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Buckling temperature of a single-walled boron nitride nanotubes using a novel nonlocal beam model

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Abstract. In this paper, the critical buckling temperature of single-walled Boron Nitride nanotube (SWBNNT) is estimated using a new nonlocal first-order shear deformation beam theory. The present model is capable of capturing both small scale effect and transverse shear deformation effects of SWBNNT and is based on 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. Results indicate the importance of the small scale effects in the thermal buckling analysis of Boron Nitride nanotube.

Keywords: single walled boron nitride nanotube; critical buckling temperature; small scale effect

1. Introduction

One of the most promising materials for nanotechnology is boron nitride nanotubes (BNNTs) due to the coupling characteristics of electromechanics field. This promising material were theoretically predicted in 1994 (Rubio *et al*. 1994, Blase *et al*. 1994) and experimentally realized in the following year (Chopra *et al*. 1995). BNNT is a structural analog of a Carbon Nanotube (CNT) in nature: (Iijima 1991, Oberlin *et al*. 1976) alternating B and N atoms entirely substitute for C atoms in graphitic like sheet with almost no change in atomic spacing (Fig. 1) (Panchal and Upadhyay 2013a). Such BNNTs possess many of the superior properties of the CNTs (Santosh *et al*. 2009) such as exceptional elastic properties (Goldberg *et al*. 2010, Moon and Hwang 2004, Pokropivny *et al*. 2008, Verma *et al*. 2007, Li and Chou 2006), high mechanical strength (Jeon and Mahan 2009, Ghassemi and Yassar 2010, Suryavanshi *et al*. 2004, Chopra and Zettl 1998), chemical inertness (Zhi *et al*. 2008) and structural stability (Ciofani *et al*. 2009), high heat conduction and piezoelectricity (Oh, 2010). In addition, BNNT has a wide band-gap independent of geometrical/atomic configuration. These factors make BNNT particularly suitable for biological and medical applications (Zhi *et al*. 2005, Kumar *et al*. 2014, Genchi *et al*. 2016, Rocca *et al*.

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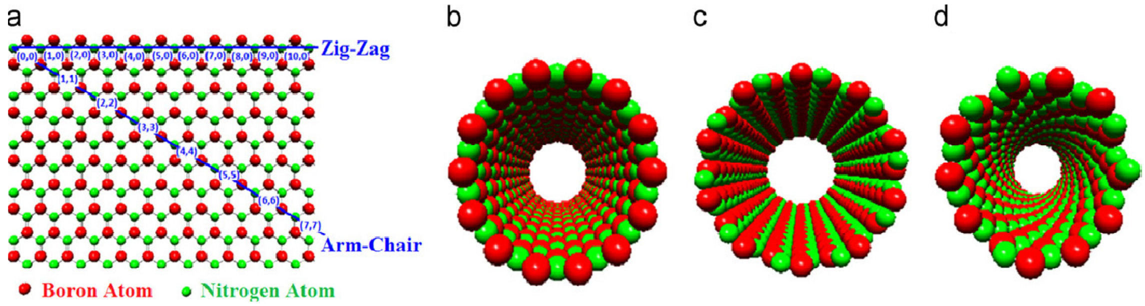

Fig. 1 (a) Plane BN sheet with possible wrapping of zigzag and armchair chiralities and structural models of single walled BNNTs made of a wrapped BN layer; (b) zigzag; (c) armchair; and (d) chiral (Panchal and Upadhyay 2013a)

2016). Also, potential applications of BNNTs include various materials reinforcements such as polymer, ceramic, and metal based composites, and key parts of nanomechanical systems. Unlike CNTs, BNNTs are expected to be semi-conducting material, with predictable electronic properties that are independent of tube diameter and number of layers.

In recent years, a large amount research works have been carried out on the buckling and vibration of the nanotubes. Lu *et al*. (2007) investigated the wave propagation and vibration properties of single- or multi-walled CNTs based on nonlocal beam model. Reddy (2007) developed nonlocal theories for Euler–Bernoulli, Timoshenko, Reddy, and Levinson beams. Analytical bending, vibration and buckling solutions are obtained which bring out the nonlocal effect on bending deformation, buckling load, and natural frequencies. Heireche *et al*. (2008a) studied the Sound wave propagation in single-walled carbon nanotubes using nonlocal elasticity. Heireche *et al*. (2008b) discussed the scale effect on wave propagation of double–walled carbon nanotubes with initial axial loading. Benguediab *et al*. (2014) investigated the Chirality and scale effects on mechanical buckling properties of zigzag double-walled carbon nanotubes. Besseghier *et al*. (2015) examined the nonlinear vibration properties of a zigzag single-walled carbon nanotube embedded in a polymer matrix. Rakrak *et al*. (2016) investigated the free vibration problem for chiral double-walled carbon nanotube using the non-local elasticity theory and Euler Bernoulli beam model. Furthermore, Tounsi *et al*. (2009a, b) derived the consistent governing equation of motion for the free vibration of fluid- conveying CNTs with nonlocal effect, which is an important application of nonlocal elastic theory in CNTs. More recently, Tounsi *et al*. (2013a, b) investigated the thermal buckling of nanobeams using an efficient higher-order nonlocal beam theory. Considering the effects of the transverse shear deformation and rotary inertia, Tounsi *et al*. (2013a, b) studied the thermal buckling properties of double walled carbon nanotube with the classical Timoshenko beam model. The characteristics of the critical buckling temperature were presented.

All the above mentioned references were considered CNTs, but few studies dealing with BNNTs can be found in the published literature. Recently, Panchal and Upadhyay (2013b) used molecular structural mechanics based FE model to simulate the atomic structure of SWBNNT considering the presence of extended defect/dislocation line. Panchal *et al*. (2013a) employed 3-dimensional atomistic finite element model to simulate the atomic structure of the defective SWBNNT considering point defects (VB – boron vacancy, VN – nitrogen vacancy, and VBN – divacancies). The potentials of single walled BNNTs as nanomechanical resonators considering both cantilevered and bridged nanotubes are investigated by Panchal *et al*. (2012) using continuum mechanics based analytical approach and finite element model. The vibration response analysis of SWBNNTs treated as thin walled tube has been done by Panchal *et al*. (2013b) using finite element method (FEM). Using the FE modelling-based simulation approach the feasibility of SWBNNT-based biosensor in terms of detection as well as identification of intermediate landing position of the biological object having mass of zeptogram-scale is exploded by Panchal and Upadhyay (2014). Panchal *et al*. (2014) presented an ultra-sensitive biosensor based on a single-walled boron nitride nanotube (SWBNNT) structure for acetone detection.

The buckling of structures is an important topic of researches. Indeed, Jabbari *et al*. (2014) examined the thermal buckling response of porous circular plate with piezoelectric actuators based on first order shear deformation theory. Chen *et al*. (2014) studied the buckling of a piezo-electric viscoelastic nano beam subjected to vander Waals forces. Nasihatgozar *et al*. (2016) discussed the buckling behaviour of piezoelectric cylindrical composite panels reinforced with CNTs. Belkorissat *et al*. (2015) analyzed vibration properties of functionally graded nano-plate using a new nonlocal refined four variable model. Bounouara *et al*. (2016) presented a nonlocal zeroth-order shear deformation theory for free vibration of functionally graded nanoscale plates resting on elastic foundation. Eltaher *et al*. (2016) studied the static stability of nonlocal nanobeams using higher-order beam theories. To the best of authors' knowledge the thermal buckling of BNNTs using nonlocal beam theory is not studied in the open literature.

In this research, the nonlinear thermal buckling of SWBNNTs is investigated using a new nonlocal first-order shear deformation beam theory basing on the local beam model developed recently by Bouremana *et al*. (2013). The displacement field of the proposed theory is chosen based on the following assumptions: (1) the transverse displacement consists 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; (2) the bending component of axial displacement is similar to that given by the Euler–Bernoulli beam theory. Based on the nonlocal constitutive relations of Eringen (1983) and the von Karman nonlinear kinematic relations, the governing equations of SWBNNTs are derived using the principle of virtual work. The scale effects on the thermal buckling properties of BNNT 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. The results presented in this paper can provide useful guidance for the study and design of the next generation of nanodevices that make use of the thermal buckling properties of Boron Nitride nanotubes.

2. Atomic structure of SWBNNT

Fig. 1 presents the lattice indices of translation (n, m) along the base vectors, $\vec{a}_1$ and $\vec{a}_2$ (Panchal and Upadhyay 2013a, b, 2014, Panchal *et al*. 2012). The n and m are the indices of translation which decide the structure around the circumference. The value of index translation $m = 0$ and $m = n$ results in zigzag and armchair forms of SWBNNTs, respectively.

3. Analysis

SWBNNTs have an equivalent Young's modulus E, shear modulus G, length L, average radius r and thickness h. The first-order shear deformation beam theory developed by Bouremana *et al*.

(2013) is utilized to analyze the thermal buckling response for the SWBNNTs subjected to a uniform temperature rise. The displacement field of the present model is given as follows (Bouremana *et al*. 2013)

$$u(x,z) = -z\frac{\partial w_b}{\partial x} \tag{1a}$$

$$w(x,z) = w_b(x) + w_s(x) \tag{1b}$$

where the transverse displacement w is portioned into bending (w_b) and shear parts (w_s). u is the axial displacement.

The non zero strains associated with the displacements in Eq. (1) are (Bouremana *et al*. 2013)

$$\varepsilon_x = -z\frac{\partial^2 w_b}{\partial x^2} \quad \text{and} \quad \gamma_{xz} = \frac{\partial w_s}{\partial x} \tag{2}$$

where ε_x is the axial strain and γ_{xz} the shear strain.

3.1 Constitutive relations

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

$$\sigma_x - \mu\frac{d^2\sigma_x}{dx^2} = E\varepsilon_x \tag{3a}$$

$$\tau_{xz} - \mu\frac{d^2\tau_{xz}}{dx^2} = G\gamma_{xz} \tag{3b}$$

where σ_x is the axial stress, τ_{xz} the shear stress, E Young's modulus, G the shear modulus and $\mu = (e_0a)^2$ is the nonlocal parameter. e_0 is a constant appropriate to each material and a is an internal characteristic length.

3.2 Governing equations

The principle of virtual works of the considered nanobeam is expressed as (Bourada *et al*. 2015, 2016, Ait Amar Meziane *et al*. 2014, Belabed *et al*. 2014, Ait Yahia *et al*. 2015, Bourada *et al*. 2016)

$$\delta U + \delta V = 0 \tag{4}$$

where δU is the virtual strain energy and δV is the external virtual works due to the external load applied to the nanobeam. The variation of the strain energy of the beam can be stated as (Hebali *et al*. 2014, Bourada *et al*. 2015)

$$\delta U = \int_0^L \int_A (\sigma_x \delta\varepsilon_x + \tau_{xz}\delta\gamma_{xz}) dA dx = \int_0^L \left(-M_b \frac{d^2\delta w_b}{dx^2} + Q\frac{d\delta w_s}{dx} \right) dx \tag{5}$$

where M_b and Q are the stress resultants defined as (Bourada *et al*. 2015)

$$M_b = \int_A z\,\sigma_x dA \qquad \text{and} \qquad Q = \int_A \tau_{xz} dA \tag{6}$$

The variation of the potential energy by the applied loads can be written as (Bourada *et al*. 2015)

$$\delta V = -\int_0^L N_0 \frac{d(w_b + w_s)}{dx}\frac{d\delta(w_b + w_s)}{dx} dx \tag{7}$$

where N_0 is the axial loads.

Substituting the expressions for δU and δV from Eqs. (5) and (7) into Eq. (4) and integrating by parts, and collecting the coefficients of δw_b, and δw_s, the following governing equations of the proposed beam theory are obtained

$$\delta w_b : \frac{d^2 M_b}{dx^2} - N_0 \frac{d^2 (w_b + w_s)}{dx^2} = 0 \tag{8a}$$

$$\delta w_s : \frac{dQ}{dx} - N_0 \frac{d^2 (w_b + w_s)}{dx^2} = 0 \tag{8b}$$

when the shear deformation effect is neglected (w_s = 0), the equilibrium equations in Eq. (8) recover those derived from the Euler–Bernoulli beam theory.

By substituting Eq. (2) into Eq. (3) and the subsequent results into Eq. (6), the stress resultants are obtained as

$$M_b - \mu \frac{d^2 M_b}{dx^2} = -D \frac{d^2 w_b}{dx^2} \tag{9a}$$

$$Q - \mu \frac{d^2 Q}{dx^2} = A_s \frac{dw_s}{dx} \tag{9b}$$

where

$$D = \int_A z^2 E dA\,, \qquad A_s = K_s \int_A G dA \tag{10}$$

where K_s is the shear correction factor employed to compensate for the error due to constant shear stress assumption.

By substituting Eq. (9) into Eq. (8), the nonlocal governing equations can be expressed in terms of displacements (w_b, w_s) as

$$(D - \mu N_0)\frac{d^4 w_b}{dx^4} + N_0\left(\frac{d^2(w_b + w_s)}{dx^2} - \mu \frac{d^4 w_s}{dx^4}\right) = 0 \tag{11a}$$

$$(N_0 - A_s)\frac{d^2 w_s}{dx^2} + N_0\left(\frac{d^2 w_b}{dx^2} - \mu \frac{d^4 (w_b + w_s)}{dx^4}\right) = 0 \tag{11b}$$

The governing equations of local beam theory can be obtained from Eq. (11) by setting the scale parameter μ equal to zero.

For the present model, the nonlocal governing equation for the buckling of SWBNNT considering thermal effects can be rewritten as

$$(D-\mu N_0)\frac{d^4 w_b}{dx^4}+N_{th}\left(\frac{d^2(w_b+w_s)}{dx^2}-\mu\frac{d^4 w_s}{dx^4}\right)=0 \tag{12a}$$

$$(N_{th}-A_s)\frac{d^2 w_s}{dx^2}+N_{th}\left(\frac{d^2 w_b}{dx^2}-\mu\frac{d^4(w_b+w_s)}{dx^4}\right)=0 \tag{12b}$$

Based on the theory of thermal elasticity mechanics, the axial load $N_{th} = N_0$ can be expressed as

$$N_{th}=\frac{EA}{1-2\nu}\alpha_x T \tag{13}$$

where α_x is the coefficient of thermal expansion in the direction of x-axis, and ν is Poisson's ratio, respectively. T presents the change in temperature. In the present work, it is supposed that only axial force due to temperature change exists on the SWBNNT.

3.3 Analytical solutions

An explicit solution of critical buckling temperature versus geometrical parameters, material constants, thermal load, and nonlocal scale parameter is illustrated in this section. The supposed displacement field in the case of SWBNNT hinged at two ends can be described by the following harmonic functions that respect the boundary conditions

$$\begin{Bmatrix} w_b \\ w_s \end{Bmatrix}=\sum_{n=1}^{\infty}\begin{Bmatrix} W_{bn}\sin(\beta x) \\ W_{sn}\sin(\beta x) \end{Bmatrix} \tag{14}$$

where W_{bn}, and W_{sn} are arbitrary parameters to be determined, ω is the eigenfrequency associated with nth eigenmode, and $\beta = n\pi / L$.

Substituting the expansions of w_b and w_s from Eq. (14) into Eq. (12), the closed-form solutions can be obtained from the following equations

$$\left(\begin{bmatrix} S_{11} & S_{12} \\ S_{12} & S_{22} \end{bmatrix}-\lambda N_{th}\alpha^2\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\right)\begin{Bmatrix} W_{bn} \\ W_{sn} \end{Bmatrix}=\begin{Bmatrix} 0 \\ 0 \end{Bmatrix} \tag{15}$$

where

$$S_{11}=D\beta^4, \qquad S_{12}=0, \qquad S_{22}=A_s\beta^2, \qquad \lambda=1+\mu\beta^2 \tag{16}$$

Then, the thermal critical buckling load with the nonlocal continuum theory can be derived as

$$N_{th}=\frac{S_{11}S_{22}}{\lambda\beta^2(S_{11}+S_{22})} \tag{17}$$

The critical temperature with the nonlocal continuum theory can be obtained as

$$T_{cr} = \frac{\beta^2 K_s GI(1-2\upsilon)}{\alpha_x(1+\mu\beta^2)(\beta^2 EI + K_s GA)} \tag{18}$$

The non-dimensional critical temperature can be written as the following form

$$P_{cr} = \alpha_x \frac{AL^2}{I} T_{cr} \tag{19}$$

I represents the moment of area of the cross-section.

4. Numerical results and discussion

The dimensions and characteristics employed in numerical results for the SWBNNTs with zigzag structure are considered as follows: the wall thickness h = 0.075 mm, mean radius r = 0.313 nm, Poisson's ratio v = 0.34, elastic modulus E = 1.8 TPa, and the values of thermal expansion is $\alpha_x = 1.2\times10^{-6}$.

The variation of the non-dimensional critical temperature and the axial mode number is illustrated in Fig. 2. The results obtained using the present nonlocal first-order shear deformation beam theory (PFSDT) coincides with those predicted using the conventional Timoshenko beam theory (TBT). It can be seen that the results based on local and nonlocal theories are almost the same for small mode numbers. However, by increasing the mode number, the difference becomes obvious. In addition, it can be observed that the increasing of nonlocal parameter causes the decreasing in critical temperature.

The comparison of non-dimensional critical temperature buckling of zigzag SWBNNTs with different slenderness ratios for the first six modes based on nonlocal conventional TBT and nonlocal PFSDT is shown in Fig. 3. As depicted in the figure, the two theories provide identical results. It can be seen that the effect of the slenderness ratio on the critical temperature buckling, is

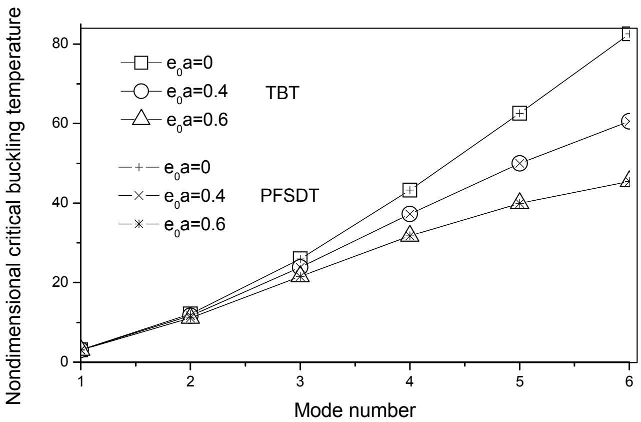

Fig. 2 Relation between the non-dimensional critical buckling temperature and the mode number for different scale coefficients (e_0a) and $L/d = 20$

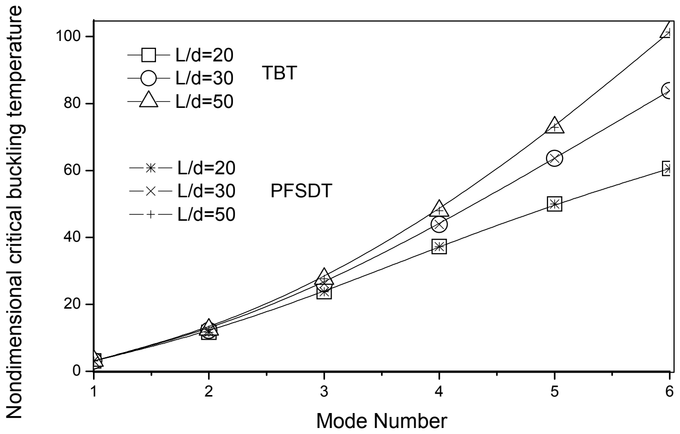

Fig. 3 Relation between the non-dimensional critical buckling temperature and the mode number for different values of L/d and e_0a = 0.4 nm

significant at higher modes and the decrease of the slenderness ratio reduces the critical temperature of zigzag SWBNNTs.

The dependence of the non-dimensional critical buckling temperature on the slenderness ratio of the zigzag SWBNNT is also shown in Fig. 4 for various values of nonlocal parameter. It is found that both the nonlocal conventional TBT and nonlocal PFSDT predict similar results. It can be concluded from the results of this figure that an increase in nonlocal scale parameter gives rise to a decrement in the critical buckling temperature. Furthermore, it can be seen that when the slenderness ratio is small, the nonlocal scale effects are significant. However, the nonlocal scale effects on the non-dimensional critical buckling temperature will diminish with the slenderness ratio increasing. It implies that the nonlocal effects on the thermal buckling characteristics are not obvious for slender SWBNNT but should be taken into consideration for short SWBNNT.

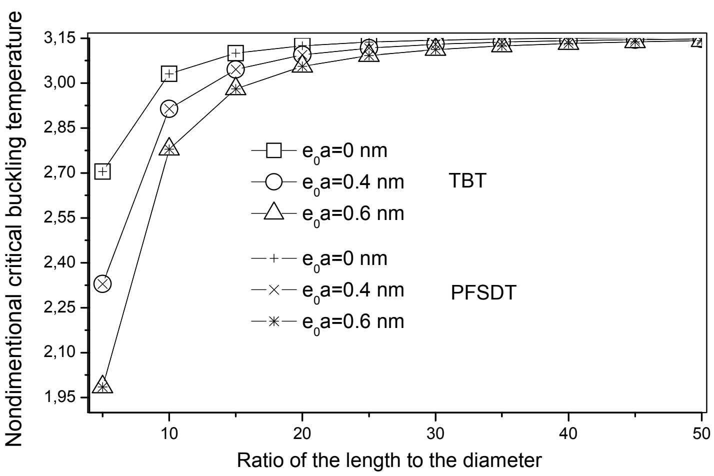

Fig. 4 Relation between the non-dimensional critical buckling temperature and L/d for different values of e_0a and n = 1

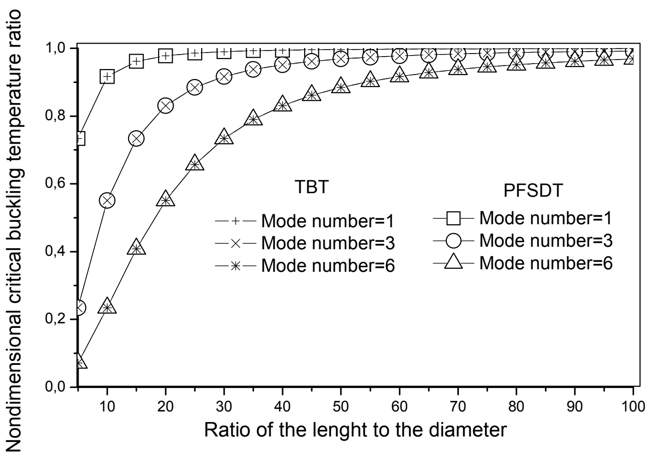

Fig. 5 Ratio of the critical buckling temperature by (TBT, PFSDT) to the nonlocal EBT vs. ratio of the length to the diameter for different mode numbers (e_0a = 0.6 nm)

In order to demonstrate the effects of the transverse shear deformation, the critical buckling temperature of the zigzag SWBNNT by both the present nonlocal PFSDT and the nonlocal conventional TBT to the nonlocal Euler–Bernoulli beam model with different slenderness ratios is presented in Fig. 5. The mode number n = 1, 3, 6 and the scale coefficient e_0a = 0.6 nm are considered. From Fig. 5, it can be observed that for different mode numbers, all of the ratios are smaller than 1.0. It means that because of the effects of the transverse shear deformation, the critical buckling temperature of the nonlocal PFSDT is lower than that of the nonlocal Euler–Bernoulli beam model. This phenomenon is more obvious for higher mode numbers and smaller slenderness ratios. It means that the effects of the transverse shear deformation should be considered and the nonlocal PFSDT is more accurate for short boron nitride nanotube.

5. Conclusions

In this work, the critical buckling temperature of zigzag SWBNNTs subjected to a uniform temperature rise is investigated using a new nonlocal first-order shear deformation beam theory. An analytical solution is derived and an explicit equation for the prediction of critical buckling temperature is obtained. From the examined examples, it can be concluded that the nonlocal scale effects should be considered for the thermal buckling responses, especially for higher mode numbers and short SWBNNT. The non-dimensional critical buckling temperature can be modified by different slenderness ratios of the SWBNNT. The results demonstrated in this work can provide useful guidance for the investigation and design of the next generation of nanodevices that make use of the thermal buckling characteristics of SWBNNTs.

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