Nonlinear free and forced vibration analysis of a single-walled carbon nanotube using shell model

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ABSTRACT

In this Paper, the nonlinear free and force vibration of a single-walled carbon nanotube (SWCNT) with simply supported ends is investigated based on von Karman's geometric nonlinearity. The SWCNT described as an individual shell and the Donnell's equations of cylindrical shells are used to obtain the governing equations. The Galerkin's procedure is used to discretized partial differential equations of the governing into the ordinary differential equations of motion. The method of averaging is applied to analyze the nonlinear vibration of (10, 0), (20, 0) and (30, 0) zigzag SWCNTs in the analytical calculations. The effects of the nonlinear parameters, different aspect ratios, different circumferential wave numbers and longitudinal half-wave numbers are investigated. Both free and forced motions (due to harmonic excitation) are considered. It is shown that (30, 0) zigzag SWCNT has less nonlinear behavior than the other CNTs for a constant aspect ratio. The type of nonlinearity is determined by the aspect ratio. It is seen from the results that for Small values of aspect ratios, the vibration behavior is softening type for the low amplitudes, and it is hardening type for the large amplitudes. And for large value of the aspect ratio, the vibration behavior is hardening type for all amplitudes.

Key words: Nonlinear Vibration, CNT, Donnell Shell Model, Averaging Method

INTRODUCTION

In recent years, extensive research has been carried out on CNTs because of their novel mechanical, physical, and electrical properties. The mechanical properties of CNTs have been extensively investigated by researchers in mechanical fields. Experimental measurements and theoretical analyses have shown that CNTs possess excellent mechanical stiffness and strength. The study of vibration in CNTs is currently a major topic of interest, which can be used to further understand their dynamic mechanical behavior. There are three major methods for simulating the mechanical properties of CNTs: experiments, molecular dynamics (MD) and the continuum mechanics. Due to the experimental calculations at the nanoscale are difficult and the MD simulations remain difficult for large-scale systems, continuum mechanical models have been effectively used to study mechanical behaviors of carbon

nanotubes. Recently, many elastic continuum models have been widely and successfully used for studying the bending, buckling and vibrational behaviors of CNTs, including beam models and cylindrical shell models. The beam models employed are often developed on the basis of the Euler–Bernoulli theory and the Timoshenko beam theory. And the shell models are often developed on the basis of Flügge theory and Donnell theory. For example, (Yokobson et al, 1996) used a traditional continuum shell model to predict the buckling of a single-walled Carbon nanotube (SWCNT) and compared it with the MD simulation. (Ru, 2005) proposed the buckling analysis of the CNTs with shell models. (Sun and Liu, 2007) investigated the free vibration of the multi-walled carbon nanotubes (MWCNTs), by using Donnell's shell equations. (Zhang et al 2009) investigated critical buckling strains of axially loaded SWCNTs for both beam and cylindrical shell model. (Wang and Zhang, 2008) used continuum shell model to investigate the deformation of SWCNT. Up until now, most

of the shell model investigations were limited to the linear vibration of nanotube, but investigations of the geometric nonlinearities behavior are seldom. Nanotubes can undergo large deformations within the elastic limit, so the nonlinear analysis is clearly essential. Therefore, nonlinear analysis is high important for getting better predictive models to study the vibration behavior of the CNTs. (Yan et al, 2008) modeled the nonlinear free vibration behaviors of double-walled carbon nanotubes in the context of the Donnell's cylindrical shell and used the harmonic balance method to find the amplitudes-frequency relationship. In this paper, free and forced vibrations of a SWCNT based on the shell model are investigated. The geometrical nonlinearity has been used in the continuum models for getting an accurate vibration behavior of a nanotube. The Galerkin's procedure and the method of averaging are employed in order to reduce the problem to the solution of nonlinear algebraic and nonlinear differential equations. The influences of the nonlinear parameters, different aspect ratios and the vibration modes on the nonlinear vibration behavior are examined analytically. The results show that nonlinear parameter controls the strength of nonlinearity. So, increasing in the nonlinear parameter causes the increment of nonlinear behavior. Another important parameter which influences on the nonlinear vibration is an aspect ratio, which changes the nonlinearity type of CNTs into softening or hardening types. It is seen from the results that small values of the aspect ratio generally effects on softening type and the large value of the aspect ratio causes the behavior to hardening type.

MATHEMATICAL FORMULATION

Consider a thin-walled simply supported shell with radius of R, thickness h and length l. The cylindrical coordinate system (O; x, r, θ) is chosen, with the origin O placed at the center of one end of the shell. The displacements of the shell are denoted by u, v, and w, in the axial, circumferential and radial directions respectively.
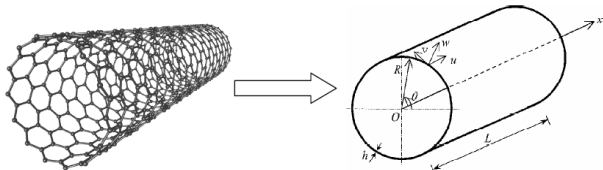

Figure1. Cylindrical shell representation of SWCNT

When the shell deflection w is of the same order of the magnitude as the shell thickness h, results obtained by using the linear theories become quite inaccurate. Therefore, a theory of large deflections (Von Karman theory) developed in cylindrical coordinates. In Donnell's nonlinear theory, only nonlinear terms that depend on w are retained, and all other nonlinear terms are neglected. The relationships between the strain and the displacement of Donnell's nonlinear shell can be written as follows:

$$\varepsilon_x = \varepsilon_{x,0} + zk_x, \qquad \varepsilon_\theta = \varepsilon_{\theta,0} + zk_\theta, \qquad \gamma_{x\theta} = \gamma_{x\theta,0} + k_{x\theta}.$$
(1)

Where ε_x, ε_θ and $\gamma_{x\theta}$ are shell strains and $\varepsilon_{x,0}$, $\varepsilon_{\theta,0}$, $\gamma_{x\theta,0}$ are middle surface strains and z is the distance of the arbitrary point of the shell from the middle surface.

$$\varepsilon_{x,0} = \frac{\partial u}{\partial x} + \frac{1}{2}(\frac{\partial w}{\partial x})^2, \qquad \varepsilon_{\theta,0} = \frac{1}{R}\frac{\partial v}{\partial \theta} + \frac{w}{R} + \frac{1}{2R^2}(\frac{\partial w}{\partial \theta})^2,$$
$$\gamma_{x\theta,0} = \frac{1}{R}\frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial x} + \frac{1}{R}(\frac{\partial w}{\partial \theta})(\frac{\partial w}{\partial x}).$$
(2)

$$k_x = -\frac{\partial^2 w}{\partial x^2} \qquad k_\theta = -\frac{\partial^2 w}{R^2 \partial \theta^2} \qquad k_{x\theta} = -\frac{2}{R}\frac{\partial^2 w}{\partial \theta \partial x}$$
(3)

Where k_x, k_θ and $k_{x\theta}$ change in curvature and torsion of the middle surface. The elastic strain energy U of a circular cylindrical shell is given by

$$U = \frac{1}{2}\iiint (\sigma_x \varepsilon_x + \sigma_\theta \varepsilon_\theta + \sigma_z \varepsilon_z + \tau_{x\theta}\gamma_{x\theta} + \tau_{z\theta}\gamma_{z\theta} + \tau_{zx}\gamma_{zx}) dx R d\theta dz.$$
(4)

$$\frac{\partial F}{\partial u} - \frac{\partial}{\partial x}(\frac{\partial F}{\partial u_{,x}}) - \frac{\partial}{\partial \theta}(\frac{\partial F}{\partial u_{,\theta}}) = 0, \qquad \frac{\partial F}{\partial v} - \frac{\partial}{\partial x}(\frac{\partial F}{\partial v_{,x}}) - \frac{\partial}{\partial \theta}(\frac{\partial F}{\partial v_{,\theta}}) = 0,$$

$$\frac{\partial F}{\partial w} - \frac{\partial}{\partial x}(\frac{\partial F}{\partial w_{,x}}) - \frac{\partial}{\partial \theta}(\frac{\partial F}{\partial w_{,\theta}}) + \frac{\partial^2}{\partial x^2}(\frac{\partial F}{\partial w_{,xx}}) + \frac{\partial^2}{\partial \theta^2}(\frac{\partial F}{\partial w_{,\theta\theta}}) + \frac{\partial^2}{\partial x \partial \theta}(\frac{\partial F}{\partial w_{,x\theta}}) = 0.$$
(5)

By using Eqs. (1~5) the stress resultants and moment resultants can be written in the following form:

$$N_x = \frac{EH}{1-\upsilon^2}[-\frac{\upsilon w}{R} + \frac{1}{2}(\frac{\partial w}{\partial x})^2 + \frac{\upsilon}{2}(\frac{\partial w}{R\partial \theta})^2 + \frac{\partial u}{\partial x} + \frac{\upsilon}{R}\frac{\partial \upsilon}{\partial \theta}]$$

$$N_\theta = \frac{EH}{1-\upsilon^2}[-\frac{w}{R} + \frac{v}{2}(\frac{\partial w}{\partial x})^2 + \frac{1}{2}(\frac{\partial w}{R\partial \theta})^2 + \upsilon\frac{\partial u}{\partial x} + \frac{1}{R}\frac{\partial \upsilon}{\partial \theta}]$$

$$N_{x\theta} = \frac{EH}{2(1+\upsilon)}[\frac{w}{R}\frac{\partial u}{\partial \theta} + \frac{1}{R}\frac{\partial w}{\partial x}\frac{\partial w}{\partial \theta} + \frac{\partial \upsilon}{\partial x}]$$
(6)

$$M_x = -D(\frac{\partial^2 w}{\partial x^2} + v\frac{\partial^2 w}{R^2 \partial \theta^2})$$

$$M_\theta = -D(\frac{\partial^2 w}{R^2 \partial \theta^2} + v\frac{\partial^2 w}{\partial x^2})$$

$$M_x = -D(1-v)(\frac{\partial^2 w}{\partial x R \partial \theta})$$
(7)

With Substituting Eqs. (6)and (7) into Eq. (5),the governing equations of the equilibriums base on the Donnell's shell theory can be obtained as follows (Amabili,1999 ; Amabili, 1999):

$$D\nabla^4 w + \rho h \ddot{w} + q = \frac{1}{R}\frac{\partial^2 w}{\partial x^2} + \frac{1}{R^2}(\frac{\partial^2 F}{\partial \theta^2}\frac{\partial^2 w}{\partial x^2} - 2\frac{\partial^2 F}{\partial x \partial \theta}\frac{\partial^2 w}{\partial x \partial \theta} + \frac{\partial^2 F}{\partial x^2}\frac{\partial^2 w}{\partial \theta^2})$$
(8)

$$\frac{1}{Eh}\nabla^4 F = -\frac{1}{R}\frac{\partial^2 w}{\partial x^2} + \left[\left(\frac{\partial^2 w}{R\partial x\partial\theta}\right)^2 - \frac{\partial^2 w}{\partial x^2}\frac{\partial^2 w}{R^2\partial\theta^2}\right] \tag{9}$$

F is the in-plane Airy stress function; q is the external excitation and the biharmonic operator in Eqs. (12), (13) is defined as:

$$\nabla^4 w = \left(\frac{\partial^2 w}{\partial x^2} + \frac{1}{R^2}\frac{\partial^2 w}{\partial\theta^2}\right)^2.$$

The forces per unit length in the axial, circumferential directions and shear force are given by:

$$N_x = \frac{1}{R^2}\frac{\partial^2 F}{\partial\theta^2}, \quad N_\theta = \frac{\partial^2 F}{\partial x^2}, \quad N_{x\theta} = -\frac{1}{R}\frac{\partial^2 F}{\partial x\partial\theta}. \tag{10}$$

In this study, the attention is focused on a finite, simply supported ends, circumferentially closed circular cylindrical shell with length *l*. The following boundary conditions are imposed as:

$$\upsilon = w = 0, \qquad N_x = 0, \qquad M_x = 0. \tag{11}$$

MATERIALS AND METHODS

The radial displacement *w* is expanded by using the linear shell eigen modes as the basis; in particular, the flexural response may be written as follows (Nash;Watawala 1983; Amabili 2003):

$$w(x,\theta,t) = A(t)\cos(n\theta)\sin(\frac{m\pi x}{l}) + \frac{n^2}{4R}A(t)^2\sin(\frac{m\pi x}{l})^2. \tag{12}$$

Where *m* is the axial wave number (equal to the number of half-waves along the shell), and *n* is the circumferential wave number. The amplitude functions, A is an Unknown generalized time function of the vibration. Substituting the expansion of *w*, Eq. (16), in the right-hand side of Eq. (13), and solving for the particular solution, we have (F. Pellicano 2002)

$$F_p = EH(A_1\cos(2n\theta) + A_2\cos(n\theta)\sin(\frac{3m\pi x}{L}) + A_3\cos(n\theta)\sin(\frac{m\pi x}{L})). \tag{13}$$

A_1, A2 and A_3 values are not reported here for the sake of brevity. For solving Eq. (12) substitute Eqs. (16) and (17) into Eq.(12). But direct on is impossible. Thus, the Galerkin's technique was employed to obtain an approximate solution.

GALERKIN'S METHOD

The Galerkin's method employs any set of basic functions φ, approximates the nonlinear partial differential equation (PDE) by transforming it into a finite set of coupled ordinary differential equations (ODEs). The Galerkin projection of the equation of motion (12), in this case, may be expressed as (Amabili 2008):

$$\left(D\nabla^4 w + \rho h\ddot{w} = ..., \varphi\right) = \int_0^{2\pi}\int_0^l (D\nabla^4 w + \rho h\ddot{w} = ...)\times\varphi. \tag{14}$$

Where the Galerkin's weighting function is

$$\varphi = \cos(n\theta)\sin(\frac{m\pi x}{l}) + \frac{n^2}{2R}A(t)\sin(\frac{m\pi x}{l})^2. \tag{15}$$

After the evaluation of the integrals, an ordinary non-linear differential equation is obtained.

$$\tilde{\alpha}_1 A(t) + \tilde{\alpha}_2 A(t)^3 + \tilde{\alpha}_3 A(t)^2(\frac{d^2}{dt^2}A(t)) + \tilde{\alpha}_4 A(t)(\frac{d^2}{dt^2}A(t)) + \tilde{\alpha}_5 A(t)(\frac{d}{dt}A(t))^2 + \bar{q}(t) = \tilde{\alpha}_6 A(t)^3 + \tilde{\alpha}_7 A(t) + \tilde{\alpha}_8 A(t)^5 \tag{16}$$

$\tilde{\alpha}$ values are not reported here for the sake of brevity.

AVERAGING METHOD

The ordinary non-linear differential equation (20) cannot yet be solved exactly. But, an approximate solution can be obtained by the procedure known as the method of averaging (Ali hasan nayfe 1995). The unknown function $A(t)$ is taken to be in the form,

$$A(t) = a(t)\cos(\omega t + \beta(t)),$$
$$\dot{A}(t) = -a(t)w\sin(\omega t + \beta(t)),$$
$$\ddot{A}(t) = -a(t)\omega^2\cos(\omega t + \beta(t)) - \dot{a}(t)\omega\sin(\omega t + \beta(t)) - a(t)\dot{\beta}(t)\cos(\omega t + \beta(t)). \tag{17}$$

In this paper the steady-state vibrations are considered, which means the average values A and ϕ remain steady with time. In this case, the average derivative $\dot{\beta}(t)$ is identically zero, and equation (20) can be reduced to:

$$\bar{\bar{\alpha}}_1 A + \bar{\bar{\alpha}}_2 A^3 + \bar{\bar{\alpha}}_3 A^3 w^2 + \bar{\bar{\alpha}}_4 A w^2 + \bar{q} = \bar{\bar{\alpha}}_5 A^3 + \bar{\bar{\alpha}}_6 A + \bar{\bar{\alpha}}_7 A^5 \tag{18}$$

$\bar{\bar{\alpha}}$ values are not reported here for the sake of brevity. The resulting of non-linear algebraic equations may conveniently be represented in terms of the dimensionless variables:

$$\tilde{A} \equiv \frac{A}{h},$$

$$w_{mn}^2 = \frac{E}{\rho R + \mu^2(\xi^2+1)}\left[\frac{\xi^4}{(\xi^2+1)^2 + \mu^2(\xi^2+1)^3} + \frac{\varepsilon(\xi^2+1)^2}{12(1-\upsilon^2)}\right], \tag{19}$$

$$\xi \equiv \frac{m\pi R}{nl}, \varepsilon \equiv (\frac{n^2 h}{R})^2, \Omega = \frac{w}{w_{mn}}.$$

Where, w_{mn} is linear vibration frequency, ε is nonlinearity parameter, ξ and Ω is non dimensional nonlinear vibration changes to linear vibration as $\varepsilon = 0$. With the increment of ε values the nonlinearity of vibration increases (Evensen 1967)

$$-\Omega^2(\alpha_1\tilde{A}+\alpha_2\tilde{A}^3)+\alpha_3\tilde{A}+\alpha_4\tilde{A}^3+\alpha_5\tilde{A}^5=\bar{q}. \qquad (20)$$

α values are not reported here for the sake of brevity

RESULTS AND DISCUSSION

Zigzag (10, 0), (20, 0) and (30,0) SWCNT have been investigated to analyse nonlinear vibration. The geometries of SWCNTs has been reported by Gupta *et al* (S.S. Gupta 2010).

Table 1: Geometries of SWCNTs

Tube (n, m)	Radius (R) (Å)	υ	h (Å)
(10,0)	3.713	0.265	0.878
(20,0)	7.420	0.238	1.251
(30,0)	11.129	0.227	1.340

Fig.2 shows the influence of large amplitudes on the free vibration frequencies of (10, 0), (20, 0) and (30, 0) zigzag CNTs with an aspect ratio $\xi=1/4$. The axial and circumferential wave numbers are m=1 and n=1 respectively. The Figure shows that the vibration behavior is softening type for the low vibration amplitudes, and it is hardening type for the large amplitudes for each three nanotubes. The radius increasing makes the nonlinear parameter decreased. The (30, 0) CNT has the biggest radius among two others CNTs. So, it has less nonlinear behavior than the other CNTs.
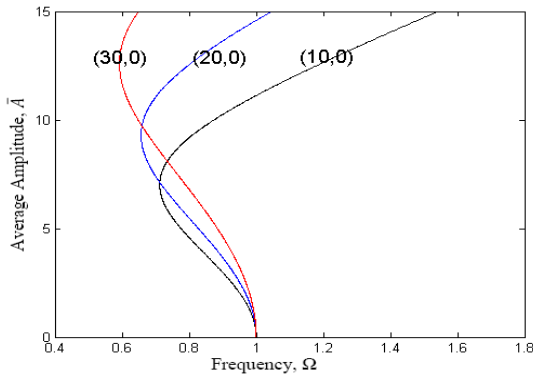

Figure 2. Influence of the large amplitudes on the vibration frequency for different nanotubes.
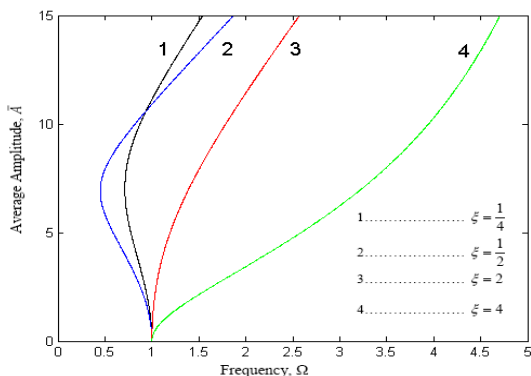

Figure 3. Shows an influence of the large amplitudes on the free vibration frequencies (10, 0) zigzag SWCNT nanotubes with the different aspect ratios ($\xi=1/2,1/4,2,4$)

The axial and circumferential wave numbers are m = n =1. It is seen from the figure that for the small values of the aspect ratios ($\xi<1/2$), the vibration behavior is softening type in small amplitudes and hardening type in large amplitudes and shows that for ($\xi>2$), the vibration behavior is hardening type for all amplitudes
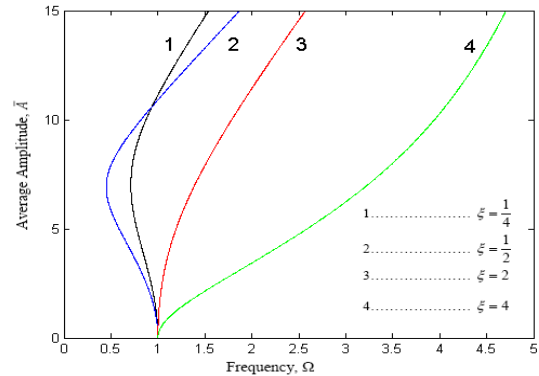

Figure 3. Influence of aspect ratio on vibration frequency ($\xi=1/2,1/4,2,4$).

Small values of the aspect ratios correspond to the long circumferential wave numbers and/or short axial wave numbers and/or increasing the length of the CNT. So, the CNTs with the length $l=4\pi R$ and circumferential wave number n=1 and an axial wave number m=1, 2, 8, 16 have the same results with figure 3. Fig. 4 shows the influence of large amplitudes on the free vibration frequencies of (10, 0) zigzag SWCNT with the different circumferential wave numbers (n=1, 2, 5). Consider the CNT with the length $l=4\pi R$ and axial wave number m=1. An increasing in the circumferential wave numbers causes the nonlinear parameter increased and decreases the aspect ratio. Therefore, as it is seen in Fig.4, the SWCNT has the more nonlinear behavior and more softening behavior in n = 5.
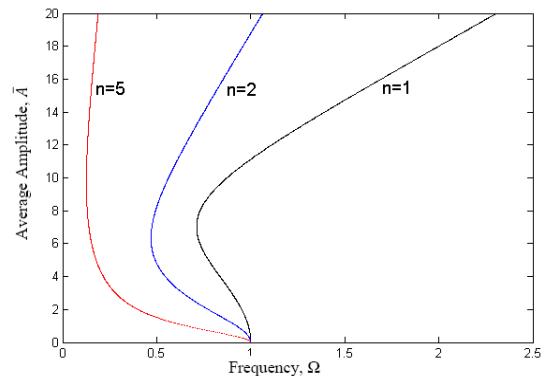

Figure 4. Influence of the different circumferential wave numbers on the vibration frequencies.

In Fig. 5, the amplitude is plotted against the frequency for the forced vibration of (10, 0) zigzag SWCNT The axial and circumferential wave numbers are respectively m=1 and n=1 and average excitation $\bar{q} = 0.1$. In the fig.5a the dotted lines denote the frequency-amplitude relationships for free vibration (also known as the backbone curve) and the solid lines represent the forced response for $(\xi = 1/4)$. The results show that the nonlinear behavior of CNT is the softening type. Fig 5b is plotted for $(\xi = 2)$ and shows that the nanotube behavior is hardening type.
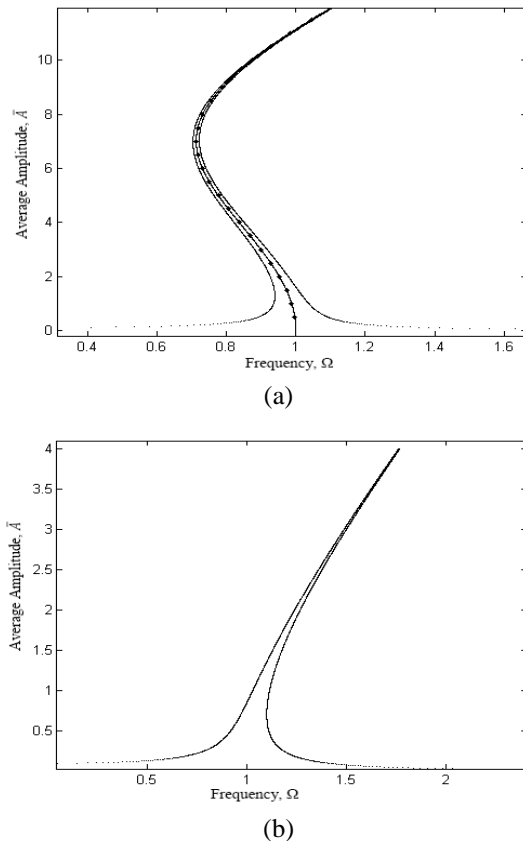

(a)

(b)

Figure 5. Amplitude of forced vibration versus frequency of excitation for (a) $\bar{q} = 0.1, \xi = 1/4$ and (b) $\bar{q} = 0.1, \xi = 2$.

CONCLUSIONS

In this paper, the nonlinear free vibrations of a SWCNT investigated based on von Karman's geometric nonlinearity. The SWCNT is considered as a thin circular cylindrical shell with simply supported ends. Governing equations are obtained by Donnell's shell theory. The Galerkin's procedure and the method of averaging are employed for solving nonlinear equations. The influences of the nonlinear parameters, different aspect ratios and the vibration mode on the nonlinear vibration behavior are considered. Both free and forced motions (due to harmonic excitation) are considered. The results show that (30, 0) zigzag SWCNT has less nonlinear behavior than the other

CNTs for a constant aspect ratio. The degree of nonlinearity is dependent on wall thickness of CNTs, number of circumferential waves and radius of CNTs.

The type of nonlinearity is determined by the aspect ratio. It is seen from the results that for Small values of the aspect ratio, the vibration behavior is softening type for the low amplitudes, and it is hardening type for the large amplitudes. And for large value of the aspect ratio, the vibration behavior is hardening type for all amplitudes. Small values of the aspect ratios correspond to the long circumferential wave numbers and/or short axial wave numbers and/or increasing the length of the CNT. The other considered parameters were an axial and the circumferential wave numbers. Decreasing of the axial wave number causes the increment of the aspect ratio and changes the CNT's behavior. An increasing in the circumferential wave numbers causes the nonlinear parameter increased and decreases the aspect ratio. So, increasing in the circumferential wave numbers causes the increment of nonlinear behavior and softening behavior of CNT.

Nomenclature

R	Radius of single-walled carbon nanotube
h	Nanotube wall thickness
l	Length of nanotube
x, θ, z	axial, circumferential and radial coordinates
u, v, w	axial, circumferential and radial displacements
$\varepsilon_x, \varepsilon_\theta, \gamma_{x\theta}$	Axial, circumferential and shear strains
$\varepsilon_{0,x}, \varepsilon_{0,\theta}, \gamma_{0,x\theta}$	middle surface strains
$\sigma_x, \sigma_\theta, \tau_{x\theta}$	Kirchhoff stresses
U	Strain energy
$N_x, N_\theta, N_{x\theta}$	stress resultants
$M_x, M_\theta, M_{x\theta}$	Couple resultants
∇^4	Biharmonic operator
$F(x, \theta, t)$	Stress function
ν	Poissen 's ratio
ρ	Mass density
E	Young's modulus
D	flexural rigidity
m, n	Axial and circumferential wave number
φ	weighting function
ε	Nonlinear parameter
ξ	Aspect ratio
w_{mn}	Linear vibration frequency
Ω	Non-dimensional frequency
q	External excitation

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