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Scale Effects on Thermal Buckling Properties of Single-Walled Carbon Nanotube

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Abstract-*In this Paper, the thermal buckling properties of carbon nanotube with small scale effects are studied. Based on the nonlocal continuum theory and the Timoshenko beam model, the governing equation is derived and the nondimensional critical buckling temperature is presented. The influences of the scale coefficients, the ratio of the length to the diameter, the transverse shear deformation and rotary inertia are discussed. It can be observed that the small scale effects are significant and should be considered for thermal analysis of carbon nanotube. The nondimensional critical buckling temperature becomes higher with the ratio of length to diameter increasing. Also, for smaller ratios of the length to the diameter and higher mode numbers, the transverse shear deformation and rotary inertia have remarkable influences on the thermal buckling behaviors.*

Keywords - single-walled carbon nanotubes, thermal buckling, Timoshenko beam, Scale Effects, Shear Deformation

1.0 INTRODUCTION

Since the invention of carbon nanotubes CNTs by Iijima, a new area of research is in growth for the proper and accurate understanding of nanosize structures. These nanosize structures exhibit remarkable physical, mechanical, chemical, electronic, and electrical properties. These outstanding properties of CNTs have lead to its usage in the emerging field of nanoelectronics, nanodevices, nanocomposites, etc.

Experiments at the nanoscale are extremely difficult and atomistic modeling remains prohibitively expensive for large-sized atomic system. Consequently continuum models continue to play an essential role in the study of CNTs. effective method for calculation [1]. However, in the classical elastic model, the small scale effects are not considered. The nonlocal continuum theory initiated by Eringen [2], assumes the stress at a reference point is considered as a function of the strain at every point in the body. Here, it should mention some pioneer work on the mechanical behaviors of carbon nanotube with the nonlocal continuum theory. Sudak firstly developed the nonlocal multi-beam model to discuss the buckling properties [3]. Zhang et al. firstly presented the nonlocal multi-shell model [4] and estimated a value of the scale effect parameter e0for nanotubes [5]. As a result, the nonlocal continuum theory can present the more reliable analysis and show accurate results [6]. Furthermore, some researches indicate that the mechanical behaviors of carbon nanotube are sensitive to the thermal effects in the external environment [7]. Recently, considering the effects of the transverse shear deformation and rotary inertia, Hsu et al. [8] and Lee and Chang [9] studied the thermal buckling properties of carbon nanotube with the classical Timoshenko beam model. The characteristics of the critical buckling temperature were presented. However, the small scale effects are not taken into account for the thermal buckling properties. In the present Letter, based on the nonlocal Timoshenko beam theory, the governing equation is derived. The scale effects on the thermal buckling properties of carbon nanotube are investigated. The influences of the scale coefficients, the ratio of the length to the diameter, the transverse shear deformation and rotary inertia are discussed. From the results, some interesting and valuable conclusions can be drawn.

2.0 WAVE MOTION EQUATION

The carbon nanotube with the length L is presented in Figure. 1. Based on the nonlocal continuum theory [10], which accounts for the scale effects by assuming the stress at a reference point as a function of the strain at every point in the body, the basic equations are of the beam. Based on this theory, the equilibrium equations are

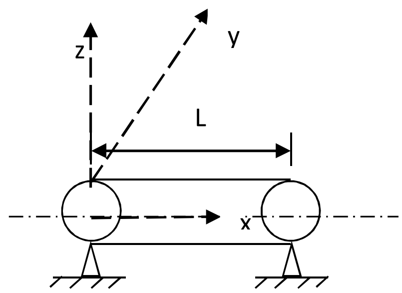

Figure 1: SWCNT with hinged boundary conditions for the nonlocal Timoshenko beam model.

$$\sigma_{ij,j}=0$$

$$\sigma_{ij}=\int_V K(|x-x'|,\ \tau)C_{ijkl}\varepsilon_{kl}(x')dV(x'),\qquad \forall x\in V \tag{1}$$

$$\varepsilon_{ij,j}=\frac{1}{2}(u_{i,j}+u_{j,i})$$

where C_{ijkl}'s are the elasticity tensor components of classical isotropic elasticity and σ_{ij} and ε_{ij} are the components of stress and strain tensors, respectively. $K(|x-x'|,\ \tau)$ is the kernel function and τ is a material constant that depends on internal and external characteristic length or attenuation function which considers the nonlocal effects at the reference point x produced by the local strain at the source x' and can be expressed as

$$\lambda(|x|,\tau)=(2\pi l^2\tau^2)^{-1}K_0(x.\frac{x}{l\tau}) \tag{2}$$

where K_0 is the modified Bessel function, $\tau = e_0a/l$ the material constant, a the internal characteristic lengths (e.g. lattice parameter, granular size, distance between C–C bonds), l the external characteristic lengths (e.g. crack length, wavelength), e_0 the constant for adjusting the model in matching with experimental results and by other models, $|x-x'|$ the distance in the

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Euclidean form and V the entire body considered. For the nonlocal Timoshenko beam theory, the Hook's law of carbon nanotube can be expressed as the following partial differential forms:

$$\left[\sigma_x - (e_0 a)^2 \frac{\partial^2 \sigma_x}{\partial x^2}\right] = E\varepsilon_x$$

$$\left[\tau_{xy} - (e_0 a)^2 \frac{\partial^2 \tau_{xy}}{\partial x^2}\right] = G\gamma_{xy} \quad (3)$$

where σ_x is the axial stress, ε_x is the axial strain and γ_{xy} denotes the shear strain, E and G are Young's and shear modulus, respectively. The expressions of the axial strain and the shear strain are

$$\varepsilon_x = z\frac{\partial \psi}{\partial x}$$

$$\gamma_{xy} = \frac{\partial w}{\partial x} - \psi \quad (4)$$

ψ is the rotation angle and $\boldsymbol{w}$ is the transverse displacement. For the Timoshenko beam model with the thermal stress, the following relation can be derived:

$$\frac{dS}{dx} = -N_T \frac{d^2 w}{dx^2}$$

$$\frac{dM}{dx} + S = 0 \quad (5)$$

M and S are the resultant bending moment and the resultant shear force, respectively. N_T is the thermal force which can be expressed as

$$N_T = -\frac{E\alpha T A_c}{1-2\upsilon} \quad (6)$$

A is the cross-section area of the beam, where α is the thermal expansion coefficient, T the temperature change, υ the Poisson's ratio.

Table 1: Relation between the nondimensional critical buckling temperature (P_{cr}) and the mode number (k) with different scale coefficients (e_0a). The value of L/d is 10.

L/d=10	*e₀a=0*				
Mode Number	0	2	4	6	8
P_{cr}	0	13.676	39.029	59.431	72.738
	$e_0a=1$				
Mode Number	0	2	4	6	8
P_{cr}	0	13.567	37.811	55.412	64.432
	$e_0a=2$				
Mode Number	0	2	4	6	8
P_{cr}	0	13.249	34.572	46.068	47.991
	$e_0a=5$				
Mode Number	0	2	4	6	8
P_{cr}	0	11.338	21.614	21.128	17.225

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The bending moment and the shear force can be defined by

$$M = \int_{A_c} z\sigma_x dA_c \qquad S = \int_{A_c} \tau_{xy} dA_c \tag{7}$$

According to Eqs. (3), (4), and (7), we can obtain the following relation

$$M - (e_0 a)^2 \frac{\partial^2 M}{\partial x^2} = EI \frac{d\psi}{dx}$$

$$S - (e_0 a)^2 \frac{\partial^2 S}{\partial x^2} = k\, A_c G\left(\psi - \frac{dw}{dx}\right) \tag{8}$$

I is the moment of inertia, and κ the shear correction factor which is used to compensate for the error due to the constant shear stress assumption. Based on Eqs. (5) and (8), the following relation can be obtained

$$M = EI \frac{d\psi}{dx} - (e_0 a)^2 (-\frac{\partial^2 S}{\partial x^2}) \tag{9}$$

Substituting Eq. (5) into Eq. (9), we can obtain

$$M = EI \frac{d\psi}{dx} - (e_0 a)^2 (N_T \frac{\partial^2 w}{\partial x^2}) \tag{10}$$

Based on Eqs. (5) and (8), it can be derived that

$$S = k\, A_c G\left(\psi - \frac{dw}{dx}\right) + (e_0 a)^2 (-N_T \frac{\partial^3 w}{\partial x^3}) \tag{11}$$

Substituting Eq. (11) into Eq. (5), we can obtain

$$k\, A_c G\left(\frac{\partial^2 w}{\partial x^2} - \frac{\partial \psi}{\partial x}\right) + (e_0 a)^2 (-N_T \frac{\partial^4 w}{\partial x^4}) = -N_T \frac{\partial^2 w}{\partial x^2} \tag{12}$$

Based on Eqs. (5), (10) and (11), the following relation can be derived:

$$EI \frac{\partial \psi}{\partial x} + k\, A_c G\left(\psi - \frac{\partial w}{\partial x}\right) \tag{13}$$

It can be observed that Eqs. (12) and (13) are the governing equations. For the hinged boundary condition, the solution of carbon nanotube can be expressed as

$$w = W \sin(\lambda x) \qquad \psi = \Psi \cos(\lambda x) \tag{14}$$

where W is the amplitude of the deflection and the slope, $\lambda = \frac{k\pi}{L}$, k a positive integer which is related to the buckling modes. Substituting Eq. (14) into Eqs. (12) and (13), we can obtain

$$\left[1 + (e_0 a)^2 \lambda^2\right] \lambda^2 N_T W + \lambda^2 k\, G\, A_c\, W - \lambda k\, G\, A_c \Psi = 0$$

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$$\lambda k\, G\, A_c\, W - (\lambda^2 EI + k\, G\, A_c)\Psi = 0 \tag{15}$$

Then, the critical temperature with the nonlocal continuum theory can be derived as

$$T_{cr}^{non} = \frac{(\lambda)^2 k\, G\, I(1-2\upsilon)}{\alpha\left(1+(e_0 a)^2 \lambda^2\right)\left(\lambda^2 E\, I + k\, G\, A_c\right)} \tag{16}$$

Table 2: Relation between the nondimensional critical buckling temperature (P_{cr}) and the mode number (k) with different values of *L/d*. The scale coefficient e_0a = 1 nm.

e_0a=2	*L/d*=10				
Mode Number	0	2	4	6	8
P_{cr}	0	13.249	34.572	46.068	47.991
	L/d=20				
Mode Number	0	2	4	6	8
P_{cr}	0	15.082	52.999	98.315	138.291
	L/d=30				
Mode Number	0	2	4	6	8
P_{cr}	0	15.469	58.269	119.249	187.451
	L/d=100				
Mode Number	0	2	4	6	8
P_{cr}	0	15.761	62.696	139.766	245.298

As a result, the nondimensional critical temperature can be expressed as the following form [11]

$$P_{cr} = \frac{\alpha\, A_c\, L^2}{I} T_{cr}^{non} \tag{17}$$

3.0 Numerical examples and discussions

In this section, numerical calculations for the thermal buckling properties of carbon nanotube are carried out. The material constants used in the calculation are the Young's modulus E = 1 TPa, the mass density ρ = 2.3 g/cm3, the Poisson's ratio υ = 0.3, the shear modulus G = 0.4 TPa, the shear coefficient κ = 0.8 and the temperature expansion coefficient α = 1.1×10−6K−1which is for the case of the high temperature [12-13]. It should be noted that according to the previous discussions about the values of e0 and a in detail, e0a is usually considered as the single scale coefficient which is smaller than 2.0 nm for nanostructures [14]. The relation between the nondimensional critical temperature (P_{cr}) and the mode number (k) is presented in Table. 2. The ratio of the length to the diameter, *L/d*, is 10. The scale coefficients e_0a = 0, 1 and 2 nm are considered. The most notable feature is that the results based on the two theories are almost the same for small mode numbers [15-16]. However, the difference becomes obvious with the mode number increasing. The classical elastic (i.e. the local) model, which does not consider the small scale effects, will give a higher approximation for the nondimensional critical buckling temperature. But the nonlocal continuum theory will present

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an accurate and reliable result [17]. The influences of the ratio of the length to the diameter, L/d, on the nondimensional critical buckling temperature are shown in Table. 2.

Table 3(a): Relation between the nondimensional critical buckling temperature (P_{cr}) and the value of L/d with different scale coefficients (e_0a). k = 1.

k=1	$e_0a=0$			
L/d	10	40	70	100
P_{cr}	3.800	3.938	3.944	3.946
	$e_0a=1$			
L/d	10	40	70	100
P_{cr}	3.793	3.937	3.944	3.946
	$e_0a=2$			
L/d	10	40	70	100
P_{cr}	3.770	3.936	3.944	3.945
	$e_0a=5$			
L/d	10	40	70	100
P_{cr}	3.618	3.925	3.940	3.944

Table 3(b): Relation between the nondimensional critical buckling temperature (P_{cr}) and the value of L/d with different scale coefficients (e_0a). k = 5

k=5	$e_0a=0$			
L/d	10	40	70	100
P_{cr}	50.191	93.075	96.787	97.751
	$e_0a=1$			
L/d	10	40	70	100
P_{cr}	47.788	92.783	96.688	97.702
	$e_0a=2$			
L/d	10	40	70	100
P_{cr}	41.780	91.918	96.391	97.555
	$e_0a=5$			
L/d	10	40	70	100
P_{cr}	22.221	86.286	94.363	96.536

Table 3(c): Relation between the nondimensional critical buckling temperature (P_{cr}) and the value of L/d with different scale coefficients (e_0a). k = 10.

k=10	$e_0a=0$			
L/d	10	40	70	100
P_{cr}	81.148	317.974	365.921	380.093
	$e_0a=1$			
L/d	10	40	70	100
P_{cr}	67.543	314.021	364.423	379.329
	$e_0a=2$			
L/d	10	40	70	100
P_{cr}	44.940	302.730	360.002	377.055
	$e_0a=5$			
L/d	10	40	70	100
P_{cr}	13.455	241.857	331.821	361.871

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Table 4: Ratio of the critical buckling temperature by the nonlocal Timoshenko beam model to the nonlocal Euler–Bernoulli beam model. Ratio of the length to the diameter with different mode numbers (*k*). The scale coefficient e_0a = 2 nm.

$e_0a=2$	$k=1$			
L/d	10	40	70	100
P_{cr}	0.062	0.997	0.9992	0.9996
	$k=5$			
L/d	10	40	70	100
P_{cr}	0.507	0.942	0.980	0.990
	$k=10$			
L/d	10	40	70	100
P_{cr}	0.204	0.804	0.926	0.962

The scale coefficient is 1 nm. From Table. 2, it can be seen that when the mode number is less than 4, the difference is not obvious [18]. When the mode number is larger than 5, this influence becomes remarkable. Moreover, the nondimensional critical buckling temperatures for all of the three ratios become larger with the mode number increasing. The larger the ratio of the length to the diameter is, the higher the nondimensional critical buckling temperature becomes [19]. It means that the ratio of the length to the diameter has significant influence on the nondimensional critical buckling temperature for larger mode numbers [20-21]. The relation between the nondimensional critical buckling temperature and the ratio of the length to the diameter are shown in Table. 3(a)–(c). The scale coefficients e_0a = 0, 1, 2 and 4 nm and the mode number k = 1, 5 and 10 are considered, respectively. It can be seen that the ranges of the nondimensional critical buckling temperature for these mode numbers are quite different. In Table. 4(a), the range is the smallest for k = 1, but the range is the largest for k = 10 in Table. 3(c). It means that the larger the mode number is, the higher the nondimensional critical buckling temperature becomes [22-23]. Furthermore, it can be observed that when the ratio of the length to the diameter is small, the scale effects are significant. However, the scale effects on the nondimensional critical buckling temperature will diminish with the ratio (i.e. L/d) increasing [24]. It implies that the scale effects on the thermal buckling properties are not obvious for slender carbon nanotube but should be taken into account for short nanotube. In order to shown the influences of the transverse shear deformation and rotary inertia, the critical buckling temperature by the nonlocal Timoshenko beam model to the nonlocal Euler–Bernoulli beam model with different ratios of the length to the diameter is presented in Table. 4 [25-26]. The mode number k = 1,3,6 and the scale coefficient e_0a = 2 nm are considered. From Table. 4, it can be seen that for different mode numbers, all of the ratios are smaller than 1.0. It means that because of the influences of the transverse shear deformation and rotary inertia [27-28], the critical buckling temperature of the nonlocal Timoshenko beam model is lower than that of the nonlocal Euler–Bernoulli beam model. This phenomenon is more obvious for higher mode numbers and smaller ratios of the length to the diameter. It implies that the influences of the transverse shear deformation and rotary inertia should be considered and the nonlocal Timoshenko beam model is more accurate for short carbon nanotube [29].

4.0 CONCLUSION

In this study, based on the nonlocal continuum theory, the governing equation is presented and the nondimensional critical buckling temperature of carbon nanotube is derived. The influences of the scale coefficient, the ratio of the length to the diameter, the transverse shear deformation

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and rotary inertia on the thermal buckling properties are discussed. From the results, it can be concluded that the small scale effects should be considered for the thermal buckling behaviors, especially for higher mode numbers and short carbon nanotube. The nondimensional critical buckling temperature can be changed by different ratios of the length to the diameter. The influences of the transverse shear deformation and rotary inertia are obvious for higher mode numbers and smaller ratios of the length to the diameter. This work is expected to be useful to design and analyze the thermal buckling properties of nanoscale physical devices.

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