

Small-scale effects on buckling of multiwalled carbon nanotubes under axial compressionY. Q. Zhang,¹ G. R. Liu,^{1,2} and J. S. Wang^{1,3}¹*Singapore-MIT Alliance, National University of Singapore, E4-04-10, 4 Engineering Drive 3, Singapore 117576, Singapore*²*Centre for Advanced Computations in Engineering Science, Department of Mechanical Engineering, National University of Singapore, 10 Kent Ridge Crescent, Singapore 119260, Singapore*³*Department of Computational Science, National University of Singapore, 3 Science Drive 2, Singapore 117543, Singapore*

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Based on the theory of nonlocal continuum mechanics, a multiple shell model is developed for the axial buckling of multiwalled carbon nanotubes under axial compression. The effects of small length scale are incorporated in this model. In particular, an explicit expression is derived for the axial buckling strain for a double-walled carbon nanotube. On the basis of this expression, the influence of the small length scale on the axial buckling strain is discussed. As a result, the effect of small length scale on the axial buckling strain is related to the buckling mode and the length-to-radial ratio.

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I. INTRODUCTION

It is known that carbon nanotubes (CNTs) are cylindrical macromolecules composed of carbon atoms in a periodic hexagonal arrangement. They can be produced by an array of techniques, such as arc discharge, laser ablation and chemical vapor deposition. Depending on the synthesis conditions, nanotubes can be single-walled or multiwalled. Due to their remarkable mechanical, physical, and chemical properties, CNTs have emerged as potentially attractive materials as reinforcing elements in composite materials and have drawn a great deal of attention and a good many stimulated extensive studies.¹⁻⁵ As most potential applications of CNTs are heavily based on a thorough understanding of their mechanical behavior,^{6,7} mechanical behavior of CNTs has been the subject of much recent research.⁸⁻¹²

For the sake of the difficulties in experimental characterization of nanotubes, investigation of mechanical response of CNTs by theoretical modeling has been pursued.^{13,14} The modeling for the theoretical analysis is classified into two main categories. The first one is the atomistic modeling, including the techniques such as classical molecular dynamics (MD), tight-binding molecular dynamics (TBMD), and density functional theory (DFT). However, being very time consuming and computationally expensive for large-sized atomic systems, practical applications of these atomistic modeling techniques are very limited. In order to derive theoretical analysis for large-sized atomic systems, it is desirable to develop continuum theories that may overcome the limitations of atomistic simulations concerning both time and length scales. Recently, continuum mechanics models have been widely used to study carbon nanotubes.^{8,10,11,15-18}

When CNTs are subjected to external loads, the phenomenon of buckling is often observed. Hence, buckling of CNTs has been one of the topics of primary interest,^{8,16,19,20} and quite a few continuum buckling models have been presented. Yakobson *et al.*⁸ compared the results of atomistic modeling for axially compressed buckling of single-walled nanotubes (SWNTs) with a simple continuum shell model, and found that the properties of buckling given by the molecular-dynamics simulations can be predicted satisfactorily by the continuum shell model. Ru²¹ developed a multiple-elastic

beam model to study column buckling of multiwalled carbon nanotubes (MWNTs) embedded within an elastic medium. This model assumes that each of the nested, originally concentric SWNTs is an individual elastic beam, and the deflections of all elastic beams are coupled through the van der Waals interaction between adjacent nanotubes. Wang *et al.*²² gave a systematic analysis of axially compressed buckling of MWNTs subjected to radial internal or external pressure based on a multiple-elastic shell model.²³ It was shown that the predicted increase of the critical axial stress due to an internal radial pressure appears to be in qualitative agreement with some known results obtained by molecular dynamics simulations.

Although the classic continuum models, especially the elastic models, provide simple formulas in many important cases which clearly identify major factors affecting mechanical behavior of carbon nanotubes, the applicability of these classical continuum models to CNTs in many cases of practical and academic interest is questionable. This has raised a major challenge to the classic continuum mechanics. To solve this issue, one can extend the continuum approach to smaller length scales by incorporating information regarding the behavior of material microstructure. This is carried out quite readily by the use of the theory of nonlocal continuum mechanics. The theory of nonlocal continuum mechanics was formally initiated by the papers of Eringen²⁴ and Eringen and Edelen²⁵ on nonlocal elasticity. While the classical (local) continuum mechanics assumes that the stress state at a given point is dependent uniquely on the strain state at that same point, the theory of nonlocal continuum mechanics regards the stress state at a given point as a function of the strain states of all points in the body. Thus, the theory of nonlocal continuum mechanics contains information about the long range forces between atoms, and the internal length scale is introduced into the constitutive equations simply as a material parameter.

The theory of nonlocal continuum mechanics has been applied to a wide variety of fields such as lattice dispersion of elastic waves, fracture mechanics, dislocation mechanics, wave propagation in composites, and surface tension in fluids, among others. Very recently, Peddieson *et al.*²⁶ employed the nonlocal elasticity theory to develop a nonlocal

Benoulli/Euler beam model, and it was concluded that the nonlocal continuum mechanics could potentially play a useful role in analysis related to nanotechnology applications. Based on the theory of nonlocal continuum mechanics, Sudak²⁷ derived a multiple-elastic beam model to study column buckling of MWNTs, and the significance of small-scale effects were demonstrated. In this study, the assumption that the beam consists of fibers which are in a state of uniaxial compression or tension was adopted.

In recent years, elastic beam models have been effectively applied to CNTs by many researchers. However, they are valid only for those with large aspect ratios. When aspect ratios of CNTs are small, or local deformation is concerned, CNTs should be treated as elastic shell rather than elastic beam. In this article, basic equations for axially compressed cylindrical shell are formulated on the basis of nonlocal continuum mechanics. Then, based on these nonlocal basic equations, a multiple shell model is developed for the axial buckling of MWNTs under axial compression, which includes the effect of small length scale. Finally, an explicit expression is derived for the axial buckling strain for a double-walled carbon nanotube (DWNT).

II. NONLOCAL CONTINUUM SHELL MODEL

A. Constitutive relation of the nonlocal elasticity

In the theory of nonlocal elasticity,²⁸ the stress at a reference point \mathbf{x} in the body is dependent not only on the strains at \mathbf{x} but also on strains at any other points of the body, which is in accordance with atomic theory of lattice dynamics and experimental observations on phonon dispersion. Ignoring the effects of strains at points other than \mathbf{x} , the classical (local) theory of elasticity is obtained. The most general form of the constitutive equation for nonlocal elasticity involves an integral over the entire region of interest. This integral contains a kernel function which describes the relative influences of strains at various locations on the stress at a given location.

For homogeneous and isotropic elastic solids, the constitutive equation is given by

$$\boldsymbol{\sigma}(\mathbf{x}) = \int_V \alpha(|\mathbf{x}' - \mathbf{x}|, \tau) \mathbf{t}(\mathbf{x}') dV(\mathbf{x}') \quad (1)$$

with

$$\mathbf{t}(\mathbf{x}') = \mathbf{C} : \boldsymbol{\varepsilon}(\mathbf{x}'),$$

where the symbol “:” is the inner product with double contraction, \mathbf{C} is the elastic stiffness tensor of classical isotropic elasticity, $\boldsymbol{\sigma}(\mathbf{x})$ denotes the nonlocal stress tensor at \mathbf{x} , and $\mathbf{t}(\mathbf{x}')$ is the macroscopic (classical) stress tensor at any points \mathbf{x}' in the body which is a function of the strain tensor $\boldsymbol{\varepsilon}(\mathbf{x}')$. The kernel function $\alpha(|\mathbf{x}' - \mathbf{x}|, \tau)$ is the nonlocal modulus, $|\mathbf{x}' - \mathbf{x}|$ is the Euclidean distance, and $\tau = e_0 a / l$, where e_0 is a constant appropriate to each material, a is an internal characteristic length (e.g., length of C-C bond, lattice spacing, granular distance), and l is an external characteristic length (e.g., crack length, wavelength). It should be noted that the value of e_0 needs to be determined from experiments or by

matching dispersion curves of plane waves with those of atomic lattice dynamics. In addition, the volume integral in Eq. (1) is over the region V occupied by the body.

As the constitutive equation of nonlocal elasticity involves spatial integrals which represent weighted averages of the contributions of the strain tensors of all points in the body to the stress tensor at the given point, it is difficult mathematically to get the solution of nonlocal elasticity problems. However, it is pointed out by Eringen²⁸ that the integral constitutive equation can be converted exactly into an equivalent differential form for some kernels. This, of course, provides a great deal of simplicity and convenience for the application of the theory of nonlocal elasticity. In what follows, the following form for the kernel function:

$$\alpha(|\mathbf{x}|, \tau) = (2\pi l^2 \tau^2)^{-1} K_0(\sqrt{\mathbf{x} \cdot \mathbf{x}} / l \tau)$$

will be adopted, which was suggested by Eringen.²⁸ In this equation, K_0 is the modified Bessel function. With this form of the kernel function, we have

$$(1 - \tau^2 l^2 \nabla^2) \boldsymbol{\sigma} = \mathbf{t}. \quad (2)$$

This is the singular differential constitutive equation developed by Eringen.²⁸

B. Basic equations of cylindrical shells

In this section, we consider infinitesimal axially compressed buckling of a single-layer cylindrical shell with radius of curvature R and thickness h . In the derivation of the shell equations, we assume that the shell is thin, lateral deflections are small compared to the thickness of the shell, and lines normal to the middle surface of the shell before bending remain straight and normal during bending. The material of the shell is regarded as homogeneous, isotropic, and elastic. The coordinate system is chosen so that the origin is in the middle surface of the shell, the x direction is parallel to the axis of the cylinder, the θ direction is tangent to a circular arc, and the z direction is normal to the median surface. Regarding the behavior of thin shells, it is customary to suppose that the normal stress σ_z , the corresponding strain ε_z , and the shear strains ε_{xz} and $\varepsilon_{\theta z}$ are negligible. As a consequence, the thin shell can be treated as a two-dimensional stress problem.²⁹

Let ε_x^0 and ε_θ^0 be the membrane strains due to uniform axial pressures prior to buckling. If u , v , and w denote the additional displacements of the middle surface due to buckling, along x , θ , and the inward normal direction of the shell, respectively, the total membrane strains can be expressed as³⁰

$$\varepsilon_x = \varepsilon_x^0 + \frac{\partial u}{\partial x}, \quad \varepsilon_\theta = \varepsilon_\theta^0 + \frac{1}{R} \frac{\partial v}{\partial \theta} - \frac{w}{R}, \quad \varepsilon_{x\theta} = \frac{1}{2} \left[\frac{1}{R} \frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial x} \right]. \quad (3)$$

In order to capture the essential features and the analytical solutions for the buckling of cylindrical shells by the use of theory of nonlocal elasticity, simplifying assumptions are obviously required. To this end, we assume that $\partial \sigma_x / \partial \theta = \partial \sigma_\theta / \partial x = 0$. Thus, it follows from Eq. (2) that

$$\sigma_x - (e_0a)^2 \frac{\partial^2 \sigma_x}{\partial x^2} = \frac{E}{1-\nu^2} (\varepsilon_x + \nu \varepsilon_\theta), \quad (4a)$$

$$\sigma_\theta - (e_0a)^2 \frac{1}{R^2} \frac{\partial^2 \sigma_\theta}{\partial \theta^2} = \frac{E}{1-\nu^2} (\varepsilon_\theta + \nu \varepsilon_x), \quad (4b)$$

$$\sigma_{x\theta} - (e_0a)^2 \left(\frac{\partial^2 \sigma_{x\theta}}{\partial x^2} + \frac{1}{R^2} \frac{\partial^2 \sigma_{x\theta}}{\partial \theta^2} \right) = \frac{E}{1+\nu} \varepsilon_{x\theta}, \quad (4c)$$

where E and ν are the Young's modulus and Poisson's ratio of the material, respectively. As can be seen, Eq. (4) reverts to Hooke's law of classical elasticity for a two-dimensional stress problem when the small scale parameter a vanishes. Following Eq. (4), the total membrane forces can be obtained by

$$N_x - (e_0a)^2 \frac{\partial^2 N_x}{\partial x^2} = K(\varepsilon_x + \nu \varepsilon_\theta), \quad (5a)$$

$$N_\theta - (e_0a)^2 \frac{1}{R^2} \frac{\partial^2 N_\theta}{\partial \theta^2} = K(\varepsilon_\theta + \nu \varepsilon_x), \quad (5b)$$

$$N_{x\theta} - (e_0a)^2 \left(\frac{\partial^2 N_{x\theta}}{\partial x^2} + \frac{1}{R^2} \frac{\partial^2 N_{x\theta}}{\partial \theta^2} \right) = K(1-\nu) \varepsilon_{x\theta}, \quad (5c)$$

where

$$N_x = \sigma_x h, \quad N_\theta = \sigma_\theta h, \quad N_{x\theta} = \sigma_{x\theta} h \quad (6)$$

and

$$K = \frac{Eh}{1-\nu^2}. \quad (7)$$

Substituting Eq. (3) into Eq. (5) gives

$$N_x = K \left(\frac{\partial u}{\partial x} + \frac{\nu}{R} \frac{\partial v}{\partial \theta} - \nu \frac{w}{R} \right) + (e_0a)^2 \frac{\partial^2 N_x}{\partial x^2} + K(\varepsilon_x^0 + \nu \varepsilon_\theta^0) = N'_x + N_{x^0}, \quad (8a)$$

$$N_\theta = K \left(\nu \frac{\partial u}{\partial x} + \frac{1}{R} \frac{\partial v}{\partial \theta} - \frac{w}{R} \right) + (e_0a)^2 \frac{1}{R^2} \frac{\partial^2 N_\theta}{\partial \theta^2} = N'_\theta, \quad (8b)$$

$$N_{x\theta} = \frac{1}{2} K(1-\nu) \left(\frac{1}{R} \frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial x} \right) + (e_0a)^2 \left(\frac{\partial^2 N_{x\theta}}{\partial x^2} + \frac{1}{R^2} \frac{\partial^2 N_{x\theta}}{\partial \theta^2} \right) = N'_{x\theta}, \quad (8c)$$

where N'_x , N'_θ , and $N'_{x\theta}$ are the membrane forces due to buckling, and N_{x^0} is the only nonzero membrane force prior to buckling under a uniform axial compression.

The moments M_x , M_θ , and $M_{x\theta}$ are caused by normal and shear stresses, and their magnitude is proportional to the distance of the stress from the middle surface. Consequently,

$$M_x = \int_{-h/2}^{h/2} \sigma_x z dz, \quad M_\theta = \int_{-h/2}^{h/2} \sigma_\theta z dz, \quad (9)$$

$$M_{x\theta} = - \int_{-h/2}^{h/2} \sigma_{x\theta} z dz.$$

Substitution of Eq. (4) into Eq. (9) yields

$$M_x = -D \left(\frac{\partial^2 w}{\partial x^2} + \frac{\nu}{R^2} \frac{\partial^2 w}{\partial \theta^2} \right) + (e_0a)^2 \frac{\partial^2 M_x}{\partial x^2}, \quad (10a)$$

$$M_\theta = -D \left(\frac{1}{R^2} \frac{\partial^2 w}{\partial \theta^2} + \nu \frac{\partial^2 w}{\partial x^2} \right) + (e_0a)^2 \frac{1}{R^2} \frac{\partial^2 M_\theta}{\partial \theta^2}, \quad (10b)$$

$$M_{x\theta} = D(1-\nu) \frac{1}{R} \frac{\partial^2 w}{\partial x \partial \theta} + (e_0a)^2 \left(\frac{\partial^2 M_{x\theta}}{\partial x^2} + \frac{1}{R^2} \frac{\partial^2 M_{x\theta}}{\partial \theta^2} \right), \quad (10c)$$

where use is made of

$$\varepsilon_x = -z \frac{\partial^2 w}{\partial x^2}, \quad \varepsilon_\theta = -z \frac{1}{R^2} \frac{\partial^2 w}{\partial \theta^2}. \quad (11)$$

In Eq. (10), the parameter D is the effective bending stiffness of the shell, which is expressed as

$$D = \frac{Eh^3}{12(1-\nu^2)}. \quad (12)$$

It should be pointed out that it is questionable if Eq. (12) is applied directly as the effective bending stiffness of nanotubes in elastic shell model. As noted by Yakobson *et al.*,⁸ the actual bending stiffness of SWNTs is much lower than that given by Eq. (12) if the thickness h is substituted by the representative thickness $h=0.34$ nm. From the study of SWNTs, the effective bending stiffness is $D=0.85$ eV while the in-plane stiffness is $Eh=360$ J/m².^{8,31}

The condition that the sum of the moments about the x direction must vanish gives²⁹

$$\frac{1}{R} \frac{\partial M_\theta}{\partial \theta} - \frac{\partial M_{x\theta}}{\partial x} - Q_\theta = 0, \quad (13)$$

where Q_θ is the component in the z direction of the shearing force in the transverse section perpendicular to θ direction. Similarly, moment equilibrium about the θ direction leads to

$$\frac{\partial M_x}{\partial x} - \frac{1}{R} \frac{\partial M_{x\theta}}{\partial \theta} - Q_x = 0, \quad (14)$$

where Q_x is the component in the z direction of the shearing force in the transverse section perpendicular to x axis. The equation of equilibrium in the z direction is expressed as

$$\frac{\partial Q_x}{\partial x} + \frac{1}{R} \frac{\partial Q_\theta}{\partial \theta} + (N'_x + N_{x^0}) \frac{\partial^2 w}{\partial x^2} + N'_\theta \frac{1}{R} \left(1 + \frac{1}{R} \frac{\partial^2 w}{\partial \theta^2} \right) + 2N'_{x\theta} \frac{1}{R} \frac{\partial^2 w}{\partial x \partial \theta} + p = 0, \quad (15)$$

where p denotes the net (inward) normal pressure at buckling. In Eq. (15) the initial curvature and the primary middle-surface forces are quantities of finite magnitude. By compari-

son, the curvatures due to bending and the secondary middle-surface forces are infinitesimally small. It is therefore possible to neglect some of the terms in Eq. (15) and reduce it to the form

$$\frac{\partial Q_x}{\partial x} + \frac{1}{R} \frac{\partial Q_\theta}{\partial \theta} + N_x^0 \frac{\partial^2 w}{\partial x^2} + \frac{1}{R} \frac{Eh}{1-\nu^2} \left(\frac{1}{R} \frac{\partial v}{\partial \theta} - \frac{w}{R} + \nu \frac{\partial v}{\partial x} \right) + p = 0. \quad (16)$$

A combination of Eqs. (8), (10), (13), (14), and (16) yields

$$D \nabla_R^8 w + (e_0 a)^2 \nabla_R^4 \eta - N_x^0 \frac{\partial^2}{\partial x^2} \nabla_R^4 w + \frac{Eh}{R^2} \frac{\partial^4 w}{\partial x^4} - \nabla_R^4 p = 0, \quad (17)$$

where

$$\eta = \nabla_R^2 p + N_x^0 \left(\frac{\partial^4 w}{\partial x^4} + \frac{1}{R^2} \frac{\partial^4 w}{\partial x^2 \partial \theta^2} \right), \quad \nabla_R^2 = \frac{\partial^2}{\partial x^2} + \frac{1}{R^2} \frac{\partial^2}{\partial \theta^2}, \quad (18)$$

and use is made of the following relations:

$$\nabla_{Ru}^4 = \frac{\nu}{R} \frac{\partial^3 w}{\partial x^3} - \frac{1}{R^3} \frac{\partial^3 w}{\partial \theta^2 \partial x}, \quad \nabla_{Rv}^4 = \frac{\nu+2}{R^2} \frac{\partial^3 w}{\partial x^2 \partial \theta} + \frac{1}{R^4} \frac{\partial^3 w}{\partial \theta^3}. \quad (19)$$

It can be observed that when the small scale parameter a vanishes, Eq. (17) reduces to the classical result.¹¹

C. Multiple shell model

The present work studies axially compressed buckling of a thin MWNT (the innermost radius-to-thickness ratio is larger than five) under axial pressure. It is known that MWNTs are distinguished from traditional elastic shells by their hollow multilayer structure and the associated van der Waals forces. As all nested tubes are originally concentric and the initial interlayer spacing is equal or very close to the equilibrium spacing, the initial van der Waals interaction between two tubes of undeformed MWNTs can be overlooked. When the external load applies, the interlayer spacing changes, and any increase (or decrease) in the interlayer spacing will cause an attractive (or repulsive) van der Waals interaction. Assuming $p_{i(i+1)}$ denotes the pressure on tube i due to tube $i+1$, which is positive inward and can be expressed by¹¹

$$p_{i(i+1)} = c(w_{i+1} - w_i) \quad (i = 1, 2, \dots, N-1), \quad (20)$$

where the subscripts $1, 2, \dots, N$ denote the quantities of the innermost tube, its adjacent tube, ... and the outermost tube, respectively, w_i is the (inward) deflection of the i th tube, and c is the van der Waals interaction coefficient, which can be estimated by²²

$$c = \frac{320 \text{ erg/cm}^2}{0.16d^2} \quad (d = 0.142 \text{ nm}). \quad (21)$$

Let $p_{(i+1)i}$ stand for the pressure on tube $i+1$ due to tube i , it can be obtained by

$$p_{(i+1)i} = -\frac{R_i}{R_{i+1}} p_{i(i+1)}, \quad (22)$$

where R_i is the radius of tube i .

In what follows, all nested tubes are assumed to have the same thickness and effective material constants. Applying Eq. (17) to each concentric tube of a MWNT, the buckling is governed by the N coupled equations

$$D \nabla_j^8 w_j = \nabla_j^4 \left[p_{j(j+1)} - \frac{R_{j-1}}{R_j} p_{(j-1)j} \right] - (e_0 a)^2 \nabla_j^4 \eta_j + N_x^0 \frac{\partial^2}{\partial x^2} \nabla_j^4 w_j - \frac{Eh}{R_j^2} \frac{\partial^4 w_j}{\partial x^4} \quad (23)$$

with

$$\eta_j = \nabla_j^2 \left[p_{j(j+1)} - \frac{R_{j-1}}{R_j} p_{(j-1)j} \right] + N_x^0 \left(\frac{\partial^4 w_j}{\partial x^4} + \frac{1}{R_j^2} \frac{\partial^4 w_j}{\partial x^2 \partial \theta^2} \right), \quad (24)$$

where $j=1, 2, \dots, N$, and the values of R_0 , p_{01} , and $p_{N(N+1)}$ are defined to be zero. In addition, the axial force N_x^0 is uniform over all nested tubes, and

$$\nabla_j^2 = \frac{\partial^2}{\partial x^2} + \frac{1}{R_j^2} \frac{\partial^2}{\partial \theta^2}. \quad (25)$$

Combining Eqs. (20), (23), and (24) gives N coupled linear equations for N deflections w_j .

III. BUCKLING ANALYSIS

In what follows, the buckling of a double-walled carbon nanotube (DWNT) is studied, and a condition for its critical axial buckling strain is derived. For DWNTs, it follows from Eqs. (20), (23), and (24) that

$$D \nabla_1^8 w_1 = c \nabla_1^4 (w_2 - w_1) - (e_0 a)^2 \nabla_1^4 \eta_1 + N_x^0 \frac{\partial^2}{\partial x^2} \nabla_1^4 w_1 - \frac{Eh}{R_1^2} \frac{\partial^4 w_1}{\partial x^4}, \quad (26a)$$

$$D \nabla_2^8 w_2 = c \frac{R_1}{R_2} \nabla_2^4 (w_1 - w_2) - (e_0 a)^2 \nabla_2^4 \eta_2 + N_x^0 \frac{\partial^2}{\partial x^2} \nabla_2^4 w_2 - \frac{Eh}{R_2^2} \frac{\partial^4 w_2}{\partial x^4}, \quad (26b)$$

with

$$\eta_1 = c \nabla_1^2 (w_2 - w_1) + N_x^0 \left(\frac{\partial^4 w_1}{\partial x^4} + \frac{1}{R_1^2} \frac{\partial^4 w_1}{\partial x^2 \partial \theta^2} \right), \quad (27a)$$

$$\eta_2 = c \frac{R_1}{R_2} \nabla_2^2 (w_1 - w_2) + N_x^0 \left(\frac{\partial^4 w_2}{\partial x^4} + \frac{1}{R_2^2} \frac{\partial^4 w_2}{\partial x^2 \partial \theta^2} \right). \quad (27b)$$

It is seen that the van der Waals interaction makes Eqs. (26a) and (26b) coupled. When the small length scale parameter a vanishes, Eq. (26) reduces to the known local result at the same condition.¹¹

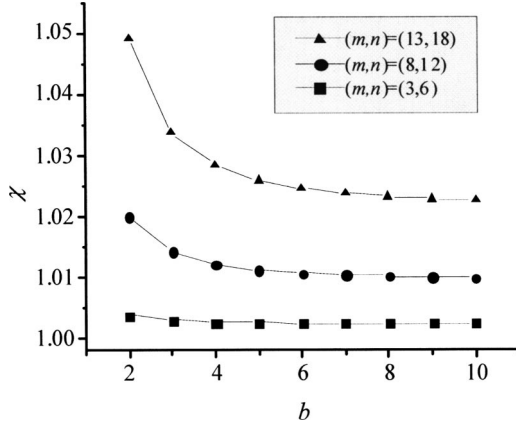


FIG. 1. Effect of the small length scale on the axial buckling strain for various buckling modes.

Considering the boundary conditions corresponding to simply supported ends, we have

$$w_1 = A_1 \sin \frac{m\pi x}{L} \sin n\theta, \quad w_2 = A_2 \sin \frac{m\pi x}{L} \sin n\theta, \quad (28)$$

where A_1 and A_2 are real constants, L is the length of the DWNT, m is the number of half-waves in the longitudinal direction, and n is the number of half-waves in the circumferential direction. Substitution of Eq. (28) into Eqs. (26) and (27) yields

$$\left[D\lambda_1^4 + c\lambda_1^2 + (e_0a)^2 c\lambda_1^3 + \frac{Eh}{R_1^2} \omega^4 + (1 + e_0^2 a^2 \lambda_1) N_x^0 \omega^2 \lambda_1^2 \right] A_1 - c\lambda_1^2 (1 + e_0^2 a^2 \lambda_1) A_2 = 0, \quad (29a)$$

$$c \frac{R_1}{R_2} \lambda_2^2 (1 + e_0^2 a^2 \lambda_2) A_1 - \left[D\lambda_2^4 + c \frac{R_1}{R_2} \lambda_2^2 + (e_0a)^2 c \frac{R_1}{R_2} \lambda_2^3 + \frac{Eh}{R_2^2} \omega^4 + (1 + e_0^2 a^2 \lambda_2) N_x^0 \omega^2 \lambda_2^2 \right] A_2 = 0, \quad (29b)$$

with

$$\lambda_1 = \frac{m^2 \pi^2}{L^2} + \frac{n^2}{R_1^2}, \quad \lambda_2 = \frac{m^2 \pi^2}{L^2} + \frac{n^2}{R_2^2}, \quad \omega = \frac{m\pi}{L}. \quad (30)$$

In order to determine the critical axial compressive buckling strain, it is necessary to obtain the nontrivial solution of Eq. (29), which leads to the following relation:

$$X \left(\frac{N_x^0}{Eh} \right)^2 + Y \frac{N_x^0}{Eh} + Z = 0 \quad (31)$$

with

$$X = E^2 h^2 (1 + e_0^2 a^2 \lambda_1)^2 \omega^4 \lambda_1^4, \quad (32a)$$

$$Y = 2Eh\omega^2 \Delta (1 + e_0^2 a^2 \lambda_1) \lambda_1^2, \quad (32b)$$

$$Z = \Delta^2 - c^2 \lambda_1^4 (1 + e_0^2 a^2 \lambda_1)^2, \quad (32c)$$

where

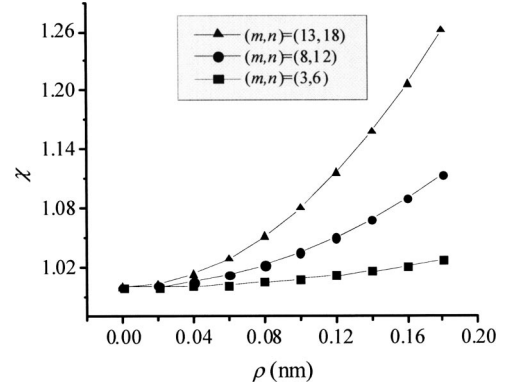


FIG. 2. Relationship between the effect of the small length scale and parameter ρ .

$$\Delta = D\lambda_1^4 + c\lambda_1^2 + e_0^2 a^2 c\lambda_1^3 + \frac{Eh}{R_1^2} \omega^4. \quad (33)$$

As the radii of MWNTs are usually not less than a few nanometers and thus at least one order of magnitude larger than the interlayer spacing which is about 0.34 nm,^{9,32,33} all terms proportional to the ratio $(R_2 - R_1)/R_1$ can be assumed to be small, and then have been ignored in Eq. (32). Combining Eqs. (31) and (32), the axial compressive buckling strain can be obtained by

$$-\frac{N_x^0}{Eh} = \frac{\Delta - c\lambda_1^2 (1 + \lambda_1 e_0^2 a^2)}{Eh(1 + \lambda_1 e_0^2 a^2) \omega^2 \lambda_1^2} \quad (34)$$

which includes the small length scale effect. Thus, the critical axial compressive buckling strain can be determined by minimizing the right-hand side of the above equation with respect of the integers m and n .

IV. DISCUSSION

To illustrate the influence of the small length scale on the axial buckling strain of a DWNT, the van der Waals forces are ignored for simplicity. For this case, Eq. (34) reduces to

$$-\frac{N_x^0}{Eh} = \frac{DR_1^2 \lambda_1^4 + Eh\omega^4}{EhR_1^2 \omega^2 \lambda_1^2 (1 + \lambda_1 e_0^2 a^2)}. \quad (35)$$

Neglecting the small length scale effect, the above equation reduces to the classic (local) result²⁹

$$-\frac{N_x^0}{Eh} = \frac{DR_1^2 \lambda_1^4 + Eh\omega^4}{EhR_1^2 \omega^2 \lambda_1^2}. \quad (36)$$

It can be observed that Eq. (35) gives a smaller axial buckling strain than the classic result given by Eq. (36). In other words, the classic result could overestimate the axial buckling strain.

To further examine the effect of the small length scale on the axial buckling strain, let us consider the ratio χ of the buckling strain predicted by Eq. (36) to that given by Eq. (35). It follows from these two equations that

$$\chi = 1 + (\pi^2 m^2 + n^2 b^2) \frac{e_0^2 a^2}{b^2 R_1^2}, \quad (37)$$

where b is the length-to-radial ratio, which is defined as

$$b = L/R_1. \quad (38)$$

It should be pointed out that the value of parameter e_0 has not been obtained for carbon nanotubes at present. The value of parameter a can be chosen to be the length of a C-C bond which is equal to 0.142 nm. If we assume that $R_1=6.8$ nm and the value of parameter e_0 is 0.39 which was given by Eringen,²⁸ the influence of the small length scale on the axial buckling strain can be obtained from Eq. (37), as shown in Fig. 1. It is found that the effect of the small length scale on the axial buckling strain is dependent on the buckling mode and the length-to-radial ratio. With the same buckling mode, the degree of influence of the small length scale on the axial buckling strain decreases with increasing the length-to-radius ratio. If the tube length is assumed to be 40 nm, the relation between the ratio χ and parameter ρ ($\rho=e_0 a$) is obtained from Eq. (37), which is shown in Fig. 2. As can be seen, the axial buckling strain decreases compared to the classical result as the small length scale parameter ρ increases in magnitude. In other words, the effect of the small length scale on the axial buckling strain becomes more significant as parameter ρ becomes larger. As parameter a remains fixed, parameter e_0 increases with increasing parameter ρ . Consequently,

a larger value of e_0 implies a more significant influence of small length scale on the axial buckling strain.

V. CONCLUSIONS

Based on the theory of nonlocal continuum mechanics, basic equations for axially compressed cylindrical shell are formulated. Following these nonlocal basic equations, a multiple shell model is developed for the axial buckling of MWNTs under axial compression, which takes account of the effects of small length scale. An explicit expression is derived for the axial buckling strain for a double-walled carbon nanotube.

The influence of the small length scale on the axial buckling strain is discussed. The effect of small length scale on the axial buckling strain is related to the buckling mode and the length-to-radial ratio. The degree of influence of the small length scale varies with the buckling mode and the length-to-radius ratio. Although the value of parameter e_0 remains unknown for carbon nanotubes, it is clear from the results that a larger value of e_0 implies a more significant effect of the small length scale.

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