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Curvature effects on axially compressed buckling of a small-diameter double-walled carbon nanotube

H. Qian, K.Y. Xu *, C.Q. Ru [1]

Shanghai Institute of Applied Mathematics and Mechanics, Department of Mechanics, Shanghai University, 99 Shangda Road, Shanghai 200444, China

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Abstract

The curvature effects of interlayer van der Waals (vdW) forces on axially compressed buckling of a double-walled carbon nanotube (DWNT) of diameter down to 0.7 nm are studied. Unlike most existing models which assume that the interlayer vdW pressure at a point between the inner and outer tubes depends merely on the change of the interlayer spacing at that point, the present model considers the dependence of the interlayer vdW pressure on the change of the curvatures of the inner and outer tubes at that point. A simple expression is derived for the curvature-dependence of the interlayer vdW pressure in which the curvature coefficient is determined. Based on this model, an explicit formula is obtained for the axial buckling strain. It is shown that neglecting the curvature effect alone leads to an under-estimate of the critical buckling strain with a relative error up to −7%, while taking the average radius of two tubes as the representative radius and the curvature effect leads to an over-estimate of the critical buckling strain with a relative error up to 20% when the inner radius downs to 0.35 nm. Therefore, the curvature effects play a significant role in axially compressed buckling problems only for DWNTs of very small radii. In addition, our results show that the effect of the vdW interaction pressure prior to buckling of DWNTs under pure axial stress is small enough and can be negligible whether the vdW interaction curvature effects are neglected or not.

Keywords: Carbon nanotube; Buckling; Curvature effects; van der Waals forces

* Corresponding author. Tel.: +86 2166134972; fax: +86 2166134080.
E-mail address: kyxu@staff.shu.edu.cn (K.Y. Xu).
[1] On leave from University of Alberta, Edmonton, Canada T6G 2G8.

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1. Introduction

Carbon nanotubes (CNTs) are the most promising new material and expected to play a pivotal role in nanotechnology (Ball, 2001; Baughman et al., 2002). Mechanical behavior of CNTs, including axially compressed elastic buckling, has been one of recent topics of considerable interest (Treacy et al., 1996; Yakobson et al., 1996; Wong et al., 1997; Falvo et al., 1997; Poncharal et al., 1999; Ru, 2000a,b, 2001a,b). Elastic shell models have been effectively used to study mechanical deformation of CNTs (Qian et al., 2002; Ru, 2004), especially axially compressed buckling of CNTs (Yakobson et al., 1996; Ru, 2000a, 2001b). Previous work has shown that critical loading and the associated buckling mode predicted by simple isotropic elastic shell models are generally in reasonable agreement with available experiments and molecular dynamics simulations of single-walled nanotubes (SWNTs) (Ru, 2000a; Wang et al., 2003). On the other hand, axially compressed buckling of large-diameter multi-walled nanotubes (MWNTs) has been studied based on a multiple shell model (Ru, 2000b, 2001a,b; Wang et al., 2003), although a comparison is still not available due to the lack of relevant experimental results or molecular dynamics simulations for axially compressed MWNTs. Furthermore, Wang et al. (2003) have recently studied elastic buckling of individual MWNTs under external radial pressure based on the multiple-elastic shell model (Ru, 2000b, 2001a,b). Wang et al.'s results showed that the multiple-shell model is in reasonably good agreement with the experimental results of Tang et al. (2000) for a specific group of MWNTs of about 20 layers, which suggests that the multiple-elastic shell model can be used to study buckling behavior of MWNTs.

So far, almost all previous work for axial buckling of MWNTs has been limited to CNTs of larger radii for which the curvature effects of the interlayer vdW forces and the difference of the inner and outer radii of DWNTs are neglected (Ru, 2001a,b; Feng et al., 2004). The curvature effects of the interlayer vdW forces on axial buckling of small-diameter MWNTs is an interesting tropic for further work. By analyzing the high resolution transmission electron microscopy images, Kiang et al. (1998) have shown that the interlayer equilibrium spacing between adjacent layers of MWNTs increases with decreasing radii. They have attributed this increase in the interlayer spacing to the high curvature of MWNTs of small radii, resulting in a repulsive vdW force due to the decreased radii of the nanotube shells.

In order to study the curvature effects, a more accurate model is required for the interlayer vdW forces to account for the curvature-dependence of the interlayer vdW forces between two adjacent deformed tubes. Such a model will be suggested in the present paper. Here, it should be stated that an attempt has been made by Feng et al. (2004) to study the curvature effects of the interlayer vdW forces. Unlike Feng et al. (2004) where an assumed model with an undetermined curvature coefficient was used, the model developed in the present paper is based on a theoretical derivation. In particular, based on the data of Kiang et al. (1998), the present model gives a reliable estimate of the curvature coefficient. In addition, almost all previous work on axial buckling of DWNTs have assumed that the inner and outer radii of DWNTs are much larger than the interlayer spacing (0.34 nm) (Feng et al., 2004), and thus the difference between the inner and outer radii is negligible compared to the radii. This simplification is not true for small-diameter DWNTs (such as DWNTs of the inner radius about 1 nm or less) (Wang et al., 2004). Therefore, a more detailed study is needed to examine axial buckling of small-diameter DWNTs. In particular, it is known that the curvature effects are likely relevant for MWNTs of smaller radii (Kiang et al., 1998).

The present paper studies axially compressed buckling of DWNTs with smaller radii. Based on a theoretical model for the curvature dependence of the interlayer vdW forces, an explicit formula is derived for the axial buckling strain. The axial buckling strain is calculated for various radii, with detailed comparison to the results which neglect the difference of the two radii of the inner and outer tubes or the curvature effects of the interlayer vdW forces. The relative error (defined by (approximate solution-exact solution)/exact solution) due to these approximate simplifications is calculated.

2. Basic equations

The elastic-shell models have been effectively applied to SWNTs and multi-walled carbon nanotubes (MWNTs) (Yakobson et al., 1996; Falvo et al., 1997; Ru, 2000a,b, 2001a,b). For MWNTs, a multiple-elastic shell model has been developed by Ru (2000b, 2001a,b), which assumes that each of the concentric nanotubes is described as an individual elastic shell, and the interlayer friction is negligible between any two adjacent tubes. In the absence of any tangential external force, elastic buckling of a cylindrical shell of radius R is governed by (Timoshenko and Gere, 1961; Calladine, 1983; Ru, 2000b, 2001a,b)

$$D_0\nabla^8 w = \nabla^4 p(x,\theta) + F_x\frac{\partial^2}{\partial x^2}\nabla^4 w + \frac{F_\theta}{R^2}\frac{\partial^2}{\partial\theta^2}\nabla^4 w - \frac{Et}{R^2}\frac{\partial^4 w}{\partial x^4}, \tag{1}$$

where x and θ are axial coordinate and circumferential angular coordinate, respectively, w is the radial (inward) deflection due to buckling, $p(x,\theta)$ is the net normal (inward) pressure due to buckling, F_x and F_θ are the uniform axial and circumferential membrane forces prior to buckling, D_0 and t are the effective bending stiffness and thickness of the shell, and E is Young's modulus. Here, the effective bending stiffness D_0 can be independent of the thickness t, and thus not necessarily proportional to t^3.

The present work studies elastic buckling of a DWNT under axial compression, as shown in Fig. 1. Applying Eq. (1) to each of the two concentric tubes of a DWNT, elastic buckling of a DWNT is governed by the two coupled equations

$$\begin{aligned} D_1\nabla_1^8 w_1 &= \nabla_1^4 p_{12} + F_x^{(1)}\frac{\partial^2}{\partial x^2}\nabla_1^4 w_1 + \frac{F_\theta^{(1)}}{R_1^2}\frac{\partial^2}{\partial\theta^2}\nabla_1^4 w_1 - \frac{Et_1}{R_1^2}\frac{\partial^4 w_1}{\partial x^4},\\ D_2\nabla_2^8 w_2 &= \nabla_2^4 p_{21} + F_x^{(2)}\frac{\partial^2}{\partial x^2}\nabla_2^4 w_2 + \frac{F_\theta^{(2)}}{R_2^2}\frac{\partial^2}{\partial\theta^2}\nabla_2^4 w_2 - \frac{Et_2}{R_2^2}\frac{\partial^4 w_2}{\partial x^4}, \end{aligned} \tag{2}$$

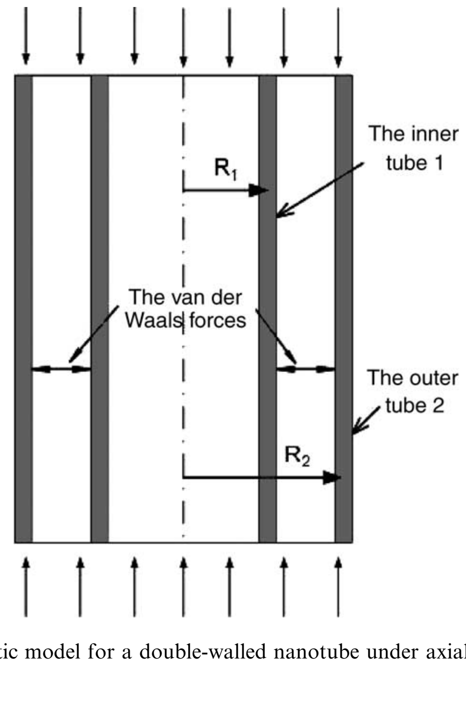

Fig. 1. Elastic model for a double-walled nanotube under axial compression.

where $w_k(k=1,2)$ is the (inward) deflection of the kth tube, D_k and t_k are the bending stiffness and thickness of the kth tube, the subscripts 1, 2 denote the quantities of the inner tube and outer tube, respectively, E is Young's modulus of CNTs, R_k is the radius of the kth tube, $F_x^{(k)}$ and $F_\theta^{(k)}$ $(k=1,2)$ are the uniform axial and circumferential membrane forces of the kth tube prior to buckling, and

$$\nabla_k^2 = \frac{\partial^2}{\partial x^2} + \frac{1}{R_k^2}\frac{\partial^2}{\partial \theta^2} \quad (k=1,2). \tag{3}$$

In addition, p_{12} is the (inward) pressure on inner tube due to outer tube, p_{21} is the (inward) pressure on outer tube due inner tube, and they are related by

$$p_{21} = -\frac{R_1}{R_2}p_{12}. \tag{4}$$

Since the two tubes are originally concentric and the initial interlayer spacing is equal or very close to the equilibrium spacing, the initial vdW interaction pressure between two tubes of undeformed DWNTs is negligible. When the axial loading is applied, however, the interlayer spacing changes which causes the interlayer vdW forces. Here, since infinitesimal buckling of DWNT is studied, the vdW interaction pressure (per unit area) at any point between the two tubes can be assumed to depend linearly on the change of the interlayer spacing and the change of the curvatures of the inner and outer tubes at that point. It is well known that the change of the curvature of the kth tube due to the deflection w_k is $\frac{w_k}{R_k^2} + \nabla_k^2 w_k$, thus the interlayer vdW pressure due to the deflections is given by

$$p_{12}(x,\theta) = c[w_2 - w_1] + c_1\left[\frac{w_2}{R_2^2} + \nabla_2^2 w_2\right] - c_1\left[\frac{w_1}{R_1^2} + \nabla_1^2 w_1\right]. \tag{5}$$

Here the vdW interaction coefficient c can be estimated as the second derivative of the energy-interlayer spacing relation of DWNTs as (Wang et al., 2003, 2004)

$$c = \frac{320 \times \mathrm{erg/cm^2}}{0.16d^2}(d = 1.42 \times 10^{-8}\ \mathrm{cm}), \tag{6}$$

where d is the C–C bond length. On the other hand, the vdW interaction curvature coefficient c_1 can be estimated by studying the dependence of the interlayer vdW pressure on the curvature radii. According to Kiang et al. (1998), the interlayer equilibrium spacing between adjacent layers of MWNTs increases with decreasing radii. For example, the interlayer equilibrium spacing of two concentric tubes is about 0.4 nm when the radius of the inner tube downs to 0.35 nm (Kiang et al., 1998) (Fig. 2(a)). Thus, when two flat graphite sheets (with the initial equilibrium spacing 0.34 nm (Treacy et al., 1996; Ru, 2000b)) (Fig. 2(b)) are rolled into a DWNT of the inner radius R_1 and the outer radius R_2, the interlayer equilibrium spacing increase by $\Delta\delta$ and the difference of two curvature changes by $(1/R_1 - 1/R_2)$. Because the interlayer vdW pressure remains zero at the new interlayer equilibrium spacing, the attractive vdW forces due to increasing spacing is compensated by the impulsive vdW forces due to increasing curvatures. Thus, we have

$$p = c\Delta\delta + c_1\left(\frac{1}{R_1} - \frac{1}{R_2}\right) = 0, \tag{7}$$

where $\Delta\delta = 0.4\ \mathrm{nm} – 0.34\ \mathrm{nm} = 0.06\ \mathrm{nm}$, $R_1 = 0.35\ \mathrm{nm}$, $R_2 = 0.35\ \mathrm{nm} + 0.4\ \mathrm{nm} = 0.75\ \mathrm{nm}$, then it is estimated that

$$c_1 = -c(0.2\ \mathrm{nm})^2 \cong -4\ \mathrm{kg/s^2}. \tag{8}$$

Substitution of (5) into (2) leads to two coupled linear equations for deflection w_1 and w_2. The condition for existence of a non-zero solution determines buckling strain of a DWNT under axial stress.

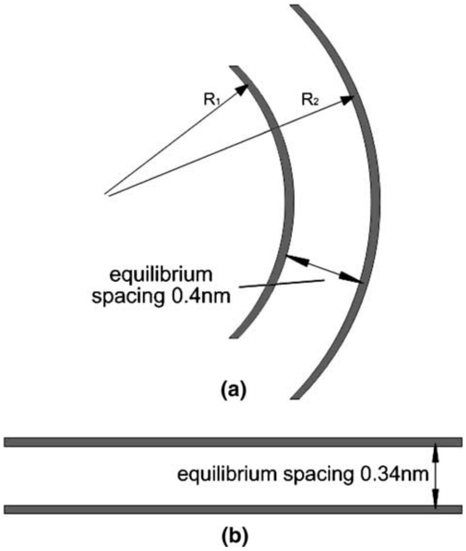

Fig. 2. The interlayer equilibrium spacing of a double-walled nanotube: (a) when the radius of the inner tube is 0.35 nm (Kiang et al., 1998) and (b) when the radii of the two tubes are infinite.

3. Pre-buckling analysis

Constrains for the ends of cylindrical shell are usually ignored in pre-buckling analysis (Timoshenko and Gere, 1961; Calladine, 1983). As a result, under uniform axial stress, the axial and circumferential membrane force $F_x^{(k)}$ and $F_\theta^{(k)}(k = 1, 2)$ prior to buckling are some constants. The equilibrium conditions prior to buckling give (Wang et al., 2003)

$$\sigma_\theta^{(k)} = \frac{F_\theta^{(k)}}{t_k} = -\frac{p_k R_k}{t_k}, \quad \sigma_x^{(k)} = \frac{F_x^{(k)}}{t_k} = \sigma_{\text{axial}} \quad (k = 1, 2), \tag{9}$$

where $\sigma_\theta^{(k)}$ and$\sigma_x^{(k)}$ are the pre-buckling axial and circumferential membrane stresses in the kth tube, p_k is the net (inward) pressure to the kth tube prior to buckling, and σ_{axial} is the axial stress applied to the DWNT. Here

$$p_1 = p_{12}, \quad p_2 = p_{21}. \tag{10}$$

Note that (Hooke's relation) (Wang et al., 2003)

$$\varepsilon_\theta^{(k)} = \frac{\Delta R_k}{R_k} = \frac{1}{E}(\sigma_\theta^{(k)} - v\sigma_x^{(k)}) \quad (k = 1, 2), \tag{11}$$

where ΔR_k is the increase of the radius of the kth tube prior to buckling, and v is Poisson's ratio. Prior to buckling, the deflection of the kth tube is $w_k = -\Delta R_k$, and prior to buckling, we have

$$\nabla_k^2 w_k = 0 \quad (k = 1, 2), \tag{12}$$

Combining Eqs. (4), (5), (9), (10), (12) with Eq. (11) gives two conditions which allow us to determine ΔR_k $(k = 1, 2)$

$$\Delta R_1\left[\left(c+\frac{c_1}{R_1^2}\right)\left(-\frac{R_1}{Et_1}\right)-\frac{1}{R_1}\right]+\Delta R_2\left(c+\frac{c_1}{R_2^2}\right)\left(\frac{R_1}{Et_1}\right)-\frac{v}{E}\sigma_{\text{axial}}=0,$$
$$\Delta R_1\left[\left(c+\frac{c_1}{R_1^2}\right)\left(-\frac{R_1}{Et_2}\right)\right]+\Delta R_2\left[\left(c+\frac{c_1}{R_2^2}\right)\left(\frac{R_1}{Et_2}\right)+\frac{1}{R_2}\right]+\frac{v}{E}\sigma_{\text{axial}}=0. \tag{13}$$

Once $\Delta R_k (k = 1, 2)$ are known, all membrane forces and pressure distribution prior to buckling can be determined.

4. Buckling analysis

Because the critical axial strain is usually not sensitive to the boundary conditions, we consider the hinged nanotubes. The ends of both tubes of DWNTs are simply supported. Thus, the buckling mode is given by

$$w_1 = A\sin\frac{m\pi x}{L}\cos n\theta,$$
$$w_2 = B\sin\frac{m\pi x}{L}\cos n\theta, \qquad (m \geqslant 1) \tag{14}$$

where A and B are two real constants, L is the length of the DWNT, m is the axial half wavenumber, and n is the circumferential wavenumber. For the DWNT, the bending stiffness is same for two tubes, i.e., $D_1 = D_2 = D$, and the thickness is constant, i.e., $t_1 = t_2 = t$. Thus, Eq. (9) gives $F_x^{(1)} = F_x^{(2)} = F_x$. Introducing (14), together with the known net pressure distribution (see Section 3) and Eqs. (4) and (5) into Eq. (2) gives

$$\left[DJ_1^4+\left(c+\frac{c_1}{R_1^2}\right)J_1^2-c_1J_1^3+\frac{Et}{R_1^2}\left(\frac{m\pi}{L}\right)^4+J_1^2F_x\left(\frac{m\pi}{L}\right)^2+J_1^2\frac{F_\theta^{(1)}}{R_1^2}n^2\right]A-\left[\left(c+\frac{c_1}{R_2^2}\right)J_1^2-c_1J_1^2J_2\right]B=0,$$
$$-\frac{R_1}{R_2}J_2^2\left[\left(c+\frac{c_1}{R_1^2}\right)-c_1J_1\right]A+\left\{DJ_2^4+\frac{R_1}{R_2}\left(c+\frac{c_1}{R_2^2}\right)J_2^2-\frac{R_1}{R_2}c_1J_2^3+\frac{Et}{R_2^2}\left(\frac{m\pi}{L}\right)^4+J_2^2F_x\left(\frac{m\pi}{L}\right)^2+J_2^2\frac{F_\theta^{(2)}}{R_2^2}n^2\right\}B=0, \tag{15}$$

where

$$J_1=\left(\frac{m\pi}{L}\right)^2+\left(\frac{n}{R_1}\right)^2,\quad J_2=\left(\frac{m\pi}{L}\right)^2+\left(\frac{n}{R_2}\right)^2. \tag{16}$$

Evidently, axial buckling of the DWNT is prohibited if there is a zero solution of the Eq. (15).

Accordingly, the critical axial strain can be determined by the existence condition for a non-zero solution of Eq. (15), which leads to a quadratic equation for membrane force F_x

$$F_x^2 + XF_x + Y = 0, \tag{17}$$

where

$$X=\left(\frac{L}{m\pi}\right)^2\left[DJ_1^2+\left(c+\frac{c_1}{R_1^2}\right)-c_1J_1+\frac{Et}{R_1^2}\left(\frac{m\pi}{L}\right)^4\frac{1}{J_1^2}+\frac{F_\theta^{(1)}}{R_1^2}n^2\right]$$
$$+\left(\frac{L}{m\pi}\right)^2\left[DJ_2^2+\frac{R_1}{R_2}\left(c+\frac{c_1}{R_2^2}\right)-\frac{R_1}{R_2}c_1J_2+\frac{Et}{R_2^2}\left(\frac{m\pi}{L}\right)^4\frac{1}{J_2^2}+\frac{F_\theta^{(2)}}{R_2^2}n^2\right], \tag{18}$$

$$
\begin{aligned}
Y = \left(\frac{L}{m\pi}\right)^4 \Bigg\{ & \left[DJ_1^2 + \left(c + \frac{c_1}{R_1^2}\right) - c_1 J_1 + \frac{Et}{R_1^2}\left(\frac{m\pi}{L}\right)^4 \frac{1}{J_1^2} + \frac{F_\theta^{(1)}}{R_1^2} n^2\right] \\
& \times \left[DJ_2^2 + \frac{R_1}{R_2}\left(c + \frac{c_1}{R_2^2}\right) - \frac{R_1}{R_2} c_1 J_2 + \frac{Et}{R_2^2}\left(\frac{m\pi}{L}\right)^4 \frac{1}{J_2^2} + \frac{F_\theta^{(2)}}{R_2^2} n^2\right] \\
& - \frac{R_1}{R_2}\left[\left(c + \frac{c_1}{R_2^2}\right) - c_1 J_2\right]\left[\left(c + \frac{c_1}{R_1^2}\right) - c_1 J_1\right]\Bigg\}.
\end{aligned} \tag{19}
$$

It can be verified that

$$
\begin{aligned}
X^2 - 4Y = \left(\frac{L}{m\pi}\right)^4 \Bigg[& D(J_1^2 - J_2^2) + c\left(1 - \frac{R_1}{R_2}\right) + c_1 R_1\left(\frac{1}{R_1^3} - \frac{1}{R_2^3}\right) - c_1\left(J_1 - \frac{R_1}{R_2} J_2\right) \\
& + Et\left(\frac{m\pi}{L}\right)^4\left(\frac{1}{R_1^2 J_1^2} - \frac{1}{R_2^2 J_2^2}\right) + n^2\left(\frac{F_\theta^{(1)}}{R_1^2} - \frac{F_\theta^{(2)}}{R_2^2}\right)\Bigg]^2 \\
& + 4\left(\frac{L}{m\pi}\right)^4 \frac{R_1}{R_2}\left[\left(c + \frac{c_1}{R_2^2}\right) - c_1 J_2\right]\left[\left(c + \frac{c_1}{R_1^2}\right) - c_1 J_1\right].
\end{aligned} \tag{20}
$$

If all terms proportional to $(R_1 - R_2)/R_1$ are small and negligible, then $J_1 \approx J_2$ and

$$
\left[\left(c + \frac{c_1}{R_2^2}\right) - c_1 J_2\right]\left[\left(c + \frac{c_1}{R_1^2}\right) - c_1 J_1\right] \approx \left[\left(c + \frac{c_1}{R_2^2}\right) - c_1 J_2\right]^2 \geqslant 0. \tag{21}
$$

Generally, because $c_1 = -c(0.2\ \mathrm{nm})^2$ (see Eq. (8)) and $c + \frac{c_1}{R_k^2} > 0$ $(k = 1, 2)$ for $R_k > 0.2$ nm, $X^2 - 4Y$ is positive. The axial buckling membrane force F_x is determined by the smallest root of Eq. (17) which gives

$$
-F_x = \frac{X - \sqrt{X^2 - 4Y}}{2}. \tag{22}
$$

Thus the axial buckling strain is determined by

$$
\begin{aligned}
\varepsilon = -\frac{F_x}{Et} = & \frac{1}{2Et}\left(\frac{L}{m\pi}\right)^2\left[DJ_1^2 + \left(c + \frac{c_1}{R_1^2}\right) - c_1 J_1 + \frac{Et}{R_1^2}\left(\frac{m\pi}{L}\right)^4 \frac{1}{J_1^2} + \frac{F_\theta^{(1)}}{R_1^2} n^2\right] \\
& + \frac{1}{2Et}\left(\frac{L}{m\pi}\right)^2\left[DJ_2^2 + \frac{R_1}{R_2}\left(c + \frac{c_1}{R_2^2}\right) - \frac{R_1}{R_2} c_1 J_2 + \frac{Et}{R_2^2}\left(\frac{m\pi}{L}\right)^4 \frac{1}{J_2^2} + \frac{F_\theta^{(2)}}{R_2^2} n^2\right] \\
& - \frac{1}{2Et}\sqrt{\left(\frac{L}{m\pi}\right)^4\left[D(J_1^2 - J_2^2) + c\left(1 - \frac{R_1}{R_2}\right) + c_1 R_1\left(\frac{1}{R_1^3} - \frac{1}{R_2^3}\right) - c_1\left(J_1 - \frac{R_1}{R_2} J_2\right) + Et\left(\frac{m\pi}{L}\right)^4\left(\frac{1}{R_1^2 J_1^2} - \frac{1}{R_2^2 J_2^2}\right) + n^2\left(\frac{F_\theta^{(1)}}{R_1^2} - \frac{F_\theta^{(2)}}{R_2^2}\right)\right]^2 + 4\left(\frac{L}{m\pi}\right)^4 \frac{R_1}{R_2}\left[\left(c + \frac{c_1}{R_2^2}\right) - c_1 J_2\right]\left[\left(c + \frac{c_1}{R_1^2}\right) - c_1 J_1\right]}.
\end{aligned} \tag{23}
$$

This determines a relationship between the axial buckling strain and the wave-numbers (m, n). Thus, the critical axial strain for axially compressed buckling can be obtained by minimizing the right-hand side of Eq. (23) with respect to the integers m and n.

If we consider the vdW interaction curvature coefficient $c_1 = 0$ and neglect all terms proportional to $(R_1 - R_2)/R_1$, Eq. (23) becomes Eq. (19) of Ru (2000b). On the other hand, if we assume all terms proportional to $(R_1 - R_2)/R_1$ are small and can be neglected, Eq. (23) becomes

$$
\begin{aligned}
-\frac{F_x}{Et} = & \frac{1}{Et}\left(\frac{L}{m\pi}\right)^2\left[DJ^2 + \left(c + \frac{c_1}{R^2}\right) - c_1 J + \frac{Et}{R^2}\left(\frac{m\pi}{L}\right)^4 \frac{1}{J^2}\right] - \frac{1}{Et}\left(\frac{L}{m\pi}\right)^2 \\
& \times \sqrt{\left(\frac{n^2 P_0}{R^2}\right)^2 + \left[\left(c + \frac{c_1}{R^2}\right) - c_1 J\right]^2},
\end{aligned} \tag{24}
$$

where $J = (\frac{m\pi}{L})^2 + (\frac{n}{R})^2$. It is similar to Eq. (24) in Feng et al. (2004) with a minor difference which is caused by the present more accurate curvature expression (5) compared to Feng et al. (2004). Moreover, if the interlayer vdW forces prior to buckling is neglected, then Eq. (24) reduces to the classical result for single-layer elastic shell

$$-\frac{F_x}{Et} = \frac{1}{Et}\left(\frac{L}{m\pi}\right)^2\left[DJ^2 + \frac{Et}{R^2}\left(\frac{m\pi}{L}\right)^4\frac{1}{J^2}\right], \tag{25}$$

where $J = (\frac{m\pi}{L})^2 + (\frac{n}{R})^2$. In this case, the critical axial strain for the double-walled nanotube is approximated equal to that for a single-walled nanotube under otherwise identical condition (Timoshenko and Gere, 1961).

In what follows, detailed numerical results are shown to examine the curvature effects on axial buckling of smaller radii DWNTs. Throughout the paper, we assume that $L = 12R_2$ or $L = 20R_2$ (the outer radius), $v = 0.3$ (Falvo et al., 1997), $D = 0.85$ eV, and $Et = 360$ J/m^2 (Yakobson et al., 1996; Ru, 2000a), and the interlayer spacing between the inner and outer tubes of DWNTs is 0.34 nm.

4.1. The relative errors due to neglecting the vdW interaction pressure prior to buckling

Since both nested tubes are originally concentric and the initial interlayer spacing is equal to or very close to the equilibrium spacing, the initial vdW interaction pressure between two tubes of undeformed DWNTs is negligible. When the axial loading is applied, however, the interlayer spacing changes, which cause the vdW interaction pressure. If the interaction pressure prior to buckling is considered, the critical axial buckling strain can be calculated exactly using an iterative method. But if the vdW interaction pressure prior to buckling is neglected, the critical axial buckling strain can be calculated based on Eq. (23) directly by taking $F_\theta^{(1)} = F_\theta^{(2)} = 0$.

As shown in Fig. 3, the results show that the relative errors of the critical strain due to neglecting the vdW interaction pressure prior to buckling are limited to 0.5%. Based on this result, it is concluded that the vdW interaction pressure prior to buckling for DWNTs under pure axial stress is negligible. So, the axial buckling strain will be calculated without considering the vdW interaction pressure prior to buckling in what follows.

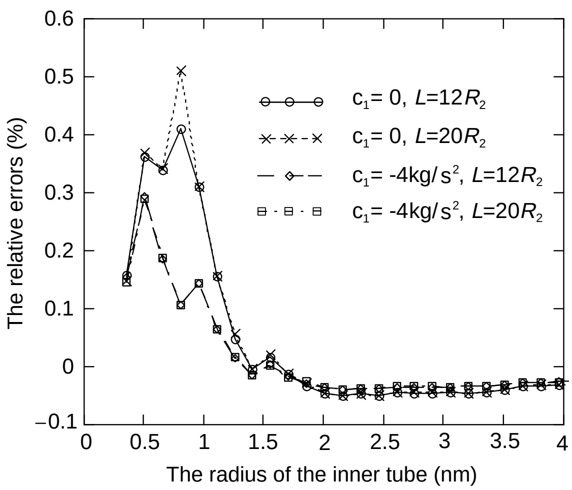

Fig. 3. The relative errors of the critical strain due to neglecting the van der Waals interaction pressure prior to buckling.

4.2. The relative errors due to neglecting the difference of the radii of the inner and the outer tubes when $c_1 = 0$

The axial buckling strain is calculated for various radii, with detailed comparison to the results which do not consider the difference of the radii of the inner and the outer tubes. The relative errors of the critical strain due to neglecting the difference of the two radii can be calculated when $c_1 = 0$, as shown in Fig. 4. Here, when the difference of the radii of the inner and the outer tube is neglected, we take the average radius of two tubes as the representative radius. It is seen from Fig. 4 that the relative error of the critical strain, defined by the solutions neglecting and not neglecting the difference of two radii (both with $c_1 = 0$), is 29%, 5% or 0.3% when the radius of the inner tube is 0.35 nm, 0.95 nm or 2 nm, respectively. Thus, neglecting the difference of the inner and outer radii when $c_1 = 0$ leads to an over-estimate of the critical axial buckling strain if the average radius of the inner and outer radii is used as the representative radius of DWNTs. In particular, this relative error is negligible (less than 1%) when the inner radius of DWNTs is larger than 1.5 nm.

On the other hand, the present model shows that if the outer radius, instead of the average radius, is used as the representative radius of DWNTs, neglecting the difference of the inner and outer radii will lead to an under-estimate of the critical axial buckling strain with a relative error −7% when the radius of the inner tube is 2 nm. This can explain the inconsistency between the present conclusion and those of He et al. (2005) where they used the outer radius as the representative radius of DWNTs and found that neglecting the difference of two radii leads to an under-estimate of the critical strain. In particular, these results are consistent with Wang et al. (2003) where it is shown that the critical axial buckling strain of a MWNT is bounded from above and below by the critical strains of the innermost and the outermost SWNTs.

4.3. The dependence of the axial buckling strain on (m, n) when $c_1 = 0$

Let us examine elastic buckling of DWNTs under pure axial stress when the vdW interaction curvature coefficient c_1 is neglected. The dependence of the axial buckling strain on the wavenumbers (m,n) is shown in Fig. 5(a) and (b) for small or large inner radius. An interesting general result is that, similar to the classical results of axially compressed buckling of elastic thin shells (Timoshenko and Gere, 1961; Calladine, 1983), the wavenumbers corresponding to the minimum axial buckling strain are not unique. More precisely, there always is more than one combination of (m,n) which corresponds to the same minimum (critical) axial buckling strain. As a result, the wavenumbers of the buckling modes of DWNTs under pure

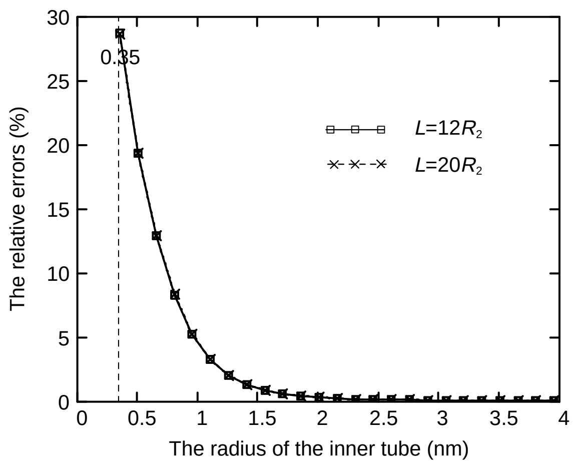

Fig. 4. The relative errors of the critical strain due to neglecting the difference of the radii of the inner and the outer tubes when $c_1 = 0$.

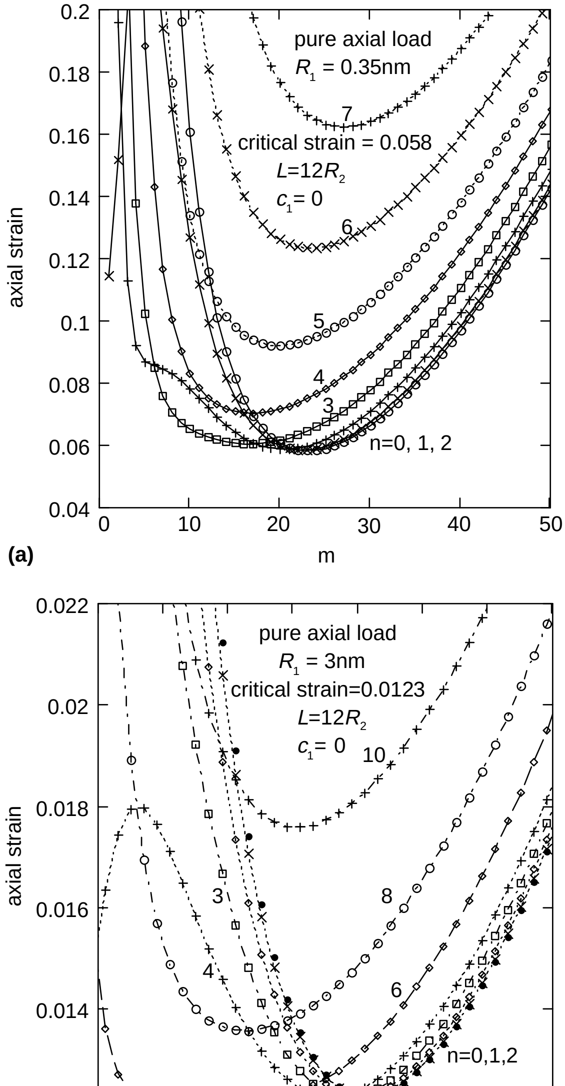

Fig. 5. The dependence of axial strain on the wavenumbers (m,n) when the vdW interaction curvature coefficient c_1 is neglected: (a) when the radius of the inner tube is 0.35 nm and (b) when the radius of the inner tube is 3 nm.

axial stress cannot be determined uniquely when the vdW interaction curvature coefficient c_1 is neglected. Similar results are obtained for MNWTs (Wang et al., 2003).

4.4. The relative errors due to neglecting the vdW interaction curvature coefficient c_1 when all terms proportional to $(R_1 - R_2)/R_1$ are not neglected

The previous models (Ru, 2000b, 2001a,b), which neglect the vdW interaction curvature coefficient c_1, assume that the interlayer vdW pressure at any point between the inner and outer tubes depends merely on the change of the interlayer spacing at that point. Instead, the present model also considers the dependence of the interlayer vdW pressure on the change of the curvatures of the inner and outer tubes at that point. The relative errors of the critical buckling strain due to neglecting the vdW interaction curvature coefficient c_1 alone when all terms proportional to $(R_1 - R_2)/R_1$ are retained is shown in Fig. 6. It is seen from Fig. 6 that the relative error of the critical buckling strain, defined by the solutions neglecting and not neglecting the curvature coefficient c_1 is −7%, −2.7% or −0.13% when the radius of the inner tube is 0.35 nm, 0.95 nm or 1.7 nm, respectively. It is seen from Fig. 6 that the critical axial strain without the curvature effects ($c_1 = 0$) is lower than that with the curvature effects ($c_1 \neq 0$). This can be explained by the fact that the vdW interaction curvature coefficient c_1 increases the interlayer vdW energy and thus promotes the critical strain for buckling. And Fig. 6 also shows that the curvature effects on the critical axial strain are more significant for DWNTs of smaller radii, because the buckling mode of DWNTs of smaller radii has

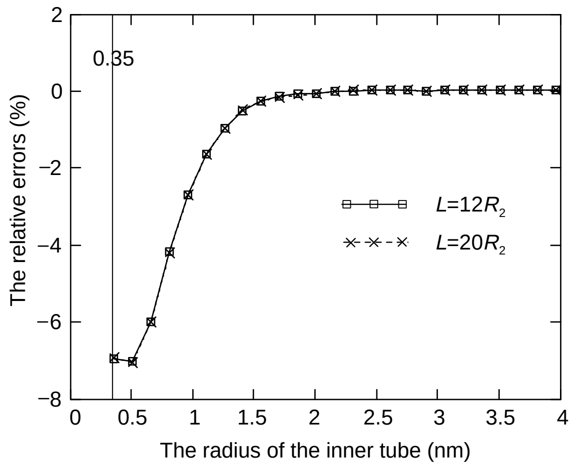

Fig. 6. The relative errors of the critical strain due to neglecting the vdW interaction curvature coefficient c_1 when all terms proportional to $(R_1 - R_2)/R_1$ are not neglected.

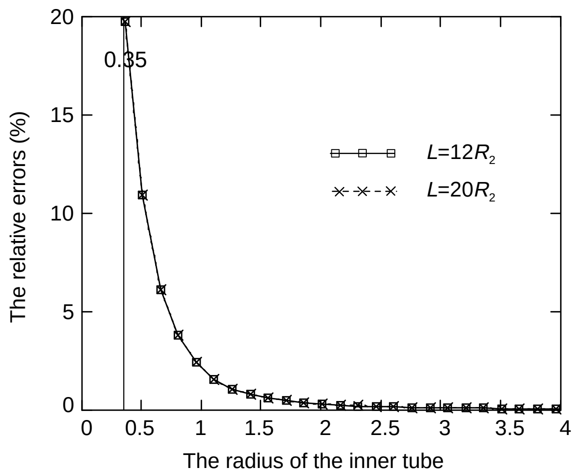

Fig. 7. The relative errors of the critical strain due to neglecting the vdW interaction curvature coefficient c_1 and all terms proportional to $(R_1 - R_2)/R_1$.

shorter wave-lengths. The result agrees with Feng et al. (2004) where it is shown that the curvature effects play a more significant role in elastic buckling of DWNTs of smaller radii.

4.5. The relative errors due to neglecting both the vdW interaction curvature coefficient c_1 and all terms proportional to $(R_1 - R_2)/R_1$

Prior related works (Ru, 2000b, 2001a; Feng et al., 2004) study the critical buckling strain of DWNTs when the all terms proportional to $(R_1 - R_2)/R_1$ are neglected. The critical axial strain is given by Eq. (25)

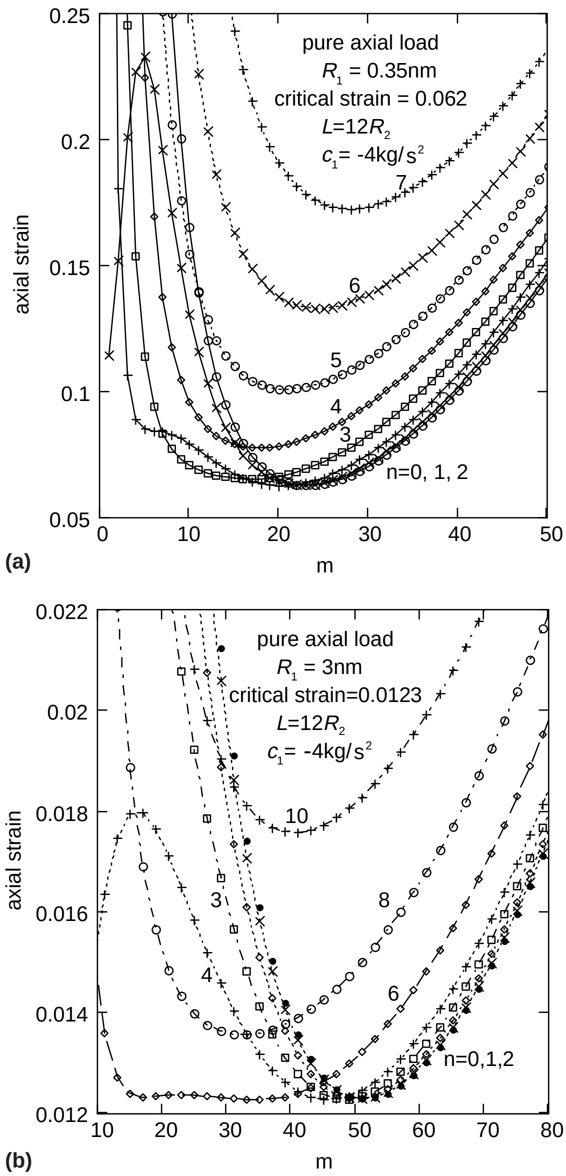

Fig. 8. The dependence of axial strain on the wavenumbers (m, n) when the vdW interaction curvature coefficient c_1 is not neglected: (a) when the radius of the inner tube is 0.35 nm and (b) when the radius of the inner tube is 3 nm.

when both the vdW interaction curvature coefficient c_1 and all terms proportional to $(R_1 - R_2)/R_1$ are neglected. Here, the critical axial strain is calculated for various radii, with comparison to the results which neglect both the difference of two radii of the inner and outer tubes and the vdW interaction curvature coefficient c_1. The relative errors of the critical strain, defined by the solutions neglecting and not neglecting the curvature coefficient c_1 and all terms proportional to $(R_1 - R_2)/R_1$, are shown in Fig. 7. It is seen from Fig. 7 that the relative error of the critical strain is 19.7%, 2.4% or 0.26% when the radius of the inner tube is 0.35 nm, 0.95 nm or 2 nm, respectively. As shown above, neglecting all terms proportional to $(R_1 - R_2)/R_1$ leads to an over-estimate of the critical strain (Fig. 4), and neglecting the vdW curvature coefficient c_1 leads to an under-estimate of the critical strain (Fig. 6). Since the relative error of the critical strain due to neglecting all terms proportional to $(R_1 - R_2)/R_1$ is larger than those due to neglecting the vdW curvature coefficient c_1, neglecting both the vdW curvature coefficient c_1 and all terms proportional to $(R_1 - R_2)/R_1$ leads to an over-estimate of the critical strain, as shown in Fig. 7.

4.6. The dependence of the axial buckling strain on (m, n) when the vdW interaction curvature coefficient c_1 is not neglected

Let us now examine elastic buckling of DWNTs under pure axial stress when the vdW interaction curvature coefficient c_1 is not neglected. The dependence of axial buckling strain on the wavenumbers (m, n) is shown in Fig. 8(a) and (b). Similar to the axial buckling strain when the vdW interaction curvature coefficient c_1 is neglected, the buckling modes associated with the minimum axial strain are not determined uniquely for DWNTs whether the inner radius is small or large.

4.7. The dependence of the critical buckling strain on the value of the coefficient c_1

Finally, let us examine the effect of the value of the curvature coefficient c_1 on the critical buckling strain. To this end, let us consider the coefficient c_1 around $c_1 = -c(0.2\ \text{nm})^2 \cong -4\ \text{kg/s}^2$. The critical buckling

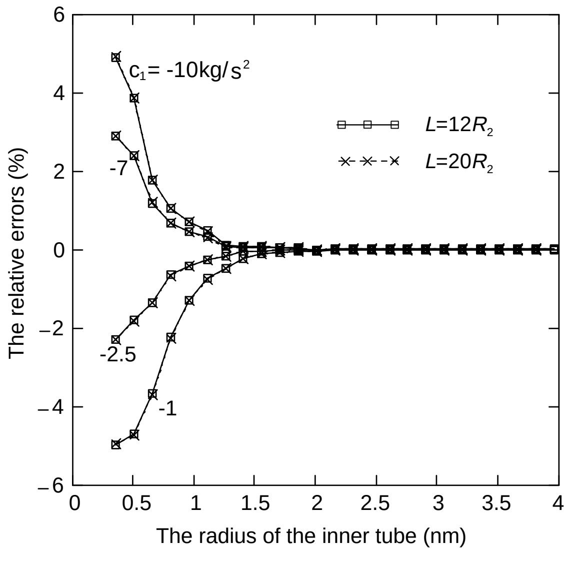

Fig. 9. The dependence of the critical buckling strain on the value of the vdW interaction curvature coefficient c_1.

strain for different vdW interaction curvature coefficient c_1 is compared to the results for $c_1 = -4$ kg/s^2 in Fig. 9. It is seen from Fig. 9 that the relative error of the critical axial strain is limited to 5% when the vdW interaction curvature coefficient c_1 varies from -1 kg/s^2 to -10 kg/s^2 for even small inner radii down to 0.35 nm. On the other hand, for the inner radii larger than 1.5 nm, the effects of different values of the coefficient c_1 are negligible.

5. Conclusions

A new model is developed to study the curvature effects of the interlayer vdW forces on axial buckling of DWNTs of inner radius down to 0.35 nm. The interlayer vdW pressure at a point is assumed to depend linearly not only on the change of the interlayer spacing at that point but also the change of the curvatures of the inner and outer tubes at that point. In particular, the curvature coefficient is estimated based on some relevant data available in the literature. The axial buckling strain is calculated for various radii, with detailed comparison to the results which neglect the difference of the two radii of the inner and outer tubes or the curvature effects of the interlayer vdW forces. Our main results are summarized as follows:

(1) The effect of the vdW interaction pressure prior to buckling under pure axial stress is small and can be negligible whether the vdW interaction curvature coefficient c_1 is neglected or not.
(2) Neglecting the difference of the inner and outer radii alone leads to an over-estimate of the critical axial buckling strain if the average radius of the inner and outer tubes is used as the representative radius. However, the relative error is negligible (less than 1%) if the inner radius of DWNTs is larger than 1.5 nm.
(3) The specific value of the curvature coefficient c_1 has a negligible influence on the critical buckling strain when the inner radius is larger than 1.5 nm.
(4) Similar to the classical results of axially compressed buckling of elastic thin shells, the buckling modes associated with the minimum axial strain are not determined uniquely for DWNTs under pure axial stress whether the vdW interaction curvature coefficient c_1 is neglected or not.
(5) The critical axial strain given by the simplified model without the curvature effects ($c_1 = 0$) is lower than that predicted by the present model with the curvature effects ($c_1 \neq 0$). The curvature effects play a significant role in axially compressed buckling problems of DWNTs of inner diameter around or smaller than 1 nm.

Although the present results are limited to axially compressed buckling of DWNTs, similar results are expected for the role of the curvature effects in other problems of MWNTs of smaller radii, such as radial buckling of MWNTs of smaller innermost radius. In addition, the model for curvature dependence of the interlayer vdW forces developed here could be used to study other short-wavelength deformation of MWNTs, such as highly localized deformation under bending or large-deflection post-buckling of MWNTs.

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