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Calibration of the analytical nonlocal shell model for vibrations of double-walled carbon nanotubes with arbitrary boundary conditions using molecular dynamics

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ABSTRACT

In the present study, the free vibration response of double-walled carbon nanotubes (DWCNTs) is investigated. Eringen's nonlocal elasticity equations are incorporated into the classical Donnell shell theory accounting for small scale effects. The Rayleigh–Ritz technique is applied to consider different sets of boundary conditions. The displacements are represented as functions of polynomial series to implement the Rayleigh–Ritz method to the governing differential equations of nonlocal shell model and obtain the natural frequencies of DWCNTs relevant to different values of nonlocal parameter and aspect ratio. To extract the proper values of nonlocal parameter, molecular dynamics (MD) simulations are employed for various armchair and zigzag DWCNTs, the results of which are matched with those of nonlocal continuum model through a nonlinear least square fitting procedure. It is found that the present nonlocal elastic shell model with its appropriate values of nonlocal parameter has the capability to predict the free vibration behavior of DWCNTs, which is comparable with the results of MD simulations.

1. Introduction

As one of the stable families of carbon nanostructures, carbon nanotubes (CNTs) have been the subject of intensive studies about their possible applications in different emerging fields of scientific research. This is due to their extraordinary mechanical, electrical, and physical properties that make them as an essential part for various nanodevices [1–6]. Owing to the small scale of CNTs, there are some difficulties to investigate the responses of them using experimental methods that causes copious tendency for analyzing based on theoretical study of nanostructures.

Different theoretical methods such as molecular mechanics and atomistic modeling are employed in order to investigate about mechanical behaviors of nanotubes. However, modified continuum models have been one of the most applied analytical methods in nanomechanics due to their computational efficiency and their capability to produce accurate results which are comparable to those of atomistic models. One approach for including nanoscale size-effects into classical continuum mechanics is the use of modified continuum models based on the concept of nonlocal elasticity. The application of nonlocal continuum mechanics allowing for the small scale effects to the vibrational analysis of nanomaterials has been recommended by many research workers.

Song et al. [7] studied the dispersion relation of waves propagating in one-dimensional nanostructures with initial axial stress based on nonlocal elastic model. Aydogdu [8] developed a nonlocal elastic rod model and applied it to investigate the small scale effect on axial vibration of nanorods. He concluded that size-effects have a significant role on the values of axial vibration frequencies. Ke et al. [9] studied the nonlinear free vibration of embedded DWCNTs based on nonlocal Timoshenko beam theory and von Karman geometric nonlinearity. Axial vibration of CNT heterojunctions was studied by Filiz and Aydogdu [10] using nonlocal rod theory. They found that by joining CNTs good vibrational properties can be obtained by suitable selection of parameters. Xie et al. [11] investigated the effect of small size on dispersion characteristics of waves in multi-walled CNTs. They formulated dynamic governing equations of the CNT on the basis of nonlocal elasticity shell model. Recently, Ansari et al. [12] developed a nonlocal finite element plate model which accounts for the small scale effects to study the vibrational characteristics of multi-layered graphene sheets with different boundary conditions.

There are so many other works in which the nonlocal continuum elasticity is utilized to predict the behavior of CNTs under various loading conditions [13–25], which indicates the popularity of this type of theoretical solution.

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