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Scale effect on wave propagation of double-walled carbon nanotubes

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Abstract

Scale effect on transverse wave propagation in double-walled carbon nanotubes (DWNTs) is studied via nonlocal elastic continuous models. The nonlocal Euler–Bernoulli and Timoshenko beam models are proposed to study the small-scale effect on wave dispersion results for DWNTs with respect to the variation of DWNT's wavenumbers and diameters by theoretical analyses and numerical simulations. The cut-off frequency, asymptotic phase velocity, and asymptotic frequency are also derived from the nonlocal continuum models. A rough estimation on the scale coefficient used in the nonlocal continuum models is proposed for the study of carbon nanotubes (CNTs) in the manuscript. The diameter-dependent dispersion relations for DWNTs via the nonlocal continuum models are observed as well. In addition, the applicability of the two beam models is explored by numerical simulations. The research work reveals the significance of the small-scale effect on wave propagation in multi-walled carbon nanotubes.

Keywords: Carbon nanotubes; Wave propagation; Nonlocal continuum mechanics; Euler–Bernoulli beam; Timoshenko beam; Cut-off frequency; Asymptotic velocity; Dispersion relations

1. Introduction

Carbon nanotubes (CNTs) have become one of the most promising new materials for nanotechnology (Ball, 2001; Baughman et al., 2002; Ajayan and Zhou, 2001) due to their novel electronic and mechanical properties. Some of the examples of CNTs applications are atomic-force microscope, field emitters, nano-fillers for composite materials, nanoscale electronic devices, and even frictionless nano-actuators, nano-motors, nano-bearings, and nano-springs (Lau, 2003). The modeling for CNTs is classified into two main categories. The first one is the atomic modeling, including the techniques such as classical molecular dynamics, tight binding molecular dynamics and density functional model (Iijima et al., 1996; Yakobson et al., 1997; Hernandez et al., 1998; Sanchez-Portal et al., 1999). These atomic methods are only limited to systems with a small

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number of molecules and atoms and therefore only restrained to the study of small-scale modeling. Unlike classical molecular dynamics, continuum model is practical in analyzing CNTs for large-scale systems. Yakobson et al. (1996) studied the unique features of fullernes and developed a continuum shell model in studying different instability patterns of a CNT under different compressive load. Ru (2000b) proposed the buckling analysis of CNTs with shell models. Krishnan et al. (1998) estimated Young's modulus of singled-walled carbon nanotubes (SWNTs) by observing their freestanding room-temperature vibrations in a transmission electron microscope. Wang (2004) proposed the effective in-plane stiffness and bending rigidity of armchair and zigzag CNTs through the analysis of a representative volume element of the graphene layer via continuous elastic models. Wang et al. (2005) studied the bending instability characteristics of DWNTs of various configurations using a hybrid approach. The research showed that the bending instability may take place through the formation of a single kink in the midpoint of a DWNT or two kinks, placed symmetrically about the midpoint, depending upon both the tube length and diameters.

The small-size scales associated nanotechnology are often sufficiently small to call the applicability of classical continuum models into question for nano-structures with very small dimensions. Classical or local continuum models, such as beam and shell models, do not admit intrinsic size dependence in the elastic solutions of inclusions and inhomogeneities. At nanometer scales, however, size effects often become prominent, the cause of which need to be explicitly addressed with an increasing interest in the general area of nanotechnology (Sharma et al., 2003). The modeling of such a size-dependent phenomenon has become an interesting subject of some researches in this field (Sheehan and Lieber, 1996; Yakobson and Smalley, 1997). It is thus concluded that the applicability of classical continuum models at very small scales is questionable, since the material microstructure at small size, such as lattice spacing between individual atoms, becomes increasingly important and the discrete structure of the material can no longer be homogenized into a continuum. Therefore, newly proposed continuum model rather than the classical continuum models may be an alternative to take into account the scale effect in the studies of nanomaterials.

The scale effect was accounted for in elasticity by assuming the stress at a reference point is considered to be a functional of the strain field at every point in the body by theory of NONLOCAL elasticity (Eringen, 1976). In this way, the internal size scale could be considered in the constitutive equations simply as a material parameter. The application of nonlocal elasticity models in nanomaterials was proposed by Peddieson et al. (2003). They applied the nonlocal elasticity to formulate a nonlocal version of Euler–Bernoulli beam model, and concluded that nonlocal continuum mechanics could potentially play a useful role in nanotechnology applications. Further applications of the nonlocal continuum mechanics have been employed in studying the mechanical behavior of CNTs. Sudak (2003) studied the infinitesimal column buckling of multi-walled nanotubes (MWNTs) incorporating not only van der Waals forces but also the effects of small length scales. His results showed that as the small length scale increases in magnitude the critical axial strain decreases compared to the results with classical continuum mechanics. Zhang et al. (2004) proposed a nonlocal multi-shell model for the axial buckling of MWNTs under axial compression. Their results showed that the influence of the small scale on the axial buckling strain is related to the buckling mode and the length of tubes.

Growing interest in terahertz physics of nanoscale materials and devices (Sirtori, 2002; Jeon and Kim, 2002; Antonelli and Maris, 2002; Brauns et al., 2002) opens a new topic on wave characteristics of CNTs, especially on the terahertz frequency range. Yoon et al. (2003, 2004) studied the wave propagation of MWNTs. In their studies, van der Waals force was modeled via their multiple-beam model. In structural analysis of one-dimensional beam-like structures, two models are usually employed, namely Euler–Bernoulli and Timoshenko beam models. Both models assume that plane sections remain plane. But in Euler–Bernoulli beam model, the sections remain perpendicular to the neutral axis whereas this assumption is removed in Timoshenko beam model (1921) to account for the effect of shear and rotary effect. Euler–Bernoulli beam model normally provides over-estimated wave phase velocity at higher wavenumber. Timoshenko beam model, on the other hand, is proved to be able to provide more accurate wave solution even at higher frequency range, although it is more complicated than Euler–Bernoulli beam model. The above investigations conducted the feasibility of the two local beam models in analysis of wave propagation of CNTs on terahertz frequency range. However, the small-scale effect was never considered in the published results. Since terahertz physics of nanoscale materials and devices are the main concerns in the wave characteristic of CNTs, the small-scale effect must be obvious as the wavelength in the frequency domain is in the order of *nanometer*.