Determination of Non-local Elasticity Constants for the Torsional Buckling of Single-Wall Carbon Nanotubes Using Molecular Dynamics

F. Khademolhosseini*, N. Rajapakse** and A. Nojeh**

*University of British Columbia, Department of Mechanical Engineering, Vancouver, Canada, V6T 1Z4, khadem@interchange.ubc.ca
** University of British Columbia, Vancouver, Canada, rajapakse@mech.ubc.ca
*** University of British Columbia, Vancouver, Canada, anojeh@ece.ubc.ca

ABSTRACT

Recently, devices have been developed which use Carbon Nanotubes (CNTs) as torsional spring elements [1]. In order to define the range of applicability of CNTs in such devices, it is important to fully understand their torsional response, and to investigate failure modes such as the torsional buckling limit. Currently available continuum models are inaccurate as they are unable to account for the size effects that inevitably exist in such devices. In this work, a modified nonlocal continuum shell model for the torsional buckling of CNTs is proposed. This is done through modifying classical continuum models by incorporating basic concepts from nonlocal elasticity. Furthermore, molecular dynamics (MD) simulations are performed on a range of Zigzag and Armchair nanotubes with different diameters. It is easily seen that compared to classical models, the modified nonlocal model provides a much better fit to MD simulation results. Values of the nonlocal constants are calculated as 0.6 and 0.8 for Zigzag and Armchair CNTs respectively.

.

Keywords: carbon nanotube, torsion, nonlocal elasticity, shell, molecular dynamics

1 INTRODUCTION

Carbon nanotubes (CNTs) have been the subject of ongoing research. These interesting nano-structures exhibit superior mechanical, electrical, thermal, magnetic and optical properties, and could provide the means for development of novel devices at the nano-scale. Ever since their discovery, much work has been done on the characterization and modeling of CNT properties, ranging from experimental observations to numerical simulations. Among the different approaches, continuum modeling is of special interest in defining the mechanical properties of CNTs. Continuum models are simple and efficient, however, in their classical sense, they are unable to account for the size effects that arise due to the discrete nature of matter at the nano-scale. To overcome such problems, modified continuum models have been proposed. One such model is based on the non-local elasticity theory proposed by Eringen [2] which has recently been successfully used to show size effects in nano-scale structures [3]. Using the same approach, in this paper, a modified nonlocal continuum shell model for the torsional buckling of carbon nanotubes is proposed to account for the size effects and provide an efficient and accurate method for the prediction of CNT torsional properties. The proposed non-local shell model is validated through comparison with results from molecular dynamics simulations and consistent values for the shell thickness and non-local constants of zigzag and armchair nanotubes are determined.

2 NON-LOCAL CONTINUUM SHELL MODEL

In this section, the basic concepts of non-local elasticity as proposed by Eringen in the 1970's are briefly presented. These basic equations are used to develop a non-local shell model to predict the buckling torque of single-walled carbon nanotubes (SWCNTs).

2.1 Non-local Theory of Elasticity

This theory states that the stress at a reference point X in a body depends not only on the strain at point X, but also on the strains at all other points X' in the body [2]. The basic equations of the non-local elasticity theory are;

$$t_{kl,k} + \rho(f_l - \ddot{u}_l) = 0 \quad ,$$

$$t_{kl}(X) = \int_v \alpha\left(\left|X' - X\right|, \tau\right)\sigma_{kl}(X')dv(X'),$$

$$\sigma_{kl}(X') = \lambda e_{rr}(X')\delta_{kl} + 2\mu e_{kl}(X'),$$

$$e_{kl}(X') = \frac{1}{2}\left(\frac{\partial u_k(X')}{\partial X'_l} + \frac{\partial u_l(X')}{\partial X'_k}\right) \tag{1}$$

where t_{kl}, ρ, f, u_l are the stress tensor, mass density, body force density and the displacement vector at x respectively. $\sigma_{kl}(x')$ is the classical stress tensor at x' which is related to the linear strain tensor $e_{kl}(x')$ at point x' through the lame constants λ and μ. The kernel function $\alpha(|x'- x|,\tau)$ is the nonlocal modulus and $|x'- x|$ is the Euclidean distance between points x' and x, $\tau=e_0d/l$ where d is an internal

characteristic length of the system (such as the carbon-carbon bond length), l is an external characteristic length (such as the CNT radius or the CNT length) and e_0 represents Eringen's nonlocal constant which has to be determined for each material independently.

For a special class of physically admissible kernel, the above integro-partial differential equations of non-local elasticity can be reduced to singular partial differential equations. In the case of homogenous, isotropic elastic bodies the above equations reduce to:

$$(1-e_0^2 d^2 \nabla^2)\sigma = C_0 : \varepsilon \tag{2}$$

where C_0 is the elastic stiffness tensor of classical (local) isotropic elasticity, σ is the nonlocal stress tensor, ε is the strain tensor and ':' denotes the inner product of tensors [4].

2.2 Modified Timoshenko Continuum Shell Model

In this approach a CNT is modeled as a thin cylindrical shell with thickness h and radius a. A cylindrical coordinate system (r, θ, x) is used with the x-axis along the centre of the cylinder and r *and* θ corresponding to the radial and circumferential directions, respectively. The displacements in the axial, circumferential and radial directions of the shell denoted by u, v and w respectively are functions of only x and θ. Note that these are small displacements measured from the twisted equilibrium state of the shell. For the case of torsional buckling, the non-zero strains can be expressed in terms of displacements as [5];

$$\begin{aligned}
\varepsilon_{xx} &= \frac{\partial u}{\partial x} \\
\varepsilon_{\theta\theta} &= \frac{1}{a}\frac{\partial v}{\partial \theta} - \frac{w}{a} \\
\varepsilon_{x\theta} &= \frac{1}{2}\left(\frac{1}{a}\frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial x}\right)
\end{aligned} \tag{3}$$

Based on equation (2), the nonlocal form of Hooke's law for the stress-strain relations in a cylindrical coordinate system can be expressed in the following form;

$$\begin{aligned}
\sigma_x - \varepsilon\, \nabla_R^2\, \sigma_x &= \frac{E}{1-\nu^2}(\varepsilon_x + \nu\varepsilon_\theta) \\
\sigma_\theta - \varepsilon\, \nabla_R^2\, \sigma_\theta &= \frac{E}{1-\nu^2}(\varepsilon_\theta + \nu\varepsilon_x) \\
\sigma_{x\theta} - \varepsilon\, \nabla_R^2\, \sigma_{x\theta} &= \frac{E}{1+\nu}\varepsilon_{x\theta}
\end{aligned} \tag{4}$$

The above stress-strain relations can be substituted into the equilibrium equations proposed by Timoshenko [5] to find the modified governing differential equations for the torsional buckling of a cylindrical shell. The buckling mode-shape is assumed to be of the following form;

$$\begin{aligned}
&u = A\ \cos(\frac{\lambda x}{a} - n\theta) \quad ; \quad v = B\ \cos(\frac{\lambda x}{a} - n\theta) \\
&w = C\ \sin(\frac{\lambda x}{a} - n\theta) \quad , \quad \lambda = \frac{m\pi a}{l}
\end{aligned} \tag{5}$$

where m is the number of half waves in the axial direction; and n is the number of waves in the circumferential direction. Substitution of equation (5) in the modified governing differential equations and the solution of the resulting eigenvalue problem yields the following solution for the non-dimensional form of the non-local buckling torque of a cylindrical shell;

$$\bar{M}_{Cr}^{NT} = \frac{M_{Cr}^{NT}}{E\sqrt{ah^5}} = \frac{\dfrac{\pi\sqrt{2}}{3(1-\upsilon^2)^{3/4}}}{1+n^2 e_0{}^2 (\dfrac{d}{a})^2} \tag{6}$$

For comparison, the non-dimensional form of the buckling torque corresponding to the classical thin shell model based on ideal elasticity is;

$$\bar{M}_{Cr}^{T} = \frac{M_{Cr}^{T}}{E\sqrt{ah^5}} = \frac{\pi\sqrt{2}}{3(1-\upsilon^2)^{3/4}} \tag{7}$$

Therefore,

$$\frac{\bar{M}_{Cr}^{T}}{\bar{M}_{Cr}^{NT}} = \frac{M_{Cr}^{T}}{M_{Cr}^{NT}} = 1 + n^2 e_0{}^2 (\frac{d}{a})^2 \tag{8}$$

The results of equations (6) and (7) are based on the following critical buckling wavelength (λ_{cr}) given by Timoshenko and Gere [4];

$$\lambda_{cr} = \sqrt{\frac{2h}{a\sqrt{1-\nu^2}}} \tag{9}$$

2.3 Comparison of Classical and Nonlocal Models for Buckling Torque

It is clear from equations (6) and (7) the former is size-dependent due to the presence of the shell radius in the denominator. Thus, the non-local model provides a method to bring size effects into account when calculating the buckling torque. Looking at equation (8), the ratio of the classical to non-local critical torques increases with decreasing values of the nanotube radius and the number of waves in the circumferential direction of the buckled shape. This ratio is also significantly affected by the value of the

NSTI-Nanotech 2009, www.nsti.org, ISBN 978-1-4398-1784-1 Vol. 3, 2009

nonlocal constant e_0 (Figure 1). Note that when $e_0=0$, the ratio equals to one and obviously the non-local model result reduces to the classical solution.

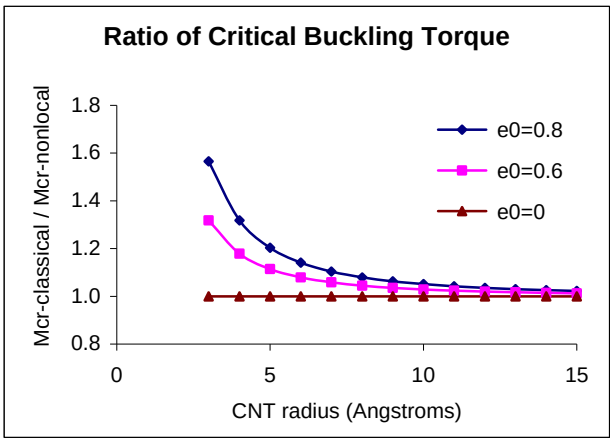


Figure 1: Ratio of the classical to nonlocal buckling torque for three different values of the nonlocal constant.

It is seen from Figure 1 that for CNTs with radii smaller than 0.7 nm, classical shell models can substantially overestimate the buckling torque.

3 DETERMINATION OF THE NON-LOCAL CONSTANT

It is interesting to compare the nonlocal models derived here with classical models to see if a substantial improvement is achieved in the prediction of CNT buckling torques. Ideally, it is best to compare both models with experimental results; however, currently no such experimental results for the buckling torque of SWCNTs have been reported. Thus, molecular dynamics is used to calculate the buckling torque of CNTs.

3.1 MD Simulation of CNT Torsion

The software package Nanohive1 [6], incorporated with the AIREBO potential field is used to perform quasi-static molecular dynamic simulations on a range of nanotubes in order to determine the equivalent continuum properties applicable to the current continuum shell models and assess their validity in CNT modeling. The Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential is an extension of the commonly used second generation REBO potential developed for solid carbon and hydrocarbon molecules.

To determine the buckling state of a certain nanotube under torsion, the modeling is started from an initial non-twisted configuration followed by uniform twists (φ) applied incrementally along the nanotube. The new atomic coordinates are subsequently used as the input to the MD simulator. MD is used to perform relaxation on the twisted CNT until equilibrium is reached and the potential energy of the system converges to a minimum value. For each nanotube, the above simulation is conducted at different values of twist / shear strain and it is seen that above a certain value of twist, which is identified as the critical twist for buckling (φ_{cr}), the nanotube collapses into a buckled shape when allowed to relax for a sufficient amount of time. The outputs of the MD simulations are then analyzed to find the CNT torsional properties such as the buckling torque, buckling strain and the surface shear modulus. MD simulations are performed on a range of zigzag and armchair nanotubes. The results obtained for zigzag nanotubes with different diameters are depicted in Table 1.

Chiral Indices	Diam.(Å)	G.h (GPa nm)	M_{cr} (N.m)	γ_{cr}
(10,0)	7.75	136.15	6.53E-18	0.052
(12,0)	9.30	131.19	7.22E-18	0.041
(14,0)	10.8	127.28	7.67E-18	0.034
(16,0)	12.4	123.34	8.20E-18	0.029
(20,0)	15.5	116.00	9.00E-18	0.022

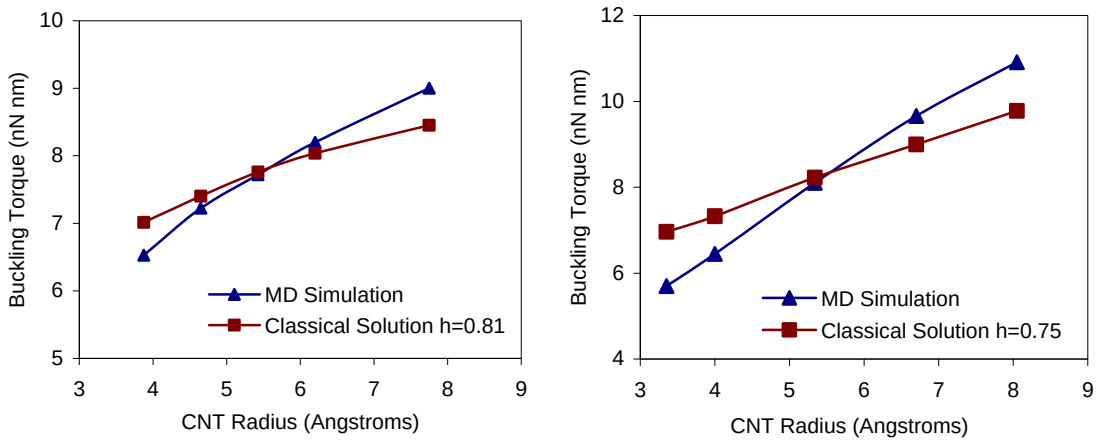
Table 1: MD simulation results for the torsional buckling of a number of zigzag CNTs with different diameters (γcr is the buckling shear strain).

3.2 Non-local Constant

A non-linear least squares optimization technique is used to fit the classical and nonlocal solutions to the MD simulation results. In the case of the classical solution, the thickness h is the optimization variable and for the case of the non-local solution, both the non-local constant e_0 and the thickness h are the optimization variables. The results are shown in Table 2 and Figures 2 and 3.

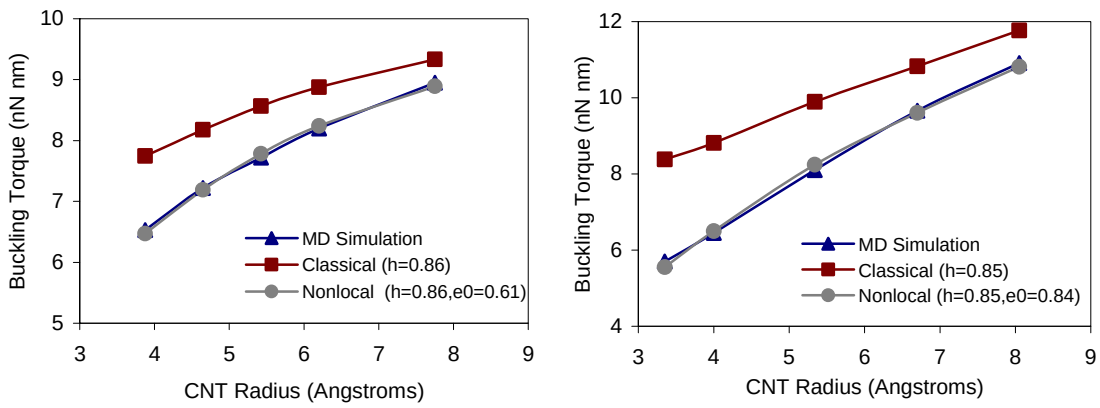
ARMCHAIR			
	h(Å)	e0	Residual Norm ($nN^2.nm^2$)
Classical	0.75	—	4.11
Non-local	0.85	0.85	0.09
ZIGZAG			
	h(Å)	e0	Residual Norm ($nN^2.nm^2$)
Classical	0.81	—	5.9
Non-local	0.86	0.61	0.04

Table 2: Values of non-local constant and thickness obtained by fitting of non-local and classical solutions to MD results for torsional buckling.



(a) (b)

Figure 2: Comparison of critical buckling torque from classical solution with MD simulations using optimized values for thickness ; (a) Zigzag SWCNTs (10,0), (12,0), (14,0), (16,0), (20,0) (b) Armchair SWCNTs (5,5), (6,6), (8,8), (10,10), (12,12)



(a) (b)

Figure 3: Comparison of critical buckling torque from classical and modified non-local solutions with MD simulations using optimized values of thickness and non-local constant; (a) for a Zigzag SWCNTs (b) for Armchair SWCNTs.

4 CONCLUSIONS

It is easily seen that compared to classical models, the modified nonlocal model provides a much better fit to MD simulation results (Figures 2&3). The classical models are unable to show the correct rate of change in buckling torque with the change in CNT radius. This is due to ignoring the existing size effects at these scales. Based on the obtained results, a global thickness of 0.085 nm for CNTs subject to torsion is proposed. Values of the nonlocal constants are calculated as 0.6 and 0.8 for Zigzag and Armchair CNTs respectively. Through comparison of classical and modified non-local models it is concluded that classical approaches can overestimate the critical buckling torque of CNTs by as much as 30 percent and this error becomes more significant for CNTs with smaller diameters. For CNTs with large diameters (several nanometers or more), size effects are insignificant and both the classical and nonlocal models predict the same values for the buckling torque.

Acknowledgement: this work was funded by NSERC.

REFERENCES

[1] A.R. Hall, M.R. Falvo, R. Superfine, S. Washburn, Nature Nanotechnology 2, 413-416, 2007
[2] A. C. Eringen, J. Phys. D 10, 671-678, 1977
[3] J. Peddison, J.; R. Buchanan and R.P. McNitt, Int. J. Eng. Sci. 41, 305-312, 2003
[4] Y.Q. Zhang, G.R. Liu and X. Han, Phys. Lett. A. 349, 370-376, 2006
[5] S.P. Timoshenko and J.M. Gere, "Theory of Elastic Stability", 2nd ed., McGraw Hill, 500-510, 1961
[6] NanoHive-1, v.1.2.0-b1., Nanorex Inc., 2005