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Bending vibration of single-walled carbon nanotubes using doublet mechanics

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Abstract

This paper investigates the bending vibration of single-walled carbon nanotubes based on a new theory called doublet mechanics with a scale parameter. A sixth order partial differential equation that governs the bending vibration for such nanotubes is derived. 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 models. However, with increasing the tube length, the scale effect on the natural frequency decreases. It is the first time that DM is used to model the bending vibration of carbon nanotube.

Keywords

doublet mechanics, natural frequency, free bending vibration, scale parameter, single-walled carbon nanotubes

1. Introduction

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. In order to overcome this limitation, various elegant modifications to continuum mechanics have been proposed to incorporate scale and microstructural features into the theory.

One particular theory that has recently been applied to granular materials is the DM model. This approach originally developed by Granik (1978) [1], has been applied to granular materials by Granik, Ferrari (1993) [2] and Ferrari et al. (1997) [3]. 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 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 [4]. Some application of DM in biomedical and nanomechanics is given in [5-7] and for civil engineering is given in [8, 9]. Fang et al. [10] studied the plane wave propagation in a cubic tetrahedral assembly with DM. Some other application of D is given in [11, 12].

One of the most popular theories in micromechanics is nonlocal theory. The nonlocal elasticity theory was first developed by Eringen [13]. Unlike DM, the nonlocal theory is developed following a simplified

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pattern without considering a particular microstructure. Under such an approach the parameters of the microstructure are not included in the mathematical model directly as in DM. Also, the total number of elastic macroconstants in the nonlocal theory is considerably larger than that in DM [3]. Another popular theory in micromechanics is molecular dynamics (MD) theory which studies vibrations of the atomic nuclei of solid crystals. DM 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) [3].

Carbon nanotubes (CNTs) have been invented by Iijima in 1991 [14]. Nanotubes have great potential for wide applications as components in nano-electronic-mechanical systems (NEMS). These components are subjected to external loadings during work operation and then, their resonant properties are of much concern. Bending vibration of SWCNTs is studied in [15-18] using nonlocal and MD theories. In this paper, the bending vibration of SWCNTs is studied based on a new theory called DM.

2. Brief review of DM

In this section a brief review of DM has been given. 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. 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. 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 (respectively $p_\alpha, m_\alpha, t_\alpha$ in Fig. 1). A pair of such particles represents a doublet as shown in Fig. 1.

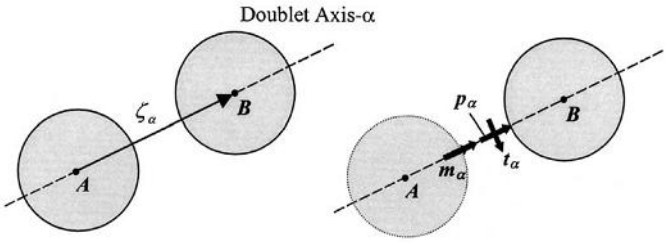

Fig. 1. doublet

Corresponding to the doublet *(A, B)* there exists a doublet or branch vector $\boldsymbol{\zeta}_\alpha$ connecting the adjacent particle centers and defining the doublet axis. The magnitude of this vector $\eta_\alpha = |\boldsymbol{\zeta}_\alpha|$ is simply the particle diameter for particles in contact. The internal characteristic scale for the crystal lattice parameter of carbon is $\eta_a = 1.421\, a$ [17]. For simplicity, it is assumed that the shear and torsional micro deformations and microstresses are negligible whereby only extensional strains and stresses exist. The unit vectors for initial branch vector $\boldsymbol{\zeta}_\alpha^0$ and current branch vector $\boldsymbol{\zeta}_\alpha$ are defined by $\boldsymbol{\tau}_\alpha^0$ and $\boldsymbol{\tau}_\alpha$, respectively. In the linear theory of DM, it is assumed that the relative displacement is small compared to the doublet separation distance η_α so that the initial and final configurations of the system can be assumed to coincide and then $\boldsymbol{\tau}_\alpha = \boldsymbol{\tau}_\alpha^0$ [19].

The extensional microstrain scalar measure ϵ_α, representing the axial deformation of the doublet vector, is expanded in a Taylor series as [3]

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

where $\boldsymbol{\nabla}$ is the gradient operator. In the isotropic media with local interaction, the relation between microstrees and macrostress is written by [3]:

$$p_\alpha = A_0 \epsilon_\alpha \tag{2}$$

The relation between microstress and macrostress can be written as [3]:

$$\sigma_{ij}^{(M)} = \sum_{\alpha=1}^{n} \tau_{\alpha i}^0 \tau_{\alpha j}^0 \sum_{\chi=1}^{M} \frac{(-\eta_\alpha)^{\chi-1}}{\chi!} (\boldsymbol{\tau}_\alpha^0 . \boldsymbol{\nabla})^{\chi-1} p_\alpha \tag{3}$$

Superscript *M* indicates that macrostresses incorporate scale effect. The three-dimensional equation of motion in DM is written by the following equation [3]

$$\frac{\partial \sigma_{ji}^{(M)}}{\partial x_j} + F_i = \rho \frac{\partial^2 u_i}{\partial t^2} \tag{4}$$

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

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 is the two-dimensional hexagonal packing without internal atoms which is nano structure. Consider a SWCNT of 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 [18].

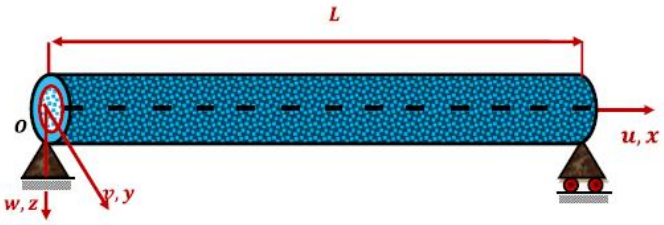

Fig. 2. A SWCNT

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

$$\frac{\partial^2 M_{xx}}{\partial x^2} = \rho A \frac{\partial^2 w}{\partial t^2} - \rho I \frac{\partial^4 w}{\partial x^2 \partial t^2}, \qquad M_{xx} = \int_{-\frac{t}{2}}^{\frac{t}{2}} z \sigma_{xx}^{(M)} dA \ , I = \int_A z^2 dA \tag{5}$$

A nanotube is constructed from three doublets have equal lengths and angles. Consider a Zigzag nanotube shown in Fig. 3. Using Eq. (1)- (3) and Euler–Bernoulli kinematics relations in beam model along with considering three terms in series (1) and (3), the macrostresses $\sigma_{xx}^{(M)}$ in Eq. (1) can be obtained as

$$\sigma_{xx}^{(M)} = -A_0 z \left(\frac{\partial^2 w}{\partial x^2} + \frac{1}{12} \eta^2 \frac{\partial^4 w}{\partial x^4}\right) \tag{6}$$

If Eq. (6) is substituted into the Eq. (5), the following equation of motion in term of *w* can be obtained

$$-EI\left(\frac{\partial^4 w}{\partial x^4} + \frac{1}{12} \eta^2 \frac{d^6 w}{dx^6}\right) - \rho A \frac{\partial^2 w}{\partial t^2} + \rho I \frac{\partial^4 w}{\partial x^2 \partial t^2} = 0 \tag{7}$$

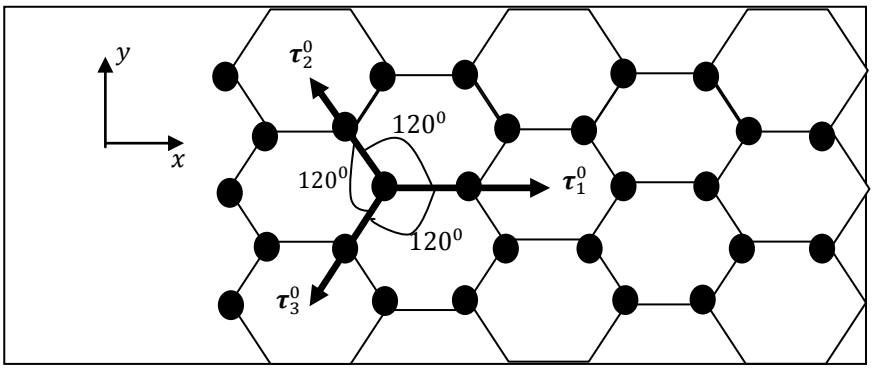

Fig. 5. A Zigzag SWCNT

According to Eq. (7) a six-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 terms of order and lower in the infinite series in Eq. (1) and (3) are retained.

It is assumed that the boundaries forces of the tubes are simple and independent to scale. Then, the frequency equation for bending vibration of nanotube with scale effect can be written by:

$$\left(\omega_n^{(\eta)}\right)^2 = \frac{EI\left[\left(\frac{n\pi}{L}\right)^4 - \frac{1}{12}\eta^2\left(\frac{n\pi}{L}\right)^6\right]}{\rho A + \rho I\left(\frac{n\pi}{L}\right)^2} \tag{8}$$

For Armchair nanotubes, similar calculations yields

$$\left(\omega_n^{(\eta)}\right)^2 = \frac{EI\left[\left(\frac{n\pi}{L}\right)^4 - \frac{1}{16}\eta^2\left(\frac{n\pi}{L}\right)^6\right]}{\rho A + \rho I\left(\frac{n\pi}{L}\right)^2} \tag{9}$$

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, the 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.

4. Results and discussion

To validate the present approach, MD and nonlocal simulations are conducted for a simply-supported (8, 8) SWCNT with different aspect ratios ranging from 8.3 to 39.1 [19]. 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 [18].

Results predicted by the present model in Table.1 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. 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 ratio of length-to-diameter increases, the discrepancy between various models decreases so that the frequencies tend to converge at an aspect ratio of approximately 40.

The numerical results for free vibrating nanotubes are given in graphical form in Figs. 6 - 11. In Fig. 6, the effect of scale parameter on frequency ratios in different vibration mode are shown for (8, 8) Armchair SWCNTs. The boundary conditions of the nanotubes are simply support. 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 mode.

Table1: Fundamental frequencies (THz) for (8, 8) Armchair SWCNTs with simple boundaries

L/D	DM	MD [18]	Nonlocal [18]
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

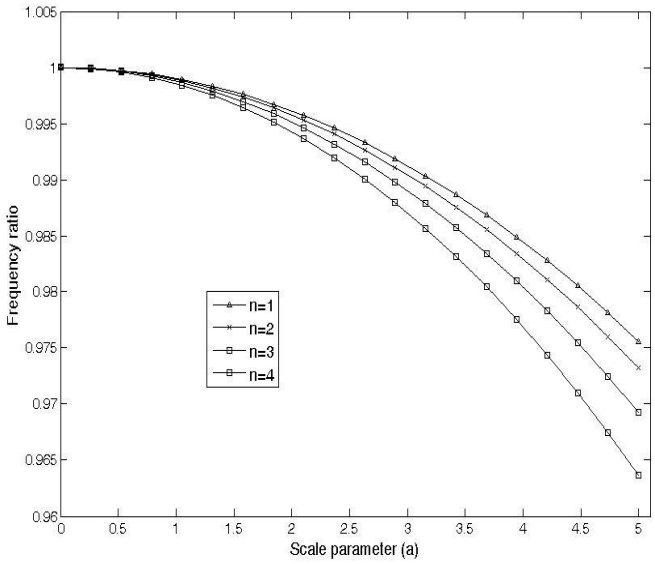

Fig. 6. Variation of frequency ratio with scale parameter for (8, 8) Armchair nanotube with L=100 nm for different bending vibration mode

Variation of frequency ratio of the SWCNTs as a function of tube radius for different mode numbers for Armchair and Zigzag nanotubes are investigated. It is proven that frequency ratio is increasing with increase in tube radius. This is more apparent for lower tube radius. Variation of frequency ratio with tube length is also studied for different vibration mode for such nanotubes. It is shown that with increasing in the length of the nanotubes, frequency ratio increases. This increasing is more pronounced for higher vibration modes. Since scale effects are more effective for smaller wave lengths, after a certain tube length *L*, frequency ratios approaches to a certain valueit is also shown that the difference between different vibration mode becomes more pronounced for very short SWCNTs.

5. Conclusions

The DM theory has been employed to model the bending vibration of SWCNTs. The governing equation of motion in bending mode was obtained in terms of lateral displacement and was solved analytically to

obtain a closed form expression for the natural frequency of such a nanotube. 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 classical continuum 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.

References

[1] V. T. Granik, 1978, Microstructural mechanics of granular media, Technique Report IM/MGU 78-241, Institute of Mechanics of Moscow State University, in Russian.
[2] V. T. Granik , M. Ferrari, Microstructural mechanics of granular media, Mechanics of Materials, 15, 301-322, 1993
[3] Ferrari M., Granik V.T., Imam A., Nadeau J., Advances in Doublet Mechanics, Berlin, Springer, 1997
[4] Kojic M., Vlastelica I., Decuzzi P., Granik V.T., Ferrari M., A finite element formulation for the doublet mechanics modeling of microstructural materials, Comput. Methods Appl. Mech. Engrg, 200, 1446–1454, 2011
[5] Xin J., Zhou L.X., Ru W.J., Ultrasound Attenuation in Biological Tissue Predicted by the Modified Doublet Mechanics Model, Chin. Phys. Lett, 26(7), 074301.1-074301.4, 2009
[6] Ferrari M., Nanomechanics, and Biomedical Nanomechanics: Eshelby's Inclusion and Inhomogeneity Problems at the Discrete Continuum Interface, Biomedical Microdevices, 2(4), 273-281, 2000
[7] Gentile F., Sakamoto J., Righetti R., Decuzzi P., Ferrari M., A doublet mechanics model for the ultrasound characterization of malignant tissues, J. Biomedical Science and Engineering, 4, 362-374, 2011
[8] Lin S.S., Shen Y.C., Stress fields of a half-plane caused by moving loads-resolved using doublet mechanics, Soil Dynamics and Earthquake Engineering 25, 893–904, 2005
[9] Sadd M.H., Dai Q., A comparison of micro-mechanical modeling of asphalt materials using finite elements and doublet mechanics, Mechanics of Materials 37, 641–662, 2005
[10] Fang J. Y., Jue Z., Jing F ., Ferrari M., Dispersion analysis of wave propagation in cubic-Tetrahedral assembly by doublet mechanics, Chin.Phys.Lett, 21(8),1562-1565 ,2004
[11] Sadd M. H., Elasticity theory, applications, and numeric, New York, Elsevier, 2005
[12] Ferrari M., BioMEMS and Biomedical Nanotechnology, Volume I Biological and Biomedical Nanotechnology, New York, Springer, 2006
[13] A. C. Eringen, Nonlocal polar elastic, International Journal of Engineering Science, 1972, 10, l-16
[14] Iijima S., Helical microtubes of graphitic carbon, Nature (London), 354, 56–58, 1991
[15] Bocko J., Lengvarský P., Bending Vibrations of Carbon Nanotubes by using Nonlocal Theory, Procedia Engineering 96,21 – 27 , 2014
[16] Ghorbanpour Arani A., Karamali Ravandi A., Roudbari M.A, Azizkhani M.B., Hafizi Bidgoli A., Axial and Transverse Vibration of SWBNNT System Coupled Pasternak Foundation Under a Moving Nanoparticle Using Timoshenko Beam Theory, Journal of solids mechanics, 7(3), 239-254, 2015
[17] Gupta S.S., Batra R.C., Continuum structures equivalent in normal mode vibrations to single-walled carbon nanotubes, Computational Materials Science, 43, 715–723, 2008
[18] Ansari R, Gholami R., Rouhi H., Vibration analysis of single-walled carbon nanotubes using different gradient elasticity theories, Composites: Part B, 43, 2985–2989, 2012