NATURAL FREQUENCIES OF TRIPLE-WALLED CARBON NANOTUBES

Angelo Oreste Andrisano
Department of Engineering "Enzo Ferrari",
University of Modena and Reggio Emilia, Italy
E-mail: angelooreste.andrisano@unimore.it

Francesco Pellicano
Department of Engineering "Enzo Ferrari",
University of Modena and Reggio Emilia, Italy
E-mail: francesco.pellicano@unimore.it

Matteo Strozzi
Department of Engineering,
University of Ferrara, Italy
E-mail: strmtt@unife.it

Abstract. *In this paper, the linear vibrations of Triple-Walled Carbon Nanotubes (TWNTs) are analysed. A multiple elastic shell model is considered. The shell dynamics is studied in the framework of the Sanders-Koiter shell theory. The van der Waals (vdW) interaction between two layers of the TWNT is modelled by a radius-dependent function. The circular cylindrical shell deformation is described in terms of longitudinal, circumferential and radial displacements. Simply supported, clamped and free boundary conditions are considered. The three displacement fields are expanded by means of a double mixed series based on Chebyshev orthogonal polynomials for the longitudinal variable and harmonic functions for the circumferential variable. The Rayleigh-Ritz method is applied to obtain approximate natural frequencies and mode shapes. The present model is validated in linear field by means of data derived from the literature. This study is focused on determining the effect of the geometry and boundary conditions on the natural frequencies of TWNTs.*

Keywords: *carbon nanotubes, multiple elastic shell model, van der Waals interaction*

1. INTRODUCTION

Single-Walled Carbon Nanotubes (SWNTs) were discovered in 1991 by Iijima [1], who first analysed molecular carbon structures in the form of fullerenes and then reported the preparation of the carbon nanotubes, as helical microtubules of graphitic carbon.

The analogies between the continuous shells and the discrete SWNTs led to a very large application of the elastic shell theories for the SWNT structural analysis [2-7].

Triple-Walled Carbon Nanotubes (TWNTs) can be described as systems composed by three concentric SWNTs, whereby each SWNT is treated as a cylindrical shell continuum; an elastic multiple shell model is used for the vibration analysis of the TWNT and the van der Waals interaction between any two layers of the system can be modelled by means of a radius-dependent function [8-10].

In this paper, the linear vibrations of TWNTs are investigated. The shell dynamics is studied in the framework of the Sanders-Koiter shell theory and a multiple elastic shell model is considered. The van der Waals (vdW) interaction between any two layers of the TWNT is modelled by a radius-dependent function.

The shell deformation is described in terms of longitudinal, circumferential and radial displacements. Simply supported, clamped and free boundary conditions are considered. The three displacement fields are expanded by means of a double mixed series based on Chebyshev polynomials and harmonic functions. The Rayleigh-Ritz method is applied to obtain approximate natural frequencies and mode shapes.

The model proposed in the present paper is validated in linear field by means of data derived from the literature. This study is focused on determining the effect of the geometry and boundary conditions on the natural frequencies of TWNTs.

2. SANDERS-KOITER LINEAR SHELL THEORY EXTENDED TO TWNTS

In Figure 1, a circular cylindrical shell having radius R_i, length L_i and thickness h_i is shown; a cylindrical coordinate system (O; x, θ, z) is considered where the origin O of the reference system is located at the centre of one end of the circular shell. Three displacement fields are represented: longitudinal u_i (x, θ, t), circumferential v_i (x, θ, t) and radial w_i (x, θ, t), where (x, θ) are the longitudinal and angular coordinates of the circular cylindrical shell, z is the radial coordinate along the thickness h_i and t is the time.

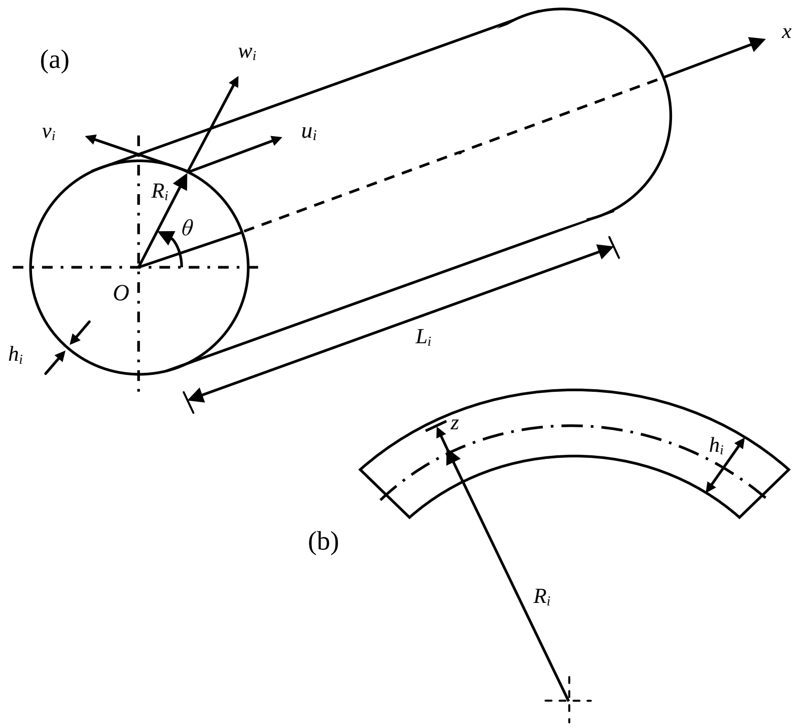

Figure 1. Geometry of the *i*-th shell. (a) Complete shell; (b) cross-section of the shell.

Strain-Displacement Relationships

The three nondimensional displacement fields ($\tilde{u}_i$,$\tilde{v}_i$,$\tilde{w}_i$) of the i-th cylindrical shell can be written in the following form [2]

$$\tilde{u}_i = \frac{u_i}{R_i} \qquad \tilde{v}_i = \frac{v_i}{R_i} \qquad \tilde{w}_i = \frac{w_i}{R_i} \qquad i = (1,3) \tag{1}$$

where (u_i,v_i,w_i) are the three dimensional displacement fields and R_i is the radius of the i-th shell.

The nondimensional middle surface strains of the i-th cylindrical thin shell are given as [2]

$$\tilde{\varepsilon}_{x,0,i} = \alpha_i \frac{\partial \tilde{u}_i}{\partial \eta} \qquad \tilde{\varepsilon}_{\theta,0,i} = \frac{\partial \tilde{v}_i}{\partial \theta} + \tilde{w}_i \qquad \tilde{\gamma}_{x\theta,0,i} = \frac{\partial \tilde{u}_i}{\partial \theta} + \alpha_i \frac{\partial \tilde{v}_i}{\partial \eta} \qquad i = (1,3) \tag{2}$$

where $\eta = x/L$ is the nondimensional longitudinal coordinate of the shell and $\alpha_i = R_i/L$.

The nondimensional middle surface changes in curvature and torsion of the i-th cylindrical shell are expressed as [2]

$$\tilde{k}_{x,i} = -\alpha_i^2 \frac{\partial^2 \tilde{w}_i}{\partial \eta^2} \qquad \tilde{k}_{\theta,i} = \frac{\partial \tilde{v}_i}{\partial \theta} - \frac{\partial^2 \tilde{w}_i}{\partial \theta^2}$$
$$\tilde{k}_{x\theta,i} = -2\alpha_i \frac{\partial^2 \tilde{w}_i}{\partial \eta \partial \theta} + \frac{3\alpha_i}{2}\frac{\partial \tilde{v}_i}{\partial \eta} - \frac{1}{2}\frac{\partial \tilde{u}_i}{\partial \theta} \qquad i = (1,3) \tag{3}$$

Elastic Strain and Kinetic Energy

The nondimensional elastic strain energy of the i-th cylindrical shell is written in the following form [7]

$$\tilde{U}_i = \frac{1}{2}\frac{1}{(1-\nu^2)}\int_0^1\int_0^{2\pi}\left[\tilde{\varepsilon}_{x,0,i}^2 + \tilde{\varepsilon}_{\theta,0,i}^2 + 2\nu\tilde{\varepsilon}_{x,0,i}\tilde{\varepsilon}_{\theta,0,i} + \frac{(1-\nu)}{2}\tilde{\gamma}_{x\theta,0,i}^2\right]d\eta d\theta +$$
$$\frac{1}{2}\frac{\beta_i^2}{12(1-\nu^2)}\int_0^1\int_0^{2\pi}\left[\tilde{k}_{x,i}^2 + \tilde{k}_{\theta,i}^2 + 2\nu\tilde{k}_{x,i}\tilde{k}_{\theta,i} + \frac{(1-\nu)}{2}\tilde{k}_{x\theta,i}^2\right]d\eta d\theta \qquad i = (1,3) \tag{4}$$

where $\beta_i = h/R_i$.

The nondimensional kinetic energy of the i-th cylindrical shell is given by [4]

$$\tilde{T}_i = \frac{1}{2}\gamma_i \int_0^1\int_0^{2\pi}(\tilde{u}_i'^2 + \tilde{v}_i'^2 + \tilde{w}_i'^2)d\eta d\theta \qquad i = (1,3) \tag{5}$$

where $\gamma_i = \rho R_i^2 \omega_0^2/E$.

Van der Waals Interaction Energy

The nondimensional pressure $\tilde{p}_i$ exerted on the i-th shell due to vdW interaction between two different layers can be written as a function of the nondimensional radial displacements ($\tilde{w}_i$,$\tilde{w}_j$) of the shells in the following form [8,9]

$$\tilde{p}_i(\eta,\theta) = \sum_{j=1}^{3} \tilde{c}_{ij} \left(\delta_i \tilde{w}_i - \delta_j \tilde{w}_j \right) \qquad i = (1,3) \qquad (6)$$

where $\delta_i = R_i / \hat{R}$, $\delta_j = R_j / \hat{R}$, $\hat{R} = R_1$.

The nondimensional vdW interaction coefficient $\tilde{c}_{ij}$ is expressed as [10]

$$\tilde{c}_{ij} = -\left(\frac{1001\pi\tilde{\varepsilon}\tilde{\sigma}^{12}}{3\tilde{a}^4} \tilde{E}_{ij}^{13} - \frac{1120\pi\tilde{\varepsilon}\tilde{\sigma}^{6}}{9\tilde{a}^4} \tilde{E}_{ij}^{7} \right) \delta_j \qquad (i,j) = (1,3) \qquad (7)$$

The nondimensional elliptical integral $\tilde{E}_{ij}^m$ is given by [10]

$$\tilde{E}_{ij}^m = (\delta_j + \delta_i)^{-m} \int_0^{\pi/2} \frac{d\theta}{(1 - \tilde{k}_{ij}\cos^2\theta)^{m/2}} \qquad (i,j) = (1,3) \qquad (8)$$

The nondimensional coefficient $\tilde{k}_{ij}$ is expressed in the form [10]

$$\tilde{k}_{ij} = \frac{4\delta_j\delta_i}{(\delta_j + \delta_i)^2} \qquad (i,j) = (1,3) \qquad (9)$$

3. LINEAR VIBRATION ANALYSIS

A modal vibration, i.e., a synchronous motion, can be formally written in the form [6]

$$\tilde{u}_i(\eta,\theta,\tau) = \tilde{U}_i(\eta,\theta) f_i(\tau) \qquad \tilde{v}_i(\eta,\theta,\tau) = \tilde{V}_i(\eta,\theta) f_i(\tau) \qquad \tilde{w}_i(\eta,\theta,\tau) = \tilde{W}_i(\eta,\theta) f_i(\tau) \qquad i = (1,3) \qquad (10)$$

where $\tilde{U}_i(\eta,\theta)$, $\tilde{V}_i(\eta,\theta)$, $\tilde{W}_i(\eta,\theta)$ are the mode shape of the i-th shell, $f_i(\tau)$ is the time law, which is supposed to be the same for each displacement field in the modal analysis.

The mode shape ($\tilde{U}_i$, $\tilde{V}_i$, $\tilde{W}_i$) is expanded by means of a double series in terms of m-th order Chebyshev polynomials $T_m^*(\eta)$ in the longitudinal direction and harmonic functions ($\cos n\theta$, $\sin n\theta$) in the circumferential direction, in the following form [6]

$$\tilde{U}_i(\eta,\theta) = \sum_{m=0}^{M_u}\sum_{n=0}^{N} \tilde{U}_{i,m,n} T_m^*(\eta)\cos n\theta \qquad \tilde{V}_i(\eta,\theta) = \sum_{m=0}^{M_v}\sum_{n=0}^{N} \tilde{V}_{i,m,n} T_m^*(\eta)\sin n\theta \qquad \tilde{W}_i(\eta,\theta) = \sum_{m=0}^{M_w}\sum_{n=0}^{N} \tilde{W}_{i,m,n} T_m^*(\eta)\cos n\theta \qquad i = (1,3) \qquad (11)$$

where $T_m^* = T_m(2\eta - 1)$, m is the polynomials degree, n is the number of nodal diameters and ($\tilde{U}_{i,m,n}$, $\tilde{V}_{i,m,n}$, $\tilde{W}_{i,m,n}$) are unknown coefficients of the boundary conditions.

Rayleigh-Ritz Method

The maximum number of variables needed for describing a general vibration mode with n nodal diameters is obtained by the relation ($N_p = 3\times(M_u + M_v + M_w + 3 - p)$), where ($M_u = M_v = M_w$) are the degree of the Chebyshev polynomials and p is the number of equations which are needed to satisfy the boundary conditions.

For a multi-mode analysis including different values of nodal diameters n, the number of degrees of freedom of the system is computed by the relation ($N_{max} = N_p \times (N + 1)$), where N represents the maximum value of the nodal diameters n considered.

Equations (10) are inserted in the expressions of the elastic strain energy (4) and kinetic energy (5) in order to compute the Rayleigh quotient; after imposing the stationarity to the Rayleigh quotient, one obtains the eigenvalue problem [6]

$$(-\omega_i^2 \tilde{\mathrm{M}}_i + \tilde{\mathrm{K}}_i)\tilde{\mathrm{q}}_i = \tilde{0} \qquad i = (1,3) \qquad (12)$$

which furnishes the approximate natural frequencies and mode shapes, where $\tilde{\mathrm{q}}_i$ denotes a vector containing all the unknown variables in the form [6]

$$\tilde{\mathrm{q}}_i = \begin{bmatrix} \dots \\ \tilde{U}_{i,m,m} \\ \tilde{V}_{i,m,n} \\ \tilde{W}_{i,m,n} \\ \dots \end{bmatrix} \qquad i = (1,3) \qquad (13)$$

4. NUMERICAL RESULTS

The mechanical parameters of the TWNT analysed in this paper are shown in Table 1.

Table 1. Mechanical parameters of the TWNT [10].

Young's modulus *E*	5.5 TPa
Poisson's ratio *ν*	0.19
Mass density *ρ*	11700 kg/m^3
Thickness *h*	0.066 nm
Innermost radius R_1	5.00 nm
Intermediate radius R_2	5.34 nm
Outermost radius R_3	5.68 nm
Length *L*	56.8 nm

Table 2. Natural frequencies (THz) of a simply-simply TWNT with R_1 = 5.00 nm, R_3 = 5.68 nm and L/R_3 = 10 with vdW interaction. Circumferential flexural modes. Comparisons between Sanders-Koiter (present model) and Donnell-Mushtari (Ref. [10]) shell theories.

Mode	**Displacement**	**Radius**	**Natural frequency (THz)**		**Difference %**
(*j*,*n*)	**(*u*,*v*,*w*)**	***R***	**Present model**	**Ref. [10]**	
1,2	*w*	R_3	0.0149	0.0150	0.67
	w	R_1	2.0557	2.0550	0.03
	w	R_2	3.3479	3.3480	0.00
2,2	*w*	R_3	0.0466	0.0469	0.64
	w	R_1	2.0586	2.0580	0.03
	w	R_2	3.3481	3.3490	0.03
3,2	*w*	R_3	0.0944	0.0942	0.21
	w	R_1	2.0638	2.0630	0.04
	w	R_2	3.3483	3.3490	0.02

Validation of the Present Method in Linear Field

In Table 2, comparisons between the natural frequencies of a simply supported TWNT obtained by considering the Sanders-Koiter shell theory (present model) and the Donnell-Mushtari shell theory (Ref. [10]) are reported.

The mechanical parameters of Table 1 are used. The vdW interaction is taken into account. The circumferential flexural modes (n=2) are studied. The radial displacement w is considered. The three concentric SWNTs which give the TWNT are denoted by innermost radius R_1, intermediate radius R_2 and outermost radius R_3, respectively.

From these comparisons, it can be noted that the present model is in good accordance with the results from the pertinent literature, the differences between the natural frequencies being less than 1%.

Effect of the Boundary Conditions

In Figure 2, comparisons between the natural frequencies of a TWNT obtained considering the Sanders-Koiter shell theory are reported. The mechanical parameters of Table 1 are used. The vdW interaction is taken into account. The circumferential flexural modes (n=2) are studied. The radial displacement w is considered. The SWNT with outermost radius R_3 is analysed.

Free-free, simply supported-free, clamped-free, simply supported-simply supported, clamped-simply supported and clamped-clamped boundary conditions are considered.

From these comparisons, it can be noted that, for the value of the radius R_3, the natural frequency for the clamped-clamped TWNT is the highest, followed by the clamped-simply supported, simply supported-simply supported, clamped-free, simply supported-free and free-free natural frequencies.

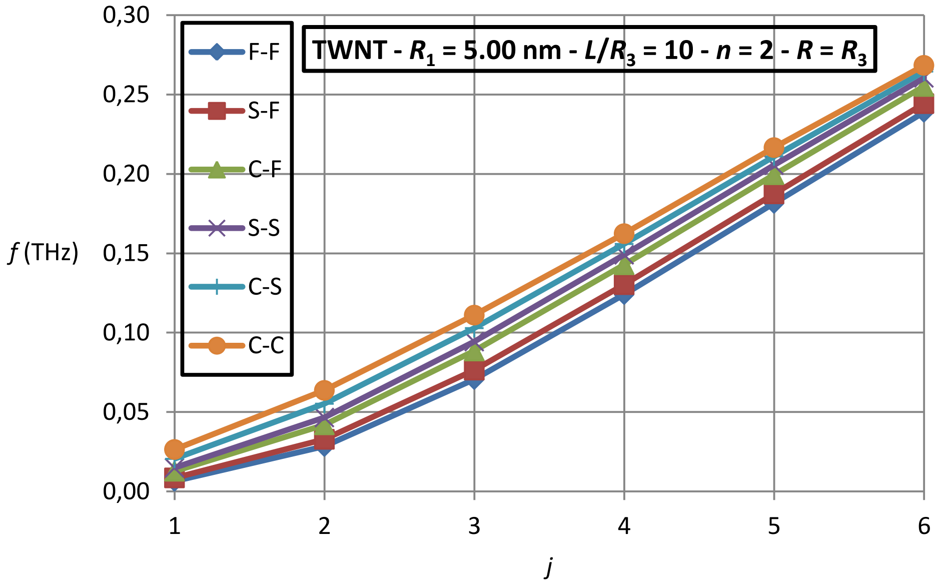

Figure 2. Natural frequencies (THz) of a TWNT with vdW interaction. Mode (n=2). Radial displacement w. Radius R_3. Sanders-Koiter shell theory. Mechanical parameters of Table 1.

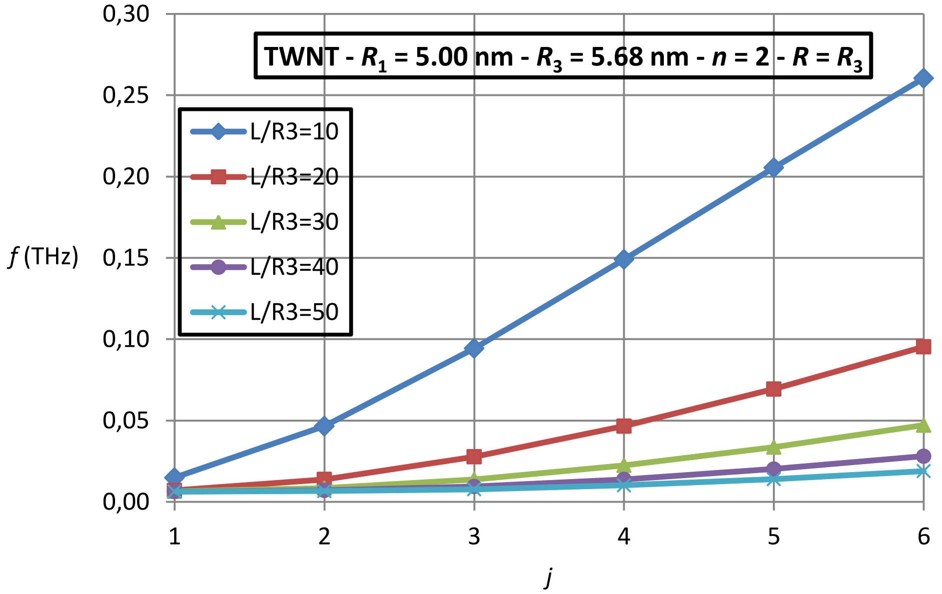

Figure 3. Natural frequencies (THz) of a simply supported TWNT with vdW interaction. Mode (n=2). Radial displacement w. Radius R_3. Sanders-Koiter shell theory. Mechanical parameters of Table 1.

Effect of the Aspect Ratio

In Figure 3, comparisons between the natural frequencies of a simply supported TWNT obtained considering the Sanders-Koiter shell theory are given. The mechanical parameters of Table 1 are used. The vdW interaction is taken into account. The circumferential flexural modes (n=2) are investigated. The radial displacement w is considered. The SWNT with outermost radius R_3 is analysed. Five different aspect ratios L/R_3 = (10,20,30,40,50) are compared.

From this Figure, it is confirmed that the natural frequency of a vibrational mode (j, n) increases with the number of longitudinal half-waves j and decreases with increasing length L. In particular, it can be seen that the natural frequencies for the lower aspect ratio L/R_3=10 increase almost linearly with j, while the natural frequencies for the higher aspect ratio L/R_3=50 tend to an horizontal asymptote.

5. CONCLUSIONS

In this paper, the linear vibrations of TWNTs are analysed considering a multiple elastic shell model. The shell dynamics is studied in the framework of the Sanders-Koiter theory, where the vdW interaction between any two layers of the TWNT is modelled by a radius-dependent function. Simply supported, clamped and free boundary conditions are applied. The circumferential flexural modes are studied. The radial displacement is considered. The Rayleigh-Ritz method is used in order to obtain approximate natural frequencies and mode shapes.

The present model is validated in linear field by means of data derived from the literature. From comparisons between the natural frequencies of a simply supported TWNT obtained by considering the Sanders-Koiter and Donnell-Mushtari shell theories, it can be noted that the present model is in good accordance with the results retrieved from the literature.

The effect of the boundary conditions on the natural frequencies of a TWNT obtained by considering the Sanders-Koiter shell theory is investigated. The outermost radius is analysed. From these comparisons, it can be noted that the natural frequency of the clamped-clamped TWNT is the highest, followed by the clamped-simply supported, simply supported-simply supported, clamped-free, simply supported-free and free-free natural frequencies, respectively.

The influence of the aspect ratio on the natural frequencies of a TWNT obtained by considering the Sanders-Koiter shell theory is studied. The outermost radius is investigated. From these comparisons, it is confirmed that the natural frequency of a vibrational mode increases with the number of the longitudinal half-waves and decreases with increasing the length. Moreover, it can be noted that the natural frequencies for the lower aspect ratio increase almost linearly with the longitudinal half-waves, while the natural frequencies for the higher aspect ratio tend to an horizontal asymptote.

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