Chapter 5

Vibrational Behavior of Single-Walled Carbon Nanotubes Based on Donnell Shell Theory Using Wave Propagation Approach

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Additional information is available at the end of the chapter

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Abstract

This chapter is concerned with the vibration analysis of single-walled carbon nanotubes (SWCNTs). This analysis is based on the Donnell thin shell theory. The wave propagation approach in standard eigenvalue form has been employed in order to derive the characteristic frequency equation describing the natural frequencies of vibration in SWCNTs. The axial modal dependence is measured by the complex exponential functions implicating the axial modal numbers. Vibration frequency spectra are gained and evaluated for physical parameter like length-to-diameter ratios. The dimensionless frequency is also investigated in armchair and zigzag SWCNTs with in-plane rigidity and mass density per unit lateral area for armchair and zigzag SWCNTs. These frequencies of the SWCNTs are computed with the aid of the computer software MATLAB. These results are compared with those obtained using molecular dynamics (MD) simulation and the results are somewhat in agreement.

Keywords: vibration analysis, wave propagation approach, Donnell thin shell theory, single-walled carbon nanotube

1. Introduction

Iijima [1] discovered the carbon nanotubes (CNTs) in 1991 and the uses of carbon nanotubes (CNTs) have been originate in various areas such as electronics, optical, medicine, charge detectors, sensors, field emission devices, aerospace, defense, construction and even fashion. To study their remarkable properties, a bulk of research work was performed for their high springiness and characteristic ratio [2], a very effective Young modulus and tensile potency [3], well-bonding

strength and superconductivity between carbon atoms [4]. Study of free vibrations of these tube have has been examined with regard to their properties and material behavior. For their useful applications, it needs more explorations to examine vibration characteristics of SWCNTs.

Poncharal et al. [5] and Treacy et al. [6] conducted the experiments, the resonance frequency of multi-walled carbon nanotubes for clamped-free excited by electrical loads or thermal were detected in a transmission electron microscope (TEM). Thermal vibrations of SWCNTs have been performed for natural frequencies by Molecular dynamics (MD) to predict the Young's modulus by Zhao et al. [7].

The behaviors and material properties of CNTs using either or continuum mechanics modeling or atomistic modeling have been conducted in Wang et al. [8]. For the analysis of CNTs, when compared to continuum mechanics modeling, atomistic modeling is an easy approach and relatively inexpensive. Consequently, the development of continuum mechanics model has attracted much attention of researchers; especially after Yakobson et al. [9] showed that the results obtained using continuum mechanics modeling and molecular dynamics (MD) simulations are in good agreement.

A comprehensive molecular dynamics (MD) study for the contraction and thermal expansion behaviors on different mode of vibration analysis carried by Cao et al. [10]. The fundamental frequency for deformed clamped-clamped shift of SWCNTs under torsion, bending and axial loadings investigated by them. Lordi and Yao [11] performed molecular dynamic (MD) simulations to determine the Young's modulus and thermal vibration frequencies of SWCNTs using the universal force field with various clamped-free conditions based on the Euler beam theory. Carbon nanotubes model of chiral SWCNTs for analyzing their resonant frequency are developed by Hsu et al. [12] and these tubes were observed under a thermal vibration. The model used for implicating the shear deformation and rotatory inertia was Timoshenko beam model. Chawis et al. [13] and Bocko et al. [14] used nonlocal theory of elasticity for the vibration analysis of SWCNTs. An analysis of vibration characteristics of SWCNTs was examined by Yang et al. [15] and initiated this analysis is based on Timoshenko beam model for nonlocal theory. A number of end conditions have interpreted by Azrar et al. [16–17] for the vibrations of these tubes. Recently, vibration behaviors of SWCNTs have been investigated by some researchers [18, 19, 20].

To examine the feasibility of SWCNTs as a nano-resonator, the molecular structural mechanics method was employed by Li and Chou [21] .The predicted fundamental frequencies were perceptive to dimensions such as diameter, length along with boundary conditions clamped-free or clamped SWNTs, but the frequencies are correlatively imperceptive to chirality of the tubes. The vibration and buckling aspects of carbon nanotubes using nonlocal Donnell shell theory was examined by Ansari et al. [22, 23].

Vibration analysis of SWCNTs is examined by using the present approach with clamped-clamped and clamped-free vibration. Single-walled carbon nanotubes (SWCNTs) have three distinctive structures as: (i). armchair (ii). zigzag (iii) chiral. These structures have different properties but their vibrational behavior is less clear according to the regarding situation. Vibration analysis of armchair and zigzag type of carbon nanotubes is executed for following boundary conditions: clamped-clamped (C-C), and clamped-free (C-F). Variations of dimensionless frequencies are attained for length-to-diameter ratio.

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Here an analytical investigation of single-walled carbon nanotubes is conducted for extracting their vibration characteristics. The study of free vibration of SWCNTs is done based on cylindrical shell model. This analysis based on the Donnell thin shell theory. These shell dynamics equations are solved by wave propagation approach. The Donnell shell theory based on WPA is, therefore, another choice of powerful research technique of CNTs whose results are applicable in the limit of acceptable statistical errors than the earlier used BM and other approaches [3–6, 22, 23]. The shell frequency equation is formulated in the eigenvalue form. To provide the complete characteristic of vibrational behavior of SWCNTs by using wave propagation approach is studied in the present chapter. Results are obtained for various material parameters. The dimensionless frequency is also investigated in armchair and zigzag SWCNTs with in-plane rigidity. Now the gape is that there is no research to find directly the dimensionless frequencies of SWCNTs based on cylindrical shell model by using wave propagation approach. However, to the best of authors' knowledge, to find the frequency of SWCNTs, there is no research works on the vibration analyses of zigzag, armchair SWCNTs based on cylindrical shell using wave propagation approach. These frequencies of the SWCNTs are computed with the aid of the computer software MATLAB and these results are compared against MD simulation results in order to assess the accuracy and validity of the cylindrical shell model for predicting the vibration frequencies of SWCNTs.

2. Theoretical formation

2.1. Cylindrical shell model for the vibration of SWCNT

Carbon nanotubes have two kinds, which are single-walled carbon nanotubes and multi-walled carbon nanotubes. Actually multi-walled carbon nanotubes are singled walled carbon nanotubes that are coaxially interposed with different radii. When a graphene sheet rolled up into one time, then it becomes a SWCNTs to produce a hollow cylinder but with end caps. A schema of graphene sheet and single-walled carbon nanotube are shown in **Figure 1**.

Armchair and zigzag nanotubes are made when chiral angle is equal to 0 and 30 respectively and both are the limiting cases with (m, m) and (m, 0). The structure of single-walled carbon nanotubes is similar to the circular cylinders with regard to geometrical shapes as shown in **Figure 2**. So, the motion equations for cylindrical shells are utilized for studying the free vibrations of SWCNTs. According to the Donnell thin shell theory (He et al. [24]), the governing equation of motion for free vibration of a CNTs is used. Where v_1, v_2, and v_3 are the longitudinal, circumferential, and radial displacements of the shell, R is the radius of the shell, Eh is the in-plane rigidity, ρh is the mass density per unit lateral area, t is the time and ν is the Poisson ratio.

It is assumed that for the representation of the modal deformation displacement functions in the axial, circumferential and radial directions are $v_1(x, \theta, t)$, $v_2(x, \theta, t)$ and $v_3(x, \theta, t)$ correspondingly. The three unknown displacement functions for SWCNTs executing vibration, a system of PDE is given as:

$$\frac{\partial^2 v_1}{\partial x^2}+\frac{1-\nu}{2R^2}\frac{\partial^2 v_1}{\partial \theta^2}+\frac{1+\nu}{2R}\frac{\partial^2 v_2}{\partial x \partial \theta}-\frac{\nu}{R}\frac{\partial v_3}{\partial x}=\frac{(1-\nu^2)\rho h}{Eh}\frac{\partial^2 v_1}{\partial t^2} \tag{1}$$

$$\frac{1+\nu}{2R}\frac{\partial^2 v_1}{\partial x \partial \theta}+\frac{1-\nu}{2}\frac{\partial^2 v_2}{\partial x^2}+\frac{1}{R^2}\frac{\partial^2 v_2}{\partial \theta^2}-\frac{1}{R^2}\frac{\partial v_3}{\partial \theta}=\frac{(1-\nu^2)\rho h}{Eh}\frac{\partial^2 v_2}{\partial t^2} \tag{2}$$

$$\frac{\nu}{R}\frac{\partial v_1}{\partial x}+\frac{1}{R^2}\frac{\partial v_2}{\partial \theta}-\left(\frac{1}{R^2}+\frac{(1-\nu^2)}{Eh}.D\left(\frac{\partial^4 v_3}{\partial x^4}+2.\frac{1}{R^2}\frac{\partial^4 v_3}{\partial x^2 \partial \theta^2}+\frac{1}{R^4}\frac{\partial^4 v_3}{\partial \theta^4}\right)\right)=\frac{(1-\nu^2)\rho h}{Eh}\frac{\partial^2 v_3}{\partial t^2} \tag{3}$$

where $D=\frac{Eh^3}{12(1-v^2)}$ denotes the effective bending stiffness.

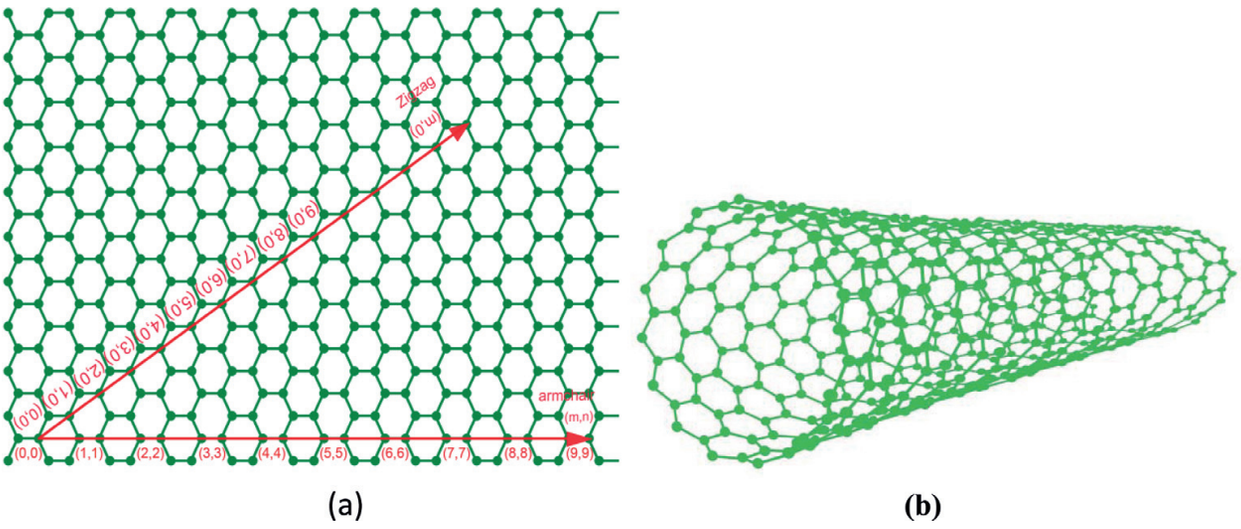

Figure 1. Hexagonal lattice (a) graphene sheet (b) single-walled carbon nanotube.

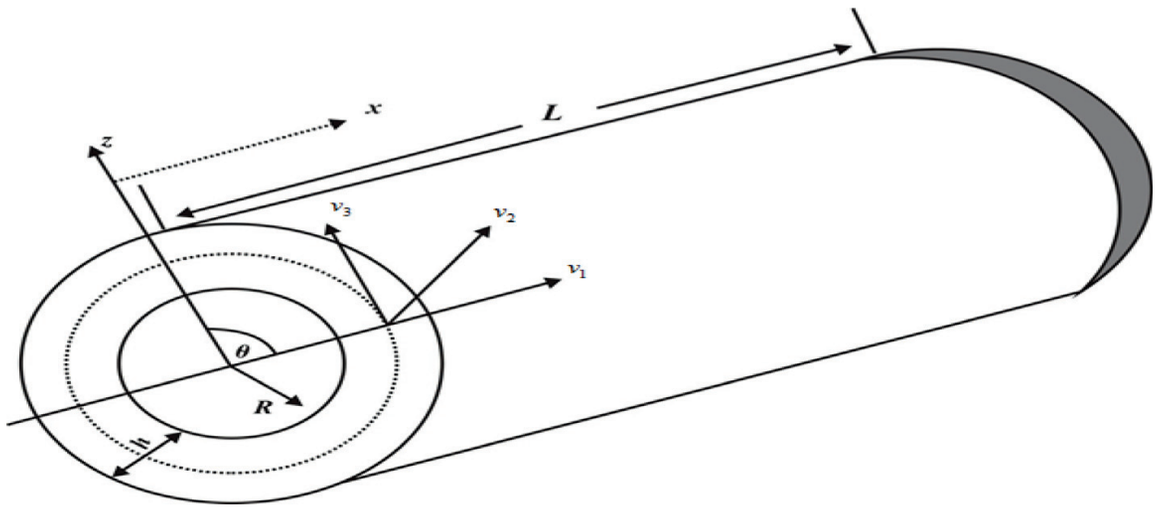

Figure 2. Geometry of SWCNTs.

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2.2. Applications of the wave propagation approach

An efficient and a simple technique which corporate as wave propagation approach is employed for the solution of CNT problem in the form of differential equation. Before this, present method has been successively used for the study of shell vibrations [25–27]. The axial coordinate and time variable are denoted by x, t correspondingly and the circumferential coordinate signifies by θ. The functions $v_1(x,\theta,t)$, $v_2(x,\theta,t)$ and $v_3(x,\theta,t)$ are used to designate their respective displacement deformation function. So for modal deformation displacements are written in the assumed expression as:

$$v_1(x,\theta,t) = p_m e^{-ik_m x}\cos(n\theta)e^{\omega t} \tag{4}$$

$$v_2(x,\theta,t) = q_m e^{-ik_m x}\sin(n\theta)e^{\omega t} \tag{5}$$

$$v_3(x,\theta,t) = r_m e^{-ik_m x}\cos(n\theta)e^{\omega t} \tag{6}$$

where p_m, q_m and r_m stand for three vibration amplitude coefficients in the axial, circumferential and radial directions. The axial half and the circumferential wave numbers are denoted by m and n respectively and angular frequency is designated by ω. The formula for fundamental frequency f which is written as: $f = \omega/2\pi$. Where k_m is the axial wave number related with an end conditions. Using the expressions for $v_1(x,\theta,t)$, $v_2(x,\theta,t)$, $v_3(x,\theta,t)$ and their partial derivatives in applying the product method by substituting the modal displacement functions for partial differential equations, the space and time variable are split.

After putting Eqs. (4)–(6), into Eqs. (1)–(3), the above equations is transmuted in matrix representation after the arrangement of terms, and to designate the vibration frequency equation for SWCNTs, an eigenvalue problem is formed:

$$\begin{bmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{bmatrix} \begin{pmatrix} p_m \\ q_m \\ r_m \end{pmatrix} = \frac{(1-\nu^2)\rho h}{Eh}\omega^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{pmatrix} p_m \\ q_m \\ r_m \end{pmatrix} \tag{7}$$

The form of non-zero solution of (p_m, q_m, r_m) yields the vibration frequency and associated modes for SWCNTs. The expressions for the terms L_{ij} 's are given in the Appendix-I. Where the roots of the equation furnish the frequencies. The lowest root corresponds to the frequency of vibration. It is clear that the frequency should be minimized with respect to the wave numbers m, n in order to obtain the frequency of vibration.

3. Result and discussion

The vibration frequency spectra for SWCNTs are evaluated by Eq. (3) based on Donnell thin cylindrical shell theory. Variations of the frequencies are obtained with regard to the material properties and tube thickness. Keeping in view of this aspect, the natural frequencies of the

longitudinal clamped-free vibration of SWCNTs with a length 6.92 nm are first determined by the MD simulation. The E/ρ ratio as measured from molecular dynamic simulation is $3.6481 \times 10^8 m^2/s^2$. By applying this ratio on the longer tube having length 14.4 nm is simulated by MD simulation. The results were found to be same, demonstrating the unconventionality of the ratio on the length. We shall adopt the material properties and tube thickness as suggested by Zhang et al. [18], i.e. the in-plane rigidity Eh =278.25 Gpa·nm, E/ρ=$3.6481 \times 10^8 m^2/s^2$, Poisson's ratio ν = 0.2. The in-plane stiffness or rigidity is computed as Eh = 278.25 GPa.nm which is based on the E/ρ ratio, to calculate the natural and dimensional frequencies of vibration using wave propagation approach, the ratio E/ρ= 3.6481×10^8 m^2/s^2 is used throughout this study. For example, the range of reported thickness is from 0.0612 to 0.69 nm in [9, 28–29] and v varies from 0.14 to 0.34. Considering a diameter d = 6.86645×10^{-10} m, the vibration frequencies for Single-walled carbon nanotubes of various length-to-diameter ratios are calculated using Eq. (3). In present model, the effects of different length-to-diameter ratio for clamped-clamped and clamped-free boundary condition have been considered and matched quantitatively with MD results as well as for the validity and to assure the accuracy. In this study, all frequency results are presented in THz unless otherwise stated. In present study, the frequencies of SWCNTs are obtained by using the some parameters which are compared with MD simulation and continuum shell. However the MD results were obtained for a clamped-clamped SWCNT. Two sets of result are compared as shown in the **Tables 1** and **2**.

It can be observed that the results which are obtained from present model, the values are nearer to the molecular dynamics results when the length-to-diameter ratio is greater than 10.26. From **Table 1**, one can notice that the average percentage error between MD results is approximately 3.6%. This fact shows that the results obtained by present method and earlier MD simulation model are in good agreement.

3.1. Vibration of clamped-clamped and clamped-free SWCNTs

In the application of micro-oscillators and micro or nano-strain sensors, the carbon nanotube sensor is generally clamped with both ends [30]. The clamped-clamped and clamped-free single-walled carbon nanotubes have been performed by atomistic simulations [20–21, 31]. In this section, the distinctive first and third mode frequencies for the set of clamped-clamped single-walled carbon nanotubes is given by present models for their vibration frequencies and

L/d	Frequencies (THz)		
	Present	MD	Percentage error
6.67	0.67832	0.64697	4.85
8.47	0.44146	0.43335	1.87
10.26	0.30922	0.30518	1.32
13.89	0.17360	0.18311	−5.19

Table 1. Comparison of frequencies of C-C SWCNT with MD simulation for the first vibration mode.

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L/d	Frequencies (THz)		
	Present	MD	Percentage error
4.67	0.17074	0.23193	−26.38
6.47	0.09048	0.12872	−29.70
7.55	0.06678	0.1000	−31.61
8.28	0.05566	0.07935	−29.85
10.07	0.03777	0.05493	−31.23

Table 2. Comparison of frequencies of clamed-free SWCNT for the first vibration mode.

compared with molecular dynamic simulations and Timoshenko beam model with thicknesses h = 0.34 nm. The results are in good agreement with the MD and Timoshenko beam model results showing same trend in the open literature.

The first and third mode natural frequencies accessed by present model and compared with MD simulations are depicted graphically in **Figure 3** respectively. It can be observed from **Tables 1** and **2** that the length-to-diameter ratio of the set of C-C SWCNTs is somewhat dissimilar from that of C-F SWCNTs. For the prediction of mechanical characters [7, 19–21] from atomistic studies and the experimental studies [5, 6, 33–38] are often used for the clamped-free carbon nanotubes. The frequencies for the first and third modes obtained from present model which is compared with molecular dynamic simulation and Timoshenko beam model are shown in **Figure 3**. It can be readily seen that higher frequencies are produced by higher modes and when length-to-diameter ratio rises at each mode then frequency falls down smoothly as shown in **Figure 3**. The relationship between the length-to-diameter ratios and

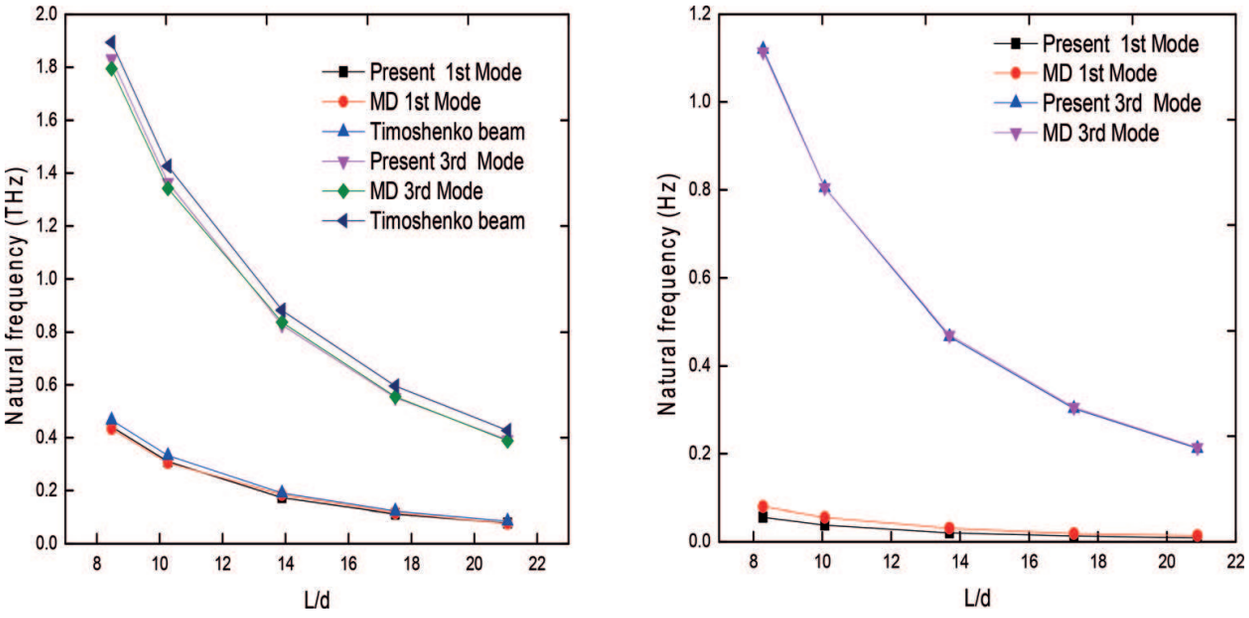

Figure 3. Comparison of numerically obtained results for clamped-clamped and clamped-free frequencies of SWCNTs for first and third mode versus length-to-diameter ratio L/d with MD by Cao et al. [32] and Timoshenko beam model [18].

natural frequencies is inversely proportional indicates that the vibrations are very sensitive due to long tube and since the SWCNTs are of almost the same diameter. The results for SWCNTs given by MD are little bit higher than the frequencies investigated by the present model. In MD simulation, the frequencies of length-to-radius ratio are 8.28 is 0.0793 and at 20.89 is 0.0138. But in the present model, the frequencies at 8.28 are 0.05566 and at 20.89 is 0.00883, when compared to the MD results.

3.2. Vibration of SWCNTs with dimensionless frequency

Furthermore, the parametric study for the vibrational behavior of SWCNTs with dimensionless is carried out and presented in **Figure 4**. Alibeigloo et al. [39, 40] and Soldatos et al. [41] used the dimensionless frequency for multi-walled carbon nanotubes and for thin cylindrical shell with respect to length-to-radius ratio respectively. This frequency is associated with frequency Ω through the following formula: $\Omega = \omega R\sqrt{\frac{\rho}{E}}$. A variation of non-dimensional frequency versus length-to-diameter ratio is presented in **Figure 4**. This figure shows that, increasing the value of length-to-diameter ratio as well as there is a decrease in dimensionless frequency. From the physical point of view, it is noted that when the length of SWCNTs becomes small, the effect of the atomic interactions among a reference point and all other atoms becomes significant.

Figure 4 shows an armchair and zigzag CNT, vary the length-to-diameter ratio from 8.3 to 20.9 will change the dimensionless frequency from 0.0385 to 0.0063 THz in case of clamped-clamped boundary condition. Likewise, in clamped-free condition it changes from 1.2827 to 0.5094 THz in armchair case. It may be seen from the above **Figure 4** that the resulting value of dimensionless frequency decreases with the increase in length-to-diameter ratio. Now in

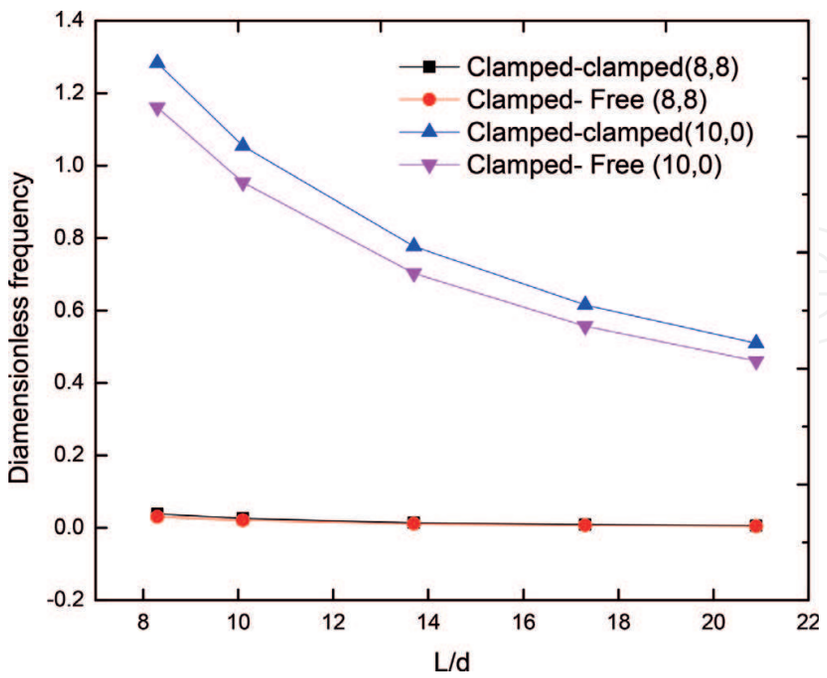

Figure 4. Variations of dimensionless frequencies of CC and CF armchair and zigzag SWCNTs.

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zigzag CNT, changing the length-to-diameter ratio from 4.86 to 35.53, the dimensionless frequency changes from 0.0303 to 0.0049 THz in case of clamped-clamped boundary condition. Likewise, in clamped-free condition it varies from 1.16605 to 0.4609 THz.

3.3. Vibration of SWCNTs with in-plane rigidity

For the results generated so far, the nanotube in-plane rigidity has been taken to be *Eh* =278.25 Gpa·nm. However, there exist some inconsistencies concerning this quantity in the literature. The reported CNT in-plane stiffness is largely scattered, ranging from *Eh* =300 Gpa·nm to *Eh* = 400 Gpa·nm [42]. Both set of **Figure 5** is presented to investigate the influence of the in-plane rigidity *Eh* variation on the dimensionless frequency of a (7, 7) armchair and (9, 0) Zigzag SWCNT with different boundary conditions likewise as clamped-clamped and clamped-free boundary conditions. These figures shows that for all the selected boundary conditions, dimensionless frequency calculated via shell model are sensitive to the nanotube in-plane rigidity *Eh* and also the larger the in-plane rigidity in-plane rigidity *Eh*, the higher the dimensionless frequency. The difference is more considerable for shorter length CNTs.

Previous study reveals that the bending rigidity of SWCNTs should be considered as an independent material parameter not linked to the representative thickness by the classic bending rigidity formula, i.e., $D = Eh^3/12(1-\nu^2)$ and the actual bending rigidity of SWCNTs is lesser than its classical counterpart [43, 44]. For shorter length-to-diameter ratio, the value of dimensionless frequencies for clamped-clamped at *Eh* = 300 Gpa·nm, *Eh* = 400 Gpa·nm is 0.04863, 0.05788, respectively which shows that a slight increase in frequency due to increase of in-plane rigidity *Eh*. Same trend is observed for dimensionless frequency. For the present shell model with in-plane rigidity *Eh*, the values of the C-F single-walled carbon nanotubes respectively, which are a little lower than those of corresponding CC SWCNTs with bending rigidity are plotted in **Figure 5**.

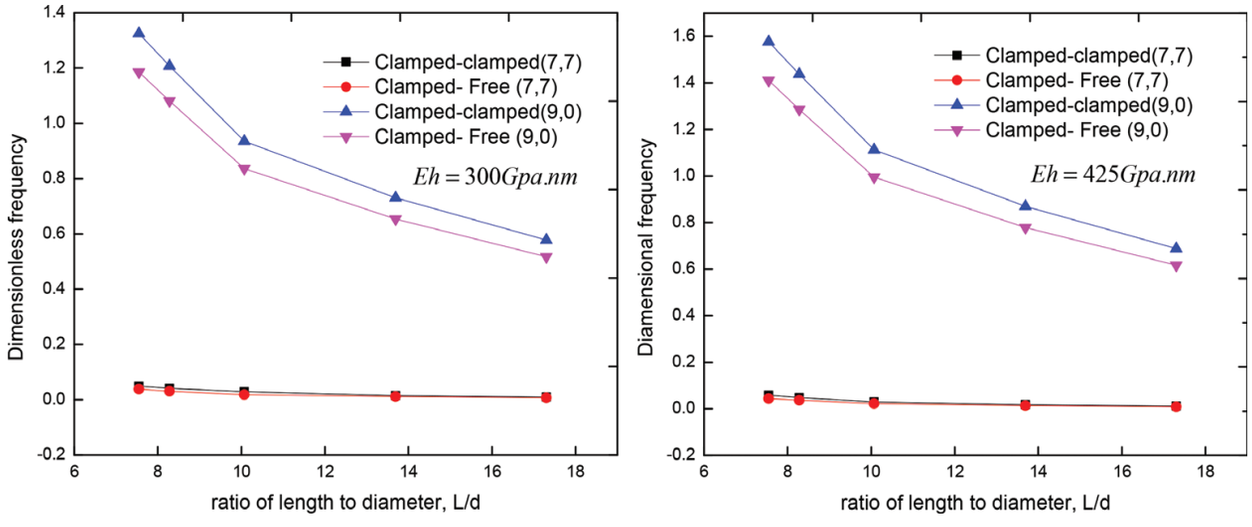

Figure 5. Variations of dimensionless frequencies Ω of CC and CF armchair and zigzag SWCNTs when *Eh* = 300 GPa.Nm and *Eh* = 425Gpa.Nm.

3.4. Vibration with mass density per unit lateral area

Figure 6 is presented to investigate the influence of the mass density per unit lateral area variation on the dimensionless frequency of a (12, 12) armchair and (14, 0) zigzag SWCNT with boundary conditions: clamped-clamped and clamped-free. These figures shows that for all the selected boundary conditions, the frequency calculated via shell model are sensitive to the nanotube mass density and also the larger the mass density per unit lateral area ρh, lower the frequency. It is observed that applying the mass density per unit lateral area ρh to the present shell model, yields the slight decrease of the frequency. For shorter length-to-diameter ratio, the value of dimensionless frequencies at ρh =740.52 nm, 800.64 nm and 820.80 nm is 0.3667, 0.03342, 0.03128 respectively for clamped-clamped and 1.74285, 1.71298, 1.6001 respectively for clamped-free, which shows that decreases in frequency. For the present shell model, the values of length-to-diameter ratio for C-C SWCNTs, which are a little higher than those corresponding C-F SWCNTs values with mass density per unit lateral area are plotted in **Figure 6**.

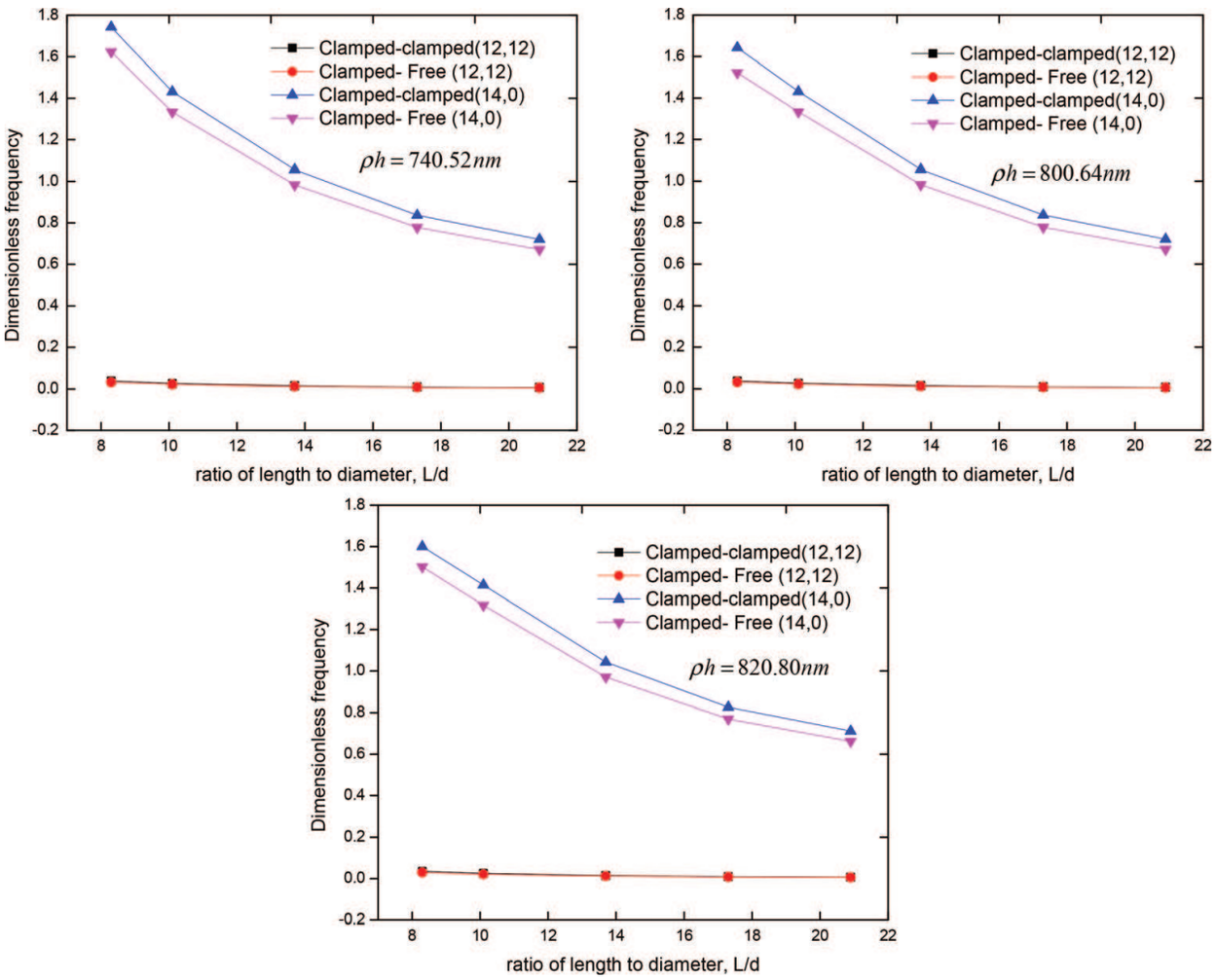

Figure 6. Variations of dimensionless frequencies of CC and CF armchair and zigzag SWCNTs when $\rho h = 740.52nm$, $\rho h = 800.64nm$ and $\rho h = 820.80nm$.

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4. Conclusions

The vibration behavior of CF and CC SWCNTs are extensively investigated by present model compared with MD simulation. With properly chosen parameters, the present models can reproduce satisfactory frequencies that are in reasonable agreement with those results obtained by MD simulations and Timoshenko beam model. The effects of the length-to-diameter ratio for armchair and zigzag CNTs with in-plane rigidity, mass density per unit lateral area on the dimensionless frequencies are also examined with present models. It is found that the frequencies decreases smoothly when length-to-diameter ratio would increases and higher mode of vibration occurred when the frequencies are higher. For a clamped-free SWCNT, their exist an inverse proportionality which is observed between the resulting frequency and length-to-diameter ratio. For clamped-clamped SWCNTs, the results took a similar trend but in this case frequency values are much higher. The results are obtained numerically for different boundary conditions and plotted in graphical forms. In the field of CNTs vibrations, wave propagation approach presents a good application. A better cylindrical shell model is needed to furnish more accurate prediction of the vibration frequencies of SWCNTs, such as the nonlocal shell theory that incorporates the effect of small length scale effect.

Appendix 1

$L_{11} = {k^2}_m + \frac{1-v}{2R^2}n^2$, $L_{12} = ik_m \frac{1+v}{2R}n$, $L_{13} = ik_m \frac{v}{R}$, $L_{21} = -n\frac{1+v}{2R}ik_m$, $L_{22} = \frac{1-v}{2}{k^2}_m + \frac{n^2}{R^2}$.

$L_{23} = \frac{n}{R^2}$, $L_{31} = -\frac{v}{R}ik_m$, $L_{32} = \frac{n}{R^2}$, $L_{33} = \frac{1}{R^2} + \frac{\left(1-\nu^2\right)}{Eh}D\left({k^4}_m + 2\frac{1}{R^2}{k_m}^2n^2 + \frac{n^4}{R^4}\right)$.

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