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Inextensional vibration of zig-zag single-walled carbon nanotubes using nonlocal elasticity theories

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A B S T R A C T

We study inextensional vibrations of zig-zag single-walled carbon nanotubes using nonlocal elasticity theories and molecular mechanics simulations employing MM3 potential. We find that the frequency expressions for the Rayleigh and Love modes of inextensional vibrations, predicted by the stress and strain gradient theories, differ from the classical continuum theory expressions by a multiplicative factor only. The factor is different for stress and strain gradient theories. We also observe that the strain gradient theory with positive sign exhibits a *saturation-like* behavior of the inextensional mode frequency with the circumferential wave number. Using this fact and molecular mechanics simulation data we derive an expression for the nonlocal parameter.

1. Introduction

After the discovery of single-walled carbon nanotubes (SWCNTs) (Iijima and Ichihashi, 1993) many researchers have used the classical continuum theory based thin shell models to characterize their mechanical properties and behavior (Yakobson et al., 1996; Pantano et al., 2004; Sears and Batra, 2004; Wang et al., 2004; Zhang et al., 2005; Guo et al., 2006; Wang and Zhang, 2008; Gupta et al., 2010; Silvestre et al., 2011). The radius and the length in the thin shell model have been considered to be the mean radius and length of the SWCNT. The thickness of the shell is either assumed (Wang et al., 2004; Robertson et al., 1992; Hernández et al., 1998; Lier et al., 2000; Sanchez-Portal et al., 1999; Guo et al., 2006) to be approximately 0.34 nm, the interlayer separation in bulk graphite, or computed (Yakobson et al., 1996; Pantano et al., 2004; Sears and Batra, 2004; Gupta et al., 2010; Wang et al., 2005; Xin et al., 2000; Tu and Ou-Yang, 2002) by matching various modes of deformations obtained from molecular simulations/experiments with those of a thin shell. It is also noted that the static deformation of SWCNTs has been studied using a membrane model by incorporating a modified Cauchy–Born rule (Arroyo and Belytschko, 2002). This model does not require estimation of the wall thickness of the SWCNTs. Further, a SWCNT can be thought of as a rolled graphene sheet. The graphene lattice has sixfold symmetry in its basal plane therefore, the material for the shell model of SWCNTs is assumed to be isotropic (Lee et al., 2008). Often, these models of SWCNTs are termed as equivalent continuum structures (ECSs). The shell models based on continuum theory are computationally efficient compared to atomistic models to study deformations of SWCNTs. However, the ECSs based on classical continuum theory can not predict the true dispersion relation in carbon nanotubes (Chen et al., 2004). It is shown by Chen et al. (2004) that a dynamic equivalence between the crystal lattices and their continuum analogue is possible through nonlocal elasticity models. The nonlocal elasticity theories are capable of accounting for long range inter-atomic interactions in the form of a size dependent parameter which renders the constitutive model a partial differential equation unlike classical Hooke's law in which the relationship between stresses and strains is algebraic.

The most popular nonlocal constitutive models employed to study deformations of carbon nanotubes (CNTs) have two different forms. The one due to Eringen (1983): $[1-(e_0a)^2\nabla^2]\mathbf{T}=\mathbf{C}\,\boldsymbol{\varepsilon}$, where $e_0,\ a,\ \nabla^2,\ \mathbf{T},\ \mathbf{C}$ and $\boldsymbol{\varepsilon}$ are the nonlocal parameter, lattice parameter, Laplacian operator, nonlocal stress tensor, elasticity tensor and strain tensor, respectively. The other form is known as the strain gradient model (Mindlin and Eshel, 1986; Aifantis, 1999; Askes et al., 2002; Peddieson et al., 2003): $\mathbf{T}=\mathbf{C}[1\pm(e_0a)^2\nabla^2]\boldsymbol{\varepsilon}$. If e_0 is set equal to zero, one recovers the classical Hooke's law in both the cases. Choosing positive or negative sign in the strain gradient model leads to significant change in the dynamic behavior of the ECS of a SWCNT. For example, Shi et al. (2009b) found that for a given SWCNT and for the positive sign the radial breathing mode

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(RBM) frequency increased with (e_0a) and the reverse happened when the negative sign was considered. It has also been observed that the strain gradient model with positive sign predicts frequency and dispersion behavior that agrees with experiments and crystal lattice model (Papargyri-Beskou et al., 2009). However, it exhibits dynamic/thermodynamic instabilities, whereas the one with negative sign is stable (Askes and Aifantis, 2011; Maranganti and Sharma, 2007). The nonlocal elasticity based shell models have been used extensively to investigate dynamic behavior of SWCNTs and multi-walled carbon nanotubes (Wang et al., 2006, 2012; Wang and Varadan, 2007; Hu et al., 2008; Shi et al., 2009a; Arash and Ansari, 2010; Fazelzadeh and Ghavanloo, 2012). Table 1 summarizes the salient features of a few such studies.

In the absence of traction and displacement boundary conditions a thin shell made of a linearly elastic, homogeneous and isotropic material exhibits Rayleigh and Love inextensional modes of vibration (Love, 1927). In the similar scenario, molecular mechanics (MM) simulations on SWCNTs also predict Rayleigh and Love inextensional modes in the eigenspectrum (Gupta et al., 2010). In the present study, we derive the frequency expressions for the Rayleigh and Love inextensional modes of vibration in an ECS of a SWCNT using nonlocal elasticity. The material of a SWCNT and, hence, that of the ECS is assumed to be linearly elastic, homogeneous and isotropic. The rest of the paper is organized as follows. In Section 2, we briefly discuss the kinematics of inextensional modes in a thin cylindrical shell. In Section 3, we first outline the derivation of Rayleigh and Love mode frequency expressions using classical elasticity and subsequently, we obtain the frequency expressions using the two forms of nonlocal elasticity theories. We compare the behavior of the frequency of the inextensional modes for various continuum theories and MM simulation in Section 4. Further, in this section we derive an expression for the nonlocal parameter. In Section 5, we present conclusions from our findings.

2. Inextensional deformation of a thin cylindrical shell

The displacements of a material point on the middle surface of the cylindrical shell in axial, circumferential and radial directions are u, v and w, respectively (see Fig. 1). For a cylindrical shell, the strain–displacement relations at a generic point, according to Flügge shell theory (Blevins, 1979), are

$$\epsilon_{xx} = \frac{\partial u}{\partial x} + z\frac{\partial^2 w}{\partial x^2}, \tag{1}$$

$$\epsilon_{\theta\theta} = \frac{1}{R}\left(\frac{\partial v}{\partial \theta} - w\right) + \frac{z}{R^2}\left(\frac{\partial^2 w}{\partial \theta^2} + w\right) \tag{2}$$

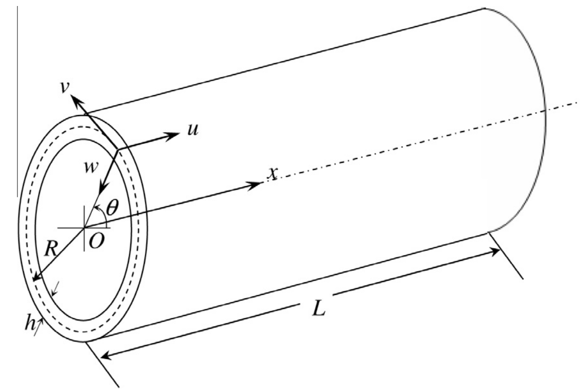

Fig. 1. Schematic of the ECS of a SWCNT (half length) showing the coordinate system and the mid-surface displacements. The SWCNT spans from x = -L to +L.

and

$$\epsilon_{x\theta} = \left(\frac{1}{R}\frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial x}\right) - \frac{z}{R}\left(\frac{1}{R}\frac{\partial u}{\partial \theta} - \frac{\partial v}{\partial x} - 2\frac{\partial^2 w}{\partial x \partial \theta}\right). \tag{3}$$

In case of inextensional deformation of the cylindrical shell, the middle surface $(z = 0)$ strains are zero. Thus, we have the relations,

$$\frac{\partial u}{\partial x} = 0, \quad \frac{\partial v}{\partial \theta} - w = 0, \quad \text{and} \quad \frac{1}{R}\frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial x} = 0. \tag{4}$$

The following general solution (Love, 1927) satisfies the relations in Eq. (4)

$$u = -\sum_{n=2}^{\infty}\frac{R}{n}B_n\sin(n\theta), \tag{5}$$

$$v = \sum_{n=2}^{\infty}[A_n\cos(n\theta) + B_n x\cos(n\theta)], \tag{6}$$

$$w = -\sum_{n=2}^{\infty}n[A_n\sin(n\theta) + B_n x\sin(n\theta)], \tag{7}$$

where A_n and B_n denote amplitudes and n is the circumferential mode number. Note that the inextensional modes correspond to $n \geqslant 2$. In the case of vibration of the cylindrical shell the displacements are harmonic functions of time. Accordingly, we consider A_n and B_n to be harmonic functions of time. The strain terms are now expressed using Eq. (4) as,

$$\epsilon_{xx} = z\frac{\partial^2 w}{\partial x^2} \equiv z\kappa_1, \quad \epsilon_{\theta\theta} = \frac{2}{R^2}\left(\frac{\partial^2 w}{\partial \theta^2} + w\right) \equiv z\kappa_2 \tag{8}$$

Table 1
Summary of some of the literature based on nonlocal continuum theories.

Research groups	Nonlocal model/Shell theory	Contributions
Wang et al. (2006)	Strain gradient (+ sign)	Compared longitudinal wave propagation in nonlocal ECSs with that from MD simulations (Tersoff–Brenner potential)
Wang and Varadan (2007)	Eringen's/Flügge shell	Wave propagation (longitudinal and circumferential) in nonlocal ECS for different values of nonlocal parameters
Hu et al. (2008)	Eringen's/Flügge shell	Compared wave propagation (transverse and torsional) in nonlocal ECSs with that from MD simulations (2nd generation REBO Potential). Different values of e_0 found for different mode of deformations
Narendar et al. (2011)	Eringen's/Molecular structural mechanics	Studied wave propagation (longitudinal and torsional) using a combination of molecular structural mechanics and Eringen's nonlocal theory. The parameter e_0 was found to be dependent on diameter of tube and mode
Shi et al. (2009a)	Strain gradient (− sign)/ Goodier–McIvor shell	Studied transition from radial breathing mode to circumferential mode: MD simulations (COMPASS force field) and study of ECS of a SWCNT
Arash and Ansari (2010)	Eringen's/Shear deformable shell	Comparison of frequency of fundamental mode of ECS for different boundary conditions and comparison with available MD simulations. Different values of e_0 were considered
Fazelzadeh and Ghavanloo (2012)	Eringen's/Flügge shell	Studied wave propagation (longitudinal and circumferential) in nonlocal ECS for different values of nonlocal parameters and aspect ratios
Wang et al. (2012)	Eringen's/Donnell shell	Studied wave propagation (longitudinal and circumferential) in nonlocal ECS for different values of nonlocal parameters and aspect ratios