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Research article

A new method for determination of natural frequency in bending vibration mode of single-walled carbon nanotubes

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Abstract

This paper investigates the bending vibration of single-walled carbon nanotubes (SWCNTs) based on a new theory called doublet mechanics (DM) with a scale parameter. A sixth order partial differential equation that governs the bending vibration for such nanotubes is derived. It is the first time that DM is used to model the bending vibration of carbon nanotube. Euler-Bernoulli beam model is used in this paper. Using DM, the relation between natural frequency and scale parameter is derived in the bending vibration mode. It is proven that scale parameter plays significant role in the vibration behavior of such nanotubes in lateral direction. Such effect decreases the natural frequency compared to the predictions of the classical continuum mechanics (CCM) models. However, with increasing the tube length, the scale effect on the natural frequency decreases. To show the accuracy and capability of this method, the results obtained herein are compared with the existing nonlocal and molecular dynamics (MD) results and good agreement is observed. It is notable that the results generated herein are new and can be used as a benchmark for future works.

Keywords: Doublet mechanics; Natural frequency; Scale parameter; Bending vibration; Single-walled carbon nanotubes

1- Introduction

The mechanical behavior of heterogeneous solids is divided in two general viewpoints depending on whether the material phases are distributed as either continuous or discrete. Under continuous distribution, theories are based on continuum mechanics and have provided many useful solutions to problems of engineering interest. However, these theories generally develop models that do not contain scaling effects and this is normally regarded as a limitation to predicting micromechanical material behavior.

At nanoscale, the mechanical characteristics of nanostructures are often significantly different from their behavior at macroscopic scale due to the inherent size effects. Such effects are essential for nanoscale materials or structures and the influence on nanoinstruments is great. Size effects exist not only for mechanical

properties but also for electronic, optical and some other properties. Classical continuum mechanics (CCM) [1] used to study vibration of nanostracture do not consider scale effects. In order to overcome this limitation, various elegant modifications to CCM have been proposed to incorporate scale and microstructural features into the theory. On the other hand, discrete modeling develops particular microforce–deformation relations between the various material phases within the solid. Discrete models normally lead to theories with one or more length scales resulting in nonlocal behavior where the stress at a point will depend on the deformation in a neighborhood about the point. These length scales may represent the sizes and/or separations of particles, dimensions of internal cells, characteristic ranges of particle or phase interactions, etc. One of the most popular theories in micromechanics is nonlocal theory. The nonlocal elasticity theory was first developed by Eringen [2] and it assumes that the stress tensor at a point is a function of strains at all points in the continuum. The nonlocal theory is developed following a simplified pattern without considering a particular microstructure. Under such an approach the parameters of the microstructure are not included in the mathematical model directly. The microstructural parameters enter the non local theory indirectly because it is implicitly contained in the macro tensors of elasticity. Consequently, the total number of elastic macroconstants in the nonlocal theory is considerably large [3]. Another popular theory in micromechanics is molecular dynamics (MD) theory. This theory studies vibrations of the atomic nuclei of solid crystals, the nuclei being considered as material points (particles) mutually bonded by elastic interatomic forces. MD is based on the following far-reaching. First, any crystal is an infinite lattice structure and second, the crystal obeys some devised periodic boundary conditions (PBC). It is seen that MD can exist as a general theory only on the basis of a particular boundary condition (the PBC) and it is, in general, incompatible with arbitrary boundary conditions [3].

One particular theory that has recently been applied to granular materials is the DM model. This approach originally developed by Granik (1978) [4], has been applied to granular materials by Granik, Ferrari (1993) [5] and Ferrari et al. (1997) [3]. DM is a micromechanical discrete model whereby solids are represented as arrays of points, particles or nodes at finite distances. The theory has shown promise is predicting observed behaviors that are not predictable using continuum mechanics. These behaviors include the so-called Flamant paradox (Ferrari et al., 1997) [3], where in a half-space under compressive boundary loading, continuum theory predicts a completely compressive stress field but observations indicate regions of tensile stress. Other anomalous behaviors include dispersive wave propagation. Ferrari et al. reformulated DM using a finite element approach with the aim of expanding even more the potential applications of such an approach [6]. Some application of doublet mechanics in biomedical and nanomechanics is given in [7-9] and for civil engineering is given in [10, 11]. Fang et al. [12] studied the plane wave propagation in a cubic tetrahedral assembly with DM. Some other application of doublet mechanics is given in [13, 14]. There are few works that investigate vibrations of nanostructure with DM.

Fatahi-Vajari and Imam studied axial and radial vibration of single-walled carbon nanotubes using DM in [15] and [16], respectively. They obtained a theoretical formula for natural frequency dependent to scale parameter.

Carbon nanotubes (CNTs) have been invented by Iijima in 1991 [17]. CNTs have many unique properties. Their electro-mechanical property has explained in [18, 19]. Owing to nanoscale dimensions of CNTs, it is difficult to set up controlled experiments to measure the properties of an individual CNT [20, 21]. Also, atomistic methods [22-24] are costly and time consuming to implement particularly for large-scale systems. With rapid development in nanotechnology, nanotubes have great potential for wide applications as components in nano-electronic-mechanical systems (NEMS). Some method for producing CNTs are given in [25- 27]. Such nanostructures have received growing interest recently. Very often, these components are subjected to external loadings during work operation and then, their resonant properties are of much concern. As a result, nanotechnological research on free vibration properties of nanotubes under certain support conditions is important because such components can be used as design components in nanosensors and nanoactuators. Elishakoff and Pentaras evaluated the fundamental natural frequencies of double-walled carbon nanotubes under various boundary conditions [27]. Ansari et al. investigated the vibrational characteristics of SWCNTs based on the gradient elasticity theories [28]. Sohani and Eipakchi derived the governing equations of a vibratory beam with moderately large deflection using the first order shear deformation theory [29]. Hosseini–Hashemi et al. considered surface effects including surface elasticity, surface stress and surface density, on the free vibration analysis of Euler-Bernoulli and Timoshenko nanobeams using nonlocal elasticity theory [30]. Ghorbanpour Arani et al. studied nonlinear free vibration of double-walled carbon nanotubes (DWCNTs) embedded in an elastic medium based on classical (local) Euler-Bernoulli beam theory [31]. Bocko and Lengvarský studied the free bending vibration and natural frequency of SWCNTs based on nonlocal theory of beam bending [32]. Ranjan studied the development of alternative beam finite elements using hp-spectral nodal expansions to eliminate shear and membrane locking [33].

However, most of the previous works on the vibration analysis methods of SWCNTs are usually restricted to the nonlocal theory and atomistic methods which are time consuming and have voluminous calculations. The purpose of this work is to present a modeling for bending vibration of SWCNTs using DM. First, the basic equation of motion for bending vibration of SWCNTs which considers small scale effect is derived using DM and then the governing equation is solved to obtain the frequency equation for bending vibration mode of SWCNTs.

2- Brief review of DM

Originally developed by Granik (1978) [1], DM is a micromechanical theory based on a discrete material model whereby solids are represented as arrays of points or nodes at finite distances. A pair of such nodes is referred to as a doublet, and the nodal spacing distances introduce length scales into the microstructural theory. Each node in the array is allowed to have a translation and rotation, and increments of these variables are expanded in a Taylor series

about the nodal point. This allowable kinematics develops microstrains of elongation, shear and torsion (about the doublet axis). Through appropriate constitutive assumptions, these microstrains can be related to corresponding elongational, shear and torsional microstresses. Applications of this theory to geomechanics problems have been given by Granik and Ferrari (1993) [2] and Ferrari et al. (1997) [3]. For these applications, a granular interpretation of DM has been employed, in which the material is viewed as an assembly of circular or spherical particles. A pair of such particles represents a doublet as shown in Fig. 1. Corresponding to the doublet (A, B) there exists a doublet or branch vector $\boldsymbol{\zeta}_a$ connecting the adjacent particle centers and defining the doublet axis. The magnitude of this vector $\eta_a = |\boldsymbol{\zeta}_a|$ is simply the particle diameter for particles in contact. However, in general the particles need not be in contact, and for this case the length scale η_a could be used to represent a more general microstructural feature. For example, the internal characteristic scale for the crystal lattice parameter of carbon is $\eta_a = 1.421\ a$ [23]. As mentioned, the kinematics allow relative elongational, shearing and torsional motions between the particles, and this is used to develop an elongational microstress p_a, shear microstress t_a, and torsional microstress m_a as shown in Fig. 1.

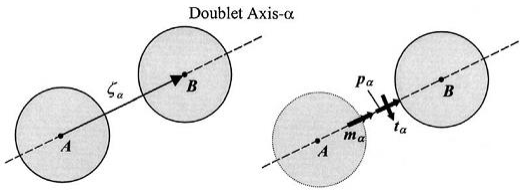

Fig. 1 Doublet.

It should be pointed out that these microstresses are not second order tensors in the usual continuum mechanics sense. Rather, they are vector quantities that represent the elastic microforces and microcouples of interaction between doublet particles. Their directions are dependent on the doublet axes which are determined by the material microstructure. These microstresses are not continuously distributed but rather exist only at particular points in the medium being simulated by DM.From Fig. 2, suppose doublet (a, b_α) converts to doublet (a', b'_α) because of kinematic translation. The superscript 0 for vectors indicates the initial state. If $\boldsymbol{u}(\boldsymbol{x},t)$ is the displacement field coinciding with a particle displacement, then the increment function at $\boldsymbol{x}=\boldsymbol{x}_A$ is written as [3]:

$$\Delta\boldsymbol{u}_\alpha = \boldsymbol{u}\left(\boldsymbol{x}+\boldsymbol{\zeta}_\alpha^0, t\right) - \boldsymbol{u}(\boldsymbol{x},t) \tag{1}$$

where $\boldsymbol{x}_A$ is the position vector of the particle A and $\boldsymbol{\zeta}_\alpha^0$ is the initial branch vector.

Here, $\alpha = 1,...,n$ while n is referred to the numbers of doublets. In many practical applications, it can be assumed that the shear and torsional microdeformations and microstresses are negligible and thus only extensional strains and stresses will exist.

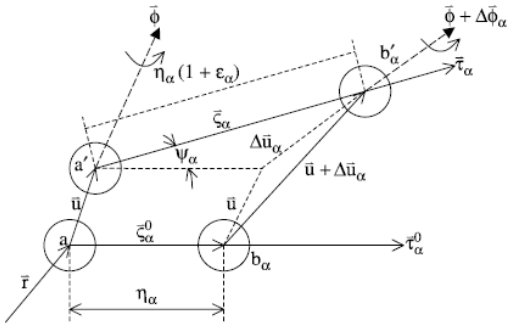

Fig. 2 Translations of the doublet nodes $a \in A$, $b_\alpha \in B_\alpha$.

As in linear elasticity, it is assumed that the relative displacement $\Delta \boldsymbol{u}_\alpha$ is small compared to the doublet separation distance η_α ($|\Delta \boldsymbol{u}_\alpha| \ll \eta_\alpha$) so that the initial and final configuration of the system can be assumed to coincide. That means that $\boldsymbol{\tau}_\alpha = \boldsymbol{\tau}_\alpha^0$.

The extensional microstrain scalar measure ϵ_α, representing the axial deformation of the doublet vector, is defined as [3]:

$$\epsilon_\alpha = \frac{\boldsymbol{\tau}_\alpha . \Delta \boldsymbol{u}_\alpha}{\eta_\alpha} \tag{2}$$

This can be interpreted as the compatibility equation within the linear DM. The increment function in Eq. (2) can be expanded in a Taylor series as [15]:

$$\epsilon_\alpha = \sum_{\chi=1}^{M} \frac{(\eta_\alpha)^{\chi-1}}{\chi!} \boldsymbol{\tau}_\alpha^0 . \left(\boldsymbol{\tau}_\alpha^0 . \nabla\right)^\chi \boldsymbol{u} \tag{3}$$

where ∇ is the Del operator in general coordinate and η_α is the internal characteristic length scale. The order at which the series is truncated defines the degree of approximation employed. The lowest order case using only a single term in the series will not contain any length scales, while using more than one term will produce a multi length scale theory.

It may be written that $\boldsymbol{\tau}_\alpha^0 = \tau_{\alpha j}^0 \boldsymbol{e}_j$ where $\tau_{\alpha j}^0$ are the cosines of the angles between the directions of microstress and the coordinates.

In DM with such assumptions and neglecting temperature effect, the relation between microstrain and microstress for the linear elasticity is written by the following equation [3]

$$p_\alpha = \sum_{\beta=1}^{n} A_{\alpha\beta} \epsilon_\beta \tag{4}$$

where p_α is axial microstress along doublet axes in the case of linear and homogeneous inter nodal central interactions. Eq. (4) can be interpreted as the constitutive equation in the linear and homogeneous DM theory, and $A_{\alpha\beta}$ is the matrix of the micromodules of the doublet.

In the isotropic media with local interaction, Eq. (4) is reduced to [3]

$$p_\alpha = A_0 \epsilon_\alpha \tag{5}$$

The relation between microstress and macrostress can be written as [16]:

$$\sigma_{ij}^{(M)} = \sum_{\alpha=1}^{n} \tau_{\alpha i}^0 \tau_{\alpha j}^0 \sum_{\chi=1}^{M} \frac{(-\eta_\alpha)^{\chi-1}}{\chi!} \left(\boldsymbol{\tau}_\alpha^0 . \nabla\right)^{\chi-1} p_\alpha \tag{6}$$

Superscript M indicates that macrostresses incorporate scale effect.

The three-dimensional equation of motion in DM is written by the following equation [34]

$$\frac{\partial \sigma_{ji}^{(M)}}{\partial x_j} + F_i = \rho \frac{\partial^2 u_i}{\partial t^2} \tag{7}$$

where ρ is the mass density, u_i are the displacement vector, F_i body force and t is the time.

Now, the form of matrix [$\boldsymbol{A}$] in Eq. (4) containing elastic macroconstant for plane problem (two-dimensional) is obtained. For this reason, consider Fig. 3. According to Fig. 3, in the $x_1 - x_2$ plane, there are only three doublets with equal angels between them. The solution for the scale-less condition can be calculated directly from the associated CCM problem for an isotropic material.

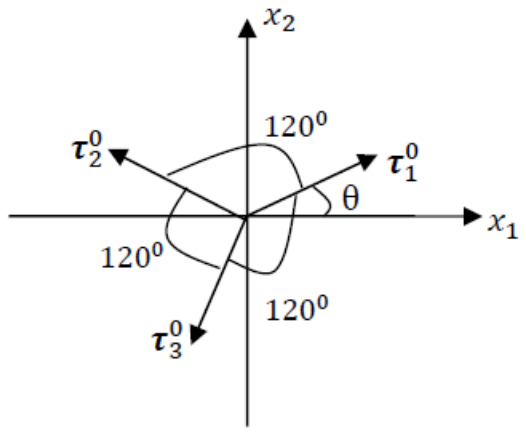

Fig. 3 Three doublets with equal angle 120^0 between them.

For the plane problems in the homogeneous media, $[\boldsymbol{A}]$ is a symmetric matrix of order 3 with the most general form [35]

$$[\boldsymbol{A}]=\begin{bmatrix} a & b & b \\ b & a & b \\ b & b & a \end{bmatrix} \tag{8}$$

It can be shown that the coefficients of matrix $[\boldsymbol{A}]$ are independent to chirality of doublets rendering the material isotropic. Furthermore, the coefficients a and b in matrix $[\boldsymbol{A}]$ for plane stress conditions are found to be [3]:

$$a=\frac{4}{9}\mu\frac{7\lambda+10\mu}{\lambda+2\mu},b=\frac{4}{9}\mu\frac{\lambda-2\mu}{\lambda+2\mu} \tag{9}$$

One could use $b=0$ as a quantitative guide to the applicability of the simpler constitutive relations such as Eq. (5). If $\lambda=2\mu$ (or $\nu=\frac{1}{3}$) in plane stress condition from Eq. (9), it is concluded that [36]

$$a=A_0=\frac{8\mu}{3}=E \tag{10}$$

3- DM model for bending vibration of SWCNTs

Specific applications of DM have been developed for two-dimensional problems with regular particle packing microstructures. One case that has been studied in this paper is the two-dimensional hexagonal packing without internal atoms as shown in Fig. 3. This geometrical microstructure establishes three doublet axes with equal angles between them. This structure is coincident with nanostructure.

Now, consider a SWCNT with length L, mean radius R, Young's modulus E, Poisson's ratio ν, mass density ρ, cross-sectional area A and cross-sectional moment of inertia I as shown in Fig. 4.

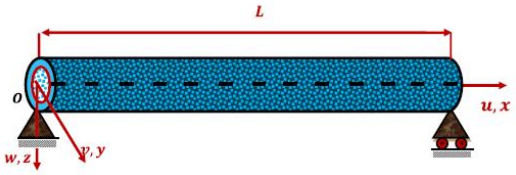

Fig. 4 A schematic of SWCNT.

Using the Euler–Bernoulli beam model in conjunction with DM, the governing equations for the bending vibration of SWCNTs are derived as follows.

The Euler–Bernoulli beam theory (EBT) is the simplest beam theory in which it is assumed that the straight lines which are vertical to the mid-plane will remain straight and vertical to the mid plane after deformation. Based on the EBT, the displacement field at any point can be written as [28]:

$$u(x,z,t)=-z\frac{\partial w}{\partial x} \tag{11}$$

$$v(x,z,t)=0 \tag{12}$$

$$w(x,z,t)=w(x,t) \tag{13}$$

wherein u, v and w are the displacements of the tube in x, y and z directions, respectively. The strain–displacement relations corresponding to EBT can be given as [28]:

$$\varepsilon_{xx} = -z\frac{\partial^2 w}{\partial x^2} \tag{14}$$

And other macrostrains are zero.

$$\gamma_{xz} = 2\varepsilon_{xz} = 0 \tag{15}$$

Expanding Eq. (7) in Cartesian coordinate in the absence of body forces in the *x* and *y* directions yields

$$\frac{\partial \sigma_{xx}^{(M)}}{\partial x} + \frac{\partial \sigma_{yx}^{(M)}}{\partial y} + \frac{\partial \sigma_{zx}^{(M)}}{\partial z} = \rho\frac{\partial^2 u}{\partial t^2} \tag{16}$$

$$\frac{\partial \sigma_{xy}^{(M)}}{\partial x} + \frac{\partial \sigma_{yy}^{(M)}}{\partial y} + \frac{\partial \sigma_{zy}^{(M)}}{\partial z} = \rho\frac{\partial^2 v}{\partial t^2} \tag{17}$$

$$\frac{\partial \sigma_{xz}^{(M)}}{\partial x} + \frac{\partial \sigma_{yz}^{(M)}}{\partial y} + \frac{\partial \sigma_{zz}^{(M)}}{\partial z} + f_z = \rho\frac{\partial^2 w}{\partial t^2} \tag{18}$$

Integration of Eq. (16) and Eq. (17) with respect to the cross-area of the tube (*A*) and neglecting shear macrostresses $\sigma_{yx}^{(M)}, \sigma_{zy}^{(M)}$ in the upper and lower planes of the tube with considering Eq. (12) yield

$$\frac{\partial N_{xx}}{\partial x} + \frac{\partial N_{xz}}{\partial z} = \rho h\frac{\partial^2 u}{\partial t^2} \tag{19}$$

where

$$N_{xx} = \int_A \sigma_{xx}^{(M)} dA\ , N_{xz} = \int_A \sigma_{xy}^{(M)} dA \tag{20}$$

Eq. (19) is the equation of motion of the tube in longitudinal (*x*) direction. Now, the equation of motion in the lateral (*z*) direction is obtained. Differentiating Eq. (16), Eq. (17) and Eq. (18) with respect to *x* ,*y* and *z* respectively and using Eqs. (11)-(15) along with combining the results, it is found that

$$\frac{\partial^2 \sigma_{xx}^{(M)}}{\partial x^2} - \frac{\partial^2 \sigma_{zz}^{(M)}}{\partial z^2} = \frac{\partial f_z}{\partial z} - \rho\frac{\partial^3 w}{\partial z \partial t^2} - \rho z\frac{\partial^4 w}{\partial x^2 \partial t^2} \tag{21}$$

Multiplication both side of Eq. (21) by *z* and then integrating it according to cross-area of the beam and neglecting $\sigma_{zz}^{(M)}$ yields

$$\frac{\partial^2 M_{xx}}{\partial x^2} = \rho A\frac{\partial^2 w}{\partial t^2} - \rho I\frac{\partial^4 w}{\partial x^2 \partial t^2} \tag{22}$$

where

$$M_{xx} = \int_{-\frac{t}{2}}^{\frac{t}{2}} z\sigma_{xx}^{(M)} dA\ , I = \int_A z^2 dA \tag{23}$$

and $q = \int_{-\frac{h}{2}}^{\frac{h}{2}} z\frac{\partial f_z}{\partial z} dA$ is the transverse force per unit length of the tube.

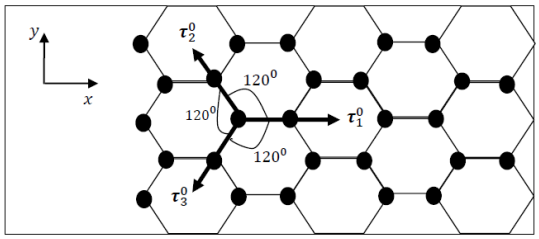

Fig. 5 A Zigzag SWCNT.

As is known, the nanotube is constructed with three doublets arranged with equal lengths and angles. Now, for example consider a Zigzag nanotube ($\theta = 0$ in Fig. 3) shown in Fig. 5. From this figure, the director vectors in Cartesian coordinates are written as:

$$\tau_{1x}^0 = 1\ , \tau_{2x}^0 = -cos60\ , \tau_{3x}^0 = -cos60 \tag{24}$$

$$\tau_{1y}^0 = 0, \tau_{2y}^0 = cos30\ , \tau_{3y}^0 = -cos30 \tag{25}$$

$$\tau_{1z}^0 = 0\ , \tau_{2z}^0 = -cos30\ , \tau_{3z}^0 = cos30 \tag{26}$$

If Eq. (3) is substituted into Eq. (5) and then the result is substituted into Eq. (6) and neglecting the terms with order $O(\eta^3)$ and higher, it can be found that

$$\boldsymbol{\sigma}^{(M)}=\sum_{\alpha=1}^{n}\boldsymbol{\tau}_{\alpha}^{0}\boldsymbol{\tau}_{\alpha}^{0}\left\{\boldsymbol{\tau}_{\alpha}^{0}.\left[\boldsymbol{\tau}_{\alpha}^{0}.\nabla\boldsymbol{u}+\frac{1}{12}\eta^{2}\left(\boldsymbol{\tau}_{\alpha}^{0}.\nabla\right)\left(\boldsymbol{\tau}_{\alpha}^{0}.\nabla\right)\left(\boldsymbol{\tau}_{\alpha}^{0}.\nabla\boldsymbol{u}\right)\right]\right\} \quad (27)$$

This equation is the relation between macrostress and displacement with order $O\left(\eta^{2}\right)$. Noting that in Cartesian coordinate $\nabla=\frac{\partial}{\partial x_{i}}\boldsymbol{e}_{i}$, Eq. (27) can be reduced to:

$$\sigma_{ij}^{(M)}=\sum_{\alpha=1}^{n}A_{0}\tau_{\alpha i}^{0}\tau_{\alpha j}^{0}\tau_{\alpha m}^{0}\tau_{\alpha n}^{0}\left(\varepsilon_{mn}+\frac{1}{12}\eta^{2}\tau_{\alpha t}^{0}\tau_{\alpha s}^{0}\frac{\partial^{2}\varepsilon_{mn}}{\partial x_{t}\partial x_{s}}\right) \quad (28)$$

where ε_{mn} is the linear elastic macrostrain tensor defined by $\varepsilon_{mn}=\frac{1}{2}\left(\frac{\partial u_{m}}{\partial x_{n}}+\frac{\partial u_{n}}{\partial x_{m}}\right)$ in Cartesian coordinate.

It is further assumed that all doublets originating from a common node have the same magnitudes; i.e. $\eta_{a}=\eta\left(a=1,2,\ldots,n\right)$ and the interactions are purely axial (no shear or torsional microstresses is present). For local interaction in the plane, there will be two micromoduli a ,b and the constitutive relationship between elongation microstress and microstrain is expressed by Eq. (4). If $\nu=\frac{1}{3}$, matrix $\left[\boldsymbol{A}\right]$ will be diagonal and there will be one micromodulus A_{0} and the constitutive relationship between elongation microstress and microstrain is expressed by Eq. (5). In this paper, Eq. (5) is used because volume of calculation with two micromoduli is overbearing.

It can be seen from Eq. (28) that nonlocal behavior enters into the problem through the constitutive relations. Expanding Eq. (28) and setting $i, j = x$ and using Eqs. (14) and (15) along with Eqs. (23)- (25), it is found that

$$\sigma_{xx}=-A_{0}z\left(\frac{\partial^{2}w}{\partial x^{2}}+\frac{1}{12}\eta^{2}\frac{\partial^{4}w}{\partial x^{4}}\right) \quad (29)$$

This equation is relation between macrostress and displacement.

It is clear that the nanotube in bending vibration mode is in plane stress condition then from Eq. (10), it is concluded that $A_{0}=E$. If Eq. (29) is substituted into the first part of Eq. (23) and integrating is performed, the following equations for moments can be obtained

$$M_{z}=-EI\left(\frac{\partial^{2}w}{\partial x^{2}}+\frac{1}{12}\eta^{2}\frac{d^{4}w}{dx^{4}}\right) \quad (30)$$

If Eq. (30) is substituted into the Eq. (21), the following equation of motion in term of *w* can be obtained

$$-EI\left(\frac{\partial^{4}w}{\partial x^{4}}+\frac{1}{12}\eta^{2}\frac{d^{6}w}{dx^{6}}\right)-\rho A\frac{\partial^{2}w}{\partial t^{2}}+\rho I\frac{\partial^{4}w}{\partial x^{2}\partial t^{2}}=0 \quad (31)$$

According to Eq. (31) a sixth order governing equation is obtained. However, the governing equation derived from the DM principle turns out to be an infinite order differential equation in terms of η. Because it is almost impossible to solve the infinite order differential equation, only lower order terms in the infinite series in Eq. (3) and Eq. (6) are retained.

For the general case which the scale parameter is present, Eq. (30) is the basic equation of motion with scale effect for bending vibration of Zigzag SWCNTs.

It is assumed that the boundaries forces of the tubes are independent to scale. Then the

displacement fields can be written by the following equation [3]

$$w = w_0 + \eta^2 w_2 \tag{32}$$

Suppose that the boundaries of the tube are simply supported. Then it can be concluded that

$$w(x,t) = M_{xx}^{(M)}(x,t) = 0 \, at \, x = 0, L \tag{33}$$

Substituting Eq. (32) in to Eq. (33) yields

$$w_0(x,t) = 0, \frac{\partial^2 w_0(x,t)}{\partial x^2} = 0 \, at \, x = 0, L \tag{34}$$

$$w_2(x,t) = 0, \frac{\partial^2 w_2(x,t)}{\partial x^2} = 0 \, at \, x = 0, L \tag{35}$$

To find the frequency of lateral vibration of nanotube, the following solution for the lateral vibrations of nanotube is considered as

$$w = \left(A_n + \eta^2 B_n\right).sin\frac{n\pi}{L} y.sin\omega_n^{(\eta)} t \tag{36}$$

wherein A_n and B_n are the amplitudes of lateral vibration, $\omega_n^{(\eta)}$ is the frequency of lateral vibration and n is mode number, respectively. Substituting Eq. (36) into Eq. (31) yields

$$\left(\omega_n^{(\eta)}\right)^2 = \frac{EI\left[\left(\frac{n\pi}{L}\right)^4 - \frac{1}{12}\eta^2\left(\frac{n\pi}{L}\right)^6\right]}{\rho A + \rho I\left(\frac{n\pi}{L}\right)^2} \tag{37}$$

This is the frequency equation of lateral vibration of nanotube considering scale effect.

For Armchair nanotubes, similar calculations yield

$$\left(\omega_n^{(\eta)}\right)^2 = \frac{EI\left[\left(\frac{n\pi}{L}\right)^4 - \frac{1}{16}\eta^2\left(\frac{n\pi}{L}\right)^6\right]}{\rho A + \rho I\left(\frac{n\pi}{L}\right)^2} \tag{38}$$

The advantage of these simple expressions is that they show the dependency of the bending natural frequency on the mechanical and geometrical properties of the SWCNT. In particular, these expressions show that by increasing the Young's modulus (E) and the moment of area (I) of the SWCNT, their bending frequency increases; however by increasing the mass density (ρ), the scale parameter (η), their bending frequency decreases.

In the scale-less condition where $\eta = 0$, from Eq. (36) and/or Eq. (38), it is found that

$$\omega_n^2 = \frac{EI\left(\frac{n\pi}{L}\right)^4}{\rho A + \rho I\left(\frac{n\pi}{L}\right)^2} \tag{39}$$

This equation is exactly in agreement with frequency obtained in [22, 23] for lateral vibration with simply supported beam.

It is evident from Eqs. (37)- (39) that using a continuum beam model in the frequency analysis of nanotube can cause an overestimate. However as the length of the tube increases, the difference between natural frequency of lateral vibration with and without scale parameter becomes smaller and the frequencies of the two models converge to a single value. It is also seen that the presence of the nanoscale η decreases the natural frequency but as the length of the tube increases the effect of scale decreases.

4- Results and discussion

To validate the present approach, the result obtained herein using DM are compared

with available MD and nonlocal simulation results for simply-supported (8, 8) SWCNT with different aspect ratios ranging from 8.3 to 39.1 [28]. In the current study, the effective thickness of the SWCNTs is assumed to be equal to the spacing of graphite ($h = 0.34\ nm$). In addition, Poisson's ratio ν, mass density ρ and Young's modulus E are assumed to be 0.3, $2300\frac{Kg}{m^3}$ and 1.1 *TPa*, respectively [28].

Table 1 present the values of fundamental frequency obtained from DM, MD simulations and the nonlocal stress gradient elasticity theory for (8, 8) Armchair nanotube with different aspect ratios (length to diameter; L/D). The results predicted by the present model are found to be in good agreement with the ones obtained from MD and nonlocal simulation which indicates the capability of the present approach in accurately predicting frequencies of SWCNTs.

Table 1: Fundamental frequencies (THz) for (8, 8) Armchair SWCNTs with simply support boundary condition

L/D	DM	MD [28]	Nonlocal [28]
8.3	0.5378	0.5299	0.5376
10.1	0.3639	0.3618	0.3638
13.7	0.1982	0.1931	0.1982
17.3	0.1244	0.1103	0.1244
20.9	0.0853	0.0724	0.0853
24.5	0.0621	0.0519	0.0621
28.1	0.0472	0.0425	0.0472
31.6	0.0373	0.0358	0.0373
35.3	0.0299	0.0287	0.0299
39.1	0.0244	0.0259	0.0244

From Table. 1, it is observed that employing DM leads to highly accurate results which are comparable to those obtained by MD simulations and nonlocal results particularly for low aspect ratios. As the aspect ratio increases, the discrepancy between various vibration modes decreases so that the fundamental frequencies tend to converge at an aspect ratio of approximately 40.

The free vibration frequency ratio is defined as

$$Frequency\ Ratio = \frac{[natural\ frequency]_{DM\ theory}}{[natural\ frequency]_{local\ theory}}$$

Then from Eq. (37) and Eq. (39) for bending mode vibration, Frequency Ratio (*F.R.*) for Zigzag SWCNTs becomes

$$F.R. = \frac{\omega_n^{(\eta)}}{\omega_n} = \sqrt{1 - \frac{1}{12}\eta^2\left(\frac{n\pi}{L}\right)^2} \qquad (40)$$

And for Armchair SWCNTs, from Eq. (38) and Eq. (39), it becomes

$$F.R. = \frac{\omega_n^{(\eta)}}{\omega_n} = \sqrt{1 - \frac{1}{16}\eta^2\left(\frac{n\pi}{L}\right)^2} \qquad (41)$$

The numerical results for free vibrating nanotubes are given in graphical form in Figs. 6-11. The unit of length and radius is given in angstrom (a). In Figs. 6 and 7, the effect of scale parameter on frequency ratio in different vibration modes is shown for (8, 8) Armchair and (16, 0) Zigzag SWCNTs, respectively. The boundary conditions of the nanotubes are considered to be simply support.

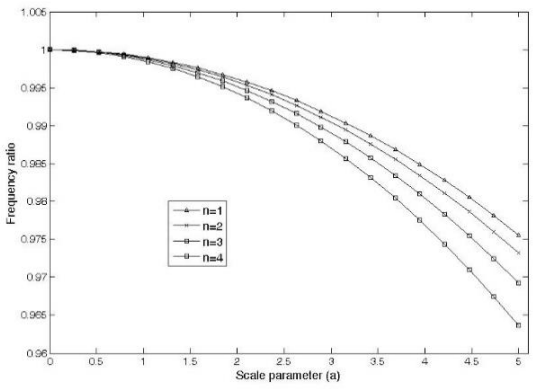

Fig. 6 Variation of frequency ratio with scale parameter for (8, 8) Armchair nanotube with L=100 a for different bending vibration mode.

It is found that the frequency ratio decreases with increasing in scale parameter for all vibration modes. This decreasing is more apparent for higher vibration modes.

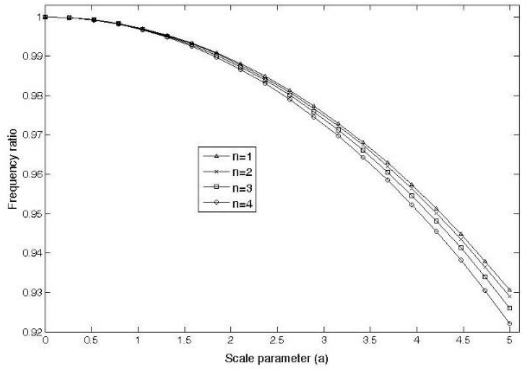

Fig. 7 Variation of frequency ratio with scale parameter for (16, 0) Zigzag nanotube with L=70 a for different bending vibration mode

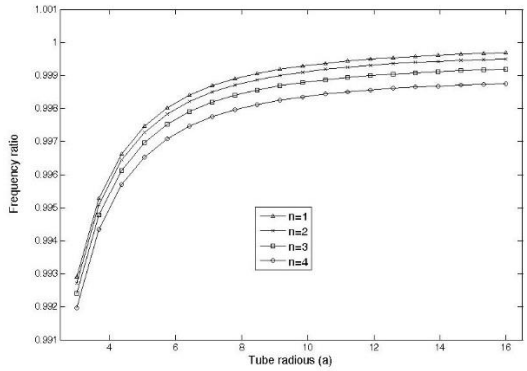

Fig. 8 Variation of frequency ratio with tube radius for Armchair nanotube with L=100 a for different bending vibration.

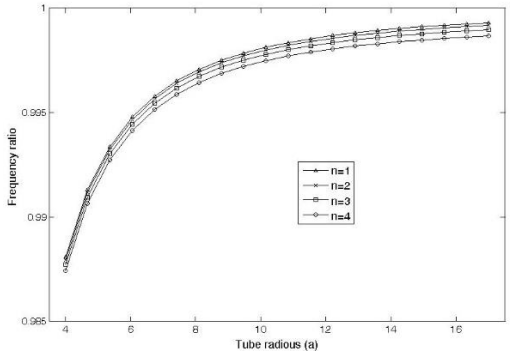

Fig. 9 Variation of frequency ratio with tube radius for Zigzag nanotube with L=70 a for different bending vibration mode.

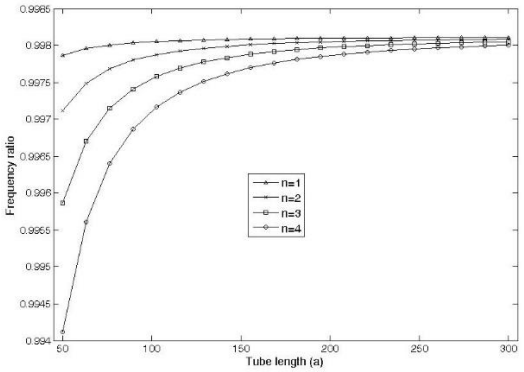

Fig. 10 Variation of frequency ratios with tube length for (8, 8) Armchair nanotube for different bending vibration mode.

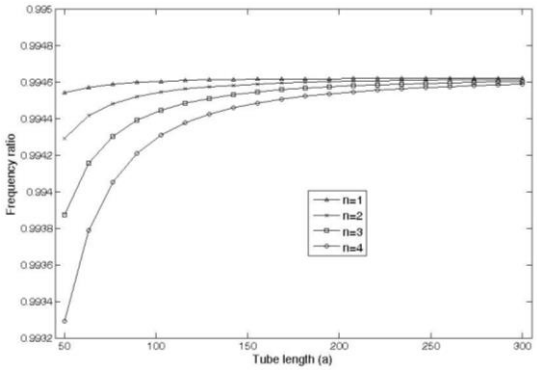

Fig. 11 Variation of frequency ratios with tube length for (16, 0) Zigzag nanotube for different bending vibration mode.

Variation of frequency ratio of the SWCNTs as a function of tube radius for different mode numbers for Armchair and Zigzag nanotubes are plotted in Fig. 9 and Fig. 10, respectively. The boundary conditions of the nanotubes are simply supported. According to these figures, frequency ratio is increasing with increase in tube radius. This is more apparent for lower tube radius.

In Figs. 10 and 11, variation of frequency ratio with tube length *L* is given for different vibration mode for (8, 8) Armchair and (16, 0) Zigzag SWCNTs, respectively with simply supported boundary conditions. According to these figures, with increasing in the length of the nanotubes, frequency ratio increases. This increasing is more pronounced for higher modes of

vibration. Since scale effects are more effective for smaller wave lengths, after a certain tube length *L*, frequency ratios approaches to a certain value. These figures also reveal that the difference between different vibration modes becomes more pronounced for very short SWCNTs.

5- Conclusion

The DM theory has been employed to model the bending vibration of simply supported SWCNTs. The governing equation of motion in bending mode was obtained in terms of lateral displacement using DM and was solved analytically to obtain a closed form expression for the natural frequency of such a nanotube. To the best of authors' knowledge, there is no prior work reported in the literature before this study. Then, availability of present paper gives a possibility of an appropriate and effective evaluation of the natural frequency in bending vibration mode for SWCNTs. The following points are particularly noted in this work. Firstly, the scale effects decrease natural frequency of a nanotube in bending mode vibration based on DM model presented here, or the nanotube stiffness is lessened in comparison with the CCM theory. Secondly, for a nanotube with sufficient Aspect ratio, the nanoscale effect becomes insignificant and thus the governing equation can be reduced to the classical equation and both DM and classical solutions are in complete agreement, and validity of the DM model developed here for vanishing nonlocal effect is established. Then the scale parameter is more effective in higher modes of vibration and lower Aspect ratios. Lastly, with increase in tube length and/or in tube radios, frequency ratio increases. This increasing is more apparent in higher modes of vibration.

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