Free torsional vibrations of carbon nanotube based on nonlocal elasticity of bi-Helmholtz type

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Abstract. In this paper, the theory of nonlocal elasticity of bi-Helmholtz type is applied to analyze the problem of torsional vibrations of single walled carbon nanotube with higher order boundary conditions containing two nonlocal nano scale parameters. The effect of different parameters on the angular frequencies of vibrations are explained.

1. Introduction
The classical linear theory of elasticity is intrinsically size independent and it is valid only for small wave numbers with no dispersions. In this theory, the stress at any point of the body is uniquely determined by the strain at the same point. The constitutive equations of classical elasticity are simply algebraic relations between the stress-strain components. This theory cannot be applied to study of Mechanical properties of special type bodies with carbon nanomaterials that are used in the design of MEMS and NEMS devices. The nonlocal elasticity theory used in this paper, was first developed by Eringen [1-5] and his associates. It assumes that the stress at a reference point in the elastic continuum is a function of elastic strain field at every point in that model. This theory is based on the atomic theory of lattice dynamics and on phonon dispersions. In this theory the nonlocal stress is represented by a spatial integral of weighted averages of all local stresses within the domain. The spatial weight is specified by a nonlocal modulus is known as an attenuation function which depends on a single dimensionless nonlocal parameter. This parameter is proportional to the ratio internal characteristic length to the external characteristic length. The dynamic properties of materials at nanoscale are significantly different from their behaviors at larger scales due to the influence of surfaces stress and size effects. Usually the variational principles are applied to derive for the equation of motion and corresponding higher order boundary conditions which contain a nonlocal nanoscale parameter. The constitutive equations of nonlocal elasticity for isotropic medium involve not only two elastic constants but also the nonlocal kernel with a single nonlocal parameter. In literature [6] this theory is known as nonlocal theory of Helmholtz type. Recently the theory of nonlocal elasticity of bi-Helmholtz type for isotropic materials are under discussion[7-10]. In the theory of nonlocal elasticity of bi-Helmholtz type the kernel involves two nonlocal parameters which are functions of internal characteristic length scale. The nonlocal elasticity of bi-Helmholtz type involves two limits the first limit reduces bi-Helmholtz to Helmholtz type and the second limit...
from Helmholtz type to classical theory of elasticity. The nonlocal elasticity of bi-Helmholtz type is mentioned in the paper of Eringen[11] but not discussed in detail.

The main objective of this paper is to study the problem of free torsional vibration of carbon nanotubes using the theory of nonlocal elasticity of bi-Helmholtz type. The governing differential equation of fourth order is derived and a closed form solution for angular displacement involving nonlocal parameters is obtained. The frequencies of vibrations are obtained as the roots of dispersive relation which is a fourth order polynomial. The general solution is simplified by considering higher order boundary conditions at each end of the body. The effect of different nonoscale parameters on the free angular frequency are explained numerically. The corresponding problems of nonlocal elasticity of bi-Helmholtz type and of classical elasticity can be derived as special case.

2. Basic equations of nonlocal elasticity

The nonlocal elastic stress field theory first proposed by Eringen [2] concerns the state of stress at a reference point \( x' \) within domain. The nonlocal stress depends not only on the strain at that location but also on the strain at all other points within the domain in a diminishing influence away from the reference location. The nonlocal elastic field theory for homogeneous and isotropic solids is described using the following basic equations given as [13-16]

\[
\sigma_{ij,t} + \rho (f_j - u_j) = 0, \tag{1}
\]

\[
\sigma_{ij}(r) = \int_V \phi(|r' - r|, \alpha) t_{ij}(r') dv(r'), \tag{2}
\]

\[
t_{ij}(r') = \lambda \delta_{kk}(r') \delta_{ij} + 2 \mu e_{ij}(r'), \tag{3}
\]

\[
e_{ij}(r') = \frac{1}{2} \left[ \frac{\partial u_j(r')}{\partial r'_i} + \frac{\partial u_i(r')}{\partial r'_j} \right], \tag{4}
\]

where \( \sigma_{ij}(r) \), \( \rho \), \( f_j \) and \( u_j \) are the nonlocal stress tensor, mass density, body force density and displacement vector at time \( t \) respectively at a reference point \( r \) in the body. Here the indices \( i, j \) take the values 1\((or)1, 2\((or)1, 2, 3 \) depending on the dimensions of the body. The linear relationship between the local stress tensor \( t_{ij} \) and classical strain tensor \( e_{ij}(r') \) at any arbitrary point \( r' \) is shown in eqn(3). The Lame constants are \( \lambda \), \( \mu \) and \( \delta_{ij} \) is the Kronnecker delta. The nonlocal kernal function denoted by \( \phi(|r' - r|, \alpha) \) depends on the Euclidean distance \( |r' - r| \) between the reference point \( r \) and the arbitrary point \( r' \) and on the dimensionless nanolength scale \( \alpha \). The dimensionless nanolength scale \( \alpha \) is described in [3] as

\[
\alpha = \frac{e_0 a}{L}, \tag{5}
\]

here \( a \) is the internal characteristic length (Ex. Lattice parameter, \( C - C \) bond length, granular distance), and \( L \) is an external characteristic length (Ex. Crack length, Wave length etc.) of the nanotube. Also, we take \( e_0 \) as nonlocal scaling parameter which is assumed to be constant appropriate to continuum model. The parameter \( e_0 \) is estimated such that the relations on the nonlocal elasticity model could provide satisfactory approximations to the atomic dispersion curves of the plane waves with those obtained from the atomistic lattice dynamics. The above equations is in partial integral form and generally difficult to solve analytically. Thus a differential form of nonlocal elasticity equation is often used. According to Eringen’s [3] the expression of nonlocal modulus can be given as

\[
\phi(|x|, \alpha) = (2\Pi l^2 \alpha^2)^{-1} k_0(\sqrt{x, x/l}, \alpha), \tag{6}
\]
where $k_0$ is the modified Bessel function, using equations \([1 - 4]\) and \((6)\), the nonlocal constitutive equations can be approximated as

\[
\left[1 - \epsilon^2 \nabla^2 + \gamma^4 \nabla^4\right] \sigma_{ij} = t_{ij},
\]

where $\epsilon = \epsilon_0 a$ and $\gamma = \gamma_0 a$ are constants and $\nabla^2$ is the Laplacian operator.

3. Nonlocal elasticity of bi-Helmholtz type

In the theory of nonlocal elasticity of bi-Helmholtz type the linear differential operator is in the form of

\[
L = 1 - \epsilon^2 \nabla^2 + \gamma^4 \nabla^4,
\]

where $\epsilon$ and $\gamma$ are nonnegative parameters of nonlocality. These two parameters have the dimension of lengths and it satisfies the equation as

\[
L\phi(|x' - x|) = \delta(|x' - x|),
\]

where $\phi$ is the attenuation function and $\delta$ is the usual Dirac delta function. Here $\nabla^2$ is the harmonic operator and $\nabla^4$ is the bi-harmonic operator. In the above definition $\epsilon$ and $\gamma$ are two nonlocal parameters having the dimensions of lengths. These parameters can be represented in terms of characteristic length $a$ as

\[
\epsilon = \epsilon_0 a, \quad \epsilon_0 \geq 0, \quad \gamma = \gamma_0 a, \quad \gamma_0 \geq 0.
\]

The nonlocal elasticity of bi-Helmholtz type has two types of limits. The first limit from $\gamma \to 0$ reduces from bi-Helmholtz type elasticity to Helmholtz type. The second limit is obtained by $\epsilon \to 0$ which is followed by first limit. The second limit reduces nonlocal elasticity of bi-Helmholtz type to classical theory of elasticity. The constitutive equations for the nonlocal elasticity of bi-Helmholtz type can be written as

\[
\left[1 - \epsilon^2 \nabla^2 + \gamma^4 \nabla^4\right] \sigma_{ij} = t_{ij}.
\]

The bi-Helmholtz operator can be factorized as

\[
L = \left[1 - \epsilon^2 \nabla^2 + \gamma^4 \nabla^4\right] = \left[1 - d_1 \nabla^2\right] \left[1 - d_2 \nabla^2\right],
\]

where $d_1 + d_2 = \epsilon^2$, $d_1 d_2 = \gamma^4$. Solving the equation for $d_1, d_2$, we obtain

\[
d_1 = \frac{\epsilon^2}{2} \left[1 + \sqrt{1 - \frac{4\gamma^4}{\epsilon^4}}\right]
\]

and

\[
d_2 = \frac{\epsilon^2}{2} \left[1 - \sqrt{1 - \frac{4\gamma^4}{\epsilon^4}}\right].
\]

For the validity of the roots to be real we have the condition

\[
1 - \frac{4\gamma^4}{\epsilon^4} \geq 0.
\]
In order to have the roots $d_1, d_2$ to be distinct non-negative and satisfy the condition as $\epsilon > \sqrt{2}\gamma$. We can observe that the nonlocal elasticity of Helmholtz type due to Eringen’s is obtained to the limit form $d_1 \to \epsilon^2, \ d_2 \to 0$.

In this paper we describe a nonlocal model of lattice dynamics with next nearest neighborhood interactions. In this model we consider the interacting with the first and second neighbours in the homogeneous chain of the Brillouin zone from the dispersive relation. For such model the values of the nonlocal parameters $\epsilon_0, \gamma_0$ are taken as $\epsilon_0 = 0.318, \ \gamma_0 = 0.450$. These values satisfy the required condition $\epsilon_0 > \sqrt{2}\gamma_0$. It is described in the literature that the best physical result for the dispersive relations of nonlocal elasticity of bi-Helmholtz type with two different parameters can be obtained only from the lattice theory with next nearest neighborhood interactions.

4. Nonlocal torsional vibration of nanotube with bi-Helmholtz type operator

Consider a single walled carbon nanotube with two fixed ends undergoing torsional vibration. The influence of forces applied at one end, the nanotube is assumed to be of length $L$. Using by-Helmholtz type operator given by Eq.(11), the Eringen’s nonlocal stress can be represented in one dimensional differential equation form as

$$\tau - (e_0a)^2 \frac{\partial^2 \tau}{\partial x^2} + (\gamma_0a)^4 \frac{\partial^4 \tau}{\partial x^4} \sigma_{ij} = G\gamma,$$

where $G$ is the shear modulus, $\gamma$ is the shear strain and $\tau$ is the shear stress of the nanotube. The resultant stress due to shear force can be written as

$$S = \int_A \tau dA,$$

where $A$ is the area of the cross section of nanotube. The torque relation $T$ due to torsional vibration can be given as

$$T = \int_A \tau z dA.$$

By using the equations(16)and (18) we get the constitutive relation as

$$S - (e_0a)^2 \frac{\partial^2 S}{\partial x^2} + (\gamma_0a)^4 \frac{\partial^4 S}{\partial x^4} = GA\gamma,$$

$$T - (e_0a)^2 \frac{\partial^2 T}{\partial x^2} + (\gamma_0a)^4 \frac{\partial^4 T}{\partial x^4} = GIp \frac{d\Theta}{dx},$$

where $\Theta$ and $Ip$ are the angular displacement and the polar moment of inertia of the cross section respectively. By ignoring the external force, the equation of motion at an element of length $dx$ can be written as

$$\left[ T + \frac{\partial T}{\partial x} dx \right] - T = \rho Ip \frac{\partial^2 \Theta}{\partial t^2} dx,$$

where $T$ is the induced torque per unit length and the term $\rho Ip \frac{\partial^2 \Theta}{\partial t^2} dx$ represents the inertia torque acting on element of the carbon nanotube. Here $\rho$ represents the density of carbon nanotube and $t$ indicates time respectively. From the equations(20) and (21) we have

$$T = GI_p \frac{\partial \Theta}{\partial x} + (e_0a)^2 \rho Ip \frac{\partial^2 \Theta}{\partial t^2} dx - (\gamma_0a)^4 \rho Ip \frac{\partial^4 \Theta}{\partial x^4 \partial t^2} dx.$$ 

Using the equation of equilibrium (21) we obtain the governing differential equation as

$$\epsilon^2 \frac{\partial^2 \Theta}{\partial x^2} - (e_0a)^2 \frac{\partial^4 \Theta}{\partial x^2 \partial t^2} + (\gamma_0a)^4 \frac{\partial^6 \Theta}{\partial x^4 \partial t^2} = 0.$$


where the shear speed of sound \( c = \sqrt{G/\rho} \). It can be observe that small scale effects \((e_0 a = 0\) and \(\gamma_0 a = 0\) we get the conventional equation for torsional vibration of cylindrical tube.

We assume the solution of equation (23) as

\[
\Theta(x, t) = \psi(x) e^{i\omega t},
\]

where \( \omega \) is the angular frequency. Introducing the normalized coordinate \( X = x/L \) in the above Eqn.(23) can be transformed to space variables form as

\[
\frac{d^4\psi}{dX^4} + \left( \frac{\alpha^2 - \tau^2_1}{\tau^2_2} \right) \frac{d^2\psi}{dX^2} + \left( \frac{\tau^2_1}{\tau^2_2} \right) \psi = 0,
\]

where \( \tau_1 = \frac{e_0 a}{L}, \tau_2 = \frac{\gamma_0 a}{L} \), and \( \alpha^2 = \frac{c^2 \omega^2}{L^2}. \)

For the torsional vibration of a carbon with bi-Helmholtz operator the governing equation of motion can be put in the form as

\[
\tau^4_2 \frac{d^4\psi}{dX^4} + \left( \alpha^2 - \tau^2_1 \right) \frac{d^2\psi}{dX^2} + \psi = 0.
\]

We assume that for the single walled carbon nanotube is fixed at both ends so that a soft clamped boundary conditions [18] for the problem can be taken as

\[
\Theta|_{X=0} = 0, \quad \Theta|_{X=1} = 0, \quad T|_{X=0} = 0, \quad T|_{X=1} = 0.
\]

The general solution of the differential equation can be expressed as

\[
\psi(X) = \left[ c_1 e^{i\beta_1 X} + c_2 e^{i\beta_2 X} + c_3 e^{i\beta_3 X} + c_4 e^{i\beta_4 X} \right] e^{i\omega t},
\]

where \( c_i \) (for \( i = 1, 2, 3, 4 \)) are the arbitrary constants and \( \beta_i \) (for \( i = 1, 2, 3, 4 \)) are the roots of the dispersion relation.

\[
\tau^4_2 \beta^4 + \left( \alpha^2 - \tau^2_1 \right) \beta^2 + 1 = 0.
\]

The above equation is obtained by substituting \( \psi(X) = Ce^{i\beta X} \) into Eq(26) where \( C \) is a nonzero constant.

5. Solution using higher order boundary conditions

The governing equations of motion consider the boundary conditions of the nanotube by Eq.(27) and the arbitrary constants \( c_i \) for most significant terms of the nonlocal effect \( \tau \) by the equation (29) can be represented as

\[
\begin{pmatrix}
1 & 1 & 1 & 1 \\
k_1 & e^{i\beta_1} & e^{i\beta_2} & e^{i\beta_3} \\
k_1 e^{i\beta_1} & k_2 & e^{i\beta_2} & e^{i\beta_3} \\
k_1 e^{i\beta_1} & k_2 e^{i\beta_2} & k_3 e^{i\beta_3} & e^{i\beta_4}
\end{pmatrix}
\begin{pmatrix}
C_1 \\
C_2 \\
C_3 \\
C_4
\end{pmatrix} = 0,
\]

where \( k_i = \frac{GL}{L^2} \beta_i - \frac{(e_0 a)^2 \rho}{L^3} \beta_i \omega^2 - \frac{(\gamma_0 a)^2 \rho}{L^3} \beta_i^2 \omega^2 (i = 1, 2, 3, 4) \). For nontrivial solution of \( C_i, (i = 1, 2, 3, 4) \) the determinant of coefficient matrix must vanish.

\[
\begin{vmatrix}
1 & 1 & 1 & 1 \\
k_1 & e^{i\beta_1} & e^{i\beta_2} & e^{i\beta_3} \\
k_1 e^{i\beta_1} & k_2 & e^{i\beta_2} & e^{i\beta_3} \\
k_1 e^{i\beta_1} & k_2 e^{i\beta_2} & k_3 e^{i\beta_3} & e^{i\beta_4}
\end{vmatrix} = 0.
\]
From Eqs.(29) and (31), the relation of dimensional natural frequency and nonlocal nanoscale can be established.

6. Results and discussion

Numerical results are presented using the properties of carbon nanotubes. The following values of the parameters are used [14]: $\rho = 2300 kg/m^3$, $L = 10 nm$, $E = 1000 Gpa$, $I_p = 4.91 \times 10^{-38} m^4$, $A = 7.85 \times 10^{-19} m^2$. The nonlocal effects on the torsional vibration of carbon nanotubes are presented in this section. The derived expressions for torsional vibration are discussed. From Figure 1, it is found that the different values of nonlocal scale parameter ($e_0a$) by increasing the wave number ($K$) there is an increase of nonlocal frequency ($\omega$). Also, it is observe that higher values of an nonlocal scaling parameter then the angular frequency decreases with the increase of wave number. It shows that for very small wave numbers then the influence of the nonlocal effect is also very small.

7. References

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