

Thermal Buckling of Multi-Walled Carbon Nanotubes by Nonlocal Elasticity

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The small internal length scales of nanomaterials/nano-devices may call the direct application of classical continuum models into question. In this research, a nonlocal elastic shell model, which takes the small scale effects into account, is developed to study the thermal buckling behavior of multi-walled carbon nanotubes. The multi-walled carbon nanotubes are considered as concentric thin shells coupled with the van der Waals forces between adjacent nanotubes. Closed form solutions are formulated for two types of thermal buckling of a double-walled carbon nanotube: Radial thermal buckling (as in a shell under external pressure) and axial thermal buckling. The effects of small scale effects are demonstrated, and a significant influence of internal characteristic parameters such as the length of the C-C bond has been found on the thermal buckling critical temperature. The study interestingly shows that the axial buckling is not likely to happen, while the "radial" buckling may often take place when the carbon nano-tubes are subjected to thermal loading. Furthermore, a convenient method to determine the material constant, " e_0 " and the internal characteristic parameter, " a ," is suggested.

[DOI: 10.1115/1.2200656]

1 Introduction

The discovery of carbon nanotubes by Ijima [1] has inspired the promise of a new generation of novel composites and devices such as nano-electronics, nano-devices, and nano-composites [2,3]. Attention has been attracted to the subject of understanding the material properties of carbon nanotubes and their applications [4–7]. In most of the studies, experimental and molecular-dynamics simulation approaches are often employed and many relevant results have been obtained. However, the experiments at the nano-scale are often hard to control, and the simulations by molecular-dynamics are difficult to accurately formulate and extremely expensive for large-scale atomic systems [8]. Therefore, many researchers have attempted to expand the classical continuum mechanics approach to the atomic or molecular-based discrete systems [8–11]. For example, adding the van der Waal's forces to the classical shell models in order to simulate the carbon nanotubes, etc. The classical continuum models are efficient and accurate in computations for a material system in large length scales. But the length scales at nano-meters such as in nanomaterials or nano-devices may not be sufficiently big enough to homogenize the discrete structure into a continuum [12]. The assumption upon which the classical continuum mechanics is built may no longer be fully satisfied. Therefore, modifications which would take the small scale effect into account are needed in order to make use of the virtues of the well-developed classical continuum mechanics.

In 1972, Eringen proposed a theory, called nonlocal continuum mechanics [13], in an effort to deal with the small-scale structure problems. In the classical (local) continuum elasticity, the material particles are assumed to be continuously distributed and the stress tensor at a reference point is uniquely determined by the strain tensor at the same point. On the contrary, the nonlocal continuum

mechanics is based on the constitutive functionals being functionals of the past deformation histories of all material points of the body concerned. The small length scale effects are counted by incorporating the internal characteristic length such as the length of the C-C bond into the constitutive relationship. Solutions from various problems support this theory [13–15]. For examples, the dispersion curves by the nonlocal model are in excellent agreement with those by the Born-Karman theory of lattice dynamics; the dislocation core and cohesive stress predicted by the nonlocal theory are close to those known in the physics of solids [14,15]. Recently, some researchers such as Peddieson et al. [16] and Sudak [17] applied Eringen's theory to the nano-scales structures. In particular, Peddieson et al. [16] illustrated by the Benoulli/Euler beam model that the small scale effects manifest themselves in the range of nano-meters. Sudak in [17] applied the nonlocal elasticity to the column buckling study of the axial buckling of carbon nano-tubes. The results in these papers indicate that the small length scales would have significant influences and the nonlocal continuum model can effectively capture these influences in the study of nano-structures.

The importance and significant results of thermal buckling for conventional structures such as plates and shells have been reported by many researchers [18]. But in our literature search, the study of thermal buckling of nano-tubes has received relatively little attention. In the current paper, a nonlocal multiple shell model is developed to investigate the thermal buckling problems of multi-walled carbon nanotubes. In this model, not only the terms concerning the van der Waals forces between adjacent nanotubes are incorporated into the Donnell shell model [19], but the full nonlocal constitutive relationship is also adopted in the derivation of the formulas. Therefore, this model includes both the interactions from the van der Waals forces and the effects from the internal small scales of the nano-devices. Compared with some nonlocal models in the literature for nano-tubes subjected to mechanical loading, our model is a comprehensive nonlocal elastic model in the sense that no approximation has been made in the use of the nonlocal elastic constitutive equations and each tube is treated as a shell, not a one-dimensional column. Since the thermal expansion coefficients of the carbon nano-tube are negative [7], the tube usually contracts when its temperature is elevated. Therefore, its thermal buckling modes are different from those of

Contributed by the Applied Mechanics Division of ASME for publication in the ASME JOURNAL OF APPLIED MECHANICS. Manuscript received August 31, 2005; final manuscript received March 15, 2006. Review conducted by S. Mukherjee. Discussion on the paper should be addressed to the Editor, Prof. Robert M. McMeeking, Journal of Applied Mechanics, Department of Mechanical and Environmental Engineering, University of California – Santa Barbara, Santa Barbara, CA 93106-5070, and will be accepted until four months after final publication in the paper itself in the ASME JOURNAL OF APPLIED MECHANICS.

conventional shell structures. For example, a simply supported conventional shell structure often shows axial buckling modes under increased temperature without radial constraints [18]. However, a fixed simply supported nano-tube is in tension in the axial direction, but may fall into a “radial” buckling mode because of the contraction, like a traditional shell under external radial compressive pressure. In this study two cases of temperature variations are investigated under fixed simply edge-supported boundary conditions: Radially elevated temperature and uniformly reduced temperature. Closed form expressions for the critical temperatures are obtained and numerical results for double-walled nanotubes are presented. The results show that the internal small scales have significant effects on the critical buckling temperature. A method to determine the internal characteristic parameter, “ a ” and material constant, “ e_0 ” (defined in see Sec. 2) is also proposed.

This paper is organized as follows: Section 2 is a brief summary of the nonlocal continuum mechanics; Sec. 3 is the derivation of a nonlocal continuum elastic shell model for the multi-walled nanotubes; in Sec. 4, the thermal buckling for two types of temperature distributions are analyzed under simply end-supported boundary conditions, and closed form solutions are formulated for the double-walled nano-tubes; numerical results for double-walled nano-tubes and discussions are presented in Sec. 5; and some conclusions are suggested in Sec. 6.

2 Summary of the Nonlocal Elasticity

In the classical (local) theory of elasticity, the stress tensor at a reference point x of a body can be determined by the strain tensor at that point. However, Eringen [13,14] pointed out that when we deal with a small scale structure, the media may no longer be considered continuously distributed and the internal characteristic length such as the length of the C-C bond in carbon nano-tubes should be considered. Based on this motivation, he developed a theory of nonlocal elasticity. The nonlocal mechanics says that the stress tensor at a reference point x in a body depends not only on the strain tensor at that point x , but also on the strain tensor at all other points, x' of this body. The constitutive equations of nonlocal elasticity read as

$$\sigma_{ij}(x) = \int_v \alpha(|x' - x|, \tau) c_{ijkl} \epsilon_{kl}(x') dv(x') \quad (1)$$

where, $\alpha(|x' - x|, \tau)$ is the nonlocal moduli; $\tau = e_0 a / l$ with a an internal characteristic length (e.g., lattice parameter, granular distance, length of C-C bonds), l an external characteristic length (e.g., crack length, wave-length), and e_0 a constant appropriate to each material and being determined by experiment or by matching dispersion curves of plane waves with those of atomic lattice dynamics; c_{ijkl} the elastic moduli tensor; $\epsilon_{kl}(x')$ the strain tensor.

Sometimes, it is hard to find an explicit expression for the kernel, $\alpha(|x' - x|, \tau)$ and do the integration of (1). In 1983, Eringen [15] developed some differential forms for practical use. For the two-dimensional nonlocal elasticity, a differential form corresponding to Eq. (1) is expressed as:

$$(1 - \tau^2 l^2 \nabla^2) \sigma_{ij} = c_{ijkl} \epsilon_{kl} \quad (2)$$

One may see that when the internal characteristic length a is neglected, i.e., the particles of a medium are considered to be continuously distributed, then τ , which is defined as $a e_0 / l$ is zero, and Eq. (2) reduces to the constitutive equation of classical elasticity. Also, it should be noted that, through Eq. (2), the ℓ is cancelled from the rest of the analysis, leaving a and e_0 as the internal characteristic constants.

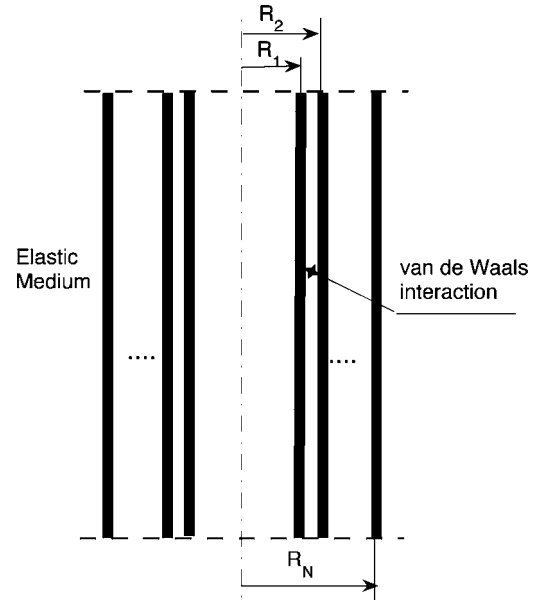


Fig. 1 A shell model of multi-walled nanotubes in an elastic medium

3 A Nonlocal Continuum Model for Multi-Walled Carbon Nanotubes

Let x, s, z be the axial, circumferential and radial coordinates of the nanotube (Fig. 1), respectively. If the Donnell's assumptions [19] are used, then the strains and displacements of a nanotube have the following relations:

$$\epsilon_x = \epsilon_{0x} - z w_{,xx}, \quad \epsilon_s = \epsilon_{0s} - z w_{,ss}, \quad \gamma_{xs} = \gamma_{0xs} - z w_{,xs} \quad (3)$$

where ϵ_{0x} , ϵ_{0s} , and γ_{0xs} are the mid-surface strains. These are:

$$\begin{aligned} \epsilon_{0x} &= u_{,x} + \frac{1}{2} w_{,x}^2 \\ \epsilon_{0s} &= v_{,s} + \frac{1}{2} w_{,s}^2 + \frac{w}{R} \end{aligned} \quad (4)$$

$$\gamma_{0xs} = u_{,s} + v_{,x} + w_{,x} w_{,s}$$

in which, u and v are, respectively, the axial and circumferential displacements of mid-surface, and w is the radial displacement; R is the radius of the mid-surface; the comma denotes differentiation with the corresponding coordinates. From Eq. (2), the nonlocal constitutive equations can be written as:

$$\begin{aligned} (1 - \tau^2 l^2 \nabla^2) \sigma_x &= \frac{E}{1 - \nu^2} (\epsilon_x + \nu \epsilon_s) - \frac{E \alpha \Delta T}{1 - \nu} \\ (1 - \tau^2 l^2 \nabla^2) \sigma_s &= \frac{E}{1 - \nu^2} (\nu \epsilon_x + \epsilon_s) - \frac{E \alpha \Delta T}{1 - \nu} \end{aligned} \quad (5)$$

$$(1 - \tau^2 l^2 \nabla^2) \sigma_{xs} = \frac{E}{2(1 + \nu)} \gamma_{xs}$$

in which $\nabla^2 = \partial^2 / \partial x^2 + \partial^2 / \partial s^2$; $E, \nu, \alpha, \Delta T$ are the elastic modulus, Poisson's ratio, thermal expansion coefficient, and increase in temperature, respectively.

From Eqs. (3) and (5), one can have the following resultant forces and moments:

$$(1 - \tau^2 l^2 \nabla^2) N_x = K (\epsilon_{0x} + \nu \epsilon_{0s}) - \frac{N^T}{1 - \nu}$$

$$(1 - \tau^2 l^2 \nabla^2) N_s = K(\nu \epsilon_{0x} + \epsilon_{0s}) - \frac{N^T}{1 - \nu} \quad (6)$$

$$(1 - \tau^2 l^2 \nabla^2) N_{xs} = \frac{1 - \nu}{2} K \gamma_{0xs}$$

and

$$(1 - \tau^2 l^2 \nabla^2) M_x = -D(w_{,xx} + \nu w_{,ss}) - \frac{M^T}{1 - \nu}$$

$$(1 - \tau^2 l^2 \nabla^2) M_s = -D(w_{,ss} + \nu w_{,xx}) - \frac{M^T}{1 - \nu} \quad (7)$$

$$(1 - \tau^2 l^2 \nabla^2) M_{xs} = -(1 - \nu) D w_{,xs}$$

where, $K = Eh/(1 - \nu^2)$ and $D = Eh^3/12(1 - \nu^2)$, with h being the thickness of the nano-tube; $N^T = \int E\alpha\Delta T dz$, and $M^T = \int E\alpha\Delta T z dz$ are the thermal resultant force and moment, respectively.

The nonlinear equilibrium equations, $\sigma_{ij,j} + f_i = 0$, with $f_1 = f_2 = 0$ and $f_3 = p(x, s)$, can be expressed in terms of resultant forces and moments as:

$$(1 - \tau^2 l^2 \nabla^2) N_{x,x} + (1 - \tau^2 l^2 \nabla^2) N_{s,xs} = 0$$

$$(1 - \tau^2 l^2 \nabla^2) N_{s,x} + (1 - \tau^2 l^2 \nabla^2) N_{s,s} = 0 \quad (8)$$

$$(1 - \tau^2 l^2 \nabla^2) M_{x,xx} + 2(1 - \tau^2 l^2 \nabla^2) M_{xs,xs} + (1 - \tau^2 l^2 \nabla^2) M_{s,ss}$$

$$- (1 - \tau^2 l^2 \nabla^2) N_L - (1 - \tau^2 l^2 \nabla^2) \frac{1}{R} N_s + (1 - \tau^2 l^2 \nabla^2) p(x, s) = 0$$

where the N_L is a nonlinear operator defined as

$$N_L = N_x w_{,xx} + 2N_{xs} w_{,xs} + N_s w_{,ss} \quad (9)$$

and $p(x, s)$ is the force acting in the radial direction. For nano-tubes, it is the van der Waals interaction from an adjacent tube. This interaction is considered to be proportional to the radial displacement difference between two neighboring nano-tubes [8,11,17].

To study the buckling behavior of the nanotubes, the perturbation technique [20,21] is employed here. Let u_0, v_0, w_0 be the pre-buckling state of displacements, which satisfy equilibrium equations, u^1, v^1, w^1 a neighboring state, and the ξ is very small constant, then one has:

$$u = u_0 + \xi u^1, \quad v = v_0 + \xi v^1, \quad w = w_0 + \xi w^1 \quad (10)$$

The corresponding resultant forces and moments can be written as:

$$N_x = N_{0x} + \xi N_{1x}, \quad N_s = N_{0s} + \xi N_{1s}, \quad N_{xs} = N_{0xs} + \xi N_{1xs} \quad (11)$$

$$M_x = M_{0x} + \xi M_{1x}, \quad M_s = M_{0s} + \xi M_{1s}, \quad M_{xs} = M_{0xs} + \xi M_{1xs}$$

Considering the w_0 to be zero in the pre-buckling state [22,23] and substituting Eqs. (10) into Eq. (11), then into Eq. (8), leads to the following stability equation for nonlocal continuum elasticity of a nano-tube:

$$\nabla^8 w + 4k^4 w_{,xxxx} + \frac{1}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 N_L^0 = \frac{1}{D} [(1 - \tau^2 l^2 \nabla^2) \nabla^4 p(x, s)] \quad (12)$$

where $k^4 = 3(1 - \nu^2)/(R^2 h^2)$, and the N_L^0 operator reads as:

$$N_L^0 = N_{0x} w_{,xx} + 2N_{0xs} w_{,xs} + N_{0s} w_{,ss} \quad (13)$$

N_{0x}, N_{0xs}, N_{0s} are the resultant forces at the pre-buckling state that satisfy the equilibrium equation (8). For convenience of writing, the superscript "1" is omitted in Eqs. (12) and (13).

Our structure is a multi-walled nano-tube and we shall denote by $w_j, j = 1, 2, \dots, N$ the transverse displacements of each of the N walls. Also, we denote by $p_{j,(j+1)}$ the interaction pressure exerted

on the tube j from the tube $j + 1$. Applying Eq. (12) to each of the nano-tubes of the multi-walled carbon nanotube structure, one can obtain a set of nonlocal equations for the multi-walled carbon nanotube (i.e., w_1 is the displacement of the first nano-tube; w_2 is the displacement of the second nano-tube, etc.):

$$\nabla^8 w_1 + 4k_1^4 w_{1,xxxx} + \frac{1}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 N_{L1}^0$$

$$= \frac{1}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 p_{12}(x, s)$$

$$\nabla^8 w_2 + 4k_2^4 w_{2,xxxx} + \frac{1}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 N_{L2}^0$$

$$= \frac{1}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 \left[p_{23}(x, s) - \frac{R_1}{R_2} p_{12}(x, s) \right] \quad (14)$$

$$\nabla^8 w_N + 4k_N^4 w_{N,xxxx} + \frac{1}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 N_{LN}^0$$

$$= \frac{1}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 \left[p_N(x, s) - \frac{R_{N-1}}{R_N} p_{(N-1)N}(x, s) \right]$$

where,

$$p_{12}(x, s) = c[w_2(x, s) - w_1(x, s)]$$

$$p_{N(N-1)}(x, s) = c[w_N(x, s) - w_{N-1}(x, s)] \quad (15)$$

$$p_N(x, s) = -k_0[w_N(x, s) - w_{N-1}(x, s)]$$

in which, $p_{j(j+1)}(x, s)$ is the interaction pressure exerted on the tube j from the tube $j + 1$, while $p_{(j+1)j}(x, s)$ is the interaction pressure exerted on the tube $j + 1$ from the tube j ; these have the following relationship:

$$R_j p_{j(j+1)}(x, s) = -R_{j+1} p_{(j+1)j}(x, s), \quad j = 1, 2, \dots, N - 1 \quad (16)$$

p_N is the interaction pressure between the outmost tube and the surrounding elastic medium; k_0 is the spring constant of the surrounding elastic medium; c is the van der Waals interaction coefficient and can be estimated from the data given in [12,24], and it reads as:

$$c = \frac{200}{0.16\pi d^2} \text{ erg/cm}^2, \quad d = 0.142 \text{ nm} \quad (17)$$

where d is the bond distance between carbon atoms in a graphite sheet. One may realize that the buckling phenomenon can be described as an infinitesimal deflection perturbation, so the van der Waals interaction and interaction between the outer tube and the elastic surrounding media can be estimated from a linear function of the deflection jump at two points, and the interactions in the tangential direction can be neglected, as discussed in Ref. [17]. But for post-buckling behavior, the nonlinear higher order terms and effects from the tangential force should be included in these interaction expressions.

Substitution of (15) into Eq. (14) yields the nonlocal model for the multi-walled nano-tubes:

$$\nabla^8 w_1 + 4k_1^4 w_{1,xxxx} + \frac{1}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 N_L^0$$

$$= \frac{c}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 [w_2 - w_1]$$

$$\nabla^8 w_2 + 4k_2^4 w_{2,xxxx} + \frac{1}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 N_L^0$$

$$= \frac{c}{D} (1 - \tau^2 l^2 \nabla^2) \nabla^4 \left[w_3 - w_2 - \frac{R_1}{R_2} (w_2 - w_1) \right]$$

$$\begin{aligned} & \nabla^8 w_{N-1} + 4k_{N-1}^4 w_{N-1,xxxx} + \frac{1}{D}(1 - \tau^2 l^2 \nabla^2) \nabla^4 N_L^0 \\ &= \frac{c}{D}(1 - \tau^2 l^2 \nabla^2) \nabla^4 \left[w_N - w_{N-1} - \frac{R_{N-2}}{R_{N-1}}(w_{N-1} - w_{N-2}) \right] \end{aligned} \quad (18)$$

$$\begin{aligned} & \nabla^8 w_N + 4k_N^4 w_{N,xxxx} + \frac{1}{D}(1 - \tau^2 l^2 \nabla^2) \nabla^4 N_L^0 \\ &= \frac{c}{D}(1 - \tau^2 l^2 \nabla^2) \nabla^4 \left[-\frac{k_0}{c} w_N - \frac{R_{N-1}}{R_N}(w_N - w_{N-1}) \right] \end{aligned}$$

Here in the set of Eqs. (18), one can clearly see that if the internal characteristic parameter, a is negligible, then $1 - \tau^2 l^2 \nabla^2 = 1$, and this model returns to the classical continuum elastic shell model including the van de Waals interaction via the coefficient c , and the interaction from the surrounding elastic medium via the coefficient k_0 .

4 Thermal Buckling of the Multi-Walled Carbon Nanotubes

In the set of Eqs. (18), the thermal stress is related through the pre-buckling terms such as N_{0x} and N_{0s} in N_L^0 . The edges of the nano-tubes are assumed to be simply supported and the buckling of the carbon nanotubes under two types of temperature distributions will be analyzed in the following study: (a) Radially elevated temperature and (b) uniformly reduced temperature. Without loss of generality, let us first consider the double-walled carbon nanotubes (DWCNT), i.e., $N=2$.

4.1 Radially Elevated Temperature. The thermal expansion coefficient of carbon nanotubes depends on the temperature range, radius, the number of layers and helix [6]. But in most cases, they are likely negative [7]. Hence, the nano-tubes contract when the temperature rises, while the surrounding media expands. Therefore, the tube can be viewed as a shell under external compressive pressure.

If the temperature rise varies linearly across the nano-tube thickness as

$$\Delta T(z) = \Delta T_0 \frac{z + h/2}{h}, \quad -\frac{h}{2} < z < \frac{h}{2} \quad (19)$$

then from pre-buckling equilibrium, one can have $N_{0x} = N_{0xs} = 0$ in the operator N_L^0 , and

$$N_{0s} = -\frac{E\alpha h}{1-\nu} \int_{-h/2}^{h/2} \Delta T(z) dz = -\frac{E\alpha h}{2(1-\nu)} \Delta T_0 \quad (20)$$

The stability equations from (18) can then be written as:

$$\begin{aligned} & \nabla_{R1}^8 w_1 + 4k_1^4 w_{1,xxxx} = -\frac{N_{0s}}{D}(1 - \tau^2 l^2 \nabla_{R1}^2) \nabla_{R1}^4 w_{1,ss} \\ & \quad + \frac{1}{D}(1 - \tau^2 l^2 \nabla_{R1}^2) \nabla_{R1}^4 [c(w_2 - w_1)] \end{aligned} \quad (21)$$

$$\begin{aligned} & \nabla_{R2}^8 w_2 + 4k_2^4 w_{2,xxxx} = -\frac{N_{0s}}{D}(1 - \tau^2 l^2 \nabla_{R2}^2) \nabla_{R2}^4 w_{2,ss} \\ & \quad - \frac{1}{D}(1 - \tau^2 l^2 \nabla_{R2}^2) \nabla_{R2}^4 \left[k_0 w_2 + c \frac{R_1}{R_2} (w_2 - w_1) \right] \end{aligned}$$

where,

$$\nabla_{Rj}^2 = \frac{\partial^2}{\partial x^2} + \frac{1}{R_j^2} \frac{\partial^2}{\partial \theta^2}, \quad j = 1, 2 \quad (22)$$

One can see that a solution for each of the concentric nanotubes can take the form:

$$w_1 = A_1 \sin\left(\frac{m\pi}{L}x\right) \sin(n\pi\theta), \quad w_2 = A_2 \sin\left(\frac{m\pi}{L}x\right) \sin(n\pi\theta) \quad (23)$$

which satisfies the edge conditions

$$w_1 = w_{1,xx} = 0, \quad w_2 = w_{2,xx} = 0 \quad (24)$$

where m is the axial half wave-number, and n the circumferential half wave-number.

If one defines:

$$\begin{aligned} & \Lambda_{R1} = \frac{m^2 \pi^2}{L^2} + \frac{n^2 \pi^2}{R_1^2}, \quad \Lambda_{R2} = \frac{m^2 \pi^2}{L^2} + \frac{n^2 \pi^2}{R_2^2} \\ & \beta_1 = \frac{D}{(1 + \tau^2 l^2 \Lambda_{R1}) \Lambda_{R1}^2} \left(\Lambda_{R1}^4 + \frac{m^4 \pi^4}{L^4} 4k_1^4 \right) \\ & \beta_2 = \frac{D}{(1 + \tau^2 l^2 \Lambda_{R2}) \Lambda_{R2}^2} \left(\Lambda_{R2}^4 + \frac{m^4 \pi^4}{L^4} 4k_2^4 \right) \end{aligned} \quad (25)$$

Then, substitution of (23) into Eq. (21) yields:

$$\begin{aligned} & \left[\beta_1 + c - \left(\frac{n\pi}{R_1} \right)^2 N_{0s} \right] A_1 - c A_2 = 0 \\ & -c \frac{R_1}{R_2} A_1 + \left[\beta_2 + c \frac{R_1}{R_2} + k_0 - \left(\frac{n\pi}{R_2} \right)^2 N_{0s} \right] A_2 = 0 \end{aligned} \quad (26)$$

For non-trivial solutions of A_1 and A_2 , the determinant of Eq. (26) must vanish, i.e.,

$$\left[\beta_1 + c - \left(\frac{n\pi}{R_1} \right)^2 N_{0s} \right] \left[\beta_2 + c \frac{R_1}{R_2} + k_0 - \left(\frac{n\pi}{R_2} \right)^2 N_{0s} \right] - \frac{R_1}{R_2} c^2 = 0 \quad (27)$$

which leads to:

$$\begin{aligned} \Delta T_0^{NL} = & \frac{1-\nu}{E\alpha h} \left(\frac{1}{n\pi} \right)^2 \left[\left(\beta_1 R_1^2 + \beta_2 R_2^2 + k_0 R_2^2 + c R_1^2 + \frac{R_1}{R_2} c R_2^2 \right) \right. \\ & \left. - \sqrt{\left(\beta_2 R_2^2 - \beta_1 R_1^2 + k_0 R_2^2 - c R_1^2 + \frac{R_1}{R_2} c R_2^2 \right)^2 + 4c R_1^2 \frac{R_1}{R_2} c R_2^2} \right] \end{aligned} \quad (28)$$

If the effects of small scale are neglected, the constants β_1 and β_2 in (25) are redefined as:

$$\begin{aligned} \beta_1^o &= D \left(\Lambda_{R1}^2 + \frac{m^4 \pi^4}{L^4 \Lambda_{R1}^2} 4k_1^4 \right) \\ \beta_2^o &= D \left(\Lambda_{R2}^2 + \frac{m^4 \pi^4}{L^4 \Lambda_{R2}^2} 4k_2^4 \right) \end{aligned} \quad (29)$$

and the buckling temperature variation reads:

$$\begin{aligned} \Delta T_0^L = & \frac{1-\nu}{E\alpha h} \left(\frac{1}{n\pi} \right)^2 \left[\left(\beta_1^o R_1^2 + \beta_2^o R_2^2 + k_0 R_2^2 + c R_1^2 + \frac{R_1}{R_2} c R_2^2 \right) \right. \\ & \left. - \sqrt{\left(\beta_2^o R_2^2 - \beta_1^o R_1^2 + k_0 R_2^2 - c R_1^2 + \frac{R_1}{R_2} c R_2^2 \right)^2 + 4c R_1^2 \frac{R_1}{R_2} c R_2^2} \right] \end{aligned} \quad (30)$$

To investigate the effects of small length scale on the thermal buckling temperature variation, the ratio $\phi(a, e_0, c, k_0, R_1, R_2, L, E, \alpha)$ can be defined as:

$$\phi(a, e_0, c, k_0, R_1, R_2, L, E, \alpha) = \frac{\Delta T_0^{NL}}{\Delta T_0^L} \quad (31)$$

The superscripts NL and L denote the results obtained by the nonlocal elastic model and the classical model, respectively.

4.2 Uniformly Reduced Temperature. Now let us consider the case that the temperature of the nano-tubes uniformly decreases by:

$$T(x) = \Delta T_0, \quad 0 < x < L \quad (32)$$

Due to this temperature change, a compressive axial force is developed at the fixed ends of the nano-tubes. In the radial direction, the surrounding elastic medium contracts away from the nano-tubes while the tubes expand. Therefore, the pre-buckling forces are: $N_{0s} = N_{0xs} = 0$ in the operator N_L^0 , and

$$N_{0x} = \frac{E\alpha h}{1-\nu} \Delta T_0 \quad (33)$$

Now, the stability equations become:

$$\begin{aligned} \nabla_{R1}^8 w_1 + 4k_1^4 w_{1,xxxx} = & -\frac{N_{0x}}{D} (1 - \tau^2 l^2 \nabla_{R1}^2) \nabla_{R1}^4 w_{1,xx} \\ & + \frac{1}{D} (1 - \tau^2 l^2 \nabla_{R1}^2) \nabla_{R1}^4 [c(w_2 - w_1)] \end{aligned} \quad (34)$$

$$\begin{aligned} \nabla_{R2}^8 w_2 + 4k_2^4 w_{2,xxxx} = & -\frac{N_{0x}}{D} (1 - \tau^2 l^2 \nabla_{R2}^2) \nabla_{R2}^4 w_{2,xx} \\ & - \frac{1}{D} (1 - \tau^2 l^2 \nabla_{R2}^2) \nabla_{R2}^4 \left[k_0 w_2 + c \frac{R_1}{R_2} (w_2 - w_1) \right] \end{aligned}$$

$$\begin{bmatrix} a_{1,1} + \left(\frac{n\pi}{R_1}\right)^2 N_{0s} & -c & 0 & \dots & 0 \\ -c \frac{R_1}{R_2} & a_{2,2} - \left(\frac{n\pi}{R_2}\right)^2 N_{0s} & -c & 0 & \dots \\ 0 & \dots & \dots & \dots & \dots \\ \dots & 0 & -\frac{R_{N-2}}{R_{N-1}} c & a_{N-1,N-1} - \left(\frac{n\pi}{R_{N-1}}\right)^2 N_{0s} & -c \\ 0 & \dots & 0 & -\frac{R_{N-1}}{R_N} c & a_{N,N} - \left(\frac{n\pi}{R_N}\right)^2 N_{0s} \end{bmatrix} \quad (37)$$

where,

$$\begin{aligned} a_{1,1} = \beta_1 + c; \quad a_{2,2} = \beta_2 + \left(1 + \frac{R_1}{R_2}\right) c \\ a_{N-1,N-1} = \beta_{N-1} + \left(1 + \frac{R_{N-2}}{R_{N-1}}\right) c; \quad a_{N,N} = \beta_N + \frac{R_{N-1}}{R_N} c + k_0 \end{aligned} \quad (38)$$

Setting the determinant of (37) to zero results in an N th polynomial equation in terms of ΔT_0 , which can be solved numerically for $N > 2$. The minimum of the solutions for ΔT_0 is the desired critical solution.

5 Results and Discussion

Numerical results are presented here for double-walled carbon nano-tubes in an elastic medium. The original data are chosen as: The length of a C-C bond is $a = 1.42$ nm [13]; the material thermal expansion coefficient $\alpha = -1.60 \times 10^{-6} / ^\circ\text{K}$, $E = 742$ GPa, $\nu = 0.17$ [7]; the radius of the inner carbon tube $R_1 = R_1^0 = 0.35$ nm and the radius of the outer carbon tube $R_2 = R_2^0 = 0.79$ nm (Fig. 1), the thickness of each nano-tube $h = (R_2 - R_1) / 4$, the length of the

The expression (23) can also be a solution to this case. The argument similar to the one used in obtaining (26) yields:

$$\begin{aligned} \left(\beta_1 + c - \frac{m^2 \pi^2}{L^2} N_{0x}\right) A_1 - c A_2 = 0 \\ -c \frac{R_1}{R_2} A_1 + \left(\beta_2 + c \frac{R_1}{R_2} + k_0 - \frac{m^2 \pi^2}{L^2} N_{0x}\right) A_2 = 0 \end{aligned} \quad (35)$$

which leads to:

$$\begin{aligned} \Delta T_0 = \frac{1-\nu}{2E\alpha h} \left(\frac{L}{m\pi}\right)^2 \left\{ \beta_1 + \beta_2 + k_0 + \left(1 + \frac{R_1}{R_2}\right) c \right. \\ \left. - \sqrt{\left[\beta_2 - \beta_1 + k_0 - \left(1 - \frac{R_1}{R_2}\right) c\right]^2 + 4 \frac{R_1}{R_2} c^2} \right\} \end{aligned} \quad (36)$$

A ratio similar to (31) can also be defined for this case, in order to compare with the classical (as opposed to the nonlocal elastic) model.

4.3 Number of the Carbon Nanotubes, $N > 2$. Though the above study is for $N = 2$, the procedure can be extended to multi-walled carbon nanotubes ($N > 2$). For example, if the multi-walled nano-tube is subjected to the thermal loading defined in Eq. (19), the critical temperature variation ΔT_0 , through Eq. (20), is found by setting equal to zero the determinant of the following matrix:

nano-tubes $L = 10 \times R_2$; the van de Waals interaction coefficient $c = 0.0694$ TPa, the spring constant from the surrounding elastic medium $k_0 = 0.001 \times c$.

Presented in Fig. 2 is the influence of the internal characteristic parameter, $a: \phi(a, e_0, \dots, \alpha)$, defined in Eq. (31), versus a for different sizes of the nano-tubes. Both the axial half wave-number, m and circumferential half wave-number, n are 1, which corresponds to the critical value of ΔT_0 (see Fig. 5 for details). Here, the material constant, e_0 is assumed as 0.39 [15].

Three observations can be made here: First, for each of the tubes (except the one with $R_1 = 300R_1^0, R_2 = 300R_2^0$), the $\phi(a, e_0, \dots, \alpha)$ decreases notably as the internal characteristic parameter, a increases. This means that the classical shell model may give over-estimated predictions for the thermal buckling temperature when a structure is in the scope of nanometers. Second, when the inner tube diameter of the multi-walled carbon tube is larger than 1.05×10^{-8} m (out of the nanometer range), the length of the C-C bond (an internal characteristic parameter) does not have an influence on the thermal buckling behavior (see the dotted curve of Fig. 2). In other words, if the structure considered falls above the nanometer range, the nonlocal model and classical shell model will give very close predictions. Third, for carbon nano-tubes, the internal parameter a ($= 1.42$ nm) has a significant influ-

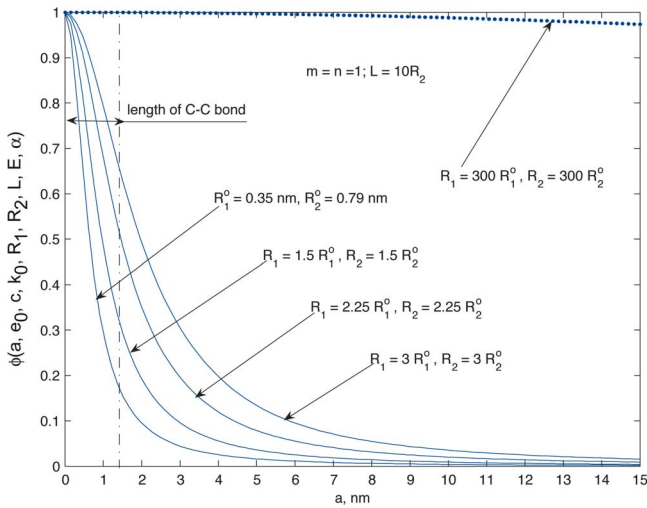


Fig. 2 The influence of the internal characteristic parameter, “a”

ence on the thermal buckling point. For example, if the inner radius of the double-walled carbon nanotubes is 0.35 nm and the outer radius is 0.79 nm, the ratio function $\phi(a, e_0, \dots, \alpha) = 0.18$.

Plotted in Fig. 3 are the influences from the combination of the internal characteristic parameter and the material constant, ae_0 , while the curves depicted in Fig. 4 are the influences of the internal parameter a under different material constants, e_0 . The decreasing tendency similar to the one in Fig. 2 is also shown in Figs. 3 and 4, i.e., the value of $\phi(a, e_0, \dots, \alpha)$ decreases as the value of ae_0 increases (Fig. 3), or as the internal length parameter, a increases for each given e_0 (Fig. 4). One may further observe that the curves in Figs. 3 and 4 together can provide a convenient way to determine the values of the material constant, e_0 and the internal characteristic parameter, a for each material. Here is the procedure: (1) Experimentally find the critical buckling temperature variation ΔT_0^{NL} , then calculate the value of $\phi_{ae_0} = \phi(a, e_0, c, k_0, R_1, R_2, L, E, \alpha)$ via dividing ΔT_0^{NL} by ΔT_0^L ; (2) Using the ϕ_{ae_0} to locate the value of ae_0 from the curves in Fig. 3; (3) Using the same ϕ_{ae_0} to locate the values of the pair (a, e_0) from the curves in Fig. 4; (4) the values of the pair (a, e_0) , whose product equals the value of ae_0 in step two are the values for a and e_0 of the material, respectively. Sudak [17] discussed the de-

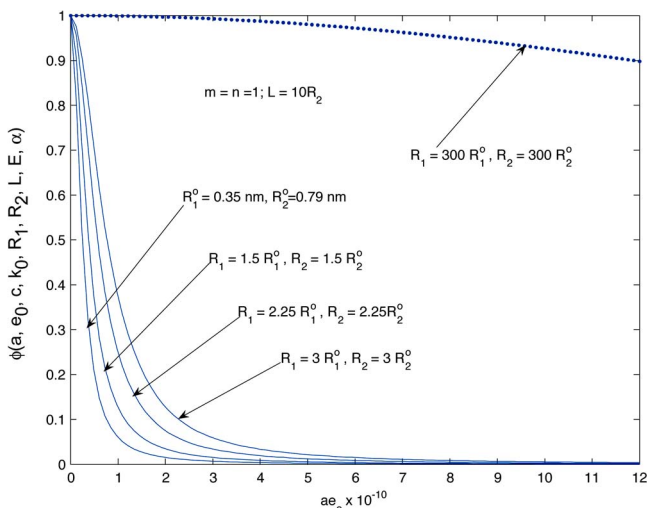


Fig. 3 The influence of the combined parameter “ ae_0 ”

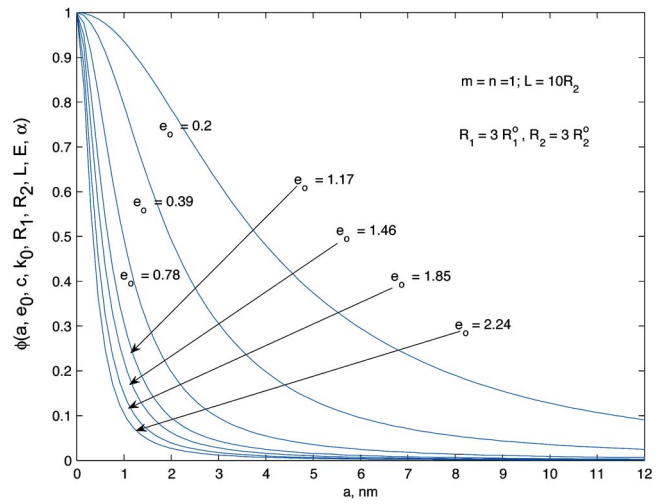


Fig. 4 The influence of the internal parameter “a” or various values of “ e_0 ”

termination of the material constant e_0 for the known a . But the suggested procedure solves for the e_0 and a simultaneously.

Results in Figs. 5 and 6 are the critical ΔT_0 s of two types of thermal buckling modes (radial buckling due to elevated radial temperature and axial buckling due to reduced temperature [18]) versus the axial half wave-number, m and the circumferential half wave-number, n . The material constant e_0 used in Figs. 5 and 6 is assumed to be 0.78, which is very close to the estimated value of 0.775 from the data given in [25]. The other data are the original ones described in the beginning of the section. Figure 5 shows that thermal buckling happens when both the axial half wave-number, m and circumferential half wave-number are 1, and the ΔT_0 is increased by 840.25 °C for this double-walled nano-tubes. However, from the result in Fig. 6, one can see that the absolute value of ΔT_0 (“-” means temperature decreased) is very big. Physically speaking, this type of buckling mode will never happen for the carbon nano-tubes, which by itself is an interesting observation.

Finally, it should be mentioned that in this paper we study buckling and therefore, as is well known in bifurcation theory, we do not need to consider the geometric nonlinearities. Of course, if post-buckling is studied, nonlinearities need to be included, as in [26,27].

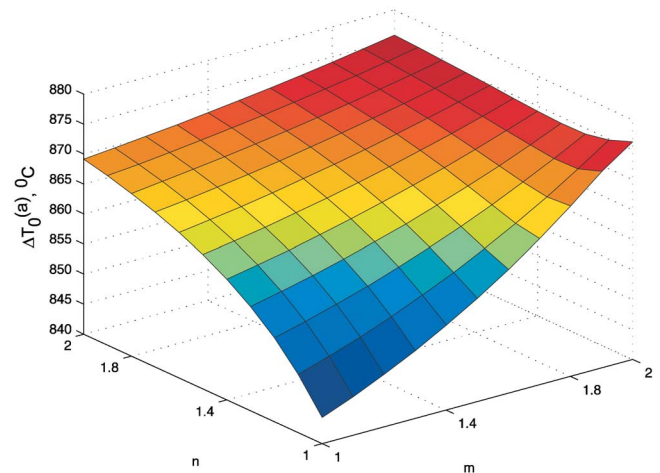


Fig. 5 Critical temperature ΔT_0^a versus (m, n)

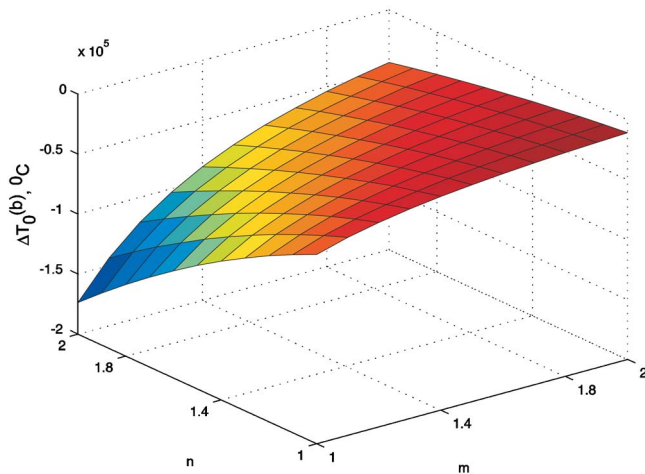


Fig. 6 Critical temperature $\Delta T_0^{(b)}$ versus (m, n)

6 Conclusions

In this paper, a nonlocal multi-walled shell model is developed to investigate the thermal buckling phenomenon of multi-walled carbon nano-tubes in an elastic medium. The tubes are considered concentric shells coupled by the van der Waals' interaction between adjacent tubes. Closed form expressions for the critical temperature variation are formulated for double-walled carbon nano-tubes, and numerical results are presented to demonstrate the influences of the small length scales in the study of nano-devices. Observations in this research suggest the following conclusions: (1) When the structure considered falls into the nano-meter range, the material internal characteristic parameter has a significant influence on the outcomes of this study. The nonlocal mechanics model is an appropriate model. But when the geometrical sizes of the structure are bigger than nano-meter scales, the classical elastic model is valid; (2) the curves of $\phi(a, e_0, \dots, \alpha)$ versus ae_0 and $\phi(a, e_0, \dots, \alpha)$ versus a under different e_0 can be used to determine the internal parameter a , and the material constant, e_0 ; (3) for carbon nano-tubes, the possible thermal buckling mode is the "radial" buckling mode (as in a shell under external pressure).

Acknowledgments

The financial support of the Office of Naval Research, Ship Structures and Systems, S and T Division, Grants Nos. N00014-90-J-1995 and N00014-0010323, and the interest and encouragement of the Grant Monitor, Dr. Y.D.S. Rajapakse, are both gratefully acknowledged.

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