Torsional Buckling of Double-Walled Carbon Nanotubes

S. H. Soong

Engineering Science Programme, National University of Singapore
Kent Ridge, Singapore 119260

ABSTRACT

This paper is concerned with the torsional buckling of double-walled carbon nanotubes (DWCNT). A double-cylindrical shell continuum model is presented for the torsional buckling analysis and this model takes into consideration the effects of the van der Waals forces between the inner and outer nanotubes. The critical torques of DWCNT with different diameters were obtained using the continuum shell model and they were found to be comparable to the results furnished by molecular dynamics simulations.

INTRODUCTION

In the open literature, one finds many papers written on the buckling analysis of CNTs under axial compression by using either continuum mechanics (beam and cylindrical shell) models or molecular dynamics simulations (see literature survey paper by Wang et al. 2007). However, relatively few papers have been published on the torsional buckling of CNTs, for example the paper by Yao and Han (2006). It is well-known that carbon nanotubes can be used as torsional springs in resonators or rotational bearings in actuators. Therefore, it is of great significance to understand the torsional buckling behaviours of CNTs. There exist three primary methods for determining the torsional buckling behaviour of CNTs, namely, the experimental approach, the atomistic simulations method and the continuum mechanics method. Conducting experiments on CNTs remain a great challenge and the cost is still expensive. As for the atomistic simulations, intensive computing is required for a large system comprising thousands of atoms. As for the continuum mechanics models, the computational effort is relatively easy and their applicability for CNTs was confirmed by Yakobson et al. (1996) by comparing the results with those obtained from molecular dynamics simulation and experiments. Since then, researchers have resorted to the continuum mechanics models for solution. In the last few decades, one can observe many proposed continuum shell models, beam models and space truss/frame models for the analysis of CNTs (Batra and Sears, 2007).

The objective of this paper is to present a double-cylindrical shell model for the torsional buckling analysis of DWCNTs. In the double-shell model, the inner and outer tubes in the DWCNTs are treated as thin cylindrical shells and the shells are connected by lateral (Winkler) springs to simulate the van der Waals interactions. The critical torques of the DWCNTs are calculated and compared with those obtained from molecular dynamics simulations. The two sets of results have been found to be within
several percentages difference, indicating the reasonable validity of the continuum shell models for the torsional buckling analysis of CNTs.

ELASTIC CYLINDRICAL SHELL MODEL

A cylindrical shell with a radius $r$, thickness $h$, Young’s modulus $E$ and Poisson’s ratio $\nu$ has been shown to be able to simulate the bending and torsional behaviour of single-walled carbon nanotubes (Yakobson et al., 1996). Based on Donnell’s Shell Theory (1976), the equilibrium equation in the radial direction is given by:

$$\frac{\partial^4 w}{\partial r^4} - \frac{1}{r^2} \frac{\partial w}{\partial r} = 2N_{r} \frac{\partial^2 w}{\partial r^2} + P$$

(1)

where $D = \frac{Eh^3}{12(1-\nu^2)}$ is the flexural rigidity of the shell, and $x$ and $y$ denote the axial and circumferential coordinates of the shell, respectively, $w(x, y)$ is the displacement of the middle surface of the shell along the inward normal direction and $P$ is the normal pressure.

Considering the equilibrium of inplane forces in the cylindrical shell, one obtains the following equilibrium equations

$$\frac{\partial N_r}{\partial x} + \frac{\partial N_{r'y}}{\partial y} = 0$$

(2)

$$\frac{\partial N_y}{\partial y} + \frac{\partial N_{ry}}{\partial x} = 0$$

(3)

In order to satisfy Eq. (2), there must be a function $A(x,y)$ such that

$$N_r = \frac{\partial A}{\partial y}$$

(4)

$$N_{ry} = -\frac{\partial A}{\partial x}$$

(5)

Similarly, in order to satisfy Eq. (3), there must be a function $B(x,y)$ such that
From Eqs. (5) and (7), we have

\[ A(x,y) = \frac{\partial \phi(x,y)}{\partial y}, \quad B(x,y) = \frac{\partial \phi(x,y)}{\partial x} \]  

(8a,b)

where the stress function \( \phi(x,y) \) is introduced in Eqs. (8a) and (8b) so that the inplane forces may also be written as

\[ N_x = \frac{\partial \phi}{\partial y}, \quad N_y = \frac{\partial \phi}{\partial x}, \quad N_{xy} = \frac{\partial^2 \phi}{\partial x \partial y} \]  

(9a,b,c)

Since the inplane strains are given by

\[ \varepsilon_x = \frac{1}{Eh} (N_x - vN_y), \quad \varepsilon_y = \frac{1}{Eh} (N_y - vN_x), \quad \gamma_{xy} = \frac{2(1+v)}{Eh} N_{xy} \]  

(10a,b,c)

Using Eqs. (9a) to (9c), we can rewrite Eqs. (10a) to (10c) as

\[ \varepsilon_x = \frac{1}{2h} \left( \frac{\partial^2 \phi}{\partial y^2} - v \frac{\partial^2 \phi}{\partial x^2} \right), \quad \varepsilon_y = \frac{1}{2h} \left( \frac{\partial^2 \phi}{\partial x^2} - v \frac{\partial^2 \phi}{\partial y^2} \right), \quad \gamma_{xy} = \frac{2(1+v)}{2h} \left( - \frac{\partial^2 \phi}{\partial x \partial y} \right) \]  

(11a,b,c)
Based on the Donnell shell theory (Donnell, 1976), the compatibility condition of a thin shell is given by

$$\frac{\partial E_{xx}}{\partial x} + \frac{\partial E_{yy}}{\partial y} - \frac{\partial \gamma_{xy}}{\partial x} - \frac{1}{\rho} \frac{\partial \gamma_{xy}}{\partial y} = 0$$

(12)

By substituting Eqs. (11a), (11b) and (11c) into Eq. (12), one obtains

$$\nabla^4 \varphi = -\frac{Eh}{\rho} \frac{\partial^2 w}{\partial y^2}$$

(13)

In view of Eqs. (1) and (13), the governing equation can be written in the following form:

$$D \nabla^4 w = \frac{1}{\rho} \frac{\partial^2 w}{\partial y^2} - 2N_{xy} \frac{\partial^2 w}{\partial x \partial y} = R$$

(14)

The stress function $\varphi(x, y)$ in Eq. (14) can be eliminated by using Eq. (13). This result in a single equation in terms of the radial displacement $w(x, y)$ given by:

$$D \nabla^4 w + \frac{Eh}{\rho} \frac{\partial^2 w}{\partial y^2} - \nabla^4 2N_{xy} \frac{\partial^2 w}{\partial x \partial y} = \nabla^4 P(x, y)$$

(15)

Equation (15) is the governing equation of a thin cylindrical shell subjected to a torque $M = 2m^4 N_{xy}$. In the following, we extend Eq. (15) for the torsional buckling analysis of DWCNT by allowing for the effect of the van der Waals interactions.

**VAN DER WAALS FORCE BETWEEN ADJACENT NANOTUBES**

The Lennard-Jones model can be used to describe the van der Waals force between any two carbon atoms. As described by Ru (2000a), the van der Waals force exerted on any atom on a tube can be estimated by adding up all forces between the atom and all atoms on the other tube. Figure 1 shows the double-shell model for a DWCNT with the van der Waals forces. The pressure $P_1$ expresses the van der Waals force exerted by the outer tube on the inner tube. On the other hand, the pressure $P_2$ expresses the van der Waals force exerted by the inner tube on the outer tube. Since the interaction forces between the two tubes are equal and opposite, the pressure $P_1$ and $P_2$ exerted on the corresponding points on the inner tube ($1^{st}$) tube and the outer ($2^{nd}$) tube should be related by
where $r_1$ and $r_2$ are the radii of the 1st and 2nd tubes, respectively.

![Image of a double shell model for a DWCNT]

Fig. 1 Double shell model for a DWCNT

The pressure caused by the van der Waals forces at any point $(x, y)$ on the 1st tube could be assumed to be a function of the distance between the two tubes at that point, denoted by $\bar{d}(x, y)$, namely,

$$P_1(x, y) = G(\bar{d}(x, y))$$

(17)

where $G(\bar{d})$ is a nonlinear function of the intertube spacing $\bar{d}$ as given by Ru (2000b, 2001). After buckling, the pressure caused by the van der Waals forces at any point $(x, y)$ on the 1st tube becomes

$$P_1(x, y) = c\left[\bar{d}(x, y) - \bar{d}_1\right]$$

(18)

where $c$ is a constant which is defined below. The equilibrium distance between a carbon atom and a flat monolayer is around 0.34 nm. If the interlayer spacing is 0.34 nm, the van der Waals force between the inner and outer tubes will be zero. In this case, any increase (or decrease) in the interlayer spacing at a point will cause an attractive (or repulsive) van der Waal interaction at that point, and then $c$ should be a positive number. According to the data given in Saito et al. (2001), one can find

$$c = \frac{320 \times 10^{-3}}{0.16 \bar{d}^2} = 9.918667 \frac{10^{14} \text{N}}{\text{m}^2}$$

(19)

where $\bar{d} = 1.63 \times 10^{-10} \text{m}$ is the inter-wall spacing between the tubes.
In view of Eqs. (16) and (18), the pressures exerted on each tube of the double-walled carbon nanotubes are given by

\[ R_1 = \sigma (W_2 - W_1) \quad (20a) \]

\[ R_2 = \frac{R_1}{n_2} (W_2 - W_1) \quad (20b) \]

**CRITICAL BUCKLING CONDITION**

Equation (15) and Eqs. (20a) and (20b) can now be used to express the torsional buckling problem of DWCNT:

For the inner tube

\[ D \frac{\partial^2 W_1}{\partial x^2} + \frac{E_h}{n_1^2} \frac{\partial^4 W_1}{\partial x^4} - \frac{K_1}{n_1^2} \left[ 2N_{xy} \frac{\partial^2 W_1}{\partial x \partial y} \right] = \sigma \left( W_2 - W_1 \right) \quad (21a) \]

For the outer tube

\[ D \frac{\partial^2 W_2}{\partial x^2} + \frac{E_h}{n_2^2} \frac{\partial^4 W_2}{\partial x^4} - \frac{K_2}{n_2^2} \left[ 2N_{xy} \frac{\partial^2 W_2}{\partial x \partial y} \right] = \frac{R_1}{n_2} \left( W_2 - W_1 \right) \quad (21b) \]

where the bending stiffness \( D \) is assumed to be the same for the two tubes having the same effective material constants and thickness. It is clear that the van der Waals interaction makes the Eqs. (21a) and (21b) coupled through the parameter \( c \).

The torque applied to the first tube is denoted by \( M_1 = 2\pi r_1^2 N_{xy1} \), while the torque applied to the 2nd tube is denoted by \( M_2 = 2\pi r_2^2 N_{xy2} \), where

\[ N_{xy1} N_{xy2} = n_1 n_2 \quad (22) \]

Let \( N_{xy} = N_{xy1} \), then

\[ N_{xy2} = \frac{n_2}{n_1} N_{xy} \quad (23) \]

The critical torque given by the continuum shell model is

\[ M = M_1 + M_2 \quad (24) \]
In view of Eqs. (22) and (23), Equations (21a) and (21b) can be rewritten as

\[
D V^2 W_1 - \frac{E k^4}{r_1^2} \frac{\partial^4 W_1}{\partial x^4} - 2 N_{xv} V^4 \left[ \frac{\partial^2 W_1}{\partial x \partial y} \right] = \sigma V^4 W_2 - c V^4 W_1
\]

(25a)

\[
D V^2 W_2 - \frac{E k^4}{r_2^2} \frac{\partial^4 W_2}{\partial x^4} - 2 N_{xv} \frac{r_2}{r_1} V^4 \left[ \frac{\partial^2 W_2}{\partial x \partial y} \right] = \sigma \frac{r_1}{r_2}(V^4 W_2 - V^4 W_1)
\]

(25b)

The torsional buckling mode is assumed to be a periodic, low-amplitude rippling of the shell wall and to take on the following function for simply supported ends:

\[
W_k = f_k \sin \left( \frac{\pi k}{L} \right), \quad k = 1, 2
\]

(26)

The expression indicates that the nanotubes have the buckling modes with sinusoidal wave shape both in the axial and circumferential directions, where \( r_1 \) and \( r_2 \) the radii of the inner and the outer nanotubes, respectively, \( L \) is the length of the nanotube, \( f_k \) the amplitude, \( m \) and \( n \) are the wave numbers in the axial and circumferential directions, respectively. By substituting Eq. (26) into Eqs. (25a) and (25b), one obtains

\[
A \left[ D \left( \frac{(m/n)^4}{r_1^2} + \frac{(m/n)^4}{r_2^2} \right) - 2 N_{xv} \left( \frac{(m/n)^4}{r_1^2} + \frac{(m/n)^4}{r_2^2} \right) + c \left( \frac{(m/n)^4}{r_1^2} + \frac{(m/n)^4}{r_2^2} \right) \right] = f_k \sigma \left( \frac{(m/n)^4}{r_1^2} + \frac{(m/n)^4}{r_2^2} \right)
\]

(27a)

\[
f_k \sigma ^2 (\frac{2(\pi k)^4}{L^2} + (\pi k^2)^4) (\frac{m/n}{L})^4 - 2 N_{xv} \frac{n_2}{n_1} (\frac{m/n}{L})(n/m) + \frac{E h}{r_2^2} (\frac{m/n}{L})^4 = 0
\]

(27b)

Equations (27a) and (27b) may be written in a matrix form as
\[
\begin{bmatrix}
G_{11} & G_{12} \\
G_{21} & G_{22}
\end{bmatrix}
\begin{bmatrix}
\delta_1 \\
\delta_2
\end{bmatrix} = 0
\]  

where

\[
G_{11} = \rho \left[ \left( \frac{M_m}{L} \right)^2 + \left( \frac{n}{L} \right)^2 \right] + \frac{\pi h}{2} \left( \frac{M_m}{L} \right)^2 - 2N_{xy} \left( \frac{M_m}{L} \right)^2 \times \left[ \left( \frac{n}{L} \right)^2 + \left( \frac{n}{L} \right)^2 \right] + \frac{\pi h}{2} \left[ \left( \frac{M_m}{L} \right)^2 + \left( \frac{n}{L} \right)^2 \right],
\]

\[
G_{12} = -\rho \left[ \left( \frac{M_m}{L} \right)^2 + \left( \frac{n}{L} \right)^2 \right], 
\]

\[
G_{21} = -\frac{\pi h}{2} \left[ \left( \frac{M_m}{L} \right)^2 + \left( \frac{n}{L} \right)^2 \right],
\]

\[
G_{22} = \frac{\pi h}{2} \left[ \left( \frac{M_m}{L} \right)^2 + \left( \frac{n}{L} \right)^2 \right].
\]

For non-trivial solutions, the determinant of \([G]\) must vanish, i.e.

\[
\text{det } G = 0
\]

By solving the characteristic Eq. (30) for the lowest value of \(N_{xy}\) with respect to \(m\) and \(n\), one can obtain the critical torque.

**NUMERICAL RESULTS AND CONCLUDING REMARKS**

Various DWCNTs with different outer and inner diameters are considered. For the computation, it is assumed that the Young’s modulus= \(5.735 \times 10^{10}\) Pa, thickness \(h=0.06 \times 10^{-10} m\), and Poisson’s ratio \(\nu=0.2\). The critical torques are computed using both the continuum cylindrical shell model and molecular dynamics simulations. The mode numbers \(m = n = 3\) furnish the lowest torque value. The results are presented in Table 1.

<table>
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<th>Cases</th>
<th>(d_1 \times 10^{-10} m)</th>
<th>(d_2 \times 10^{-10} m)</th>
<th>(L \times 10^{-10} m)</th>
<th>Critical Torque (\times 10^{-17} Nm) (from MD)</th>
<th>Critical Torque (\times 10^{-17} Nm) (from CS)</th>
<th>%age Error</th>
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<td>40.6701</td>
<td>3.6652</td>
<td>3.3125</td>
<td>9.624</td>
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It can be seen from Table 1 that the results obtained using the continuum shell model are on the average about 10% difference from molecular dynamics simulation results. The percentage errors in using the continuum shell model are reasonable given that the computational costs for this model are much lesser as compared to using molecular dynamics simulations. It is worth noting that the difference between using clamped-clamped boundary conditions in molecular dynamics simulation and using simply-supported boundary conditions are negligible. Figure 2 shows the torsional buckling mode of a DWCNT using molecular dynamic simulations (provided by Zhang Yingyan of the Engineering Science Programme, National University of Singapore).

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<td>10.7652</td>
<td>17.539</td>
<td>40.5760</td>
<td>6.8807</td>
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</table>

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**REFERENCES**


