Nanoscience and Nanotechnology 2014, 4(2): 27-33
DOI: 10.5923/j.nn.20140402.02

Thermal Effect on Buckling of Multiwalled Carbon Nanotubes Using Different Gradient Elasticity Theories

Mokhtar Bouazza[1,2,*], Khaled Amara[2,3], Mohamed Zidour[2,4], Tounsi Abedlouahed[2], Adda Bedia El Abbas[2]

[1]Department of Civil Engineering, University of Bechar, Bechar 08000, Algeria
[2]Laboratory of Materials and Hydrology (LMH), University of Sidi Bel Abbes, Sidi Bel Abbes 2200, Algeria
[3]Department of Civil Engineering, University centre of Ain Temouchent, Ain Temouchent 4600, Algeria
[4]Department of Civil Engineering, University of Ibn Khaldoun, BP 78 Zaaroura, 14000 Tiaret, Algeria

Abstract The present paper examines the thermal effect on axially compressed buckling of a multiwalled carbon nanotube based on the gradient elasticity theories. The small-size effect, which plays an essential role in the buckling behavior with large aspect ratios under axial compression coupling with temperature change, is captured by applying different gradient elasticity theories including stress and strain. In this model, each of the nested concentric tubes is regarded as an individual column and the deflection of all the columns is coupled together through the van der Waals interactions between adjacent tubes.

Keywords Effect of Temperature Change, Nonlocal Elasticity, Carbon Nanotubes, Buckling

1. Introduction

Carbon nanotubes (CNTs) possess many unique electrical, optical, thermal, and mechanical properties (see Dresselhaus et al [1] and references therein). They have low weight, high aspect ratio, extremely high stiffness, and sustain large elastic strain and failure strain. Such special features of CNTs make them promising candidates with excellent structural performance as novel nanometer scale electronic and mechanical devices. In particular, experimental evidence and theoretical results (Ajayan et al [2]; Chopra et al [3]; Iijima [4]; Iijima et al. [5]; Molina et al [6]; Treacy et al [7]; Yakobson et al [8]) show that carbon nanotubes hold great promise as a possible reinforcing phase in polymer composite materials. Such composite materials, reinforced with strong, high Young's modulus CNTs (fibres), are very useful due to their excellent specific mechanical properties. High aspect ratio fibres added to a polymer matrix increase Young's modulus and the strength of the composite. However, long CNTs (fibres) often easily buckle and collapse during composite manufacturing (Lourie et al [9]; Wang et al [10]). It is not possible to directly measure the mechanical properties of single nanotubes (Barber et al [11]; Yu et al [12]). Therefore, by studying the deformation and buckling modes resulting from the embedding of CNTs (fibres) in a polymer matrix, it is possible to estimate the strength of carbon nanotubes under compressive stresses.

* Corresponding author:
bouazza_mokhtar@yahoo.fr (Mokhtar Bouazza)
Published online at http://journal.sapub.org/nn

Multi-walled carbon nanotubes are composed of concentric layers of single-walled carbon nanotubes. When subjected to a compressive force, multi-walled carbon nanotubes bend at large angles and may start to elastically ripple, buckle, and form kinks. Recently, large strain deformation of single- or multi-walled carbon nanotubes involving compression, bending or/and torsion has been the subject of numerous experiments and molecular dynamic simulations [13–17]. Basically, there were two theoretical approaches to understanding the behavior of carbon nanobutes: atomistic molecular-dynamics simulations and continuum mechanics. Molecular-dynamics simulations have provided abundant results for the understanding of buckling behaviors of carbon nanotubes. However, moleculardynamics simulations are currently limited to very small length and time scales and cannot deal with the large-sized atomic system, due to the limitations of current computing power. Moreover, at the nanoscale, experiments are extremely difficult and expensive to conduct. As a result, the continuum mechanics models are expected for the theoretical analysis of buckling behavior of carbon nanotubes. Yakobson et al. [13] introduced an atomistic model for axially compressed buckling of single-walled nanotubes and also compared it with a simple continuum shell model. They found that the continuum shell model could predict all changes of buckling patterns in the atomistic molecular-dynamics simulations. However, the existing continuum shell model cannot directly be applied to investigate mechanical behavior of multi-walled nanotubes due to the presence of the van der Waals forces in multi-walled nanotubes [18–21].

The present paper examines the thermal effect on axially compressed buckling of a multi-walled carbon nanotube. The effects of temperature, surrounding van der Waals forces between the inner and outer nanotubes are taken into account. Using different gradient elasticity theories, the effect of temperature change on the properties of axially column buckling is examined.

2. Nonlocal Constitutive Equations

According to Hooke's law within continuum elasticity theory, the stress components at any point in an elastic medium depend only on the strain components at the same position. Instead, for the nonlocal theory of elasticity, the stress components at a reference point x depend not only on the strain components at the same position but also on all other points of the body [22, 23]. This theory can satisfactorily explain some phenomena related to atomic and molecular scale such as high frequency vibrations and wave dispersion [24, 25]. Mathematically, the basic constitutive equations for anisotropic, homogeneous, nonlocal elastic body can be written as:

$$\sigma_{ij}(x) = \int_V \alpha(|x'-x|)\, t_{ij}(x')\, dV(x') \tag{1}$$

$$t_{ij}(x') = \lambda\varepsilon_{kk}(x')\,\delta_{ij}\, 2\mu\varepsilon_{ij}(x') \tag{2}$$

where λ and μ are Lame's constants, ε_{ij} strain components, and t_{ij} and σ_{ij} classical and nonlocal stress components, respectively. V is the volume occupied by the elastic body.

Here α(x) is defined as the attenuation modulus of dimension length^{-3} and depends on the characteristic length ratio a/l, where a an is internal characteristic length (e.g. lattice parameter, granular distance of C–C bond length in carbon nanotubes) and l is an external characteristic length (e.g. crack length and wavelength). Alternatively, taking into account a typical characteristic of $\alpha(x)$, the constitutive equations can be written in stress gradient form [22, 23], namely,

$$\sigma_{ij} - l^2\nabla^2\sigma_{ij} = \lambda\varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij} \tag{3}$$

where l is a small scale parameter with length units describing the effects of the micro- and nano-scale on elastic behavior, and $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ is the Laplacian operator. Here $l = e_0 a$ in which e_0 is a nondimensional material constant that can be determined by experiments or numerical simulations from lattice dynamics.

In the case of stress gradient (nonlocal) theory the axial equivalent of Eq. (3) is expressed as

$$\boldsymbol{\sigma} - (e_0 a)^2 \frac{\partial^2 \boldsymbol{\sigma}}{\partial x^2} = E\boldsymbol{\varepsilon} \tag{4}$$

The differential equations for stresses shown in Eq. (4) can be solved to determine stresses as a function of displacements. Assuming $l << \mathrm{L}$, higher powers of l/L can be neglected and the solutions can be simplified to, giving [26]

$$\sigma = E\left(\varepsilon + (e_0 a)^2 \frac{\partial^2\varepsilon}{\partial x^2}\right) \tag{5}$$

Because CNTs have high thermal conductivity, it may be considered that the temperature change T is uniformly distributed in the CNTs. With the help of Eq.(5), the constitutive equations in the thermal environment are

$$\sigma = E\left(\varepsilon + (e_0 a)^2 \frac{\partial^2\varepsilon}{\partial x^2}\right) - \frac{E\,A}{1-2\nu}\alpha_x T \tag{6}$$

where ε is the axial strain, σ is the axial stress, a is the coefficient of thermal expansion in the x direction, E is Young's modulus, and u is the Poisson's ratio. For the axial force we have

$$N = \boldsymbol{\sigma} A = N_m + N_t, \tag{7}$$

where A is the cross-sectional area of the beam, and

$$N_m = \sigma_m A, \quad N_t = -\frac{E\,A}{1-2\upsilon}\alpha_x T \tag{8}$$

To derive the nonlocal deflection curve of an elastic column that will model the buckling of carbon nanotubes, we make use of the following relations [27]:

$$\begin{aligned} \frac{dV}{dx} &= -p(x) \\ V &= \frac{dM}{dx} + N\frac{dw}{dx} \end{aligned} \tag{9}$$

where V(x) is the resultant shear force and M(x) is the resultant bending moment. Using the fact that $M(x) = \int_A y\boldsymbol{\sigma}(x)dA$ and noting that the relationship between strain and curvature for small deflections is $\boldsymbol{\varepsilon} = y/R$ and that $1/R = -\left(d^2w/dx^2\right)$, where R is the radius of curvature and y is the coordinate measured positive in the direction of deflection [27], Eq. (6) can be rewritten as follows:

$$M = -EI\left(\frac{\partial^2 w}{\partial x^2} + (e_0 a)^2 \frac{\partial^4 w}{\partial x^4}\right) \tag{10}$$

Differentiating Eq. (8) twice and substituting Eq. (7) into the resulting expression the following expression can be derived for the nonlocal deflection curve of an elastic column under constant axial load and distributed lateral pressure:

$$E\,I\left(\frac{d^4w}{dx^4} + (e_0 a)^2\frac{d^6 w}{dx^6}\right) = p(x) + \left(N_m + N_t\right)\frac{d^2w}{dx^2} \tag{11}$$

Note that when parameter e_0 in Eq. (9) is set to zero, the classical Euler–Bernoulli expression with thermal effect is recovered. Here, let us assume that the lateral pressure p(x) is a continuous function of the axial coordinate x.

As CNTs have high thermal conductivity, it may be regarded that the change of temperature is uniformly distributed in the CNT. Treacy et al. [28] reported a linear relationship between the mean-square vibration amplitude of the tube's free tip displacement and the tube temperature, which implies that the tube's elastic modulus is temperature independent. Hsieh et al. [29] studied the variation of Young's modulus of SWNTs with temperature, and it was indicated that the Young's modulus of an SWNT is insensitive to temperature change in the tube at temperatures of less than approximately 1100 K, but decreases at higher temperatures. Thus, for the cases of low temperatures and high temperatures (but not very high), the Young's modulus is herein assumed to be temperature independent. In what follows, all nested tubes are supposed to have the same thickness and effective material constants. By using the same steps of Sun and Liu [30, 31], applying Eq. (9) to each layer of a MWNT under buckling, n coupled equations can be obtained as

$$\begin{aligned} E\,I_1\left(\frac{d^4 w_1}{d\,x^4}+(e_0 a)^2\frac{d^6 w_1}{d\,x^6}\right) &= p_{12}+\left(N_{m1}+N_{t1}\right)\frac{d^2 w_1}{d\,x^2} \\ E\,I_2\left(\frac{d^4 w_2}{d\,x^4}+(e_0 a)^2\frac{d^6 w_2}{d\,x^6}\right) &= p_{23}-p_{12}+\left(N_{m2}+N_{t2}\right)\frac{d^2 w_2}{d\,x^2} \\ E\,I_n\left(\frac{d^4 w_n}{d\,x^4}+(e_0 a)^2\frac{d^6 w_n}{d\,x^6}\right) &= -p_{(n-1)n}+\left(N_{mn}+N_{tn}\right)\frac{d^2 w_n}{d\,x^2} \end{aligned} \tag{12}$$

where the subscripts 1; 2; . . . ; n denote the quantities of the innermost tube, its adjacent tube, and the outermost tube, respectively, and van der Waals pressure per unit axial length on tube k due to tube k + 1 can be expressed as [32]

$$p_{i(i+1)} = c_{i(i+1)}\left(w_{i+1}-w_i\right),\ \left(i=1,2,.....,n-1\right)$$

where ck(k+1) denotes the intertube interaction coefficient, which can be estimated by [33]
where R (measured in cm) is the inner radius of each pair of nanotubes.

Substitution of Eq. (11) into Eq. (10) gives

$$\begin{aligned} E\,I_1\left(\frac{d^4 w_1}{d\,x^4}+(e_0 a)^2\frac{d^6 w_1}{d\,x^6}\right) &= c_{12}\left(w_2-w_1\right)+\left(N_{m1}+N_{t1}\right)\frac{d^2 w_1}{d\,x^2} \\ E\,I_2\left(\frac{d^4 w_2}{d\,x^4}+(e_0 a)^2\frac{d^6 w_2}{d\,x^6}\right) &= c_{23}\left(w_3-w_2\right)-c_{12}\left(w_2-w_1\right)+\left(N_{m2}+N_{t2}\right)\frac{d^2 w_2}{d\,x^2} \\ E\,I_n\left(\frac{d^4 w_n}{d\,x^4}+(e_0 a)^2\frac{d^6 w_n}{d\,x^6}\right) &= -c_{(n-1)n}\left(w_n-w_{n-1}\right)+\left(N_{mn}+N_{tn}\right)\frac{d^2 w_n}{d\,x^2} \end{aligned} \tag{13}$$

where

$$N_{mi}=\sigma_m A_i\,,\ N_{ti}=-\frac{E\,A_i}{1-2\,\upsilon}\alpha_x\theta\,,\left(i=1,2,....,n\right) \tag{14}$$

It is seen that these equations are coupled to each other due to the van der Waals interaction terms. In addition, it can be observed that with the small scale effect ignored Eqs. (13) reduce to the result presented in [34].

3. Analytical Solution for DWNT Using Stress Gradient Approach

For simplification and without loss of generality, the nonlocal axial column buckling of a DWNT with a large aspect ratio is considered. In this case, Eqs. (13) become

$$E\,I_1\left(\frac{d^4 w_1}{d\,x^4}+(e_0 a)^2\frac{d^6 w_1}{d\,x^6}\right)=c_{12}\left(w_2-w_1\right)+\left(\sigma_m-\frac{E}{1-2\upsilon}\alpha_x\theta\right)A_1\frac{d^2 w_1}{d\,x^2} \tag{15a}$$

$$E\,I_2\left(\frac{d^4 w_2}{d\,x^4}+(e_0 a)^2\frac{d^6 w_2}{d\,x^6}\right)=c_{23}\left(w_3-w_2\right)-c_{12}\left(w_2-w_1\right)+\left(\sigma_m-\frac{E}{1-2\upsilon}\alpha_x\theta\right)A_2\frac{d^2 w_2}{d\,x^2} \tag{15b}$$

Let us consider the hinged boundary conditions. For this case, we have

$$w_1=C\sin(\lambda x),\; w_2=D\sin(\lambda x) \tag{16}$$

where

$$\lambda=\frac{m\pi}{L}$$

where C and D are real constants, and m is a positive integer which is related to buckling modes. Introduction of Eqs. (16) into Eqs. (15a) and (15b) yields

$$E\,I_1\,C\left[1-(e_0 a)^2\lambda^2\right]\lambda^4=c_{12}\,(D-C)\;-\sigma_m A_1\,C\,\lambda^2+\frac{E}{1-2\,\nu}\,\alpha_x\,\theta\,A_1 C\;\lambda^2 \tag{17a}$$

$$E\,I_2\,D\left[1-(e_0 a)^2\lambda^2\right]\lambda^4=-c_{12}\,(D-C)\;-\sigma_m A_2\,D\,\lambda^2+\frac{E}{1-2\,\nu}\,\alpha_x\,\theta\,A_2 D\;\lambda \tag{17b}$$

Nontrivial solutions for the constants C and D exist only when the determinant of the coefficients in Eqs. (17a) and (17b) vanishes. In this manner, we have

$$\begin{aligned}
X&=A_1 A_2\,\lambda^4\,,\\
Y&=E\left(I_1\,A_2+I_2\,A_1\right)\lambda^6\left[1-(e_0 a)^2\,\lambda^2\right]+c_{12}\left(A_1+A_2\right)\lambda^2-2E\frac{\alpha_x\,\theta}{(1-2\,\nu)}A_1\,A_2\,\lambda^4\\
Z&=E^2 I_1\,I_2\,\lambda^8\left[1-(e_0 a)^2\,\lambda^2\right]^2+c_{12}\,E\left(I_1+I_2\right)\lambda^4\left[1-(e_0 a)^2\,\lambda^2\right]-c_{12}\,E\left(A_1+A_2\right)\frac{\alpha_x\,\theta}{(1-2\,\nu)}\lambda^2\\
&\quad-E^2\left(I_1\,A_2+I_2\,A_1\right)\frac{\alpha_x\,\theta}{(1-2\,\nu)}\lambda^6\left[1-(e_0 a)^2\,\lambda^2\right]+E^2 A_1 A_2\left(\frac{\alpha_x\,\theta}{1-2\,\nu}\right)^2\lambda^4
\end{aligned} \tag{18}$$

In consequence, the critical axial buckling strain can be obtained by

$$\begin{aligned}
\left(-\frac{\sigma_m}{E}\right)_1&=-\frac{\sqrt{\left(\frac{c_{12}}{E}\right)^2\left(A_1+A_2\right)^2\left[1+(e_0 a)^2\,\lambda^2\right]^2+2\left(\frac{c_{12}}{E}\right)\left(A_2-A_1\right)\left(I_1 A_2-I_2 A_1\right)\lambda^4\left[1+(e_0 a)^2\,\lambda^2\right]+\left(I_1 A_2-I_2 A_1\right)^2\lambda^8}}{2\,A_1\,A_2\,\lambda^2\left[1+(e_0 a)^2\,\lambda^2\right]}\\
&\quad+\frac{\left(I_1 A_2+I_2 A_1\right)\lambda^4+\left(\frac{c_{12}}{E}\right)\left(A_1+A_2\right)\left[1+(e_0 a)^2\,\lambda^2\right]}{2\,A_1\,A_2\,\lambda^2\left[1+(e_0 a)^2\,\lambda^2\right]}-\frac{\alpha_x\theta}{1-2\upsilon}.
\end{aligned} \tag{19a}$$

$$\begin{aligned}
\left(-\frac{\sigma_m}{E}\right)_2&=-\frac{\sqrt{\left(\frac{c_{12}}{E}\right)^2\left(A_1+A_2\right)^2+2\left(\frac{c_{12}}{E}\right)\left(A_2-A_1\right)\left(I_1 A_2-I_2 A_1\right)\lambda^4\left[1-(e_0 a)^2\,\lambda^2\right]+\left(I_1 A_2-I_2 A_1\right)^2\lambda^8\left[1-(e_0 a)^2\,\lambda^2\right]^2}}{2\,A_1\,A_2\,\lambda^2}\\
&\quad+\frac{\left(\frac{c_{12}}{E}\right)\left(A_1+A_2\right)+\left(I_1 A_2+I_2 A_1\right)\lambda^4\left[1-(e_0 a)^2\,\lambda^2\right]}{2\,A_1\,A_2\,\lambda^2}-\frac{\alpha_x\theta}{1-2\upsilon}.
\end{aligned} \tag{19b}$$

When the effect of temperature change is ignored, the nonlocal result for the critical axial buckling strain [33] is recovered.

4. Results and Discussion

For the case of room or low temperature, we suppose α = -1.6x10-6 K^{-1} [35]. With the aspect ratio L/d1 = 60, the scale parameter e_{0a} =0.5nm and the temperature change θ = 60 K, based on the relationship among the ratio stress/ classical and strain/ classical gradient elasticity theories, the m is indicated in Fig. 1. With m = 2 and θ = 60 K, the relationship among the ratio stress/ classical and strain/ classical gradient elasticity theories, the nonlocal parameter. With the

e_{0a}=1.5nm the aspect ratio L/d1 is shown in Fig. 2. It is clearly seen from Figs. 1 and 2 that the ratios stress/ classical and strain/ classical is less than unity. This means that the application of the local Euler–Bernoulli beam model for CNT analysis would lead to an overprediction of the critical axial buckling strain if the small length scale effect between the individual carbon atoms in CNTs is neglected. As the scale parameter m increases, the ratio strain / classical lower than value the ratio stress/ classical.

For the case of high temperature, we suppose α = 1.1x 10-6 K-1 [35]. With the aspect ratio L/d1 = 60 and the temperature change θ = 60 K, the variation of the ratio stress/ classical and strain/ classical gradient elasticity theories, with the scale parameter e_{0a}=0.5nm for various m is shown in Fig. 3. With m = 2 and θ = 60 K, the variation of the ratio stress/ classical and strain/ classical with the nonlocal parameter e_{0a}=1.5nm for various aspect ratio L/d1 is shown in Fig. 3. It is seen from Figs. 3 and 4 that the column buckling strain for the DWNT is related to the nonlocal parameter e0a. It can be seen from Figs. 3 and 4 that the ratio stress/ classical and strain/ classical is less than unity, which is similar to the case of room or low temperature. Hence the critical axial buckling strain of the nanotubes based on the classical beam theory is over estimated aspect ratio L/d_1 (length-to-diameter ratios) for m = 2 with different small scale parameter e0a. Therefore, it is clear that the small scale effect is significant for short CNTs. The comparison of small-scale effect in fig.2 and fig.4 are nearly identical.

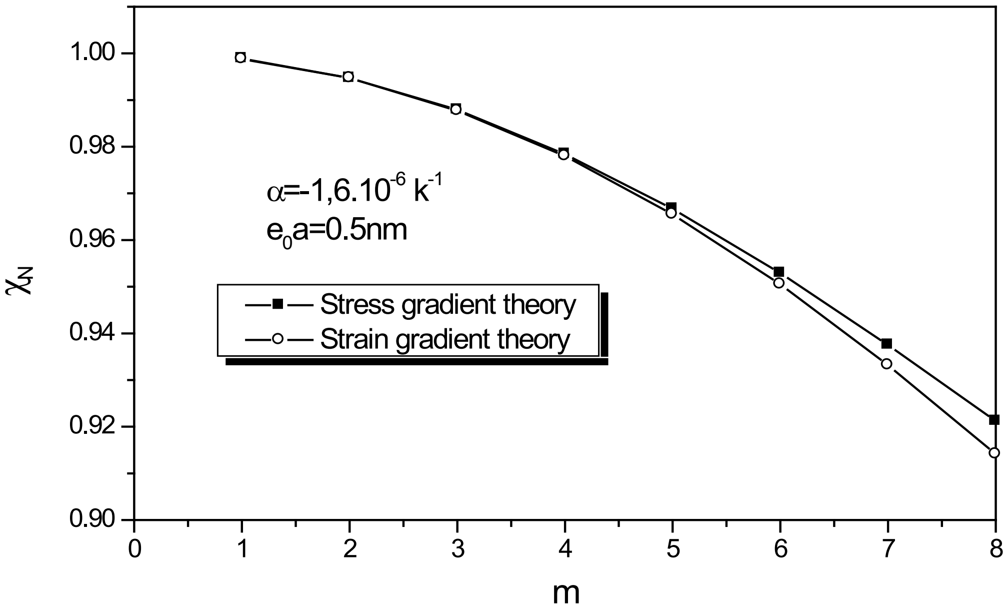

Figure 1. Small scale effect on the critical axial buckling strain ratio of DWNT with the aspect ratio L/d1 = 60 in the case of low or room temperature (θ = 60 K)

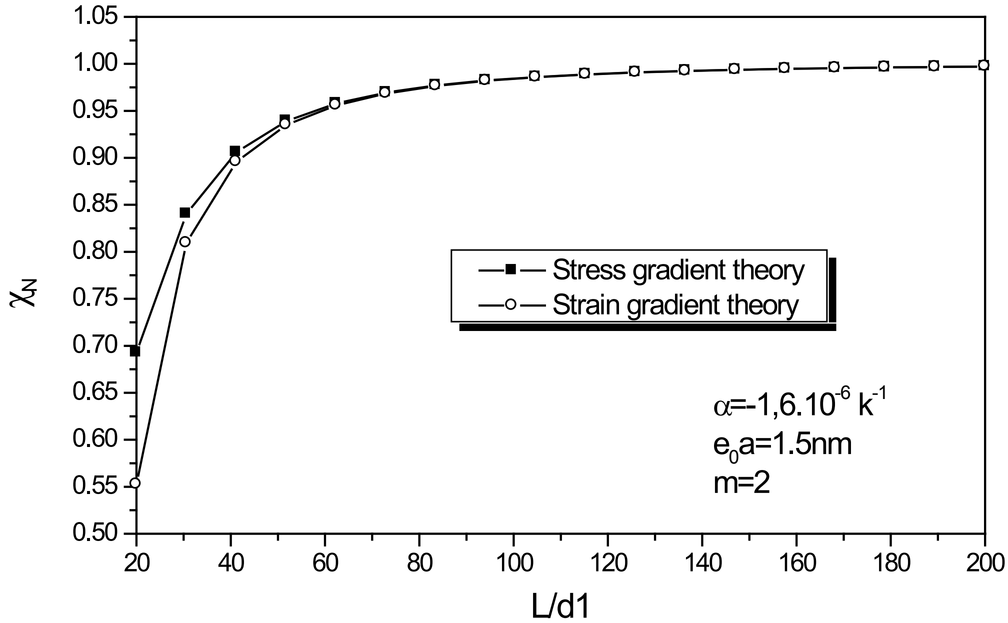

Figure 2. Small scale effect on the critical axial buckling strain ratio of DWNT in the case of low or room temperature (θ = 60 K)

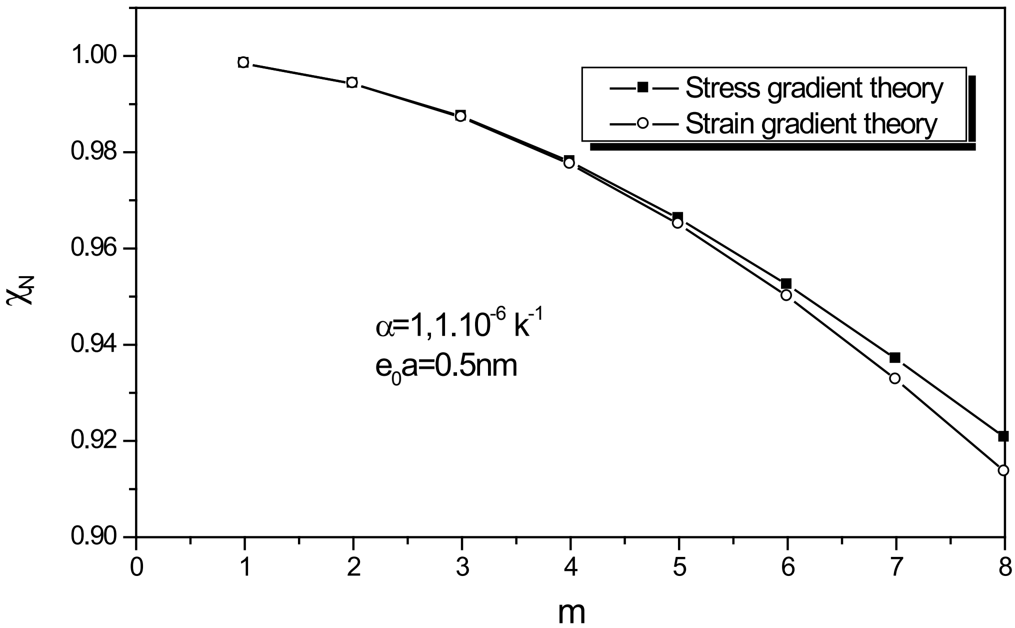

Figure 3. Small scale effect on the critical axial buckling strain ratio of DWNT with the aspect ratio L/d1 = 60 in the case of high temperature (θ = 60 K)

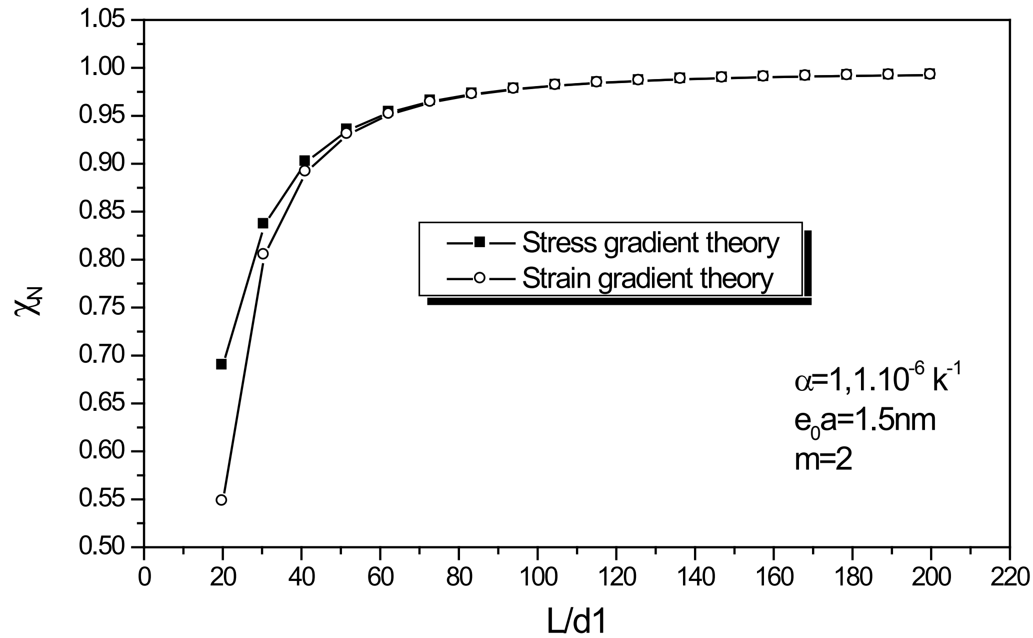

Figure 4. Small scale effect on the critical axial buckling strain ratio of DWNT in the case of high temperature (θ = 60 K)

5. Conclusions

On the basis of theory of thermal different gradient elasticity theories including stress and strain, the theoretical formulations are established, based upon both the Euler–Bernoulli beam theory, is developed for column buckling of MWNTs with large aspect ratios under axial compression coupling with temperature change, which takes into account the effect of temperature change in the formulation incorporation of small length scale effects. In particular, an explicit expression is obtained for the critical buckling strain for a double-walled carbon nanotube. It is found that the thermal effect on the buckling strain is dependent on the temperature changes, the aspect ratios, and the buckling modes of carbon nanotubes. It is hoped that the analytical buckling solutions presented herein will be useful for research work on nanostructures.

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