Computational Materials Science 49 (2010) 518–523

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Effects of initial axial stress on waves propagating in carbon nanotubes using a generalized nonlocal model

J. Song, J. Shen, X.F. Li *

School of Civil Engineering and Architecture, Central South University, Changsha 410075, China

ARTICLE INFO

Article history:
Received 27 February 2010
Received in revised form 12 May 2010
Accepted 18 May 2010
Available online 12 June 2010

Keywords:
Carbon nanotubes
Elastic waves
Dispersion relation
Initial axial stress

ABSTRACT

This paper studies the dispersion relation of waves propagating in 1D nanostructures with initial axial stress. Based on a nonlocal elastic model incorporating with strain gradient, the governing equations for longitudinal and transverse waves in bars and beams have been derived, respectively. In this equation, two scale parameters are introduced to describe size effect. The phase and group velocities of wave propagation are obtained analytically, and the effects of initial axial loading on the wave speeds are analyzed. Examples are presented for flexural waves propagating in single-walled and double-walled carbon nanotubes. Waves are always present for tensile initial axial force, while they may not exist unless the compressive axial force fulfills a certain condition. In particular, the wave speeds are sensitive to initial force for lower frequencies and insensitive to it for higher frequencies.

1. Introduction

Due to the extraordinary mechanical properties of carbon nanotubes (CNTs) such as extreme flexibility and strength, they hold substantial promise for use as super-stiff and strong nano-fibers of novel composites and devices [1]. In recent years, mechanical behaviors of CNTs including buckling, vibration, fracture, etc. have become the subject of numerous theoretical and experimental studies [2,3]. On one hand, controlled experiments in the nanometer scale are difficult to realize. On the other hand, the molecular dynamics method is feasible for systems with a small number of molecules or atoms and remains formidable for large-scale systems; therefore continuum mechanics approach has been presented and regarded as an effective method and widely used for studying the mechanical and physical properties of CNTs [4,5].

A large amount of experiment evidence has confirmed that the mechanical properties of CNTs are diameter-dependent [6,7]. This effect is usually called the size effect. The size effect seems not to be explained according to the classical elasticity theory since no scale is contained in the classical continuum mechanics. Hitherto, several non-classical elasticity theories have been formulated to capture the size effect [8–12].

In particular, the nonlocal beam model [13] developed from the nonlocal elasticity theory established by Eringen [14] has been widely adopted to investigate the size effect of the mechanical properties of CNTs. For example, the influences of the scale effects on wave propagation have been analyzed for single-walled nanotubes (SWNTs) and double-walled nanotubes (DWNTs) [15,16]. In addition, for the buckling of single-layered graphene sheets subjected to biaxial compressive loads, the scale effects have been also investigated via nonlocal continuum mechanics [17].

On the other hand, CNTs or nanowires acting as basic fillers of nanostructures often suffer from initial stresses due to residual stress, thermal effect, surface effect, mismatch between the material properties of CNTs and a surrounding medium, initial external loads, etc. As we know, initial stresses present in a medium play a key role in dominating the mechanical behaviors of the elastic medium. In this field, the effects of initial stress on the non-coaxial resonance of multi-walled nanotubes (MWNTs) have been investigated by the theories of Euler–Bernoulli and Timoshenko beams, respectively, in Wang and Cai [18] and Cai and Wang [19]. Based on the Euler–Bernoulli beam theory, Zhang et al. [20] studied the transverse vibrations of DWNTs under compressive axial load, and pointed out that natural frequencies are dependent on the axial load and decrease with increasing of the axial load, and the associated amplitude ratios of the inner to the outer tubes of DWNTs are independent of the axial load. Lu et al. [21] adopted a nonlocal Euler–Bernoulli beam model to analyze wave and vibration characteristics of one-dimensional (1D) nanostructures with axially initial stress. Furthermore, Wang et al. [22] used a nonlocal Timoshenko beam model to deal with free vibration of micro- and nano-beams with initial stress. In their model, the nonlocal effect was only considered for the normal stress, and neglected for the shear stress. Considering the simultaneous presence of the nonlocal effect both in the normal and shear stresses, Heireche et al.

* Corresponding author.
E-mail addresses: xfli@mail.csu.edu.cn, xfli25@yahoo.com.cn (X.F. Li).

0927-0256/$ - see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.commatsci.2010.05.043

[23] studied the scale effects on wave propagation of DWNTs with initial axial loading through the nonlocal beam models. The above-mentioned investigations are related to 1D beam models. From cylindrical shell models, Sun and Liu [24] also studied the dependence of resonant frequencies on the axial initial stress, and found that the intertube resonant frequencies are insensitive to the initial axial stress in MWNTs, while the natural resonant frequency is sensitive to the initial axial stress, especially for the lower ones. Using the simplified Flugge shell model, Mitra and Gopalakrishnan [25] analyzed the characteristics of wave propagation in multi-walled carbon nanotubes.

This paper deals with the effects of initial axial stress on wave propagation in SWNTs and DWNTs by generalized nonlocal beam model. For this model, the nonlocal effects in elastic stresses and strains are both considered. The phase and group velocities of transverse waves are derived in explicit form for SWNTs and DWNTs. The influences of the initial axial stress on the phase and group velocities are discussed in detail.

2. Generalized nonlocal beam model

According to Eringen's nonlocal elasticity theory, nonlocal stresses σ_{ij} and classical (local) stresses $\mathring{\sigma}_{ij}$ have the following integral relation [14]

$$\sigma_{ij}(\mathbf{r}) = \int_V \alpha_1(|\mathbf{r}-\mathbf{r}'|)\mathring{\sigma}_{ij}(\mathbf{r}')dv(\mathbf{r}'), \tag{1}$$

where α_1 is the nonlocal kernel, $\mathbf{r}$ and $\mathbf{r}'$ denote position vectors. Moreover, for an isotropic homogeneous medium, the classical stresses obey

$$\mathring{\sigma}_{ij} = \lambda\delta_{ij}\mathring{\varepsilon}_{kk} + 2\mu\mathring{\varepsilon}_{ij},$$
$$\mathring{\varepsilon}_{ij} = 0.5(u_{i,j} + u_{j,i}),$$

in which λ and μ are the Lame constants; u_i and $\mathring{\varepsilon}_{ij}$ are, respectively, the displacement vector and strain tensor. Instead of the above integral relation, (1) can be alternatively expressed via differential form [26], i.e.

$$(1 - l_m^2\nabla^2)\sigma_{ij} = \mathring{\sigma}_{ij}, \tag{2}$$

where l_m^2 is a material constant of nonlocality of length dimension, and ∇^2 denotes Laplacian operator.

On the other hand, if expanding elastic displacements up to the terms containing strain gradients, we then have the nonlocal strains in relation to the classical strains in a similar manner [27]

$$\varepsilon_{ij}(\mathbf{r}) = \int_V \alpha_2(|\mathbf{r}-\mathbf{r}'|)\mathring{\varepsilon}_{ij}(\mathbf{r}')dv(\mathbf{r}'), \tag{3}$$

or

$$(1 - l_s^2\nabla^2)\varepsilon_{ij} = \mathring{\varepsilon}_{ij}, \tag{4}$$

where α_2 and l_s are also nonlocal kernel and material constant of nonlocality of length dimension. Generally speaking, α_1 is not identical to α_2, and l_m is also not identical to l_s. Under such circumstances, the constitutive relations of the nonlocal elasticity can be further extended to a generalized form [28]

$$(1 - l_m^2\nabla^2)\sigma_{ij} = (1 - l_s^2\nabla^2)(\lambda\delta_{ij}\varepsilon_{kk} + 2\mu\varepsilon_{ij}). \tag{5}$$

Clearly, the theories of the classical nonlocal [14,26] or gradient [29] elasticity are two special cases of $l_s = 0$ or $l_m = 0$, respectively. Note that the advantage of the nonlocal elasticity theory is capable of removing the stress singularity near the dislocation core [26], but the strain field is still singular. In contrast, the gradient elasticity theory is solely capable of removing the strain singularity, rather than the stress singularity [29]. The singularity of the stress and strain fields near the dislocation core can be simultaneously removed if l_m and l_s are both present [30].

In the present study, the focus is placed on 1D nano/micro bars or beams, so it is reasonable to suppose that $\sigma_{yy} = \sigma_{zz} = \sigma_{ij} = 0$ for $i \neq j$. The only non-vanishing stress component is $\sigma_{xx} = \sigma$, which satisfies

$$\sigma - l_m^2\sigma'' = E(\varepsilon - l_s^2\varepsilon''), \tag{6}$$

according to (5), where $\varepsilon = \varepsilon_{xx}$, E is Young's modulus. Here, we use the prime to stand for differentiation with respect to the suffixed space variable x. As pointed out in [31], for dynamic problems, the negative sign in front of the second-gradient strain should be changed into the positive sign. For static problems, the negative sign ensures the uniqueness of the desired solution and the positive definiteness of the stored strain energy, while for dynamic problems, the positive sign results from approximation of discrete media or lattice dynamics. Such an analysis for flexural waves propagating in CNTs can also be found in [32]. However, when the second-gradient stress is present, the dynamic behaviors related to the constitutive equation with the negative sign in front of the second-gradient strain were investigated in [33].

3. Effects of initial stress on longitudinal waves

For longitudinal waves propagating in 1D elastic bar subjected to initial stress, the only non-vanishing displacement is $u_1 = u(x,t)$. Substituting the longitudinal strain $\varepsilon = \partial u/\partial x$ into the constitutive equation one gets

$$\sigma = l_m^2\sigma'' + E(u' - l_s^2u'''). \tag{7}$$

The equation of motion for 1D bars with initial stress takes the form

$$A\sigma' - N_0u'' = m\ddot{u} \tag{8}$$

where m is the mass per unit length, A is the cross-sectional area, and N_0 is an initial axial force, which takes positive for compressive loading and negative for tensile loading, respectively. $N_0 = 0$ corresponds to the classical case without initial axial force. A dot over a variable denotes the time derivative.

Now eliminating σ from (7) and (8) leads to

$$m\ddot{u} = (EA - N_0)u'' + (N_0l_m^2 - EAl_s^2)u^{IV} + ml_m^2\ddot{u}''. \tag{9}$$

This is the final governing equation for longitudinal waves propagating in 1D bar with initial stress. Similar wave equations with higher order derivatives u^{IV} and $\ddot{u}''$ have been derived from various motivations (see e.g. [34,35]). For microstructure materials, a wave equation with $N_0 = 0$ has been obtained by means of the variational principle [36].

Next, let us consider the effect of initial stress on longitudinal waves. To this end, u is assumed to be $u = Ue^{i(kx-\omega t)}$, where k is the wavenumber and ω is the circular frequency, and then the governing Eq. (9) becomes

$$m(1 + l_m^2k^2)\omega^2 = EA(1 + l_s^2k^2)k^2 - N_0k^2(1 + l_m^2k^2). \tag{10}$$

Solving the resulting frequency equation, the phase wave speed, $v = \omega/k$, can be found to be

$$v = \sqrt{\frac{EA(1 + l_s^2k^2)}{m(1 + l_m^2k^2)} - \frac{N_0}{m}}. \tag{11}$$

Obviously, longitudinal waves are present for initial tensile loading $N_0 < 0$. On the contrary, for an initial compressive loading, i.e., $N_0 > 0$, waves may not exist unless the compressive loading N_0 is sufficiently small, satisfying