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Thermal buckling properties of zigzag single-walled carbon nanotubes using a refined nonlocal model

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Abstract. In the present article, the thermal buckling of zigzag single-walled carbon nanotubes (SWCNTs) is studied using a nonlocal refined shear deformation beam theory and Von-Karman geometric nonlinearity. The model developed simulates both small scale effects and higher-order variation of transverse shear strain through the depth of the nanobeam. Furthermore the present formulation also accommodates stress-free boundary conditions on the top and bottom surfaces of the nanobeam. A shear correction factor, therefore, is not required. The equivalent Young's modulus and shear modulus for zigzag SWCNTs are derived using an energy-equivalent model. The present study illustrates that the thermal buckling properties of SWCNTs are strongly dependent on the scale effect and additionally on the chirality of zigzag carbon nanotube. Some illustrative examples are also presented to verify the present formulation and solutions. Good agreement is observed.

Keywords: carbon nanotube; computer modelling and simulation; thermal properties

1. Introduction

Nanotechnology is an emerging technology involving the characterization, design, production and application of materials, structures and systems via the control and manipulation of matter on the nanometer length scale, that is, at the level of atoms and molecules. A nanometer is one billionth of a meter (10^{-9} m). This is roughly four times the diameter of an individual atom. For comparison, a red blood cell is approximately 7000 nm wide and a water molecule is almost 0.3 nm across. Materials and structures with at least one dimension in 1–100 nm are within the purview of nanotechnology. In this realm, nanomaterials and nanostructures exhibit properties and phenomena that cannot be observed at macro-scale, which opens new prospects of technology innovation and engineering systems at the nanoscale.

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shear strain γ_{xz} and hence to shear stress τ_{xz} through the thickness of the nanobeam in such a way that shear stress τ_{xz} is zero at the top and bottom faces of the nanobeam. Consequently, the expression for u_s can be given as:

$$u_s = -f(z)\frac{\partial w_s}{\partial x}, \text{ with } \quad f(z) = \frac{4z^3}{3h^2} \tag{4}$$

2.2 Kinematics

Based on the assumptions made in the preceding section, the displacement field can be obtained using Eqs. (1) - (4) as

$$u(x,z) = u_0(x) - z\frac{\partial w_b}{\partial x} - f(z)\frac{\partial w_s}{\partial x} \tag{5a}$$

$$w(x,z) = w_b(x) + w_s(x) \tag{5b}$$

In the present study we wish to investigate the effect of geometric non-linearity on the response quantities. Therefore, the Von-Karman-type of geometric non-linearity is taken into consideration in the strain–displacement relations. The nonzero strains of the proposed beam theory are:

$$\varepsilon_x = \varepsilon_x^0 + z\,k_x^b + f(z)\,k_x^s \quad \text{and} \quad \gamma_{xz} = g(z)\,\gamma_{xz}^s \tag{6}$$

where

$$\varepsilon_x^0 = \frac{\partial u_0}{\partial x} + \frac{1}{2}\left(\frac{\partial w_b}{\partial x} + \frac{\partial w_s}{\partial x}\right)^2, k_x^b = -\frac{\partial^2 w_b}{\partial x^2}, \quad k_x^s = -\frac{\partial^2 w_s}{\partial x^2} \tag{7}$$

$$\gamma_{xz}^s = \frac{\partial w_s}{\partial x}, \quad g(z) = 1 - f'(z) \quad \text{and} \quad f'(z) = \frac{df(z)}{dz}$$

2.3 Constitutive relations

Response of materials at the nanoscale is different from those of their bulk counterparts. Nonlocal elasticity was historically first considered by Eringen (1972, 1983, 2002). He assumed that the stress at a reference point is a *functional* of the strain field at *every point* of the continuum. Eringen (1972, 1983, 2002) proposed a *differential* form of the nonlocal constitutive relation as:

$$\sigma_x - (e_0 a)^2 \frac{d^2\sigma_x}{dx^2} = E\left(\varepsilon_x - \frac{\alpha T}{1-2\nu}\right) \tag{8a}$$

$$\tau_{xz} - (e_0 a)^2 \frac{d^2 \tau_{xz}}{dx^2} = G\gamma_{xz} \tag{8b}$$

where 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). In addition, 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. E and G are the Young's and shear modulus, respectively; α is the thermal expansion coefficient, T the temperature change and ν the Poisson's ratio.

It is worth pointing out that the effects of small scale coefficient $e_0 a$ on the shear force are neglected in previous works (Wang 2005; Wang *et al*. 2006; Wang *et al*. 2007). It is noted that the relations (8a) and (8b) are used with the assumption of homogeneous isotropic beams (Heireche *et al*. 2008ab; Lu *et al*. 2007; Tounsi *et al*. 2013abc). However, because CNT are normally anisotropic, the properties are then direction-dependent. The justification of the identical values of e_0 at the in-plane and transverse directions in relations (8a) and (8b) is due to the symmetry of the stress tensor ($\tau_{xz} = \tau_{zx}$, x and z are in-plane and transverse direction, respectively).

Based on the link between molecular mechanics and solid mechanics, Wu *et al*. (2006) developed an energy-equivalent model for studying the mechanical properties of SWCNTs. Using the same method, the equivalent Young's modulus and shear modulus of zigzag nanotube are expressed as

$$E_z = \frac{4\sqrt{3}KC}{9Ct + 4Ka^2 t(\lambda_{z1}^2 + 2\lambda_{z2}^2)},\ G_z = \frac{2\sqrt{3}KC}{6Ct + 3Ka^2 \lambda_z^2 t} \tag{9}$$

where K and C are the force constants. t is the thickness of the nanotube and the parameters λ_{z1}, λ_{z2} and λ_z are given by

$$\lambda_{z1} = \frac{-3\sqrt{4 - 3\cos^2(\pi/2n)}\cos(\pi/2n)}{8\sqrt{3} - 2\sqrt{3}\cos^2(\pi/2n)},\ \lambda_{z2} = \frac{12 - 9\cos^2(\pi/2n)}{16\sqrt{3} - 4\sqrt{3}\cos^2(\pi/2n)}, \tag{10}$$

$$\text{and} \quad \lambda_z = \sqrt{4/3\cos^2\frac{\pi}{2n} - 1}$$

and n is the indices of translation, which dictate the structure around the circumference. The chiral vector $\vec{C}_h$ of zigzag CNT can be expressed with respect to two base vectors $\vec{a}_1$ and $\vec{a}_2$ as follows:

$$\vec{C}_h = n\vec{a}_1 + n\vec{a}_2 \tag{11}$$

The radius of the zigzag nanotube in terms of the chiral vector components can be obtained from the relation (Tokio 1995):

$$R = \frac{na}{2\pi}\sqrt{3}, \tag{12}$$

where a is the length of the carbon–carbon bond which is $1.42\,\mathrm{A}^{\circ}$.

2.4 Equations of motion

The strain energy U of the nanobeam is given by:

$$U = \frac{1}{2}\int_0^L\int_A\left[\sigma_x\left(\varepsilon_x - \frac{\alpha T}{1-2\nu}\right) + \tau_{xz}\gamma_{xz}\right]dAdx, \tag{13}$$

where σ_x is the normal stress, τ_{xz} the transverse shear stress, L the length of the SWCNT, and A its cross-sectional area.

The principle of virtual work for the present problem may be expressed as follows:

$$\left(N, M_b, M_s\right) = \int_A (1, z, f)\sigma_x dA \quad \text{and} \quad Q = \int_A g\tau_{xz}dA \tag{15}$$

where N, M, and Q are the stress resultants. Substituting Eqs. (6) and (7) into Eq. (14) and integrating by parts and then equating the coefficients of δu_0, δw_b and δw_s to zero, separately, the governing stability equations are obtained for the proposed beam theory as follows:

$$\delta u_0 : \frac{dN}{dx} = 0 \tag{16a}$$

$$\delta w_b : \frac{d^2M_b}{dx^2} + N_t\frac{d^2(w_b + w_s)}{dx^2} = 0 \tag{16b}$$

$$\delta w_s : \frac{d^2M_s}{dx^2} + \frac{dQ}{dx} + N_t\frac{d^2(w_b + w_s)}{dx^2} = 0 \tag{16c}$$

Here N_t is the thermal force which can be expressed as:

$$N_t = -\frac{E_z\,\alpha\,T\,A}{1-2\nu} \tag{17}$$

When the shear deformation effect is neglected ($w_s = 0$), the equilibrium equations in Eq. (16) recover those derived from the Euler–Bernoulli beam theory. By substituting Eq. (7) into Eq. (8) and the subsequent results into Eq. (15), the stress resultants are obtained as

$$N-(e_0a)^2\frac{d^2N}{dx^2}=A_m\left[\frac{du_0}{dx}+\frac{1}{2}\left(\frac{dw_b}{dx}+\frac{dw_s}{dx}\right)^2\right]+N_t \tag{18a}$$

$$M_b-(e_0a)^2\frac{d^2M_b}{dx^2}=-D\frac{d^2w_b}{dx^2}-D_s\frac{d^2w_s}{dx^2} \tag{18b}$$

$$M_s-(e_0a)^2\frac{d^2M_s}{dx^2}=-D_s\frac{d^2w_b}{dx^2}-H_s\frac{d^2w_s}{dx^2} \tag{18c}$$

$$Q-(e_0a)^2\frac{d^2Q}{dx^2}=A_s\frac{dw_s}{dx} \tag{18d}$$

where

$$\left(A_m,D,D_s,H_s\right)=\int_A\left(1,z^2,z\ f,f^2\right)E_z dA,\ A_s=\int_A g^2G_z dA \tag{19}$$

By substituting Eq. (18) into Eq. (16), the nonlocal equations of motion can be expressed in terms of displacements (w_b , w_s) as:

$$-D\frac{d^4w_b}{dx^4}-D_s\frac{d^4w_s}{dx^4}+N_t\left(\frac{d^2(w_b+w_s)}{dx^2}-(e_0a)^2\frac{d^4(w_b+w_s)}{dx^4}\right)=0 \tag{20a}$$

$$-D_s\frac{d^4w_b}{dx^4}-H_s\frac{d^4w_s}{dx^4}+A_s\frac{d^2w_s}{dx^2}+N_0\left(\frac{d^2(w_b+w_s)}{dx^2}-(e_0a)^2\frac{d^4(w_b+w_s)}{dx^4}\right)=0 \tag{20b}$$

The equations of buckling of *local* beam theory can be retrieved as a special case from Eq. (20) by setting the nonlocal parameter e_0a equal to zero. Eqs. (20) are effectively the governing equations for the present nano-structural problem. For the hinged boundary condition case, the solution of these eqs. for a carbon nanotube can be expressed as follows:

$$w_b=W_b\sin(\beta x)\ \text{ and }\ w_s=W_s\sin(\beta x) \tag{21}$$

where $\beta=m\pi/L$ and m denotes a positive integer which is related to the buckling modes.

Inserting equation (21) into equations (20), one can easily obtain:

$$\left(\begin{bmatrix}K_{11} & K_{12}\\ K_{12} & K_{22}\end{bmatrix}+\lambda N_t\beta^2\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}\right)\begin{Bmatrix}W_b\\ W_s\end{Bmatrix}=\begin{Bmatrix}0\\ 0\end{Bmatrix} \tag{22}$$

where

$$K_{11}=D\beta^4,\quad K_{12}=D_s\beta^4,\quad K_{22}=H_s\beta^4+A_s\beta^2,\quad \lambda=1+(e_0a)^2\beta^2 \tag{23}$$

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

$$T_{cr}^{non} = \frac{(1-2\nu)\left(K_{11}K_{22}-(K_{12})^2\right)}{E_z\beta^2\alpha\, A\,\lambda\left(K_{11}+K_{22}-2K_{12}\right)} \tag{24}$$

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

$$P_{cr} = \frac{T_{cr}^{non}}{I/\alpha\ AL^2} \tag{25}$$

3. Numerical examples and discussion

Based on the formulations obtained above with the present nonlocal refined shear deformation beam theory, the effect of the lattice indices of translation n on the thermal buckling properties of zigzag single-walled nanotubes are discussed here. The parameters used in calculations for the zigzag SWCNTs are given as follows: the effective thickness of CNTs taken to be 0.258 nm (Wu *et al*. 2006), the force constants (Cornell *et al*. 1995) *K*/2= 46900 kcal/mol/nm^2 and *C*/2= 63 kcal/mol/rad^2, the mass density ρ = 2.3 g cm^{-3} (Heireche *et al*. 2008a; Zidour *et al*. 2012) and the temperature expansion coefficient α = 1.1×10^{-6} K^{-1} which is for the case of the high temperature (Yao and Han 2006; Zidour *et al*. 2012). This data represents realistic CNTs.

Fig. 1 shows the *non-dimensional* critical buckling temperature of zigzag (15, 0) SWCNT versus the ratio of the length to the diameter. The obtained results are compared with those obtained using nonlocal Timoshenko beam model. The appropriate shear correction factor used in the Timoshenko beam model is $k=(2+2\nu)/(4+3\nu)$ i.e. that for a thin-walled tube (Cowper, 1996). It can be seen that the results of present theory are in excellent agreement with those predicted by the Timoshenko beam model.

Fig. 2 depicts the critical buckling temperature of zigzag (15, 0) SWCNT with different nonlocal values and $L/d=10$ for different modes based on present refined shear deformation beam theory. The parameter value of $e_0a=0$ implies that the *nonlocal effect is neglected*. Evidently the influence of nonlocal parameter e_0a on the critical buckling temperature is significant, especially at higher order modes. Increasing the nonlocal effect markedly *decreases* the critical buckling temperature.

The influences of the aspect ratio i.e. ratio of the length to the diameter (L/d), on the *non-dimensional* critical buckling temperature are shown in Fig. 3. The nonlocal parameter is e_0a =1 nm. From Fig. 3, *it is apparent that* when the mode number is less than 3, the difference is not obvious. This influence becomes considerable when the mode number is larger than 4. Moreover, the non-dimensional critical buckling temperatures for all of three aspect ratios are elevated with the mode number increasing. With a rise in aspect ratio i.e. the greater the ratio of the length to the diameter is, the higher the non-dimensional critical buckling temperature becomes. This implies that the ratio of the length to the diameter has significant influence on the non-dimensional critical buckling temperature for larger mode numbers, and this is a key consideration in nano-structural design exploiting CNTs.

The relation between the nondimensional critical buckling temperature, the chirality of zigzag

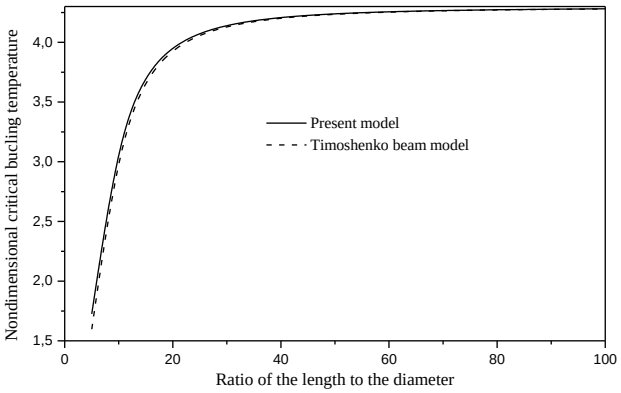

Fig. 1 Variations of critical buckling temperature of zigzag (15, 0) SWCNT with respect to the ratio of the length to the diameter (L/d) for nonlocal parameter $e_0a = 2\,nm$ and the number mode $m = 1$

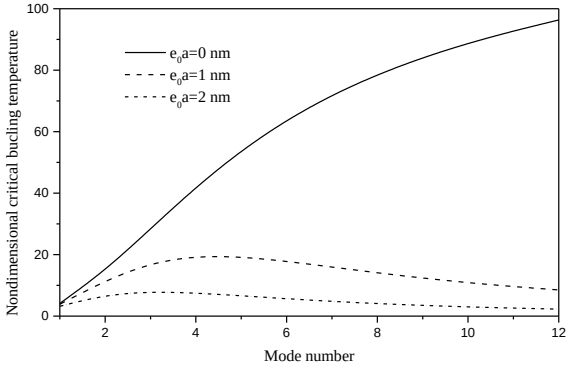

Fig. 2 Critical buckling temperature of zigzag (15, 0) SWCNT with different nonlocal parameters and $L/d = 10$ for different modes based on refined shear deformation beam theory

carbon nanotube n and the nonlocal parameter e_0a is shown in Figs. 4 and 5 for the mode number $m = 1$ and 5, respectively. It can be seen that the ranges of the non-dimensional critical buckling temperature for these mode numbers are quite different. In Fig. 4, the range is the smallest for $m = 1$, but the range is the largest for $m = 5$ in Fig. 5. This indicates that the larger the mode number is, the higher the non-dimensional critical buckling temperature becomes. Furthermore, it can be observed that the critical buckling temperature is enhanced with increasing the index of translation (n) whereas, conversely it is decreased with the nonlocal parameter increasing.

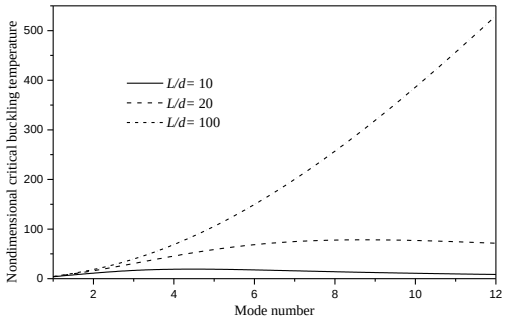

Fig. 3Critical buckling temperature of zigzag (15, 0) SWCNT with different ratios of the length to the diameter (L/d) and $e_0a=1nm$ nm for different modes based on refined shear deformation beam theory

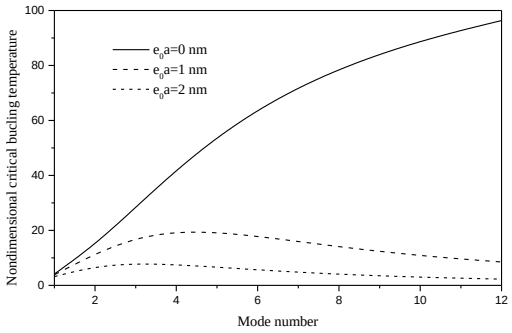

Fig. 4 Relationship between the critical buckling temperature, chirality of zigzag carbon nanotube n and the nonlocal parameter e_0a for mode number $m=1$ and aspect ratio $L/d=10$

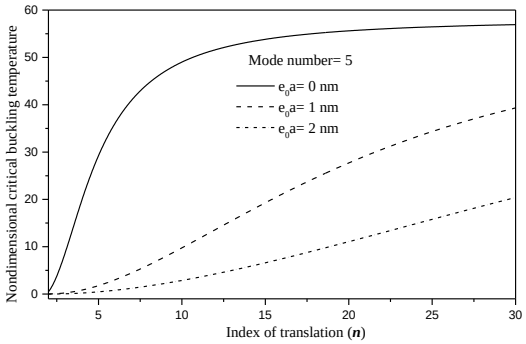

Fig. 5: Relationship between the critical buckling temperature, chirality of zigzag carbon nanotube n and the nonlocal parameter e_0a for mode number $m=5$ and aspect ratio $L/d=10$

4. Conclusions

A nonlocal shear deformation beam theory has been proposed for thermal buckling of zigzag single-walled carbon nanotubes. The geometric nonlinearity is considered using von Karman's strain– displacement relations. The present model is capable of capturing the small scale effect, chirality of zigzag SWCNT and transverse shear deformation effects of nanobeams, and does not require shear correction factors. The formulation lends itself particularly well to other analytical methods including for example, the Homotopy Perturbation Method (Anwar Bég and Islam 2011), which will be considered in the near future. This work is expected to be useful in the design and analyze the thermal buckling properties of nanoscale physical devices.

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