C. R. Mecanique 345 (2017) 158–168

Contents lists available at ScienceDirect

Comptes Rendus Mecanique

www.sciencedirect.com

Prediction of the critical buckling load of multi-walled carbon nanotubes under axial compression

Prédiction de la charge critique de flambage des nanotubes de carbone multi-parois sous compression axiale

Abdelaziz Timesli [a], Bouazza Braikat [b,*], Mohammad Jamal [b], Noureddine Damil [b]

[a] *Département de génie civil et environnement, École nationale des sciences appliquées (ENSA), Université Mohammed-Premier, BP 03, Ajdir Al Hoceima, Morocco*

[b] *Laboratoire d'Ingénierie et Matériaux LIMAT, Faculté des Sciences Ben M'Sik, Université Hassan-II de Casablanca, Sidi Othman, Casablanca, Morocco*

ARTICLE INFO

Article history:
Received 16 November 2016
Accepted after revision 20 December 2016
Available online 6 January 2017

Keywords:
Buckling
Multi-walled carbon nanotubes
Van der Waals interaction
Axial compression
Elastic multiple Donnell shell

Mots-clés :
Flambage
Nanotubes de carbone multi-parois
Interaction de van der Waals
Compression axiale
Coque élastique multiple de Donnell

ABSTRACT

In this paper, we propose a new explicit analytical formula of the critical buckling load of double-walled carbon nanotubes (DWCNT) under axial compression. This formula takes into account van der Waals interactions between adjacent tubes and the effect of terms involving tube radii differences generally neglected in the derived expressions of the critical buckling load published in the literature. The elastic multiple Donnell shells continuum approach is employed for modelling the multi-walled carbon nanotubes. The validation of the proposed formula is made by comparison with a numerical solution. The influence of the neglected terms is also studied.

RÉSUMÉ

Cet article a pour objectif la proposition d'une formule analytique explicite de la charge critique de flambage des nantubes de carbone à double parois (DWCNT) soumis à une compression axiale. Cette formule prend en compte les interactions de van der Waals entre les tubes adjacents et l'influence des rayons, généralement negligée dans les formules donnant la charge critique de flambage publiées dans la littérature. L'approche continue des coques multiples de Donnell est utilisée pour la modélisation des nanotubes de carbone multi-parois. La validation de la formule proposée est faite par une comparaison avec une solution numérique. L'effet des termes négligés a aussi été étudié.

* Corresponding author.
E-mail address: b.braikat@gmail.com (B. Braikat).

http://dx.doi.org/10.1016/j.crme.2016.12.002

1. Introduction

Carbon nanotubes are tubular carbon molecules of diameters of a few tens of nanometers and of a length of several microns. These ultra-fine tubular carbon structures exhibit superior mechanical, electronic and thermal properties and have potential applications in nano-technology and nano-electronics. Since their discovery by Iijima in 1991 [1], carbon nanotubes have led to several innovations in nano-technology and caused profound impacts on almost all existing industries ranging from medicine, agriculture, environment and biotechnology to information technology, aeronautics, and energy. The performance of the new materials based on carbon nanotubes depends essentially on their outstanding mechanical properties.

Several research studies have been conducted to determine these properties in order to better understand their various static and dynamic behaviors such as rupture, vibration, wave propagation, and in particular their buckling behavior.

In view of their high aspect ratio and their very thin hollow cylindrical geometry, buckling of carbon nanotubes has become a very important attractive topic of research in the community of scientists who are interested in studying the instability phenomena of carbon nanotubes.

Buckling analysis of carbon nanotubes, observed in recent works, is performed using two methods: molecular dynamics simulations (classical molecular dynamics tight molecular dynamics and ab initio) and methods based on continuous models of beams, shells and truss of the continuum media mechanics. The applicability of continuum mechanics for analyzing the mechanical behavior of carbon nanotubes (CNTs) has been suggested in 1996 by Yakobson et al. [2]. Since this date, great efforts have been devoted, using the continuum mechanics approaches [3–6], to explore and simulate the buckling instability of single and multi-walled carbon nanotubes. The buckling of carbon nanotubes with single or multi walls axially compressed has been the subject of many works [7–13] based on mono- or multi-Euler–Bernoulli or Timoshenko beams [14] and Donnell or Sanders cylindrical circular-shell elastic continuum models [15–17].

The beam continuum model is valid for slender long CNTs. The buckling in this case is global. However, when the CNTs are short and have large diameters, their buckling is local and their modelling is better using shell continuum approaches. During the last recent years, buckling of double-walled carbon nanotubes (DWCNTs) under axial compression with simply supported ends is intensively studied using Donnell's cylindrical continuum shell model, taking into account van der Walls forces between the layers [7,11,12,18–20].

Analytical formulae for the buckling load of DWCNTs have been derived in the literature. These proposed formulae are based on approximations consisting in neglecting the terms involving the difference between the radii of the inner and outer tubes. Furthermore, the critical buckling load is always obtained numerically [7,11,12,18].

The aim of this paper is to propose a new explicit analytical formula for the critical buckling load of DWCNTs under axial compression for fixed aspect ratios without any assumption on radii tubes. This expression is obtained using Donnell's cylindrical continuum model taking into account the van der Waals interaction. The critical buckling load is derived by an analytical minimization procedure. A comparison with numerical result is performed to validate the proposed formula. The effect of omitting terms on the critical buckling load is also investigated.

2. Basic equations

Thin-shell theories based on continuum mechanics have been successfully applied to predict several mechanical properties of single and multi-walled carbon nanotubes (SWCNTs, DWCNTs). The Donnell elastic shell models have been applied to single-walled and multi-walled carbon nanotubes [7,8,18,19,21–25].

2.1. Donnell's cylindrical elastic shell continuum model

Consider an axially compressed buckling of a single circular cylindrical elastic shell of radius R, thickness h, Young's modulus E and Poisson's ratio ν. The equilibrium equation of the shell is given by [3,4,26–28]:

$$k^2\Delta^2 w-\rho\frac{N_y}{Eh}-\frac{1}{Eh}\left(N_x\frac{\partial^2 w}{\partial x^2}+2N_{xy}\frac{\partial^2 w}{\partial x\partial y}+N_y\frac{\partial^2 w}{\partial y^2}\right)-\frac{p}{Eh}=0 \tag{1}$$

where $k^2=D/Eh$; with $D=Eh^3/12(1-\nu^2)$ is the bending stiffness of the shell, $\rho=1/R$ is the curvature, w is the radial displacement of the middle area, $N_x=K(\epsilon_{xx}+\nu\epsilon_{yy})$ is the axial membrane force, $N_y=K(\epsilon_{yy}+\nu\epsilon_{xx})$ is the circumferential membrane force, $N_{xy}=K(1-\nu)\epsilon_{xy}$ is the shear membrane force, p is the total radial pressure, ϵ_{xx}, ϵ_{yy} and ϵ_{xy} are the strains, x and y denote the axial and circumferential coordinates of the shell respectively, $w(x,y)$ is the radial displacement of the middle surface of the shell along the normal direction, $\Delta^2(.)=\left(\frac{\partial^2(.)}{\partial x^2}+\frac{\partial^2(.)}{\partial y^2}\right)^2$ is the bi-Laplacian operator and $K=Eh/(1-\nu^2)$.

To investigate the possible existence of adjacent equilibrium configurations, we use the adjacent equilibrium criterion [3,29]. We examine the two adjacent configurations represented by the displacements before and after increments, as follows:

$$\begin{cases} u = u_0 + u_b \quad , \quad v = v_0 + v_b \\ w = w_0 + w_b \quad , \quad N_x = N_{x0} + N_{xb} \\ N_y = N_{y0} + N_{yb} \quad , \quad N_{xy} = N_{xy0} + N_{xyb} \\ p = p_0 + p_b \end{cases} \tag{2}$$

where the index 0 indicates the pre-buckling quantities and the index b indicates those of post-buckling. The pre-buckling solution $(u_0, v_0, w_0, N_{x0}, N_{y0}, N_{xy0})$ verifies the following equation [29–33]:

$$k^2\Delta^2 w_0 - \rho\frac{N_{y0}}{Eh} - \frac{1}{Eh}\left(N_{x0}\frac{\partial^2 w_0}{\partial x^2} + 2N_{xy0}\frac{\partial^2 w_0}{\partial x\partial y} + N_{y0}\frac{\partial^2 w_0}{\partial y^2}\right) - \frac{p_0}{Eh} = 0 \tag{3}$$

We remark that $(w_0 = 0, N_{y0} = -p_0/\rho)$ is a solution to Eq. (3). According to the shell theory, the membrane forces N_{xb}, N_{yb} and N_{xyb} are connected to the stress function Φ by the following relations [29]:

$$\begin{cases} N_{xb} = Eh\dfrac{\partial^2\Phi}{\partial y^2} \\ N_{yb} = Eh\dfrac{\partial^2\Phi}{\partial x^2} \\ N_{xyb} = -Eh\dfrac{\partial^2\Phi}{\partial x\partial y} \end{cases} \tag{4}$$

Inserting Eqs. (2) and (4) in Eq. (1) and neglecting the terms of second order in index b, we obtain the following equation:

$$k^2\Delta^2 w_b - \rho\frac{\partial^2\Phi}{\partial x^2} - \frac{1}{Eh}\left(N_{x0}\frac{\partial^2 w_b}{\partial x^2} + 2N_{xy0}\frac{\partial^2 w_b}{\partial x\partial y} + N_{y0}\frac{\partial^2 w_b}{\partial y^2}\right) - \frac{p_b}{Eh} = 0 \tag{5}$$

The stress function $\Phi(x, y)$ verifies the following compatibility condition [29]:

$$\Delta^2\Phi + \rho\frac{\partial^2 w_b}{\partial x^2} = 0 \tag{6}$$

If the shear membrane forces are neglected $(N_{xy0} = 0)$, the equations (5) and (6) are reduced to:

$$\begin{cases} k^2\Delta^2 w_b - \rho\dfrac{\partial^2\Phi}{\partial x^2} - \dfrac{N_{x0}}{Eh}\dfrac{\partial^2 w_b}{\partial y^2} - \dfrac{N_{y0}}{Eh}\dfrac{\partial^2 w_b}{\partial y^2} - \dfrac{p_b}{Eh} = 0 \\ \Delta^2\Phi + \rho\dfrac{\partial^2 w_b}{\partial x^2} = 0 \end{cases} \tag{7}$$

As $N_{x0} = P$, P is the axial compression and denoting by $F = N_{y0}$ the circumferential membrane force, the system (7) giving the Donnell equations becomes:

$$\begin{cases} k^2\Delta^2 w_b - \rho\dfrac{\partial^2\Phi}{\partial x^2} - \lambda\dfrac{\partial^2 w_b}{\partial y^2} - \dfrac{F}{Eh}\dfrac{\partial^2 w_b}{\partial y^2} - \dfrac{p_b}{Eh} = 0 \\ \Delta^2\Phi + \rho\dfrac{\partial^2 w_b}{\partial x^2} = 0 \end{cases} \tag{8}$$

where $\lambda = P/Eh$ is the load parameter.

2.2. Donnell's multiple-shell continuum model

Consider a multi-walled carbon nanotubes (MWCNT), consisting of N tubes of radius R_j $(j = 1, \ldots, N)$, length L, same thickness h, Young's modulus E, Poisson's ratio ν, subjected to an axial compression P. The walls of adjacent tubes interact through van der Waals forces as shown in Fig. 1. The modelling of MWCNT is performed by the use of continuum Donnell concentric multi-shells. Each tube j $(j = 1, \ldots, N)$ is modeled by an elastic homogeneous and isotropic circular cylindrical shell of length L, thickness h, radius R_j, Young's modulus E, and Poisson's ratio ν, coupled by van der Waals interaction. Let us note by $u_i(x,\theta)$, $v_i(x,\theta)$ and $w_i(x,\theta)$ the components of the displacement vector, x the axial coordinate and θ the

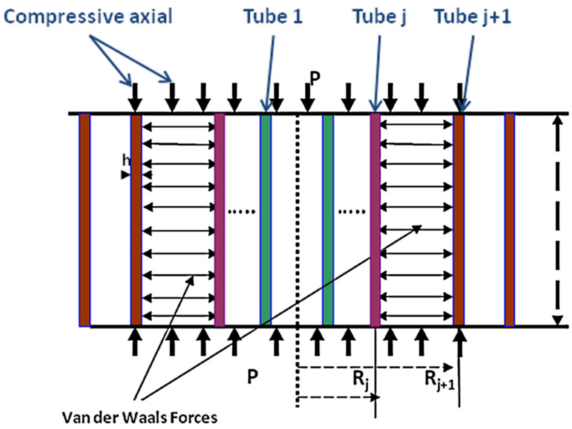


Fig. 1. Multi-Walled Carbone NanoTubes (MWCNT) under axial compression.

circumferential coordinate. Within Donnell's theory and if the pre-buckling rotations are neglected, the transverse displacements $w_i(x,\theta)$ and the corresponding additional stress functions $\Phi_j(x,\theta)$ of MWCNT are solutions to the following $2N$ coupled linear equations system [2,13,21].

$$\begin{cases} k^2\Delta_j^2 w_j - \lambda\dfrac{\partial^2 w_j}{\partial x^2} - \rho_j\dfrac{\partial^2\phi_j}{\partial x^2} - \dfrac{F_j^{\text{vdw}}}{Eh} = 0 \\ \Delta_j^2\phi_j + \rho_j\dfrac{\partial^2 w_j}{\partial x^2} = 0 \end{cases} \quad j = 1,\ldots,N \tag{9}$$

where $\rho_j = \frac{1}{R_j}$ is the curvature of jth tube, $\Delta_j^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{1}{R_j^2}\frac{\partial^2}{\partial\theta^2}\right)^2$ is the bi-Laplacian operator, ϕ_j is the stress function of jth tube. The van der Waals force F_j^{vdw} is expressed by:

$$F_j^{\text{vdw}} = \frac{F_j}{R_j^2}\frac{\partial^2 w_j}{\partial\theta^2} - p_j \tag{10}$$

with F_j are the forces by length unit in the circumferential direction of jth tube prior buckling and p_j is the pressure due to van der Waals interaction between layers of MWCNT given by [13]:

$$p_j = w_j\sum_{k=1}^{N} c_{jk} - \sum_{k=1}^{N} c_{jk}w_k \tag{11}$$

The van der Waals coefficients c_{jk} are given by He et al. [13]:

$$c_{jk} = -\left[\frac{1001\pi\epsilon\sigma^{12}}{3a^4}E_{jk}^{13} - \frac{1120\pi\epsilon\sigma^6}{9a^4}E_{jk}^{7}\right]R_k \tag{12}$$

where the coefficient a is the C–C bond, ϵ is the depth of Lennard–Jones potential, σ is a parameter being determined by the equilibrium distance [34] and E_{jk}^m is the elliptic integrals expressed as:

$$E_{jk}^s = \frac{1}{(R_j+R_k)^s}\int_0^{\frac{\pi}{2}}\frac{\mathrm{d}\theta}{(1-K_{jk}\cos^2(\theta))^{s/2}}R_k \tag{13}$$

with s is an integer and $K_{jk} = \frac{4R_jR_k}{(R_j+R_k)^2}$.

Using the cylindrical coordinates (x,θ) with $y = R_j\theta$ and taking into account Eqs. (10) and (11), the system (9) can be written in the following form:

$$\begin{cases} k^2\Delta_j^2 w_j + \lambda\dfrac{\partial^2 w_j}{\partial x^2} - \dfrac{1}{Eh}\left(\dfrac{F_j}{R_j^2}\dfrac{\partial^2 w_j}{\partial\theta^2} - \left(w_j\displaystyle\sum_{k=1}^{N} c_{jk} - \sum_{k=1}^{N} c_{jk}w_k\right)\right) = 0 \\ \Delta_j^2\phi_j + \rho_j\dfrac{\partial^2 w_j}{\partial x^2} = 0 \end{cases} \quad j = 1,\ldots,N \tag{14}$$

The solution to the problem (14) is sought in the following form [6,30,31,33,35,36]:

$$\begin{cases} w_j(x,\theta) = A_j \exp(\mathrm{i}\dfrac{m\pi}{L}x)\cos(n\theta) + cc \\ \phi_j(x,\theta) = D_j \exp(\mathrm{i}\dfrac{m\pi}{L}x)\cos(n\theta) + cc \end{cases} \quad j = 1, \ldots, N \tag{15}$$

where m and n are respectively the axial and circumferential half wavenumbers of the jth tube, A_j and D_j are arbitrary complex constants and cc denotes the complex conjugate. The expression (15) indicates that the carbon nanotubes have buckling modes with sinusoidal wave pattern both in the axial and circumferential directions. The substitution of (15) into (14) leads to the following equations:

$$\begin{cases} k^2\left(p^2+q_j^2\right)^2 A_j - \lambda p^2 A_j + \rho_j p^2 D_j - \dfrac{1}{Eh}\left(-q_j^2 F_j A_j + A_j \displaystyle\sum_{k=1}^{N} c_{jk} A_k\right) = 0 \\ \left(p^2+q_j^2\right)^2 D_j - \rho_j p^2 A_j = 0 \end{cases} \quad j = 1, \ldots, N \tag{16}$$

The second equation of (16) gives:

$$D_j = \frac{\rho_j p^2}{\left(p^2+q_j^2\right)^2} A_j \tag{17}$$

where p and q_j are defined by:

$$p = \frac{m\pi}{L}, \quad q_j = \frac{n}{R_j}, \quad j = 1, \ldots, N \tag{18}$$

By inserting equation (17) into first equation of equation (16), we obtain the following homogeneous matrix system:

$$\left(k^2[B]p^4 - \lambda[I]p^2 + [R] + \frac{1}{Eh}[C]\right)\begin{Bmatrix} A_1 \\ A_2 \\ \cdot \\ \cdot \\ \cdot \\ A_N \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{Bmatrix} \tag{19}$$

where $[I]$ is the unit matrix, the matrices $[B]$, $[R]$ and $[C]$ are defined by:

$$\begin{cases} B_{ij} = \left(1+\beta_i^2\right)^2 \delta_i^j \\ R_{ij} = \left(1+\beta_i^2\right)^2 \delta_i^j \\ C_{ij} = -c_{ij} + \left[F_i q_i^2 + \sum_{k\neq i}^{N} c_{ik}\right]\delta_{ij} \end{cases} \quad i, j = 1, 2, 3, \ldots, N \tag{20}$$

with δ_{ij} is a Kronecker symbol and the coefficients β_j $(j = 1, \ldots, N)$ are the aspect ratios defined by:

$$\beta_j = \frac{nL}{m\pi R_j} \tag{21}$$

The equation (21) allows us to write $\beta_{j+1} = \left(R_j/R_{j+1}\right)\beta_j$. The coupled system of N equations (19) and N unknowns $(A1, A2, \ldots, A_N)$ has a nonzero solution if and only if:

$$\det\left(k^2[B]p^4 - \lambda[I]p^2 + [R] + \frac{1}{Eh}[C]\right) = 0 \tag{22}$$

The expression of the determinant (22) is a polynomial of degree N in λ. Its resolution gives the buckling loads λ and the smallest value is the critical buckling load noted by λ_{cr}.

The next section is devoted to derivation of an explicit analytical expression of the critical buckling load λ_{cr} of a double-walled carbon nanotube (DWCNT) in terms of its mechanical and geometrical characteristics.

3. Buckling analysis of double-walled carbon nanotubes (DWCNTs)

3.1. Buckling load λ

In the case of a double-walled carbon nanotube (DWCNT) ($N=2$), the expression of the buckling loads λ as a function of β_1, β_2, ρ_1, ρ_2, c_{12} and c_{21} is easily deduced from the characteristic equation (22) and can be written as follows:

$$\lambda = \frac{1}{2p^2}\left((\alpha_1+\alpha_2) \pm \sqrt{(\alpha_1-\alpha_2)^2 + \frac{4c_{12}c_{21}}{(Eh)^2}}\right) \tag{23}$$

where α_1 and α_2 are given by:

$$\begin{cases} \alpha_1 = k^2\left(1+\beta_1^2\right)^2 p^4 - \dfrac{\beta_1^2 F_1}{Eh}p^2 + \dfrac{\rho_1^2}{\left(1+\beta_1^2\right)^2} - \dfrac{c_{12}}{Eh} \\ \alpha_2 = k^2\left(1+\beta_2^2\right)^2 p^4 - \dfrac{\beta_2^2 F_2}{Eh}p^2 + \dfrac{\rho_2^2}{\left(1+\beta_2^2\right)^2} - \dfrac{c_{21}}{Eh} \end{cases} \tag{24}$$

The smallest value of the buckling loads λ in (23) is obtained by taking the negative sign in the expression (23) because of the following relation:

$$\left((\alpha_1+\alpha_2) - \sqrt{(\alpha_1-\alpha_2)^2 + \frac{4c_{12}c_{21}}{(Eh)^2}}\right) > 0 \tag{25}$$

and in view of the relations

$$\alpha_1 > -\frac{c_{12}}{Eh}\ , \ \alpha_2 > -\frac{c_{21}}{Eh} \tag{26}$$

where

$$c_{12} < 0\ ,\ c_{21} < 0\ ,\ (\alpha_1+\alpha_2)^2 - (\alpha_1-\alpha_2)^2 = 4\alpha_1\alpha_2 > \frac{4c_{12}c_{21}}{(Eh)^2} \tag{27}$$

Let us note that the most formulae published in the literature [8,9] are simplified expressions. They are derived by assuming all terms involving the ratio $(R_2-R_1)/R_1$ are very small and they are neglected in the expression (30). Let us introduce a set of coefficients a_i $(i=1,\dots,10)$ defined by:

$$\begin{cases} a_1 = k^2\left(\left(1+\beta_1^2\right)^2 + \left(1+\beta_2^2\right)^2\right)\ ,\ a_2 = \dfrac{\rho_1^2}{\left(1+\beta_1^2\right)^2} + \dfrac{\rho_2^2}{\left(1+\beta_2^2\right)^2} - \dfrac{c_{12}+c_{21}}{Eh} \\ a_3 = k^2\left(\left(1+\beta_1^2\right)^2 - \left(1+\beta_2^2\right)^2\right)\ ,\ a_4 = \dfrac{\rho_1^2}{\left(1+\beta_1^2\right)^2} - \dfrac{\rho_2^2}{\left(1+\beta_2^2\right)^2} - \dfrac{c_{12}-c_{21}}{Eh} \\ a_5 = 2\,a_3\,a_4 + a_8^2 \qquad ,\ a_6 = a_4^2 + \dfrac{4\,c_{12}\,c_{21}}{(Eh)^2} \\ a_7 = \dfrac{1}{Eh}\left(\beta_1^2F_1 + \beta_2^2F_2\right) \qquad ,\ a_8 = \dfrac{1}{Eh}\left(\beta_1^2F_1 - \beta_2^2F_2\right) \\ a_9 = 2\,a_3\,a_8 \qquad ,\ a_{10} = 2\,a_4\,a_8 \end{cases} \tag{28}$$

We remark that $\beta_1 = \frac{n}{pR_1}$ and $\beta_2 = \frac{n}{pR_2}$ then $\beta_1^2F_1 = \left(\frac{n}{p}\right)^2\left(\frac{F_1}{R_1}\right)^2$ and $\beta_2^2F_2 = \left(\frac{n}{p}\right)^2\left(\frac{F_2}{R_2}\right)^2$. As $\left(\frac{F_1}{R_1}\right)^2 = \left(\frac{F_2}{R_2}\right)^2 = \text{constant}$, then:

$$\begin{cases} a_7 = \dfrac{2}{Eh}\beta_1^2F_1\ ,\ a_5 = 2a_3a_4 \\ a_8 = 0 \qquad ,\ a_9 = 0 \\ a_{10} = 0 \end{cases} \tag{29}$$

Taking into account the definition of the coefficients in (29) and the fact of $\beta_1^2 F_1 = \beta_2^2 F_2$ (see [13]), we can write the expression of the buckling loads (23) in terms of the axial wave number p as follows:

$$\lambda = \frac{1}{2p^2}\left(a_1 p^4 + a_2 - \sqrt{(a_3^2 p^8 + a_5 p^4 + a_6)}\right) + \frac{a_7}{2} \tag{30}$$

We can also rewrite the expression (23) according to m and n ($\lambda = \lambda(m, n)$). Let us note that the critical buckling load is generally determined by searching numerically the values of m and n, which gives the minimal value of the critical load λ as in [8,13]. We propose in the next section an explicit analytical expression of the critical buckling load for fixed aspect ratio β_1 and β_2 using a theoretical minimization with respect to axial number wave p. In this study, we consider that the buckling load is given according to β_1, β_2 and p ($\lambda = \lambda(\beta_1, \beta_2, p)$). A comparison of the obtained analytical solution with the numerical solution computed by the minimization procedure with respect to integer numbers m and n will be also presented.

3.2. Determination of the critical buckling load of the double-walled carbon nanotubes

The critical buckling load λ_{cr} is obtained by minimizing the expression of the buckling loads $\lambda(\beta_1, \beta_2, p)$ given by the equation (30) with respect to the axial wave number p for fixed aspect ratio β_1 and β_2:

$$\frac{\partial \lambda(\beta_1, \beta_2, p)}{\partial p}\Big|_{\beta_1 \text{ or } \beta_2 \text{fixed}} = 0 \tag{31}$$

Equation (31) leads to the following polynomial of degree 16 in p, that we can rewrite in the form of a polynomial of degree 4 in Λ by putting $\Lambda = p^4$:

$$b_4\Lambda^4 + b_3\Lambda^3 + b_2\Lambda^2 + b_1\Lambda + b_0 = 0 \tag{32}$$

where the coefficients b_i $(i = 0, 1, 2, 3, 4)$ are given by:

$$\begin{cases} b_0 = a_6(a_2^2 - a_6) \quad , \; b_1 = a_2^2 a_5 - 2a_1 a_2 a_6 \\ b_2 = a_2^2 a_3^2 - 2a_1 a_2 a_5 + a_1^2 a_6 + 2a_3^2 a_6 \; , \; b_3 = a_1^2 a_5 - 2a_1 a_2 a_3^2 \\ b_4 = a_1^2 a_3^2 - a_3^4 \end{cases} \tag{33}$$

To access the critical buckling load of a double-walled carbon nanotube, we must find the roots of the polynomial (32). The only real root of equation (32) (more details are given in the appendix) is given by:

$$p_{cr} = \left(\frac{B}{2(u - A)} - \frac{b_3}{4b_4}\right)^{\frac{1}{4}} \tag{34}$$

where

$$A = -\frac{3}{8}\frac{b_3^2}{b_4^2} + \frac{b_2}{b_4} \;,\; B = \frac{1}{8}\frac{b_3^3}{b_4^3} - \frac{1}{2}\frac{b_2 b_3}{b_4^2} + \frac{b_1}{b_4} \;,\; u = \frac{A}{3} + \sqrt[3]{-\frac{D_0}{2} + \sqrt{\frac{D_0^2}{4} + \frac{D_1^3}{27}}} + \sqrt[3]{-\frac{D_0}{2} - \sqrt{\frac{D_0^2}{4} + \frac{D_1^3}{27}}} \tag{35}$$

with

$$D_0 = -\frac{2}{27}A^3 + \frac{3}{8}AC - B^2 \;,\; D_1 = -\left(\frac{A^2}{3} + 4C\right) \;,\; C = -\frac{3}{256}\frac{b_3^4}{b_4^4} + \frac{b_2 b_3^2}{16 b_4^3} - \frac{b_1 b_3}{4b_4^2} + \frac{b_0}{b_4} \tag{36}$$

Finally the proposed critical buckling load λ_{cr} of double-walled carbon nanotubes (DWCNT), taking into account van der Waals interactions is expressed by the following explicit analytical formula:

$$\lambda_{cr} = \lambda(p = p_{cr}) = \frac{1}{2p_{cr}^2}\left(a_1 p_{cr}^4 + a_2 - \sqrt{(a_3^2 p_{cr}^8 + a_5 p_{cr}^4 + a_6)}\right) + \frac{a_7}{2} \tag{37}$$

where the axial wave number p_{cr} is given by Eq. (34).

To our knowledge, there is no explicit analytical formula of the form (37) in the literature. Furthermore, this expression has been obtained without the assumption on the radius of tubes, that is to say the terms containing $(R_2 - R_1)/R_1$ are not neglected in the formula (37). This approximation ($R_1 \approx R_2$) has been adopted in [7] by assuming that these terms are small and their effects are negligible.

Let us note that the most formulae published in the literature [8,13] are simplified expressions. They are derived by assuming that all terms involving the ratio $\frac{R_1 - R_2}{R_1}$ are very small and that they are neglected in the expression (30). This

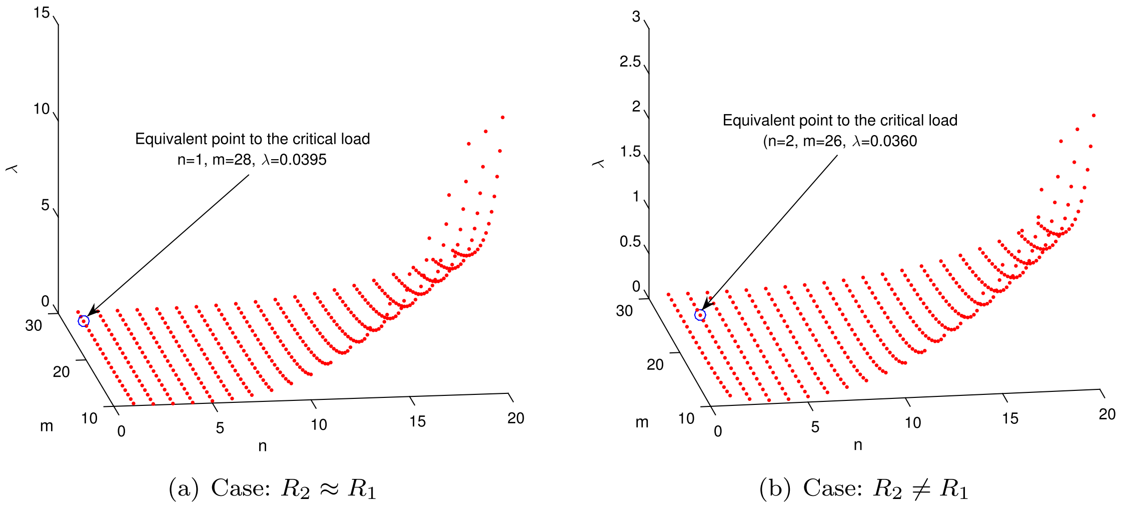


Fig. 2. Buckling loads λ versus (m, n) for equal and different radii.

simplification is based by assuming $\rho_1 = \rho_2$. As a consequence, we have $q_1 = q_2$, $\beta_1 = \beta_2$ and $F_1 = F_2$. Adopting this simplification, the expressions of coefficients a_i $(i = 1, ..., 7)$ given by (28) are reduced to:

$$\begin{cases} a_1 = 2k^2 \left(1 + \beta_1^2\right)^2 & , \; a_2 = 2\dfrac{\rho_1^2}{\left(1 + \beta_1^2\right)^2} - \dfrac{c_{12} + c_{21}}{Eh} \\ a_3 = 0 & , \; a_4 = -\dfrac{c_{12} - c_{21}}{Eh} \\ a_5 = 0 & , \; a_6 = \left(\dfrac{c_{12} + c_{21}}{Eh}\right)^2 \\ a_7 = \dfrac{-\beta_1^2 F_1}{Eh} \end{cases} \tag{38}$$

Inserting (38) in (30) gives the following simplified expression:

$$\lambda = \frac{1}{2p^2}\left(a_1 p^4 + a_2 - \sqrt{a_6}\right) + \frac{a_7}{2} \tag{39}$$

which is identical to the expression given by the formula given in [13], when the forces in the circumferential direction $p_1 = -\frac{N_\theta}{R_1}$ and $p_2 = -\frac{N_\theta}{R_2}$ prior to buckling are equal to zero and putting $\rho_1 = \rho_2 = \frac{1}{R_2}$, $p = \frac{m\pi}{L}$, $q_1 = q_2 = \frac{n}{R_2}$, $\beta_1 = \beta_2 = \frac{q_2}{p}$.

The analytical minimization of (39) gives the following critical buckling load:

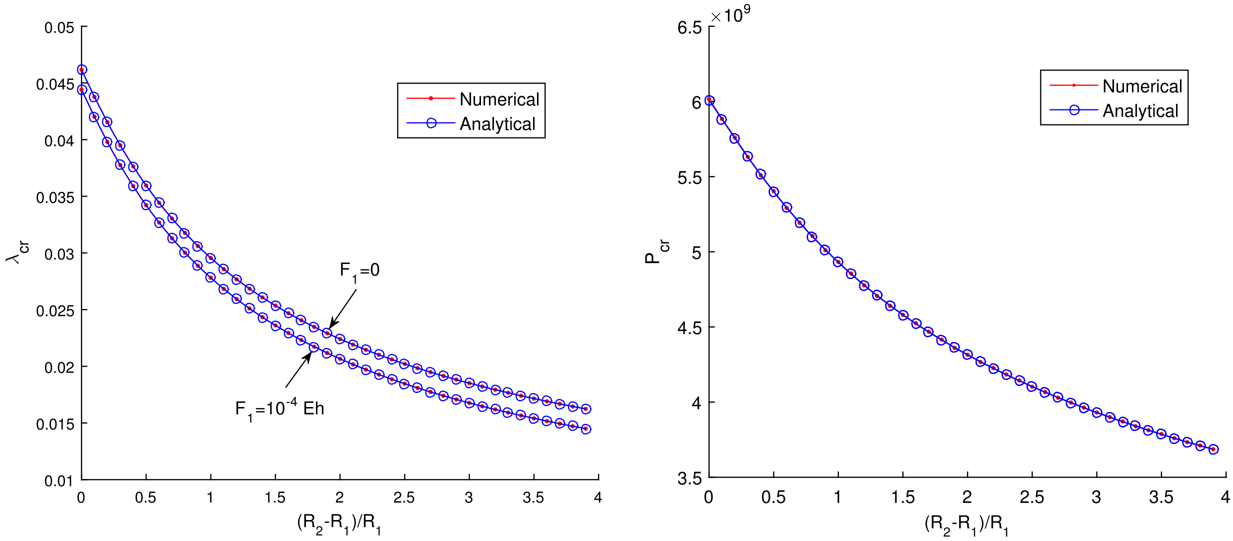
$$\lambda_{\text{cr}} = \sqrt{a_1\left(a_2 - \sqrt{a_6}\right)} + \frac{a_7}{2} \tag{40}$$

where a_1, a_2, a_6 and a_7 are given by (38). This expression (40) is a particular case of the proposed formula (37) in this work.

4. Numerical comparison and discussion

Numerical results are presented in this section for validating the proposed analytical expression of the critical buckling load of double-walled carbon nanotubes (DWCNT) under axial compression. We adopt the same data used in [37]. The considered experimental values of tubes radii R_1 and R_2 are: $0.45\text{ nm} \le R_1 \le 1\text{ nm}$, $1.5\text{ nm} \le R_2 \le 5.4\text{ nm}$. In numerical tests, we choose the following numerical values: $R_1 = 1$ nm, $R_2 = 1.5$ nm, $L/R_2 = 10$, $E = 1.7$ TPa, $\nu = 0.34$, $h = 0.075$ nm, $c_{12} = -9.9187 \times 10^{19}$ N/m^3, $c_{21} = (R_1/R_2)c_{12}$, $F_1 = 0$ and for F_1 different from zero. The numerical validation consists in comparing the obtained result by minimization of the expression (30) with the new analytical formula given by the equation (37).

The buckling loads $\lambda(m, n)$, given by Eq. (30), are plotted in Fig. 2 versus the half wave numbers (m, n) in the axial and circumferential directions. Fig. 2a illustrates the case used in [7,38], and we represent in Fig. 2b the buckling loads for R_1



(a) Comparison between the analytical formula and numerical result of the critical buckling loads

(b) Comparison between the analytical formula and numerical result of wave number p_{cr} in axial direction

Fig. 3. Numerical and analytical solution versus the ratio $(R_2 - R_1)/R_1$.

different from R_2. The critical buckling load λ_{cr} is obtained by searching numerically the minimal value of the buckling loads $\lambda(m, n)$ given by Eq. (30).

These results show that the approximate formula given in Ru [8], in which the terms involving the ratio $(R_2 - R_1)/R_1$ are omitted, gives a higher critical buckling load.

To validate the proposed formula of the critical buckling load for fixed values of aspect ratios β_1 and β_2, we consider the values of aspect ratios given by $\beta_1 = 0.37$ and $\beta_2 = 0.24$. These values are equivalent to the critical values $(m = 26, n = 2)$ of the numerical test as shown in Fig. 2b.

The analytical solution $\lambda_{cr} = 0.036$ of critical buckling loads obtained by using formula (37) is equal to the minimal value of the buckling load of the curve given by solving numerically the equation (30) as shown in Fig. 2. On the other hand, the numerical and analytical half wave numbers m in axial direction are equal to 26. Consequently, this result validates the proposed analytical formula for double-walled carbon nanotubes (DWCNT).

In Fig. 3a, we give the critical buckling load of double-walled carbon nanotubes (DWCNT) estimated numerically using Eq. (30) and that analytically computed by the proposed formula (37) versus the ratio $(R_2 - R_1)/R_1$. It is clear that the critical load decreases for increasing values of the ratio $(R_2 - R_1)/R_1$. In addition, when the force by length unit F_1 in the circumferential direction is considered ($F_1 \neq 0$), the Donnell cylindrical circular shell elastic continuum models give small values for the critical buckling load. Fig. 3b presents the wave number p_{cr} in the axial direction versus the ratio; the wave number p_{cr} and the axial half wavenumbers m are not affected by the force F_1. One observe that, in the cylindrical Donnell shell models where $L >> R_2$, the forces by length unit in the circumferential direction are affected in their directions. Figs. 3a and 3b show that the two solutions obtained numerically and by the proposed formula are in good agreement. According to experimental data [24], the smallest experimental value of the ratio $(R_2 - R_1)/R_1$ is equal to 0.5, then the approximation $(R_2 - R_1)/R_1 \approx 0$ is not reasonable.

In the following, we will analyze the critical buckling load parameter λ_{cr} under the effect of aspect ratio β_1 for three values of the force F_1 ($F_1 = 0$, $10^{-5} \times Eh$, $2.10^{-5} \times Eh$). In Fig. 4, the analytical formula of the critical buckling load parameter λ_{cr} is given for various forces versus the aspect ratio β_1 compared to the numerical critical buckling load parameter. It is seen that critical load buckling presents a minimum for $F_1 = 0$, $10^{-5} \times Eh$ and decreases monotonically from $F_1 = 2.10^{-5} \times Eh$. The comparison of the proposed analytical formula (37) and of the minimized expression (30) varying the aspect ratio β_1 for various values of F_1 is depicted in Fig. 4. It is important to note that for the three distinct forces and for a fixed β_1, we obtain the same values of critical buckling loads. This plot shows that there is a certain value F of the force F_1 such that for all force less than F, the critical buckling load in term of aspect ratio presents a minimum and increases from this aspect ratio corresponding to this minimum. Beyond this value, the critical buckling load decreases with increasing the aspect ratio.

5. Conclusion

An exact explicit analytical formula of the critical buckling load of double-walled carbon nanotubes (DWCNTs) under axial compression for fixed values of the aspect ratio has been established without any assumption on tube radii. The derivation

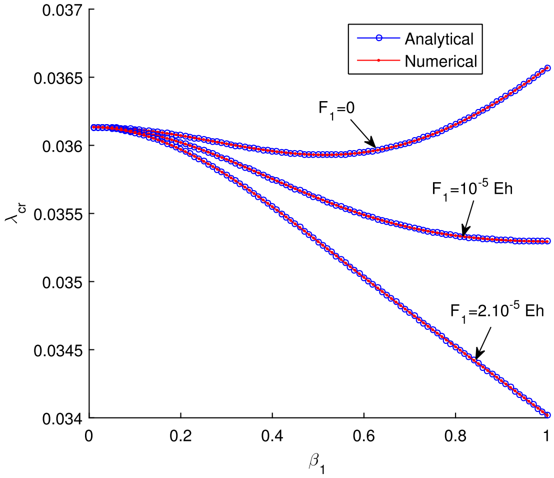


Fig. 4. Comparison between the analytical formula and the numerical calculation of the critical buckling load λ_{cr} versus the aspect ratio β_1 for $F_1 = 0$, $10^{-5} \times Eh$, $2.10^{-5} \times Eh$.

of the formula is performed by using the elastic circular cylindrical shell Donnell model. This proposed expression permits to recover the results published in the literature. In addition, it shows that the omission of tubes radii difference leads to an overestimation of the critical buckling load and to erroneous buckling modes. These terms have a significant effect on the critical buckling load and must be taken into account for its realistic prediction. This approximation is legitimate if the ratio $(R_2 - R_1)/R_1$ is very small.

Appendix A

Let us search the solution to (32), first we eliminate the term in $\wedge^3$ by introducing the following change of variable:

$$\wedge = x - \frac{b_3}{4b_4} \tag{41}$$

Inserting (41) into (32), we get:

$$x^4 + Ax^2 + Bx + C = 0 \tag{42}$$

where A, B and C are defined by Eqs. (35) and (36). We transform the polynomial of degree 4 in a polynomial of degree 3 by introducing an auxiliary variable u such that:

$$\left(x + \frac{u}{2}\right)^2 = (u - A)x^2 - Bx + \left(\frac{u^2}{4} - C\right) \tag{43}$$

with $u \neq A$. Let us note that the polynomial (43) is equivalent to (42). Imposing that the discriminant of the right-hand side of (43) is zero and putting:

$$u = v + \frac{A}{3} \tag{44}$$

we obtain:

$$u^3 + D_1 v + D_0 = 0 \tag{45}$$

where D_0 and D_1 are defined by Eq. (36). Equation (45) is a polynomial of an odd degree, then it has at least a real root. Its root is obtained using Cardan's formulae. For $4D_1^3 + 27D_0^2 > 0$, it is given by:

$$v_{cr} = \sqrt{3} - \frac{D_0}{2} + \sqrt{\frac{D_0^2}{4} + \frac{D_1^3}{27}} + \sqrt{3} - \frac{D_0}{2} - \sqrt{\frac{D_0^2}{4} + \frac{D_1^3}{27}} \tag{46}$$

The equation (44) gives:

$$u_{cr} = v_{cr} + \frac{A}{3} \tag{47}$$

Taking into account Eq. (41) and $\wedge = p^4$, we get Eq. (32). The local critical buckling load λ_{cr} (40) of the double-walled carbon nanotubes is obtained using Eqs. (30) and (34).

References

[1] S. Iijima, Helical microtubes of graphitic carbon, Nature 354 (6348) (1991) 56–58.
[2] B.I. Yakobson, C.J. Brabec, J. Bernholc, Nanomechanics of carbon tubes: instabilities beyond linear response, Phys. Rev. Lett. 76 (14) (1996) 2511–2514.
[3] W.T. Koiter, On the stability of elastic equilibrium, Ph.D. thesis, English translation, NASA Technology Transfer Programme, 1945.
[4] N. Yamaki, Elastic Stability of Circular Cylindrical Shells, North-Holland, Amsterdam, 1984.
[5] W.T. Koiter, The effect of axisymmetric imperfections on the buckling of cylindrical shells under axial compression, Proc. K. Ned. Akad. Wet., Ser. B, Phys. Sci. 66 (1963) 265–279.
[6] G.W. Hunt, N. Lucena, Localized buckling in long axially loaded cylindrical shells, J. Mech. Phys. Solids 39 (7) (1991) 770–783.
[7] C.Q. Ru, Effective bending stiffness of carbon nanotubes, Phys. Rev. B 62 (15) (2000) 9973–9976.
[8] C.Q. Ru, Effect of van der Waals forces on axial buckling of a double-walled carbon nanotube, J. Appl. Phys. 87 (10) (2000) 7227–7231.
[9] L. Sudak, Column buckling of multiwalled carbon nanotubes using nonlocal continuum mechanics, J. Appl. Phys. 94 (11) (2003) 7281–7287.
[10] C.Y. Wang, C.Q. Ru, A. Mioduchowski, Axially compressed buckling of pressured multiwall carbon nanotubes, Int. J. Solids Struct. 40 (15) (2003) 3893–3911.
[11] J.T. Feng, K.Y. Xu, C.Q. Ru, Curvature effect of interlayer van der Waals forces on axial buckling of a double-walled carbon nanotubes, Int. J. Struct. Stab. Dyn. 4 (2004) 515–526.
[12] Y.Q. Zhang, G.R. Liu, J.S. Wang, Small-scale effects on buckling of multiwalled carbon nanotubes under axial compression, Phys. Rev. B 70 (20) (2004) 2054301.
[13] X.Q. He, S. Kitipornchai, K.M. Liew, Buckling analysis of multi-walled carbon nanotubes: a continuum model accounting for van der Waals interaction, J. Mech. Phys. Solids 53 (2) (2005) 303–326.
[14] T. Natsuki, Q.Q. Ni, M. Endo, Stability analysis of double-walled carbon nanotubes as afm probes based on a continuum model, Carbon 49 (2011) 2532–2537.
[15] A.R. Ranjbartoreh, G.X. Wang, A. GhorbanpourArani, A. Loghman, Comparative consideration of axial stability of single and double-walled carbon nanotube and its inner and outer tubes, Physica E 41 (2008) 202–208.
[16] T. Natsuki, T. Tsuchiya, Q.Q. Ni, M. Endo, Torsional elastic instability of double-walled carbon nanotubes, Carbon 48 (15) (2010) 4362–4368.
[17] J. Wu, Q. Cheng, B. Liu, Y.W. Zhang, W.B. Lu, K.C. Hwang, Study on the axial compression buckling behaviors of concentric multi-walled cylindrical shells filled with soft materials, J. Mech. Phys. Solids 60 (2012) 803–826.
[18] C.Q. Ru, Degraded axial buckling strain of multiwalled carbon nanotubes due to interlayer slips, J. Appl. Phys. 89 (6) (2001) 3426–3433.
[19] C.Q. Ru, Axially compressed buckling of a double-walled carbon nanotube embedded in an elastic medium, J. Mech. Phys. Solids 49 (6) (2001) 1265–1279.
[20] C.Q. Ru, Elastic models for carbon nanotubes, in: H.S. Nalwa (Ed.), Encyclopedia of Nanoscience and Nanotechnology, vol. 2, American Scientific, Stevenson Ranch, CA, USA, 2004, pp. 731–744.
[21] E.W. Wong, P.E. Sheehan, C.M. Lieber, Nanobeam mechanics elasticity, strength, and toughness of nanorods and nanotubes, Science 277 (1977) 1971–1975.
[22] B.I. Yacobson, C.J. Brabec, J. Bernhole, Nanomechanics of carbon nanotubes: instabilities beyond linear response, Phys. Rev. Lett. 76 (1996) 2511–2514.
[23] M.M.J. Treacy, T. Ebbesen, J.M. Gibson, Exceptionally high Young's modulus observed for individual carbon nanotubes, Nature 381 (1996) 678–680.
[24] M.R. Falvo, G.J. Clary, R.M. Taylor, V. Chi, F.P. Brooks, S. Washburn, R. Superfine, Bending and buckling of carbon nanotubes under large strain, Nature 389 (1997) 582–584.
[25] P. Poncharal, Z.L. Wang, D. Ugarte, W.A. De Heer, Electrostatic deflexions and electromechanical resonances of carbon nanotubes, Science 283 (1999) 1513–1516.
[26] L.H. Donnell, A new theory of the buckling of thin cylindrical shells under compression and bending, ASME Trans. 56 (1934) 795–806.
[27] S.P. Timoshenko, J.M. Gere, Theory of Elastic Stability, McGraw-Hill, New York, 1961.
[28] C. Calladine, Theory of Shell Structures, Cambridge University Press, Cambridge, UK, 1983.
[29] D. Brush, B. Almroth, Buckling of Bars, Plates and Shells, McGraw-Hill, New York, 1975.
[30] R. Abdelmoula, N. Damil, M. Potier-Ferry, Influence of distributed and localized imperfections on the buckling of cylindrical-shells under external-pressure, Int. J. Solids Struct. 29 (1992) 1–25.
[31] N. Damil, M. Potier-Ferry, Amplitude equation for cellular instability, Dyn. Stab. Syst. 7 (1992) 1–34.
[32] M. Jamal, M. Midani, N. Damil, M. Potier-Ferry, Influence of localized imperfections on the buckling of cylindrical shells under axial compression, Int. J. Solids Struct. 36 (3) (1999) 441–464.
[33] M. Jamal, L. Lahlou, M. Midani, H. Zahrouni, A. Limam, N. Damil, M. Potier-Ferry, A semi-analytical buckling analysis of imperfect cylindrical shells under axial compression, Int. J. Solids Struct. 40 (2003) 1311–1327.
[34] R. Saito, R. Matsuo, T. Kimura, G. Desselhaus, M.S. Dresselhaus, Anomalous potential barrier of double-wall carbon nanotube, Chem. Phys. Lett. 348 (3–4) (2001) 187–193.
[35] N. Damil, M. Potier-Ferry, A new method to compute perturbed bifurcations: application to the buckling of imperfect elastic structures, Int. J. Eng. Sci. 28 (1990) 943–957.
[36] M. Jamal, M. Midani, N. Damil, M. Potier-Ferry, Influence of localized imperfections on the buckling of cylindrical shells under axial compression, Int. J. Solids Struct. 25 (1999) 330–353.
[37] M. Endo, H. Muramatsu, T. Hayashi, Y.A. Kim, M. Terrones, M.S. Dresselhaus, Nanotechnology: 'buckypaper' from coaxial nanotubes, Nature 433 (7025) (2005) 476.
[38] Y.G. Sun, X.H. Yao, Q. Han, Combined torsional buckling of double-walled carbon nanotubes with axial load in the multi-field coupled condition, Sci. China, Ser. G, Phys. Mech. Astron. 54 (9) (2011) 1659–1665.