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Simulating vibration of single-walled carbon nanotube using Rayleigh-Ritz's method

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Abstract. In this paper, a new method based on the Sander theory is developed for SWCNTs to predict the vibrational behavior of length and ratio of thickness-to-radius according to various end conditions. The motion equation for this system is developed using Rayleigh-Ritz's method. The proposed model shows the vibration frequencies of armchair (5, 5), (7, 7), (9, 9), zigzag (12, 0), (14, 0), (19, 0) and chiral (8, 3), (10, 2), (14, 5) under different support conditions namely; SS-SS, C-F, C-C, and C-SS. The solutions of frequency equations have been given for different boundary condition, which have been given in several graphs. Several parameters of nanotubes with characteristic frequencies are given and vary continuously in length and ratio of thickness-to-radius. It has been illustrated that an enhancing the length of SWCNTs results in decreasing of the frequency range. It was demonstrated by increasing of the height-to-radius ratio of CNTs, the fundamental natural frequency would increase. Moreover, effects of length and ratio of height-to-radius with different boundary conditions have been investigated in detail. It was found that the fundamental frequencies of C-F are always lower than that of other conditions, respectively. In addition, the existence of boundary conditions has a significant impact on the vibration of SWCNTs. To generate the fundamental natural frequencies of SWCNTs, computer software MATLAB engaged. The numerical results are validated with existing open text. Since the percentage of error is negligible, the model has been concluded as valid.

Keywords: Rayleigh's method; Sander's shell theory; carbon nanotubes; MATLAB

1. Introduction

Carbon nanotubes have been firstly reported by Iijima (1991), and they contain very unique properties. Treacy *et al*. (1996) estimated through an experiment that carbon nanotubes might be useful as lightweight composite material. Due to the small dimensions of carbon nanotubes, their mechanical properties, thermal vibrations, high Young's moduli were measured by transmission electron microscope (TEM) and in tera-pascal (TPa) range. Yakobson *et al*. (1996) used continuum model for getting the reason able results with properly chosen parameters.

Since the discovery of CNTs, has become very important and interest of research due to considerable observation and research publications every year. CNTs have a variety of uses and applications in potential looking fields, some of which are charge detectors, electronics, communication, composite materials, biotechnology, environment, energy storage, chemical, and optical (Iijima 1991). Therefore, in order to effectively use of CNTs in each of these fields, it is important that their vibration characteristics are examined. Owing to the small sizes of the micro beams, they are very appropriate for designing small instruments like sensors and actuators. Large deformation of CNTs related to morphological design corresponds to the release of energy in strains-stress curve. This idea provides an accurate roadmap of nanotube behavior for researchers. Lordi and Yao (1998) started the molecular dynamic simulation using inter atomic potential function to develop a formula for approximating the tube radii. The vibration of chiral SWCNTs was calculated by Timoshenko beam model (TBM), which involves rotary inertia and shear deformation. The calculations that were performed with the cylindrical shell model differ slightly from those obtained with the MD simulation. Second method that is experimental method was used by Krishnan *et al*. (1998) for studying the properties of CNTs. Harik (2002) studied the behaviors of CNTs using beam models. He concluded that beam model can be used for the qualitative exploration of CNTs with the condition of nanotube aspect ratio is greater than 10 nm. The behavior of elements become more complicated using experimental,

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molecular dynamics and continuum models. Zhao *et al*. (2002) predicted natural frequencies by applying MD simulations. Li and Chou (2003) established a connection between structural and molecular mechanics to produce deformation in CNTs. Wang *et al*. (2005) found the frequencies of cantilever SWCNT and the results were compared with earlier computations (Krishnan *et al*. 1998). Elongated CNTs can be prepared with the extension of MWCNTs like Russian dolls (Hong *et al*. 2005). These elongated can be shortened with the oxidation of CNTs (Liu *et al*. 1998). Lu *et al*. (2007) explored new form of nanotubes and investigated the frequencies of cantilevered SWCNTs and it is concluded that the frequency can reach the GHz level when the diameter of the tube is very small. The vibrational modes and the frequency results compared with earlier researchers. Grupta and Barta (2008) the resulting frequencies of first mode which was found equal to second and third mode of SWCNTs for axial and torsional vibrations. It was observed that with the changing of diameter, the shear modulus also varies.

Murmu and Pradhan (2009) investigated the vibrational frequencies with different modes along temperature change using nonlocal small scale effects. On the other side, for length scale coefficient and soft elastic medium with embedded carbon nanotube, the nonlocal frequencies are comparatively lower. It is also found that the frequencies of the nonlocal model at different stages of temperature are higher than the nonlocal with same temperature. Sakhaee-Pour *et al*. (2009) used formulism of FEM to explore the vibration of SWCNTs. By taking the different diameter and length side, the vibration of cantilever and bridge SWCNTs is calculated. The fundamental frequencies of different categories of SWCNTs are performed by atomistic simulation and a good agreement found with MSM. Yang *et al*. (2010) demonstrated the frequencies of CNTs using nonlocal theory and geometric theory. Vibrational frequencies of zigzag SWCNTs (5, 0), (8, 0), (9, 0) and (11, 0), with different boundary conditions are considered and calculated numerically through MD simulation. The influence of nonlocal parameter on height and radius is studied in detail. Ansari *et al*. (2011) engaged Eringen's nonlocal theory based on Rayleigh-Ritz technique to obtain the frequencies of the DWCNT association with different values of ratios and parameters. The results were presented for different zigzag and armchair DWCNTs. Rafiee and Moghadam (2012) employed a 3D-FEM with reinforced polymer CNT. The shear deformation of CNTs is implicated as using TBM and results are compared with earlier simulations. The behavior of reinforced polymer CNT is evaluated both in axial and transverse direction subject to high strain loading and impact of buckling are stimulated at micro-scale. Alibeigloo and Shaban (2013) investigated the impact of nonlocal parameters on the vibration of CNTs by using the three-dimensional elastic theory based on the Fourier series expansion. It was concluded that the frequency decreased when nonlocal parameters increased. Rana *et al*. (2016) introduced the Buongiorno model analytically and numerically based on perturbation theory. The dispersion relation with applying normal modes, various parameters has been derived such as the Brownian diffusion parameters and the influence of thermophoresis.

Chawis *et al*. (2013) reported a nonlocal theory with scale length to conduct vibration of SWCNTs with Euler beam theory using nonlocal parameter. The results are obtained by classical solutions and compared with the results of FEM. In this study, effects of different geometrical boundary condition and tube chirality have been considered. They reported that different variation in the frequency observed with increasing the length, diameter and atomic arrangements. Moreover, a new pattern of frequencies observed with increasing the nonlocal parameter. Recently, CNTs are used on large scale applying synthesis method with various lengths, diameters, and chirality. There are many methods for the production of SWCNTs for the distribution of diameter and chiralities which are used in transistors and sensors (Smalley *et al*. 2006, Sanchez-Valencia *et al*. 2014). Akbaş (2016a, b, c) analyzed the size effect of nano structure plate , edge cracked microbeams and viscoelastic nanobeam using couple and modified couple stress theory. He found that if length scale parameter is set to be zero then this new classical model can attain the total energy. New expressions were gained for cracked segment of microbeam through a rotational spring by integration method. He also studied the Winkler-Pasternak foundation with the attachment of coupled theory for investigation of size effect of beam model. Besseghier *et al*. (2015) presented the nonlinear vibration of zigzag SWCNTs based on Winkler-type model. The energy-equivalent model was used for the derivation of general equation. Akbaş (2017a, b) presented the response of free and forced vibration of functionally graded nonobeam and micro beam using CST and MCST. According to exponential distribution, the material properties changes at high direction and using the Kelvin–Voigt formulation, finite element modeling within beam theory for the determination of damping effect. Mehar and Panda (2016a, b, 2018a) computed the vibration behavior, bending and dynamic response of FG reinforced CNT using shear deformation theory and finite element method. For the sake of generality, the mathematical model was presented with the mixture of Green Lagrange method. The convergence of these methodologies has been checked for the variety of results. The composite paltes with differenct greded was investigated with isotropic and core phase. Hussain and Naeem (2017) examined the frequencies of armchair tubes using proposed approach based on Flügge's shell model. The effect of length and thickness-to-radius ratios against fundamental natural frequency with different indices of armchair tube. The increment and decrement of frequency observed on increasing the thickness-to-radius ratio and length.

Akbaş (2018a, b, c) investigated the bending and cracked cantilever FG nanobeam for the damping effect, rotational effect based on coupled stree theory. He examined and discussed the solution of the dynamic problem with finite element ang Kelvin-Voigt model with the combination of Timishenko beam theory. The results were verified with the earliear published results from different theories. The effect of various geometric and material properties was investigated said theory. This investigation has opened a new window for the material researchers. Bouadi *et al*. (2018) developed the new model displacement field for the nonlocal buckling properties of single graphene sheet. The Eringen relation was used for the theoretical formation with length scale parameter. Mehar *et al*. (2018a, b, c) evaluated the frequency behavior of nanolpate structure using FEM including the nonlocal theory of elasticity. Computer generated results are created by using the software first time roubustly to check the vibration of nanoplate. The efficiency was checked by comparing the results of available data. Ebrahimi and Mahmoodi (2018) presented the static analysis of SWCNTs and vibration of CNTs using Eringen's beam theory. The bending moment and function of strain were performed with different boundary conditions. Mehar and Panda (2018b) investigated the curved shell and CNT vibration with thermal environment using higher order deformation theory. This CNT was mixed with different configurations of the layers. The results have been verified with the earlier investigations. Recently some material researchers explained the axially vibration analysis, bukling response and effect of nanofluid with cracked nanorod using nonlocal theory with coupled nonlinear equation (Akbaş 2019, Malikan 2019, Olofinkua 2018). The thermal conductivity of carbon nanotubes , analysis of Bernoulli nanobeams and wave propagation in microbeam had been investigated in detail (Ansari *et al*. 2018, Attarnejad and Ershadbakhsh 2016, Kocaturk and Akbas 2013). Boutaleb *et al*. (2019) performed the dynamic analysis of nanosize rectangular plates and beams with nonlocal quasi 3D HSDT and surface elasticity theory. The effect of various parameters such as thickness-radius ratio, aspect ratio, beam thickness, material index, surface density and surface elastic constants. Mehar *et al*. (2017a, b, c, d) studied the freqncy response of FG CNT and reinforced CNT using the simple deformation theory, finite element modeling, Mori-Tanaka scheme. They investigated a new frequency phenomenon with the combination of Lagrange strain, Green-Lagrange, for double curved and curved panel of FG and reinforced FG CNT. The charactrictics of sandwich and grades CNT Bwas found with labeling the temperarure environ. The thermoelastic frequency of single shaollow panel was determined using Mori-Tanake formaulation.The research of these authore have opened a new frequency spectrum for other material researchers. Ehyaei and Daman (2017) and Eltaher *et al*. (2019) investigated the vibration characteristics of SWCNTs and DWCNTs using initial perfection and continuum mechanics approach. The general equation of motion was obtained by Hamiltonian principle and energy equivalent model. The numerical frequencies of DWCNTs and SWCNTs were determined by Navier method and finite element method. Semmah *et al*. (2019) investigated the buckling analysis of zigzag single walled boron nitride based on Winkler foundation. The governing equation was taken into account with the shear deformation theory. Effect of different nonlocal parameter was investigated with closed form solution. Hussain and Naeem (2017) examined the frequencies of armchair tubes using proposed approach based on Flügge's shell model. The effect of length and thickness-to-radius ratios against fundamental natural frequency with different indices of armchair tube. The increment and decrement of frequency observed on increasing the thickness-to-radius ratio and length.

Many material researchers calculated the frequency of CNTs using different techniques, for example, Timoshenko beam element (Banerjee and Williams 1992), classical molecular dynamics (Han *et al*. 1997), strain gradient higher order shell and shear deformation theory (Karami *et al*. 2018, Zine *et al*. 2018); continuum models (Duan *et al*. 2007), Galerkin's method (Elishakoff and Pentaras 2009), axially loaded double beam system (Natsuki *et al*. 2009), Ritz method (Emdadi *et al*. 2019), MD simulation (Rafiee and Mahdavi 2016), Euler-Bernoulli beam mode (Bensattalah *et al*. 2018), nonlocal Timoshenko beam theory (Wu *et al*. 2018), Euler-Bernoulli's elastic beams (Kumar 2018), deformation theory (Mehar *et al*. 2016), nonlocal elasticity theory (Mehar *et al*. 2018a, b, c), Multiscale modeling approach (Mehar and Panda 2019, Mehar *et al*. 2019, Das *et al*. 2013), nonlocal elastic theory (Lee and Chang 2008, Soltani *et al*. 2016), Finite Element Method (Mungra and Webb 2015, Tserpes and Papanikos 2005), dynamic response for plates (Bakhadda *et al*. 2018, Medani *et al*. 2019, Draoui *et al*. 2019), nonlocal continuum mechanics (Narendar and Gopalakrishnan 2011), and wave propagation (El-sherbiny *et al*. 2013). The suggested method to investigate the solution of fundamental eigen relations is Rayleigh's method (RRM), which is a well-known and efficient technique to develop the fundamental frequency equations. It is keenly seen from the literature, no evidence is found regarding present model where such problem has been studied so it gave impetus to conduct present work. The proposed models are quite straightforward for the vibrational analysis of these structures of SWCNTs. Recently Hussain and Naeem (2019a, b, c, d) performed the vibration of SWCNTs based on wave propagation approach and Galerkin's method.

In this paper, based on Sander shell theory aims to investigate the vibration of SWCNTs considering the clamped-simply supported (C-SS), clamped-free (C-F), clamped-clamped (C-C), and simply supported-simply supported (SS-SS) end conditions. After developing the governing equation of the objective system, the Rayleigh's method is implemented for the purpose of obtaining the frequency equation in the eigen form. In addition, the applicability of this model for the analysis of vibration of CNTs is examined with the effect of length and ratio of height-to-radius. It has been illustrated that an enhancing the length of SWCNTs results in decreasing of the frequency range. It is demonstrated by increasing of the height-to-radius ratio of CNTs, the fundamental natural frequency would increase. The proposed model shows the vibration frequencies of armchair (5, 5), (7, 7), (9, 9), zigzag (12, 0), (14, 0), (19, 0) and chiral (8, 3), (10, 2), (14, 5) under different support conditions namely; SS-SS, C-F, C-C, and C-SS. Moreover, effects of length and ratio of height-to-radius with different boundary conditions have been investigated in detail. It is found that the fundamental frequencies of C-F are always lower than that of other conditions, respectively. In addition, the existence of

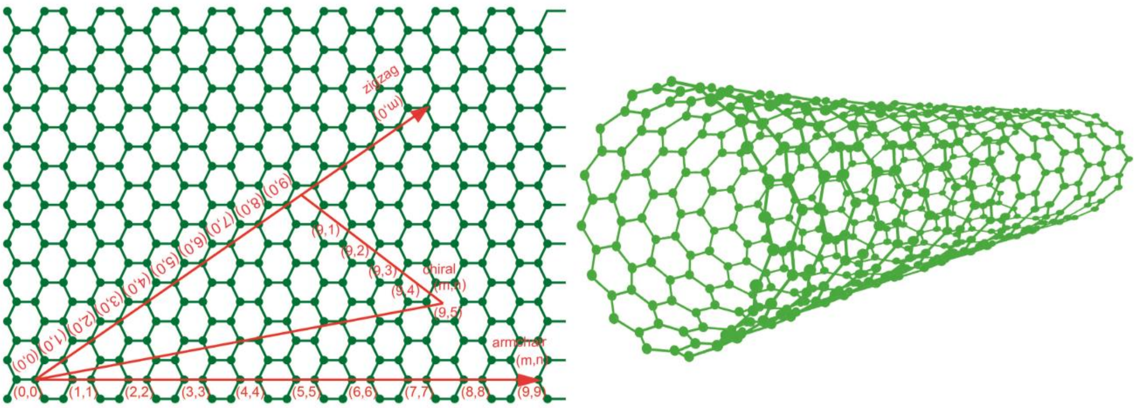

Fig. 1 Graphene sheet with indices

boundary conditions has a significant impact on the vibration of SWCNTs. To generate the fundamental natural frequencies of SWCNTs, computer software MATLAB engaged.

2. Theoretical assumptions

When a graphene sheet is rolled with its hexagonal cells, the structure can be conceptualized as SWCNTs and its circumference and quantum properties depend upon the chirality and diameter described as a pair of (n, m). In addition, the integers n and m represent the orientation of the graphene honeycomb lattice. Fig. 1 shows the orientation of the graphene sheet as, the nanotubes are zigzag, if m = 0 and nanotubes become chiral, if $n \neq m$.

The tube is assumed to have length L, thickness h and the radius R for SWCNTs with its coordinate system (x, θ, z) as shown in Fig. 2. An orthogonal system (x, θ, t) is setup for the reference surface (middle surface). The x, θ co-ordinate are assumed to be along longitudinal and circumferential direction, respectively and z-co-ordinates are taken in its radial directions.

When the material and geometrical parameters are

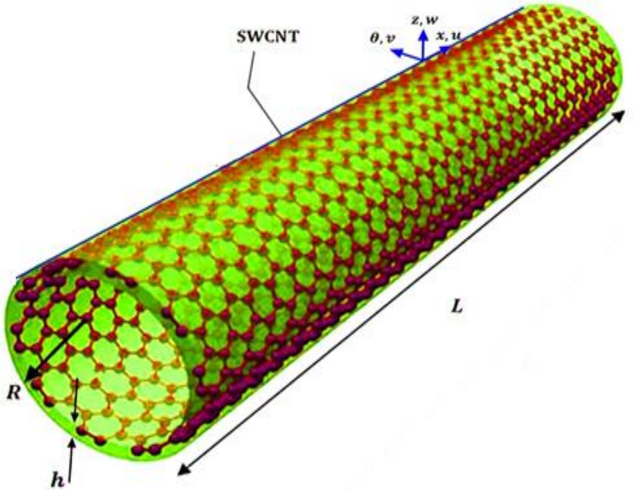

Fig. 2 Geometry of SWCNTs

considered, the formula for a strain energy, S of a vibrating cylindrical shell is expressed as

$$S = \frac{R}{2}\int_0^L\int_0^{2\pi} [A_{11} e_1^2 + A_{22}e_2^2 + 2A_{12}e_1e_2 + A_{66}e_{12}^2 \\ +2(B_{11}e_1k_1 + B_{11}e_1k_1 + B_{11}e_1k_1 \\ +B_{11}e_1k_1 + 2B_{66}e_{12}k_{12}) + D_{11}k_1^2 \\ +D_{22}k_2^2 + 2D_{12}k_1k_2 + D_{66}^2k_{12}^2]d\theta dx \quad (1)$$

where e_1, e_2 and e_3 designate the reference surface strains and k_1, k_2 and k_3 denote the reference surface curvatures respectively. The extensional stiffness, A_{ij}, coupling stiffness, B_{ij} and bending stiffness, D_{ij} are written as

$$\{A_{ij}, B_{ij}, D_{ij}\} = \int_{h/2}^{h/2} Q_{ij}\{1, z, z^2\}dz \quad (2)$$
$$(i, j = 1,2,6)$$

Here the reduced stiffness, Q_{ij}'s are written as

$$Q_{11} = Q_{22} = \frac{E}{1-v^2}, \\ Q_{12} = \frac{vE}{1-v^2}, \qquad Q_{66} = \frac{E}{2(1+v)} \quad (3)$$

for an isotropic cylindrical tube.

2.1 Application of Budiansky and Sanders' shell theory

There are found many shell/tube theories which are used to study a tube problem. A proper shell/tube theory is taken to analyze vibration of CNT. Here the strain - displacement and curvature - displacement relations are used from Budiansky and Sanders (1963) first-order linear thin shell theory. The strain-displacement relations are furnished as

$$e_{12} = \frac{\partial y}{\partial x}, \quad e_{22} = \frac{1}{R}\left(\frac{\partial v}{\partial \theta} - w\right), \quad e_{12} = \frac{\partial v}{\partial x} + \frac{1}{R}\frac{\partial u}{\partial \theta} \quad (4)$$

and the expressions for the curvature - displacement relations are represented as

$$k_{11} = \frac{\partial^2 w}{\partial x^2}, \quad k_{22} = \frac{1}{R^2}\left(\frac{\partial^2 w}{\partial \theta^2} + \frac{\partial v}{\partial \theta}\right),$$
$$k_{12} = \frac{1}{R}\left(\frac{\partial^2 w}{\partial x \partial \theta} + \frac{3}{4}\frac{\partial v}{\partial x} - \frac{1}{4R}\frac{\partial u}{\partial \theta}\right) \quad (5)$$

Making substitutions of these relations from the expression (4) and (5) into the formula (1), the tube strain energy, S takes the following forms

$$\begin{aligned} S = \frac{1}{2}\iint_{0\,0}^{2\pi L} \Bigg[& A_{11}\left(\frac{\partial u}{\partial x}\right)^2 + A_{22}\frac{1}{R^2}\left(\frac{\partial v}{\partial \theta} + w\right)^2 \\ & + 2A_{12}\frac{1}{R}\frac{\partial u}{\partial x}\left(\frac{\partial v}{\partial \theta} + w\right) + A_{66}\left(\frac{\partial v}{\partial \theta} + \frac{1}{R}\frac{\partial u}{\partial x}\right)^2 \\ & - 2B_{11}\left(\frac{\partial u}{\partial x}\right)\left(\frac{\partial^2 w}{\partial x^2}\right) - 2B_{12}\frac{1}{R^2}\left(\frac{\partial u}{\partial x}\right)\left(\frac{\partial^2 w}{\partial \theta^2} - \frac{\partial v}{\partial \theta}\right) \\ & - 2B_{12}\frac{1}{R}\left(\frac{\partial v}{\partial \theta} + w\right)\left(\frac{\partial^2 w}{\partial x^2}\right) \\ & - 2B_{22}\frac{1}{R^3}\left(\frac{\partial v}{\partial \theta} + w\right)\left(\frac{\partial^2 w}{\partial \theta^2} - \frac{\partial v}{\partial \theta}\right) \\ & - 4B_{66}\frac{1}{R}\left(\frac{\partial v}{\partial \theta} + \frac{1}{R}\frac{\partial u}{\partial x}\right)\left(\frac{\partial^2 w}{\partial x \partial \theta} - \frac{3}{4}\frac{\partial v}{\partial x} + \frac{1}{4R}\frac{\partial u}{\partial \theta}\right) \\ & + D_{11}\left(\frac{\partial^2 w}{\partial x^2}\right)^2 + \frac{D_{22}}{R^4}\left(\frac{\partial^2 w}{\partial \theta^2} - \frac{\partial v}{\partial \theta}\right)^2 \\ & + 2D_{12}\frac{1}{R^2}\left(\frac{\partial^2 w}{\partial x^2}\right)\left(\frac{\partial^2 w}{\partial \theta^2} - \frac{\partial v}{\partial \theta}\right) \\ & + 4D_{66}\frac{1}{R^2}\left(\frac{\partial^2 w}{\partial x \partial \theta} - \frac{3}{4}\frac{\partial v}{\partial x} + \frac{1}{4R}\frac{\partial u}{\partial \theta}\right)^2 \Bigg] R\,dx\,d\theta \end{aligned} \quad (6)$$

The tube kinetic energy, K of the tube is written as

$$K = \frac{1}{2}\iint_{0\,0}^{2\pi L} \rho_t \left[(\frac{\partial u}{\partial t})^2 + (\frac{\partial v}{\partial t})^2 + (\frac{\partial w}{\partial t})^2 \right] R\,dx\,d\theta \quad (7)$$

at any time, t and ρ_t designates the mass density per unit length and is written as

$$\rho_t = \int_{h/2}^{h/2} \rho\,dz \quad (8)$$

where ρ stands for the mass density and remains constant for an isotropic material. The Lagrange energy functional $\prod$ for a vibrating tube is stated as the difference between kinetic and strain energies and is expressed as

$$\prod = K - S \quad (9)$$

3. Solution methodology

Here Rayleigh's method is used to solve the CNT problem of differential equations in an efficient and comprehensive way. This method needs the axial modal approximates dependence on the characteristic function. The governing equation was formulated based on Sander's thin shell theory with energy functional. In present work, the current method is used to find the vibration of FG zigzag and chiral SWCNTs. Over the past several years vibration of tube structures of various configurations and boundary conditions have been extensively studied (Ghavanloo and Fazelzadeh 2012, Hsu *et al.* 2008, Hu *et al.* 2008, Ke *et al.* 2009, Kiani 2014, Kulathunga *et al.* 2009, Hussain *et al.* 2018a, b, c, 2019a, b, Hussain and Naeem 2018a). The RRM is very powerful technique for the prediction of vibration of shells/tubes.

3.1 Modal displacement expressions

The modal deformation displacement functions which are involved in the strain and kinetic energy expressions for a tube, depend on two space variables, x and θ and time variable, *t*. These functions u, v and w are split and assumed in the following modal displacement relations

$$\begin{aligned} u(x,\theta,t) &= U(x)\sin(n\theta)\sin(\omega t) \\ v(x,\theta,t) &= V(x)\cos(n\theta)\sin(\omega t) \\ w(x,\theta,t) &= W(x)\sin(n\theta)\sin(\omega t) \end{aligned} \quad (10)$$

where n gives number of circumferential wave modes, ω designates the natural circular frequency for a vibrating tube. $U(x)$, $V(x)$ and $W(x)$ represent for the axial modal deformation functions in the axial, circumferential and radial directions respectively and meet end conditions. For generality, the following non-dimension parameters are adopted as

$$\begin{aligned} \bar{U} &= \frac{U}{h}, & \bar{V} &= \frac{V}{h}, & \bar{W} &= \frac{W}{R}, \\ a &= \frac{L}{R}, & b &= \frac{h}{R}, & X &= \frac{x}{L} \end{aligned} \quad (11)$$

Using these quantities, the expressions designate in the Eq. (10) is re-framed as

$$\begin{aligned} u(x,\theta,t) &= h\bar{U}\sin(n\theta)\sin(\omega t) \\ v(x,\theta,t) &= h\bar{V}\cos(n\theta)\sin(\omega t) \\ w(x,\theta,t) &= R\bar{W}\sin(n\theta)\sin(\omega t) \end{aligned} \quad (12)$$

3.2 Axial modal dependence

In the expression (12) the function $\bar{U}$, $\bar{V}$ and $\bar{W}$ approximate the dimensionless axial modal deformations in the longitudinal, tangential and transverse directions respectively. Axial, circumferential and radial direction is related only to the axial displacement function. The unknown functions involving the tube dynamical equations are functions of shape linear variables. The independent variables are separated by employing prescribed method. They are supposed in the form of the product of separate functions of independent variables. The displacement function was first invoked by Flügge (1962) to clarify the problem of shells and then used by Forsberg (1964) and Warburton (1965). The following expressions for Ritz polynomial functions are taken for measuring the axial modal deformations: $\bar{U}$, $\bar{V}$ and $\bar{W}$ that fulfill the edge conditions

Table 1 Powers n_u , n_v , n_w of Eq. (13)

	Boundary conditions							
	C_1	C_2	C_3	C_4	S_1	S_2	S_3	S_4
n_u	0	0	1	1	0	0	1	1
n_V	1	0	0	1	1	0	0	1
n_W	2	2	2	2	1	1	1	1

$$\begin{aligned}\bar{U} &= \sum_{i=1}^{N} a_i\,\bar{U}_i = \sum_{i=1}^{N} a_i\,X^{i-1}X^{n_u^0}\,(1-X)^{n_u^1}\\ \bar{V} &= \sum_{i=1}^{N} b_i\,\bar{V}_i = \sum_{i=1}^{N} b_i\,X^{i-1}X^{n_v^0}\,(1-X)^{n_v^1}\\ \bar{W} &= \sum_{i=1}^{N} c_i\,\bar{W}_i = \sum_{i=1}^{N} c_i\,X^{i-1}X^{n_w^0}\,(1-X)^{n_w^1}\end{aligned} \tag{13}$$

where the exponents n_u^0 , n_u^1 , n_v^0 , n_v^1 , n_w^1 and n_w^0 are given in Table 1. The superscripts of the powers (i.e., 0 and 1) are associated with boundary conditions specified at ends of a tube.

3.3 Derivation of frequency equation

The assumed expressions for u, v and w from the Eq. (12) and their partial derivatives along with modal forms: $\bar{U}$, $\bar{V}$ and $\bar{W}$ from Eq. (13) are written in the Eq. (9) and the Lagrange function is achieved in the dimensionless quantities given in Eq. (9) as follows

$$\begin{aligned}\prod = \int_0^1 \Bigg\{ &\frac{\pi hLR^3}{2}\Bigg[\left(b^2\sum_{i=1}^{N} a_1\,\bar{U}_i\right)^2 + \left(b^2\sum_{i=1}^{N} b_i\,\bar{V}_i\right)^2 \\ &+ \left(b^2\sum_{i=1}^{N} c_i\,\bar{W}_i)^2\right]\bar{\rho}_t\omega^2 cos^2\omega t \\ &-\frac{\pi hLR}{2}\Bigg[a^2b^2\bar{A}_{11}\left(\sum_{i=1}^{N} a_i\frac{d\bar{U}_i}{dX}\right)^2 \\ &+\bar{A}_{22}\left(-nb\sum_{i=1}^{N} b_i\bar{V}_i + \sum_{i=1}^{N} c_i\,\bar{W}_i\right)^2 \\ &+2ab\bar{A}_{12}\left(\sum_{i=1}^{N} a_i\frac{d\bar{U}_i}{dX}\right)\left(-nb\sum_{i=1}^{N} b_i\,\bar{V}_i + \sum_{i=1}^{N} c_i\,\bar{W}_i\right. \\ &+\bar{A}_{66}\left(ab\sum_{i=1}^{N} b_i\frac{d\bar{V}_i}{dX}s + nb\sum_{i=1}^{N} a_i\,\bar{U}_i\right)^2 \\ &-2a^3b^2\bar{B}_{11}\left(\sum_{i=1}^{N} a_i\frac{d\bar{U}_i}{dX}\right)\left(\sum_{i=1}^{N} c_i\frac{d^2\bar{W}_i}{dX^2}\right) \\ &-2ab^2\bar{B}_{12}\left(\sum_{i=1}^{N} a_i\frac{d\bar{U}_i}{dX}\right)\left(-n^2\sum_{i=1}^{N} c_i\,\bar{W}_i + nb\sum_{i=1}^{N} b\bar{V}_i\right) \\ &-2a^2b\bar{B}_{12}\left(-nb\sum_{i=1}^{N} b_i\bar{V}_i + \sum_{i=1}^{N} c_i\,\bar{W}_i\right)\left(\sum_{i=1}^{N} c_i\frac{d^2\bar{W}_i}{dX^2}\right) \\ &-2b\bar{B}_{22}\left(-nb\sum_{i=1}^{N} b_i\bar{V}_i + \sum_{i=1}^{N} c_i\,\bar{W}_i\right) \\ &\left(-n^2\sum_{i=1}^{N} c_i\,\bar{W}_i + nb\sum_{i=1}^{N} b_i\bar{V}_i\right) \\ &-4b\bar{B}_{66}\left(ab\sum_{i=1}^{N} b_i\frac{d\bar{V}_i}{dX} + nb\sum_{i=1}^{N} a_i\,\bar{U}_i\right) \\ &\left(na\sum_{i=1}^{N} c_i\frac{d\bar{W}_i}{dX} - \frac{3ab}{4}\sum_{i=1}^{N} b_i\,\bar{V}_i + \frac{nb}{4}\sum_{i=1}^{N} a_i\,\bar{U}_i\right) \\ &+a^4b^2\bar{D}_{11}\left(\sum_{i=1}^{N} c_i\frac{d^2\bar{W}_i}{dX^2}\right)^2 \\ &+b^2\bar{D}_{22}\left(-n^2\sum_{i=1}^{N} c_i\,\bar{W}_i + nb\sum_{i=1}^{N} b_i\,\bar{V}_i\right)^2 \\ &+2a^2b^2\bar{D}_{12}\left(\sum_{i=1}^{N} c_i\frac{d^2\bar{W}_i}{dX^2}\right) \\ &\left(-n^2\sum_{i=1}^{N} c_i\,\bar{W}_i + nb\sum_{i=1}^{N} b_i\,\bar{V}_i\right) \\ &+4b^2\bar{D}_{66}\Bigg(na\sum_{i=1}^{N} c_i\frac{d\bar{W}_i}{dX} - \frac{3ab}{4}\sum_{i=1}^{N} b_i\,\bar{V}_i \\ &+\frac{nb}{4}\sum_{i=1}^{N} a_i\,\bar{U}_i\Bigg)^2\Bigg] sin^2\,\omega t\Bigg\}dX\end{aligned} \tag{14}$$

3.4 Use of the Rayleigh-Ritz procedure

The Rayleigh-Ritz technique has used has employed to frame the eigenvalue frequency equation in the generalized form. To obtain necessary extreme conditions the Lagrangian functional $\prod$ is differentiated with regard to the generalized Fourier coefficients a_i , $b_{i,}$ c_i. The flowing conditions are obtained

$$\frac{\partial\prod}{\partial a_i} = \frac{\partial\prod}{\partial b_i} = \frac{\partial\prod}{\partial c_i} = 0 \quad \text{where} \quad i = 1,2,\ldots\ldots\ldots\ldots N. \tag{15}$$

These equations are written in the following complete forms after concealing a huge amount of algebraic process

$$\begin{aligned}&\sum_{j=1}^{N} a_j\Bigg[a^2b^2\bar{A}_{11}\int_0^1 \frac{d\bar{U}_i}{dx}\frac{d\bar{U}_j}{dx}dX \\ &+n^2b^2\left(\bar{A}_{66} - b\bar{B}_{66} + \frac{b^2\bar{D}_{66}}{4}\right)\int_0^1 \bar{U}_i\bar{U}_j\,dX\Bigg] \\ &+\sum_{j=1}^{N} b_j\,\Bigg[-nab^2(\bar{A}_{12} + b\bar{B}_{12})\int_0^1 \frac{d\bar{U}_i}{dX}\bar{V}_j dX \\ &+nab^2\left(\bar{A}_{66} + b\bar{B}_{66} - \frac{3b^2\bar{D}_{66}}{4}\right)\int_0^1 \bar{U}_i\frac{d\bar{V}_j}{dX}dX\Bigg]\end{aligned} \tag{16}$$

$$+\sum_{j=1}^{N} c_j \left[ab(\bar{A}_{12} + n^2 b\bar{B}_{12}) \int_0^1 \frac{d\bar{U}_i}{dX} \bar{W}_j dX \right.$$
$$+n^2ab^2(-2\bar{B}_{66} + b\bar{D}_{66}) \int_0^1 \bar{U}_i \frac{d\bar{W}_j}{dX} dX$$
$$\left. -a^3b^2\bar{B}_{11} \int_0^1 \frac{d\bar{U}_j}{dX}\frac{d^2\bar{W}_j}{dX^2} dX \right] \tag{16}$$
$$= R^2\bar{\rho}_t\omega^2 \sum_{j=1}^{N} a_j\, b^2 \int_0^1 \bar{U}_i\bar{U}_j\, dX$$

$$\sum_{j=1}^{N} a_j \left[-nab^2(\bar{A}_{12} + b\bar{B}_{12}) \int_0^1 \frac{d\bar{U}_j}{dX} \bar{V}_i dX \right.$$
$$+nab^2 \left(\bar{A}_{66} + b\bar{B}_{66} - \frac{3b^2\bar{D}_{66}}{4} \int_0^1 \bar{U}_j \frac{d\bar{V}_i}{dX} dX \right.$$
$$+\sum_{j=1}^{N} b_j \left[a^2b^2 \left(\bar{A}_{66} + 3b\bar{B}_{66} + \frac{9b^2\bar{D}_{66}}{4} \right) \int_0^1 \frac{d\bar{V}_i}{dX}\frac{d\bar{V}_j}{dX} dX \right.$$
$$+(\bar{A}_{22} + 2b\bar{B}_{22} + b^2\bar{D}_{22}) \int_0^1 \bar{V}_i\, \bar{V}_j dX]$$
$$+\sum_{j=1}^{N} c_j\, [-nb(\bar{A}_{22} + (n^2+1)b\bar{B}_{22} + n^2b^2\bar{D}_{22}) \tag{17}$$
$$\int_0^1 \bar{V}_i\, \bar{W}_j d - n^2b^2(2\bar{B}_{66} + 3b\bar{D}_{66}) \int_0^1 \frac{d\bar{V}_j}{dX}\frac{d\bar{W}_j}{dX} dX$$
$$+nab^2(\bar{B}_{12} + b\bar{D}_{66}) \int_0^1 \bar{V}_i \frac{d^2\bar{W}_i}{dX^2} dX]$$
$$= R^2\bar{\rho}_t\omega^2 \sum_{j=1}^{N} b_j\, b^2 \int_0^1 \bar{V}_i\, \bar{V}_j dX$$

$$\sum_{j=1}^{N} a_j\, [ab(\bar{A}_{12} + n^2b\bar{B}_{12}) \int_0^1 \frac{d\bar{U}_j}{dX} \bar{W}_j dX$$
$$+n^2ab^2(-2\bar{B}_{12} + b\bar{D}_{66}) \int_0^1 \bar{U}_j \frac{d\bar{W}_i}{dX} dX$$
$$-n^2b^2\bar{B}_{11} \int_0^1 \frac{d\bar{U}_j}{dX}\frac{d^2\bar{W}_i}{dX} dX]$$
$$+\sum_{j=1}^{N} b_j\, [-nb(\bar{A}_{12} + (n^2 + 1b\bar{B}_{22} + n^2b^2\bar{D}_{22})$$
$$\int_0^1 \bar{V}_i\, \bar{W}_i dX - na^2b^2(2\bar{B}_{66} + 3b\bar{D}_{66}) \int_0^1 \frac{d\bar{V}_j}{dX}\frac{d\bar{W}_j}{dX} dX$$
$$+na^2b^2(2\bar{B}_{12} + 3b\bar{D}_{66}) \int_0^1 \frac{d\bar{V}_j}{dX}\frac{d\bar{W}_i}{dX} dX$$
$$+n \int_0^1 \frac{d\bar{V}_j}{dX}\frac{d\bar{W}_j}{dX} dX b^2(\bar{B}_{12} + b\bar{D}_{12}) \int_0^1 \bar{V}_j \frac{d^2\bar{W}_i}{dX^2} dX]$$
$$+\sum_{j=1}^{N} c_j\, [(\bar{A}_{22} + 2n^2b\bar{B}_{22} + n^4b^2\bar{D}_{22}) \int_0^1 \bar{W}_i\, \bar{W}_j dX$$
$$+4n^2a^2b^2\bar{D}_{66} \int_0^1 \frac{d\bar{W}_i}{dX}\frac{d\bar{W}_j}{dX} dX - a^2b(\bar{B}_{12} + n^2b\bar{D}_{12}) \tag{18}$$
$$\int_0^1 (\,\bar{W}_i \frac{d^2\bar{W}_j}{dX^2} + \frac{d^2\bar{W}_i}{dX^2}\bar{W}_i) dX$$
$$+a^4b^2\bar{D}_{11} \int_0^1 \frac{d^2\bar{W}_i}{dX^2}\frac{d^2\bar{W}_j}{dX^2} dX]$$
$$= R^2\bar{\rho}_t\omega^2 \sum_{j=1}^{N} c_j\, b^2 \int_0^1 \bar{W}_i\, \bar{W}_j dX$$

After the ordering of above equations, the tube vibration frequency is expressed by the generalized eigenvalue relation as

$$\{[K] - \Delta[M]\}[\underline{x}]^T = 0 \tag{19}$$

where $[K]$ and $[M]$ represent the stiffness and mass matrices for the tube and

$$[\underline{x}]^T = (a_1, a_2, \ldots\ldots\ldots, a_N, b_2, \ldots\ldots.\, b_N, c_1, c_2, \ldots\ldots\ldots.\,., c_N) \tag{20}$$

and

$$\Delta_1 = R^2\bar{\rho}_t\omega^2 \tag{21}$$

Eq. (19) yields tube frequencies and mode shapes for isotropic CNT. Coupling stiffness, B_{ij} become zero for isotropic materials. The eigenvalues represent with the tube frequencies and the corresponding eigenvectors designate the mode shapes. This procedure is used for any edge condition.

4. Numerical results and discussions

The obtained results for the different boundary conditions (BCs) likewise: SS-SS, C-C, C-F and C-S for armchair, zigzag and chiral SWCNTs are parametrically studied in this part. The results for length and ratio of thickness-to-radius are presented versus fundamental frequencies f (THz × 10^4) and f (THz × 10^6), respectively. For obtaining new results, the appropriate tube thickness and material properties are a challenge. For present study, the material properties and tube thickness are chosen here, which was suggested by Wang and Zhang (2007), the reported effective thickness of SWCNTs in the range of 0.0612 nm ~ 0.69 nm (Yakobson *et al.* 1996, Tu and Yang 2002, Vodenitcharova and Zhang 2003) whose magnitude difference is more than an order. In most of previous studies, the value of $K_{extension}$ is obtained and lies in the range of 330 to 363 J/m^2 [see Yakobson *et al.*

Table 2 Comparison of C-C first mode SWCNTs frequencies with MD simulation

Length-to-diameter ratio	*f* (THz)			
	Zhang *et al.* (2009)	Present	Wang *et al.* (2006)	Present
4.68	1.06812	1.15234	1.17470	1.18245
6.67	0.64697	0.65756	0.59090	0.60324
8.47	0.43335	0.47564	0.46250	0.47968
10.26	0.30518	0.37132	0.34940	0.32546
13.89	0.18311	0.18576	0.19380	0.21564

Table 3 Comparison of frequencies of C-F first mode SWCNTs with MD simulation based on Sander shell theory

Length-to-diameter ratio	*f* (THz)	
	Zhang *et al.* (2009)	Present
4.67	0.23193	0.24041
6.47	0.12872	0.14431
7.55	0.1000	0.11868
8.28	0.07935	0.08943
10.07	0.05493	0.05728
13.69	0.03052	0.03640

1996, Robertson *et al*. 1992, Chen and Cao 2006) and Poisson's ratio ν arises from 0.14 ~ 0.34.

In this paper, we have obtained and discussed the variation of the vibrational frequency of length and ratio of thickness-to-radius under different nanotube boundary conditions. Frequency spectra using formula $f = \omega/2\pi$ for SWCNT versus length/diameter ratio using Rayleigh's method with same reference parameters (Zhang *et al*. 2009) are determines as 1.23445 ~ 0.17360 (THz) for the C-C end condition and 0.17074 ~ 0.02051 for C-F end condition, found a satisfactory agreement. It is noted that from Tables 2-3, the frequency value of present model has the large values as the values followed by the Zhang *et al*. (2009) and Wang *et al*. (2006) show a frequency difference between these studies. It can be seen that the error percentage is negligible, hence showing high rate of convergence. It is concluded that the frequency decreased as aspect ratio increased. The proposed model based on Rayleigh's method can incorporate in order to accurately predict the acquired results of material data point. Fig. 3 show the frequency response of armchair (5, 5), (7, 7), (9, 9) against length with radii 678 nm, 1356 nm, 2034 nm, respectively. The frequency curves are sketched with different BCs of the type C-F, C-C, SS-SS and C-SS. Particularly, the natural frequencies corresponding to length (L = 10 nm) for armchair indices (5, 5), (7, 7), (9, 9) are 0.4849, 0.9099, 1.460, for the C-C end condition, and 0.4460, 0.8503, and 1.384, for the C-SS end condition, and 0.4045, 0.7926, 1.310, for the SS–SS end condition, and 0.3277, 0.6834, 1.169, for the C-F support condition, respectively. Similarly, the frequencies corresponding to length (L = 100 nm) for armchair indices (5, 5), (7, 7), (9, 9) are 0.0095, 0.0095, 0.0147, for the C-C end condition, and 0.0093, 0.0089, 0.0140, for the C-SS end condition, and 0.0091, 0.0084, 0.0133 for the SS-SS end condition, and 0.0088, 0.0074, 0.0110, for the C-F end condition, respectively. It is noted that highest frequency pattern of C-C armchair (5, 5), (7, 7), (9, 9) SWCNTs is observed than other boundary condition. It can be seen that the frequency curves with C-F BCs are the lowest for changing the length.

Variation of frequencies versus length for indices (12, 0), (14, 0) and (19, 0) with BCs has been plotted in graph of Fig. 4. The value of fundamental frequency decreases on increasing the length of the tube. In addition, when the tube length increases from 10 nm to 20 nm, the frequency decreases rapidly, while for the length (L = 20 nm ~ 30 nm), the frequency is gently parallel. In present result, the frequencies are insignificant at length (L = 70 nm). It shows that natural frequencies decrease as L is increased, for these boundary conditions. For long SWCNTs, it can be seen that the effect of BCs is insignificant and more prominent at shorter length (L = 10 nm ~ 40 nm) and moderately negligible at length (L = 80~100 nm).

Fig. 5 shows the variation of frequencies versus length of chiral (8, 3), (10, 2) and (14, 5) with First, the frequencies fall down, then, become parallel and, after it seem linear for all BCs. It is observed that there is minute difference with different boundary conditions. The frequencies are more visible as compared to zigzag case. It is found that from these figure that the FNF outcomes of chiral (14, 5), are higher than those of (8, 3) and (10, 2).

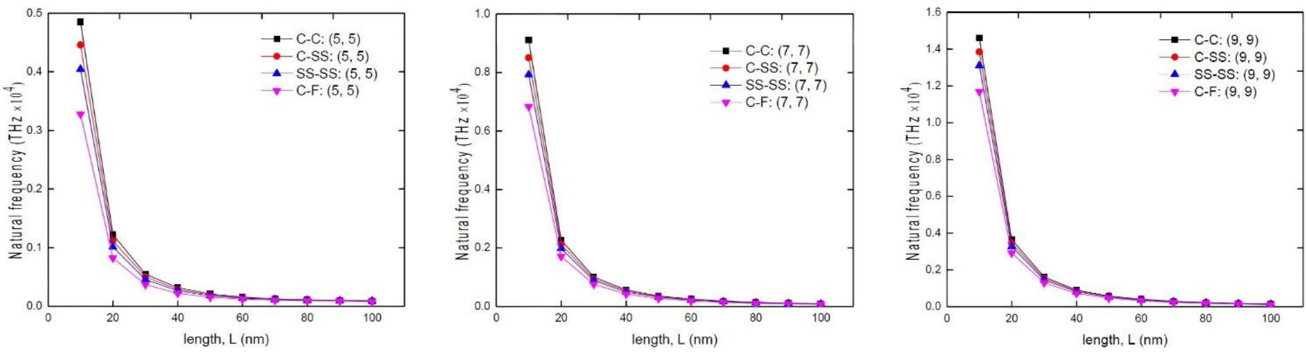

Fig. 3 Effect of length on the frequency-response of armchair SWCNTs (5, 5), (7, 7), (9, 9) different boundary conditions with h = 0.1 nm

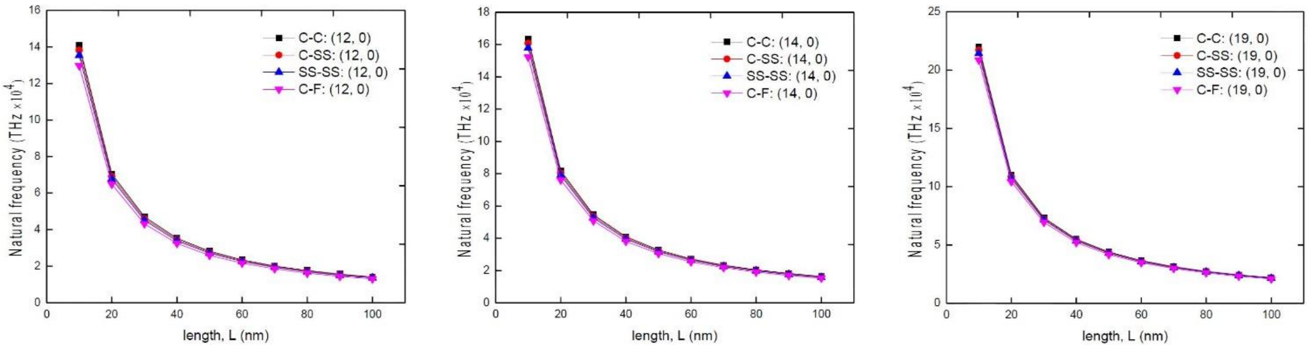

Fig. 4 Effect of length on the frequency-response of zigzag SWCNTs (12, 0), (14, 0), (19, 0), for different boundary conditions with h = 0.1 nm

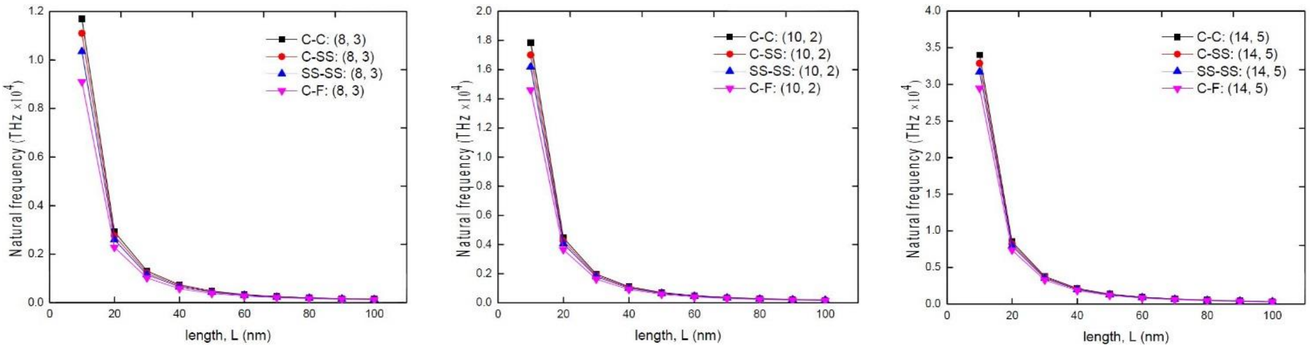

Fig. 5 Effect of length on the frequency-response of chiral SWCNTs (8, 3), (10, 2), (14, 5), for different boundary conditions with h = 0.1 nm

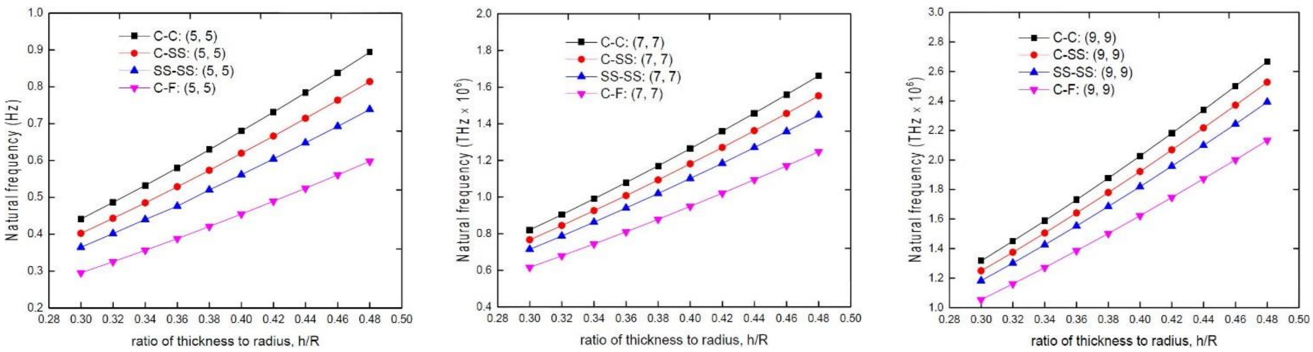

Fig. 6 Frequency response of armchairs SWCNTs (5, 5), (7, 7), (9, 9), versus *h/R* for different boundary conditions with L = 2.4 nm

The variations of tube ratio h/R versus frequencies (Hz) of carbon nanotubes for BCs have been sketched in graph of Fig. 6. As evidenced by this figure, the fundamental natural frequency would slightly increase by increasing the h/R for different BCs. When fundamental natural frequencies seem parallel for all calculated values of ratio *h/R* varies as 0.30 ~ 0.48. For initial values, the gap between frequency curves are little significant and for bigger values of ratio h/R, the frequency curves moderately pronounced. As shown by this figure, the boundary conditions C-C have the highest frequency curves. Fig. 6 shows the frequency response of armchair (5, 5), (7, 7), (9, 9) against ratio of thickness-to-radius with length 2.4 nm with specified boundary conditions. The investigated values of frequencies with different boundary conditions are at *h/R* = 0.30 as C-C = (5, 5) *f*~0.4414, (7, 7) *f*~0.8208, (9, 9) *f*~1.3171, and for C-S = (5, 5) *f*~0.4022, (7, 7) *f* ~0.7670, (9, 9) *f*~1.2486, and for SS-SS = (5, 5) *f*~0.3648, (7, 7) *f*~0.7150, (9, 9) *f*~1.1821, and for C-F = (5, 5) *f* ~0.2955, (7, 7) *f*~0.6165, (9, 9) *f*~1.0544, respectively. Once again, the frequencies outcomes with proposed boundary conditions at *h/R* = 0.48 as C-C = (5, 5) *f*~0.8934, (7, 7) *f* ~1.3457, (9, 9) *f*~2.6655, and for C-S = (5, 5) *f*~0.8140, (7, 7) *f*~1.5524, (9, 9) *f*~2.5271, and for SS-SS = (5, 5) *f*~0.7383, (7, 7) *f*~1.4472, (9, 9) *f*~2.3923, and for C-F = (5, 5) *f*~0.5980, (7, 7) *f*~1.2479, (9, 9) *f*~2.1339, respectively. It can take into account that the armchair SWCNTs (5, 5), (7, 7), (9, 9) with C-C condition have the prominent and highest frequencies

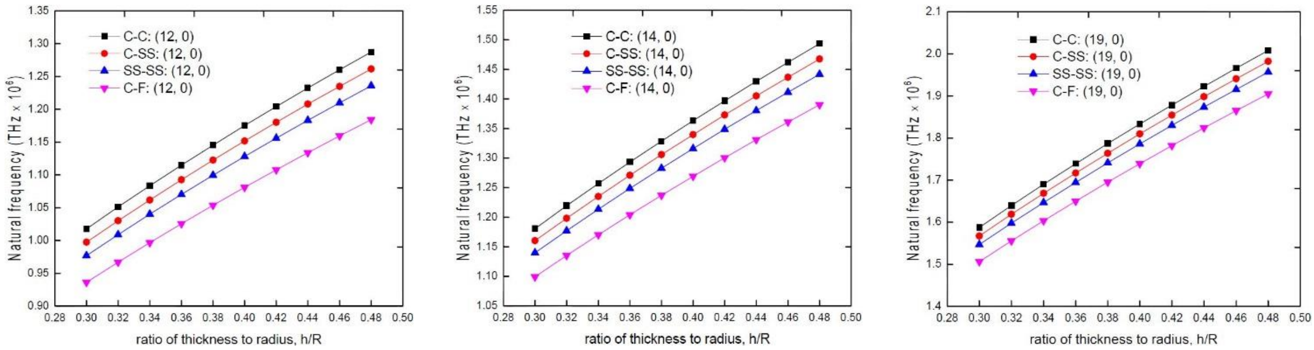

Fig. 7 Frequency response of zigzag SWCNTs (12, 0), (14, 0), (19, 0), versus *h/R* for different boundary conditions with L = 2.4 nm

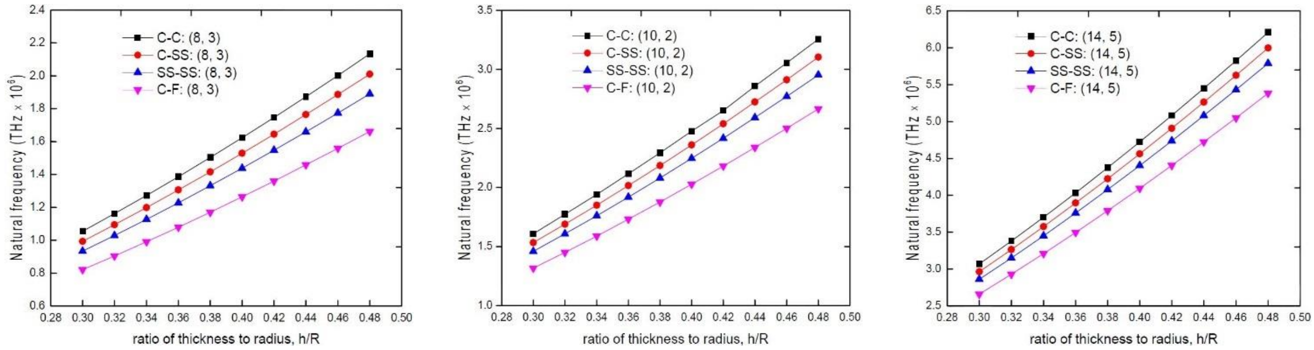

Fig. 8 Frequency response of chiral SWCNTs (8, 3), (10, 2), (14, 5), versus *h/R* for different boundary conditions with L = 2.4 nm

and other BCs followed as C-S, SS-SS and C-F. It is also concluded that the frequency curves with changing the values of *h/R* of C-F boundary condition are the lowest outcomes. The frequency pattern with all boundary conditions are seems to be parallel for overall values of *h/R* (= 0.30 ~ 0.48).

The variations of tube ratio h/R versus frequencies (Hz) of carbon nanotubes for BCs have been sketched in graph of Figs. 7-8 for zigzag and chiral indices, As evidenced by this figure, the fundamental natural frequency would slightly increase by increasing the h/R for different BCs. When fundamental natural frequencies seem parallel for all calculated values of ratio *h/R* varies as 0.30 ~ 0.48. For initial values, the gap between frequency curves are little significant and for bigger values of ratio h/R, the frequency curves moderately pronounced. As shown by this figure, the boundary conditions C-C have the highest frequency curves.

5. Conclusions

The governing equation of motion using Rayleigh's method is written in the form of eigen value to extract the frequencies of CNTs. The effects of different physical and material parameters on the fundamental frequencies are investigated for armchair, zigzag and chiral SWCNTs invoking Sander shell theory. However, for the analysis of structures at higher frequencies of length and ratio of thickness-to-radius under different boundary conditions.

Hence, it is concluded that for each data point curve, frequency value for armchair is greater than that of zigzag and chiral values and frequency curves decreases as the length with specific value of radius increases. Also, the Flügge shell model based on the wave propagation method for estimating fundamental natural frequency has been developed to converge more quickly than other methods and models. The presented vibration modeling and analysis of carbon nanotubes may be helpful especially in applications such as oscillators and in non-destructive testing. The vibrations of the piezoelectric based SWCNTs resonators using the developed theory for the curved structure and piezoelectric based on FGM carbon nanotubes can be also investigated as a new topic for the future researchers.

Declariation of conflicting interests

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