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Accurate modeling of buckling of single- and double-walled carbon nanotubes based on shell theories

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Abstract
The accuracy of widely employed classical shell-theory-based formulae to calculate the buckling strain of single- and double-walled carbon nanotubes is assessed here. It is noted that some simplifications have been made in deriving these widely employed formulae. As a result critical buckling strains calculated from these formulae are independent of aspect ratio (length/diameter). However, molecular dynamics simulation results in the literature show an aspect ratio dependence of buckling strain. Therefore, analytical expressions are derived in this paper to calculate buckling strains of single- and double-walled carbon nanotubes based on classical shell theory without simplifications. Applicability of these expressions is further verified through molecular dynamics simulations based on the COMPASS force field. In addition, improvement in results achieved through a refinement of classical shell theory is assessed by calculating buckling strains based on first-order shell theory. Results show that simplified formulae introduce a significant error at higher aspect ratios and smaller diameters. The formulae derived here show reasonable agreement with the molecular dynamics results at all aspect ratios and diameters. First-order shell theory is found to produce a slight improvement in results for CNTs with smaller diameters and lower aspect ratios.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In the last decade, there have been many studies that were devoted to the mechanical characterization of carbon nanotubes (CNTs). Experiments, quantum mechanics and continuum mechanics were the major tools employed in these studies. Due to the nanometer size, conducting experiments on CNTs has become a difficult task and hence a limited number of studies based on experiments can be found in the literature. With the development of suitable force fields, quantum mechanics has become an accurate tool for analyzing CNTs. Moreover, the development in the field of computers has make quantum mechanics a feasible option. However, quantum mechanics still remains an expensive tool for CNTs with a larger number of atoms such as multi-walled carbon nanotubes (MWCNTs). Therefore, developing continuum mechanics models to analyze CNTs is a primary interest of researchers. However, the accuracy of the results provided by continuum mechanics models is still questionable. Continuum mechanics modeling of CNTs involve beam or shell models associated with analytical or numerical techniques. In this paper, we will concentrate only on analytical shell modeling of CNTs.

Buckling of CNTs is one of the areas subjected to a great deal of attention by researchers. Many studies can be found based on atomistic simulations, continuum mechanics modeling as well as a molecular structural mechanics approach. However, there are many discrepancies among the existing results. One such major discrepancy is that most of the MDS-based studies (Li and Chou 2004, Liew *et al* 2004, Wang *et al* 2005, Sears and Batra 2006, Zhang *et al* 2009) report an aspect ratio dependence of buckling strain while hardly any of the continuum-shell-model-based studies capture this point. Most of the previous studies involving shell theory employed the formula given in equation (1) to calculate axial buckling strain of single-walled carbon nanotubes (Yokobson *et al* 1996, Xiao *et al* 2004):

$$\varepsilon_{\text{cr}} = \frac{2}{\sqrt{3(1-\nu^2)}}\frac{h}{d} \tag{1}$$

where ε_{cr} is the axial buckling strain, h is the thickness, d is the diameter and ν is Poisson's ratio.

This formula is for axisymmetric buckling of thin cylindrical shells. However, it is evident from MDS results that buckling of single-walled carbon nanotubes (SWCNT) is mostly non-axisymmetric (Yokobson *et al* 1996, Cornwell and Wille 1997, Buehler *et al* 2004, Wang *et al* 2005). Moreover, this formula is clearly independent of aspect ratio.

Ru (2000a) employed a formula derived by Timoshenko and Gere (1961) to calculate non-axisymmetric buckling strain of simply supported SWCNTs. This formula is given in equation (2):

$$\frac{N_x}{Eh} = \frac{D}{Eh\alpha^2}[\alpha^2+\beta^2]^2 + \frac{1}{\alpha^2 R^2}\left[\frac{\alpha^2}{\alpha^2+\beta^2}\right]^2. \tag{2}$$

Based on similar derivations as for equation (2), expressions given in equations (3) and (4) have been developed by several researchers (He *et al* 2005a, Zhang *et al* 2006) to calculate the buckling strain of double-walled carbon nanotubes (DWCNTs):

$$\frac{\hat{N}}{Eh} = \frac{\left[\frac{\Delta_1}{\lambda_1^2}+\frac{\Delta_2}{\lambda_2^2}\right] - \sqrt{\left[\frac{\Delta_1}{\lambda_1^2}-\frac{\Delta_2}{\lambda_2^2}\right]^2 + 4c_{12}c_{21}}}{2Eh\alpha^2} \tag{3}$$

where

$$\begin{gathered}\Delta_1 = D\lambda_1^4 + c_{12}\lambda_1^2 + \frac{Eh}{R_1^2}\alpha^4,\\ \Delta_2 = D\lambda_2^4 + c_{21}\lambda_2^2 + \frac{Eh}{R_2^2}\alpha^4\\ \lambda_1 = \alpha^2 + (\beta_1)^2, \qquad \lambda_2 = \alpha^2 + (\beta_2)^2\\ \alpha = \frac{m\pi}{L}, \qquad \beta_1 = \frac{n}{R_1}, \qquad \beta_2 = \frac{n}{R_2}.\end{gathered} \tag{4}$$

Here, $\hat{N}$ is the axial load per unit circumferential length, E is the Young's modulus, D is the bending stiffness, R_1 and R_2 are the inner and outer tube radii, L is the length of tube, m and n are the longitudinal and circumferential wavenumbers, and c_{12} and c_{21} are the vdW coefficients of inner and outer tubes.

It is noted that, in deriving these formulae given in equations (2)–(4), several terms have been omitted assuming that the ratio (longitudinal wavenumber/aspect ratio) is a large value (Timoshenko and Gere 1961). As a result of these simplifications, at larger aspect ratios these simplified expressions lead to a significant error. Moreover, in contrast to the MDS results, minimum buckling strain values calculated from these formulae appear to be almost insensitive to the aspect ratio of the tube. In order to assess the error introduced by these simplifications, in this paper, analytical expressions are derived for buckling strain based on classical shell theory without simplifications. Moreover, analytical expressions based on first-order shell theory are also derived here. First-order shell theory accounts for shear deformation and hence improvement of results can be expected for CNTs with smaller diameters and lower aspect ratios in which shear deformation is significant. Molecular dynamics simulations based on the COMPASS force field are also conducted to verify the accuracy of the derived expressions.

Table 1. Strain–displacement relations.

Strains	Classical shell theory	First-order shell theory
ε_x^0	$\frac{\partial u}{\partial x}$	$\frac{\partial u}{\partial x}$
ε_θ^0	$\frac{1}{R}\frac{\partial v}{\partial \theta} + \frac{w}{R}$	$\frac{1}{R}\frac{\partial v}{\partial \theta} + \frac{w}{R}$
$\varepsilon_{x\theta}^0$	$\frac{\partial v}{\partial x} + \frac{1}{R}\frac{\partial u}{\partial \theta}$	$\frac{\partial v}{\partial x} + \frac{1}{R}\frac{\partial u}{\partial \theta}$
$\varepsilon_{\theta z}^0$	—	$\varphi_\theta + \frac{1}{R}\frac{\partial w}{\partial \theta} - \frac{v}{R}$
ε_{xz}^0	—	$\varphi_x + \frac{\partial w}{\partial x}$
ε_x^1	$-\frac{\partial^2 w}{\partial x^2}$	$\frac{\partial \varphi_x}{\partial x}$
ε_θ^1	$\frac{1}{R^2}\left(\frac{\partial v}{\partial \theta} - \frac{\partial^2 w}{\partial \theta^2}\right)$	$\frac{1}{R}\frac{\partial \varphi_\theta}{\partial \theta}$
$\varepsilon_{x\theta}^1$	$\frac{1}{R}\left(\frac{\partial v}{\partial x} - 2\frac{\partial^2 w}{\partial x \partial \theta}\right)$	$\frac{\partial \varphi_\theta}{\partial x} + \frac{1}{R}\frac{\partial \varphi_x}{\partial \theta}$

2. Axial buckling strain of SWCNTs based on shell theories

The analytical expressions for buckling strain are derived in this paper starting from the equilibrium equations, stress–strain relations and strain–displacement relations. Stress resultants–strain relations and strain–displacement relations employed in this paper for two shell theories are given in tables 1 and 2, respectively. Equilibrium equations for two shell theories are given in equations (5)–(12). All these equations were taken from Reddy (2004, 2007). x, θ and z represent the axial, circumferential and thickness directions, respectively (z positive in the outward direction). u, v and w are the displacements in the x, θ and z directions while φ_x and φ_θ are rotations of the transverse normal about the θ and x axes. ε_i^0 denotes membrane strains while ε_i^1 denotes flexural strains.

For isotropic shells

$$Q_{11} = Q_{22} = \frac{E}{(1-\upsilon^2)}, \qquad Q_{12} = \frac{\upsilon E}{(1-\upsilon^2)},$$

$$Q_{44} = Q_{55} = Q_{66} = \frac{E}{2(1+\upsilon)}$$

$$(A_{ij}, B_{ij}, D_{ij}, E_{ij}, F_{ij}, H_{ij}) = \int_{-h/2}^{h/2} Q_{ij}(1, z, z^2, z^3, z^4, z^6)\,\mathrm{d}z$$

for $i, j = 1, 2, 4, 5, 6$.

Equilibrium equations from classical shell theory are

$$\frac{\partial N_{xx}}{\partial x} + \frac{1}{R}\frac{\partial N_{x\theta}}{\partial \theta} = 0 \tag{5}$$

$$\frac{\partial N_{x\theta}}{\partial x}+\frac{1}{R}\frac{\partial N_{\theta\theta}}{\partial\theta}+\frac{1}{R}\left(\frac{\partial M_{x\theta}}{\partial x}+\frac{1}{R}\frac{\partial M_{\theta\theta}}{\partial\theta}\right)=0 \tag{6}$$

$$\frac{\partial}{\partial x}\left(\frac{\partial M_{xx}}{\partial x}+\frac{1}{R}\frac{\partial M_{\theta x}}{\partial\theta}\right)+\frac{1}{R}\frac{\partial}{\partial\theta}\left(\frac{\partial M_{x\theta}}{\partial x}+\frac{1}{R}\frac{\partial M_{\theta\theta}}{\partial\theta}\right)$$
$$-\frac{N_{\theta\theta}}{R}-\hat{N}\frac{\partial^2 w}{\partial x^2}+p=0. \tag{7}$$

Equilibrium equations from first-order shell theory are

$$\frac{\partial N_{xx}}{\partial x}+\frac{1}{R}\frac{\partial N_{x\theta}}{\partial\theta}=0 \tag{8}$$

$$\frac{\partial N_{x\theta}}{\partial x}+\frac{1}{R}\frac{\partial N_{\theta\theta}}{\partial\theta}+\frac{Q_\theta}{R}=0 \tag{9}$$

$$\frac{\partial Q_x}{\partial x}+\frac{1}{R}\frac{\partial Q_\theta}{\partial\theta}-\frac{N_{\theta\theta}}{R}-\hat{N}\frac{\partial^2 w}{\partial x^2}+p=0 \tag{10}$$

$$\frac{\partial M_{xx}}{\partial x}+\frac{1}{R}\frac{\partial M_{\theta x}}{\partial\theta}-Q_x=0 \tag{11}$$

$$\frac{\partial M_{x\theta}}{\partial x}+\frac{1}{R}\frac{\partial M_{\theta\theta}}{\partial\theta}-Q_\theta=0. \tag{12}$$

Here, $\hat{N}$ is the axial compressive load per unit circumferential length and p is the radial pressure.

In deriving buckling strain solutions, firstly the equilibrium equations based on each shell theory are rewritten in terms of displacements by substituting strain–displacement and stress resultants–strain relations into equilibrium equations. Then, to solve the resulting equilibrium equations, the assumed displacement field given in equation (13) is substituted into the equilibrium equations. These assumed displacement functions satisfy simply supported boundary conditions given by $v=0$; $w=0$; $\frac{\partial^2 w}{\partial x^2}=0$; $\varphi_\theta=0$ at $x=0$ and L:

$$u=\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}U_{mn}\cos\alpha x\sin n\theta$$
$$v=\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}V_{mn}\sin\alpha x\cos n\theta$$
$$w=\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}W_{mn}\sin\alpha x\sin n\theta \tag{13}$$
$$\phi_x=\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}X_{mn}\cos\alpha x\sin n\theta$$
$$\phi_\theta=\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}Y_{mn}\sin\alpha x\cos n\theta$$

where $\alpha=\frac{m\pi}{L}$ and $\beta=\frac{n}{R}$.

Here, m and $2n$ are the number of half-waves along the length and circumference respectively.

The equilibrium equations after substitution by the displacement field are given in equations (14)–(29). Here, i represents the ith wall of a CNT and R_i represents the radius of the ith wall.

From classical shell theory

$$C_{11}^iU_{mn}^i+C_{12}^iV_{mn}^i+C_{13}^iW_{mn}^i=0 \tag{14}$$

Table 2. Stress resultants–strain relations.

Stress resultants	Classical shell theory	First-order shell theory
N_x	$A_{11}\varepsilon_x^0+A_{12}\varepsilon_\theta^0$	$A_{11}\varepsilon_x^0+A_{12}\varepsilon_\theta^0$
N_θ	$A_{12}\varepsilon_x^0+A_{22}\varepsilon_\theta^0$	$A_{12}\varepsilon_x^0+A_{22}\varepsilon_\theta^0$
$N_{x\theta}$	$A_{66}\varepsilon_{x\theta}^0$	$A_{66}\varepsilon_{x\theta}^0$
M_x	$D_{11}\varepsilon_x^1+D_{12}\varepsilon_\theta^1$	$D_{11}\varepsilon_x^1+D_{12}\varepsilon_\theta^1$
M_θ	$D_{12}\varepsilon_x^1+D_{22}\varepsilon_\theta^1$	$D_{12}\varepsilon_x^1+D_{22}\varepsilon_\theta^1$
$M_{x\theta}$	$D_{66}\varepsilon_{x\theta}^1$	$D_{66}\varepsilon_{x\theta}^1$
Q_x	—	$K_sA_{55}\varepsilon_{xz}^0$
Q_θ	—	$K_sA_{44}\varepsilon_{\theta z}^0$

$$C_{21}^iU_{mn}^i+C_{22}^iV_{mn}^i+C_{23}^iW_{mn}^i=0 \tag{15}$$

$$C_{31}^iU_{mn}^i+C_{32}^iV_{mn}^i+(C_{33}^i-\hat{N}\alpha^2)W_{mn}^i+p_i=0 \tag{16}$$

where

$$C_{11}^i=A_{11}\alpha^2+A_{66}\beta_i^2,\qquad C_{12}^i=(A_{12}+A_{66})\alpha\beta_i,$$
$$C_{13}^i=-A_{12}\frac{\alpha}{R_i} \tag{17}$$

$$C_{21}^i=C_{12}^i$$

$$C_{22}^i=A_{66}\alpha^2+A_{22}\beta_i^2+\frac{D_{22}\beta_i^2}{R_i^2}+\frac{D_{66}\alpha^2}{R_i^2} \tag{18}$$

$$C_{23}^i=-\left[\frac{A_{22}\beta_i}{R_i}+\frac{(2D_{66}+D_{12})\alpha^2\beta_i}{R_i}+\frac{D_{22}\beta_i^3}{R_i}\right]$$

$$C_{31}^i=C_{13}^i,\ C_{32}^i=C_{23}^i$$

$$C_{33}^i=D_{11}\alpha^4+D_{22}\beta_i^4+2(D_{12}+2D_{66})\alpha^2\beta_i^2+\frac{A_{22}}{R_i^2}. \tag{19}$$

From first-order shell theory

$$F_{11}^iU_{mn}^i+F_{12}^iV_{mn}^i+F_{13}^iW_{mn}^i=0 \tag{20}$$

$$F_{21}^iU_{mn}^i+F_{22}^iV_{mn}^i+F_{23}^iW_{mn}^i+F_{25}^iY_{mn}^i=0 \tag{21}$$

$$F_{31}^iU_{mn}^i+F_{32}^iV_{mn}^i+(F_{33}^i-\alpha^2\hat{N})W_{mn}^i+F_{34}^iX_{mn}^i$$
$$+F_{35}^iY_{mn}^i+p_i=0 \tag{22}$$

$$F_{43}^iW_{mn}^i+F_{44}^iX_{mn}^i+F_{45}^iY_{mn}^i=0 \tag{23}$$

$$F_{52}^iV_{mn}^i+F_{53}^iW_{mn}^i+F_{54}^iX_{mn}^i+F_{55}^iY_{mn}^i=0 \tag{24}$$

where

$$F_{11}^i=A_{11}\alpha^2+A_{66}\beta_i^2,\qquad F_{12}^i=(A_{12}+A_{66})\alpha\beta_i,$$
$$F_{13}^i=-A_{12}\frac{\alpha}{R_i} \tag{25}$$

$$F_{21}^i=F_{12}^i,\qquad F_{22}^i=\left(A_{66}\alpha^2+A_{22}\beta_i^2+\frac{K_sA_{66}}{R_i^2}\right)$$

$$F_{23}^i=-\left[\frac{\beta_i}{R_i}(A_{22}+K_sA_{66})\right],\qquad F_{25}^i=-\frac{K_sA_{66}}{R_i}=F_{52}^i \tag{26}$$

$$F_{31}^i=F_{13}^i,\qquad F_{32}^i=F_{23}^i$$

$$F_{33}^i=\left[K_sA_{66}(\alpha^2+\beta_i^2)+\frac{A_{22}}{R_i^2}\right] \tag{27}$$

$$F_{34}^i=K_sA_{66}\alpha,\qquad F_{35}^i=K_sA_{66}\beta_i$$

$$F^i_{43} = F^i_{34} \qquad F^i_{44} = (D_{11}\alpha^2 + D_{66}\beta_i^2 + K_s A_{66})$$
$$F^i_{45} = (D_{12} + D_{66})\alpha\beta_i \tag{28}$$

$$F^i_{53} = F^i_{35}, \qquad F^i_{54} = F^i_{45}$$
$$F^i_{55} = (D_{66}\alpha^2 + D_{22}\beta_i^2 + K_s A_{66}). \tag{29}$$

By solving the equilibrium equations, the expressions given in equations (30)–(37) can be obtained for the buckling strain of SWCNTs. Only the external axial compressive force is considered here and hence the radial pressure $p = 0$ for SWCNTs.

From classical shell theory

$$\frac{\hat{N}}{Eh} = \frac{1}{Eh\alpha^2}(C_{31}C_{uw} + C_{32}C_{vw} + C_{33}) \tag{30}$$

where

$$C_{uw} = \frac{C_{12}C_{23} - C_{22}C_{13}}{C_{11}C_{22} - C_{12}C_{21}} \quad \text{and}$$
$$C_{vw} = \frac{C_{21}C_{13} - C_{11}C_{23}}{C_{11}C_{22} - C_{12}C_{21}} \tag{31}$$

and $C_{kl} = C^1_{kl}$ is given in equations (17)–(19).

From first-order shell theory

$$\frac{\hat{N}}{Eh} = \frac{1}{Eh\alpha^2} \times \left[P_{11} - \frac{P_{21}P_{12}P_{33} - P_{21}P_{13}P_{32} - P_{31}P_{12}P_{23} + P_{31}P_{13}P_{22}}{(P_{22}P_{33} - P_{23}P_{32})}\right] \tag{32}$$

where

$$P_{11} = (F_{31}S_{uw} + F_{32}S_{vw} + F_{33}),$$
$$P_{12} = (F_{31}S_{uy} + F_{32}S_{vy} + F_{35}), \qquad P_{13} = F_{34} \tag{33}$$
$$P_{21} = F_{43}, \qquad P_{22} = F_{44}, \qquad P_{23} = F_{45} \tag{34}$$
$$P_{31} = F_{52}S_{vw} + F_{53}, \qquad P_{32} = F_{54},$$
$$P_{33} = F_{52}S_{vy} + F_{55} \tag{35}$$
$$S_{uw} = \frac{F_{12}F_{23} - F_{22}F_{13}}{F_{11}F_{22} - F_{12}F_{21}}, \qquad S_{uy} = \frac{F_{12}F_{25}}{F_{11}F_{22} - F_{12}F_{21}} \tag{36}$$
$$S_{vw} = \frac{F_{21}F_{13} - F_{11}F_{23}}{F_{11}F_{22} - F_{12}F_{21}}, \qquad S_{vy} = \frac{-F_{11}F_{25}}{F_{11}F_{22} - F_{12}F_{21}} \tag{37}$$

$F_{kl} = F^1_{kl}$ is given in equations (25)–(29).

3. Axial buckling strain of DWCNTs based on shell theories

In deriving the buckling strain for DWCNTs, van der Waals (vdW) interactions should be taken into account. Several vdW interaction models can be found in the literature (Ru 2000a, 2001, Wang *et al* 2003, He *et al* 2005a, 2005b). In this paper the vdW model proposed by Ru (2000a, 2001) and Wang *et al* (2003) is adopted. According to Ru (2000a, 2001) and Wang *et al* (2003), vdW pressure at any point on a wall is linearly proportional to the difference between radial deflections at that point. Thus, radial pressure due to vdW interactions on the outer and inner tubes can be given as shown in equations (38) and (39).

Consider a double-walled carbon nanotube of outer radius R_1 and inner radius R_2. Let w_i be the generalized radial displacements (z direction) and p_i be the vdW pressure associated with the ith tube ($i = 1$ and 2 refer to the outer and inner walls, respectively). c_i is the vdW coefficient of the ith wall:

$$p_1 = c_1(w_1 - w_2) \tag{38}$$
$$p_2 = c_2(w_2 - w_1). \tag{39}$$

By considering the equilibrium of forces in the z direction:

$$c_2 = c_1\frac{R_1}{R_2} \tag{40}$$

$$c_1 = \frac{320 \text{ ergs cm}^{-2}}{0.16t^2} = \frac{320 \times 10^{-7} \text{ Nm cm}^{-2}}{0.16(0.142 \text{ nm})^2}$$
$$= 99.19 \text{ GPa nm}^{-1}. \tag{41}$$

The same equilibrium equations (equations (14)–(29)) can be applied for the two walls of DWCNTs separately where p_i is replaced by equations (38) and (39). It is clear that, due to p_i, the third equilibrium equations for inner and outer walls are coupled. As in the case of SWCNTs, by solving the equilibrium equations, the following buckling strain solutions for DWCNTs based on classical and first-order theories can be obtained.

From classical shell theory

$$\frac{\hat{N}}{Eh} = \frac{(H_{11} + H_{22}) - \sqrt{(H_{11} - H_{22})^2 + 4H_{12}H_{21}}}{2Eh\alpha^2} \tag{42}$$

$$H_{11} = C^1_{31}C^1_{uw} + C^1_{32}C^1_{vw} + C^1_{33} + c_1 \qquad H_{12} = -c_1$$
$$H_{22} = C^2_{31}C^2_{uw} + C^2_{32}C^2_{vw} + C^2_{33} + c_2 \qquad H_{21} = -c_2 \tag{43}$$

C^i_{kl} is given in equations (17)–(19).

Also

$$C^i_{uw} = \frac{C^i_{12}C^i_{23} - C^i_{22}C^i_{13}}{C^i_{11}C^i_{22} - C^i_{12}C^i_{21}}, \qquad C^i_{vw} = \frac{C^i_{21}C^i_{13} - C^i_{11}C^i_{23}}{C^i_{11}C^i_{22} - C^i_{12}C^i_{21}}. \tag{44}$$

From first-order shell theory

$$\frac{\hat{N}}{Eh} = \frac{(K_{11} + K_{22}) - \sqrt{(K_{11} - K_{22})^2 + 4K_{12}K_{21}}}{2Eh\alpha^2} \tag{45}$$

where

$$K_{11} = F^1_{31}S^1_{uw} + F^1_{32}S^1_{vw} + F^1_{33} + [F^1_{31}S^1_{uy} + F^1_{32}S^1_{vy} + F^1_{35}]P^1_{yw} + F^1_{34}P^1_{xw} + c$$
$$K_{22} = F^2_{31}S^2_{uw} + F^2_{32}S^2_{vw} + F^2_{33} + [F^2_{31}S^2_{uy} + F^2_{32}S^2_{vy} + F^2_{35}]P^2_{yw} + F^2_{34}P^2_{xw} + c\frac{R_1}{R_2} \tag{46}$$
$$K_{12} = -c \qquad K_{21} = -c\frac{R_1}{R_2}$$

F^i_{kl} is given in equations (25)–(29):

$$S^i_{uw} = \frac{F^i_{12}F^i_{23} - F^i_{22}F^i_{13}}{F^i_{11}F^i_{22} - F^i_{12}F^i_{21}}, \qquad S^i_{uy} = \frac{F^i_{12}F^i_{25}}{F^i_{11}F^i_{22} - F^i_{12}F^i_{21}}$$
$$S^i_{vw} = \frac{F^i_{21}F^i_{13} - F^i_{11}F^i_{23}}{F^i_{11}F^i_{22} - F^i_{12}F^i_{21}}, \qquad S^i_{vy} = \frac{-F^i_{11}F^i_{25}}{F^i_{11}F^i_{22} - F^i_{12}F^i_{21}} \tag{47}$$

$$P^i_{xw} = \frac{P^i_1 Q^i_{22} - P^i_2 Q^i_{12}}{Q^i_{11} Q^i_{22} - Q^i_{12} Q^i_{21}}, \qquad P^i_{yw} = \frac{P^i_2 Q^i_{11} - P^i_1 Q^i_{21}}{Q^i_{11} Q^i_{22} - Q^i_{12} Q^i_{21}} \tag{48}$$

$$Q^i_{11} = F^i_{44}, \qquad Q^i_{12} = F^i_{45}, \qquad Q^i_{21} = F^i_{54}, \qquad Q^i_{22} = F^i_{52} S^i_{vy} + F^i_{55}, \tag{49}$$

$$P^i_1 = -F^i_{43}, \qquad P^i_2 = -(F^i_{52} S^i_{vw} + F^i_{53}). \tag{50}$$

4. Axial buckling strain based on molecular dynamics simulations

Molecular dynamic simulations (MDS) are conducted at 0 K using the COMPASS force field. The COMPASS force field (condensed-phase optimized molecular potentials for atomistic simulation studies) has been proven as a better force field for analyzing mechanical behavior of CNTs and has been used by many researchers (Cao and Chen 2006a, 2006b, Chen and Cao 2006, Wang *et al* 2007a, 2007b, 2008a, 2008b). This force field accounts for the cross-term interacting energy and nonbond energy as well while the other widely used force fields such as the Tersoff–Brenner potential account only for valence energy (bond energy). Moreover, parameters of the COMPASS force field are obtained from the *ab initio* quantum mechanics calculations while parameters of an empirical force field, such as Tersoff–Brenner, are obtained from experiments. Moreover, a Berendsen thermostat is employed with a displacement step of $0.05A^0$, time step of 0.5 fs and a total of 10 000 time steps.

5. Results and discussion

In order to assess the accuracy of simplified formulae given in equations (2) and (3), analytical expressions are derived here based on classical shell theory without simplifications. Moreover, expressions are derived based on first-order shell theory to investigate the effect of refinement of classical shell theory on the accuracy of buckling strain solutions. Molecular dynamic simulations are also conducted to verify the accuracy of these analytical expressions.

In these calculations, a wall thickness of 0.066 nm and Young's modulus of 5.5 TPa are used, as suggested by Yokobson *et al* (1996). Shear modulus, axial stiffness and bending stiffness are calculated based on their respective classical formulae. The nterlayer spacing of DWCNTs is considered as 0.34 nm.

5.1. Critical buckling strain of SWCNTs

Critical buckling strains calculated from the simplified formula (equation (2)), formulae derived here based on classical shell theory (equation (30)) and first-order shell theory (equation (32)) and molecular dynamic simulation (MDS) results for (8, 0) and (7, 7) SWCNTs with various aspect ratios have been plotted in figure 1.

It can be seen from the figure that the simplified formula is almost insensitive to aspect ratio, while the other two analytical expressions are highly sensitive to aspect ratio. Agreeing with the previous MDS-based work (Li and Chou 2004, Liew *et al* 2004, Wang *et al* 2005, Sears and Batra 2006, Zhang *et al* 2009), the MDS results obtained in this study are also sensitive to aspect ratio. Moreover, the critical buckling strain values obtained by Yokobson *et al* (1996) and Zhang *et al* (2009) for (7, 7) SWCNTs agree well with the value shown in figure 1(b) for the same SWCNTs. Also, the critical buckling strain value (0.073) obtained by Wang *et al* (2008a) for (8, 0) SWCNTs with an aspect ratio 3.78 agrees well with the value shown in figure 1(a) for the same SWCNTs. Thus, the MDS results obtained in this study appear to be in good agreement with the available MDS results in the literature.

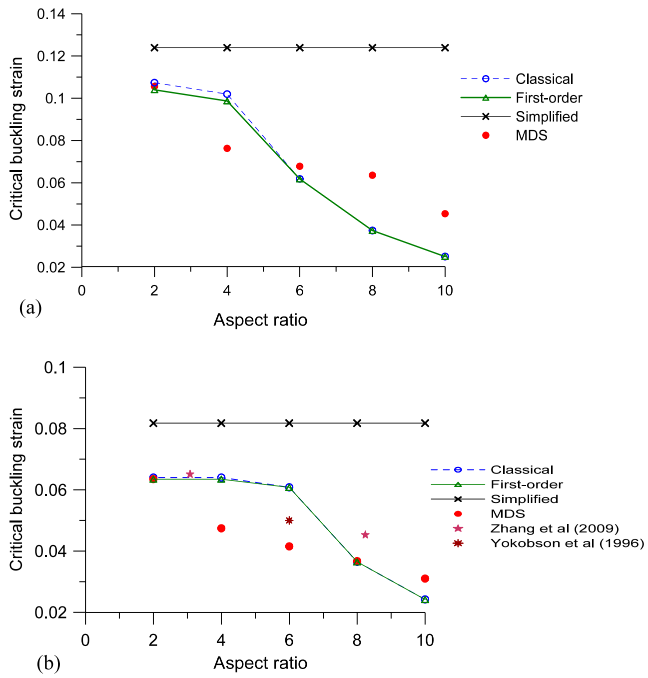

Figure 1. Critical buckling strain versus aspect ratio for SWCNTs: (a) 8, 0 and (b) 7, 7.

Buckled shapes for (7, 7) SWCNTs with aspect ratios 2, 4, 6, 8 and 10 are shown in figure 2. All the tubes in this figure show a shell buckling mode. Hence it is further convinced that aspect ratio is an important parameter for buckling strains of SWCNTs not only for beam buckling but also for shell buckling.

Also, it is noteworthy that the error introduced by the simplified formula is very significant for CNTs with higher aspect ratios (table 3 and figure 1). Moreover, a marginal improvement from the first-order shell theory can be seen for CNTs at lower aspect ratio where the effect of shear deformation is usually significant.

In figure 3, critical buckling strains of SWCNTs with different diameters are shown for aspect ratios 2 and 10. It is clear from the figure that, at aspect ratio 2, the simplified formula, the formulae derived by the authors and the MDS results show the same trend. The maximum percentage difference between the simplified formula and the MDS results shown in figure 3(a) is 46%. In contrast, at aspect ratio 10 results from the simplified formula deviate greatly from the results of analytical expressions derived in this paper. It can be seen from figure 3(b) that critical buckling strain values calculated from the formulae derived here are less sensitive

Figure 2. Buckled shapes for (7, 7) SWCNTs obtained from MDS.

Table 3. Error percentages correspond to the simplified formula and formulae derived by the authors based on classical and first-order shell theories.

		Error % w.r.t MDS		
SWCNT	Aspect ratio	Simplified	Classical	First-order
(8, 0)	2	−17	−2	2
	4	−67	−37	−33
	6	−83	9	9
	8	−95	41	41
	10	−173	45	45
(7, 7)	2	−29	−1	0
	4	−72	−35	−34
	6	−97	−46	−46
	8	−123	1	1
	10	−164	22	22

to diameter at aspect ratio 10 while those calculated from the simplified formula are highly sensitive to diameter even at aspect ratio 10. It is well understood that diameter plays a significant role in shell buckling while aspect ratio plays a significant role in beam buckling. Therefore, it is clear that, as the aspect ratio increases, the effect from diameter should be reduced while the effect from aspect ratio increases. Thus, the formulae derived here give more meaningful results compared to the simplified formula.

Interestingly, MDS results are also less sensitive to diameter at this aspect ratio and are closer to the results obtained from the formulae derived here. For example, the maximum difference between buckling strain values produced by the simplified formula and MDS is 263% while that between the formulae derived here and MDS is 48%. Therefore, the formulae derived here can be considered as a more accurate solution for buckling strain. However, it should be noted that the formulae derived here under-estimates the buckling strain compared to MDS.

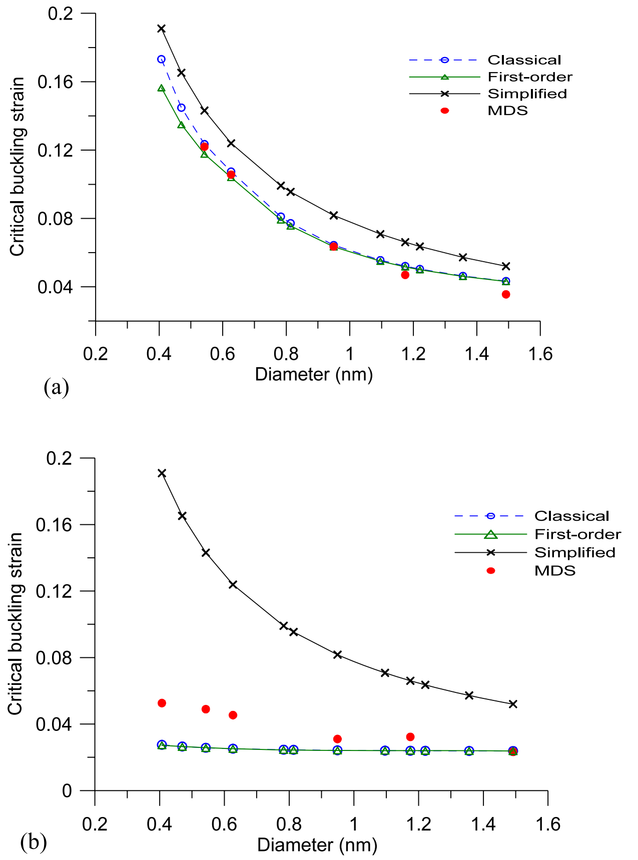

Figure 3. Variation of critical buckling strain with diameter (a) at aspect ratio 2 and (b) at aspect ratio 10.

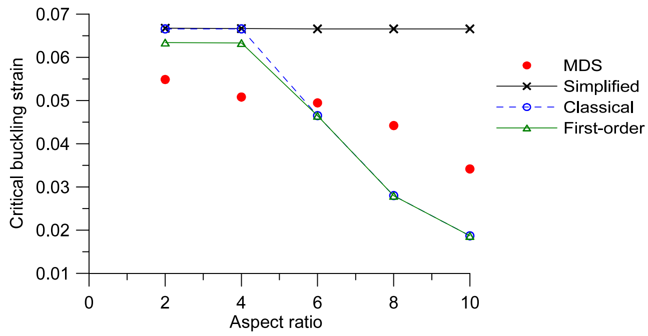

Figure 4. Variation of critical buckling strain of DWCNTs (4, 4) (9, 9).

5.2. *Critical buckling strains of DWCNTs*

Figure 4 shows the critical buckling strains of (4, 4) (9, 9) DWCNTs with different aspect ratios. Similar to the results of SWCNTs, critical buckling strains of DWCNTs calculated from the simplified formula given in equation (3) are not sensitive to the aspect ratio while buckling strains calculated from the formulae derived here based on classical shell theory (equation (42)) and first-order shell theory (equation (45)) are highly sensitive to aspect ratio. MDS results are also sensitive to aspect ratio and closer to the values obtained from the formulae derived here. Moreover, at lower aspect ratios, an improvement of about 6% can be observed in results obtained

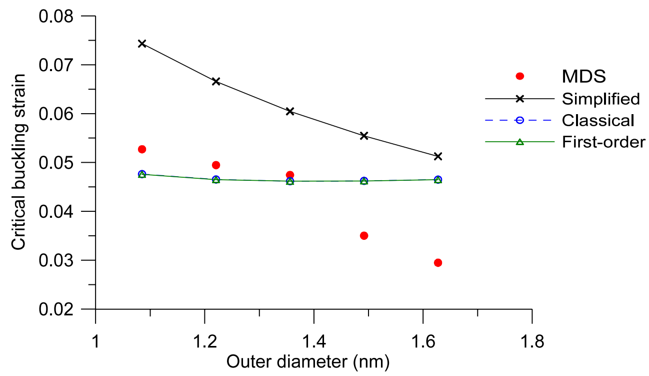

Figure 5. Variation of critical buckling strain with outer diameter for DWCNTs at aspect ratio 6.

from first-order shell theory compared with classical shell theory.

Figure 5 shows the variation of critical buckling strain with the diameter of the outer tube at aspect ratio 6. It is seen from the figure that, similar to SWCNTs, buckling strain of DWCNTs obtained from the formulae derived in this study show less sensitivity to the diameter at higher aspect ratios. MDS results seem to follow the same trend for outer diameter up to 1.36 nm. However, beyond that diameter, a higher reduction of buckling strain can be observed. Very few MDS-based studies on DWCNTs can be found in the literature. However, a buckling strain value (i.e. 0.06) obtained by Liew *et al* (2004) for (5, 5) (10, 10) DWCNTs of aspect ratio 4.4 and the value (0.05) obtained by Zhang *et al* (2007) for the same DWCNTs of aspect ratio 5.5 agree well with the value (0.047) obtained in the present study for the same DWCNTs with aspect ratio 6. Therefore, accuracy of the authors' MDS results appears to be good. Thus, it is clear that for larger DWCNTs even the non-simplified shell theory solution cannot provide reasonable accuracy compared to MDS. However, even for such diameters the non-simplified solutions are closer to MDS results compared to the simplified solution.

6. Conclusion

It was noted that the widely employed classical-shell-theory-based analytical expressions to calculate buckling strains have been subjected to certain simplifications. As a result, the aspect ratio dependence of critical buckling strain could not be captured by these expressions. Thus analytical expressions were derived based on classical shell theory without simplifications to calculate buckling strain of SWCNTs and DWCNTs. Moreover, analytical solutions for buckling strain based on first-order shell theory are also derived to improve the accuracy of the buckling strain solution by taking the effect of shear deformation into account. Molecular dynamic simulations are also conducted to further verify the applicability of the expressions derived in this paper.

It is understood from the existing MDS results as well as the MDS results obtained in this study that buckling strain of a CNT is sensitive to aspect ratio even within the shell buckling region. The expressions derived in this paper are also sensitive to aspect ratio. However, as a result of simplifications made in the derivation, the simplified formula is almost insensitive to aspect ratio and hence leads to a significant error at higher aspect ratios. Moreover, this error increases as the diameter decreases. Therefore it is understood from the results that the simplified formulae for axial buckling of thin cylindrical shells which are widely applied to calculate the buckling strain of both SWCNTs and DWCNTs are not applicable for all CNTs. For CNTs with higher aspect ratio (approximately greater than 4) and lower diameters the simplified formulae lead to a significant error. The expressions derived here based on classical theory but without simplifications produce closer results to those produced by MDS and hence can be suggested as a better continuum mechanics solution to the buckling strain of SWCNTs and DWCNTs. Moreover, a marginal effect from first-order shell theory can be observed in buckling strains of CNTs with smaller diameters and lower aspect ratios.

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