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Free Vibration Analysis of Microtubules as Cytoskeleton Components: Nonlocal Euler-Bernoulli Beam Modeling

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Abstract. *Free vibration analysis of microtubules (MTs) is presented based on the Euler-Bernoulli beam theory. The size effect is taken into consideration using the Eringen's non-local elasticity theory. The governing differential equations for MT vibrations are being solved using the Differential Quadrature (DQ) method. Numerical results are presented to show the effect of nonlocal behavior on the frequencies of MTs. It is hoped that the results in the manuscript may present a benchmark in the study of vibration for microtubules.*

Keywords: *Microtubules; Nonlocal elasticity; Free vibration; Differential quadrature method; Euler-Bernoulli beam.*

INTRODUCTION

It is well known that microtubules (MT), microfilaments and intermediate filaments are the main components of a cytoskeleton. Microtubules (Figure 1) are proteins organized in a network that is interconnected with microfilaments and intermediate filaments to form the cytoskeleton structures [1]. The mechanical properties of microtubules play an important role in processes such as cell division and intracellular transport [2].

There have been a number of experimental and mathematical studies in the past ten years dealing with the mechanical properties of MTs. Microtubules are the most rigid of the cytoskeletal filaments and have the most complex structure. The structure of microtubules is cylindrical and it typically involves 13 parallel protofilaments that are connected laterally into hollow tubes. MTs are considered as hollow cylinders having 25 nm external and 15 nm internal diameters. The length of MTs can vary from tens of nanometers to hundreds of microns. Furthermore, MTs are considered as self-assembling biological nanotubes that are essential for cell motility, building the cytoskeleton, cell division and intracellular transport. The average Young's modulus of a microtubules is $\sim$ 2.0 GPa [2-5]. Among the three types of cytoskeletal filaments, microtubules are the most rigid. The bending rigidity of microtubules is about 100 times that of intermediate and actin filaments.

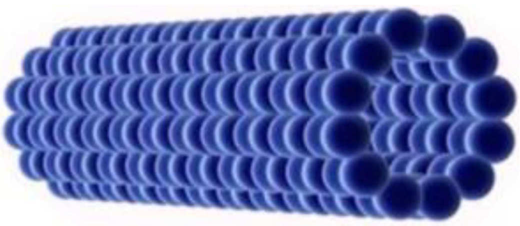

Figure 1. A typical microtubules.

Recently, much attention has been devoted to the mechanical behavior of micro/nano structures, such as nanobeams, nanorods, nanotubes and microtubules [6-19]. In general, orthotropic shell models have been applied for the modeling of MTs. In the present work, consistent governing equations for the beam model for microtubules are derived for bending analysis. Numerical results are presented to show the effect of the small-scale effect on the vibration of microtubules under different boundary conditions. To the authors' best knowledge it is the first time that the nonlocal elasticity theory has been successfully applied to microtubules for the numerical analysis of vibration. This paper is organized as follows. Nonlocal elasticity theory is investigated briefly. Then, the formulation of microtubule vibration as a nonlocal Euler-Bernoulli

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beam is given. The method of DQ and application to the title problem is given in the following section. The numerical results for free vibration of MTs are presented and discussed. Finally, the conclusion is given.

NONLOCAL ELASTICITY THEORY OF ERINGEN

It is known that the stress state of any body at point x is related to the strain state at the same point x in classical elasticity. Namely, the constitutive equations of classical (macroscopic) elasticity are an algebraic relationship between the stress and strain components. But, this theory is not in conflict with the atomic theory of lattice dynamics and experimental observation of phonon dispersion.

As stated by Eringen [20], the linear theory of nonlocal elasticity leads to a set of integropartial differential equations for the displacements field for homogeneous, isotropic bodies. The solutions of these equations are difficult, in general. But, these equations can be reduced to a set of singular partial equations for some types of kernel. Thus, these spatial integrals in constitutive equations of the nonlocal elasticity theory can be transformed to the equivalent differential constitutive equations under certain conditions.

According to the nonlocal elasticity theory of Eringen, the stress at any reference point in the body depends not only on the strains at this point, but also on strains at all points of the body. This definition of Eringen's nonlocal elasticity is based on the atomic theory of lattice dynamics and some experimental observations on phonon dispersion. In this theory, the long range force about atoms is considered, and thus an internal scale effect is introduced in the constitutive equation. In this theory, the fundamental equations involve spatial integrals that represent the weighted averages of the contributions of the related strain tensor at the related point in the body. This theory introduces the small length scale effect through a spatial integral constitutive relation. For homogenous and isotropic elastic solids, the linear theory of nonlocal elasticity is described by the following equations [21]:

$$\sigma_{kl,l} + \rho\left(f_l - \frac{\partial^2 u_l}{\partial t^2}\right) = 0, \tag{1}$$

$$\sigma_{kl}(x) = \int_V \alpha\left(|x - x'|, \chi\right) \tau_{kl}(x') dV(x'), \tag{2}$$

$$\tau_{kl}(x') = \lambda\varepsilon_{mm}(x')\delta_{kl} + 2\mu\varepsilon_{kl}(x'), \tag{3}$$

$$\varepsilon_{kl}(x') = \frac{1}{2}\left(\frac{\partial u_k(x')}{\partial x'_l} + \frac{\partial u_l(x')}{\partial x'_k}\right), \tag{4}$$

where σ_{kl} is the nonlocal stress tensor, ρ is the mass density of the body, f_l is the body (or applied) force density, u_l is the displacement vector at reference point x in the body, $\tau_{kl}(x')$ is the classical (Cauchy) or local stress tensor at any point x' in the body, $\varepsilon_{kl}(x')$ is the linear strain tensor at point x' in the body, t denotes the time, V is the volume occupied by the elastic body, $\alpha|x - x'|$ is the distance in Euclidean form, and λ and μ are the Lame constants. The non-local kernel $\alpha|x - x'|$ defines as the impact of the strain at point x' on the stress at point x in the elastic body. The value of χ depends on the ratio $(e_0 a/l)$, which is a material constant. The value a depends on the internal (granular distance, lattice parameter, distance between C-C bonds as molecular diameters) and external characteristics lengths (crack length or wave length), and e_0 is a constant appropriate to each material for adjusting the model to match reliable results by experiment or some other theories. If $\alpha|x|$ takes on a Green function of a linear differential operator given as:

$$\Re\alpha\left(|x' - x|\right) = \delta(|x' - x|), \tag{5}$$

the nonlocal constitutive relation given by Equation 2 is reduced to the following differential equation:

$$\Re\sigma_{kl} = \tau_{kl}. \tag{6}$$

Furthermore, the integropartial differential equation given by Equation 1 is also reduced to the following partial differential equation:

$$\tau_{kl,l} + \Re(f_l - \rho\ddot{u}_k) = 0. \tag{7}$$

Eringen [20] proposed a nonlocal model for this linear differential operator given as:

$$\Re = 1 - (e_0 a)^2\nabla^2 = 0, \tag{8}$$

where ∇^2 is the Laplacian. Consequently, the constitutive relations can be written as:

$$\left[1 - (e_0 a)^2\nabla^2\right]\sigma_{kl} = \tau_{kl}. \tag{9}$$

VIBRATION ANALYSIS OF MTs AS EULER-BERNOULLI BEAM MODEL

The influences of the small size effects on the mechanical properties of nanostructures cannot be properly predicted based on classical (macro) elasticity theory. In order to take into consideration the small size scale effect during the modeling and analysis stage, the theory of nonlocal elasticity proposed by Eringen [20] is used to modify the theory for vibration and buckling analyses of micro and nano scale beam devices. It is also accepted that some mechanical properties, such as vibration, bending and buckling of the beam like micro structures based on the nonlocal elasticity theory are entirely different from their counterparts based on the classical (macro) beam theory [22-28]. Thus, the theory based on the size dependent nonlocal elasticity theory could serve as a more reasonable and proper approach to the mechanical modeling of micro and nano sized components of nano mechanical devices [29-41].

The nonlocal theory of elasticity proposed by Eringen [20] has been widely used in the past five years in many nano mechanical problems including dislocation, crack, wave propagation, vibration analysis of nanobeams nanotubes, carbon nanotubes, and microtubules. The theory includes scale effects and long-range atomic interactions. General nonlocal constitutive equations for a beam can be written as [26]:

$$\sigma(x) - (e_0 a)^2 \frac{d^2\sigma(x)}{dx^2} = E\varepsilon(x), \tag{10}$$

$$\tau(x) - (e_0 a)^2 \frac{d^2\tau(x)}{dx^2} = 2G\varepsilon(x). \tag{11}$$

For a microtubule in a one dimensional case, the nonlocal constitutive relations (uniaxial Hooke's law) can be written as below:

$$\sigma_{xx} - (e_0 a)^2 \frac{\partial^2\sigma_{xx}}{\partial x^2} = E\varepsilon_{xx}, \tag{12}$$

where σ_{xx} is the axial stress, ε_{xx} is the axial strain and E is the Young modulus. Assume that the displacement of the beam along the y axial axis is $w(x,t)$ in terms of spatial coordinate x and time variable t. For transverse vibration of microtubules, the equilibrium conditions of the Euler-Bernoulli beam (Figure 2) can be written as:

$$\frac{\partial V(x,t)}{\partial x} = \rho A \frac{\partial^2 w(x,t)}{\partial t^2}, \tag{13}$$

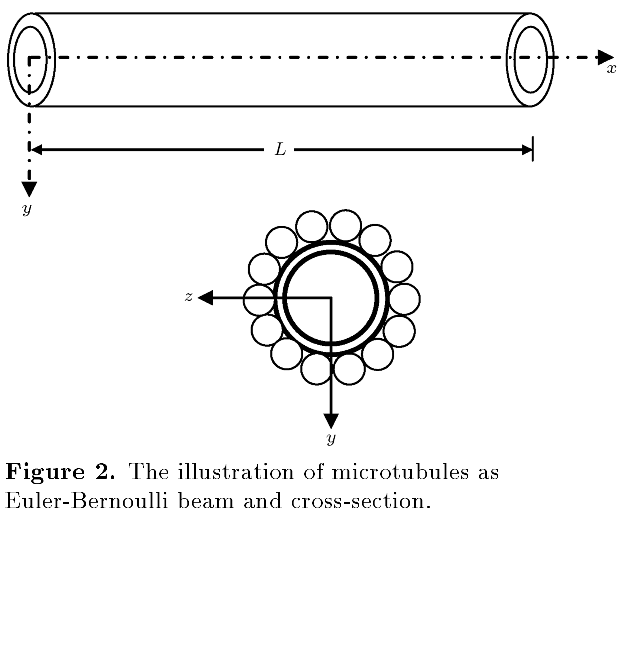

Figure 2. The illustration of microtubules as Euler-Bernoulli beam and cross-section.

$$V(x,t) = \frac{\partial M(x,t)}{\partial x}, \tag{14}$$

where $V(x,t)$ and $M(x,t)$ are resultant shear force and bending moment of the beam, ρ is the mass density, A is the area of the cross-section of the beam, $w(x,t)$ is the transverse displacement of the microtubules, and t is the time variable. We obtain the following relation from Equations 13 and 14:

$$\frac{\partial^2 M(x,t)}{\partial x^2} = \rho A \frac{\partial^2 w(x,t)}{\partial t^2}. \tag{15}$$

According to the linear theory of the Euler-Bernoulli beam, strain-displacements and the moment are given by:

$$\varepsilon = -y \frac{\partial^2 w(x,t)}{\partial x^2}, \tag{16}$$

$$M(x,t) = \int_A y\sigma dA. \tag{17}$$

At this stage, multiplying by y on both sides of Equation 12 and integrating over the cross-section area of the beam, we obtain:

$$\int_A \sigma_{xx} y dA - (e_0 a)^2 \int_A y \frac{\partial^2\sigma}{\partial x^2} dA - \int_A E y \varepsilon dA = 0. \tag{18}$$

By substituting Equations 16 and 17 into Equation 18, we have:

$$M(x,t) - (e_0 a)^2 \frac{\partial^2 M(x,t)}{\partial x^2} + EI \frac{\partial^2 w(x,t)}{\partial x^2} = 0. \tag{19}$$

By performing the differentiating of this equation, with respect to variable x, twice, we obtain:

$$\frac{\partial^2 M(x,t)}{\partial x^2} - (e_0 a)^2 \frac{\partial^4 M(x,t)}{\partial x^4} + EI \frac{\partial^4 w(x,t)}{\partial x^4} = 0. \tag{20}$$

By substituting Equation 15 into Equation 20, we obtain the below governing nonlocal equation for the motion of microtubules based on the Euler-Bernoulli beam theory:

$$EI \frac{\partial^4 w(x,t)}{\partial x^4} + \rho A \frac{\partial^2 w(x,t)}{\partial t^2} - (e_0 a)^2 \rho A \frac{\partial^4 w(x,t)}{\partial x^2 \partial t^2} = 0. \tag{21}$$

For free vibration, the transverse displacement $w(x,t)$ is assumed as:

$$w(x,t) = W(x) e^{i\omega t}. \tag{22}$$

Substituting Equation 22 into Equation 21 one obtains:

$$EI\frac{\partial^4 W(x)}{\partial x^4} - \omega^2 \rho A W(x) + (e_0 a)^2 \rho A \omega^2 \frac{\partial^2 W(x)}{\partial x^2} = 0. \qquad (23)$$

It is exactly seen from Equation 22 that the local Euler-Bernoulli beam theory is obtained when parameter e_0 is set identically to zero. In the present study, three-types of boundary condition are considered. These are:

Simply supported (S) end:

$$w = 0, \quad \text{and} \quad M = 0. \qquad (24a)$$

Clamped (C) end:

$$w = 0, \quad \text{and} \quad dw/dx = 0. \qquad (24b)$$

Free (F) end:

$$V = 0, \quad \text{and} \quad M = 0. \qquad (24c)$$

DIFFERENTIAL QUADRATURE (DQ) METHOD

In the past ten years, some new methods for numerical analysis of engineering problems have become quite popular. These are differential quadrature methods, meshless methods, and discrete singular convolution methods [42-61]. Some other numerical and analytical methods for nano scale modeling can also be possible [62-68].

The Differential Quadrature (DQ) method is a relatively new numerical technique in applied mechanics. The method of DQ can yield accurate solutions with relatively fewer grid points. It has been also successfully employed for different solid and fluid mechanic problems.

Unlike the DQ that uses polynomial functions, such as power functions, Lagrange interpolated, and Legendre polynomials as the test functions, Harmonic Differential Quadrature (HDQ) uses harmonic or trigonometric functions as the test functions. Shu and Xue [43] proposed an explicit means of obtaining the weighting coefficients for the HDQ. When $f(x)$ is approximated by a Fourier series expansion in the form [62]:

$$f(x) = c_0 + \sum_{k=1}^{N/2}\left(c_k \cos\frac{k\pi x}{L} + d_k \sin\frac{k\pi x}{L}\right), \qquad (25)$$

and the Lagrange interpolated trigonometric polynomials are taken as:

$$h_k(x) = \frac{\sin\frac{(x-x_0)\pi}{2} .. \sin\frac{(x-x_{k-1})\pi}{2} \sin\frac{(x-x_{k+1})\pi}{2} .. \sin\frac{(x-x_N)\pi}{2}}{\sin\frac{(x_k-x_0)\pi}{2} .. \sin\frac{(x_k-x_{k-1})\pi}{2} \sin\frac{(x_k-x_{k+1})\pi}{2} .. \sin\frac{(x_k-x_N)\pi}{2}}, \qquad (26)$$

for $k = 0, 1, 2, \cdots, N$. According to the HDQ, the weighting coefficients of the first-order derivatives, A_{ij}, for $i \neq j$ can be obtained by using the following formula:

$$A_{ij} = \frac{(\pi/2)P(x_i)}{P(x_j)\sin[(x_i - x_j)/2]\pi}, \quad i, j = 1, 2, 3, \cdots, N, \qquad (27)$$

where:

$$P(x_i) = \prod_{j=1, j\neq i}^{N} \sin\left(\frac{x_i - x_j}{2}\pi\right), \quad \text{for} \quad j = 1, 2, 3, \cdots, N. \qquad (28)$$

The weighting coefficients of second-order derivatives B_{ij} for $i \neq j$ can be obtained using the following formula:

$$B_{ij} = A_{ij}\left[2A_{ii}^{(1)} - \pi ctg\left(\frac{x_i - x_j}{2}\right)\pi\right], \quad i, j = 1, 2, 3, \cdots, N, \qquad (29)$$

The weighting coefficients of first-order and second-order derivatives $A_{ij}^{(p)}$ for $i = j$ are given as:

$$A_{ii}^{(p)} = -\sum_{j=1, j\neq i}^{N} A_{ij}^{(p)}, \quad p = 1 \text{ or } 2; \quad \text{for} \quad i = 1, 2, \cdots, N. \qquad (30)$$

A natural and often convenient choice for sampling points is that of equally spaced points. It was also reported that the Chebyshev-Gauss-Lobatto or non-equally sampling grid (NE-SG) points for spatial discretization as follows:

$$x_i = \frac{1}{2}\left[1 - \cos\left(\frac{i-1}{N-1}\right)\pi\right], \qquad (31)$$

performed consistently better than the equally spaced. By using DQ discretization, Equation 23 takes the following form for vibration of MTs:

$$EI\sum_{j=1}^{N} D_{ij}W_j - \omega^2 \rho A W_i + (e_0 a)^2 \rho A \omega^2 \sum_{j=1}^{N} B_{ij} W_j = 0. \qquad (32)$$

NUMERICAL RESULTS

In this section, some numerical examples related to the vibration analysis of MTs are presented. The material and geometric constants of MTs are given in Table 1. The symbol C-F, for example, represents the microtubules having a clamped edge at $x = 0$ and a free edge at $x = L$. Using the developed DQ method, as given in the above section, the free vibration of microtubules was studied under four different boundary conditions. The results are listed in Table 2 for different nonlocal parameters. It is seen from this table that the effect of nonlocal parameters on frequency values is more significant. In general, nonlocal parameters result in a decrease of the frequency values of MTs, except for the case of C-F. Under clamped boundary conditions (C-F), the frequencies increase slowly as the nonlocal parameter increases. In order to establish the accuracy and applicability of the described approach, numerical results were computed for an isolated pinned MTs vibration problem for which comparison values were available in the literature [6]. The results obtained by DQ and the results calculated by the formula given by Gu et al. [6] are presented in Table 3. The geometrical and material values are taken as Gu et al. [6] for comparison. The results obtained for the first two modes were found to be in excellent agreement with those available (obtained via given formula) in the literature [6]. The variation of frequency values of S-S microtubules for different lengths is depicted in Figure 3. Generally, it is shown that the increasing value of length always decreases the frequency parameter. Similarly, the frequency values increase considerably with mode numbers. The variation of frequency values of microtubules for different scaling effects is shown in Figures 4 to 8 for different boundary conditions. These figures indicate that for a given mode number of a microtubules, the maximum frequency values are obtained for C-C support conditions. Furthermore, the lowest frequency values are obtained for C-F support conditions. It is seen that the frequency parameters decrease as nonlocal parameters increase. Figure 9 describes the manner of variation of the frequency parameter, with respect to nonlocal parameters, under

Table 1. Material and geometric values of microtubules.

Parameter	Value
E	2×10^9 N/m^2
I	105×10^{-34} m^4
ρ	1470 kg/m^3
ν	0.3
L	$(1 \sim 8) \times 10^{-6}$ m

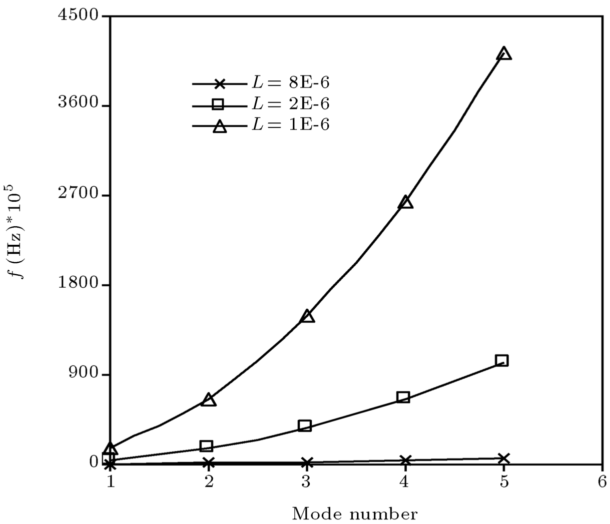

Figure 3. Variation of frequency values of S-S microtubules for different length.

Table 2. Frequency values (Hz)$\times 10^5$ of microtubules ($L = 1 \times 10^{-6}$).

$(e_o a)/L$	Boundary Conditions			
	S-S	**C-S**	**C-C**	**C-F**
0	164.93214	256.77254	373.85116	58.74609
0.1	157.58652	243.81196	349.56428	59.00957
0.2	135.78036	204.86781	290.96837	60.25963

Table 3. Comparison of first two frequencies $(\omega) \times 10^7$ of an isolated pinned microtubules ($E = 2 \times 10^9$ N/m^2; $L = 2 \times 10^{-6}$ m).

m	[6]*	Present $N = 5$	Present $N = 7$	Present $N = 9$	Present $N = 11$
1	2.5993	2.5971	2.5968	2.5968	2.5968
2	10.3972	10.3964	10.3964	10.3962	10.3962

*: Results are calculated formula $[\omega^2 = (E_x I_y/\rho A)(m\pi/L)^4]$ given this reference with the same values for I_y, A, E_x (beam model).

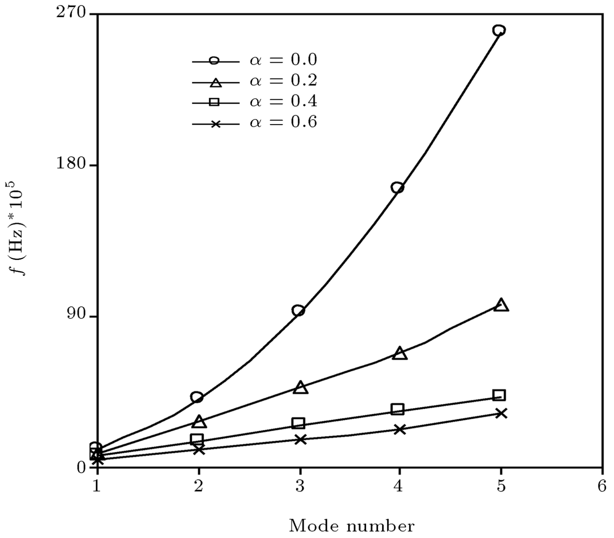

Figure 4. Variation of frequency values of S-S microtubules for different scaling effect ($L = 4$ μm).

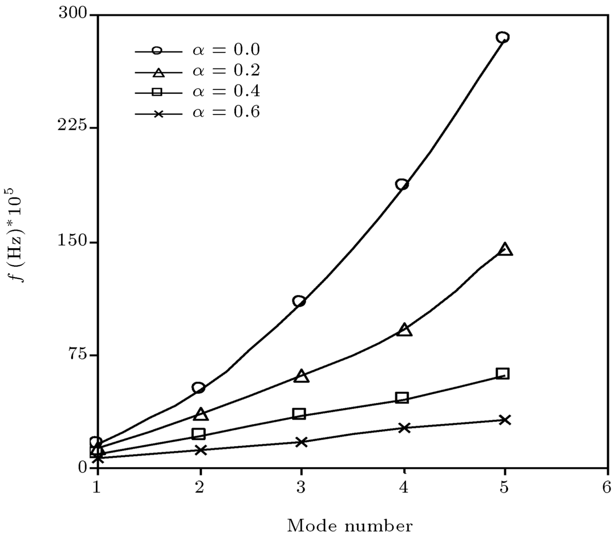

Figure 5. Variation of frequency values of C-S microtubules for different scaling effect ($L = 4$ μm).

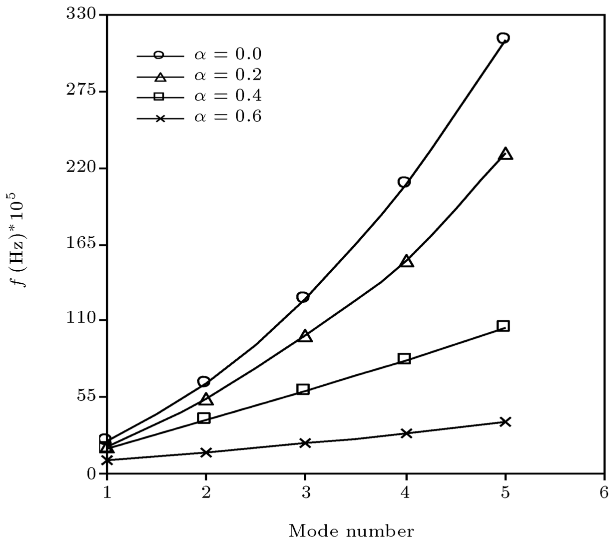

Figure 6. Variation of frequency values of C-C microtubules for different scaling effect ($L = 4$ μm).

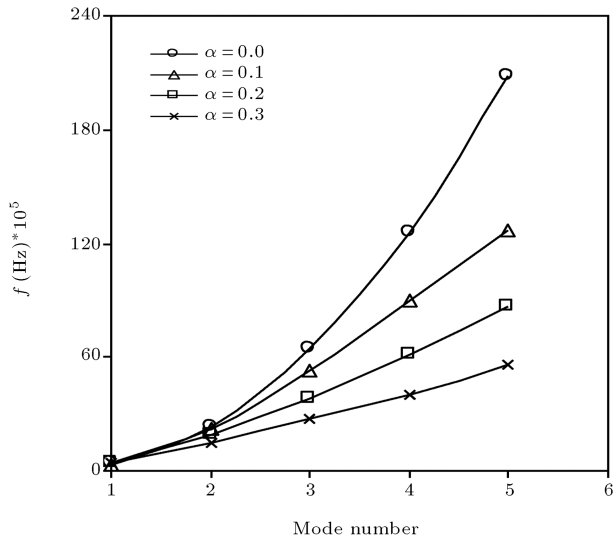

Figure 7. Variation of frequency values of C-F microtubules for different scaling effect ($L = 4$ μm).

different boundary conditions. As can be observed from this figure, the frequency parameters generally decrease with increasing the nonlocal parameter; except for C-F microtubules. Namely, the increasing value of a nonlocal parameter causes an increase for clamped MTs.

CONCLUDING REMARKS

This paper has presented a free vibration analysis of MTs in a computationally efficient manner using the nonlocal continuum beam theory. A numerical simulation is carried out to study the vibrations under different boundary conditions. The problem is analyzed using the Differential Quadrature (DQ) method. The numerical results show that the nonlocal parameter has an important effect on the vibration of microtubules. The major conclusion of this investigation is that the nonlocal continuum theory approach is superior to average (local) elasticity, especially for some boundary conditions. The method is suitable for the problem considered due to its generality, simplicity and potential for further development. Although not provided here, the method is also useful in providing the bending and buckling solutions of microtubules using the nonlocal beam theory. Even though the analysis presented is for linear static deformation cases only, the nonlinear static and vibration of microtubules based on nonlocal Euler and Timoshenko beam theories which can also be

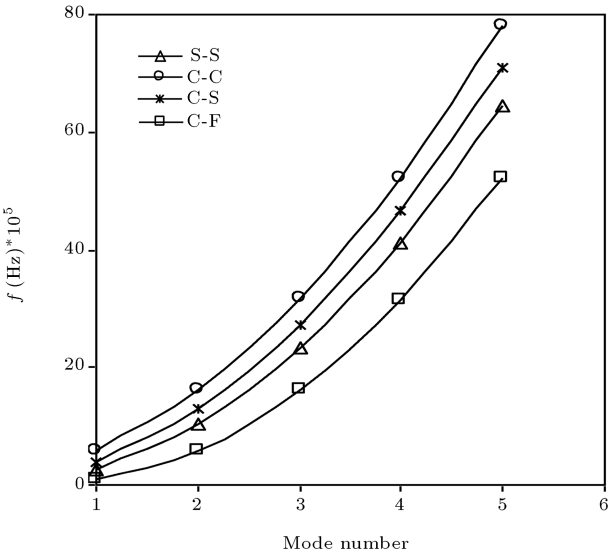

Figure 8. Variation of frequency values of microtubules with different boundary conditions ($L = 8$ μm).

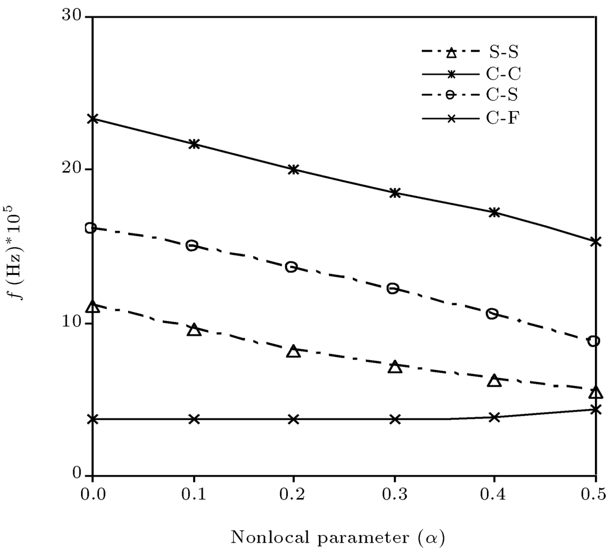

Figure 9. Variation of fundamental frequency of microtubules with nonlocal parameter for boundary conditions ($L = 4$ μm).

analyzed, using the numerical method, are presently under study.

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