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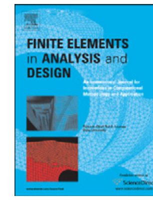

Spectral finite element and nonlocal continuum mechanics based formulation for torsional wave propagation in nanorods ☆

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ABSTRACT

Because of future promising exploration of nanotechnology, focus is being put in the miniaturization of mechanical and electromechanical devices. Attention is sought toward the development of nanodevices and nanomachines. The length scales associated with nanostructures like 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, etc. This makes a physically consistent classical continuum model formulation very challenging. So this work presents Eringen's nonlocal elasticity theory, that has been incorporated into classical torsional rod model to capture unique properties 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 torsional wave behaviors of nanorods from those of macroscopic rods. Nonlocal torsional rod model is developed for nanorods. Explicit expressions are derived for torsional wavenumbers and wave speeds of nanorods. 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 studies also shows that the nonlocal scale parameter introduces certain band gap region in torsional wave mode where no wave propagation occurs. This is manifested in the spectrum cures as the region where the wavenumber tends to infinite or wave speed tends to zero. Next, the Spectral Finite Element formulation of nanorods is performed. The exact frequency dependent shape functions and the dynamic stiffness matrix for the nanorod are obtained as a function of nonlocal scale parameter. It has been found that the nonlocal small scale has significant effect on the exact shape functions and the elements of the dynamic stiffness matrix. These effects are also captured in the present work. The results presented in this paper can provide useful guidance for the study and design of the next generation of nanodevices that make use of the wave dispersion properties of carbon nanotubes.

1. Introduction

Nanomaterials [1,2] are the base material of many nanoscale objects. Nanoscale objects are referred to as nanostructures. Recently various one-dimensional nanostructures have been realized. They include nanodots, nanorods, nanowires, nanobelts, nanotubes, nanobridges and nanonails, nanowalls, nanohelices, seamless nanorings. Among all the one-dimensional nanostructures, nanotubes, nanorods and nanowires are widely studied. This is because of the easy material formation and device applications. One-dimensional 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-opto-electronic 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 [3]. They were also proposed as elements in the biologically inspired nanoelectronic circuits. Vibrational modes will affect the properties of the inorganic–organic interface. As stated by Fonoberov and Balandin [3], pure axial vibration mode can also be observed. Axial vibration experiments can also be used to determine elastic properties of carbon nanotube. Although flexural experiments are used when determining Young's modulus axial vibrations can also be used. Nanorods can be used for microelectromechanical and nanoelectromechanical devices. During these applications axial external forces may act with nanorods and this leads to axial vibration of them. Due to this fact, understanding their axial dynamic behavior is very important task. The excellent properties of these nanomaterials have led to its multiple usages in the field of nanoelectronics, nanodevices, nanosensors, nanooscillators, nanoactuators, nanobearings, and micromechanical resonators,

☆ This work is dedicated to Prof. A. Cemal Eringen on the occasion of his 91^{st} birthday.

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transporter of drugs, hydrogen storage, electrical batteries, nanocomposites and nano-opto-mechanical systems (NOMS). However, for further effective potential applications of these nanostructures, proper physical, chemical and mechanical understanding of the nanomaterials is essential.

Conducting experiments are appropriate ways to analyze the behavior of the nanostructures. However it suffers from the drawback that controlling every parameter in nanoscale is a difficult task. Further employing the molecular dynamic (MD) simulations requires large time and high computational resources. Because of the above-mentioned limitations in the mechanical analyses of nanostructures, theoretical and mathematical modeling becomes an important issue concerning its nanoengineering applications. Continuum models of nanostructures have thus received more attention. Various reports related to the use of continuum theories in the vibration and buckling analysis of nanostructures could be found in the literature [4–6]. However though this continuum models could provide quick and approximate predictions, it fails to account for the size/scale effects. At nanometer scales, size effects often become prominent. Both experimental [7,8] and atomistic simulation results [9] have shown a significant scale/size-effect in mechanical properties when the dimensions of these structures become small. As the length scales are reduced, the influences of long-range inter-atomic and intermolecular cohesive forces on the static, dynamic and buckling properties tend to be significant and cannot be neglected. The classical theory of elasticity being the long wave limit of the atomic theory excludes these effects. The traditional classical continuum mechanics would fail to capture the small scale effects when dealing in nanostructures. The continuum theories which would reflect the size-dependency are therefore necessary for true prediction of the behavior of nanostructures. Various size-dependent continuum theories which capture this small-scale effect are therefore reported. Some theories include couple stress elasticity theory [10], strain gradient theory [11] and modified couple stress theory [12].

So, 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. In the present work the size-dependent continuum theory known as the nonlocal elasticity theory is considered. The nonlocal elasticity theory was first reported by Eringen. Nonlocal continuum field theories are concerned with the physics of material bodies whose behavior at a material point is influenced by the state of all points in the body. Eringen's nonlocal elasticity theory [13–16] 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. [16]. Recently, there has been great interest in the application of nonlocal continuum mechanics for modeling and analysis of nanostructures. Using nonlocal elasticity theory, works on vibration, bending and buckling of carbon nanotubes are numerous [17–28].

Application of the finite element method (FEM) [29] for wave propagation requires a very fine mesh to capture the mass distribution accurately. The mesh size should be comparable to the wavelengths, which are very small at high frequencies. Hence, the problem size increases enormously. Many applications in smart structure applications, such as structural health monitoring or active wave control in composite structures, require wave-based modeling since one has to use high-frequency interrogating signals. If one needs online diagnostic tools in structures, wave-based modeling is an absolute must. For such problems, the FEM by itself cannot be used as a modeling tool as it is very expensive from the computational viewpoint. Hence, one needs an alternate formulation wherein the frequency content of the exciting signal is not an issue. That is, we need a modeling tool that can give a smaller problem size for high-frequency loading, at the same time retaining the matrix structure of the FEM. Such a technique is feasible through the spectral finite element (SFEM) technique [30–32].

It is not enough to have the expressions of the wavenumbers or phase speeds with matched dispersion relation. To visualize the manifestation of these speeds it is necessary to develop a tool for analyzing the nonlocal media subjected to high frequency loading. The convolution integral form of the nonlocal theory of elasticity naturally suggests that integral transform based method of solving partial differential equation will enjoy superiority as compared to the conventional FEM. One such method is the SFEM. The SFEM, popularized by Doyle [30], is an integral transform based method with the matrix structure of FEM. The SFEM is the FEM formulated in the frequency domain and wavenumber space. That is, these elements will have interpolating functions that are complex exponentials or Bessel functions. These interpolating functions are also functions of the wavenumbers. For example, a governing partial one-dimensional wave equation, when transformed into the frequency domain using discrete Fourier transformation (DFT), removes the time derivative and reduces the governing partial differential equation (PDE) to a set of ordinary differential equations (ODEs), which have complex exponentials as solutions. In the SFEM, we use these exact solutions as the interpolating functions. As a result, the mass is distributed exactly and hence, one single element is sufficient between any two discontinuities to get an exact response, irrespective of the frequency content of the exciting pulse. That is, one SFEM can replace hundreds of FEMs normally required for wavepropagation analysis. Hence, the SFEM is an ideal candidate for developing online health monitoring software.

Spectral elements use a variation of *p*-type convergence. Spectral elements base the element interpolation functions on the eigenfunctions of the differential equation used to represent the dominant mechanics in the problem. This results in the "exact" form of the displacement field for the interpolation function. The interpolation functions of spectral elements are based on trigonometric functions, opposed to polynomial functions of conventional elements. The trigonometric functions incorporate the frequency of the response into the interpolation function. Having the interpolation function based on the eigenfunction means that a single spectral element will give the "exact" dynamic solution across the element for simple loading and boundary conditions. Even for dynamic analysis, it is only necessary to converge the geometry, loads, and boundary conditions. It is not necessary to converge the dynamics, as it is for the case with traditional finite elements. This results in a reduced number of elements, and thus a reduced model size for a spectral element model as compared to the conventional finite element model.

The formulation of various spectral elements for one-dimensional isotropic waveguides is given in Doyle [30]. Spectral elements for one-dimensional elementary and first-order shear deformable composite waveguides are given in Roy Mahapatra and Gopalakrishnan [33] and Roy Mahapatra et al. [34]. Spectral elements are also available for composite tubes [35] and functionally graded beams [36]. Spectrally formulated elements are also available for two-dimensional isotropic membrane waveguides [37] and composite waveguides [38]. In all of these works, the exact solutions to the governing equations are used as the