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Effects of strain and higher order inertia gradients on wave propagation in single-walled carbon nanotubes

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HIGHLIGHTS

- The modified strain gradient elastic shell model was developed.
- Numerical results showed good agreement with those of MD simulations.
- Effects of strain and inertia gradient parameters on dispersions were studied.
- The number of cut-off frequencies depends on the circumferential wave number.
- Asymptotic phase velocities versus gradient parameters were analytically derived.

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ABSTRACT

Dispersion relation of single-walled carbon nanotubes (SWCNTs) is investigated. The governing equations of motion of SWCNTs are derived on the basis of the gradient shell model, which involves one strain gradient and one higher order inertia parameters in addition to two Lamé constants. The present shell model can predict wave dispersion in good agreement with those of molecular dynamic (MD) simulations available in the literature. The effects of two small scale parameters on the angular frequency and phase velocity in the longitudinal, torsional and radial directions are studied in detail. The numerical results show that the angular frequency and phase velocity increase with the increase of strain gradient parameter, whereas decrease with inertia gradient parameter increases. In addition, analytical expressions of the cut-off frequencies and asymptotic phase velocities are given. It is found that the number of cut-off frequencies is dependent on the circumferential wave number, and two asymptotic phase velocities exist for nonzero value of strain gradient parameter, while only one exists when the strain gradient parameter is excluded.

1. Introduction

Carbon nanotubes (CNTs) have now gained considerable worldwide attention for a variety of applications, such as atomic force microscopes, nano-actuators and nano-fillers for composites materials, due to their unique mechanical, electrical, and chemical properties [1,2]. Therefore, a thorough understanding of their mechanical properties and behaviors by atomic simulation, experimental work and modeling is of great interest to explore their numerous potential applications.

Owing to the low dimension of CNTs, controlled experiments at the nanoscale is challenging. On the other hand, atomic modeling, including molecular MD, tight-binding MD and the density functional model, is prohibited for large-scale systems. Therefore, continuum models including one dimensional (1D) beam models and two dimensional (2D) shell models have been employed regularly to study the mechanical behaviors of CNTs in recent years. Extensive work related by the classical continuum models has been conducted for CNTs, such as buckling [3,4], vibration [5–7] and wave propagation [8–10]. These classical continuum models are not capable to characterize the micro-structure of the CNTs due to the lack of micro-structure of the material. Therefore, the application of non-classical elasticity to model the microstructure of CNTs has become an interesting issue. Examples for such size-dependent elastic theories are couple stress theory [11–13], surface elasticity [14], strain gradient elasticity [15] and stress gradient elasticity (nonlocal elasticity) [16], to name a few. Among

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those existing size-dependent elastic theories, the nonlocal elasticity has been widely used as an efficient tool to model the bending [17–19], buckling [20–24], vibration [25–27] and wave propagation [28–31] of CNTs. For example, a nonlocal Euler beam model by Peddieson et al. [18] and the nonlocal Timoshenko beam model by Wang [28] are formulated on the basis of Eringen's nonlocal elasticity [16]. Further work of nonlocal elasticity has been well documented in the study of bending, buckling, vibration and wave propagation of CNTs, either by 1D beam models or 2D shell models [32]. These existing nonlocal models result in over-prediction of deflections and under-prediction of buckling loads and free vibration frequencies. In other words, the incorporation of nonlocal parameter in the governing equation of motion softens the structures.

On the other hand, the strain gradient theory has also been widely used to the study of engineering structures (see, for example, the works of Kröner [33], Mindlin [12] and Hermann et al. [34]). However, this theory contains numerous material constants to be determined by the experiments. As a result, simplified strain gradient theory that contains fewer material constants becomes the topic of current interest. For the wave propagation problems in earlier works, one can refer to the works of Hermann et al. [34], Exadaktylos et al. [35] and Georgiadis et al. [36,37]. In recent years, the simplified strain gradient theory has also found applications in CNTs. For instance, Papargyri-Beskou et al. [38] formulated the Euler–Bernoulli beam within the context of gradient elasticity with surface energy, in which the problems of bending and stability analysis were analytically solved. The strain gradient elasticity have been widely applied to the static and dynamic analysis of micro- and nanostructures in the form of beams [19,39–42], plates [43, 44] and shells [45,46]. Recently, Polizzotto [47] addressed an elastic material featured by potential energy depending on the strain and the strain gradient, and a kinetic energy depending on the velocity and the velocity gradient; the dispersion relation for beam models were derived. Polizzotto's elastic gradient elasticity opens a new topic of current interest to explore the vibration and wave characteristics of micro/nanoscale structures. Askes et al. [48] demonstrated that the gradient elasticity and inertia gradient were shown to describe flexural wave dispersion in CNTs in a relatively wide range of wave numbers, good agreement with that predicted by MD simulations was found [39]. Later on, generalized gradient Euler–Bernoulli beam model and Timoshenko beam model were established to the analysis of flexural wave dispersion and vibration of CNTs [49–51]. These existing works are, however, limited to 1D structures. Recently, the 2D gradient models have become an increasing topic of interest. Papargyri-Beskou et al. [52] used the gradient Donnell shell model to study the wave propagation and free vibrations of elastic shells. Ghavanloo et al. [53] investigated the free vibration of orthotropic doubly-curved shallow shells based on the gradient elasticity. A first order shear deformation shell theory based on the stress and strain-inertia gradient elasticity was developed by Daneshmand et al. [54] for free vibration analysis of SWCNTs. Zeighampour et al. [55] derived the governing equations of thin shells by using modified strain gradient theory. In their work [55] , they also presented the variational-consistent boundary conditions and studied the free vibration of simply-supported shells. To our best knowledge, no work has been performed on wave propagation of SWCNTs using gradient Flügge shell models.

The paper is organized as follows. In Section 2, the Mindlin's simplified strain gradient theory is reviewed and the governing equations of motion of SWCNTs using the simplified strain gradient theory are derived. In addition, the explicit expressions of cut-off frequencies and asymptotic phase velocities are obtained. The effects of two small scale parameters on angular frequencies and phase velocities of SWCNTs are illustrated in Section 3, and conclusions are included in Section 4.

2. Linear elastic gradient shell model

2.1. Simplified strain gradient elastic theory

Within the framework of the simplified strain gradient elastic theory of Mindlin [12], the constitutive equations are given by

$$\boldsymbol{\sigma} = \boldsymbol{\tau} - \nabla\cdot\boldsymbol{\mu} = \left(1 - l_2^2\nabla^2\right)\boldsymbol{\tau},$$
$$\boldsymbol{\tau} = \lambda \mathrm{I}\ \mathrm{tr}\ \boldsymbol{\varepsilon} + 2\nu\boldsymbol{\varepsilon}, \tag{1}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ are the total and the classical Cauchy tensors, respectively, $\boldsymbol{\mu}$ is the double stress tensor, I is the unit tensor, λ and ν are the usual Lamé constants, $\boldsymbol{\varepsilon}$ is the classical strain tensor. ∇^2 is the Laplacian operator, and l_2 is the strain gradient parameter characterizing the microstructure of the material. The compatible equations are

$$\boldsymbol{\varepsilon} = \left[\nabla\,\mathrm{u} + (\nabla \mathrm{u})^{\mathrm{T}}\right]/2,\ \ \mathrm{tr}\ \boldsymbol{\varepsilon} = \nabla\cdot\mathrm{u}, \tag{2}$$

where u is the displacement vector.

2.2. Governing equations

A SWCNT is modeled by a cylindrical elastic shell with mean radius R, thickness h, as shown in Fig. 1. A cylindrical coordinate system (x, θ, z) is adopted such that the origins are set on the middle surface of the shell, x and θ denote longitudinal and angular circumferential coordinates, and z is the coordinate along the thickness direction (inward positive) of the shell. u, v and w are the displacement components in the x, θ and z directions, respectively. In the present paper, the SWCNT is assumed to be homogeneous with Young's modulus E, shear modulus G, Poisson's ratio μ and mass density ρ.

Based on the Flügge shell theory, the strain components ε_{xx}, $\varepsilon_{\theta\theta}$ and $\varepsilon_{x\theta}$ at any arbitrary point of the shell are related to the middle surface strains ε_{xx}^0, $\varepsilon_{\theta\theta}^0$ and $\varepsilon_{x\theta}^0$, and to the curvature of the middle surface κ_{xx}, $\kappa_{\theta\theta}$ and $\kappa_{x\theta}$ by

$$\{\varepsilon_{xx},\ \ \varepsilon_{\theta\theta},\ \ \varepsilon_{x\theta}\}^{\mathrm{T}} = \left\{\varepsilon_{xx}^0,\ \ \varepsilon_{\theta\theta}^0,\ \ \varepsilon_{x\theta}^0\right\}^{\mathrm{T}} + z\{\kappa_{xx},\ \ \kappa_{\theta\theta},\ \ \kappa_{x\theta}\}^{\mathrm{T}}, \tag{3}$$

where

$$\left\{\varepsilon_{xx}^0,\ \ \varepsilon_{\theta\theta}^0,\ \ \varepsilon_{x\theta}^0\right\}^{\mathrm{T}} = \left\{\frac{\partial u}{\partial x},\ \ \frac{1}{R}\frac{\partial v}{\partial \theta} - \frac{w}{R},\ \ \frac{1}{R}\frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial x}\right\}^{\mathrm{T}}, \tag{4}$$

$$\{\kappa_{xx},\ \ \kappa_{\theta\theta},\ \ \kappa_{x\theta}\}^{\mathrm{T}} = \left\{\frac{\partial^2 w}{\partial x^2},\ \ \frac{1}{R^2}\left(\frac{\partial^2 w}{\partial \theta^2} + w\right),\ \ -\frac{1}{2R^2}\left(\frac{\partial u}{\partial \theta} - R\frac{\partial v}{\partial x} - 2R\frac{\partial^2 w}{\partial x \partial \theta}\right)\right\}^{\mathrm{T}}. \tag{5}$$

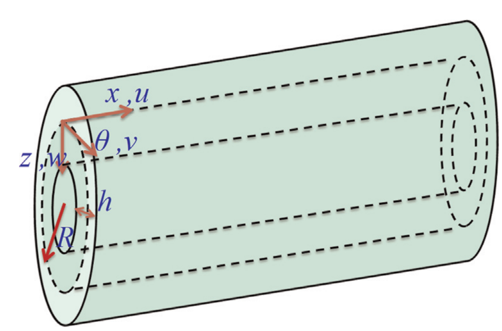

Fig. 1. Schematic illustration of the model with cylindrical coordinate system.