Physica E 43 (2011) 1015–1020

Contents lists available at ScienceDirect

Physica E

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

Terahertz wave propagation in uniform nanorods: A nonlocal continuum mechanics formulation including the effect of lateral inertia

S. Narendar *,1

Structural Test Facility, Directorate of Flight Structures, Defence Research and Development Laboratory, Defence Research and Development Organisation, Kanchanbagh (PO), Hyderabad, Andhra Pradesh 500 058, India

A R T I C L E I N F O

Article history:
Received 25 November 2010
Received in revised form
7 December 2010
Accepted 7 December 2010
This work is dedicated to my Guru
Prof. S. Gopalakrishnan, Dept. of Aerospace Engg., Indian Institute of Science, Bangalore, India.
Available online 16 December 2010

A B S T R A C T

The dynamic testing of materials and components often involves predicting the propagation of stress waves in slender rods. The present work deals with the analysis of the wave propagation characteristics of nanorods. The nonlocal elasticity theory and also the lateral inertia are incorporated into classical/local rod model to capture unique features of the nanorods under the umbrella of continuum mechanics theory. The strong effect of the nonlocal scale has been obtained which leads to substantially different wave behaviors of nanorods from those of macroscopic rods. Nonlocal rod/bar model is developed for nanorods including the lateral inertia effects. The analysis shows that the wave characteristics are highly over estimated by the classical rod model, which ignores the effect of small-length scale. The wave propagation properties of the nanorod obtained from the present formulations are compared with the continuum rod model, nonlocal second and fourth order strain gradient models, Born – *Kármán* model and the nonlocal stress gradient model. It has also been shown that, the unstable second order strain gradient model can be replaced by considering the inertia gradient terms in the formulations. The effects of both the nonlocal scale and the diameter of the nanorod on spectrum curves are highlighted in the present manuscript. The results provided in this article are useful guidance for the study and design of the next generation of nanodevices that make use of the wave propagation properties of single-walled carbon nanotubes.

1. Introduction

A nanostructure is defined as a material system or object where at least one of the dimensions lies below 100 nm. Nanostructures can be classified into three different categories: zero-dimensional (0*D*); one-dimensional (1*D*); two-dimensional (2*D*). 0*D* nanostructures are materials in which all three dimensions are at the nanoscale. A good example of these materials are buckminster fullerenes [1] and quantum dots [2]. 1*D* nanostructures are materials that have two physical dimensions in the nanometer range while the third dimension can be large, such as in the carbon nanotube [3]. 2*D* nanostructures, or thin films, only have one dimension in the nanometer range and are used readily in the processing of complimentary metal-oxide semiconductor transistors [4] and micro-electro-mechanical systems (MEMS) [5]. Since the focus of this work is on one-dimensional nanostructures, all others from this point forward will cease to be discussed. 1*D* nanostructures (here nanorods) have stimulated a great deal of interest due to their importance in fundamental scientific research and potential technological applications in nano-electronic, nano-optoelectronic and nano-electro-mechanical systems. Rod-shaped viruses, such as tobacco mosaic viruses and M13 bacteriophage, have been utilized as biological templates in the synthesis of semiconductor and metallic nanowires [6]. They were also proposed as elements in the biologically inspired nanoelectronic circuits. Vibrational and wave modes will affect the properties of the inorganic–organic interface [6].

The length scales associated with nanostructures like carbon nanotubes, nanofibers, nanowires, nanorods, graphene sheets are such that to apply any classical continuum techniques, we need to consider the small length scales such as lattice spacing between individual atoms, surface properties, grain size. This makes a physically consistent classical continuum model formulation very challenging. The Eringen's nonlocal elasticity theory [7–10] is a useful tool in treating phenomena whose origins lie in the regimes smaller than the classical continuum models. In this theory, the internal size or scale could be represented in the constitutive equations simply as material parameters. Such a nonlocal continuum mechanics has been widely accepted and has been applied to many problems including wave propagation, dislocation, crack problems, etc [10]. Recently, there has been great interest in the application of nonlocal continuum mechanics for modeling and analysis of nanostructures [11–25].

* Tel.: +91 88976 25977, +91 99493 91823, +91 40 2458 3772;
fax: +91 40 2434 2309.
E-mail addresses: nanduslns07@gmail.com, snarendar@aero.iisc.ernet.in
[1] Scientist "B", STF, DOFS, DRDL, DRDO, Kanchanbagh (PO), Hyderabad-58.

1386-9477/$ - see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.physe.2010.12.004

The study of wave propagation in nanostructures has attracted intensive attention in research because many crucial physical properties such as electrical conductance, optical transition and some dynamic behavior of carbon nanotubes (CNTs) are very sensitive to the presence of wave [21]. Among the early studies, the continuum shell model was developed by Natsuki [23] to predict wave propagation in single-walled CNT embedded in an elastic medium. Wang and Varadan [19] applied the elastic beam theory to study the wave characteristics of single-walled and double-walled CNTs base on both thin and thick beam models. Another continuum model applicable to the analysis of CNTs is the nonlocal elasticity stress field theory which was first proposed by Eringen [7–10,26]. According to this theory, the stress at a point within a continuous domain with nanoscale effects is dependent not only on the strain at that point but also it is significantly influenced by the stress of all points in the domain through a nonlocal modulus in an integral sense. With such consideration, the nonlocal forces at long-range between molecules and lattice lead to the nonlocal stress–strain equation with higher-order strain gradients. Because of its simplicity and superiority, the analysis of wave propagation in CNTs and graphene sheets using the nonlocal stress approach was recently reported [27–46]. In particular, Lu et al. [30] derived the equation of motion for a nonlocal Timoshenko beam to investigate the wave propagation characteristics in single-walled and double-walled CNTs. Other nonlocal shell models were also employed for further research in a number of studies [35–39].

The present wave propagation studies using nonlocal continuum model has shown that the wave behavior in a nanorod is drastically different compared to the behavior of local or classical model. Hence, the main objective of this paper is to bring out the main effects that the nonlocal scale parameter to the wave propagation in nanorods.

In this paper, a nonlocal rod/bar model is developed for analyzing the ultrasonic wave propagation in nanorods. The effect of nonlocal scaling parameter (e_0a) on the wave propagation in nanorods and also the variation of the escape frequency with e_0a is studied in detail. Here $e_0a=0.5$ and 1.0 nm are used (detailed description on this value is discussed in the next section), where $a=0.142$ nm ($C-C$ bond length). The present paper is organized as follows. In Section 2, Eringen's nonlocal elasticity theory is explained and the governing partial differential equation is derived for the nanorod. Wave propagation analysis in nanorods is also carried out. The explicit expressions for the wavenumbers as a function of wave frequency for the nanorod are derived for various models and theories. Also the relation between the escape frequency and nonlocal scaling parameter is derived. In Section 3, some numerical results are presented on the wave dispersion in nanorods. Finally, the paper ends with some important observations and conclusions.

2. Mathematical formulation

2.1. Theory of nonlocal elasticity

This theory assumes that the stress state at a reference point $\mathbf{x}$ in the body is regarded to be dependent not only on the strain state at $\mathbf{x}$ but also on the strain states at all other points $\mathbf{x}'$ of the body. The most general form of the constitutive relation in the nonlocal elasticity type representation involves an integral over the entire region of interest. The integral contains a nonlocal kernel function, which describes the relative influences of the strains at various locations on the stress at a given location. The constitutive equations of linear, homogeneous, isotropic, nonlocal elastic solid with zero body forces are given by [8,9]

$$\sigma_{ij,j}=0 \tag{1}$$

$$\sigma_{ij}(\mathbf{x})=\int_V \alpha(|\mathbf{x}-\mathbf{x}'|,\xi)C_{ijkl}\varepsilon_{kl}(\mathbf{x}')\,dV(\mathbf{x}'),\quad \forall \mathbf{x}\in V \tag{2}$$

$$\varepsilon_{ij}=\tfrac{1}{2}(u_{i,j}+u_{j,i}) \tag{3}$$

where C_{ijkl} is the elastic modulus tensor of classical isotropic elasticity, σ_{ij} and ε_{ij} are stress and strain tensors, respectively, and u_i is the displacement vector. $\alpha=\alpha(|\mathbf{x}-\mathbf{x}'|,\xi)$ is the nonlocal modulus or attenuation function incorporating the nonlocal effects into the constitutive equations. This nonlocal modulus is found by matching the curves of plane waves with those due to atomic lattice dynamics. Various different forms of $\alpha(|\mathbf{x}-\mathbf{x}'|)$ have been reported in Ref. [10]. $|\mathbf{x}-\mathbf{x}'|$ is the Euclidean distance, and $\xi=e_0a/\ell$ [11], where a is an internal characteristic length, e.g., length of C–C bond (0.142 nm) in CNT, granular distance etc., and ℓ is an external characteristic length e.g., wavelength (λ), crack length, size of the sample etc. e_0 is a nonlocal scaling parameter, which has been assumed as a constant appropriate to each material in published literature and V is the region occupied by the body. Choice of the value of parameter e_0a (in dimension of length) is crucial to ensure the validity of nonlocal models. This parameter was determined by matching the dispersion curves based on the atomic models [8]. For a specific material, the corresponding nonlocal parameter can be estimated by fitting the results of atomic lattice dynamics or experiment.

Generally used kernel function $\alpha(|\mathbf{x}-\mathbf{x}'|,\xi)$ (in Eq. (2)) is given as [7]

$$\alpha(|\mathbf{x}|,\xi)=\frac{1}{2\pi\xi^2\ell^2}K_0\left(\frac{\sqrt{\mathbf{x}\cdot\mathbf{x}}}{\xi\ell}\right) \tag{4}$$

where K_0 is the modified Bessel function.

For two-dimensional nonlocal elasticity, there exists a differential form for the stress–strain relation (from Eq. (2)) [7–10]

$$(1-\xi^2\ell^2\nabla^2)\sigma_{ij}=C_{ijkl}\varepsilon_{kl} \tag{5}$$

where the operator ∇^2 is the Laplacian operator. Notice that in the nonlocal elasticity, the effect of small-length scale is considered by incorporating the internal parameter length into the constitutive equation. One may also see that when the internal characteristic length a is neglected, i.e., the particles of a medium are considered to be continuously distributed, then $\xi=0$, and Eq. (5) reduces to the constitutive equation of classical elasticity. When the internal characteristic length is negligible compared to external characteristic length, ξ approaches to zero and hence nonlocal elasticity theory reduces to classical elasticity theory. While the internal characteristic length is reasonably close to external characteristic length, ξ approaches to unity and thus the nonlocal elasticity theory reduces to atomic lattice dynamics. For nanostructures, the internal and external lengths are of the same order, and one has to use the nonlocal theory for analysis.

2.1.1. Discussion on nonlocal small scale coefficient:

The identification of the small scaling parameter e_0 in the nonlocal theory has not been fully understood. Wang and Hu [27], who adopted the second order strain gradient constitutive relation, proposed $e_0=0.288$ for the flexural wave propagation study in a single-walled carbon nanotube (SWCNT) through the use of nonlocal Timoshenko beam model and molecular dynamic simulations (MDSs). Eringen [8] himself proposed e_0 as 0.39 based on the matching of the dispersion curves via nonlocal theory for plane wave and Born – *Kármán* model of lattice dynamics at the end of the Brillouin zone, $k\times a=\pi$, where a is the distance between atoms and k is the wave number in the phonon analysis. On the other hand, Eringen [9] proposed $e_0=0.31$ in his study on the comparison of the Rayleigh surface wave via nonlocal continuum mechanics and lattice dynamics. Zhang et al. [14] estimated $e_0=0.82$ from the