0 is a constant appropriate to each material; c_{ijkl} is the elastic moduli tensor. For two-dimensional nonlocal elasticity, there exists a differential form for the stress-strain relation,

$$(1-\tau^2l^2\nabla^2)\sigma_{ij}=c_{ijkl}\epsilon_{kl} \tag{1}$$

where the operator ∇^2 is the Laplacian operator and has the form $(\partial^2/x_1^2)+(\partial^2/x_2^2)$ in a rectangular coordinate system. Notice that in the nonlocal elasticity the effect of small length scale is considered by incorporating the internal parameter length into the constitutive equation. One may also see that when the internal characteristic length a is neglected, i.e., the particles of a medium are considered to be continuously distributed, then $\tau=0$, and Eq. (1) reduces to the constitutive equation of classical elasticity. Also, it should be noted that, through Eq. (1), the l is cancelled from the rest of the analysis, leaving a and e_0 as the internal characteristic constants.

The vibration of nanotubes is a important subject in the study of nanotechnology since it relates to the electronic and optical properties of MWCNT [26–28]. However, the models in the literature to-date have been exclusively based on beam theory such as these referring to thermal vibration and resonant frequencies [2,8,19,28]. But the topological structure of a nanotube can be viewed as a cylindrical shell, therefore when the multiwalled nanotubes vibrate, not one but three resonant frequencies (radial, axial, and circumferential) can be activated for each nanotube of the multiwalled carbon-nanotube assembly. Since the nanotubes of a MWCNT are coupled via the van der Waals' forces, these three resonant frequencies of each of the nanotubes may be dif-

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ferent from the ones predicted based on isolated nanotubes. The differences in resonant frequencies among the nanotubes of a MWCNT can further affect the electronic and optical properties of the nanostructure. Therefore, the study of the vibration of the MWCNT from a shell-type topological viewpoint has technological significance and in the current research, the vibration of a MWCNT is analyzed by a nonlocal elastic shell model.

We note again that although the internal characteristic length, a, may be on the same scale order as the C–C bond length, this does not mean that the nonlocal elastic theory follows each atom. This important internal characteristic parameter, a, enters into the constitutive relations to reflect the effects of the discrete character [23–25] of the nanostructures when extending the continuum theory to deal with such materials. As has been shown in the literature, experimental and molecular-dynamics simulation methods are often used in most of the studies in understanding the material properties and applications of carbon nanotubes. However, the experiments at the nano-scale are often hard to control and the simulations by molecular-dynamics are difficult to accurately formulate and quite expensive for large-scale atomic systems. Therefore, researchers have attempted to expand the classical continuum mechanics approach to the atomic or molecular-based discrete systems. The classical continuum models are efficient and accurate in computation for a material system in large length scales. But the length scales at nanometers such as in carbon nanotubes are not big enough to homogenize the discrete structure into a continuum. But by using the nonlocal theory, one would harvest the efficiency of classical continuum models and take the nanoscale effects into account at the same time, thus obtaining a satisfactory approximation [24,17,18], etc. These are the advantages of the current theory when comparing with molecular mechanics.

Therefore, in this paper, a nonlocal multiple shell model is developed to investigate the vibration characteristics of multiwalled carbon nanotubes. In this model, not only the terms concerning the van der Waals forces between adjacent nanotubes are incorporated into the Donnell shell model, but also the full nonlocal constitutive relationship is adopted in the derivation of the formulas. Therefore, this model includes both the interactions from the van der Waals forces and the effects from the internal small scales of the nanodevices. Compared with some nonlocal models in the literature for nanotubes subjected to mechanical loading, our model is a comprehensive nonlocal elastic model in the sense that no approximation has been made in the use of the nonlocal elastic constitutive equations and each tube is treated as a shell, not as a one-dimensional column. The work presented in this paper is organized as follows: in Sec. 2 we present the development of a nonlocal elastic shell model for the motion of multiwalled nanotubes; in Sec. 3 we present the analysis for the vibration of DWCNTs under simply-supported end boundary conditions and the derivation of the characteristic equation for the natural frequencies; in Sec. 4 we present numerical results and associated discussions on the vibration behavior of double-walled carbon nanotubes embedded in an elastic medium; finally, conclusions are given in Sec. 5.

2 The Nonlocal Elastic Shell Model of Multiwalled Carbon Nanotubes

Let x, θ, z be the axial, circumferential, and radial coordinates of the nanotube (Fig. 1), respectively. In terms of the the axial, circumferential, and radial displacements of mid-surface, u, v, w, respectively, the strains and displacements of a nanotube have the following relations:

$$\epsilon_{xx} = u_{,x} - z\chi_x \quad \epsilon_{\theta\theta} = \frac{1}{R}v_{,\theta} + \frac{w}{R} - z\chi_\theta$$

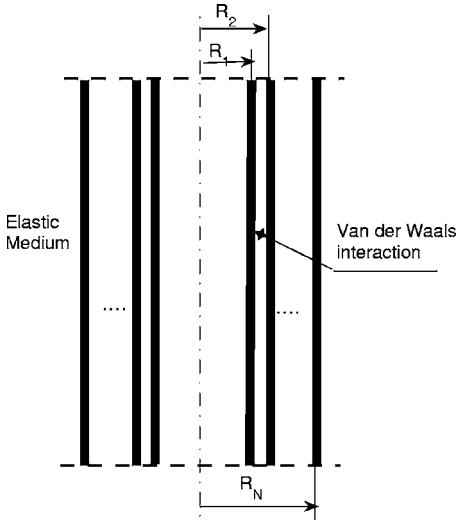

Fig. 1 A shell model of multiwalled nanotubes in an elastic medium

$$\gamma_{x_\theta} = \frac{1}{R}u_{,\theta} + v_{,x} - 2z\chi_{x\theta} \tag{2}$$

where R is the mid-surface radius; χ_x, χ_θ, and $\chi_{x\theta}$ are curvatures; the comma denotes differentiation with respect to the corresponding coordinates. We would like to emphasize that our work is a shell theory and not a 3D elasticity solution. Therefore, although three coordinates x, θ, and z are involved in Eq. (2), only two variables x and θ enter into the operators and the problem becomes a 2D problem. Similar handling of the z-direction effects can be also found in Refs. [17,18]. Hence, this problem becomes a 2D problem and the nonlocal theory is then applied onto this 2D problem.

From Eq. (1), the nonlocal stress-strain relations are written as

$$(1 - \tau^2 l^2 \nabla^2)\sigma_{xx} = \frac{E}{1-\nu^2}(\epsilon_{xx} + \nu\epsilon_{\theta\theta}) \tag{3a}$$

$$(1 - \tau^2 l^2 \nabla^2)\sigma_{\theta\theta} = \frac{E}{1-\nu^2}(\epsilon_{\theta\theta} + \nu\epsilon_{xx}) \tag{3b}$$

$$(1 - \tau^2 l^2 \nabla^2)\sigma_{x\theta} = \frac{E}{1+\nu}\gamma_{x\theta} \tag{3c}$$

in which $\nabla^2 = (\partial^2/\partial x^2) + (1/R^2)(\partial^2/\partial\theta^2)$, and E, ν, are the elastic modulus and Poisson's ratio, respectively.

From Eqs. (2) and (3), one can, respectively, write the resultant forces

$$(1 - \tau^2 l^2 \nabla^2)N_x = K\left(u_{,x} + \frac{\nu}{R}v_{,\theta} - \nu\frac{w}{R}\right) \tag{4a}$$

$$(1 - \tau^2 l^2 \nabla^2)N_\theta = K\left(\nu u_{,x} + \frac{1}{R}v_{,\theta} - \frac{w}{R}\right) \tag{4b}$$

$$(1 - \tau^2 l^2 \nabla^2)N_{x\theta} = \frac{1-\nu}{2}K\left(\frac{1}{R}u_{,\theta} + v_{,x}\right) \tag{4c}$$

and resultant moments,

$$(1 - \tau^2 l^2 \nabla^2)M_x = D(\chi_x + \nu\chi_\theta) \tag{5a}$$

$$(1 - \tau^2 l^2 \nabla^2)M_\theta = D(\chi_\theta + \nu\chi_x) \tag{5b}$$

$$(1-\tau^2 l^2\nabla^2)M_{x\theta}=(1-\nu)D\chi_{x\theta} \tag{5c}$$

where h is the thickness of the nanotube, $K=Eh/(1-\nu^2)$, and $D=Eh^3/12(1-\nu^2)$.

The governing equations in terms of resultant forces and moments may read as follows:

$$RN_{x,x}+N_{\theta x,\theta}-\rho Rh\ddot{u}=0 \tag{6a}$$

$$N_{\theta,\theta}+RN_{\theta x,x}+Q_\theta-\rho Rh\ddot{v}=0 \tag{6b}$$

$$RQ_{x,x}+Q_{\theta,\theta}+N_\theta+Rp(x,\theta)-\rho Rh\ddot{w}=0 \tag{6c}$$

$$RM_{x,x}+M_{x\theta,\theta}-RQ_x=0 \tag{6d}$$

$$RM_{x\theta,x}-M_{\theta,\theta}+RQ_\theta=0 \tag{6e}$$

If the Donnell assumptions are adopted, then substitution of Eqs. (4) and (5) into Eq. (6) leads to the following nonlocal elastic shell model of a nanotube:

$$L_1(u,v,w)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{u} \tag{7a}$$

$$L_2(u,v,w)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{v} \tag{7b}$$

$$L_3(u,v,w)=(1-\tau^2 l^2\nabla^2)[\hat{\rho}\ddot{w}-p(x,\theta)/K] \tag{7c}$$

where, $k^2=h^2/12R^2$, $\hat{\rho}=\rho(1-\nu^2)/E$, and the operators $L_j(u,v,w)(j=1,2,3)$ are defined as

$$L_1(u,v,w)=u_{,xx}+\frac{1-\nu}{2R^2}u_{,\theta\theta}+\frac{1+\nu}{2R}v_{,x\theta}-\frac{\nu}{R}w_{,x} \tag{8a}$$

$$L_2(u,v,w)=\frac{1+\nu}{2R}u_{,x\theta}+\frac{1-\nu}{2}v_{,xx}+\frac{1}{R^2}v_{,\theta\theta}-\frac{1}{R^2}w_{,\theta} \tag{8b}$$

$$L_3(u,v,w)=\frac{\nu}{R}u_{,x}+\frac{1}{R^2}v_{,\theta}-\frac{1}{R^2}w-k^2R^2\nabla^4 w \tag{8c}$$

The set of governing Eqs. (7) and (8) forms the basis of the nonlocal elastic shell model for the study of the vibration behavior of nanotubes. It is worthy to mention that the applied loading $p(x,\theta)$ plays a very important role in the study of multiwalled nanotubes. This loading usually simulates the van der Waals interactions between two adjacent nanotubes. One may readily see that the effects of the internal characteristic parameter are included in this model as reflected by the terms in the right-hand side of Eqs. (7). When the parameter τ is zero, this model returns to the classical elastic shell model.

Applying Eq. (7) to each of the multiwalled nanotubes, we have for the first nanotube,

$$L_1(u_1,v_1,w_1)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{u}_1 \tag{9a}$$

$$L_2(u_1,v_1,w_1)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{v}_1 \tag{9b}$$

$$L_3(u_1,v_1,w_1)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{w}_1-(1-\tau^2 l^2\nabla^2)\frac{1}{K}p_{12}(x,\theta) \tag{9c}$$

and for the jth wall, $j=2,\ldots,(N-1)$,

$$L_1(u_j,v_j,w_j)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{u}_j \tag{9d}$$

$$L_2(u_j,v_j,w_j)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{v}_j \tag{9e}$$

$$L_3(u_j,v_j,w_j)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{w}_j-(1-\tau^2 l^2\nabla^2)\frac{1}{K}\left[p_{j(j+1)}(x,\theta)-\frac{R_{j-1}}{R_j}p_{(j-1)j}(x,\theta)\right] \tag{9f}$$

and for the Nth wall,

$$L_1(u_N,v_N,w_N)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{u}_N \tag{9g}$$

$$L_2(u_N,v_N,w_N)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{v}_N \tag{9h}$$

$$L_3(u_N,v_N,w_N)=(1-\tau^2 l^2\nabla^2)\hat{\rho}\ddot{w}_N-(1-\tau^2 l^2\nabla^2)\frac{1}{K}\left[p_N(x,\theta)-\frac{R_{N-1}}{R_N}p_{(N-1)N}(x,\theta)\right] \tag{9i}$$

where

$$p_{j(j+1)}(x,\theta)=c[w_{j+1}(x,\theta)-w_j(x,\theta)] \quad j=1,2,\ldots,(N-1) \tag{10a}$$

$$p_N(x,\theta)=-k_0 w_N(x,\theta) \tag{10b}$$

in which, $p_{j(j+1)}(x,s)$ is the interaction pressure exerted on the tube j from the tube $j+1$, while $p_{(j+1)j}(x,s)$ is the interaction pressure exerted on the tube $j+1$ from the tube j; they have the following relationship:

$$R_j p_{j(j+1)}(x,\theta)=-R_{j+1}p_{(j+1)j}(x,\theta) \quad j=1,2,\ldots,N-1; \tag{11}$$

and p_N is the interaction pressure between the outmost tube and the surrounding elastic medium; k_0 is the spring constant of the surrounding elastic medium; and c is the van der Waals interaction coefficient and can be estimated as [22]

$$c=\frac{200}{0.16\pi d^2}\ \text{erg/cm}^2 \quad d=0.142\ \text{nm} \tag{12}$$

where d is a parameter related to the C–C bond length. One may realize that here we are dealing with a linear dynamic problem, so the van der Waals interaction and interaction between the outer tube and elastic surrounding media can be estimated from a linear function of the deflection jump at two points, and the interactions in the tangential direction can be neglected, as discussed in Refs. [18,19]. But for a nonlinear dynamic behavior, the nonlinear higher order terms and effects from the tangential force should be included in these interaction expressions.

3 Double-Walled Carbon Nanotubes

Double-walled carbon nanotubes (DWCNTs) are considered in this section to demonstrate how the nonlocal model can be used to study the dynamics of multiwalled nanotubes. For the tubes, a solution must be periodic in θ $(=s/R)$. Therefore, we can set for $j=1,2$:

$$u_j(x,\theta,t)=\sum_n u_{jn}(x,t)\cos n\pi\theta \tag{13a}$$

$$v_j(x,\theta,t)=\sum_n v_{jn}(x,t)\sin n\pi\theta \tag{13b}$$

$$w_j(x,\theta,t)=\sum_n w_{jn}(x,t)\cos n\pi\theta \tag{13c}$$

Substitution of Eq. (13) into (9) yields the following differential equations with respect to the variables x and t, for $j=1,2$,

$$\tilde{L}_1(u_{jn},v_{jn},w_{jn})=\left[1+\tau^2 l^2\left(\frac{n\pi}{R_j}\right)^2\right]\hat{\rho}\ddot{u}_{jn}-\tau^2 l^2\hat{\rho}\ddot{u}''_{jn} \tag{14a}$$

$$\tilde{L}_2(u_{jn},v_{jn},w_{jn}) = \left[1+\tau^2 l^2\left(\frac{n\pi}{R_j}\right)^2\right]\hat{\rho}\ddot{v}_{jn} - \tau^2 l^2\hat{\rho}\ddot{v}''_{jn} \quad (14b)$$

$$\tilde{L}_3(u_{jn},v_{jn},w_{jn}) = \left[1+\tau^2 l^2\left(\frac{n\pi}{R_j}\right)^2\right]\hat{\rho}\ddot{w}_{jn} - \tau^2 l^2\hat{\rho}\ddot{w}''_{jn} + F_j(w_{1n},w_{2n}) \quad (14c)$$

where

$$F_1(w_{1n},w_{2n}) = \frac{c\tau^2 l^2}{K}(w''_{2n}-w''_{1n}) - \frac{c}{K}\left[1+\tau^2 l^2\left(\frac{n\pi}{R_1}\right)^2\right](w_{2n}-w_{1n}) \quad (14d)$$

$$F_2(w_{1n},w_{2n}) = \frac{\tau^2 l^2}{K}\left[k_0 w''_{2n} + c\frac{R_1}{R_2}(w''_{2n}-w''_{1n})\right] - \frac{1}{K}\left[1+\tau^2 l^2\left(\frac{n\pi}{R_2}\right)^2\right]\left[k_0 w_{2n} + c\frac{R_1}{R_2}(w_{2n}-w_{1n})\right] \quad (14e)$$

where, the superscript $'$ denotes differentiation with respect to the variable x and the operators $\tilde{L}_1$ $\tilde{L}_2$ and $\tilde{L}_3$ are defined as

$$\tilde{L}_1(u_{jn},v_{jn},w_{jn}) = u''_{jn} - \frac{1-\nu}{2}\left(\frac{n\pi}{R_j}\right)^2 u_{jn} + \frac{1+\nu}{2}\left(\frac{n\pi}{R_j}\right)v'_{jn} - \frac{\nu}{R_j}w'_{jn} \quad (15a)$$

$$\tilde{L}_2(u_{jn},v_{jn},w_{jn}) = -\frac{1+\nu}{2}\left(\frac{n\pi}{R_j}\right)u'_{jn} + \frac{1-\nu}{2}v''_{jn} - \left(\frac{n\pi}{R_j}\right)^2 v_{jn} + \frac{1}{R_{jn}}\left(\frac{n\pi}{R_j}\right)w_{jn} \quad (15b)$$

$$\tilde{L}_3(u_{jn},v_{jn},w_{jn}) = \frac{\nu}{R}u'_{jn} + \frac{1}{R_j}\left(\frac{n\pi}{R_j}\right)v_{jn} - k_j^2 R_j^2\left\{w''''_{jn} - 2\left(\frac{n\pi}{R_j}\right)^2 w''_{jn} + \left[\left(\frac{n\pi}{R_j}\right)^4 + \frac{1}{k_j^2 R_j^4}\right]w_{jn}\right\} \quad (15c)$$

3.1 Solution for Simply Supported Tow Ends. For a simple edge-supported DWCNT, the boundary conditions read

$$v = w = N_x = M_x = 0 \text{ at } x = 0 \text{ and } x = L \quad (16)$$

or, by using $(4)_1$ and $(5)_1$,

$$v = w = 0 \quad u_{,x} + \nu v_{,s} + \nu\frac{w}{R} = 0 \quad w_{,xx} + \nu w_{,ss} - \frac{\nu}{R}v_{,s} = 0 \text{ at } x = 0, L \quad (17)$$

A solution satisfying Eqs. (17) may be expressed as

$$u_{jn} = A_1^j \cos\lambda x \cos\omega t \; v_{jn} = A_2^j \sin\lambda x \cos\omega t \; w_{jn} = A_3^j \sin\lambda x \cos\omega t \; j = 1,2 \quad (18)$$

in which $\lambda = m\pi/L$.

By substituting Eqs. (18) into the set of Eqs. (14), we obtain a system of six algebraic equations for the unknown constants A_i^j $(i=1,2,3, j=1,2)$. For nontrivial values of A_i^j, the determinant of the algebraic equations must vanish, which leads to the following characteristic equation for a double-walled carbon nanotubes:

$$\det\begin{bmatrix} \beta_1\hat{\rho}\omega^2 - a_{11} & \frac{1+\nu}{2}n\pi\hat{\lambda}_1 & -\nu\hat{\lambda}_1 & 0 & 0 & 0 \\ \frac{1+\nu}{2}n\pi\hat{\lambda}_1 & \beta_1\hat{\rho}\omega^2 - a_{22} & n\pi & 0 & 0 & 0 \\ -\nu\hat{\lambda}_1 & n\pi & \beta_1\hat{\rho}\omega^2 - a_{33} & 0 & 0 & -\frac{c}{K}\beta_1 \\ 0 & 0 & 0 & \beta_2\hat{\rho}\omega^2 - a_{44} & \frac{1+\nu}{2}n\pi\hat{\lambda}_2 & -\nu\hat{\lambda}_2 \\ 0 & 0 & 0 & \frac{1+\nu}{2}n\pi\hat{\lambda}_2 & \beta_2\hat{\rho}\omega^2 - a_{55} & n\pi \\ 0 & 0 & -\frac{k_0 + cR_1/R_2}{K}\beta_2 & -\nu\hat{\lambda}_2 & n\pi & \beta_2\hat{\rho}\omega^2 - a_{66} \end{bmatrix} = 0 \quad (19)$$

where

$$\hat{\lambda}_i = m\pi\frac{R_i}{L} \quad \beta_i = R_i^2 + \tau^2 l^2[\hat{\lambda}_i^2 + (n\pi)^2] \quad i = 1,2 \quad (20a)$$

$$a_{11} = \hat{\lambda}_1^2 + \frac{1-\nu}{2}(n\pi)^2 \quad a_{22} = \frac{1-\nu}{2}\hat{\lambda}_1^2 + (n\pi)^2 \quad (20b)$$

$$a_{33} = 1 + k_1^2[\hat{\lambda}_1^2 + (n\pi)^2]^2 - \frac{c}{K}\beta_1 \quad a_{44} = \hat{\lambda}_2^2 + \frac{1-\nu}{2}(n\pi)^2 \quad (20c)$$

$$a_{55} = \frac{1-\nu}{2}\hat{\lambda}_2^2 + (n\pi)^2 \quad a_{66} = 1 + k_2^2[\hat{\lambda}_2^2 + (n\pi)^2]^2 - \frac{k_0 + cR_1/R2}{K}\beta_2 \quad (20d)$$

The characteristic equation for a multiwalled carbon nanotube $(N>2)$ can be formulated by employing an analogous procedure. As far as a single-walled carbon nanotube, the corresponding solution is presented in the Appendix.

It is evident that Eq. (19) represents a sixth order frequency equation for the unknown ω^2, and that it has six positive, real roots for a given DWCNT. Hence, each tube of the tow tubes of a DWCNT may vibrate in three different vibrational modes, namely, radial (or bending), longitudinal (or axial), or circumferential (or

Table 1 Comparison of frequencies for a DWCNT and the corresponding to each of the nanotubes SWCNT ω/ω_{10} ($m=n=1$; $L=10R_2$)

SWCNTs	1.0000000, 1.3358769, 2.2041474	0.9258549, 1.2368282, 2.0407208
	$R=0.35$ nm	$R=0.79$ nm
DWCNT	0.99834007, 1.3358729, 2.2040182	0.41628983, 1.243199, 2.0236288
	(inner tube $R_1=0.35$ nm)	(outer tube $R_2=0.79$ nm)

torsional). The two lowest eigenfrequencies may primarily relate to the radial motions of the inner and outer tube, respectively. Because of the van der Waals' interaction between the inner and outer tubes, one can expect that the values of the frequencies pertaining to each tube would be different than the ones corresponding to a single-walled carbon nanotube with the same geometric sizes and boundary conditions, as illustrated in Table 1. More details will be discussed in the next section.

4 Numerical Results and Discussions

Results of the resonant frequencies of carbon nanotubes (Fig. 1) are presented in this section. The influence of the internal characteristic parameter on the vibration of nanotubes is also demonstrated. Unless otherwise specified, the following properties of the carbon nanotubes are used: the length of a C–C bond is $a=1.42$ nm [18]; $E=742$ GPa, $\nu=0.17$ [9]; the density $\rho=2150$ kg/m^{-3} [2]; the radius of the inner carbon tube $R_1=R_1^o=0.35$ nm and the radius of the outer carbon tube $R_2=R_2^o=0.79$ nm, the thickness of each nanotube $h=0.495(R_2-R_1)$, the length of the nanotubes $L=10\times R_2$; the van der Waals interaction coefficient c can be obtained from Eq. (12); the spring constant from the surrounding elastic medium $k_0=0.01\times c$. Also in the following discussion, Ψ_{I} and Ψ_{VI} are defined, respectively, as the lowest and highest frequencies, normalized by the corresponding values with no consideration of the inner characteristic parameter a.

Listed in Table 1 are the natural frequencies of two SWCNTs and one MWCNT for both ends simply supported. Each of the SWCNT has three natural frequencies, the lowest one corresponding to radial vibration. There are six frequencies for the MWCNT, three for the inner tube vibration and the other three for the outer tube. All values in Table 1 are normalized with the lowest value, ω_{11} of the SWCNT with $R=0.35$ nm. Geometrically, the parameters of the inner tube of the MWCNT are exactly the same as these of the SWCNT with $R=0.35$ nm while those of the outer tube of the MWCNT correspond to a SWCNT with $R=0.79$ nm. But these two nanotubes in the MWCNT are coupled via the van der Waals' force. The coupling interaction definitely has an influence on the vibration of the MWCNT, as reflected in Table 1, the radial natural frequency of the outer tube of the MWCNT reduces 55%, from 0.9258549 to 0.41628983. One can also see that variations of natural frequencies corresponding to the axial and the circumferential vibration exist but not too much because the van der Waals interactions are proportional to the displacement differences in the radial direction. The lowest is usually of primary interest in vibration, therefore, it can be concluded that the van der Waals interaction has a significant influence on the vibration analysis of multiwalled carbon nanotubes. This observation would also suggest that if a model for the vibration of MWCNTs neglects, or inadequately handles the van de Waals interaction between two adjacent nanotubes, it would significantly compromise the accuracy in the predictions of MWCNT properties.

The variation of frequencies with the ratio L/R_2 is shown in Fig. 2 and can be used to justify the current nonlocal shell model for the study of nanodynamics. One can observe that when the ratio L/R_2 is larger than 10, the results of Ψ_{I} and Ψ_{VI} are convergent. This observation is in good agreement with the classical thin shell theory. Of course, for the study of a nanostructure with the geometric parameter $L/R_2<10$, the nonlocal thick shell theory may be needed, and can be derived by a procedure similar to the one employed in the current paper.

Figure 3 shows the results of the variation of frequencies with the ratio $h/(R_2-R_1)$, i.e., the ratio of thickness over the distance in radial direction between the two nanotubes. One can see that the value of Ψ_{VI}, corresponding to the axial frequency of the inner nanotubes is not affected by the varying value of $h/(R_2-R_1)$ and the radial frequency of the outer nanotube, Ψ_{I} does not change either when the ratio $h/(R_2-R_1)$ reaches a certain value such as 0.3 in the current example.

However, the results of the radial natural frequency Ψ_{I} exhibit

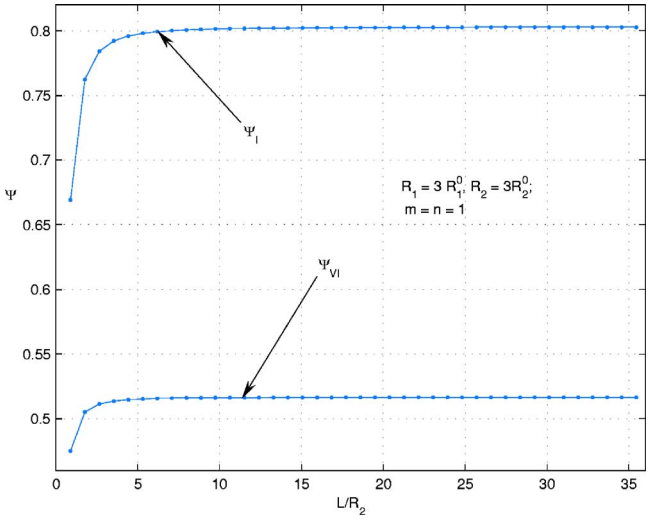

Fig. 2 Variation of frequencies with the aspect ratio, L/R_2

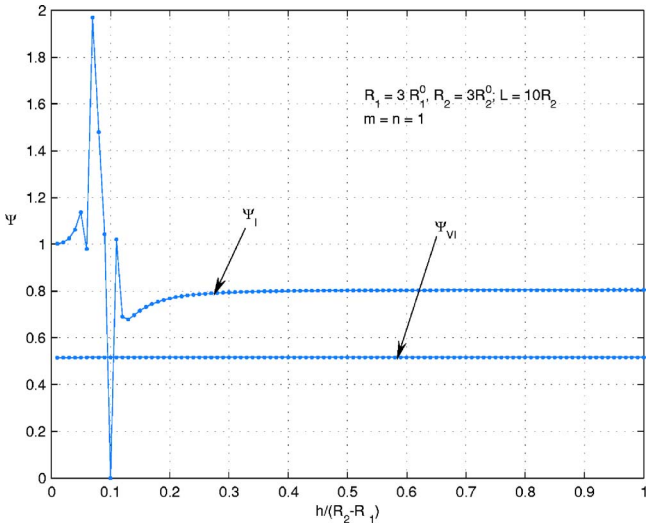

Fig. 3 Variation of frequencies with the ratio of thickness over distance between the nanotubes, $h/(R_2-R_1)$

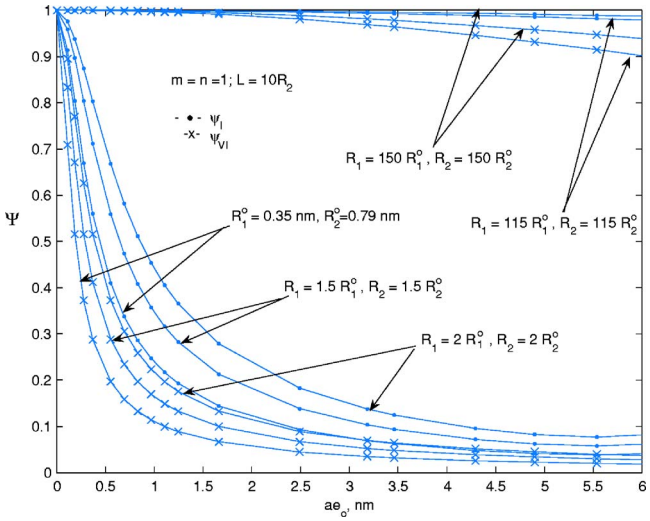

Fig. 4 The influence of the internal characteristic parameter, ae_o of the DWCNTs

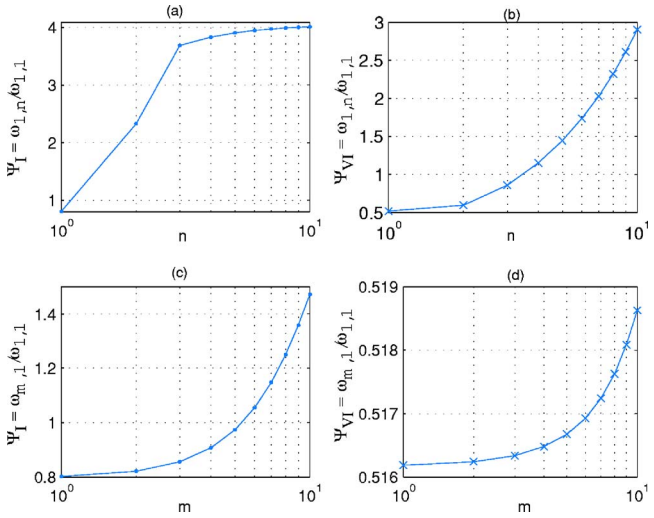

Fig. 5 The variation of the frequencies versus (m,n)

an oscillation for a value of the ratio $h/(R_2-R_1)$ of 0.1. One can further observe that at this point the scale of the nanotube thickness (around 1.3×10^{-11} m) falls into the range of molecular order. But beyond this point, the thickness of the tube enters into the range of nanoscale and the results are shown to be convergent. Therefore, this figure demonstrates that the current shell model would give a reasonable prediction in the study of nanotubes.

The curves in Fig. 4 are used to show the influences of the inner characteristic parameter a and the material constant e_0 on the natural frequencies of this simply edge-supported MWCNT. Two interesting phenomena can be observed in this figure. First, both the Ψ_I and the Ψ_{VI} decrease as the ae_0 increases. The increase of ae_0 means that the length of the C–C bond increases for a given nanomedium. Large values of the length of the C–C bond imply a big discontinuity. This observation suggests that a big error could be created by directly applying a classical continuum elastic model in nanostructures. Second, both the Ψ_I and the Ψ_{VI} increase as the geometric sizes of the MWCNT increase. Indeed, the Ψ_I and Ψ_{VI} almost reach 1 when the sizes of MWCNT reach a certain value, for example $R_1 \geqslant 0.5\times10^{-8}$ m, $R_2 \geqslant 1.2\times10^{-8}$ m, and $L \geqslant 1.2\times10^{-7}$ m, a range beyond the nanometer order (1×10^{-9} m$<L<1\times10^{-8}$ m [17]). This observation means that the classical continuum elastic model can give a good prediction if the geometric size of the nanotubes is large enough that the whole structure can be homogenized as a continuum. These two observations conclude that in the range of nanometer order 1×10^{-9} m$<L<1\times10^{-8}$ m, the inner characteristic parameter a, though small, has a significant effect on the natural frequencies predicted by the elastic model and cannot be ignored in the study of nanostructural behavior.

Presented in Fig. 5 are the variations of frequencies Ψ_I and Ψ_{VI} versus the modal numbers (m,n). Figures 5(a) and 5(b) are for the case of $m=1$ and varying n, while Figs. 5(c) and 5(d) are for $n=1$ and varying m. Here, the value of m refers to the axial modal number, and n to the circumferential modal number. One can see that the values of Ψ_I and Ψ_{VI} are more sensitive to n than to m. Since the beam model theory does not take the circumferential mode into account, this observation suggests that the beam model for the study of the dynamics of nanotubes may be inadequate and may not yield proper results.

Figure 6 shows the effects of the surrounding elastic medium on the frequencies of the MWCNTs. It can be seen that the values of Ψ_{VI} for each mode (for example for $n=1$, $m=1-5$) in the axial direction of vibration, almost do not vary with the variation of the elastic constant $\log[k_0/c]$ of the medium (Fig. 6(b)). But the values of Ψ_I corresponding to the basic radial vibration mode $(m=1,n=1)$ and higher modes in the axial direction such as $(m=2,\ldots,5,n=1)$ of the outer nanotube decrease as the value of $\log[k_0/c]$ increases, especially after $\log[k_0/c]\geqslant 1$ (Fig. 6(a)). This observation is in good agreement with the results obtained by a beam model simulation [19]. The elastic constant effects on the higher modes in the circumferential direction such as $n=2$ are shown in Fig. 7, in which a tendency similar to the one in Fig. 6 can also been found. The variation of frequencies for higher modes of $n\geqslant 2$ can only be predicted by the current shell model. Combining the results in Figs. 6 and 7, we can see that for each higher mode in the radial direction, such as $m=1$, $n=1$, 2, Ψ_I decreases while Ψ_{VI} does not change as the $\log[k_0/c]$ increases. It is obvious that the bigger the $\log[k_o/c]$ value, the stiffer the surrounding media. As a limiting case, if the surrounding elastic media is rigid, then no relative motions are possible for the outer nanotube. Therefore, the predictions of a decrease in Ψ_I in Figs. 6 and 7 are expected.

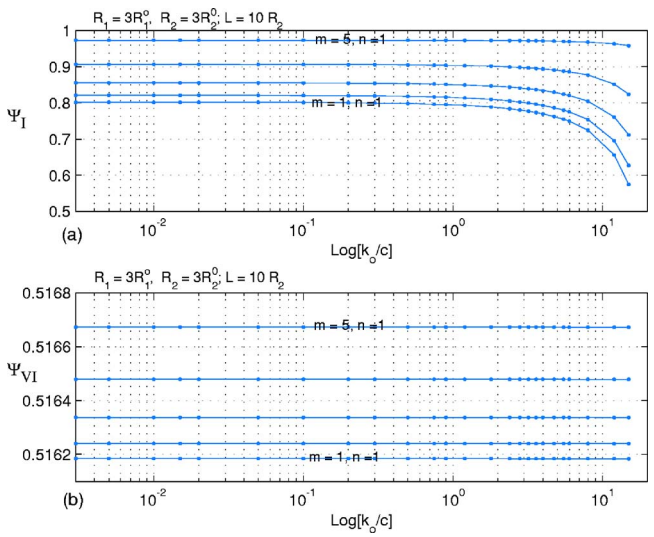

Fig. 6 The influence on the frequencies of the stiffness of the surrounding medium, k_0 versus $(m,n=1)$

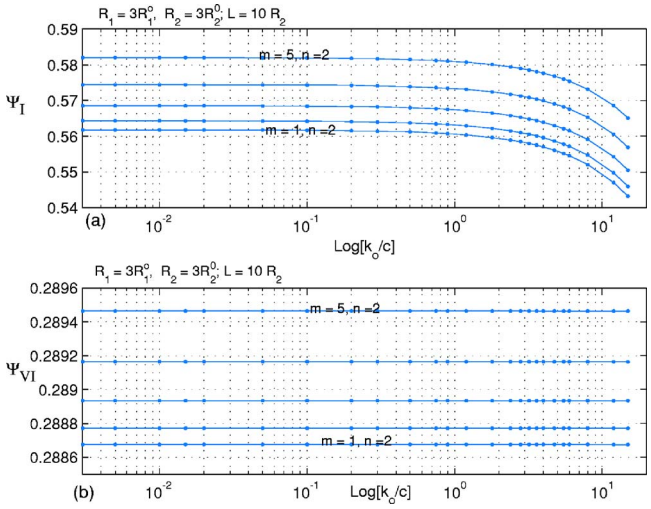

Fig. 7 The influence on the frequencies of the stiffness of the surrounding medium, k_0 versus $(m,n=2)$

5 Conclusions

In the present paper, the dynamic behavior of multiwalled carbon nanotubes embedded in elastic media is studied by a nonlocal shell model. In this model, small nanoscale parameters and the van de Waals' force between two adjacent nanotubes are included. A closed-form solution for the simply supported case is presented. The influences of the small internal parameters of the carbon nanotubes on the natural frequencies are investigated. The effects of the elastic constant of the surrounding medium are also addressed. Compared to a beam model, this shell model has the ability to capture the higher vibration modes in the radial direction. Moreover, the validation of this model is discussed. The observations in this study suggest the following specific conclusions: (1) The small internal parameters of the nanotubes have a significant influence on the natural frequencies of the MWCNTs when the structures are in the order of nanometers. These influences diminish as the geometric sizes of the structures increase. When the order of the geometric size of the structures is beyond the nanometer range, the influence from the small scale parameters could be neglected. (2) The van der Waals' interaction has a significant effect on the radial modal natural frequencies of the outer tubes of the MWCNT. Since this radial frequency is of primary interest in the vibration study of a structure, the van der Waals' force should not neglected in the study of nanodynamics. (3) When the relative stiffness, the ratio of the elastic modulus k_0 of the surrounding media and the van der Waals interaction coefficient c increases, the radial frequencies decrease significantly. This result can provide a guidance for the design of nanocomposites in order to obtain a desirable vibration behavior.

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Appendix: A Single-Walled Carbon Nanotube

The solution for the vibration of a single-walled carbon nanotube (SWCNT), simply supported at the ends, can be easily obtained from the results in Sec. 3. The external force considered is only the force from the surrounding elastic medium and it reads

$$p(x,\theta) = -k_0 w(x,\theta) \tag{A1}$$

Following a similar procedure as in Sec. 2, the governing equations can be written as

$$\tilde{L}_1(u_n,v_n,w_n) = \left[1+\tau^2 l^2\left(\frac{n\pi}{R}\right)^2\right]\hat{\rho}\ddot{u}_n - \tau^2 l^2 \hat{\rho}\ddot{u}_n'' \tag{A2a}$$

$$\tilde{L}_2(u_n,v_n,w_n) = \left[1+\tau^2 l^2\left(\frac{n\pi}{R}\right)^2\right]\hat{\rho}\ddot{v}_n - \tau^2 l^2 \hat{\rho}\ddot{v}_n'' \tag{A2b}$$

$$\tilde{L}_3(u_n,v_n,w_n) = \left[1+\tau^2 l^2\left(\frac{n\pi}{R}\right)^2\right]\hat{\rho}\ddot{w}_n - \tau^2 l^2 \hat{\rho}w_n'' + \frac{\tau^2 l^2}{K}k_0 w_n'' - \frac{1}{K}\left[1+\tau^2 l^2\left(\frac{n\pi}{R}\right)^2\right]k_0 w_n \tag{A2c}$$

The characteristic equation for natural frequencies of the SWCNT can be according derived as

$$\det\begin{bmatrix} \beta\hat{\rho}\omega^2 - a_1 & \frac{1+\nu}{2}n\pi\hat{\lambda} & -\nu\hat{\lambda} \\ \frac{1+\nu}{2}n\pi\hat{\lambda} & \beta\hat{\rho}\omega^2 - a_2 & n\pi \\ -\nu\hat{\lambda} & n\pi & \beta\hat{\rho}\omega^2 - a_3 \end{bmatrix} = 0 \tag{A3}$$

where

$$\hat{\lambda} = m\pi\frac{R}{L} \quad \beta = R^2 + \tau^2 l^2[\hat{\lambda}^2 + (n\pi)^2] \quad a_1 = \hat{\lambda}^2 + \frac{1-\nu}{2}(n\pi)^2 \tag{A4a}$$

$$a_2 = \frac{1-\nu}{2}\hat{\lambda}^2 + (n\pi)^2 \quad a_3 = 1 + k^2[\hat{\lambda}^2 + (n\pi)^2]^2 - \frac{k_0}{K}\beta \tag{A4b}$$

This model is the accurate solution for single-walled carbon nanotube reinforced composites.

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