Nonlocal effects on thermal buckling properties of double-walled carbon nanotubes

Abdelouahed Tounsi^{*1,2}, Soumia Benguediab¹, El Abbas Adda Bedia¹, Abdelwahed Semmah³ and Mohamed Zidour^{1,4}

¹Laboratoire des Matériaux et Hydrologie, Université de Sidi Bel Abbés, BP 89 Cité Ben M ^chidi, 22000 Sidi Bel Abbés, Algeria
²Département de Génie Civil, Faculté de Technologie, Université de Sidi Bel Abbés, Algeria
³Université de Sidi Bel Abbés, Département de physique, BP 89 Cité Ben M ^chidi, 22000 Sidi Bel Abbés, Algeria
⁴Université Ibn Khaldoun, BP 78 Zaaroura, 14000 Tiaret, Algérie

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Abstract. The thermal buckling properties of double-walled carbon nanotubes (DWCNTs) are studied using nonlocal Timoshenko beam model, including the effects of transverse shear deformation and rotary inertia. The DWCNTs are considered as two nanotube shells coupled through the van der Waals interaction between them. The geometric nonlinearity is taken into account, which arises from the mid-plane stretching. Considering the small-scale effects, the governing equilibrium equations are derived and the critical buckling temperatures under uniform temperature rise are obtained. The results show that the critical buckling temperature can be overestimated by the local beam model if the nonlocal effect is overlooked for long nanotubes. In addition, the effect of shear deformation and rotary inertia on the buckling temperature is more obvious for the higher-order modes. The investigation of the thermal buckling properties of DWCNTs act as basic elements.

Keywords: buckling analysis; double-walled carbon nanotubes; nonlocal effect; thermal effect

1. Introduction

Carbon nanotubes (CNTs) are among the most important nano- materials that have attracted attention of the scientific community due to their outstanding mechanical properties and wide potential applications in nanoengineering. To fully realize the potential application of carbon nanotubes, it is important to characterize the mechanical properties of these nanostructures as well as their material response. However as performing controlled experiments in nanoscale is difficult and expensive, most of researches have been mainly conducted by modelling and computational simulations. Indeed, with the difficulty for the controlled experiments at the nanometer scale, the numerical simulation has been performed widely. Two basically different approaches are available

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^{*}Corresponding author, Professor, E-mail: tou_abdel@yahoo.com

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for theoretical modelling of nanostructured materials: the atomistic approaches and the continuum mechanics. The former includes the classical molecular dynamics (TBMD) and density functional theory (DFT) (Iijima *et al.* 1996, Yakobson *et al.* 1997, Hernandez *et al.* 1998, Sanchez-Portal *et al.* 1999, Qian *et al.* 2002). These approaches are often computationally expensive, especially for large-scale CNTs with high number of walls. Hence, the continuum mechanics is increasingly being viewed as an alternative way of modelling materials at the nanometer scale. However, classical continuum mechanics theories are unable to take into account the small-size effects. The size effects are pronounced in nano-sized materials primarily due to the high surface to volume ratio. In this regard, the nonlocal elasticity theory proposed by Eringen *et al.* (1972, 1983, and 2002) has been widely applied to achieve size-dependent governing equations by incorporating an internal characteristic length in the model. This nonlocal elasticity theory has been extensively applied to analyze the bending, buckling, vibration and wave propagation of beam-like elements in micro- or nanoelectromechanical devices (Peddieson *et al.* 2003, Lu *et al.* 2006, Wang and Varadan 2006, Reddy and Pang 2008, Murmu and Pradhan 2009a, 2009b, 2009c, Şimşek 2010, 2011, Heireche *et al.* 2008a, 2008b, 2008c, Tounsi *et al.* 2008, Tounsi *et al.* 2009a, 2009b).

Due to high aspect ratio of CNTs, they are more susceptible to buckling instability when subjected to compressive loads. Hence, besides the general mechanical properties of CNTs, buckling behavior of CNTs is important to forthcoming applications like probe microscopy. Sudak (2003) studied infinitesimal column buckling of carbon nanotubes (CNTs), incorporating the van der Waals (vdW) forces and small scale effect, and showed that the critical axial strain decreases compared with the results of classical beams. Reddy (2007) reformulated different nonlocal beam theories to evaluate the static bending, vibration, and buckling responses of nanobeams. Murmu and Pradhan (2008) carried out stability analysis of beam surrounded by elastic medium using nonlocal Euler-Bernoulli beam. Further, Murmu and Pradhan (2009a) used nonlocal elasticity and Timoshenko beam theory to investigate the stability response of single-walled carbon nanotubes (SWCNTs) embedded in an elastic medium. Senthilkumar et al. (2010) investigated the smallscale effect on critical buckling load for SWCNTs based on Timoshenko beam theory using differential transformation method. Recently, Amara et al. (2010) studied the thermal effect on column buckling of MWNTs using the nonlocal beam model. To the best of the authors' knowledge, the thermal buckling of DWCNTs using nonlocal Timoshenko beam model with the geometric nonlinearity has not been studied.

The objective of the present paper is to develop, for the first time, a closed solution for the thermal buckling behavior of DWCNTs based on the nonlocal Timoshenko beam theory. The geometric nonlinearity is considered using von Karman's strain– displacement relations. The Timoshenko beam results are obtained and compared with those obtained by Euler–Bernoulli beam. In addition, the shear effect clearly indicates the importance of applying shear deformation beam models for CNTs. The results reveal also that the nonlocal parameter has significant effect on the thermal buckling behavior of nano-sized carbon nanotubes.

2. Governing equations

According to the Timoshenko beam theory, the displacement field of any point in the beam writes

$$u(x,z) = u_0(x) + z\psi(x)$$
(1a)

$$w(x,z) = w_0(x) \tag{1b}$$

where x is the longitudinal coordinate measured from the left end of the beam, z the coordinate measured from the mid-plane of the beam, w the transverse displacement, u the longitudinal displacement, $u_0(x)$ and $w_0(x)$ are the displacement components of a point located on the neutral axis and $\psi(x)$ is the section normal vector rotation about the y-axis. The nonlinear von Karman strain–displacement relations are used as follows

$$\mathcal{E}_x = \frac{du_0}{dx} + \frac{1}{2} \left(\frac{dw}{dx}\right)^2 + z \frac{d\psi}{dx}$$
(2)

$$\gamma_{xz} = \psi + \frac{dw}{dx} \tag{3}$$

where ε_x the normal strain, γ_{xz} the transverse shear strain.

For the Timoshenko beam model with the thermal stress and using the principle of virtual displacements (Fung 1965), the following relation can be derived

$$\frac{dM}{dx} - Q = 0 \tag{4a}$$

$$\frac{dQ}{dx} + N_t \frac{d^2 w}{dx^2} + q(x) = 0$$
(4b)

where Q is the shear force, M the resultant bending moment, q(x) is the van der Waals force between the inner and outer tubes, and N_t the thermal force which can be expressed as

$$N_t = -\frac{E \alpha T A}{1 - 2 \nu} \tag{5}$$

where α is the thermal expansion coefficient, T the temperature change, A the cross area and v the Poisson's ratio.

The bending moment and the shear force can be defined by

$$M = \int_{A} z \sigma_x dA, \quad Q = \int_{A} \tau_{xz} dA \tag{6}$$

where σ_x is the normal stress, and τ_{xz} the transverse shear stress.

As written, the governing buckling equations appear in the same form as the local Timoshenko beam theory, but it must be recognized that the bending moment and shear force expressions for the nonlocal beam theory are different due to the nonlocal constitutive relations as will be shown below.

The constitutive equation of classical elasticity is an algebraic relationship between the stress and strain tensors while that of Eringen's nonlocal elasticity involves spatial integrals which represent weighted averages of the contributions of strain tensors of all points in the body to the stress tensor at the given point (Eringen *et al.* 1972, 1983, and 2002). Though it is difficult mathematically to obtain the solution of nonlocal elasticity problems due to the spatial integrals in Eringen's constitutive equations, these integral-partial constitutive differential equations can be

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converted to equivalent differential constitutive equations under certain conditions. The simplified nonlocal constitutive equation for the normal stress and strain in a one-dimensional case is given by (Eringen 1983)

$$\sigma_x - (e_0 a)^2 \frac{d^2 \sigma_x}{dx^2} = E \varepsilon_x \tag{7a}$$

$$\tau_{xz} - (e_0 a)^2 \frac{d^2 \tau_{xz}}{dx^2} = G \gamma_{xz}$$
(7b)

where *E* and *G* are the Young's and shear modulus, respectively. $\mu = (e_0 a)^2$ is a nonlocal parameter revealing the nanoscale effect on the response of CNTs, e_0 is a constant appropriate to each material and *a* is an internal characteristic length (e.g. length of C–C bond, lattice spacing, granular distance). Arash and Wang (2012) showed that the value of the nonlocal parameter depends on the boundary conditions, chirality, mode shapes, number of walls, and the nature of motion. In the investigation of the nonlocal parameter effect, it is crucial to determine the magnitude of the parameter e_0 since it has a significant influence on the effect of small length scale. So far, no experiments have been conducted to predict the magnitude of e_0 for CNTs. In the open literature (Arash and Ansari 2010, Wang 2005, Wang and Wang 2007), it is suggested that the value of nonlocal parameter can be determined by using a comparison of dispersion curves from the nonlocal continuum mechanics and molecular dynamics simulation. It should be noted that according to the previous discussions about the values of the nonlocal parameter in detail, e_0a is usually considered as the single scale coefficient which is smaller than 2.0 nm for nanostructures (Wang and Wang 2007).

From relations (7a), (7b), (6), (2), and (3), the bending moment M and the shear force Q for the nonlocal model can be expressed as

$$\left[1 - (e_0 a)^2 \frac{d^2}{dx^2}\right] M = EI \frac{d\psi}{dx}$$
(8a)

$$\left[1 - (e_0 a)^2 \frac{d^2}{dx^2}\right] Q = \beta G A\left(\psi + \frac{dw}{dx}\right)$$
(8b)

where β is the form factor of shear depending on the shape of the cross section. The recommended value of β , the adjustment coefficient, is 9/10 for a circular shape of the cross area.

Substituting Eqs. (8) into Eqs. (4) and eliminating ψ yield the following differential equation

$$EI\frac{d^{4}w}{dx^{4}} - \left(1 - (e_{0}a)^{2}\frac{d^{2}}{dx^{2}}\right)\left(1 - \frac{EI}{\beta AG}\frac{d^{2}}{dx^{2}}\right)\left(N_{t}\frac{d^{2}w}{dx^{2}} + q(x)\right) = 0$$
(9)

The above equation is the equilibrium equation of a Timoshenko beam considering the non-local effects.

2.1 Double-walled carbon nanotubes

It is known that double – walled carbon nanotubes are distinguished from traditional elastic beam by their hollow two – layer structures and associated intertube van der Waals forces. The

thermal buckling load is the same for both tubes i.e. $N_{t1} = N_{t2} = N_t$. The Eq. (9) can be used to each of the inner and outer tubes of the double – walled carbon nanotubes. Assuming that the inner and outer tubes have the same thickness and effective material constants, we have

$$EI_{1}\frac{d^{4}w_{1}}{dx^{4}} - \left(1 - (e_{0}a)^{2}\frac{d^{2}}{dx^{2}}\right)\left(1 - \frac{EI_{1}}{\beta A_{1}G}\frac{d^{2}}{dx^{2}}\right)\left(N_{t}\frac{d^{2}w_{1}}{dx^{2}} + q_{12}(x)\right) = 0$$
(10a)

$$EI_{2} \frac{d^{4}w_{2}}{dx^{4}} - \left(1 - (e_{0}a)^{2} \frac{d^{2}}{dx^{2}}\right) \left(1 - \frac{EI_{2}}{\beta A_{2}G} \frac{d^{2}}{dx^{2}}\right) \left(N_{t} \frac{d^{2}w_{2}}{dx^{2}} + q_{21}(x)\right) = 0$$
(10b)

where subscripts 1 and 2 are used to denote the quantities associated with the inner and outer tubes, respectively, q_{12} and q_{21} denote the van der Waals pressure per unit axial length.

The deflection of two tubes is coupled through the van der Waals force (Reulet *et al.* 2000). The van der Waals interaction potential, as a function of the interlayer spacing between two adjacent tubes, can be estimated by the Lennard – Jones model. The interlayer interaction potential between two adjacent tubes can be simply approximated by the potential obtained for two flat graphite monolayers, denoted by $g(\Delta)$, where Δ is the interlayer spacing (Girifalco and Lad 1956, Girifalco 1991). Since the interlayer spacing is equal or very close to an initial equilibrium spacing, the initial van der Waals force is zero for each of the tubes provided they deform coaxially. Thus, for small – amplitude sound waves, the van der Waals pressure should be a linear function of the difference of the deflections of the two adjacent layers at the point as follows

$$q_{12} = tc(w_1 - w_2) \tag{11a}$$

$$q_{21} = -\frac{R_1}{R_2}c(w_1 - w_2)$$
(11b)

where t the thickness of both the inner and outer nanotubes, and c is the intertube interaction coefficient per unit length between two tubes, which can be estimated by (Sudak 2003)

$$c = \frac{320 (2R_1) erg / cm^2}{0.16 a^2} (a = 0.142 nm)$$
(12)

where R_1 and R_2 are the radius of the inner and the outer tube, respectively.

Let us assume the buckling modes as (Sears and Batra 2006, Batra 2007)

$$w_1 = A\sin\left(\frac{m\pi}{L}x\right)$$
 and $w_2 = B\sin\left(\frac{m\pi}{L}x\right)$ (13)

The above equations satisfy the simply supported boundary conditions which are

$$w_i = \frac{d^2 w_i}{dx^2} = 0$$
 at $x = 0, L$ $(i = 1, 2)$ (14)

Replacing Eq. (13) into Eq. (10), one can easily obtain

$$\begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = 0$$
(15)

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where K_{11} , K_{12} , K_{21} and K_{22} in Eq. (15) are defined as

$$K_{11} = EI_{1} \left(\frac{m\pi}{L}\right)^{4} - \left\{ t \, c - N_{t} \left(\frac{m\pi}{L}\right)^{2} \right\} \left[1 + (e_{0}a)^{2} \left(\frac{m\pi}{L}\right)^{2} \right] \left[1 + \frac{EI_{1}}{\beta A_{1}G} \left(\frac{m\pi}{L}\right)^{2} \right]$$
(16a)

$$K_{12} = t c \left[1 + (e_0 a)^2 \left(\frac{m\pi}{L} \right)^2 \right] \left[1 + \frac{EI_1}{\beta A_1 G} \left(\frac{m\pi}{L} \right)^2 \right]$$
(16b)

$$K_{21} = t c \frac{R_1}{R_2} \left[1 + (e_0 \mathbf{a})^2 \left(\frac{m\pi}{L} \right)^2 \right] \left[1 + \frac{EI_2}{\beta A_2 G} \left(\frac{m\pi}{L} \right)^2 \right]$$
(16c)

$$K_{22} = EI_2 \left(\frac{m\pi}{L}\right)^4 - \left\{ t \, c \, \frac{R_1}{R_2} - N_t \left(\frac{m\pi}{L}\right)^2 \right\} \left[1 + (e_0 a)^2 \left(\frac{m\pi}{L}\right)^2 \right] \left[1 + \frac{EI_2}{\beta A_2 G} \left(\frac{m\pi}{L}\right)^2 \right]$$
(16d)

For nontrivial solution, the determinant of the coefficient matrix in Eq. (15) must be zero. This gives the critical buckling temperature of the DWCNT in which the effects of the small scale and the van der Waals force between the inner and the outer tubes are shown.

As a result, the non-dimensional critical temperature can be expressed as the following form

$$\overline{T}_{cr} = \frac{\alpha A L^2}{I} T_{cr}$$
(17)

3. Validity and applicability of continuum beam model for CNTs

Applicability of continuum beam model for carbon nanotubes (CNTs) is examined by several authors (e.g. Wang and Hu (2005) and Harik (2001, 2002)). Harik (2001, 2002) reported ranges of applicability for the continuum beam model in the mechanics of carbon nanotubes and nanorods. Wang and Hu (2005) present a rigorous study, in which they check the validity of the beam model in studying the flexural waves, simulated by the molecular dynamics (MD), in a single – walled carbon nanotube. In this study, Wang and Hu (2005) observed that when the wave number is getting very large, the microstructure of the carbon nanotubes plays an important role in the flexural wave dispersion and significantly decreases the phase velocity of the flexural waves of high frequency.

In the present study, the numerical results for critical buckling strains obtained from this continuum mechanics theory (using nonlocal Timoshenko beam model) are compared with those obtained from MD simulations and the Sanders shell theory (Silvestre *et al.* 2011). Since the MD simulations referenced herein consider the CNTs with fixed ends, we also consider the nonlocal Timoshenko beam model with fully clamped boundary conditions (Wang *et al.* 2006). In addition, CNT (5,5) is analyzed with a diameter d = 6.71 Å and CNT (7,7) with a diameter d = 9.40 Å, for different lengths. Both nanotubes are modelled using a thickness t = 0.66 Å, Young's modulus

Table 1 Comparison between critical buckling strains of CNT (5, 5) and CNT (7, 7) obtained from MD simulations, Sanders shell theory (SST) and the present nonlocal Timoshenko beam theory (TBT)

	,			3		
	L (Å)	<i>d</i> (Å)	MD	TBT	SST	
-	16.09	6.71	0.08146	0.08216	0.08729	
	21.04	6.71	0.07528	0.07460	0.08288	
	28.46	6.71	0.06992	0.06302	0.07858	
	28.29	9.40	0.06514	0.06542	0.06582	
	40.59	9.40	0.04991	0.05763	0.05885	
	52.88	9.40	0.04710	0.04962	0.05600	

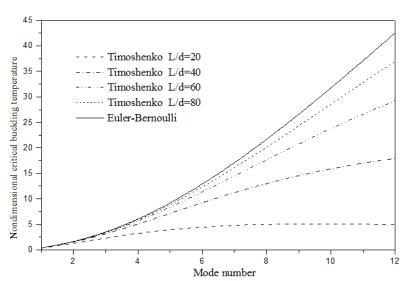


Fig. 1 Comparison of critical buckling temperature of DWCNT with different length-to-diameter ratios for different modes based on Euler beam and Timoshenko beam models ($e_0 a = 0$)

E = 5.5 TPa and Poisson's ratio v = 0.19 (Yakobson *et al.* 1996). The lengths of CNTs used in the following table are extracted from the work done by Silvestre *et al.* (2011). The results from MD simulations, nonlocal Timoshenko beam and Sanders shell models are compared in Table 1. It is seen that the critical buckling strains are in good agreement as compared with the results obtained from MD simulations as well as Sanders shell theory. Based on the MD simulation results, the value of nonlocal constant is determined for CNTs based on an averaging process. The best match between MD simulations and nonlocal formulations is achieved for a nonlocal constant value of $e_0a = 0.54$ nm for CNT (5, 5) and $e_0a = 1.05$ nm for CNT (7, 7) with good accuracy (the error is less than 10%).

4. Results and discussions

In this section, numerical calculations for the thermal buckling properties of DWCNT are carried out. The material constants used in the calculation are the Young's modulus E = 1 TPa

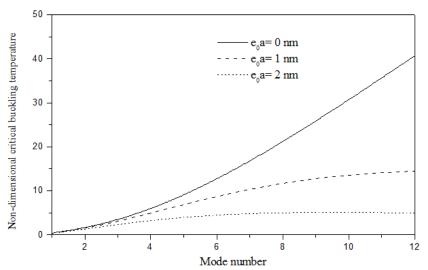


Fig. 2 Critical buckling temperature of DWCNT with different nonlocal values for different modes based on Timoshenko beam model (L/d = 20)

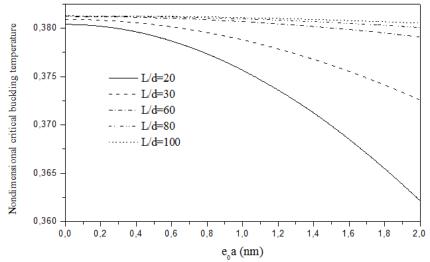


Fig. 3 Variations of critical buckling temperature of DWCNT with respect to the scale parameter for different length-to-diameter ratio with the number mode m = 1

with the effective thickness of single-walled carbon nanotubes taken to be t = 0.258 nm. The Poisson's ratio v = 0.3, the shear modulus G = 0.4 TPa, the shear coefficient $\beta = 9/10$ and the temperature expansion coefficient $\alpha = 1.1 \times 10^{-6}$ K⁻¹ which is for the case of the high temperature (Amara *et al.* 2010, Yao and Han 2006). The inner diameter $d_1 = 0.7$ nm and the outer diameter $d_2 = 1.4$ nm.

The computational results of non-dimensional critical buckling temperature T_{cr} of DWCNT are shown in Fig. 1. In this figure, we illustrate a comparison between the Euler beam model and Timoshenko beam model. It can be seen that the non-dimensional critical buckling temperature

increases with increasing the number mode and the length-to-diameter ratio L/d. The nondimensional critical buckling temperature calculated by Timoshenko beam model is lower than that obtained by Euler beam model and especially at higher buckling modes. This is because the presence of rotary inertia and shear deformation tends to make the nanotube less stiff. The effect of rotary inertia and shear deformation on the non-dimensional critical buckling temperature is significant as the value of the buckling mode becomes high.

The effect of nonlocal parameter on the non-dimensional critical buckling temperature \overline{T}_{cr} of DWCNT is shown in Fig. 2. The parameter value of $e_0a = 0$ implies that the nonlocal effect is neglected. It can be seen that the effect of nonlocal parameter e_0a on the critical buckling temperature is significant, especially at higher-order modes. Increasing the nonlocal effect decreases the critical buckling temperature.

Fig. 3 shows the variation of the non-dimensional critical buckling temperature versus the scale parameter e_0a for different values of the length-to-diameter ratio L/d. This investigation demonstrates that the non-dimensional critical buckling temperature decreases as scale parameter increases. This reduction in the critical buckling temperature is most pronounced when the carbon nanotube is short.

5. Conclusions

This paper presents closed-form solutions for the thermal buckling of double-walled carbon nanotubes within the context of the nonlocal elasticity model. The geometrical nonlinearity is modelled using von Karman's assumptions. The influences of the scale parameter, the ratio of the length to the diameter, the transverse shear deformation and rotary inertia on the critical buckling temperature are discussed. According to the analysis, the following results were obtained:

• The effects of rotary inertia and shear deformation on the critical buckling temperature of DWCNT increased with decreasing the length-to-diameter ratio, especially at higher-order modes.

• Increasing the value of nonlocal parameter decreased the critical buckling temperature, especially at higher order modes.

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