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Free vibration investigation of single walled carbon nanotubes with rotary inertia

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ABSTRACT

In present work, the free vibration dynamics of rotating single walled carbon nanotubes is investigated by using Eringen's nonlocal theory of elastic structures. Transverse flexural vibration of SWCNT embedded in an elastic medium, a rotating cantilever SWCNT and a nanorotor based SWCNTs is elaborated by using the Hamilton principle to obtain governing equations. Generalized differential quadrature method (GDQM) is employed to discretize and resolve the Eigen problem.

The effect of small scale, boundary conditions and angular velocity on the dynamic parameters is studied. Obtained results showed that SWCNTs provide exceptional structural properties. Findings of this study can be involved in the design of next generation nanomachines and nano-devices.

1. INTRODUCTION

Carbon nanotubes (CNT's) are the main subject of research in nanotechnology; developed by Iijima [1] using transmission electron microscopy, the research interest in CNT's has been enhanced by introducing them in nanoelectromechanical systems (NEMS) [2], this interest in CNTs is due the exceptional mechanical, chemical, electrical, thermal and optical properties that they offer. CNT's are increasingly being used as building parts of nano-machines such as nano-robots, nano-devices, nano-sensors and nano-actuators for NEMS, as strong reinforcement nanomaterials for nano-composite materials, as biological nanobots for drug delivery and therapy.

Researches on structural dynamics of nanoscale materials used to involve molecular dynamic (MD) simulation to investigate the nano-effect with accurate solutions for CNT's with small deflection. However, MD is limited to a number of

atoms 10^9 and it required a high cost computation. In recent years, elastic continuum models are employed as effective and successful theories to study mechanical and physical properties of CNT's [3, 4]. Nonlocal elasticity theory [5] models has been extensively used to model CNTs to study the nanoscale effects. In this theory, the small scale effects are captured by assuming that the stress at a point is a function not only of the strain at that point but also a function of the strains at all other points of the domain. Various works related to nonlocal elasticity theory are found in several references. Soltani et al. [6] considered the nonlocal Euler-Bernoulli elastic beam theory to investigate the vibrational behavior of a single-walled carbon nanotubes (SWCNTs) embedded in an elastic medium. Both Winkler-type and Pasternak-type models are employed to simulate the interaction of the SWNTs with a surrounding elastic medium more accurately, they showed that the stiffness of the medium due to both Pasternak-

type and Winkler-type increases, the bending stiffness, and the associated resonant frequency increases, consequently. Jena and Chakraverty [7] investigated the free vibration of SWCNT resting on exponentially varying Winkler elastic foundation by using DQM, they showed the effect of non-uniform parameter, nonlocal parameter, aspect ratio, Winkler modulus parameter and boundary condition on the frequency parameter.

The vibration behavior study of SWCNT's in rotation as cantilever beams has known a great interest by researchers, Narendar [8] studied the flapwise bending free vibration of a rotating cantilever SWCNT. He showed that angular velocity parameter has increased the frequency parameter, and that the nonlocal parameter effects the first mode frequency parameter increasingly and the second mode frequency parameter decreasingly.

Belhadj et al. [9] studied the SWCNT nanostructure as a rotating nanoshaft, they investigated the effect of nonlocal parameter, boundary conditions and angular velocity on the frequency by showing the Campbell diagram to evaluate critical angular velocities.

The objective of this study is to investigate the transverse vibratory behavior of SWCNT under different dynamic conditions. A nonlocal elastic Euler-Bernoulli beam model was used to study the SWCNT first in surrounding Winkler type elastic foundation, then this nanostructure was studied as a rotating cantilever beam and finally under axial rotating inertia as a nanoshaft to examine their behavior as nano-rotors for next generation rotating nano-machinery applications [10].

2. ERINGEN'S THEORY OF NONLOCAL ELASTICITY

Eringen [11] has introduced the theory of non-local elasticity to account for the small-scale effect. Unlike the classical theory of elasticity, the non-local theory consider long-range inter-atomic interaction and yields results dependent on the size of a body. In the following, the simplified form of the Eringen's nonlocal constitutive equation is employed:

$$(1 - (e_0 a)^2 \nabla^2) \sigma^{nl} = \sigma^l$$

where ∇^2 is the Laplacian operator, $(e_0 a)^2$ is nonlocal parameter,

a - internal characteristic length,
 e_0 - constant,
 nl - non local,
 l - local.

3. TRANSVERSE VIBRATION OF SWCNT

In the present paper, a single walled carbon nanotube designed using Nanotube Modeller (Figures 1, 2 and 3) is modelled mathematically based on Euler-Bernoulli beam model. The displacement field of at a point of the beam can be expressed as:

$$u_x(x, t) = u(x, t) - z \frac{\partial w(x, t)}{\partial x} \quad (1)$$

$$u_y(x, t) = 0 \quad (2)$$

$$u_z(x, t) = w(x, t) \quad (3)$$

$u_x(x, t)$, $u_y(x, t)$ and $u_z(x, t)$ are the axial and the transverse displacement component at the mid-plane respectively. The linear strain-displacement relations for the curved Euler-Bernoulli beam are expressed as:

$$\varepsilon_{xx} = \frac{\partial u}{\partial x} - z \frac{\partial^2 w}{\partial x^2} \quad (4)$$

$$\varepsilon_{zz} = \varepsilon_{xz} = 0$$

According to the nonlocal elasticity theory it is assumed that the stress at a point is a function of strains at all points in the continuum. the nonlocal constitutive behaviour of a Hooken solid is represented by the following differential constitutive relation:

$$[1 - (e_0 a)^2 \nabla^2] \sigma^{nl} = \sigma^l \quad (5)$$

where ∇^2 is the Laplacian operator, $(e_0 a)^2$ is the nonlocal parameter.

a - internal characteristic length,
 e_0 - constant,
 nl - non local,
 l - local.

The equation of motion of free vibration of a single walled carbon nanotube (SWCNT) is obtained after deriving the governing equations using Hamilton's principle as:

$$\rho A \frac{\partial^2 w}{\partial t^2} + EI \frac{\partial^4 w}{\partial x^4} = 0 \quad (6)$$

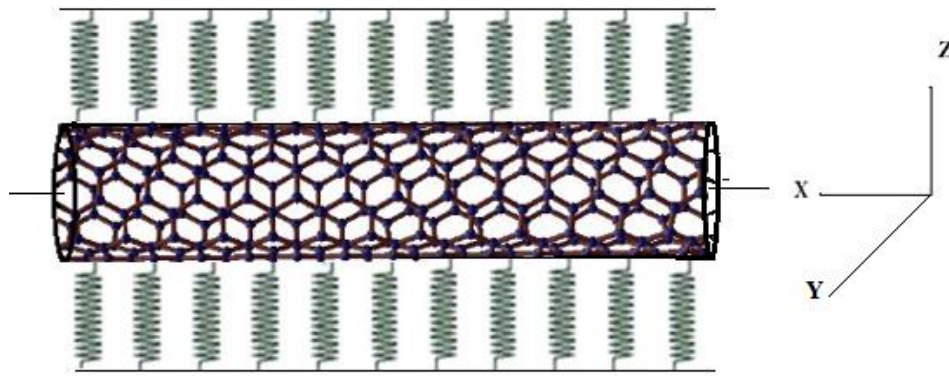


Figure 1. SWCNT embedded in an elastic medium.

$w(x, t)$ is the transverse deflection of the SWCNT, E , I and A are the elastic modulus, the moment of inertia, and the cross section respectively. Assumption the nanotube has a constant cross section, the equation (6) can be written as:

$$\phi^{(4)}(x) - \beta^4 \phi(x) = 0 \quad (7)$$

Where $\phi(x)$ is the mode shape (Eigen-shape)

$$\beta^4 = \frac{\rho A \omega^2}{EI} \quad (8)$$

The analytical solution of the equation (7) is

$$\phi(x) = C_1 \sin(\beta x) + C_2 \cos(\beta x) + C_3 \sinh(\beta x) + C_4 \cosh(\beta x) \quad (9)$$

C_1, C_2, C_3 and C_4 are the constants depending on boundary conditions.

3.1. SWCNTs embedded in an elastic medium

In this section, the SWCNT is considered to be embedded in an elastic medium of Winkler-type elastic foundation (Figure 1).

By introducing the elastic medium, the equation (6) become:

$$\rho A \frac{\partial^2 w}{\partial t^2} + EI \frac{\partial^4 w}{\partial x^4} = P(x) \quad (10)$$

$P(x)$ is the pressure acting on the CNT due to the surrounding elastic medium which is opposite to the deflections of CNT,

$$P(x) = -kw \quad (11)$$

k is the spring constant relative to the elastic medium described as a Winkler-type elastic foundation.

By introducing the non-local elasticity theory, we obtain the following governing equation:

$$\rho A \left[\frac{\partial^2 w}{\partial t^2} - (e_0 a)^2 \nabla^2 \frac{\partial^2 w}{\partial t^2} \right] + EI \frac{\partial^4 w}{\partial x^4} + K[w - (e_0 a)^2 \nabla^2 w] = 0 \quad (12)$$

Where:

$$w(x, t) = W \cdot e^{i\omega t}$$

In order to investigate the dynamic parameters we rewrite the governing equation in a dimensionless form by introducing the following no dimensionless quantities:

$$\Omega^2 = \frac{\rho A \omega^2 L^4}{EI}, \quad \bar{K} = \frac{kL^4}{EI}, \quad \mu = \frac{e_0 a}{L}, \quad \xi = \frac{x}{L}$$

3.2. SWCNTs as a rotating cantilever beam

In this section, a rotating cantilever nanobeam based SWCNT is studied (Figure 2). Flexural vibration equation based on the bending moment M and the shear force Q are expressed as:

$$\frac{\partial Q}{\partial x} = \rho A \ddot{u} \quad (13)$$

$$\frac{\partial M}{\partial x} + \left(T(x) \frac{\partial w}{\partial x} \right) = \rho A \ddot{w} \quad (14)$$

With $Q = \int_A \sigma_{xx} dA$

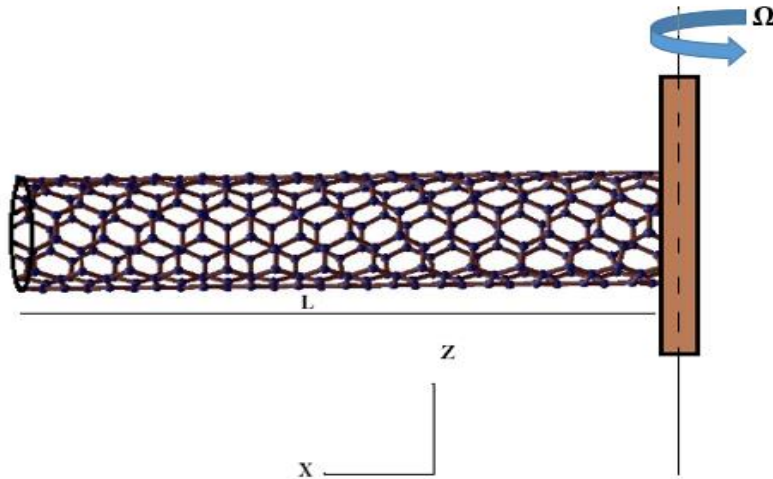


Figure 2. SWCNT as a rotating cantilever beam

$$M = \int_A z \sigma_{xx} dA \quad (15)$$

$T(x)$ the axial force due to centrifugal stiffening:

$$T(x) = \int_x^L \rho A \Omega^2 (x + R) dx \quad (16)$$

By applying nonlocal elastic theory, we obtain:

$$Q - (e_0 a)^2 \frac{d^2 Q}{dx^2} = EA \frac{du}{dx} \quad (17)$$

$$M - (e_0 a)^2 \frac{d^2 M}{dx^2} = EI \frac{d^2 w}{dx^2} \quad (18)$$

The following nondimensional parameters are employed to execute the investigation:

$$\Omega^2 = \frac{\rho A \omega^2 L^4}{EI}, \quad \mu = \frac{e_0 a}{L}, \quad \xi = \frac{x}{L}$$

The angular velocity parameter $\gamma^2 = \frac{\rho A \Omega^2 L^4}{EI}$ the hubradius $\delta = \frac{x}{L}$

3.3. SWCNTs as a rotating shaft

A SWCNT structure (Figure.3) is modelled via Euler-Bernoulli beam theory under rotating inertia, its governing equations are derived based on Hamilton's principle that considers the motion of an elastic structure during time is reduced to zero by

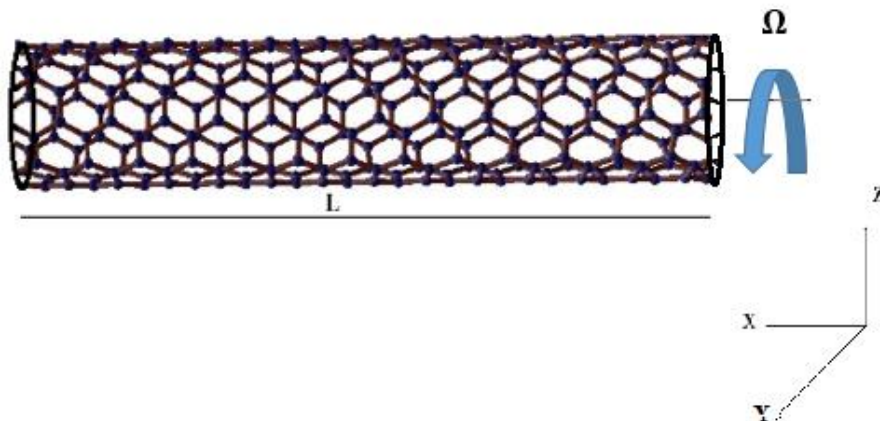


Figure 3. Geometry of a spinning SWCNT shaft.

combining the virtual displacements and virtual forces.

$$\int_{t_1}^{t_2} (\delta U + \delta V - \delta K) dt = 0 \quad (19)$$

Where:

$$\delta U = \int_0^L \left(N_{xx} \frac{\partial \delta u}{\partial x} - M_y \frac{\partial^2 \delta v}{\partial x^2} - M_z \frac{\partial^2 \delta w}{\partial x^2} \right) dx \quad (20)$$

is the variation of the strain energy. Whereas the variation of kinetic energy is:

$$K = \frac{1}{2} \int_0^L \left\{ \rho A \left[\dot{u} \frac{\partial \delta u}{\partial t} + \dot{v} \frac{\partial \delta v}{\partial t} + \dot{w} \frac{\partial \delta w}{\partial t} \right] + \rho I \left\{ \frac{\partial^2 v}{\partial t \partial x} \frac{\partial^2 \delta v}{\partial t \partial x} + \frac{\partial^2 w}{\partial t \partial x} \frac{\partial^2 \delta w}{\partial t \partial x} \right\} + 2\Omega \left(\frac{\partial \delta v}{\partial x} \frac{\partial w}{\partial x} - \frac{\partial \delta w}{\partial x} \frac{\partial v}{\partial x} \right) + 2\Omega^2 \right\} dx \quad (21)$$

ρ is the mass density, A is the cross section, I is the moment of inertia about cross section, and Ω is the angular velocity of the rotating nanostructure.

By applying the theory of nonlocal elasticity, we obtained:

$$\rho A \left[\ddot{u} - (e.a)^2 \frac{d^2 \ddot{u}}{dx^2} \right] = EA \frac{d^2 u}{dx^2} \quad (22)$$

$$\rho A \left[\ddot{v} - (e.a)^2 \frac{d^2 \ddot{v}}{dx^2} \right] + \rho I \left[\ddot{v} - (e.a)^2 \frac{d^2 \ddot{v}}{dx^2} \right] - 2\Omega \left(\dot{w} - (e.a)^2 \frac{d^2 \dot{w}}{dx^2} \right) = EI \frac{d^4 v}{dx^4} \quad (23)$$

$$\rho A \left[\ddot{w} - (e.a)^2 \frac{d^2 \ddot{w}}{dx^2} \right] + \rho I \left[\ddot{w} - (e.a)^2 \frac{d^2 \ddot{w}}{dx^2} \right] + 2\Omega \left(\dot{v} - (e.a)^2 \frac{d^2 \dot{v}}{dx^2} \right) = EI \frac{d^4 w}{dx^4} \quad (24)$$

Where, the three-directional deflection is defined as:

$$u(x, t) = ue^{i\omega t}, v(x, t) = ve^{i\omega t}, w(x, t) = we^{i\omega t}$$

4. APPLICATION OF GENERALIZED DIFFERENTIAL QUADRATURE METHOD (GDQM)

Bellman et al. [12] have firstly introduced differential quadrature method, a new partial technique called generalized differential quadrature method (GDQM) was proposed by Shu and Richard [13] to solve applied mechanics problems. In this paper, GDQM is used to discretize the differential equations.

The philosophy of DQM is based on computing the derivatives of the functions constituting the governing equation. Each derivative is formulated by a sum of values at its neighboring points.

$$\left| \frac{d^n f}{dx^n} \right|_{x=x_i} = \sum_{j=1}^N C_{ij}^{(n)} f(x_j) \quad i = 1, 2, \dots, N; n = 1, 2, \dots, N-1 \quad (25)$$

Where $C_{ij}^{(n)}$ is the weighting coefficient of the n th order derivative, and N the number of grid points of the whole domain, ($a = x_1, x_2, \dots, x_i, \dots, x_N = b$).

According to Shu and Richard rule [13], the weighting coefficients of the first-order derivatives in direction ξ , ($\xi = \frac{x}{L}$) are determined as:

$$C_{i,j}^{(1)} = \frac{P(\xi_i)}{(\xi_i - \xi_j).P(\xi_j)} \quad i, j = 1, 2, \dots, N, i \neq j \quad (26)$$

$$C_{i,j}^{(1)} = - \sum_{j \neq i}^N C_{i,j}^{(1)}$$

$$\text{Where: } P(\xi_i) = \prod_{j=1}^N (\xi_i - \xi_j) \quad i \neq j$$

The second and the higher order derivatives can be computed as:

$$C_{i,j}^{(2)} = \sum_{k=1}^N C_{i,k}^{(1)} \cdot C_{k,j}^{(1)} \quad i = j = 1, 2, \dots, N. \quad (27)$$

$$C_{i,j}^{(r)} = \sum_{k=1}^N C_{i,k}^{(1)} \cdot C_{k,j}^{(r-1)} \quad i = j = 1, 2, \dots, N. \\ r = 2, 3, \dots, m \quad (m < N)$$

Throughout the paper, the grid points are assumed based on the well-established Chebyshev-Gauss-Lobatto points

$$\xi_i = \frac{1}{2} \left(1 - \cos \frac{(i-1)\pi}{N-1} \right) \quad i = 1, 2, \dots, N \quad (28)$$

the boundary conditions used for the free vibration of rotating nonlocal shaft are:

Simply supported beam

$$w(\xi = 0) = \frac{\partial^2 w(\xi=0)}{\partial \xi^2} = 0 \quad \text{and} \quad w(\xi = 1) = \frac{\partial^2 w(\xi=1)}{\partial \xi^2} = 0 \quad (29)$$

Clamped-Clamped beam

$$w(\xi = 0) = \frac{\partial w(\xi=0)}{\partial \xi} = 0 \quad \text{and} \quad w(\xi = 1) = \frac{\partial w(\xi=1)}{\partial \xi} = 0 \quad (30)$$

Simply supported-Clamped beam

$$w(\xi = 0) = \frac{\partial^2 w(\xi=0)}{\partial \xi^2} = 0 \quad \text{and} \quad w(\xi = 1) = \frac{\partial w(\xi=1)}{\partial \xi} = 0 \quad (31)$$

5. RESULTS AND DISCUSSIONS

In this section, results of our study are reported here after solving a complex Eigen problem by developing a Matlab code using GDQM technique. The nonlocal governing differential equation is

solved using sufficient numbers of grid points which is taken as 15 as prove our previous studies. The effects of elastic medium, of small-scale parameter or nonlocal parameter, lower and higher angular velocities are investigated and the related graphs are plotted. For the present study, the properties of the nonlocal nanobeams are considered that of a SWCNT. An armchair SWCNT with chirality (5,5) is considered. With a Young's modulus $E=2.1$ TPa, the length- radius ratio is taken as $L=80d$, $d=1$ nm, a density $\rho=7800$ kg/m³, and a moment of inertia $I=\pi d^4/64$.

The validation of our results have been insured by comparing the flexural frequency parameters with Chakraverty [14] results for simply supported beam simply supported beam. Table 1 shows that the first four frequency parameters computed by as

Table 1. Comparison of First four frequency parameters of Euler-Bernoulli nanobeam for different boundary conditions and scaling effect parameters.

	$\mu^2 = 0$		$\mu^2 = 0.3$		$\mu^2 = 0.5$	
	<u>Present</u>	<u>Chakraverty[14]</u>	<u>Present</u>	<u>Chakraverty</u>	<u>Present</u>	<u>Chakraverty</u>
SS	3.1416	3.1416	2.6800	2.6800	2.3022	2.3022
	6.2832	6.2832	4.3013	4.3013	3.4404	3.4604
	9.4243	9.4248	5.4413	5.4422	4.2885	4.2941
	15.5035	15.5665	6.3646	6.3633	4.9731	4.9820

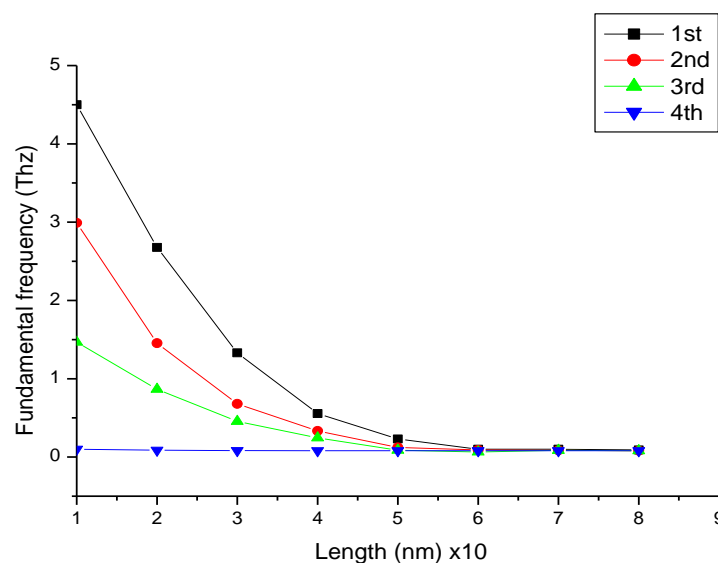


Figure 4. First four natural frequencies versus the length.

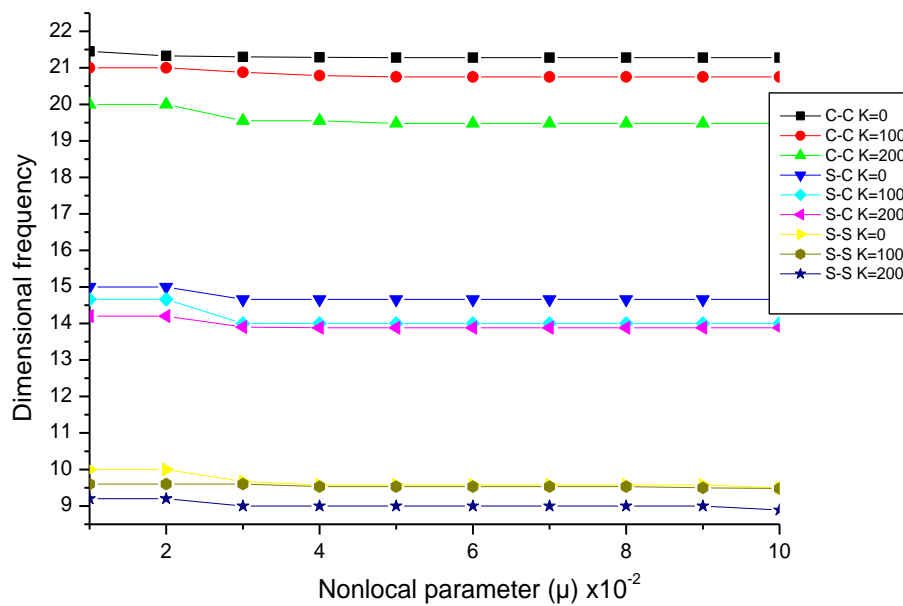


Figure 5. Variation of frequency parameters with nonlocal parameter for different elastic foundations.

present good agreement with those cited in literature.

5.1. SWCNT embedded in an elastic foundation

For the SWCNT resting on Winkler elastic foundation, natural frequencies are computed and valued to be considerably higher (Tera-hertz) due to exceptional mechanical properties that offer CNTs. The figure 4 shows the first four natural frequencies along the SWCNT for a simply supported-clamped beam boundary condition, it is remarkable that the four frequencies are distinguished in the beginning of the nanobeam, and they are converged in the end of the SWCNT. Whereas the first fundamental frequency is approximatively, uniform.

The figure.5 illustrates the effect of non-local parameter on the vibrational dimensionless frequency response for different boundary conditions, it shows that the frequency response for Clamped-Clamped beam is higher than that of simply supported-clamped and simply supported beam. The frequency response for a spring constant \bar{K} null is higher than that with a higher \bar{K} , which improves the inverse relationship between the dimensionless frequency Ω and \bar{K} .

5.2. SWCNT as a rotating cantilever nanobeam

For rotating cantilever nanobeam, as the angular velocity parameter increases the fundamental frequency parameter also increases. This observation is found to be similar for both the local and nonlocal elastic models. The increase in frequency with angular velocity is attributed to the stiffening effect of the centrifugal force, which is directly proportional to the square of the angular velocity. These remarks are valid only for the fundamental frequency parameter (Figure 6) where the frequency parameter increases with the increase of both angular velocities parameters and nonlocal parameters. For the higher mode frequency parameter, these remarks are invalid.

Figure 7 shows that the second mode frequency parameters are increasing when the angular velocity parameters increase but they decrease when the nonlocal elastic parameter increases. The small scale effect on the vibration response is amplified at high angular velocity of SWCNT. The higher frequency at amplified zone is due to the coupling effect of both rotational speed and nonlocal parameter.

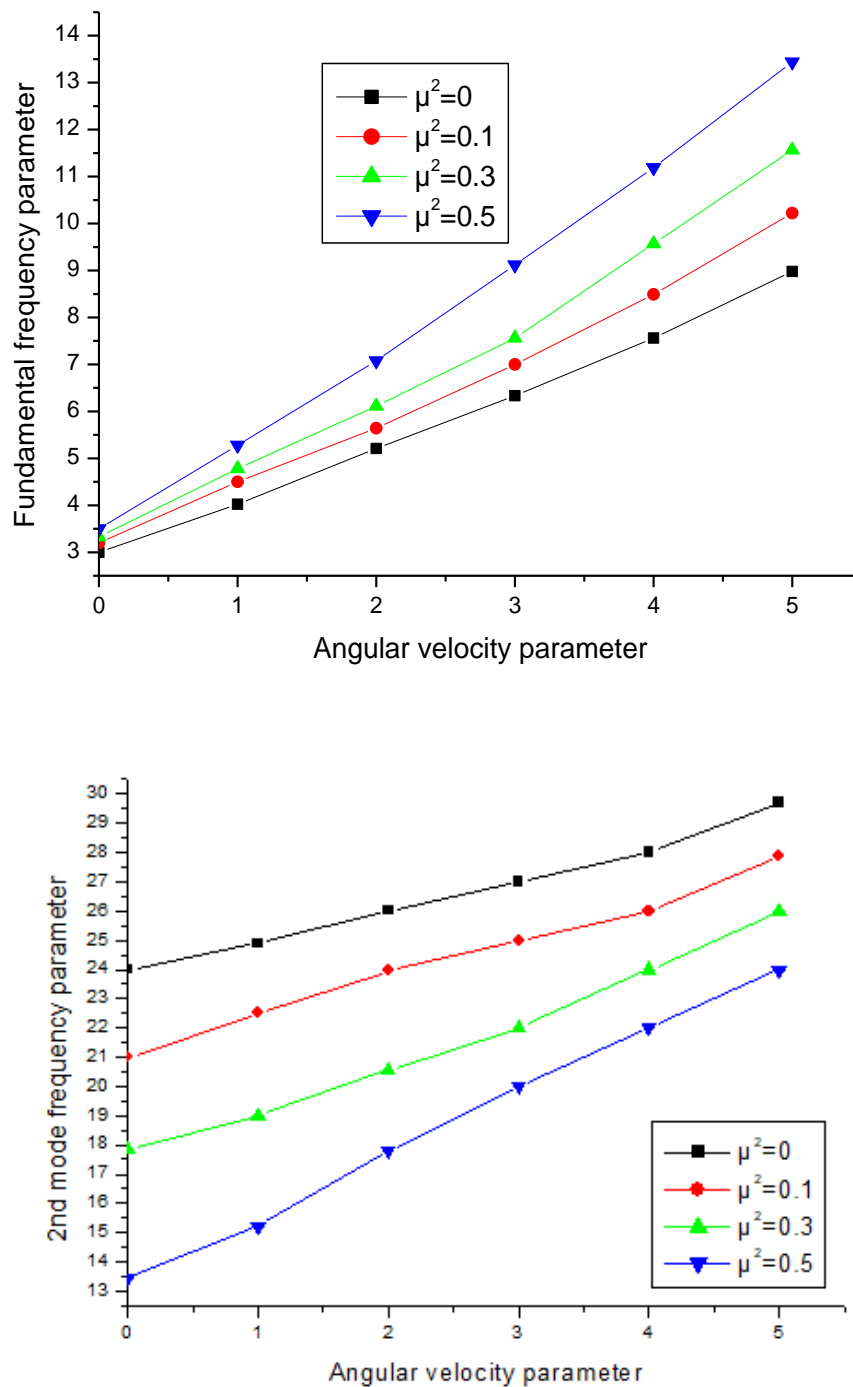


Figure 7. First frequency parameter versus angular velocity.

5.3. SWCNT as a rotating nanoshaft

In this section, the rotation of the SWCNT nanobeam is considered. The investigation of the vibration behaviour of the nanorotor [15] will be

done by solving the global Eigen problem expressed as:

$$(-\lambda^2[M] + j\lambda[G] + K).(U, V, W)^T = 0 \quad (25)$$

G is the gyroscopic matrix, $\hat{J} = -1$.

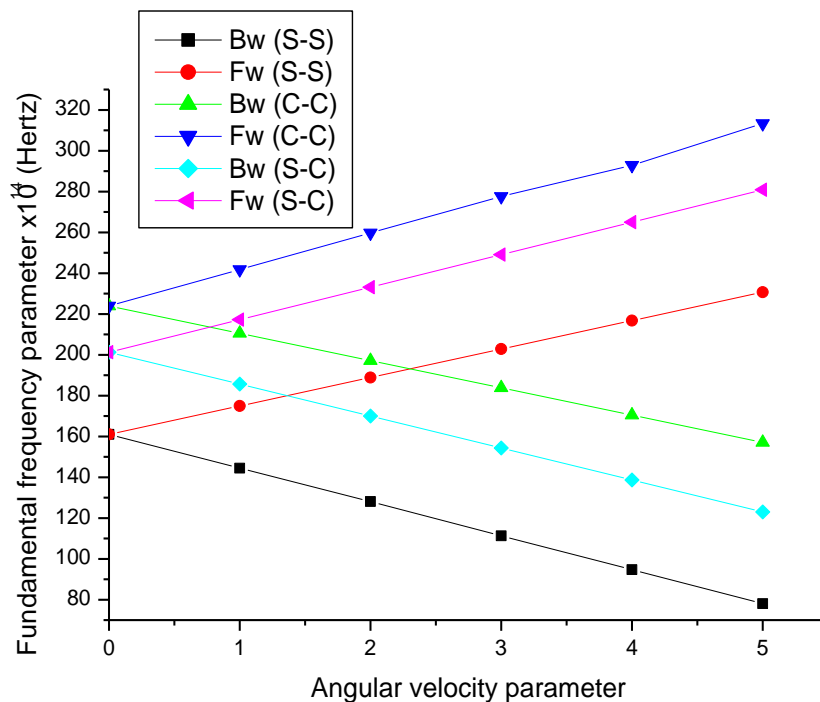


Figure 8. First frequency parameter versus angular velocity.

The Campbell diagram is employed to determine the critical speed λ_{Cr} where the nanorotor vibrates violently, it is the rotating speed correspondent to the intersection of the frequency curves and the angular velocities curves ($\lambda = \gamma$).

Figure 8 shows the Campbell diagram for different boundary conditions for a nonlocal nanobeam $\mu^2=0.3$. It is showed that the fundamental frequency have a linear relationship with angular velocities, the angular velocity parameters have increased the fundamental frequencies; the increasing frequency is the forward frequency, whereas the decreasing one is the backward frequency. It is also remarked that the C-C frequencies are higher than those of SS-C and SS boundary conditions, this difference in results is due to the effect of boundary conditions on the stiffness matrix that changes the eigenvalue decomposition of the system matrix.

5. CONCLUSION

In this paper, a computational structural dynamic analysis based on Eringen's elastic constitutive model is done to investigate the free vibration of

SWCNT nanostructure under three structural dynamic situations: first this nanostructure is studied resting on an elastic foundation of Winkler type, second the nanostructure is examined rotating around its transverse axis as a cantilever beam, then rotating as a nanoshaft around its axial axis.

The discretisation and the resolution of governing equations of motion that are derived based on Hamilton principles, is worked out by using the semi-analytical technique, generalized differential quadrature method (GDQM) that is highly recommended for structural nanomechanical problems.

Results obtained from this study are summarized as following:

- At nanoscale, nonlocal elasticity with other non-classical elastic theories are employed to model the problem.
- CNT's offer exceptional mechanical properties that are highly required in nanotechnology applications, in particularly next generation rotating nano-machinery.

- For SWCNT resting in elastic foundations, the elastic medium decreases their frequency parameters.
- For rotating cantilever nanobeam, angular velocity parameter increases the fundamental frequency parameter, so the nonlocal parameter does for fundamental frequency. A high order mode of vibration inversed the effect of nonlocal parameter.
- For the SWCNT nanorotor, Rotary inertia of the SWCNT nanostructure have split the frequency parameter to forward and backward frequencies (Campbell diagram).
- The increased critical speed parameter influences the forward frequency parameter increasingly and the backward frequency parameter decreasingly. The small scale parameter has a significant effect on the dynamic parameters, it decreases the frequency parameters as it increases.

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