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Nonlinear Vibration of Multi-walled Carbon Nanotubes

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***Abstract*—The nonlinear vibration behavior of a multi-walled carbon nanotube is investigated based on an elastic multi-layer shell model with van der Waals interaction taken into consideration. The multi-walled carbon nanotube is described as an individual elastic shell and the interlayer friction is negligible between the inner and outer tubes in the proposed model. And the Donnell equations of cylindrical shells are employed to describe the nonlinear behavior of the multi-walled carbon nanotubes. The van der Waals interaction between each layer of the nanotubes is simulated based on a new model. Numerical analyses are carried out to simulate several nonlinear vibration processes of different nanotubes. Following results show that the presence of van der Waals interaction forces can strongly influence the buckling and nonlinear vibration of the multi-walled carbon nanotubes.**

***Index Terms*—Carbon nanotubes; Nonlinear vibration; continuum shell model; van der Waals interaction.**

I. INTRODUCTION

Carbon nanotubes (CNTs) possess novel physical properties, such as high stiffness-to-weight and strength-to-weight ratios and excellent electrical and thermal conductivities make them a very promising material in nanoelectromechanical systems. A lot of methods have been employed to investigate the mechanical behavior of the CNTs during the past decades. Among those methods, elastic shell models are relatively simple and cost-effective as compared to experiments and molecular dynamic simulations. So they can offer simple general formulas in some important cases to identify major factors affecting mechanical behavior of CNTs and to explain or predict new physical phenomena. Elastic shell models have been effectively used to study mechanical deformation of CNTs [1, 2], especially buckling of CNTs under axial compression [3-5], bending [6, 4], radial pressure [7], or combined loadings [8]. The potential of using multi-walled carbon nanotubes (MWCNTs) in practical nanomechanical resonators provides the necessity for the simulation of their performance. Hence the vibration behavior of CNTs is of great interests from many scientists and engineering researchers. Noncoaxial vibration modes of MWCNTs, predicted based on a simple multiple beam model, have been confirmed by the molecular mechanics simulation. Moreover, the frequencies of CNTs for the radial breathing mode were obtained by using the multiple shell model and showed well agreement with the molecular dynamics (MD) simulation [9]. Thus, the effectiveness of dynamic simulation based on the multiple shell model was validated, and then many related investigations were performed. Yoon *et al.* [10] investigated the transverse sound wave propagation in CNTs by using Bernoulli-Euler theory of flexural beam, and the same work was also performed by Natsuki *et al.* [11] by using Flügge shell equations. Their results showed that the asymmetrical wave behavior of single- and double-walled CNTs was found to be significantly different. Further, Yoon *et al.* [12] reported the vibrational analysis of embedded MWCNTs by using the Bernoulli-Euler beam model. Their results showed that noncoaxial intertube resonance of CNTs was excited at higher natural frequency and would distort the otherwise concentric geometry of the MWCNTs. Li and Chou [13, 14] presented the vibrational analysis of single and double-walled CNTs using a truss rod model. They predicted that single-walled nanotubes (SWCNTs) could have fundamental frequency ranging from 10 GHz to 1.5 THz and the frequency depends on the diameter and length of CNTs [13]. The fundamental frequency of double-walled nanotubes (DWCNTs) was about 10% lower than that of SWCNTs with the same length and outer diameter [14]. In addition, Wang *et al.* investigated the free beamlike vibration of MWCNTs in which the applicability and limitations of simplified elastic shell equations was analyzed for various CNTs [15]. However, almost all of above vibration studies were limited to linear vibration behavior of CNTs, while the nonlinear one is seldom investigated. On the other hand, studies in [16-21] showed that the van der Waals (vdW) forces have a crucial effect on mechanical behavior of CNT ropes and MWCNTs. Thus, for the continuum shell model, the major challenge is to consider the vdW forces between adjacent tubes comparing to traditional continuum models [3-5]. Ru [4, 5] proposed a continuum shell model considering vdW interaction. He assumed that the variation of the vdW force was proportional to the normal deflection and obtained a simple relationship for the vdW interaction coefficient. Wang et al. [22] used the relationship to the buckling analysis of MWCNTs. However, as was pointed out by He et al. [23] in which they proposed a new vdW model not only for the interaction between adjacent tubes but also for the interaction between all the tubes, the simple relationship can only be applied to the analysis of DWCNTs because only the vdW interaction between two adjacent tubes is considered.

In this paper, a theoretical model for nonlinear vibration analysis of MWCNTs is developed based on the refined vdW

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interaction model [23] and the continuum elastic shell model. The influences of radius, length-radius ratio and vibration mode on the nonlinear vibration behavior are examined numerically. The key role played by the vdW interaction in such a nano-scale is also investigated. The results show that it can really change the vibration model of the MWCNTs.

II. GOVERNING EQUATIONS

In this section, a simply supported MWCNT is considered to be free of mechanical loads. The MWCNT consists of two or more single CNTs of radius R_i. Using Donnell's shallow-shell nonlinear theory, the governing equations of motion for large amplitude transverse vibrations of a circular cylindrical shell is given by [24]:

$$D\nabla^4\overline{w}_i + \rho\overline{w}_{i,tt} = p_i + \frac{N^0_{\theta i}}{R_i^2}\overline{w}_{i,\theta\theta} + \frac{1}{R_i}\bar{f}_{i,xx} + [\overline{w}_i, \bar{f}_i] \tag{1}$$

$$\frac{1}{Eh}\nabla^4 \bar{f}_i = -\frac{1}{2}[\overline{w}_i,\overline{w}_i] - \frac{1}{R_i}\overline{w}_{i,xx} \tag{2}$$

where

$$\nabla^4 = \left[\frac{\partial^2}{\partial x^2} + \frac{1}{R_i^2}\frac{\partial^2}{\partial\theta^2}\right]^2 \tag{3}$$

$$D = \frac{Eh^3}{12\left(1-v^2\right)} \tag{4}$$

$$\bar{f}_i = f_i - f_i^0 \tag{5}$$

$$[\overline{w}_i, \bar{f}_i] = \frac{1}{R_i^2}\left\{\overline{w}_{i,xx}\bar{f}_{i,\theta\theta} + \overline{w}_{i,\theta\theta}\bar{f}_{i,xx} - 2\overline{w}_{i,x\theta}\bar{f}_{i,x\theta}\right\} \tag{6}$$

$$[\overline{w}_i, \overline{w}_i] = \frac{2}{R_i^2}\left\{\overline{w}_{i,xx}\overline{w}_{i,\theta\theta} - \overline{w}_{i,x\theta}\overline{w}_{i,x\theta}\right\} \tag{7}$$

and the parameters for the vdW interaction are given by [23]:

$$p_i(x,\theta) = -\sum_{j=1}^{i-1}\overline{p}_{ij} + \sum_{j=i+1}^{N}\overline{p}_{ij} + \Delta p_i(x,\theta) \tag{8}$$

$$p_{ij} = \left[\frac{2048\varepsilon\sigma^{12}}{9a^4}\sum_{k=0}^{5}\frac{(-1)^k}{2k+1}\binom{5}{k}E_{ij}^{12} - \frac{1024\varepsilon\sigma^6}{9a^4}\sum_{k=0}^{2}\frac{(-1)^k}{2k+1}\binom{2}{k}E_{ij}^{6}\right]R_j \tag{9}$$

$$\Delta p_i = \overline{w}_i\sum_{j=1}^{N}c_{ij} - \sum_{j=1}^{N}c_{ij}\overline{w}_j \tag{10}$$

$$c_{ij} = -\left[\frac{1001\pi\varepsilon\sigma^{12}}{3a^4}E_{ij}^{13} - \frac{1120\pi\varepsilon\sigma^6}{9a^4}E_{ij}^{7}\right]R_j \tag{11}$$

$$E_{ij}^m = \left(R_i + R_j\right)^{-m}\int_0^{\pi/2}\frac{d\theta}{\left[1-K_{ij}\cos^2\theta\right]^{m/2}} \tag{12}$$

$$K_{ij} = \frac{4R_iR_j}{\left(R_i+R_j\right)^2} \tag{13}$$

where x and θ are axial and circumferential angular coordinates, respectively, $\overline{w}$ is the radial (inward) deflection, p_i is the net normal (inward) pressure due to the vdW interaction, $N^0_{\theta i}$ is the known uniform membrane forces (called "pre-stresses"), ρh is the mass density (per unit lateral area), D and h are the effective bending stiffness and thickness of the shell, and E is Young's modulus. And f_i^0 denotes the initial pre-stresses functions of the i^{th} tube to account for the vdW interaction and can be written as

$$f_i^0 = \frac{1}{2h}x^2N^0_{\theta i} = -\frac{1}{2h}x^2R_i\left(-\sum_{j=1}^{i-1}\overline{p}_{ij} + \sum_{j=i+1}^{N}\overline{p}_{ij}\right) \tag{14}$$

The subscripts $i,\ j = 1$ to N denote the i^{th} and j^{th} tubes of the MWCNT.

III. VIBRATION FREQUENCIES AND MODES

The vibration mode of i^{th} tube can be assumed as

$$\overline{w}_i = A_i(t)\cos(n\theta)\sin\left(\frac{m\pi x}{L}\right) + \frac{n^2}{4R_i}A_i^2(t)\sin^2\left(\frac{m\pi x}{L}\right) \tag{15}$$

which has been shown to give qualitative agreement with nonlinear vibration experiments and can be used for the nonlinear analysis, where m and n denote the number of axial and circumferential waves, respectively. Substituting Eq (15) into the governing equations and solving for the particular solution, we have

$$\begin{aligned}\bar{f}_i &= a_1A_i\cos n\theta\sin\beta_m x - a_2A_i^2\cos 2n\theta \\ &\quad - a_3A_i^3\cos n\theta\sin\beta_m x + a_4A_i^3\cos n\theta\sin 3\beta_m x\end{aligned} \tag{16}$$

where

$$\beta_m = \frac{m\pi}{L},\quad \beta_i = \frac{n}{R_i},\quad a_1 = \frac{\beta_m^2Eh}{R_i(\beta_m^2+\beta_i^2)^2},$$

$$a_2 = \frac{Eh\beta_m^2}{32\beta_i^2},\quad a_3 = \frac{\beta_m^2\beta_i^4R_iEh}{4\left(\beta_m^2+\beta_i^2\right)^2},\quad a_4 = \frac{\beta_m^2\beta_i^4R_iEh}{4\left(9\beta_m^2+\beta_i^2\right)^2}$$

and the force per unit length in the axial direction is given by

$$\overline{N}_{xi} = \frac{1}{R_i^2}\bar{f}_{i,\theta\theta} = -\frac{Eh}{8}\beta_m^2A_i^2\cos 2n\theta \ \text{ at } x=0 \text{ and } x=L \tag{17}$$

which means that the response modes of the dynamic state do not satisfy the classical simply supported boundary conditions ($\overline{N}_{xi}$ =0) exactly. The inaccuracy due to the violation of the boundary conditions is expected to be small for sufficiently long shells, since its effect is confined to a small edge zone. Although it does not satisfy the boundary conditions locally, it satisfies globally since

$$\int_0^{2\pi}\cos 2n\theta d\theta = 0 \quad \text{on each edge} \tag{18}$$

The unknown time-dependent function A_i can be determined by using Galerkin's method. By projecting the left-hand side of Eq (1), where Eqs (15) and (16) are used for expressing $\bar{f}_i$ and $\overline{w}_i$ in terms of A_i, and equating the result to zero, we have

$$\int_0^L\int_0^{2\pi}X\cdot Z_s(x,\theta)d\theta dx = 0 \tag{19}$$

where

$$X = D\nabla^4\overline{w}_i + \rho h\overline{w}_{i,tt} - p_i - \frac{N^0_{\theta i}}{R_i^2}\overline{w}_{i,\theta\theta} - \frac{1}{R_i}\bar{f}_{i,xx} - [\overline{w}_i, \bar{f}_i] \tag{20}$$

$$Z_s(x,\theta) = \frac{\partial w}{\partial A_i} = \cos(n\theta)\sin(\beta_m x) + \frac{n^2}{4R_i}A_i\sin^2(\beta_m x) \tag{21}$$

This yields following non-linear ordinary differential equations for unknown functions $A_i(t)$. In the nondimensional form, they are

$$\frac{d^2\zeta_i}{dt^2}+\Omega_i^2\zeta_i+\frac{3\varepsilon_i}{8}\left[\zeta_i^2\frac{d^2\zeta_i}{dt^2}+\zeta_i\left(\frac{d\zeta_i}{dt}\right)^2\right]-\varepsilon_i\gamma_i\zeta_i^3+\varepsilon_i^2\delta_i\zeta_i^5=C_i(t) \tag{22}$$

where ζ_i are vibration amplitudes defined by

$$\zeta_i=\frac{A_i}{h} \tag{23}$$

and Ω_i is the linear vibration frequency without the vdW interaction which is written as

$$\Omega_i^2=\frac{E}{\rho R_i^2}\left[\frac{\varepsilon_i\left(\xi_i^2+1\right)^2}{12(1-v^2)}+\frac{\xi_i^4}{\left(\xi_i^2+1\right)^2}+n^2\overline{N}_{\theta i}^0\right] \tag{24}$$

here

$$\overline{N}_{\theta i}^0=-\frac{\left(-\sum_{j=1}^{i-1}\overline{p}_{ij}+\sum_{j=i+1}^{N}\overline{p}_{ij}\right)R_i}{Eh} \tag{25}$$

The function $C(\tau)$ represents the generalized forces on the mode and can be written as

$$\begin{aligned}C_i(t)&=\frac{2}{\pi\rho Lh^2}\int_0^L\int_0^{2\pi}\Delta p_i\cos n\theta\sin\beta_m x\,d\theta\,dx\\&=\frac{1}{\rho h}\zeta_i\sum_{j=1}^{N}c_{ij}-\frac{1}{\rho h}\sum_{j=1}^{N}c_{ij}\zeta_j\end{aligned} \tag{26}$$

And the parameter $\varepsilon_i=\left(n^2h/R_i\right)^2$ is the basic nonlinear parameter in the problem and goes to zero when the vibrations become linear. The other parameters which influence the nonlinearities are γ_i and δ_i which are defined by

$$\gamma_i=\frac{E\xi_i^4}{\rho R_i^2}\left[\frac{1}{\left(\xi_i^2+1\right)^2}-\frac{\varepsilon_i}{12(1-v^2)}-\frac{1}{16}\right] \tag{27}$$

$$\delta_i=\frac{3E\xi_i^4}{16\rho R_i^2}\left[\frac{1}{\left(\xi_i^2+1\right)^2}+\frac{1}{\left(9\xi_i^2+1\right)^2}\right] \tag{28}$$

where ξ_i is the aspect ratio, given by

$$\xi_i=\frac{\beta_m}{\beta_i} \tag{29}$$

Eqs (22) can be solved approximately by the method of averaging [25]. Substituting Eqs (26) into (22) yields

$$\begin{aligned}&\frac{d^2\zeta_i}{dt^2}+\left(\Omega_i^2-\frac{1}{\rho h}\sum_{j=1}^{N}c_{ij}\right)\zeta_i+\frac{3\varepsilon_i}{8}\left[\zeta_i^2\frac{d^2\zeta_i}{dt^2}+\zeta_i\left(\frac{d\zeta_i}{dt}\right)^2\right]\\&\qquad-\varepsilon_i\gamma_i\zeta_i^3+\varepsilon_i^2\delta_i\zeta_i^5+\frac{1}{\rho h}\sum_{j=1}^{N}c_{ij}\zeta_j=0\end{aligned} \tag{30}$$

then applying the method of averaging leads to the approximate solution:

$$\zeta_i(t)=\overline{W_i}\cos\omega t \tag{31}$$

where the average amplitude $\overline{W_i}$ is computed from

$$\begin{aligned}&\left(\Omega_i^2-\frac{1}{\rho h}\sum_{j=1}^{N}c_{ij}-\omega^2\right)\overline{W_i}-\frac{3\varepsilon_i}{16}\omega^2\overline{W_i}^3\\&\qquad-\frac{3\varepsilon_i\gamma_i}{4}\overline{W_i}^3+\frac{5}{8}\varepsilon_i^2\delta_i\overline{W_i}^5+\frac{1}{\rho h}\sum_{j=1}^{N}c_{ij}\overline{W_j}=0\end{aligned} \tag{32}$$

The amplitude-frequency relation for free vibrations of a single mode can be written as

$$\omega^2=\frac{\left(\Omega_i^2-\frac{1}{\rho h}\sum_{j=1}^{N}c_{ij}\right)\overline{W_i}-\frac{3\varepsilon_i\gamma_i}{4}\overline{W_i}^3+\frac{5}{8}\varepsilon_i^2\delta_i\overline{W_i}^5+\frac{1}{\rho h}\sum_{j=1}^{N}c_{ij}\overline{W_j}}{\overline{W_i}+\frac{3\varepsilon_i}{16}\omega^2\overline{W_i}^3} \tag{33}$$

IV. NUMERICAL RESULTS AND DISCUSSIONS

The CNT to be considered has the thickness of graphene sheet of 0.34 nm, bending stiffness of D = 2 eV, elastic modulus of 1.059 TPa and Poisson's ratio of 0.19. The mass density of CNTs is assumed to be 1.3 g/cm^3. The vdW parameters used in the Lennard-Jones potential are taken as ε = 2.967 meV, σ = 0.34 nm [26], the in-plane stiffness is Eh = C = 360 J/m^2 as presented in [3].

What follows is to analyze nonlinear vibration behavior of a DWCNT subjected to axial compressed pressure. The influences of radii, the number of tubes, the length and the wave numbers on the nonlinear vibration pattern are examined and the results are shown as follows.

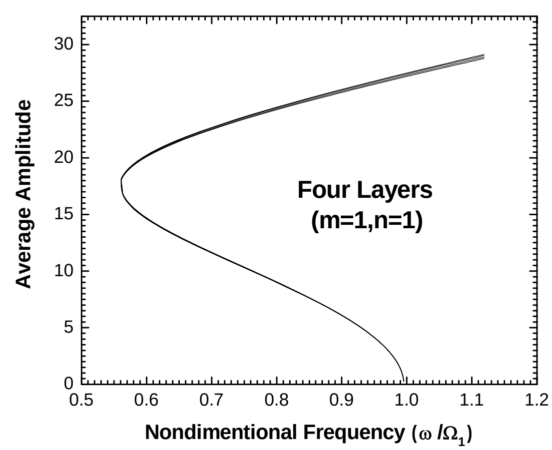

Fig. 1 Free vibrations of a four-layer carbon nanotube

Fig. 1 shows the free vibration response of a four-walled CNT. For the sake of simplicity, the nondimentional vibration frequency ω/Ω_1 is employed in which Ω_1 denotes linear free vibration frequency of innermost tube. The results indicate that all the four tubes of CNT vibrate in the same pattern. And little difference can be discriminated in their nonlinear vibration behaviors. This similarity is induced by the influence of the vdW interaction between any two tubes. If one tube vibrates, the existence of the vdW interaction will generate forces to resist the relative movement between tubes and keep the space of them unchanged, which results in the companion vibration of the other tubes due to the driven force generated from the vdW interaction. So the amplitude and the frequency of all the tubes are similar to each other. Then in the following analysis of this section, only the vibration behavior of innermost tube is shown due to this similarity.

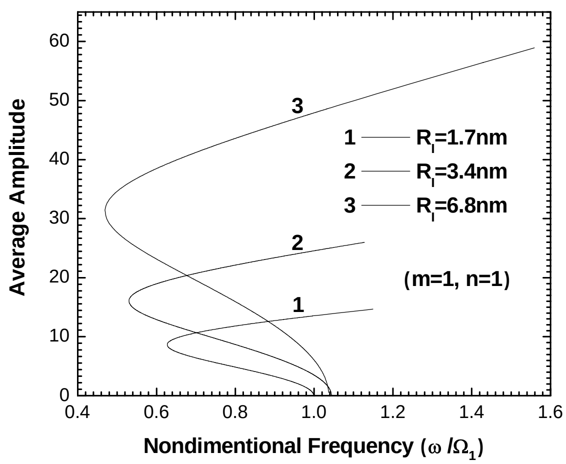

Fig. 2 Influence of large amplitudes on vibration frequency for several two-walled carbon nanotubes with different radii and the length-radius ratio L/R_O =10.

The free vibration response curves of DWCNTs shown in Fig. 2-5 illustrate a nonlinearity of the softening type. This behavior is typical for a vibration mode that involves low values of ε and ξ. For larger values of ε, the nonlinearity is stronger and for some values of ξ the nonlinearity is of the hardening type.

The manner in which the parameter ε controls the strength of the nonlinearity is shown in Figs. 2 and 5. An increase in the value of ε will increase the nonlinearity of vibration. This result is apparent from Eqs (30) and (32), which show that ε is a multiplying factor in every nonlinear term. From a physical viewpoint, small values of ε correspond to CNTs with bigger radii and/or a small number of circumferential waves, whereas large ε signifies CNTs with smaller radii or a high number of circumferential waves. Another important parameter is the aspect ratio ξ, which governs the character of nonlinearity. The way in which the type of nonlinearity varies with the aspect ratio is shown in Figs. 3-5. Actually, the parameters ε, γ and δ in Eqs (30) and (32) can be used to predict the type of nonlinearity which may occur; but both γ and δ are closely related to ξ. Small values of ξ result in small values γ and δ, and the corresponding terms in Eq (32) are relatively insignificant for small vibration amplitudes. In this case, the vibrations exhibit a softening nonlinearity for small vibration amplitudes. As the amplitude continues to increase, however, the term $\varepsilon^2\delta\overline{A}^5$ in Eq (32) finally dominates the other terms and causes an eventual hardening nonlinearity. And note that from its definition, small values of the aspect ratio ξ correspond to short circumferential and long axial wavelengths, whereas the reverse is true for large values of ξ.

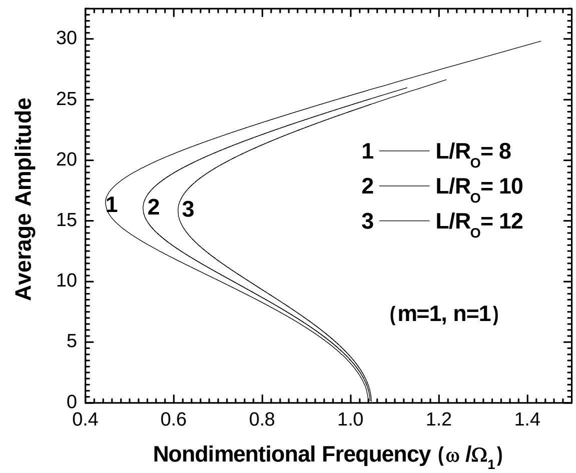

Fig. 3 Influence of large amplitudes on vibration frequency for several two-walled carbon nanotubes with different length-radius ratios and R_I =3.4nm

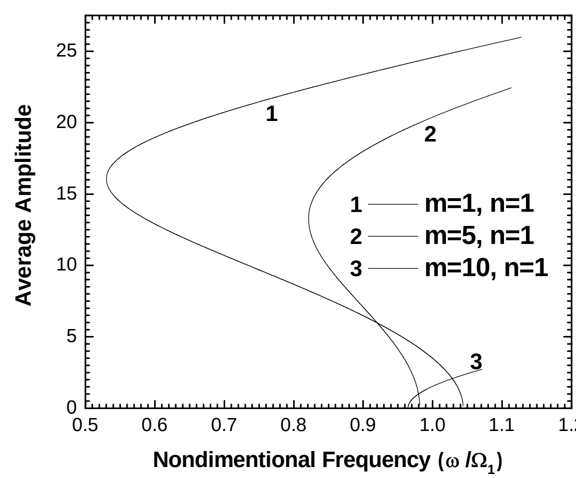

Fig. 4 Influence of large amplitudes on vibration frequency for several two-walled carbon nanotubes with different axial wave numbers and L/R_O =10, R_I =3.4nm.

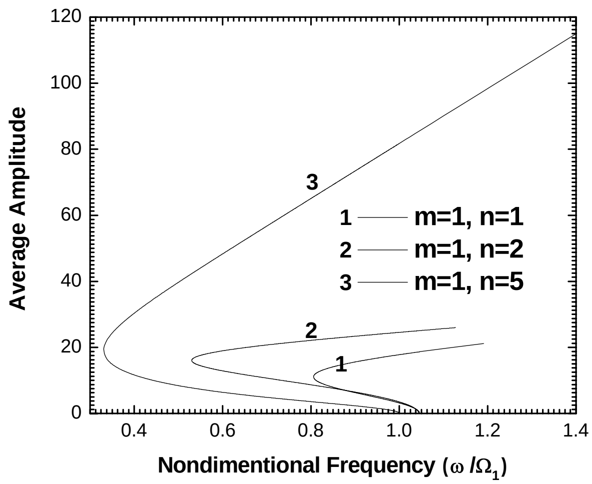

Fig. 5 Influence of large amplitudes on vibration frequency for several two-walled carbon nanotubes with different circumferential wave numbers and L/R_O =10, R_I =3.4nm.

Fig.6 shows the nonlinear vibration behavior of single-, double- and triple-walled CNTs. The results indicate that the increase of the number of the walls results in a less nonlinear vibration response. Due to the influence of the vdW interaction, all the walls of the CNT vibrate as a whole. Then the frequency can be approximated by the properties of the middle tube only. As the number of tubes increases, the effective radius of the MWCNT becomes bigger too, and thus the nonlinearity of its vibration decreases. Also, it can be seen that as the number of tubes increases, the free vibration frequency of the innermost tube increase as well. This results in the increase of the vdW forces. And the influence of vdW interaction on the vibration frequency can also be seen from the above results. Almost all the frequencies are different with the natural free vibration without the vdW interaction.

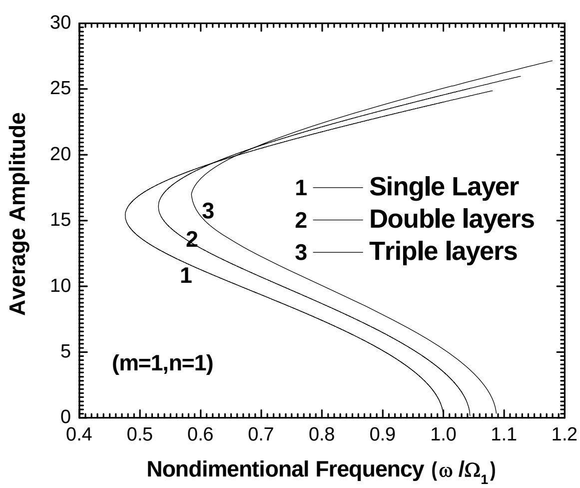

Fig. 6 Influence of amplitudes on frequency for several multi-walled carbon nanotubes with L/R_O = 10, R_I = 3.4nm.

V. CONCLUSION

Explicit formulas have been derived for predicting the nonlinear vibration behavior of MWCNTs under axial compression combining the continuum shell model and a refined vdW interaction model. Based on the proposed formulas, the nonlinear vibration behavior of a MWCNT, in which each tube is treated as an individual cylindrical shell, was analyzed numerically. The influences of radii, the number of tubes, the length and the wave numbers on the nonlinear vibration pattern are also examined. Their effects on the nonlinear vibration behavior are discussed in above sections. Then the influence of the vdW interaction between tubes on the nonlinear vibration behavior is investigated in detail. The results show that the vdW interaction plays a critical role in nano-scale mechanics. It can change the nonlinear vibration mode of the inner tubes by forcing them vibrate with a similar pattern as the outer ones. At the same time it can also influence the vibration frequency of the MWCNTs.

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