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Vibration analysis of single-walled carbon nanotubes using wave propagation approach

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Abstract. In this paper, influence of boundary conditions on free vibrations of single- walled carbon nanotubes (SWCNTs) is examined. The Flügge's shell dynamical equations are utilized for governing vibrations for carbon nanotubes. The wave propagation approach (WPA) is engaged to determine vibration frequency equation in standard eigenvalue form. The axial modal dependence is measured by the complex exponential functions implicating the axial modal numbers. These numbers are associated with boundary conditions specified at edges of a carbon nanotube. Computer programming is performed to obtain solutions of vibration frequency equation. In our new investigation, the vibration frequency spectra are obtained and analyzed for various physical parameters e.g., length and thickness-to-radius ratio. A number of results are presented to influence of different boundary conditions on SWCNTs. They are shown graphically and have been compared with those available in the literature.

1 Introduction

Carbon nanotubes (CNTs) were explored by Iijima (1991) and their uses have been found in various areas such as industry including aerospace, electronics, medicine, defense, automotive, construction, and even fashion (Iijima, 1991). A bulk of research work was performed to extract their remarkable properties e.g., a high characteristic ratio and springiness (Falvo et al., 1997; Sanchez-Portal et al., 1999), a very huge tensile potency and Young modulus (Li and Chou, 2003) superconductivity and well-bonding asset between carbon atoms (see also Falvo et al., 1997; Li and Chou, 2003; Sakhaee-Pour et al., 2009). Vibration characteristics of CNTs have been widely examined for the last fifteen years. Such characteristics are studied by thin shell (Yakobson et al., 1996), beam (Hsu et al., 2008) and ring (Vodenitcharova and Zhang, 2003) theories of continuum models (Li and Chou, 2003). Theoretical study of CNTs reflects those mechanical aspects which are difficult to observe by experimental and atomistic simulation methodologies. Study of their free vibration is an important phenomenon in dynamical science. These characteristics are impressed by their material properties. These tubes are placed in various physical environments and subject various constraints. Influence of these constraints is investigated on vibration characteristics of SWCNTs.

Carbon nanotubes (CNTs) have a vast field of applications in material strength analysis. Some worth-mentioning fields are emanation panel spectacle, chemical sensing, drug deliverance, and nano-electronics. Having a good utilization of these tubes in fields of science and industry, however, their mechanical behavior demands more understanding in this aspect of study. Use of these tubes have been found in the fields of electrical and chemical engineering and biological sciences. An experimental aspect of vibration problems of single-walled carbon nanotubes (SWCNTs) have also keen interest of researchers along with analytical study of information got through it. Three fundamental techniques are utilized to generate them, which include molecular dynamic (MD) simulations, atomistic-based modeling and the continuum approach. Mostly the continuum method is applied to fabricate them. Since these are material objects can get deformed in practical situations, so their buckling and vibration investigations are fundamental problems in CNTs motions at non-mechanical levels.

This investigation is contained some new horizons which updates the previous studies on SWCNTs with respect to theoretical and experimental methods to extract their frequency spectra. Lordi and Yao (1998) applied MD simulations to evaluate the Young's elastic modulus and determined vibration frequencies of SWCNTs using the universal force field. These results were obtained for a number of clamped-free conditions. Their analysis was based on the Euler beam theory. They inferred that frequencies obtained by a cylindrical shell model (CSM) are in somewhat agreement those ones determined by MD simulations. Hsu et al. (2008) fabricated a CNTs model for analyzing their resonant frequency of chiral SWCNTs. These tubes were studied under a thermal vibration. The Timoshenko beam model was used implicating rotatory inertia and shear deformation terms. Bocko and Lengvarský (2014) investigated vibration frequencies of CNTs for four end conditions viz.: clamped-clamped, simply supported-simply supported, clamped-simply supported and clamped-free by using the continuum approach. This study was based on the non-local beam theory and dealt with the vibrations of armchair single-walled carbon nanotube. The eigen-frequencies were given for two values of diameters of nanotubes, several nonlocal parameters and continuously changed length. Chawis et al. (2013) analyzed vibrational behavior of SWCNTs. Non-local theory with small scale effect was engaged to form the vibration frequency equation. The Euler beam theory was taken for dynamical controlling equations and frequencies for various boundary conditions were determined against aspect ratios. Yang et al. (2010) presented an investigation of free vibration characteristics of SWCNTs and founded this analysis on dynamics of non-local theory of Timoshenko beam model. Wang et al. (2013) gave a nonlinear vibration study of embedded SWCNTs by considering the aspect of geometrical imperfection. The loading response was modeled with harmonic behavior based on non-local Timoshenko beam theory. Azrar et al. (2011, 2013) have interpreted vibrations of these tubes with length scale influence for a number of end conditions. Ansari et al. (2011a, b) examined vibration and buckling aspects of carbon nanotubes and used non-local Donnell shell theory. Finite element method has been used by Swain et al. (2013) to study vibrations of SWCNTs.

Moreover, Wang and Zhang (2007) used the Flügge's shell model to investigate vibration of SWCNTs for aspects of bending stiffness and torsion stiffness. It was also found that a 3-D shell model of SWCNTs could be demonstrated with well-defined effective thickness. Ansari and Arash (2013) presented an analysis to provide the possibility of considering different combinations of layer-wise boundary conditions using nonlocal Flügge's shell model. The influences of small scale factor, layer-wise boundary conditions and geometrical parameters on the mechanical behavior of DWCNTs were fully investigated. Ansari and Rouhi (2015) developed nonlocal shell model based on the accurate Flügge's shell theory to obtain the critical axial buckling load of SWCNTs. The results were predicted for the (8, 8) armchair clamped SWCNTs for the nanotube aspect ratio against critical buckling load. Rouhi et al. (2015) developed a nonlocal Flügge shell model to study vibrations of multi-walled carbon nanotubes (MWCNTs) with various boundary conditions in a layer-wise manner. Also some new investigation was made with some non-local parameters for nanotube aspect ratio against the fundamental resonant frequency curves different boundary conditions.

Increasingly, computer simulations have been used to examine vibration characteristics of CNTs (and or SWCNTs) through different models bases (Li and Chou, 2003; Sakhaee-Pour et al., 2009; Yakobson et al., 1996; Hsu et al., 2008; Azrar et al., 2011; Elishakoff and Pentaras, 2009). Selection of a dynamical model to analyze systems related nano level is Flügge's cylindrical shell model (CSM). Numerical procedure to frame the CNT frequency equation employed is wave propagation approach (WPA), which admits to extract fundamental frequencies of SWCNTs over various combinations of parameters. Many numerical techniques been adopted for vibration problems like Galerkin's method (Azrar et al., 2011; Elishakoff and Pentaras, 2009), finite elements method (FEM) (Sakhaee-Pour et al., 2009), wave propagation approach (Xuebin, 2008; Zhang et al., 2001). On the other hand, CSM based WPA was found to be a very popular tool to compute the vibration characteristics of SWCNTs. Selim (2010) and Natsuki and Morinobu (2006) were performed Flügge's CSM to calculate the vibrational properties of SWCNTs and DWCNTs. Moreover, the novel Flügge's cylindrical shell model (CSM) based on WPA for estimating the natural frequencies of SWCNTs has been demonstrated to converge faster than the other models and other approaches. The Flügge CSM based on WPA is, therefore, another choice of powerful technique of CNTs whose results are applicable in the limit of acceptable statistical errors than the earlier used approaches (Natsuki and Morinobu, 2006; Hsu et al., 2008; Yakobson et al., 1996; Elishakoff and Pentaras, 2009; Sakhaee-Pour et al., 2009). In this work, the Flügge's CSM based on WPA for determining fundamental frequencies is extended to study vibrations of SWC-NTs, which is our particular motivation. Furthermore, up to now little is known about the vibration analyses of armchair SWCNTs, and moreover, the effects of the length (L) and height-to-radius ratio (h/R) of SWCNTs have not been investigated, by using Flügge CSM based on WPA. This is also our motivation for carrying out the present work.

Moreover CNT vibrations happen in some producing applications such as ultra-sonication in nano-composite treating and as part of certain non-destructive estimation procedures like Raman spectroscopy. An analysis of influence of boundary conditions is an important aspect on vibrations of these tubes. On such studies, various interesting results related to them are seen in literature (Wang and Zhang, 2007; Selim, 2010; Zhang et al., 2009; Eringen, 2002; Grupta and Barta, 2008; Harik, 2002; Lu et al., 2007; Muc et al., 2013; Wang and Liew, 2007).

In the present work, a theoretical analysis of single-walled carbon nanotubes is performed for various boundary condi-

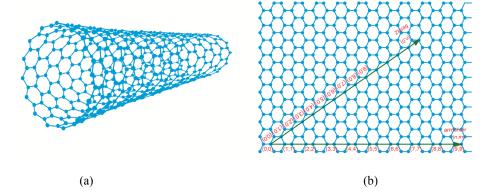


Figure 1. Hexagonal lattice (a) single-walled carbon nanotube (b) graphene sheet.

tions with an efficient and suitable mathematical procedure commonly known as wave propagation approach. This approach is applied to solve the CNT controlling motion equations which results to formulate the frequency equation. In this procedure, process of separation of modal deformation functions is done to split space and temporal variables. Axial modal dependency is measured by the complex exponential functions in the longitudinal direction and circular dependence is taken in the form of trigonometric functions in the tangential direction. The exponential functions contain the half axial wave number affiliated with a particular boundary condition. These complex functions are truncated part of characteristic beam functions which are the solutions of beam differential equation for various boundary conditions. In order to compute the frequencies of SWCNTs, the computer software MATLAB is used. Influence of various edge conditions such as clamped-clamped, clamped-simply supported, simply supported-simply supported and clamped-free on SWCNTs is numerically investigated. Results are presented in graphical forms for nano-material parameters.

2 Theoretical formation

Figure 1 represents a schema of single-walled carbon nanotube and graphene sheet.

A similarity is observed in the structures of circular cylinders and single-walled carbon nanotubes with regard to geometrical shapes as shown in the Fig. 2. So the governing equations of motion for cylindrical shells are engaged for studying free vibrations of SWCNTs. The geometrical parameters for these tubes are indicated by length (L), mean radius (R) and thickness (h). Young's modulus, mass density and Poisson's ratio being their material quantities are designated by E, ρ and v respectively.

Suppose that $u(x, \theta, t)$, $v(x, \theta, t)$ and $w(x, \theta, t)$ signify the modal deformation displacement functions in the axial, tangential and transverse direction correspondingly. A set of partial differential equations involving the three unknown displacement functions for vibration of single-walled carbon

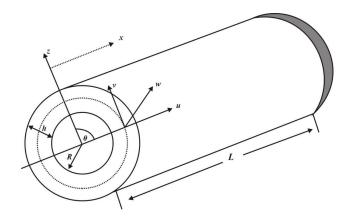


Figure 2. Geometry of SWCNTs.

nanotubes is written as:

$$\frac{\partial^{2} u}{\partial x^{2}} + \frac{1 - v}{2R^{2}} \frac{\partial^{2} u}{\partial \theta^{2}} + \frac{1 + v}{2R} \frac{\partial^{2} v}{\partial x \partial \theta} - \frac{v}{R} \frac{\partial w}{\partial x}$$

$$= \frac{\rho}{K_{\text{extension}}} \frac{\partial^{2} u}{\partial t^{2}} \qquad (1a)$$

$$\frac{1 + v}{2R} \frac{\partial^{2} u}{\partial x \partial \theta} + \frac{1 - v}{2} \frac{\partial^{2} v}{\partial x^{2}} + \frac{1}{R^{2}} \frac{\partial^{2} v}{\partial \theta^{2}} - \frac{1}{R^{2}} \frac{\partial w}{\partial \theta}$$

$$+ \frac{1}{R^{2}} K_{1} \left(K_{2} \frac{\partial^{2} v}{\partial x^{2}} + \frac{\partial^{2} v}{R^{2} \partial \theta^{2}} \right) + \frac{1}{R^{2}} K_{1} \left(\frac{1}{R^{2}} \frac{\partial^{3} w}{\partial \theta^{3}} \right)$$

$$+ (K_{2} + v) \frac{\partial^{3} w}{\partial x^{2} \partial \theta} = \frac{\rho}{K_{\text{extension}}} \frac{\partial^{2} v}{\partial t^{2}} \qquad (1b)$$

$$\frac{v}{R} \frac{\partial u}{\partial x} + \frac{1}{R^{2}} \frac{\partial v}{\partial \theta} - \frac{w}{R^{2}} - \frac{1}{R^{2}} K_{1} \left(R^{2} \frac{\partial^{4} w}{\partial x^{4}} + 2(K_{2} + v) \frac{\partial^{4} w}{\partial x^{2} \partial \theta^{2}} \right)$$

$$+ \frac{1}{R^{2}} \frac{\partial^{4} w}{\partial \theta^{4}} - \frac{1}{R^{2}} K_{1} \left((2K_{2} + v) \frac{\partial^{3} v}{\partial x^{2} \partial \theta} + \frac{1}{R^{2}} \frac{\partial^{3} v}{\partial \theta^{3}} \right)$$

$$= \frac{\rho}{K_{1}} \frac{\partial^{2} w}{\partial x^{2}} \qquad (1c)$$

where $K_1 = \frac{D_{\text{bending}}}{K_{\text{extension}}}$, $K_2 = \frac{D_{\text{torsion}}}{D_{\text{bending}}}$ and $K_{\text{extension}}$, K_{shear} , D_{bending} , D_{torsion} and G denote the in-plane stiffness, shear,

bending, torsional stiffness and shear modulus respectively. They are treated as independent parameters and are described by the followings:

$$K_{\text{extension}} = \frac{Eh}{1 - v^2}, \quad K_{\text{shear}} = Gh, \quad D_{\text{bending}} = \frac{Eh^3}{12(1 - v^2)},$$
 $D_{\text{torsion}} = \frac{Gh^3}{12} \quad \text{and} \quad G = \frac{E}{2(1 + v)}.$

There exists a unique relationship between the above quantities as:

$$\frac{D_{\text{bending}}}{K_{\text{extension}}} = \frac{D_{\text{torsion}}}{K_{\text{shear}}} = \frac{h^2}{12}$$
 (2)

3 Applications of the wave propagation approach

Various numerical techniques are applied to solve systems of partial differential equations. Since the present CNTs has been expressed in the form of differential equation, so a simple and efficient method commonly known as wave propagation approach (WPA) is employed to solve such type of differential equation. This approach has been used widely and successively for studying shell vibrations (see Sun et al., 2013; Ramezani and Ahmadian, 2009; Xuebin, 2008; Zhang et al., 2001). Forms of three modal displacement functions $u(x, \theta, t)$, $v(x, \theta, t)$ and $w(x, \theta, t)$ are assumed such that they split the independent variables. The axial and circumferential coordinates are denoted by x, θ correspondingly and t indicates time variable. So the assumed expressions for modal deformation displacements are written as:

$$u(x,\theta,t) = \alpha_m U(x) \cos n\theta e^{i\omega t}$$
(3a)

$$v(x,\theta,t) = \beta_m V(x) \sin n\theta e^{i\omega t}$$
(3b)

$$w(x,\theta,t) = \gamma_m W(x) \cos n\theta e^{i\omega t}$$
(3c)

where U(x), V(x) and W(x) stand for the axial modal dependence in the longitudinal, tangential and radial directions respectively. Here α_m , β_m and γ_m are three vibration amplitude coefficients in the three directions. The circumferential wave number is denoted by n and ω indicates natural angular frequency. This frequency is associated with fundamental frequency f through the following formula: $f = \omega/2\pi$.

Applying the product method for partial differential equations, the space and time variable are split by substituting the modal displacement functions. Now the expressions for u, v and w given in Eqs. (3a)–(3c), along with their partial derivatives are substituted into the Eqs. (1a)–(1c), and the following simplified ordinary differential equation system is achieved:

$$\[\frac{d^2 U}{dx^2} - \frac{n^2 (1 - v)}{2R^2} U(x) \] \alpha_m + \frac{n(1 + v)}{2R} \frac{dV}{dx} \beta_m$$

$$- \frac{v}{R} \frac{dW}{dx} \gamma_m = -\frac{\rho}{K_{\text{extension}}} \omega^2 U(x) \alpha_m$$
(4a)

$$-n\frac{(1+v)}{2R}\frac{dU}{dx}\alpha_{m} + \left[\frac{1-v}{2}\frac{d^{2}V}{dx^{2}} - \frac{n^{2}}{R^{2}}V(x) + \frac{K_{1}}{R^{2}}\left\{K_{2}\frac{d^{2}V}{dx^{2}} - \frac{n^{2}}{R^{2}}V(x)\right\}\right]\beta_{m} + \left[\frac{n}{R^{2}}W(x) + \frac{K_{1}}{R^{2}}\left\{\frac{n^{3}}{R^{2}}W(x)\right\}\right]$$

$$-(K_{2}+v)n\frac{d^{2}W}{dx^{2}}\right\} \gamma_{m} = -\frac{\rho}{K_{\text{extension}}}\omega^{2}V(x)\beta_{m} \quad \text{(4b)}$$

$$\frac{v}{R}\frac{dU}{dx}\alpha_{m} + \left[\frac{n}{R^{2}}V(x) - \frac{K_{1}}{R^{2}}\left\{(2K_{2}+v)\frac{d^{2}W}{dx^{2}}n - \frac{n^{3}}{R^{2}}V(x)\right\}\right]\beta_{m}$$

$$+ \left[-\frac{1}{R^{2}}W(x) - \frac{K_{1}}{R^{2}}\left\{R^{2}\frac{d^{4}W}{dx^{4}} - 2(K_{2}+v)\frac{d^{2}W}{dx^{2}}n^{2} + \frac{n^{4}}{R^{2}}W(x)\right\}\right]\gamma_{m} = -\frac{\rho}{K_{\text{extension}}}\omega^{2}W(x)\gamma_{m} \quad \text{(4c)}$$

The axial modal dependence functions: U(x), V(x) and W(x) specified by a complex exponential function, are given as:

$$U(x) = V(x) = W(x) = e^{-ik_m x}$$
 (5)

where k_m is the axial wave number for vibrating carbon nanotubes and is closely related with nature of boundary conditions applied on the ends of SWCNTs. m indicates the axial half-wave number. Values for various axial wave numbers are listed for a number of end conditions in Table 1.

Making substitutions for U(x), V(x) and W(x) along with their respective derivatives in the arrangement of differential equations, a system of simultaneous equations in α_m , β_m and γ_m is evolved as:

$$\begin{bmatrix}
k_{m}^{2} + \frac{1-v}{2R^{2}}n^{2} \\
\alpha_{m} + \left[ik_{m}\frac{1+v}{2R}n\right]\beta_{m} - ik_{m}\frac{v}{R}\gamma_{m}
\end{bmatrix} = \frac{\rho}{K_{\text{extension}}}\omega^{2}\alpha_{m}$$
(6a)
$$\begin{bmatrix}
-n\frac{1+v}{2R}ik_{m} \\
\alpha_{m} - \left[-\frac{1+v}{2}k_{m}^{2} - \frac{n^{2}}{R^{2}} \\
-\frac{K_{1}}{R^{2}}\left\{K_{2}k_{m}^{2} + \frac{n^{2}}{R^{2}}\right\}\right]\beta_{m} - \left[\frac{n}{R^{2}} + \frac{K_{1}}{R^{2}}\left\{\frac{n^{3}}{R^{2}} + (K_{2}+v)nk_{m}^{2}\right\}\right]\gamma_{m} = \frac{\rho}{K_{\text{extension}}}\omega^{2}\beta_{m}$$
(6b)
$$\frac{v}{R}ik_{m}\alpha_{m} - \left[\frac{n}{R^{2}} + \frac{K_{1}}{R^{2}}\left\{(2K_{2}+v)k_{m}^{2}n + \frac{n^{3}}{R^{2}}\right\}\right]\beta_{m}$$

$$- \left[-\frac{1}{R^{2}} - \frac{K_{1}}{R^{2}}\left\{R^{2}k_{m}^{4} + 2(K_{2}+v)k_{m}^{2}n^{2} + \frac{n^{4}}{R^{2}}\right\}\right]\gamma_{m}$$

$$= \frac{\rho}{K_{\text{extension}}}\omega^{2}\gamma_{m}$$
(6c)

After the arrangement of terms, the above system of the equation is transformed into matrix notation and an eigen-value problem is produced to designate the vibration frequency equation for SWCNTs:

Table 1. Axial wave numbers for different boundary conditions.

Boundary conditions	Wave numbers k_m
Simply supported-simply supported	$\frac{m\pi}{L}$ $(2m+1)\pi$
Clamped-clamped	$\frac{(2m+1)\pi}{2L}$ $(4m+1)\pi$
Clamped-simply supported	$\frac{(4m+1)\pi}{4L_{1}}$
Clamped-free	$\frac{(2m-1)\pi}{2L}$

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{pmatrix} \alpha_m \\ \beta_m \\ \gamma_m \end{pmatrix}$$

$$= \frac{\rho}{K_{\text{extension}}} \omega^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{pmatrix} \alpha_m \\ \beta_m \\ \gamma_m \end{pmatrix}$$
(7)

where the entries A_{ij} , (i, j = 1, 2, 3) are labeled in the Appendix A. The eigenvalues are associated with vibration frequencies of SWCNTs and the vector $(\alpha_m, \beta_m, \gamma_m)^T$ represents their mode shapes.

4 Results and discussion

In this section, the fundamental frequencies for SWCNTs are presented and analyzed for various physical parameters. The purpose of numerical study of these tubes is to predict frequencies to estimate the expected experimental values. The choice of analytical technique to study this problem is to be considered such that the procedure should be simple, easily applicable and yields results robustly. The influence of boundary conditions on free vibrations of these carbon nanotubes is investigated using wave propagation approach. This approach is capable to tackle vibration study of structure elements like beams, plates and shells. Since the structures of carbon nanotubes are similar to those of cylindrical shells. The mathematical theories and techniques which are applied for the shells equally cater for study of these tubes. There are three forms of these single-walled nanotubes as: (i) armchair, (ii) zigzag, (iii) chiral. Analysis of vibrations of armchair type of carbon nanotubes is performed for following end conditions: clamped-clamped (C-C), clamped-simply supported (C-SS), simply supported-simply supported (SS-SS) and clamped-free (C-F). However results for more boundary conditions may be determined by the present procedure. The challenge is to select the appropriate material properties and the tube thickness for obtaining new results. In the literature, one finds a range of material properties and tube thickness that researches have suggested for use. We shall adopt the material properties and tube thickness as suggested in Wang and Zhang (2007). For example, the reported operative thickness of SWCNTs ranges from 0.0612 to 0.69 nm is provided in Yakobson et al. (1996), Vodenitcharova and Zhang (2003),

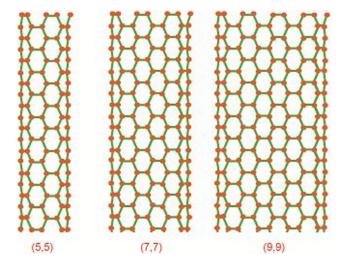


Figure 3. Shows the schematic variation of (5, 5), (7, 7) and (9, 9) armchairs nanotubes.

Hernandez et al. (1999), Tu and Ou-Yang (2002), Wang et al. (2005). The value of $K_{\text{extension}}$ obtained in most of previous studies (see Yakobson et al., 1996; Lu, 1997; Jin and Yuan, 2003; Wang et al., 2005; Chen and Gao, 2006; Robertson et al., 1992) mainly falls in the range of 330 to 363 J m⁻² and v varies from 0.14 to 0.34. Variations of vibration frequencies are obtained for length, L and tube thickness-toradius ratio, h/R of the nanotubes. The lattice translation indices (n, m) for armchair nanotubes can be inscribed as (n, n)by taking m = n. Results are obtained for a large number of parameters combinations which occurs in vibration analysis of these tubes. The eigen frequencies are calculated against length, Lfor radii 678, 1356 and 2034 nm for armchairs (5, 5), (7, 7) and (9, 9) with thickness-to-radius ratio, h/R for armchairs (5, 5), (7, 7), and (9, 9). The schema for armchairs with indices (5, 5), (7, 7) and (9, 9) are demonstrated in Fig. 3.

Figure 4 demonstrate variations of eigen-frequencies with the length, L of carbon nanotube for boundary conditions of the type: clamped-clamped (C-C), clamped-simply supported (C-SS), simply supported-simply supported (SS-SS) and clamped-free (C-F). It shows that as L is enhanced, then the natural frequencies are decreased for these boundary conditions. Chawis et al. (2013) determined frequencies against the aspect ratio (L/D) for different boundary conditions. The frequency values diminish as (L/D) is made to increase. The graphical presentation of the present results matched with those sketched by Chawis et al. (2013) demonstrating a good agreement between the two studies. At L = 10 to 20 nm, the frequencies decreased rapidly and for L = 20 to 30 nm, the frequencies are moderately parallel. The variations of natural frequencies (Hz) versus length L (nm) also shows a good agreement with those effects assessed by Bocko and Lengvarský (2014). All frequency curves meet at $L = 70 \,\mathrm{nm}$ for the boundary conditions where these curves figured by

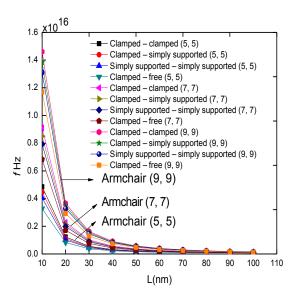


Figure 4. Variations of fundamental frequencies with length (L) for armchair (5, 5), (7, 7) and (9, 9) when radii R = 678 nm, R = 1356 nm, and R = 2034 nm, h = 0.1 nm for different boundary conditions.

Bocko and Lengvarský (2014) met at L = 80 nm. It shows a good coincidence between the two sets of results. For long single-walled carbon nanotubes, the influence of boundary conditions is insignificant. Influence of boundary conditions is prominent at small length L = 10, 20, 30,and 40nm. The influence of the boundary conditions is moderately negligible for length L = 80, 90, and 100 nm. Zhang et al. (2009) found frequencies versus the length-to-diameter ratio (L/D)which have a good agreement with the present results. The frequency curves obtained here overlapped with those curves obtained by Zhang et al. (2009). For the clamped-clamped boundary conditions, armchairs SWCNTs with indices (5, 5), (7, 7), (9, 9) have the highest frequencies followed by clamped-simply supported, simply supported-simply supported and clamped-free conditions. So lowest frequencies are associated with clamped-free end conditions, for varying length, L.

Figure 5 shows the dependencies of eigen-frequencies on the tube thickness-to-radius ratio, h/R of carbon nanotubes for boundary conditions: clamped-clamped (C-C), clamped-simply supported (C-SS), simply supported-simply supported (SS-SS) and clamped-free (C-F). As h/R is increased, the frequencies (Hz) go up for these boundary conditions correspondingly. As h/R varies from 0.30 to 0.48 nm, the corresponding four frequency curves seem to get parallel. It is perceived that for higher values of h/R ratio, the frequencies for armchairs type SWCNTs with indices (5, 5), (7, 7), (9, 9) travelling modes are always higher than those for smaller, h/R ratios. This enhancement in the frequencies with the h/R ratios is the result of the increase in the stiffness created due to carbon nanotubes thickness. The variations of

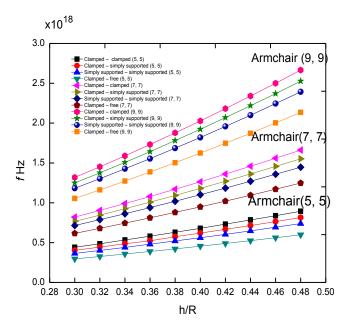


Figure 5. Variation of fundamental frequencies (Hz) with tube thickness-to-radius ratio h/R for armchairs (5, 5), (7, 7), (9, 9), L=2.4 nm for different boundary conditions.

natural frequencies (Hz) versus tube thickness-to-radius ratio h/R shows a good agreement with those results evaluated for the vibration of cylindrical shell. Behavior of these variation of natural frequencies versus tube thickness-to-radius ratios is similar to that is observed for vibrating cylindrical shells by Xiang et al. (2012), who analyzed the natural frequency versus to thickness-to-radius ratios for these shells. Effect of these boundary conditions is seen moderately more pronounced for higher values of h/R ratio. It is observed from the figure that for clamped-clamped boundary condition for armchair SWCNTs (5, 5), (7, 7), (9, 9) have the highest frequencies followed by clamped-simply supported, simply supported-simply supported and clamped-free. Frequencies associated with clamped-free conditions have lowest values. It is inferred that the follow of natural frequency curves is similar against h/R ratios for armchairs indices (5, 5), (7, 7), (9, 9) travelling modes. In the start frequency curves are more closed and seem to get wider as the values of h/R ratio are increased. The gap in the frequency curves associated with clamped-free and simply supported-simply supported boundary conditions for SWCNTs with indices (5, 5), (7, 7) and (9, 9) is more than that is seen between the adjacent curves related with clamped-simply supported, simply supportedsimply supported and clamped-clamped for the SWCNTs. This behavior is due to the physical constraints involved in these end conditions.

5 Conclusions

In the present work, influence of boundary conditions on vibrations of single-walled carbon nanotubes has been analyzed for armchair type with indices (5, 5), (7, 7), (9, 9). The problem has been investigated by the wave propagation approach (WPA). Spectra of frequencies for the armchair carbon nanotubes have calculated against for length and thickness-to-radius ratio. The eigen-frequencies are given for three values of radius of the carbon nanotubes. Variations of the natural frequencies of these are observed for the tube lengths and tube thickness-to-radius ratios and boundary conditions. Since a boundary condition is defined by adding some physical constraints, frequency variations are obvious noted for boundary conditions and they have a very promi-

nent effect on vibrations of the single-walled carbon nanotubes (SWCNTs). This influence is very visible for smaller values of length, L and larger values of h/R ratio. This investigation presents a good application of wave propagation approach in the arena of CNTs vibrations. Finally, it is concluded that the presented CSM method is an alternative best choice to examine the overall vibration behavior of SWCNTs. The present investigation may be helpful in study of MWCNTs vibrations like considering aspects of high frequency oscillators and mechanical sensors.

Data availability. All the data used in this manuscript can be obtained by requesting from the corresponding author.

Appendix A

$$\begin{split} A_{11} &= k_m^2 + \frac{1-v}{2R^2} n^2 \\ A_{12} &= i k_m \frac{1+v}{2R} n \\ A_{13} &= -i k_m \frac{v}{R} \\ A_{21} &= -n \frac{1+v}{2R} i k_m \\ A_{22} &= -\left[-\frac{1+v}{2} k_m^2 - \frac{n^2}{R^2} - \frac{K_1}{R^2} \left\{ K_2 k_m^2 + \frac{n^2}{R^2} \right\} \right] \\ A_{23} &= -\left[\frac{n}{R^2} + \frac{K_1}{R^2} \left\{ \frac{n^3}{R^2} + (K_2 + v) n k_m^2 \right\} \right] \\ A_{31} &= \frac{v}{R} i k_m \\ A_{32} &= -\left[-\frac{n}{R^2} + \frac{K_1}{R^2} \left\{ (2K_2 + v) k_m^2 n + \frac{n^3}{R^2} \right\} \right] \\ A_{33} &= -\left[-\frac{1}{R^2} - \frac{K_1}{R^2} \left\{ R^2 k_m^4 + 2(K_2 + v) k_m^2 n^2 + \frac{n^4}{R^2} \right\} \right] \end{split}$$

Appendix B

Table B1. Nomenclature.

$\alpha_m, \beta_m, \gamma_m$	The amplitudes of vibration	k_m	Axial wave number
L	Length of the tube	v	Poisson's ratio
u, v, w	Axial, circumferential and radial displacements	R	Radius of single walled carbon nanotube
(x, θ, t)	Orthogonal coordinate system	ω	Angular frequency
h/R	Thickness-to-radius ratio	G	Shear modulus
f	Vibrational natural frequency	E	Young's modulus
		ρ	Mass density

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