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Bending instability of an embedded double-walled carbon nanotube based on Winkler and van der Waals models

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Abstract

The present paper examines the instability of a double-walled carbon nanotube embedded in an elastic medium under pure bending. Effect of surrounding elastic medium and van der Waals forces between the inner and outer nanotubes is taken into consideration. From the point of view of continuum modeling, an elastic double-shell model is presented for the pure bending buckling of a double-walled carbon nanotube. Based on this model, a condition is derived in terms of the buckling modes of the shell, from which the critical bending moment can be predicted. The paper emphasizes bifurcation instability. It is shown that buckling may occur. Finally, a simplified analysis is carried out to estimate the moment causing bifurcation instability of the double-walled carbon nanotube.

Keywords: A. Nanotube; B. Buckling; C. Winkler model; van der Waals force

1. Introduction

The discovery of carbon nanotubes has stimulated, extensively, experimental and theoretical studies [1,2]. Numerous studies showed that carbon nanotubes have excellent mechanical and electronic properties. Their potential applications led to many investigations into measurements of mechanical properties of nanotubes, using techniques such as transmission electron microscopy (TEM) and atomic force microscopy (AFM) [3].

Recently, large strain deformation of single- or multi-walled carbon nanotubes involving compression, bending or/and torsion has been the subject of numerous experiments and molecular dynamic simulations [4–7]. Basically, there are two theoretical approaches to understanding the behavior of carbon nanotubes: atomistic molecular-dynamics simulations and continuum mechanics. Yakobson et al. [4] introduced an atomistic model for axially compressed buckling of single-walled nanotubes and also compared it with a simple continuum shell model. They found that the continuum shell model could predict all changes of buckling patterns in the atomistic molecular-dynamics simulations. However, the existing continuum shell model can not directly be applied to investigate mechanical behavior of multi-walled nanotubes due to the presence of the van der Waals forces in multi-walled nanotubes [8–11].

More recently, considerable attention has been turned to mechanical behavior of single- or multi-walled carbon nanotubes embedded in a polymer or metal matrix [12–14]. Ru [15] presented an elastic double-shell model for infinitesimal buckling of a double-walled carbon nanotube embedded in an elastic medium under axial compression. His analysis was based on a Winkler

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model for the surrounding elastic medium and a simplified model for the van der Waals interaction between the inner and outer nanotubes. He also studied the effect of van der Waals forces on axial buckling of a double-walled carbon nanotube and derived a simple formula for the critical axial strain, which indicated the role of the van der Waals forces between the inner and outer nanotubes [16].

Motivated by these ideas, the present paper examines the instability of a double-walled carbon nanotube embedded in an elastic medium under pure bending. The effect of surrounding elastic medium and van der Waals forces between the inner and outer nanotubes is taken into consideration. From the point of view of continuum modeling, an elastic double-shell model is presented for the pure bending buckling of a double-walled carbon nanotube. Based on these models, a condition is derived in terms of the buckling modes of the shell and the critical bending moment can be predicted. The paper emphasizes on bifurcation instability. It is shown that buckling may occur. Finally, the simplified analysis approach is also employed to estimate the moment causing bifurcation instability of the double-walled carbon nanotube.

2. The elastic shell model

Consider a circular cylindrical shell with a middle radius r, thickness t. Mechanical properties are denoted by Young's modulus E and Poisson's ratio μ. The linear Donnell's equilibrium equation in the normal direction can be given in terms of $W(x,y)$, as follows:

$$D\nabla^4 W - \frac{1}{r}N_y = N_x\frac{\partial^2 W}{\partial x^2} + 2N_{xy}\frac{\partial^2 W}{\partial x\partial y} + N_y\frac{\partial^2 W}{\partial y^2} + q, \tag{1}$$

where D is the effective bending stiffness of the shell, x and y denote the axial and circumferential coordinates of the shell, respectively. $W(x,y)$ is the radial displacement of the middle surface of the shell in the normal direction. q is the resultant inward normal pressure and (N_x, N_y, N_{xy}) denote the membrane forces.

For the post-buckling configuration, we have

$$\begin{aligned} N_x &= N_{x0} + N_{x1},\\ N_y &= N_{y0} + N_{y1},\\ N_{xy} &= N_{xy0} + N_{xy1}, \end{aligned} \tag{2}$$

$$\begin{aligned} W(x,y) &= W_0(x,y) + W_1(x,y),\\ q(x,y) &= P_0(x,y) + P(x,y), \end{aligned} \tag{3}$$

where subscript "0" pertains to the pre-buckling status, and subscript "1" means infinitesimal increments of the corresponding parameters during buckling. In Eq. (3), $P_0(x,y)$ is the normal pressure prior to buckling and $P(x,y)$ denotes the additional normal pressure after buckling.

For the pre-buckling status, the following Donnell's equation is true:

$$D\nabla^4 W_0 - \frac{1}{r}N_{y0} = N_{x0}\frac{\partial^2 W_0}{\partial x^2} + 2N_{xy0}\frac{\partial^2 W_0}{\partial x\partial y} + N_{y0}\frac{\partial^2 W_0}{\partial y^2} + P_0. \tag{4}$$

After buckling, the Donnell's equation is changed into the following form:

$$D\nabla^4 W - \frac{1}{r}N_y = N_x\frac{\partial^2 W}{\partial x^2} + 2N_{xy}\frac{\partial^2 W}{\partial x\partial y} + N_y\frac{\partial^2 W}{\partial y^2} + P_0 + P. \tag{5}$$

Combining Eqs. (4) and (5), the buckling displacement is found as

$$D\nabla^4 W_1 - \frac{1}{r}N_{y1} - \left[N_{x0}\frac{\partial^2 W_1}{\partial x^2} + 2N_{xy0}\frac{\partial^2 W_1}{\partial x\partial y} + N_{y0}\frac{\partial^2 W_1}{\partial y^2}\right] = P. \tag{6}$$

According to the shell theory, a stress function $\varphi(x,y)$ is introduced to define the membrane forces:

$$N_{x1} = \frac{\partial^2\varphi}{\partial y^2}, \quad N_{xy1} = -\frac{\partial^2\varphi}{\partial x\partial y}, \quad N_{y1} = \frac{\partial^2\varphi}{\partial x^2}, \tag{7}$$

where the stress function $\varphi(x,y)$ has to meet the compatibility condition

$$\nabla^4\varphi = -\frac{Et}{r}\frac{\partial^2 W_1}{\partial x^2}. \tag{8}$$

For simplifications, let $W_1(x,y)$ be replaced with $w(x,y)$. The buckling governing equation and the compatibility condition are re-written in the following form:

$$\begin{aligned} &D\nabla^4 w - \frac{1}{r}\frac{\partial^2\varphi}{\partial x^2} - \left[N_{x0}\frac{\partial^2 w}{\partial x^2} + 2N_{xy0}\frac{\partial^2 w}{\partial x\partial y} + N_{y0}\frac{\partial^2 w}{\partial y^2}\right]\\ &\quad = P(x,y), \end{aligned} \tag{9}$$

$$\nabla^4\varphi = -\frac{Et}{r}\frac{\partial^2 w}{\partial x^2}. \tag{10}$$

Using Eq. (10) to eliminate the stress function $\varphi(x,y)$ in Eq. (9), one obtains a single equation for the additional displacement due to buckling $w(x,y)$, which is called the buckling modes.

$$\begin{aligned} &D\nabla^8 w + \frac{Et}{r^2}\frac{\partial^4 w}{\partial x^4} - \nabla^4\left[N_{x0}\frac{\partial^2 w}{\partial x^2} + 2N_{xy0}\frac{\partial^2 w}{\partial x\partial y} + N_{y0}\frac{\partial^2 w}{\partial y^2}\right]\\ &\quad = \nabla^4 P(x,y). \end{aligned} \tag{11}$$

The above equation can be applied to buckling analysis under axial compression, bending, torsion or radial compression for cylindrical shells embedded within an infinite elastic medium. Although some studies found that elastic properties of carbon nanotubes may depend on their geometry, in what follows, it is assumed that the inner and outer nanotubes have the same thickness and effective material constants.

3. The van der Waals force between the inner and outer nanotubes

The van der Waals force between any two carbon atoms can be described by the Lennard-Jones model. Using the method described previously [16–18], the van der Waals force exerted on any atom on a tube can be estimated by adding up all forces between the atom and all atoms on the other tube.

Fig. 1 shows a double-walled nanotube embedded in an elastic medium. In what follows, the subscripts 1 and 2 denote the quantities associated with the outer tube 1 and the inner tube 2, respectively. The outer tube 1 is embedded in the elastic medium.

For the outer tube 1, the normal pressure P_1 consists of two parts, it can be described as follows:

$$P_1 = P_1^V + P_1^W, \tag{12}$$

where P_1^V is the van der Waals force between the inner and outer tubes, P_1^W denotes the interaction pressure due to the elastic medium. In particular, for the inner tube 2, the normal pressure P_2 is

$$P_2 = P_2^V. \tag{13}$$

Furthermore, because the interaction forces between the inner and outer tubes are equal and opposite, the pressure P_1^V and P_2^V, exerted on the corresponding points on the tubes 1 and 2, respectively, should be related by

$$P_1^V(x,y)r_1 = -P_2^V(x,y)r_2, \tag{14}$$

where r_1 and r_2 are the radii of the outer and inner tubes, respectively. The pressure caused by the van der Waals forces at any point (x, y) on the outer tube could be assumed to be a function of the distance between the inner and outer tubes at that point, denoted by $\delta(x, y)$, namely

$$P_1^V(x,y) = G[\delta(x,y)], \tag{15}$$

where $G(\delta)$ is a nonlinear function of the intertube spacing δ, the details of which can be found in [16,15]. In the pre-buckling situation, $\delta(x, y)\equiv\delta_0$, Eq. (15) becomes

$$P_{10}^V(x,y) = G(\delta_0), \tag{16}$$

where $P_{10}^V(x,y)$ is the van der Waals force of the outer tube prior to buckling, defined as the value of G at the initial interlayer spacing δ_0 between the inner and outer tubes. After buckling, the pressure caused by the van der Waals forces at any point (x, y) on the outer tube in the present linearized analysis becomes

$$P_1^V(x,y) = P_{10}^V + c[w_2(x,y) - w_1(x,y)], \tag{17}$$

where c is a constant, which is defined as

$$c = \left.\frac{\mathrm{d}G}{\mathrm{d}\delta}\right|_{\delta=\delta_0}. \tag{18}$$

Using Eq. (14), the pressure caused by the van der Waals forces at any point (x, y) on the inner tube 2 after buckling can be found as

$$P_2^V(x,y) = -\frac{r_1}{r_2}\left\{P_{10}^V + c[w_2(x,y) - w_1(x,y)]\right\}. \tag{19}$$

The interaction pressure due to the elastic medium, P_1^W, can be given in the following form:

$$P_1^W = P_{10}^W - dw_1(x,y) \quad \text{after buckling } (d > 0), \tag{20}$$

where d is the spring constant of Winkler-type, which is determined by the material properties of the elastic medium and the radius of the outer tube.

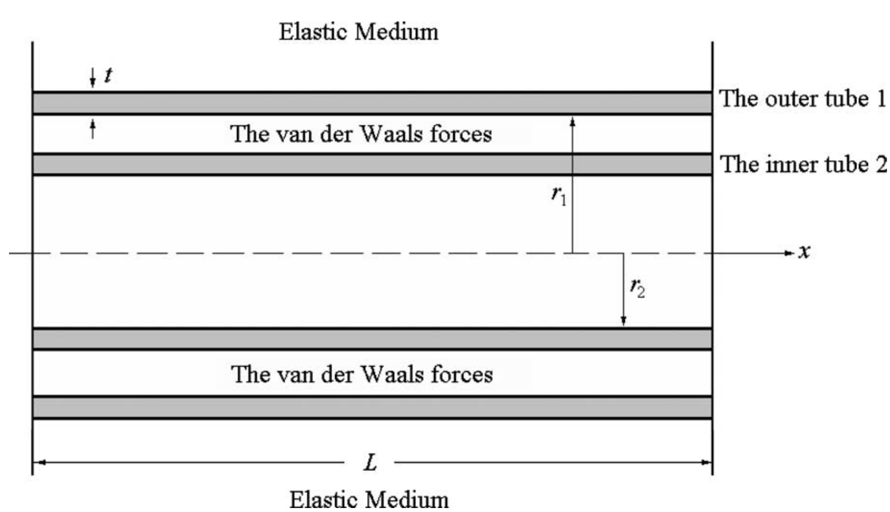

Fig. 1. A double-walled nanotube embedded in an elastic medium.

4. The critical buckling condition

Now, for each of the carbon nanotubes 1 and 2, one can use the Eq. (11), and then obtain the linear equations:

$$D\nabla^8 w_1 + \frac{Et}{r_1^2}\frac{\partial^4 w_1}{\partial x^4} - \nabla^4\left[N_{x01}\frac{\partial^2 w_1}{\partial x^2}\right] = c\nabla^4 w_2 - (c+d)\nabla^4 w_1 + \nabla^4\left[N_{y01}\frac{\partial^2 w_1}{\partial y^2}\right], \tag{21}$$

$$D\nabla^8 w_2 + \frac{Et}{r_2^2}\frac{\partial^4 w_2}{\partial x^4} - \nabla^4\left[N_{x02}\frac{\partial^2 w_2}{\partial x^2}\right] = \frac{cr_1}{r_2}\left[\nabla^4 w_1 - \nabla^4 w_2\right] + \nabla^4\left[N_{y02}\frac{\partial^2 w_2}{\partial y^2}\right], \tag{22}$$

where the bending stiffness D is the same for both tubes as they have the same effective material constants and thickness. It is clear that the van der Waals interaction makes the Eqs. (21) and (22) coupled. Furthermore, it is found from normal equilibrium conditions (21) and (22) that

$$N_{y01} = -(P_{10}^V + P_{10}^W)r_1, \tag{23}$$

$$N_{y02} = P_{10}^V r_1. \tag{24}$$

On the other hand, M, the total bending moment applied to the double-walled nanotube consists of two pares, one of which, denoted by M_1, is the bending moment applied to the outer tube 1, and the other, denoted by M_2, is the bending moment applied to the inner tube 2, namely

$$M = M_1 + M_2. \tag{25}$$

Furthermore, the bending moments M_1 and M_2 are dependent on the radii of the inner and outer tubes

$$\frac{M_1}{M_2} = \left(\frac{r_1}{r_2}\right)^3. \tag{26}$$

Combining the Eqs. (25) and (26), the bending moments M_1 and M_2 can be obtained as follows:

$$M_1 = \frac{r_1^3}{r_1^3 + r_2^3}M, \tag{27}$$

$$M_2 = \frac{r_2^3}{r_1^3 + r_2^3}M. \tag{28}$$

The membrane forces of pre-buckling is assumed as follows:

$$N_{x01} = -\frac{M_1}{\pi r_1^2}\cos\frac{y}{r_1} = -\frac{r_1 M}{\pi(r_1^3 + r_2^3)}\cos\frac{y}{r_1}, \tag{29}$$

$$N_{x02} = -\frac{M_2}{\pi r_2^2}\cos\frac{y}{r_2} = -\frac{r_2 M}{\pi(r_1^3 + r_2^3)}\cos\frac{y}{r_2}. \tag{30}$$

For the bending of an elastic cylindrical shell, prior to buckling, the Brazier effect causes the circular cross-section of the shell to become more ovalized uniformly over the whole shell length as the bending curvature increases [19]. The Brazier effect of the pre-buckling shell does not affect the buckling additional deformation in Eqs. (9) and (10). Bifurcation, on the other hand, leads to a periodic, low-amplitude rippling of the shell wall on the compressive side of the bend. Assume the buckling modes are as follows:

$$w_1 = \sin\alpha x\sum_{n=1}^{3} f_{1n}\sin\beta_1 y, \tag{31}$$

$$w_2 = \sin\alpha x\sum_{n=1}^{3} f_{2n}\sin\beta_2 y, \tag{32}$$

where

$$\alpha = \frac{m\pi}{L}, \quad \beta_1 = \frac{n}{r_1}, \quad \beta_2 = \frac{n}{r_2}. \tag{33}$$

Substitution of above equations into Eqs. (21) and (22), one can obtain

$$A_{11}f_{11} + A_{12}f_{12} + A_{14}f_{21} = 0, \tag{34a}$$

$$A_{21}f_{11} + A_{22}f_{12} + A_{23}f_{13} + A_{25}f_{22} = 0, \tag{34b}$$

$$A_{32}f_{12} + A_{33}f_{13} + A_{36}f_{23} = 0, \tag{34c}$$

$$A_{41}f_{11} + A_{44}f_{21} + A_{45}f_{22} = 0, \tag{34d}$$

$$A_{52}f_{12} + A_{54}f_{21} + A_{55}f_{22} + A_{56}f_{23} = 0, \tag{34e}$$

$$A_{63}f_{13} + A_{65}f_{22} + A_{66}f_{23} = 0. \tag{34f}$$

Using the condition for a non-zero solution of Eqs. (34a)–(34f), one can obtain the following equation which determines the critical bending moment and buckling mode:

$$\begin{vmatrix} A_{11} & A_{12} & 0 & A_{14} & 0 & 0 \\ A_{21} & A_{22} & A_{23} & 0 & A_{25} & 0 \\ 0 & A_{32} & A_{33} & 0 & 0 & A_{36} \\ A_{41} & 0 & 0 & A_{44} & A_{45} & 0 \\ 0 & A_{52} & 0 & A_{54} & A_{55} & A_{56} \\ 0 & 0 & A_{63} & 0 & A_{65} & A_{66} \end{vmatrix} = 0. \tag{35}$$

If only the first two terms are considered in Eqs. (31) and (32), namely

$$w_1 = \sin\alpha x\left[f_{11}\sin\frac{y}{r_1} + f_{12}\sin\frac{2y}{r_1}\right], \tag{36a}$$

$$w_2 = \sin\alpha x\left[f_{21}\sin\frac{y}{r_2} + f_{22}\sin\frac{2y}{r_2}\right]. \tag{36b}$$

Eq. (35) can be changed into the following form:

$$\begin{vmatrix} A_{11} & A_{12} & A_{14} & 0 \\ A_{21} & A_{22} & 0 & A_{25} \\ A_{41} & 0 & A_{44} & A_{45} \\ 0 & A_{52} & A_{54} & A_{55} \end{vmatrix} = 0, \tag{37}$$

where A_{ij} in the above equations can be given as follows:

$$A_{11} = D\left[\alpha^2 + \left(\frac{1}{r_1}\right)^2\right]^4 + \frac{Et\alpha^4}{r_1^2} + (c+d)\left[\alpha^2 + \left(\frac{1}{r_1}\right)^2\right]^2 - N_{y02}\left[\alpha^2 + \left(\frac{1}{r_1}\right)^2\right]^2\left(\frac{1}{r_1}\right)^2, \tag{38a}$$

$$A_{12} = -\frac{r_1 M\alpha^2}{2\pi(r_1^3 + r_2^3)}\left[\alpha^2 + \left(\frac{1}{r_1}\right)^2\right]^2, \tag{38b}$$

$$A_{14} = -c\left[\alpha^2 + \left(\frac{1}{r_2}\right)^2\right]^2, \tag{38c}$$

$$A_{21} = -\frac{r_1 M\alpha^2}{2\pi(r_1^3 + r_2^3)}\left[\alpha^2 + \left(\frac{2}{r_1}\right)^2\right]^2, \tag{38d}$$

$$A_{22} = D\left[\alpha^2 + \left(\frac{2}{r_1}\right)^2\right]^4 + \frac{Et\alpha^4}{r_1^2} + (c+d)\left[\alpha^2 + \left(\frac{2}{r_1}\right)^2\right]^2 - N_{y02}\left[\alpha^2 + \left(\frac{2}{r_1}\right)^2\right]^2\left(\frac{2}{r_1}\right)^2, \tag{38e}$$

$$A_{23} = -\frac{r_1 M\alpha^2}{2\pi(r_1^3 + r_2^3)}\left[\alpha^2 + \left(\frac{2}{r_1}\right)^2\right]^2, \tag{38f}$$

$$A_{25} = -c\left[\alpha^2 + \left(\frac{2}{r_2}\right)^2\right]^2, \tag{38g}$$

$$A_{32} = -\frac{r_1 M\alpha^2}{2\pi(r_1^3 + r_2^3)}\left[\alpha^2 + \left(\frac{3}{r_1}\right)^2\right]^2, \tag{38h}$$

$$A_{33} = D\left[\alpha^2 + \left(\frac{3}{r_1}\right)^2\right]^4 + \frac{Et\alpha^4}{r_1^2} + (c+d)\left[\alpha^2 + \left(\frac{3}{r_1}\right)^2\right]^2 - N_{y02}\left[\alpha^2 + \left(\frac{3}{r_1}\right)^2\right]^2\left(\frac{3}{r_1}\right)^2, \tag{38i}$$

$$A_{36} = -c\left[\alpha^2 + \left(\frac{3}{r_2}\right)^2\right]^2, \tag{38j}$$

$$A_{41} = -\frac{cr_1}{r_2}\left[\alpha^2 + \left(\frac{1}{r_1}\right)^2\right]^2, \tag{38k}$$

$$A_{44} = D\left[\alpha^2 + \left(\frac{1}{r_2}\right)^2\right]^4 + \frac{Et\alpha^4}{r_2^2} + \frac{cr_1}{r_2}\left[\alpha^2 + \left(\frac{1}{r_2}\right)^2\right]^2 + N_{y02}\left[\alpha^2 + \left(\frac{1}{r_2}\right)^2\right]^2\left(\frac{1}{r_2}\right)^2, \tag{38l}$$

$$A_{45} = -\frac{r_2 M\alpha^2}{2\pi(r_1^3 + r_2^3)}\left[\alpha^2 + \left(\frac{1}{r_2}\right)^2\right]^2, \tag{38m}$$

$$A_{52} = -\frac{cr_1}{r_2}\left[\alpha^2 + \left(\frac{2}{r_1}\right)^2\right]^2, \tag{38n}$$

$$A_{54} = -\frac{r_2 M\alpha^2}{2\pi(r_1^3 + r_2^3)}\left[\alpha^2 + \left(\frac{2}{r_2}\right)^2\right]^2, \tag{38o}$$

$$A_{55} = D\left[\alpha^2 + \left(\frac{2}{r_2}\right)^2\right]^4 + \frac{Et\alpha^4}{r_2^2} + \frac{cr_1}{r_2}\left[\alpha^2 + \left(\frac{2}{r_2}\right)^2\right]^2 + N_{y02}\left[\alpha^2 + \left(\frac{2}{r_2}\right)^2\right]^2\left(\frac{2}{r_2}\right)^2, \tag{38p}$$

$$A_{56} = -\frac{r_2 M\alpha^2}{2\pi(r_1^3 + r_2^3)}\left[\alpha^2 + \left(\frac{2}{r_2}\right)^2\right]^2, \tag{38q}$$

$$A_{63} = -\frac{cr_1}{r_2}\left[\alpha^2 + \left(\frac{3}{r_1}\right)^2\right]^2, \tag{38r}$$

$$A_{65} = -\frac{r_2 M\alpha^2}{2\pi(r_1^3 + r_2^3)}\left[\alpha^2 + \left(\frac{3}{r_2}\right)^2\right]^2, \tag{38s}$$

$$A_{66} = D\left[\alpha^2 + \left(\frac{3}{r_2}\right)^2\right]^4 + \frac{Et\alpha^4}{r_2^2} + \frac{cr_1}{r_2}\left[\alpha^2 + \left(\frac{3}{r_2}\right)^2\right]^2 + N_{y02}\left[\alpha^2 + \left(\frac{3}{r_2}\right)^2\right]^2\left(\frac{3}{r_2}\right)^2. \tag{38t}$$

To obtain an explicit formula for the critical bending moment, which indicates the effects of the surrounding elastic medium and the van der Waals forces, one can use the determinant (37) and expand it, namely

$$M = \sqrt{\frac{B - \sqrt{B^2 - 4AC}}{2A}}, \tag{39}$$

where

$$A = \frac{r_1^2 r_2^2 \alpha^8}{[2\pi(r_1^3 + r_2^3)]^4}\left[\alpha^2 + \left(\frac{1}{r_1}\right)^2\right]^2\left[\alpha^2 + \left(\frac{1}{r_2}\right)^2\right]^2 \times \left[\alpha^2 + \left(\frac{2}{r_1}\right)^2\right]^2\left[\alpha^2 + \left(\frac{2}{r_2}\right)^2\right]^2, \tag{40a}$$

$$B = \frac{\alpha^4}{[2\pi(r_1^3+r_2^3)]^2}\left\{ r_2^2 A_{11}A_{22}\left[\alpha^2+\left(\frac{1}{r_2}\right)^2\right]^2\left[\alpha^2+\left(\frac{2}{r_2}\right)^2\right]^2 + r_1^2 A_{44}A_{55}\left[\alpha^2+\left(\frac{1}{r_1}\right)^2\right]^2\left[\alpha^2+\left(\frac{2}{r_1}\right)^2\right]^2 + r_1 r_2 A_{25}A_{41}\left[\alpha^2+\left(\frac{1}{r_1}\right)^2\right]^2\left[\alpha^2+\left(\frac{2}{r_2}\right)^2\right]^2 + r_1 r_2 A_{52}A_{14}\left[\alpha^2+\left(\frac{1}{r_2}\right)^2\right]^2\left[\alpha^2+\left(\frac{2}{r_1}\right)^2\right]^2\right\}, \tag{40b}$$

$$C = A_{11}A_{22}A_{44}A_{55} + A_{14}A_{41}A_{25}A_{52} - A_{11}A_{25}A_{44}A_{52} - A_{14}A_{41}A_{22}A_{55}. \tag{40c}$$

Thus, the critical bending moment for infinitesimal buckling can be obtained by minimizing the right hand side of Eq. (39) with respect to the integer m.

5. Simplification and discussion

Now, because the radii of double-walled nanotubes are usually at least a few nanometers, the difference of the inner and outer radii should be much smaller than the radius of the double-walled nanotube. Therefore, the difference of the inner and outer tubes may be neglected, namely,

$$r_1 \approx r_2 = r. \tag{41}$$

Using this equation, Eqs. (38a), (38e), (38l), (38p) and $A_{14}A_{25}$ can be rewritten as

$$A_{11} = \left[\alpha^2+\left(\frac{1}{r}\right)^2\right]^2\left[B_1+c+d-N_{y02}\left(\frac{1}{r}\right)^2\right], \tag{42a}$$

$$A_{22} = \left[\alpha^2+\left(\frac{2}{r}\right)^2\right]^2\left[B_3+c+d-N_{y02}\left(\frac{2}{r}\right)^2\right], \tag{42b}$$

$$A_{44} = \left[\alpha^2+\left(\frac{1}{r}\right)^2\right]^2\left[B_1+c+N_{y02}\left(\frac{1}{r}\right)^2\right], \tag{42c}$$

$$A_{55} = \left[\alpha^2+\left(\frac{2}{r}\right)^2\right]^2\left[B_3+c+N_{y02}\left(\frac{2}{r}\right)^2\right], \tag{42d}$$

$$A_{14}A_{25} = c^2\left[\alpha^2+\left(\frac{1}{r}\right)^2\right]^2\left[\alpha^2+\left(\frac{2}{r}\right)^2\right]^2, \tag{42e}$$

where

$$B_1 = D\left[\alpha^2+\left(\frac{1}{r}\right)^2\right]^2 + \frac{Et\alpha^4}{r^2\left[\alpha^2+\left(\frac{1}{r}\right)^2\right]^2}, \tag{43a}$$

$$B_3 = D\left[\alpha^2+\left(\frac{2}{r}\right)^2\right]^2 + \frac{Et\alpha^4}{r^2\left[\alpha^2+\left(\frac{2}{r}\right)^2\right]^2}. \tag{43b}$$

Introduce two parameters λ_1 and λ_2

$$\lambda_1^2 = (A_{11}A_{22} - A_{44}A_{55})^2 + 4A_{14}A_{25}(A_{11}A_{22} + A_{44}A_{55}) + 4\left(A_{11}A_{44}A_{25}^2 + A_{22}A_{55}A_{14}^2\right), \tag{44a}$$

$$\lambda_2^2 = 4\left(A_{14}^2 - A_{11}A_{44}\right)\left(A_{25}^2 - A_{22}A_{55}\right). \tag{44b}$$

Eq. (39) for the critical bending moment can be rewritten as follows:

$$M = \frac{4\pi r^2}{\sqrt{2}\alpha^2\left[\alpha^2+\left(\frac{1}{r}\right)^2\right]\left[\alpha^2+\left(\frac{2}{r}\right)^2\right]}\sqrt{\sqrt{\lambda_1^2+\lambda_2^3}-\lambda_1}. \tag{45}$$

Thus, the critical bending moment should be determined by minimizing the right hand side of Eq. (45) with respect to the integer m. In what follows, the critical condition is discussed.

5.1. In the absence of the van der Waals forces and the surrounding elastic medium ($c = 0$ and $d = 0$)

In the absence of the van der Waals forces and the surrounding elastic medium, we have $c = d = 0$. Eqs. (44a) and (44b) can be simplified:

$$\lambda_1 = 0, \tag{46a}$$

$$\lambda_2 = 2\left[\alpha^2+\left(\frac{1}{r}\right)^2\right]^2\left[\alpha^2+\left(\frac{2}{r}\right)^2\right]^2 B_1 B_3. \tag{46b}$$

The relation (45) reduces to the following result:

$$M = 4\pi r^2\left\{\left\{\frac{D}{\alpha^2}\left[\alpha^2+\left(\frac{1}{r}\right)^2\right]^2 + \frac{Et\alpha^2}{r^2\left[\alpha^2+\left(\frac{1}{r}\right)^2\right]^2}\right\} \times \left\{\frac{D}{\alpha^2}\left[\alpha^2+\left(\frac{2}{r}\right)^2\right]^2 + \frac{Et\alpha^2}{r^2\left[\alpha^2+\left(\frac{2}{r}\right)^2\right]^2}\right\}\right\}^{1/2}. \tag{47}$$

In this case, the double-walled nanotubes behave like a free single-walled nanotube with a middle radius r and thickness t under the pure bending moment.

The dependency of the bending moment M on the axial half wave number m is plotted in Figs. 2 and 3. The critical bending moment for elastic buckling is defined by the lowest bending moment with m. Here, we use $E = 5.5$ Tpa, $t = 0.066$ nm.

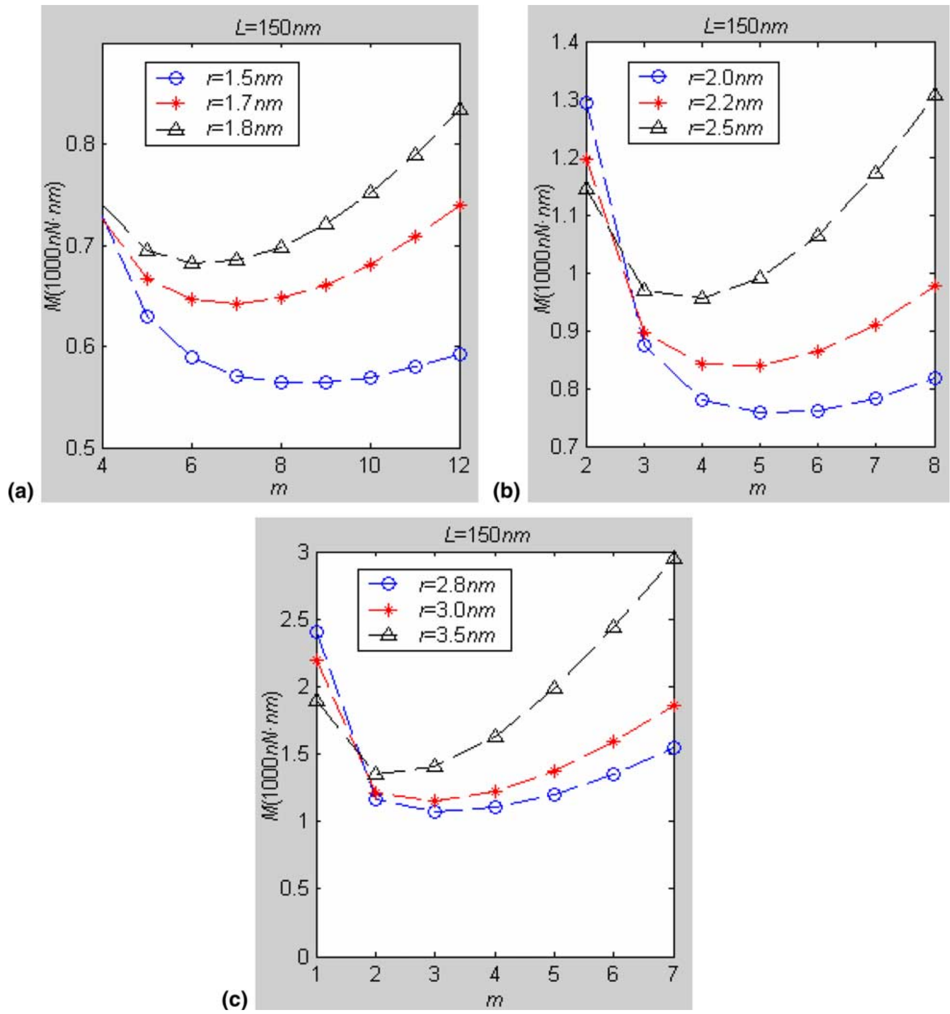

Fig. 2. Dependency of bending moment M on the axial half wave number m for three different values of r, with $L = 150$ nm.

The curves shown in Figs. 2 and 3 indicate the relationship between the bending moment M and the half wave number m. From the figures, it is seen that the critical bending moment M decreases and the axial half wave number m increases as the radius r decreases. Also the axial half wave number increases as the length L increases.

5.2. In the absence of the van der Waals forces ($c = 0$)

In the absence of the van der Waals forces, we have $c = 0$ and $d \neq 0$. Then the inner tube behaviors like a single-walled shell in which the surrounding elastic medium is also absent. This is due to the fact that the surrounding elastic medium does not affect the inner tube when the van der Waals force is absent. In this case, by minimizing the right hand side of Eq. (47) with respect to the integer m one can determine the buckling of the inner tube under the pure bending moment. But, when the inner tube buckles, buckling of the double-walled nanotube occurs.

However, the outer tube looks like a single-walled tube, but embedded in the elastic medium in the absence of the van der Waals forces. One can obtain the critical buckling moment by using the Eq. (45)

$$M = \frac{4\pi r^2}{\alpha^2}\sqrt{(B_1+d)(B_3+d)} = 4\pi r^2\left\{\left\{\frac{D}{\alpha^2}\left[\alpha^2+\left(\frac{1}{r}\right)^2\right]^2+\frac{Et\alpha^2}{r^2\left[\alpha^2+\left(\frac{1}{r}\right)^2\right]^2}+\frac{d}{\alpha^4}\right\}\times\left\{\frac{D}{\alpha^2}\left[\alpha^2+\left(\frac{2}{r}\right)^2\right]^2+\frac{Et\alpha^2}{r^2\left[\alpha^2+\left(\frac{2}{r}\right)^2\right]^2}+\frac{d}{\alpha^4}\right\}\right\}^{1/2}. \tag{48}$$

Obviously, a comparison between Eqs. (47) and (48) reveals that the surrounding elastic medium increases the critical bending moment of the outer tube.

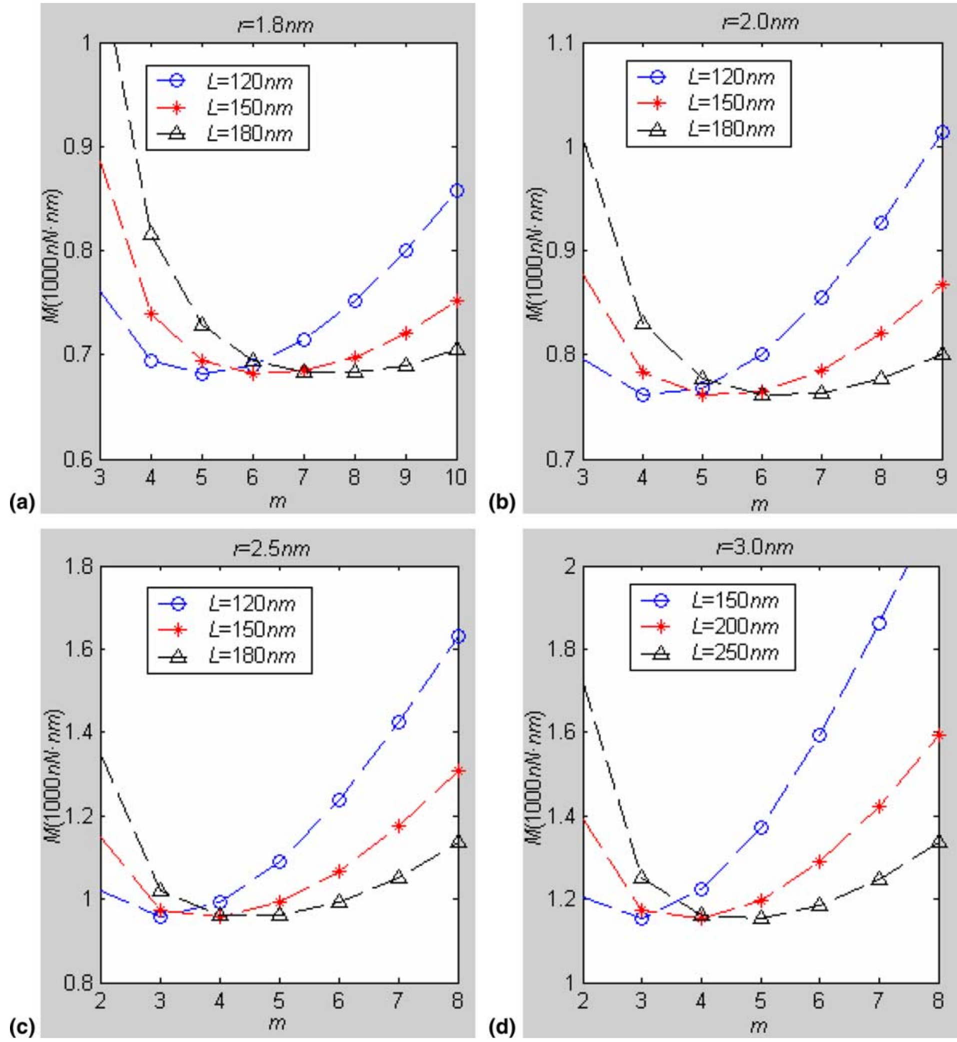

Fig. 3. Dependency of the bending moment M on the axial half wave number m for three different values of L and r.

5.3. The general case with $c \neq 0$, $d \neq 0$ and $N_{y02} = 0$

In the general case where both the van der Waals forces and the surrounding elastic medium are present, the critical bending moment can be obtained by minimizing the right-hand side of Eq. (45) with respect to the integer m.

However, due to complex of the Eq. (45), it is too difficult to discuss the effects of the surrounding elastic medium and the van der Waals forces on the critical bending moment. To analyze the effect of both the van der Waals forces and the surrounding elastic medium, let us consider a special case with $N_{y02} = 0$. Using Eq. (45), one obtains

$$M = \frac{4\pi r^2}{\sqrt{2}\alpha^2}\{2B_1B_3 + (2c+d)(B_1+B_3) + (2c+d)^2 - 2cd - (B_1+B_3+2c+d)\sqrt{4c^2+d^2}\}^{1/2}. \quad (49)$$

Let

$$F(c) = 2B_1B_3 + (2c+d)(B_1+B_3) + (2c+d)^2 - 2cd - (B_1+B_3+2c+d)\sqrt{4c^2+d^2}. \quad (50)$$

In the absence of the elastic medium ($d = 0$), Eq. (50) can be rewritten in the following form:

$$F(c) = \begin{cases} 2B_1B_3 & (d=0, c \geqslant 0), \\ 2B_1B_3 + 4c(B_1+B_3+2c) & (d=0, c<0). \end{cases} \quad (51)$$

Using Eq. (51), it is not difficult to find that the critical bending moment given by Eq. (49) is identical to Eq. (47) when $N_{y02} = d = 0$ and c is non-negative. In other words, the double-walled nanotube buckles like a single-walled one and the van der Waals forces do not affect the critical bending moment of the double-walled nanotube if $N_{y02} = d = 0$ and c is non-negative. In this case, if $w_1(x,y) = w_2(x,y)$ along the tubes, the interlayer spacing keeps unchanged and the difference of two radii of the inner and outer tubes is negligible, Eqs. (21) and (22) become identical. That is why the van der Waals forces do not affect the critical bending moment of the double-walled nanotube if $N_{y02} = d = 0$ and c is non-negative.

On the other hand, if $d \neq 0$ and $c>0$, because $\frac{dF(c)}{dc} > 0$ and $F(c)|_{c=0} = 2B_1B_3$, we have $F(c) > 2B_1B_3$, this means that the van der Waals forces increase the critical bending moment of the double-walled nanotube if $N_{y02} = 0$ and $c > 0$.

6. Conclusions

The instability of a double-walled carbon nanotube embedded in an elastic medium under pure bending is examined. The effects of surrounding elastic medium and van der Waals forces between the inner and outer nanotubes are taken into account. From the view point of continuum modeling, an elastic double-shell model is presented for the pure bending buckling of a double-walled carbon nanotube. Based on this model, a condition is derived in terms of the buckling modes of the shell from which the critical bending moment can be predicted. A simplified analysis is also performed to study, qualitatively, the effect of the van der Waals forces and the elastic medium on the critical bending moment of the double-walled carbon nanotube.

The present model is true only for infinitesimal buckling of multi-walled nanotubes whose radii are much larger than the intertube spacing (the latter is about 0.34 nm), as in the case of a study by Ru [15]. To investigate the post-buckling behavior of multi-walled nanotubes involving compression, bending and torsion, nonlinear post-buckling analysis of multi-walled carbon nanotubes has to be established. Further analysis is being carried out to explain some experimental observation. It is also noted that post-buckling analysis, model analysis, dynamic buckling and finite element technique of multi-walled carbon nanotubes are, possibly, some interesting research topics for future work.

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Appendix A. Buckling of a cylindrical shell under a pure bending moment

The governing equation of buckling of cylindrical shell under the pure bending moment is given by

$$D\nabla^8 w + \frac{Et}{r^2}\frac{\partial^4 w}{\partial x^4} + \frac{M}{\pi r^2}\nabla^4\left[\frac{\partial^2 w}{\partial x^2}\cos\frac{y}{r}\right] = 0. \tag{A.1}$$

The classical shell theory assumes the buckling modes as follows:

$$w(x,y) = \sin\frac{m\pi x}{L}\sum_{n=1} f_n \sin\frac{ny}{r}. \tag{A.2}$$

Substitution of Eq. (A.2) into Eq. (A.1), one can obtain

$$\left[\frac{D}{t}\left(\alpha^2+\beta^2\right)^4 + \frac{E}{r^2}\alpha^4\right]f_n - \frac{M}{\pi r^2 t}\cdot\frac{\alpha^2}{2}\cdot\left(\alpha^2+\beta^2\right)^2(f_{n-1}+f_{n+1}) = 0, \tag{A.3}$$

where $\alpha = \frac{m\pi}{L}, \beta = \frac{n}{r}$. For the given number of f_n, using the condition for a non-zero solution, one can obtain the critical bending moment.

It is easy to find that Eq. (47) can be obtained if only the first two terms are considered in Eq. (A.2).

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