Amirkabir University of Technology
(Tehran Polytechnic)
Vol. 46, No. 2, Winter 2014, pp. 25-27

Amirkabir Journal of Science & Research (Mechanical Engineering)
(AJSR - ME)

The Effect of Small Scale on Torsional Buckling of the Embedded Double- to Five- Walled Nanotubes Under Axial Loading and Thermal Field

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(Received 18 May 2012, Accepted 09 Feb 2014)

ABSTRACT

This paper aims at investigating the torsional buckling behavior of the embedded multi-walled nanotubes (double- to five- walled) under combined loading based on the nonlocal continuum mechanics. The governing partial differential equations are derived according to Donnel shell model assumptions and Eringen elasticity theory. The effects of the number of layers of carbon nanotube, the existence of axial force, temperature change and the existence of the elastic medium on critical shear stress are studied. Results clearly reveal that at a fixed length, the carbon nanotube which has more layers can tolerate higher critical shear stress, although the existence of compressive axial force and/or temperature change at a high temperature environment decreases the load-bearing capacity of carbon nanotube. While the existence of elastic medium and/or tensile axial force increase the critical shear stress. It is also seen that with a rise in the number of half-wave, the effects of small-scale parameter on shear stress increase. The difference in predicting critical shear stress of multi-walled nanotubes between nonlocal and local continuum mechanics is investigated as well.

KEYWORDS

Multi- Walled Nanotubes, Small Scale Effect, Torsional Buckling, Axial Force, Elastic Medium, Thermal Field.

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1- INTRODUCTION

Carbon nanotubes (CNTs) are employed in nano-electromechanical systems, such as in nano-oscillators, nano-drive devices, and actuators, which are subjected to the torsional loading and the initial stresses due to the thermal stress, mismatch between different materials, or initial external loadings. Hence, the study of the tortional buckling of carbon nanotubes under combined loading is important [1]. Although the molecular dynamics simulations are the superior methods in theoretical study of mechanical behavior of carbon nanotubes, if the buckling characteristics of long carbon nanotubes, multi-walled carbon nanotubes or carbon nanotube bundles involving a large number of atoms are under consideration, they will lose their superiority because of the limitation in time scales and length scales [2]. Therefore, some equivalent continuum models which have proved to be very efficient from the computational point of view, have been developed to study buckling characteristics of carbon nanotubes. Local and nonlocal continuum shell models are popular continuum models used by researchers to investigate the buckling behavior of the carbon nanotubes because they can predict all changes of buckling patterns in the molecular dynamic simulations [1-6].

Sun and Liu [1] investigated the torsional buckling of multi-walled carbon nanotubes under combined torque, axial loading and radial pressures based on local shell model. They showed that the axial tensile stress or the internal pressure makes the multi-walled carbon nanotubes resist higher critical buckling torque, while the axial compressive stress or external pressure leads to a lower one. They studied dynamic and static torsional buckling of the embedded double-walled carbon nanotube as well [4]. Their study showed that buckling load of the embedded double-walled carbon nanotube has been always between that of the isolated inner nanotube and that of the embedded outer nanotube for dynamic and static torsional buckling, due to the effect of the van der Waals forces [4].

Hao et al. [5] investigated the tortional buckling of the embedded multi-walled carbon nanotubes was coupled with temperature change based on nonlocal shell model. They demonstrated that critical shear force was overestimated by the local shell model and the nonlocal effect on critical buckling force decreases as the change in temperature increases at room or low temperature but increases as the change in temperature increases at higher temperature [5].

In this study, based on nonlocal shell model, the effect of small scale on the torsional buckling of the embedded carbon nanotubes (double-to five-walled carbon nanotube) is coupled with axial and the thermal loading is investigated.

2- NONLOCAL SHELL MODEL

Based on Yan et al.'s work [6], Eringen elasticity theory and Donnel shell model assumptions are used to obtain a nonlocal shell model for $0 \le e_0 a < 1$ to evaluate the torsional buckling of the embedded carbon nanotubes coupled with axial and thermal loading as follows:

$$D_e\left(\nabla_R^8 w_1^1 + (e_0 a)^2 \nabla_R^4 H_1^1\right) + \frac{Eh}{R_1^2}\frac{\partial^2}{\partial x^2}\left(\frac{\partial^2 w_1^1}{\partial x^2}\right) = \left(\gamma\frac{T_1}{2\pi R_1^2} - \frac{Eh\alpha_1 T}{1-\nu}\right)\frac{\partial^2}{\partial x^2}\left(\nabla_R^4 w_1^1\right) + \frac{2}{R_1}\frac{T_1}{\left(2\pi R_1^2\right)}\frac{\partial^2}{\partial x\partial\theta}\left(\nabla_R^4 w_1^1\right) - \frac{1}{R_1^2}\left(\frac{Eh\alpha_2 T}{1-\nu}\right)\frac{\partial^2}{\partial\theta^2}\left(\nabla_R^4 w_1^1\right) + C\nabla_R^4\left(w_2^1 - w_1^1\right) \tag{1a}$$

$$D_e\left(\nabla_R^8 w_i^1 + (e_0 a)^2 \nabla_R^4 H_i^1\right) + \frac{Eh}{R_i^2}\frac{\partial^2}{\partial x^2}\left(\frac{\partial^2 w_i^1}{\partial x^2}\right) = \left(\gamma\frac{T_i}{2\pi R_i^2} - \frac{Eh\alpha_1 T}{1-\nu}\right)\frac{\partial^2}{\partial x^2}\left(\nabla_R^4 w_i^1\right) + \frac{2}{R_i}\frac{T_i}{\left(2\pi R_i^2\right)}\frac{\partial^2}{\partial x\partial\theta}\left(\nabla_R^4 w_i^1\right) - \frac{1}{R_i^2}\left(\frac{Eh\alpha_2 T}{1-\nu}\right)\frac{\partial^2}{\partial\theta^2}\left(\nabla_R^4 w_i^1\right) + C\frac{R_{i-1}}{R_i}\nabla_R^4 w_{i-1}^1 - C\left(1+\frac{R_{i-1}}{R_i}\right)\nabla_R^4 w_i^1 + C\nabla_R^4 w_{i+1}^1 \;, i = 2,3,4 \tag{1b}$$

$$D_e\left(\nabla_R^8 w_5^1 + (e_0 a)^2 \nabla_R^4 H_5^1\right) + \frac{Eh}{R_5^2}\frac{\partial^2}{\partial x^2}\left(\frac{\partial^2 w_5^1}{\partial x^2}\right) = \left(\gamma\frac{T_5}{2\pi R_5^2} - \frac{Eh\alpha_1 T}{1-\nu}\right)\frac{\partial^2}{\partial x^2}\left(\nabla_R^4 w_5^1\right) + \frac{2}{R_5}\frac{T_5}{\left(2\pi R_5^2\right)}\frac{\partial^2}{\partial x\partial\theta}\left(\nabla_R^4 w_i^1\right) - \frac{1}{R_5^2}\left(\frac{Eh\alpha_2 T}{1-\nu}\right)\frac{\partial^2}{\partial\theta^2}\left(\nabla_R^4 w_5^1\right) + C\frac{R_4}{R_5}\left(\nabla_R^4 w_4^1 - \nabla_R^4 w_5^1\right) - K\nabla_R^4 w_5^1 \tag{1c}$$

where:

$$H_i^1 = \frac{\partial^6 w_i^1}{\partial x^6} + \frac{\partial^6 w_i^1}{{R_i}^6\partial\theta^6} + \frac{2-\nu}{{R_i}^2}\left(\frac{\partial^6 w_i^1}{\partial x^4\partial\theta^2} + \frac{\partial^6 w_i^1}{{R_i}^2\partial\theta^4\partial x^2}\right) \quad i = 1,2,\cdots,5 \tag{2}$$

In order to find the critical shear force, the buckling mode is assumed to be:

$$w_i^1 = M_i \sin\left(\frac{m\pi}{L}x - n\theta\right), i = 1,\cdots,5 \tag{3}$$

where M_i *s* are the real constants and *m, n* are two positive integers which are the wave numbers in the axial and circumferential directions. Substitution of Eq. 2 into Eq. 1, N (N=2,…,5) homogeneous equations for $M_1,\dots,M_N$ can be obtained which can be written as:

$$\begin{bmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{bmatrix}\begin{bmatrix} M_1 \\ \vdots \\ M_n \end{bmatrix} = 0, \; n = 2,3,4,5 \tag{4}$$

If the determinant of coefficient matrix ($[A_{ij}]$) is set equal to zero, the critical value of T will be found.

3- MODEL VALIDATION

The proposed formula by Sun and Liu [4] is used to verify the correctness of the results. The ratio of critical shear force obtained by Sun and Liu-to-estimated result is listed in Table 1. As seen, the predicted values are in an acceptable range.

Table (1): Comparison obtained critical shear force to Sun and Liu results [4]

R_i (nm)	$\frac{N_{x\theta}([26])}{N_{x\theta}(present)}$	(m,n)
0.76	0.97	(2,3)
1.76	0.911	(2,2)
2.712	0.974	(7,4)
3.663	0.9794	(9,5)

4. NUMERICAL RESULTS

In the numerical examples, the parameters are chosen as:

$$\nu = 0.34, De = 0.85eV, Eh = \frac{360J}{m^2}, C = 9.918667 \times \frac{10^{19}N}{m^3}, h = 0.34$$

$$\alpha_1 = 1.1\times10^{-6}, \alpha_2 = 0.8\times10^{-6}$$

The effects of the existence of axial force, temperature change and the existence of the elastic medium on critical shear stress in wave numbers (m,1) are listed in Table (2). As seen, the existence of elastic medium and/or tensile axial force increase the critical shear stress while the compressive axial force and/or temperature change at a high temperature environment decrease it.

Table (2):Effect of combined loading and number of walled on critical shear stress in (m,1), R_{in}=0.76, L=12*R_{out} , e0a=0.2

Min. Shear Stress, n=1	*Embed-ded*	*γ*	*Δ Temp. (K)*	*No. Walled*
4.8015	*N*	*0*	*0*	*2*
9.4879	*Y*	*0*	*0*	*2*
4.0483	*N*	*0*	*250*	*2*
4.8121	*N*	*+0.02*	*0*	*2*
4.7909	*N*	*-0.02*	*0*	*2*
4.0394	*N*	*-0.02*	*250*	*2*
8.7142	*Y*	*-0.02*	*250*	*2*
8.6430	*Y*	*-0.02*	*250*	*3*
7.6468	*Y*	*-0.02*	*250*	*4*
4.8268	*Y*	*-0.02*	*250*	*5*

The effect of small scale and axial force on shear stress of 4-walled CNTs in wave numbers (m,1) is shown in Fig.1. As seen, with an increase in small scale, the predicted shear stress decreases and the effect of small scale in larger value of *'m'* is more. It is also seen that the compressive axial force decreases the load-bearing capacity of CNTs and the tensile one increases it.

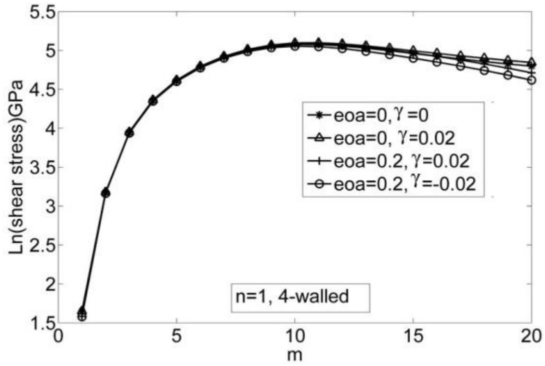

Fig. (1): The effect of small scale on shear stress of 4-walled CNT

5- CONCLUSION

This article aims at investigating the effect of small scale on the torsional buckling of the embedded carbon nanotubes (double-to five-walled carbon nanotube) is coupled with axial and the thermal loading based on nonlocal shell model. Results show that an increase in the number of half-wave 'm' increases the effects of small-scale parameter on shear stress.

The effects of the number of layers of carbon nanotube on load-bearing capacity of carbon nanotube are investigated as well. Results clearly reveal that at a fixed length, the carbon nanotube which has more layers can tolerate higher critical shear stress, although the existence of compressive axial force and/or temperature change at a high temperature environment decreases the load-bearing capacity of carbon nanotube.

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