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On the Thermal Buckling Characteristics of Armchair Single-Walled Carbon Nanotube Embedded in an Elastic Medium Based on Nonlocal Continuum Elasticity

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Abstract In this paper, the thermal buckling characteristics of armchair single-walled carbon nanotube (SWCNT) embedded in a one-parameter elastic medium are investigated using a new nonlocal first-order shear deformation theory (NNFSDT). The present model is able to consider the small-scale effect as well as the transverse shear deformation effects of nanotubes. The equivalent Young's modulus and shear modulus for armchair SWCNT are obtained by employing the energy-equivalent model. A closed-form solution for non-dimensional critical buckling temperature is obtained in this investigation. The results illustrated in this work can provide a significant guidance for the investigation and design of the novel generation of nanodevices that make use of the thermal buckling characteristics of embedded SWCNT.

Keywords Carbon nanotube · Critical buckling temperature · Scale effects

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1 Introduction

Since the seminal work of Iijima [1] about carbon nanotubes (CNTs), a new era has evolved in the field of nanotechnology. Carbon nanotubes are among the most interesting nanomaterials that have become important topics for the nano researchers due to their outstanding mechanical characteristics and wide potential applications in nanotechnology. As a result, the importance of carbon nanotube is realized, and both theoretical and exponential works are carried out [2–5].

With the difficulty for controlled experiments at the nanometer scale, numerical simulation has been carried out widely. Although the molecular dynamics (MD) simulation is an effective way to study the mechanical characteristics of nanostructures, it is time-consuming or even impossible to perform the MD simulation. Then, the elastic continuum theory has become an effective method for calculation [7–10]. However, in the classical elastic model, the small-scale effects are not considered.

Due to the inherent size effects at the nanoscale, the mechanical characteristics of nanostructures are often significantly different from their behavior at the macroscopic scale. Eringen [6] developed the nonlocal continuum theory for the investigation of small-sized structures. According to this theory, the state of the stress at a point of a nanostructure does depend on the stress state not only of that point but also those of other points. Such a dependency is introduced into the constitutive equations of the nanostructure through a so-called small-scale parameter, commonly presented by $e_0 a$. By vanishing this parameter, the nonlocal continuum theory is reduced to the classical continuum theory. Commonly, e_0a is determined by justifying the dispersion curves predicted by the nonlocal continuum theory with those of an atomic model. There are some works [7, 8] on the calibration of e_0a for the problems of SWCNTs. Such studies pointed out that e_0a relies on the aspect ratio and boundary conditions of the nanotube. The undertaken works were limited



to cantilevered and fully clamped SWCNTs, and the lack of information regarding this parameter for elastically supported SWCNTs is still obvious.

Concerning the buckling behaviors of nanostructures, Sudak [9] studied the column buckling of CNT using the nonlocal elastic continuum model. Using nonlocal beam and shell model, Wang et al. [11] examined the small-scale effect on elastic buckling of CNT. Reddy [12] developed a mathematical formulation of equilibrium equations for static, buckling, and vibration of nanoscale beams. Based on nonlocal theory of thermal elasticity mechanics, Amara et al. [13] developed an elastic multiple-column model for the linearized column buckling of multiwalled carbon nanotubes (MWNTs). Tounsi et al. [14] studied the thermal buckling properties of double-walled carbon nanotubes (DWCNTs) using nonlocal Timoshenko beam model. Tounsi et al. [15] investigated the thermal buckling behavior of nanobeams by using an efficient higher order nonlocal beam theory. Berrabah et al. [16] proposed a unified nonlocal shear deformation theory to study bending, buckling, and free vibration of nanobeams.

In this paper, the thermal buckling analysis of armchair SWCNT embedded in elastic medium is proposed using a simple nonlocal first-order shear deformation beam theory. This theory was developed recently by Bouremana et al. [17] based on the assumption that the in-plane and transverse displacements consist of bending and shear components, in which the bending components do not contribute toward shear forces, and, likewise, the shear components do not contribute toward bending moments. In this work, this theory [17] is extended to the investigation of critical buckling temperature of thin small-sized embedded armchair SWCNTs. Winklertype model is used to simulate the interaction of the armchair SWCNTs with a surrounding elastic medium. The equivalent Young's modulus and shear modulus for armchair SWCNT are obtained using an energy-equivalent model [18–20]. The influence of the scale parameter, the Winkler modulus parameter, and the effect of the chirality of armchair SWCNT are taken into account in this work. It is hoped that the present analysis will be useful to researchers and engineers working on carbon nanotubes and CNT-based composites.

2 Present Nonlocal Elasticity Theory of Beams

Contrary to the local (classical) theory, the nonlocal theory considers that the stress at a point depends not only on the strain at that point but also on strains at all other points of the body [6]. For example, in the nonlocal elasticity, the uniaxial constitutive law is expressed as [15, 21]

$$\sigma_x - \mu \frac{d^2 \sigma_x}{dx^2} = E \left(\varepsilon_x - \frac{\alpha T}{1 - 2\nu} \right) , \qquad (1a)$$



$$\tau_{xz} - \mu \frac{d^2 \tau_{xz}}{dx^2} = G \gamma_{xz} , \qquad (1b)$$

where (σ_x, τ_{xz}) and $(\varepsilon_x, \gamma_{xz})$ are the stress and strain components, respectively. E is the elasticity modulus, G is the shear modulus, α is the thermal expansion coefficient, T is the temperature change, and ν is Poisson's ratio. $\mu = (e_0 a)^2$ is a nonlocal parameter revealing the nanoscale effect on the response of nanobeams, e_0 is a constant specific to each material, and ais an internal characteristic length. Arash and Wang [22] 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 carbon nanotubes. In the literature [14, 23], it is suggested that the 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 [14].

Using an energy-equivalent model [18–20], the equivalent Young's modulus, the shear modulus, and Poisson's ratio of an armchair CNT are expressed as

$$E = \frac{4\sqrt{3}}{3} \frac{KC}{3Ct + 4Ka^2t(\lambda_{a1}^2 + 2\lambda_{a2}^2)},$$

$$G = \frac{6\sqrt{3}KC}{(18C + Ka^2\lambda_a^2)t}, \quad \nu = \frac{a^2\lambda_{a1}K - C}{a^2\lambda_{a1}K + 3C},$$
(2)

where *K* and *C* are the force constants. *t* is the thickness of the nanotube, and the parameters $\lambda_{a1}, \lambda_{a2}$ and λ_a are given by

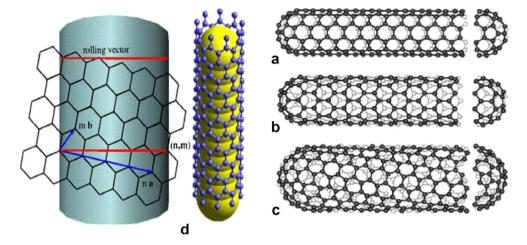
$$\lambda_{a1} = \frac{4 - \cos^{2}(\pi/2n)}{16 + 2\cos^{2}(\pi/2n)}, \quad \lambda_{a2}$$

$$= \frac{-\sqrt{12 - 3\cos^{2}(\pi/2n)}\cos(\pi/2n)}{32 + 4\cos^{2}(\pi/2n)}, \text{ and } \lambda_{a}$$

$$= \sqrt{4/\cos^{2}\frac{\pi}{2n} - 1}, \qquad (3)$$

where n is the index of translation of the armchair CNT. Figure 1 shows the lattice indices of translation (n, m) along with the base vectors. The radius of the armchair CNT in terms of the chiral vector components can be obtained from the relation [24]

Fig. 1 a An armchair, **b** a zigzag and **c** a chiral nanotube, and (**d**) a graphene being rolled into a cylinder



$$R = \frac{3na}{2\pi} \ , \tag{4}$$

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

Based on the first shear deformation beam theory developed by Bouremana et al. [17], the displacement field at any point can be written as

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

$$w(x,z) = w_b(x) + w_s(x)$$
, (5b)

where x is the longitude coordinate, z the coordinate measured from the midplane of the CNT, and u,w are displacements in the x,z, directions, respectively. u_0,w_b , and w_s are midplane displacements. The strains associated with the displacements in Eqs. (5a) and (5b) are

$$\varepsilon_{\rm x}=\varepsilon_{\rm x}^0+zk_{\rm x}^b \ \ {\rm and} \ \ \gamma_{\rm xz}=\gamma_{\rm xz}^{\rm s} \ \ , \eqno(6a)$$

where

$$\varepsilon_x^0 = \frac{\partial u_0}{\partial x}, \ k_x^b = -\frac{\partial^2 w_b}{\partial x^2}, \ \gamma_{xz}^s = \frac{\partial w_s}{\partial x}. \tag{6b}$$

The governing equations will be obtained by employing the principal of the minimum total potential energy. The variation of the strain energy of the beam can be stated as

$$\delta U = \int_{V} (\sigma_{x} \delta \varepsilon_{x} + \tau_{xz} \delta \gamma_{xz}) dV$$

$$= \int_{0}^{L} \left(N \frac{d\delta u_{0}}{dx} - M \frac{d^{2} \delta w_{b}}{dx^{2}} + Q \frac{d\delta w_{s}}{dx} \right) dx , \qquad (7)$$

where N, M, and Q are the stress resultants defined as

$$(N,M) = \int_{A} (1,z)\sigma_x dA \text{ and } Q = \int_{A} k_s \tau_{xz} dA , \qquad (8)$$

where k_s is the shear correction factor. The first variation of the work done by the external forces is given by

$$\delta V = \int_{0}^{L} q(\delta w_b + \delta w_s) dx + \int_{0}^{L} P_t \left(\frac{d\delta u_0}{dx} + \frac{d(w_b + w_s) d(\delta w_b + \delta w_s)}{dx} \right) dx ,$$
(9)

where q is the distributed transverse load and P_t is the thermal force which can be expressed as

$$P_t = -\frac{E\beta TA}{1 - 2\nu} \,,\tag{10}$$

in which β is the thermal expansion coefficient, T the temperature change, A the cross area, and ν the Poisson's ratio.

According to the minimum total potential energy principle, the first variation of the total potential energy must be zero. That is,

$$\delta \Pi = \delta(U - V) , \qquad (11)$$

in which Π is the total potential energy. Substituting Eqs. (7) and (9) in equation (11), and after performing integration by parts, we reach

$$\frac{dN}{dx} = 0 , (12a)$$

$$\frac{d^2M}{dx^2} - P_t \frac{d^2(w_b + w_s)}{dx^2} + q = 0 , \qquad (12b)$$



$$\frac{dQ}{dx} - P_t \frac{d^2(w_b + w_s)}{dx^2} + q = 0 . {12c}$$

In general, in order to reinforce the strength of composites, CNTs are commonly embedded in an elastic medium, and the surrounding elastic medium has a strong effect on mechanical behaviors of CNTs such as stability and dynamic behavior. To analyze the thermal buckling characteristics of CNTs surrounded with an elastic medium, Winkler-type elastic foundation model is employed to simulate the interaction of CNTs with the surrounding elastic medium. That is, Winkler-type foundation model can be stated as

$$q = -k_w(w_b + w_s) , \qquad (13)$$

in which k_w is the spring constant of the surrounding elastic medium.

By using Eqs. (1a), (1b), (6a), (6b), and (8), the force–strain and the moment–strain relations of the present nonlocal first-order shear deformation theory can be obtained as follows:

$$N - (e_0 a)^2 \frac{d^2 N}{dx^2} = E A \frac{du_0}{dx} , \qquad (14a)$$

$$M - (e_0 a)^2 \frac{d^2 M}{dx^2} = -EI \frac{d^2 w_b}{dx^2} , \qquad (14b)$$

$$Q - (e_0 a)^2 \frac{d^2 Q}{dx^2} = k_s G A \frac{dw_s}{dx} , \qquad (14c)$$

where

$$(A,I) = \int_{A} (1,z^{2}) dA . (15)$$

And by utilizing Eqs. (12a), (12b), (12c), (13), (14a), (14b), and (14c), the governing equation for the buckling of nonlocal first-order shear deformable beam may be obtained as below

$$-EI\frac{d^4w_b}{dx^4} = \left(1 - (e_0a)^2 \frac{d^2}{dx^2}\right) \left(P_t \frac{d^2(w_b + w_s)}{dx^2} + k_w(w_b + w_s)\right),$$
(16a)

$$k_s G A \frac{d^2 w_s}{dx^2} = \left(1 - (e_0 a)^2 \frac{d^2}{dx^2}\right) \left(P_t \frac{d^2 (w_b + w_s)}{dx^2} + k_w (w_b + w_s)\right).$$
(16b)

3 Analytical Solution of Simply Supported Nanotube

In this work, analytical solutions are given for simply supported armchair SWCNT. The following displacement field satisfies boundary conditions and governing equations.

$$\begin{cases} w_b \\ w_s \end{cases} = \sum_{n=1}^{\infty} \begin{cases} W_{bn} \sin(\alpha x) \\ W_{sn} \sin(\alpha x) \end{cases} ,$$
 (17)

where W_{bn} and W_{sn} are arbitrary parameters to be determined $\alpha = k\pi/L$ and k a positive integer which is related to the buckling modes. Substituting the expansions of w_b and w_s from equation (17) into equation (16), the closed-form solutions can be obtained from the following equations:

$$\left(\begin{bmatrix} S_{11} & 0 \\ 0 & S_{22} \end{bmatrix} - \lambda \left(k_w + P_t \alpha^2\right) \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\right) \begin{Bmatrix} W_{bn} \\ W_{sn} \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \end{Bmatrix},$$
(18)

where

$$S_{11} = EI\alpha^4, \ S_{22} = A_s\alpha^2, \ \lambda = 1 + \mu\alpha^2$$
 (19)

Then, the critical temperature with the new nonlocal firstorder shear deformation theory can be obtained as

$$T_{cr} = \frac{(1-2\nu)S_{11}S_{22}}{EA\beta\lambda\alpha^2(S_{11} + S_{22})} - k_w \frac{(1-2\nu)}{EA\beta\alpha^2} \ . \tag{20}$$

For the sake of simplicity, the following dimensionless variable is introduced for Winkler foundation parameter:

$$K_w = \frac{L^4}{EI} k_w \ . \tag{16}$$

4 Validity and Applicability of Continuum Beam Model for CNTs

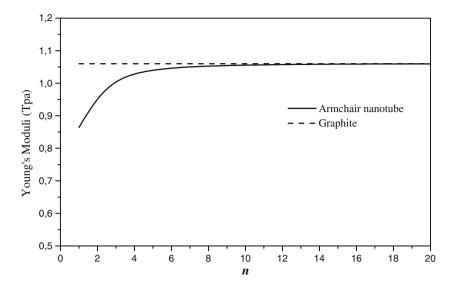
Applicability of continuum beam theory for carbon nanotubes (CNTs) is discussed by several authors (e.g., Wang and Hu [25] and Harik [26, 27]). The ranges of applicability for the continuum beam theory in the mechanics of CNTs and nanorods were reported by Harik [26, 27]. Wang and Hu [25]

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 new nonlocal first shear deformation theory (NNFSDT)

L(Å)	d (Å)	MD	NNFSDT	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. 2 The variation of Young's modulus



propose a rigorous investigation, in which they verify the validity of the beam model in examining the flexural waves, simulated by the molecular dynamics (MD), in a single-walled carbon nanotube. In their study, Wang and Hu [25] remarked that when the wave number is getting very large, the microstructure of the carbon nanotubes takes a considerable effect in the flexural wave dispersion and significantly reduces the phase velocity of the flexural waves of high frequency.

In the present work, the numerical results for critical buckling strains obtained from this continuum mechanics theory (using the new nonlocal first-order shear deformation theory (NNFSDT)) are compared with those obtained from MD simulations and the Sanders shell theory (SST) [28]. Since the MD simulations referenced herein consider the CNTs with fixed ends, we also consider the present NNFSDT with fully clamped boundary conditions [29]. In addition, CNT (5, 5) is

studied with a diameter d=6.71 Å and CNT (7, 7) with a diameter d=9.40 Å, for different lengths. Both nanotubes are modeled using a thickness t=0.66 Å, Young's modulus E=5.5 TPa, and Poisson's ratio ν =0.19 [30]. The lengths of CNTs used in the following table are extracted from the work done by Silvestre et al. [28]. The results from MD simulations, the present NNFSDT, and SST are compared in Table 1. It is seen that the critical buckling strains are in good agreement when compared to the results obtained from MD simulations as well as Sanders shell theory (SST). 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 %).

Fig. 3 The variation of Shear modulus.

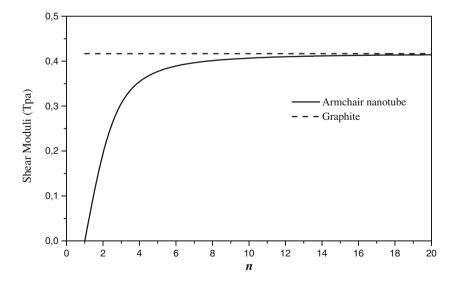
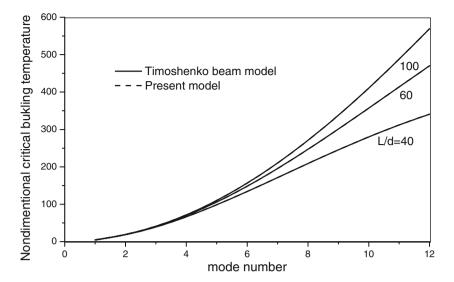




Fig. 4 Nondimensional critical buckling temperature by the nonlocal Timoshenko beam model and the present model for different mode numbers and various values of ratio of the length to the diameter ($e_0a=1$ nm, $K_w=0,n=15$)



5 Numerical Examples and Discussions

In this section, numerical computations for the thermal buckling characteristics of embedded armchair SWCNTs are carried out. The parameters used in calculations for the armchair SWCNTs are given as follows: the effective thickness of CNTs is taken to be 0.258 nm [18, 19], the force constants $K/2=46900 \text{ kcal/mol/nm}^2$ and $C/2=63 \text{ kcal/mol/rad}^2$ [31]. The temperature expansion coefficient $\beta=1.1\times10^{-6}$ K⁻¹, which is for the case of high temperature [13, 32, 33].

The variation of Young's modulus versus the structure characteristic (n) of the nanotube is presented in Fig. 2. It can be seen that increasing the lattice index of translation leads to an increase of the Young's modulus of armchair nanotubes. The same variation trend is seen for the shear modulus of carbon nanotubes in Fig. 3. From Figs. 2 and 3, it can be clearly observed that for carbon nanotubes with lattice index of translation n, Young's modulus and shear modulus exhibit a

strong dependence on the structure characteristic of nanotube n. However, for those with larger values of n, this dependence becomes very weak. The reason for this phenomenon is that a carbon nanotube with smaller lattice indices of translation n has a larger curvature, which results in a more significant distortion of C–C bonds. As the structure characteristic of nanotube n increases, the effect of curvature diminishes gradually, and all of Young's modulus and shear modulus approach the values of graphite sheet. This result has also been obtained and discussed by an earlier MD simulation [34, 35].

For verification purposes, the obtained results are compared with the conventional nonlocal Timoshenko model [21] for different ratios of the length to the diameter (L/d). For all calculations, the value of shear correction factor is taken as $k_s = (2+2\nu)/(4+3\nu)$ [36]. From Fig. 4, it can be seen that both the present new nonlocal first-order shear deformation theory and the conventional nonlocal Timoshenko model [21] give identical results. Furthermore, it is

Fig. 5 Variation of the nondimensional critical buckling temperature of armchair SWCNT with the mode number for various values of chirality numbers ($L/d=20, e_0a=1 \text{ nm}, K_w=10$)

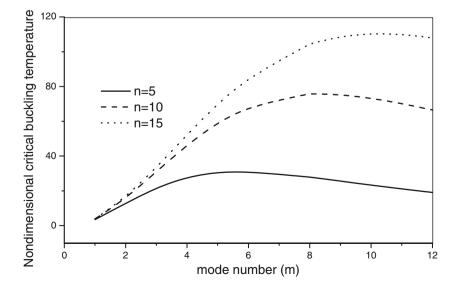
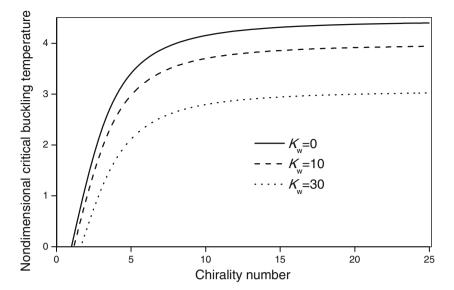




Fig. 6 Variation of the nondimensional critical buckling temperature of armchair SWCNT with chirality number for various values of Winkler foundation parameters (L/d=20, $e_0a=2$ nm, m=1)



observed that the effects of the ratio of the length to the diameter (L/d) on the nondimensional critical buckling temperature become significant when the mode number is greater than 5. Moreover, the nondimensional critical buckling temperatures for all of the three ratios become larger with the mode number increasing.

The relation between the nondimensional critical temperature and the axial mode number as well as the chirality number is illustrated in Fig. 5. The most notable feature is that the effect of the chirality number on the critical buckling temperature is relatively weak for small mode numbers. However, the difference becomes obvious with the mode number increasing.

Figure 6 illustrates the effect of the index of translation n on the critical buckling temperature of embedded armchair SWCNT with elastic medium modeled as Winkler-type

foundation. From the figure, it is observed that there is significant influence of the chirality number on the thermal buckling response of embedded SWCNT. Furthermore, it is seen that as the Winkler modulus parameter increases, the critical buckling temperature decreases. This decreasing trend is attributed to the stiffness of the elastic medium.

Figure 7 indicates the effect of the small scale on the critical buckling temperature of armchair SWCNT for various Winkler modulus parameters. As the nonlocal parameter (e_0a) increases, the critical buckling temperature decreases. Thus, it can be concluded that the classical elastic (i.e., the local) model, which does not consider the small-scale effects, will give a higher approximation for the critical buckling temperature. But the nonlocal continuum theory will present an accurate and reliable result. In addition, an interesting feature that can be deduced is that as the Winkler foundation

Fig. 7 Variation of the nondimensional critical buckling temperature of armchair SWCNT with the nonlocal small-scale parameters for various values of Winkler foundation parameters (L/d=20, n=15, m=1)

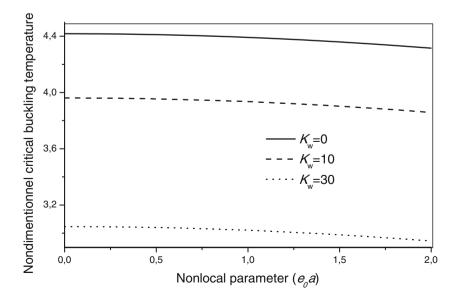
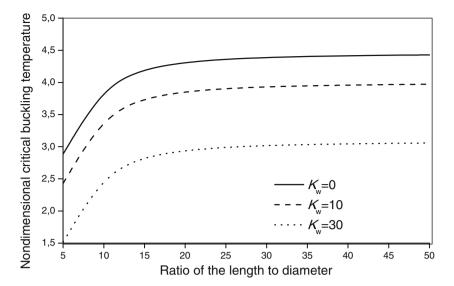




Fig. 8 Variation of the nondimensional critical buckling temperature of armchair SWCNT with the length to diameter ratio for various values of Winkler foundation parameters ($e_0a = 2$ nm,n = 15,m = 1)



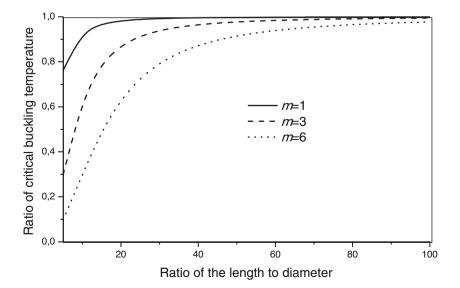
parameter increases, the value of critical buckling temperature decreases irrespective of the nonlocal parameter.

Figure 8 shows the variation of the critical buckling temperature of armchair SWCNT with aspect ratios L/d for various Winkler modulus parameters. Three different values of Winkler modulus parameter are considered for the study, viz. K_w =0, 10, and 30. In this present computation, a constant value of nonlocal parameter (e_0a =2 nm) and the index of translation (n=15) are used for the proposed model. From the figure, it is seen that as the aspect ratios (L/d) increase, the critical buckling temperature increases until taken as a constant value for higher values of L/d. Thus, for a slender SWCNT, the effect of shear deformation is less compared to short SWCNT.

In order to highlight the effect of the transverse shear deformation, the ratio of the critical buckling temperature by the present new nonlocal first-order shear deformation theory to

the nonlocal Euler-Bernoulli beam theory with different ratios of the length to the diameter is illustrated in Fig. 9. The mode number m=1,3,6, the chirality number n=8, the Winkler modulus parameter $K_w=10$, and the scale coefficient $e_0a=$ 2 nm are considered. From Fig. 9, it can be shown 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, the critical buckling temperature of the new nonlocal first-order shear deformation theory (NNFSDT) is lower than that of the nonlocal Euler-Bernoulli beam theory. 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 should be considered, and the nonlocal first-order shear deformation theory is more accurate for short carbon nanotubes.

Fig. 9 Ratio of the nondimensional critical buckling temperature by the nonlocal Timoshenko beam model to the nonlocal Euler–Bernoulli beam model vs. ratio of the length to the diameter with different mode numbers (m) $(e_0a=1\,\mathrm{nm},n=8,K_w=10)$





6 Conclusions

In this work, the thermal buckling characteristics of armchair SWCNTs, which are embedded in elastic medium, are predicted using a new nonlocal first-order shear deformation theory. The mathematical formulations include the nonlocal parameter effect, the temperature change, and the chirality of armchair carbon nanotubes. The effects of the scale coefficient, the ratio of the length to the diameter, the transverse shear deformation, the stiffness of the surrounding elastic medium, and the chirality of the thermal buckling properties are investigated. The formulation lends itself particularly well to nanostructures embedded in a Pasternak elastic medium [37–41] and/or studied with advanced shear deformation theories [42–44], which will be considered in the near future.

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