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Curvature Effects on Thermal Buckling Load of DWCNT Under Axial Compression Force

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ABSTRACT
In this article, curvature effects on elastic thermal buckling of double-walled carbon nanotubes under axially compressed force are investigated using cylindrical shell model. Also, the small scale effect is taken into account in the formulation. The dependence of the interlayer van der Waals (vdW) pressure on the change of the curvatures of the inner and outer tubes at that point is considered. The effects of the surrounding elastic medium, curvature and the vdW forces between the inner and outer tubes increase the critical buckling load under thermal and axial compression loads, while small scale effect decreases it.

Keywords: Curvature effect; Thermal buckling load; Small scale effect; Axial compression force; DWCNT.

1 INTRODUCTION

CARBON nanotubes (CNTs) discovered by Iijima in 1991 [1]. Recently, many studies on the critical buckling load of double-walled carbon nanotubes (DWCNTs) under axial compression or torsion load have been presented (Ru [2] and Ranjbartoreh et al. [3], Han and Lu [4], Wang et al. [5], and Yang and Wang [6]). Also, the effects of the small scale and curvature had not been considered in their work. Mohammadimehr et al. [7] investigated the small scale effect on the torsional buckling of a DWCNT embedded on Winkler and Pasternak foundations using the theory of nonlocal elasticity. Their results show that the surrounding elastic medium increases the critical torsional buckling, while the small scale effect decreases it. Using the non-local elasticity theory, Mohammadimehr et al. [8] investigated Timoshenko beam model to study the elastic buckling of DWCNTs embedded in an elastic medium under axial compression. The effects of the small scale, the surrounding elastic medium based on Winkler model and van der Waals (vdW) force between the inner and outer nanotubes are taken into account. Moreover, in order to estimate the non-local critical buckling load of DWCNTs under axial compression, a simplified analysis is carried out and the results are compared with those obtained using molecular mechanics (MM).Yao and Han [9] studied the thermal effect on the axially compressed buckling of a multi-walled carbon nanotube (MWCNT). Moreover, they took into account the effects of temperature change, the surrounding elastic medium and the vdW forces between two adjacent layers. Their results showed that at low temperatures, the critical axial load for infinitesimal buckling of an MWCNT increases by increasing the temperature. Ghorbanpour Arani et al. [10] investigated the torsional and axial buckling analyses of the individual embedded MWCNTs subjected to internal and external pressures. They considered both the small length-scale effect and the surrounding elastic medium. Their results showed that the internal pressure increases the critical load, whereas the external pressure tends to decrease it. Ghorbanpour Arani et al. [11] studied the buckling analysis of a DWCNT subjected to a uniform internal pressure in a thermal field. Using the continuum cylindrical shell model, they considered the

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effects of the temperature change, the surrounding elastic medium based on the Winkler model, small scale, and the vdW forces between the inner and the outer tubes. It is seen from their results that the nonlocal critical buckling load is lower than the local critical buckling load. It is also concluded that, at low temperatures, the critical buckling load for the infinitesimal buckling of a DWCNT increases as the magnitude of temperature change increases; while, at high temperatures, the critical buckling load decreases with increasing of the temperature. Qian et al. [12] investigated the curvature effects of interlayer vdW forces on axially compressed buckling of a DWCNT of diameter down to 0.7 nm. They considered the dependence of the interlayer vdW pressure on the change of the curvatures of the inner and outer tubes at that point.

However, so far, investigation on the curvature effect on thermal buckling analysis of DWCNTs embedded in an elastic medium has not been found in the literature. Motivated by these ideas, this work aims to study curvature effect on thermal buckling load of DWCNT subjected to axial compression load. The effects of the small scale, the surrounding elastic medium, the vdW pressure between the inner and the outer tube, and the curvature on the elastic thermal buckling of DWCNTs are employed in the double-continuum cylindrical shells analysis.

2 NONLOCAL CYLINDRICAL SHELL MODEL

The constitutive equation of the nonlocal elasticity theory is written as follows [13]

$$(1-e_o^2 a^2 \nabla^2)\sigma = C_o : \varepsilon \tag{1}$$

C_0 is the elastic stiffness tensor of classical isotropic elasticity, σ and ε are the stress and the strain tensors, respectively, e_0 denotes a material constant $(e_0 = 0.82)$, and a is the length of the C-C bond $(a = 0.142\,\text{nm})$ [13], which $e_0 a$ denotes the small scale effect in above equation. Consider a circular cylindrical shell with a middle radius r, the thickness h, Young's modulus E, and Poisson's ratio υ. The coordinate system is considered as the origin at the middle surface of the shell; x and θ are the axial and the circumferential coordinates of the cylindrical shell, respectively; and the z direction is the normal coordinate to the medium surface. The relationships between the strain and the displacement for cylindrical shell model are defined as the following equation [14]:

$$\varepsilon_x = \varepsilon_x^0 + \frac{\partial u}{\partial x}, \qquad \varepsilon_\theta = \varepsilon_\theta^0 + \frac{1}{r}\frac{\partial v}{\partial \theta} - \frac{w}{r}, \qquad \gamma_{x\theta} = \frac{1}{2}\left(\frac{1}{r}\frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial x}\right) \tag{2}$$

where ε_x^o and ε_θ^o are the initial normal strains prior to the buckling, the symbols ε_x, ε_θ and $\varepsilon_{x\theta}$ denote the strain components at any point through the shell wall thickness; and u, v, and w refer to the displacement components of the middle surface of the shell in the axial, circumferential, and radial directions, respectively. In this paper, the normal stress σ_z, its corresponding strain ε_z, and the shear strains ε_{xz} and $\varepsilon_{\theta z}$ are assumed to be negligible. Subsequently, the constitutive equations of the nonlocal elasticity theory are written as for the case of the plane stress [11]

$$\begin{aligned}
&\sigma_x - (e_o a)^2 \frac{\partial^2 \sigma_x}{\partial x^2} = \frac{E}{1-\upsilon^2}(\varepsilon_x + \upsilon \varepsilon_\theta) - \frac{E\alpha_1 T}{1-\upsilon} \\
&\sigma_\theta - (e_o a)^2 \frac{1}{r^2}\frac{\partial^2 \sigma_\theta}{\partial \theta^2} = \frac{E}{1-\upsilon^2}(\varepsilon_\theta + \upsilon \varepsilon_x) - \frac{E\alpha_2 T}{1-\upsilon} \\
&\sigma_{x\theta} - (e_o a)^2 \left(\frac{\partial^2 \sigma_{x\theta}}{\partial x^2} + \frac{1}{r^2}\frac{\partial^2 \sigma_{x\theta}}{\partial \theta^2}\right) = \frac{E}{1-\upsilon^2}\varepsilon_{x\theta}
\end{aligned} \tag{3}$$

where σ_x and σ_θ are the normal stresses along the x, θ directions, respectively. $\sigma_{x\theta}$ is the shear stress in the $x-\theta$ plane, α_1 and α_2 denote the thermal expansion coefficient in the axial and circumferential directions, respectively, and also, the temperature change T is also uniformly distributed in the CNTs. The resultant forces per unit length are written as the following equations

$$N_x = \sigma_x h, \qquad N_\theta = \sigma_\theta h, \qquad N_{x\theta} = \sigma_{x\theta} h \tag{4}$$

where $(N_x, N_\theta, N_{x\theta})$ are the associated total membrane forces. Substituting Eq. (3) into Eq. (4) yields the following resultant forces

$$\begin{aligned} &N_x - (e_0 a)^2 \frac{\partial^2 N_x}{\partial x^2} = C(\varepsilon_x + \upsilon \varepsilon_\theta) - \frac{Eh\alpha_1 T}{1-\upsilon} \\ &N_\theta - (e_0 a)^2 \frac{1}{r^2}\frac{\partial^2 N_\theta}{\partial \theta^2} = C(\varepsilon_\theta + \upsilon \varepsilon_x) - \frac{Eh\alpha_2 T}{1-\upsilon} \\ &N_{x\theta} - (e_0 a)^2 \left(\frac{\partial^2 N_{x\theta}}{\partial x^2} + \frac{1}{r^2}\frac{\partial^2 N_{x\theta}}{\partial \theta^2}\right) = C(1-\upsilon)\varepsilon_{x\theta} \end{aligned} \tag{5}$$

where $C = \dfrac{Eh}{1-\upsilon}$. The membrane force can be written as [15]:

$$\begin{aligned} &N_x - (e_0 a)^2 \frac{\partial^2 N_x}{\partial x^2} = N_x^M + N_x^T \\ &N_\theta - (e_0 a)^2 \frac{1}{r^2}\frac{\partial^2 N_\theta}{\partial \theta^2} = N_\theta^M + N_\theta^T \end{aligned} \tag{6a}$$

where N_x^M and N_θ^M are the membrane force caused by mechanical loads. N_x^T and N_θ^T denote the membrane force caused by thermal loads. Using Eqs. (5) and (6a), we have

$$\begin{aligned} &N_x^M = C(\varepsilon_x + \upsilon \varepsilon_\theta) \\ &N_x^T = -\frac{Eh\alpha_1 T}{1-\upsilon} \\ &N_\theta^M = C(\varepsilon_\theta + \upsilon \varepsilon_x) \\ &N_\theta^T = -\frac{Eh\alpha_2 T}{1-\upsilon} \end{aligned} \tag{6b}$$

For the post-buckling configuration, we have [7, 14, 15]

$$\begin{aligned} &N_x = N_x^1 + N_x^0 \\ &N_\theta = N_\theta^1 + N_\theta^0 \\ &N_{x\theta} = N_{x\theta}^1 + N_{x\theta}^0 \end{aligned} \tag{7}$$

where the superscript " 0 " denotes the pre-buckling state, and the superscript " 1 " refers to infinitesimal increments of the corresponding parameters during the buckling. According to Ref. [7], the governing equation is written in the following decoupling form [7]:

$$D\nabla^8 w + \frac{Eh}{r^2}\frac{\partial^4 w}{\partial x^4} + (e_o a)^2 \nabla^4 \eta - \nabla^4 \left(N_x^o \frac{\partial^2 w}{\partial x^2} + \frac{N_\theta^o}{r^2}\frac{\partial^2 w}{\partial \theta^2} \right) = \nabla^4 p(x,\theta) \tag{8}$$

where

$$\eta = \nabla^2 p + N_x^o \left(\frac{\partial^4 w}{\partial x^4} + \frac{1}{r^2}\frac{\partial^4 w}{\partial x^2 \partial \theta^2} \right) + \frac{N_\theta^o}{r^2}\left(\frac{1}{r^2}\frac{\partial^4 w}{\partial \theta^4} + \frac{\partial^4 w}{\partial x^2 \partial \theta^2} \right) \tag{9}$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}$$
$$\nabla^4 = \nabla^2.\nabla^2 = \frac{\partial^4}{\partial x^4} + \frac{2}{r^2}\left(\frac{\partial^4}{\partial x^2 \partial \theta^2}\right) + \frac{\partial^4}{\partial \theta^4} \tag{10}$$
$$\nabla^8 = \nabla^4.\nabla^4 = \frac{\partial^8}{\partial x^8} + \frac{6}{r^4}\left(\frac{\partial^8}{\partial x^4 \partial \theta^4}\right) + \frac{4}{r^2}\left(\frac{\partial^8}{\partial x^6 \partial \theta^2}\right) + \frac{4}{r^6}\left(\frac{\partial^8}{\partial x^2 \partial \theta^6}\right) + \frac{1}{r^8}\left(\frac{\partial^8}{\partial \theta^8}\right)$$

and $p(x,\theta)$ is the additional normal pressure after buckling. The surrounding elastic medium for the outer nanotube of a DWCNT is considered as follows [7]:

$$p_2^E = p_0^E - \mathrm{d}w_2 \tag{11}$$

where p_0^E is the pressure due to the surrounding elastic medium prior to the buckling and D_e and w_2 denotes the spring constant of Winkler model and radial displacement of the outer nanotube, respectively.

The vdW interaction pressure at any point between the two tubes for DWCNTs is assumed that it depends linearly on the change of the interlayer spacing and the change of the curvatures of the inner and the outer tubes at that point. It is clear that the change of the curvature of the k th tube due to the deflection w_k is $w_k / r_k{}^2 + \nabla_k^2 w_k$, thus the interlayer vdW pressure on the inner tube with considering the curvature change is written as follows [12]:

$$p_1^v(x,\theta) = c(w_2 - w_1) + c_1\left(\frac{w_2}{r_2{}^2} + \nabla^2 w_2\right) - c_1\left(\frac{w_1}{r_1{}^2} + \nabla^2 w_1\right) \tag{12}$$

in which $p_1^v(x,\theta)$ are the pressure exerted on the inner tube by the vdW force, c is a constant, w_2 and w_1 are the radial deflections of the outer and the inner tubes, respectively, r_2 and r_1 denote the radii of the outer and the inner tubes, respectively. The interaction pressures between the inner and the outer tubes are equal in magnitude and are opposite in sign; therefore, the following equation is written as [2]:

$$p_1^v(x,\theta) r_1 = -p_2^v(x,\theta) r_2 \tag{13}$$

where $p_2^v(x,\theta)$ is the pressure exerted on the outer tube by the vdW force. Substituting Eq. (12) into Eq. (13) yields the interlayer vdW pressure on the outer tube

$$p_2^v(x,\theta) = -\frac{r_1}{r_2}\left[c(w_2 - w_1) + c_1\left(\frac{w_2}{r_2{}^2} + \nabla^2 w_2\right) - c_1\left(\frac{w_1}{r_1{}^2} + \nabla^2 w_1\right)\right] \tag{14}$$

The normal pressures on the inner and the outer tubes are written as

$$p_1 = p_1^v, \qquad p_2 = p_2^v + p_2^E \tag{15}$$

Substituting Eqs. (11), (12) and (14) into Eq. (15) yield the normal pressure exerted on the inner and the outer tubes

$$p_1 = c(w_2 - w_1) + c_1\left(\frac{w_2}{r_2{}^2} + \nabla^2 w_2\right) - c_1\left(\frac{w_1}{r_1{}^2} + \nabla^2 w_1\right) \tag{16a}$$

$$p_2 = -\frac{r_1}{r_2}\left[c(w_2 - w_1) + c_1\left(\frac{w_2}{r_2^{\ 2}} + \nabla^2 w_2\right) - c_1\left(\frac{w_1}{r_1^{\ 2}} + \nabla^2 w_1\right)\right] + p_0^E - D_e w_2 \tag{16b}$$

The governing equations of the equilibrium for the inner and the outer tubes are written as

$$D\nabla^8 w_1 + \frac{Eh}{r_1^{\ 2}}\frac{\partial^4 w_1}{\partial x^4} + (e_o a)^2 \nabla^4 \eta_1 - \nabla^4\left(N_{x1}^o \frac{\partial^2 w_1}{\partial x^2} + \frac{N_{\theta 1}^o}{r_1^2}\frac{\partial^2 w_1}{\partial \theta^2}\right) = \nabla^4 p_1(x,\theta) \tag{17a}$$

$$D\nabla^8 w_2 + \frac{Eh}{r_2^{\ 2}}\frac{\partial^4 w_2}{\partial x^4} + (e_o a)^2 \nabla^4 \eta_2 - \nabla^4\left(N_{x2}^o \frac{\partial^2 w_2}{\partial x^2} + \frac{N_{\theta 2}^o}{r_2^{\ 2}}\frac{\partial^2 w_2}{\partial \theta^2}\right) = \nabla^4 p_2(x,\theta) \tag{17b}$$

where η_1 and η_2 are given by

$$\eta_1 = \nabla^2 p_1(x,\theta) + N_{x1}^o\left(\frac{\partial^4 w_1}{\partial x^4} + \frac{1}{r_1^{\ 2}}\frac{\partial^4 w_1}{\partial x^2 \partial \theta^2}\right) + \frac{N_{\theta 1}^o}{r_1^{\ 2}}\left(\frac{1}{r_1^{\ 2}}\frac{\partial^4 w_1}{\partial \theta^4} + \frac{\partial^4 w_1}{\partial x^2 \partial \theta^2}\right) \tag{18a}$$

$$\eta_2 = \nabla^2 p_2(x,\theta) + N_{x2}^o\left(\frac{\partial^4 w_2}{\partial x^4} + \frac{1}{r_2^{\ 2}}\frac{\partial^4 w_2}{\partial x^2 \partial \theta^2}\right) + \frac{N_{\theta 2}^o}{r_2^{\ 2}}\left(\frac{1}{r_2^{\ 2}}\frac{\partial^4 w_2}{\partial \theta^4} + \frac{\partial^4 w_2}{\partial x^2 \partial \theta^2}\right) \tag{18b}$$

The ends of the inner and the outer tubes for DWNTs are considered as simply supported. Therefore, the buckling modes are written as

$$w_1 = f_1 \sin\frac{m\pi x}{L}\sin n\theta, \qquad w_2 = f_2 \sin\frac{m\pi x}{L}\sin n\theta \tag{19}$$

where f_1 and f_2 are two real constants, m and n the axial half and circumferential wave numbers, respectively. Using Eqs. (16), (16) and (18), substituting Eq. (19) into Eqs. (17) yields the following equation:

$$\begin{cases} A_1 w_1 + B_1 w_2 = 0 \\ A_2 w_1 + B_2 w_2 = 0 \end{cases} \tag{20}$$

In order to obtain the critical buckling load, it is necessary to set the determinant of the coefficient matrix in Eq. (20) equal to zero:

$$A_1 B_2 - A_2 B_1 = 0 \tag{21}$$

3 RESULTS AND DISCUSSION

The mechanical, geometrical and thermal data for DWCNT are considered as follows [12, 15]

$$\begin{aligned} &r_1 = 1\ \text{nm}, \quad r_2 = 1.4\ \text{nm}, \quad L = 10r_2, \quad \upsilon = 0.34, \quad E = 10^{12}\ \text{Pa}, \quad Eh = 360\ \text{J/m}^2, \\ &D = 1.3617\times10^{-19}\ \text{J}, \quad c = 9.918667\times10^{19}\ \text{N/m}^3, \quad c_1 = -3.96\ \text{kg/s}^2, \\ &\alpha_1 = 1.1\times10^{-6}, \quad \alpha_2 = 0.8\times10^{-6}, \quad e_0 = 0.82, \quad a = 0.142\ \text{nm} \end{aligned} \tag{22}$$

3.1 Thermal buckling of DWCNTs without considering axial compression force

Substituting mechanical, geometrical and thermal data into Eq. (22) yields the critical temperature for DWCNTs without considering axial compression force. Fig. 1 shows the critical buckling temperature versus the axial half wave number for different radii. It is seen that the critical buckling temperature at the specified length decreases with increasing the outer radius for DWCNTs. Fig. 2 illustrates the curvature effect on the critical buckling temperature. It is shown from the results that the critical buckling temperature with considering the curvature effect is higher than that without considering it for $m > 50$, while this case reverses for $m < 50$. Fig. 3 depicts the small scale effect on the critical buckling temperature for DWCNTs. It is seen that the nonlocal critical buckling temperature is lower than the local critical buckling temperature.

3.2. Thermal buckling load of DWCNTs under axial compression force

The buckling load such as thermal load and axial compression force is considered as the following equation

$$N_{x1}^{0} = -\frac{Eh\alpha_1 T}{1-\upsilon} - p, \qquad N_{x2}^{0} = -\frac{Eh\alpha_2 T}{1-\upsilon} - p \tag{23}$$

Substituting Eq. (23) into Eqs. (17a) and (17b) yields the critical thermal buckling load under axial compression force. Fig. 4 shows the effect of the interlayer vdW pressure on the thermal buckling load under axial compression force. It is observed from this figure that the critical buckling load under thermal and axial compression loads increases with considering the interlayer vdW pressure. Fig. 5 depicts the curvature effect on the thermal buckling load under axial compression force.

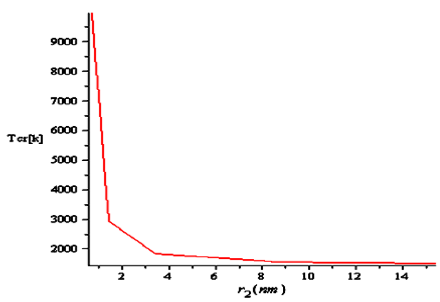

Fig. 1
The effect of the outer radius on the critical temperature (m=70, n=6).

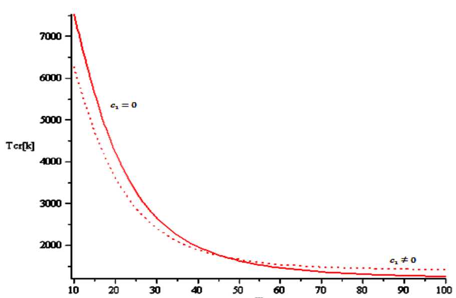

Fig. 2
The curvature effect on the critical temperature (n=6).

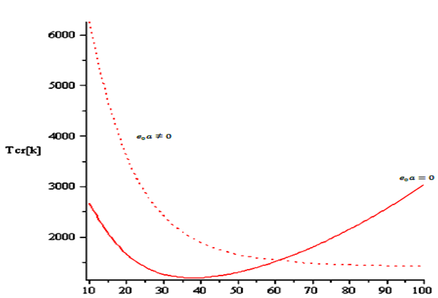

Fig. 3
The small scale effect on the critical buckling temperature for DWCNTs (n=6).

It is seen that the critical buckling load under thermal and axial compression loads increases with considering the curvature effect. Fig.6 illustrates the effect of the surrounding elastic medium based on the Winkler model on the thermal buckling load under axial compression force. It is shown that the critical buckling load under thermal and axial compression loads increases with considering the surrounding elastic medium. Fig. 7 shows the small scale effect on the thermal buckling load under axial compression force. It is seen from the results that the critical buckling load under thermal and axial compression loads decreases with considering the small scale effect.

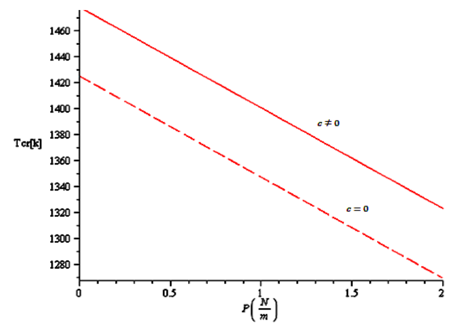

Fig. 4
The effect of the interlayer vdW pressure on the thermal buckling load under axial compression force.

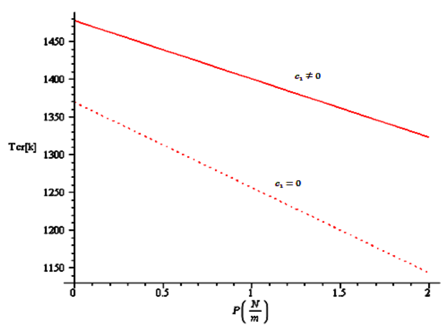

Fig. 5
The curvature effect on the thermal buckling load under axial compression force.

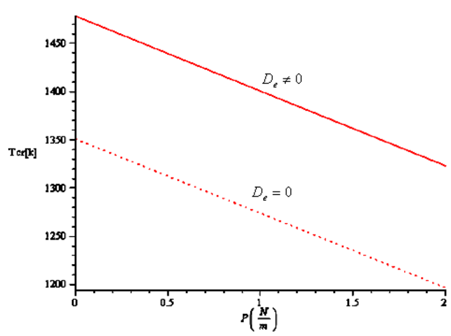

Fig. 6
The effect of the surrounding elastic medium on the thermal buckling load under axial compression force.

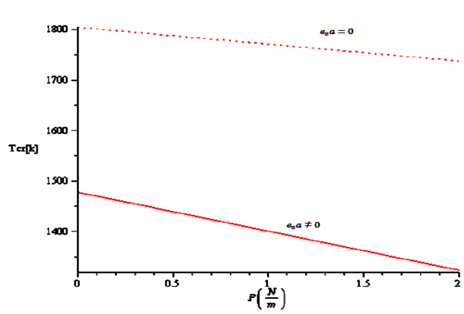

Fig.7
The small scale effect on the thermal buckling load under axial compression force.

4 CONCLUSIONS

In this paper, the effects of the small scale, the surrounding elastic medium, the interlayer vdW pressure between the inner and the outer tubes, and curvature on the elastic thermal buckling of DWCNTs under axial compression force are investigated using cylindrical shell model. The following conclusions can be obtained from the results:
1. The critical buckling load under thermal and axial compression loads increases with considering the interlayer vdW pressure.
2. The critical buckling load under thermal and axial compression loads increases with considering the curvature effect.
3. The critical buckling load under thermal and axial compression loads increases with considering the surrounding elastic medium.
4. The critical buckling load under thermal and axial compression loads decreases with considering the small scale effect.

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