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The effect of calibrated nonlocal constant on the modal parameters and stability of axially compressed CNTs

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HIGHLIGHTS

- An eigenvalue problem is defined to derive mode-dependent small scale constants.
- Estimating nonlocal parameter based on frequency domain response is presented.
- Nonlocal modal damping ratio and the nonlocal parameter are negatively correlated.

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ABSTRACT

Nowadays investigating the vibration behavior of carbon nanotubes (CNTs) has drawn considerable attention due to the superior mechanical properties of the CNTs. One of the powerful theoretical methods to study the vibration behavior of CNTs is implementing the nonlocal theory. Most of studies on the vibration behavior of CNTs have assumed a fixed value for small scale parameter for all vibration modes, however, this value is mode-dependent. Therefore, in this paper, the small scale parameter is calibrated for a single-walled carbon nanotube (SWCNT) with respect to each vibration mode. For this propose, the governing equation of motion based on the nonlocal beam theory is extracted by applying the Hamilton's principle. Then, by using the power series method, an eigenvalue problem is defined to derive the calibrated value of small scale constant and nonlocal mode shapes of the CNT. By using the expansion theory, the equation of motion is discretized, and the effect of nonlocality on the modal parameters and stability of the CNT under compressive force is investigated. Finally, the possibility of estimating nonlocal parameter based on simulated frequency domain response of the system by using modal analysis methods is studied. The results show that the calibration of small scale constant is important and the critical axial force is highly sensitive to this value.

1. Introduction

Recently, there has been great interest in the application of carbon nanotubes (CNTs) such as storing and conveying fluids in nanoscale and capsules for drug delivery due to extraordinary properties of CNTs. Therefore the dynamic behavior and stability analysis of CNTs have been investigated by many researchers. The classic beam theory can be used to estimate the key parameters of the vibration behavior [1]. However, to obtain realistic results and consider the small scale effects, the application of nonlocal continuum mechanics for modeling and analysis of nanostructures is more reliable, which has been used in different studies [2–5]. Nonlocal elasticity theory considers the scale effects by assuming the stress at a point to be a function of strain field at every other points in the body. In this theory, the small scaling parameter is a key constant, however, the identification of the parameter used in the nonlocal theory is difficult and has not been fully understood. There are some studies discussing the estimation of the small scaling parameter for various physical problems. Also in many studies by assuming a constant value for small scaling parameter and implementing the nonlocal elasticity, the dynamic behavior of nanotubes have been investigated. Wang et al. [6] proposed $e_0=0.288$ for investigating the flexural wave propagation in a single-walled carbon nanotube (SWCNT) by utilizing the continuum mechanics and molecular dynamic simulations (MDSs) based on the Terroff-Brenner potential. Zhang et al. [7] matched the nonlocal theoretical results with those calculated by molecular mechanics simulations and predicted that the value of e_0 is equal to 0.82 for the CNT. Then based on this value, the buckling of

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SWCNT has been analyzed by implementing Donnell shell theory and molecular mechanics simulations. Boumia et al. [8] studied the dynamic properties of a single-walled carbon nanotube by considering a constant small scale parameter. They used the nonlocal continuum theory and the Timoshenko beam model to derive the equation of motion and showed that as the mode number increases, the effect of small scale parameter on the frequency ratios increases. Rafiei et al. [9] discussed the effect of the constant small scale parameter on the CNTs linear vibration. Their results revealed that the natural frequencies obtained from the nonlocal theory are less than those based on the local one. Liang and Su [10] studied the stability of a single-walled carbon nanotube conveying pulsating and viscous fluid with nonlocal theory. They showed that decrease of nonlocal parameter and increase of viscosity both increase the fundamental frequency and critical flow velocity in the system. Murmu et al. [11] studied the axial vibration of embedded nanorods under transverse magnetic field effects via nonlocal elastic continuum theory. They showed that the frequency parameter increases with increasing the stiffness of the elastic medium. The aforementioned studies are also based on an assumed fixed nonlocal constant.

In addition, there are some other investigations on the dynamic behavior of CNTs in which different theories than nonlocal theory have been used. Cigeroglu and Samandari [12] investigated the nonlinear free vibration of curved double-walled carbon nanotubes embedded in an elastic medium. They considered the presence of van der Waals forces and utilized differential quadrature method (DQM) to obtain the dynamic response of the CNT. They showed that as the nonlinear resonance frequency increases, the vibration amplitude rises. Koh et al. [13] studied the thermally induced nonlinear vibration of single-walled carbon nanotubes by deriving the bending equation of motion by using the strain energy. Other major categories for simulating the mechanical properties of CNTs are molecular dynamic simulations and experiments. However, MDS is expensive, complex, and time consuming, especially for large-sized atomic systems, and a controlled experiment at nanoscale is difficult. So, nonlocal continuum mechanics models can be widely applied. This theory has gradually demonstrated its effectiveness in the prediction of mechanical characteristics of CNTs. Once the mechanical characteristics are predicted, the dynamic behavior can be investigated by a mathematical model. Large number of studies on the vibration and buckling behavior of CNTs have been done by assuming a fixed nonlocal constant for all vibration modes and as shown by Kiani [14], and Rafiei et al. [9] an assumed fixed nonlocal constant has more effect on higher vibration modes. However, Duan et al. [15] found that the small scaling parameter is function of length-to-diameter ratio, mode shape and boundary conditions. Therefore, a large value of scaling constant for lower vibration modes might have different results than those found by Kiani [14] and Rafiei et al. [9]. So, calibration of this parameter for each mode is essential to obtain more realistic results from vibration behavior of CNTs.

The dynamic characteristics of a structure highly depends on modal parameters and it is important to consider the effect of calibrated small scale parameter on the modal parameters of CNT. On the other hand, in order to model the vibration behavior of CNTs mathematically, modal parameters should also be estimated. In this regard, in the present study by considering that the calibration constant is function of mode shape, an eigenvalue problem based on power series method is established to find the nonlocal parameter. The calibration is based on natural frequencies obtained from MDSs results reported in the literature. To this end, first the nonlocal elasticity theory is utilized and equation of motion of CNT in the presence of axial force is derived by implementing the Hamilton's principle. Second, the governing equation is discretized and an exclusive e_0 constant for each vibration mode is obtained. Then, the effect of calibrated small scale nonlocal constant on the modal parameters and stability of CNT is investigated. Finally, the experimental frequency response of the system is simulated mathematically and the possibility of estimating modal parameters as well as nonlocal constant based on this frequency domain response is discussed.

2. The governing equation of motion

As shown in Fig. 1, a single-walled carbon nanotube clamped at both ends is considered. It is assumed that the CNT has Young's modulus E, cross-sectional area moment of inertia I, length L, inner radius r_1 and thickness h. In addition, $\widehat{w}(\widehat{x},\widehat{t})$ is planar motion of the CNT in the $\widehat{z}$ direction, at the location of $\widehat{x}$ and time $\widehat{t}$.

In this study, in order to investigate the transverse vibration behavior of the CNT, the gravity effect is neglected and by using the nonlocal beam theory and applying the Hamilton's principle, the governing equation of motion is derived. The kinetic energy of the system, K_e, can be expressed as

$$K_e = \frac{1}{2}\int_0^L \rho_{nt}A_{nt}\left(\frac{\partial \widehat{w}}{\partial \widehat{t}}\right)^2 d\widehat{x} \tag{1}$$

where $\rho_{nt}A_{nt}$ is the mass per unit length of the nanotube. The nonlocal beam theory is used to consider the small scale effects. This theory is an agreement between the atomic theory of lattice dynamics and experimental observations or molecular simulations. According to this theory, the stress at a point of a body is dependent on the strain at all the points in the body. For a homogenous isotropic material, based on nonlocal theory and considering Kelvin–Voigt damping model, the stress field can be expressed as [4]:

$$\sigma_x^{nl} - (e_0 a)^2 \frac{\partial^2 \sigma_x^{nl}}{\partial \widehat{x}^2} = E\varepsilon_x + \eta\frac{\partial \varepsilon_x}{\partial \widehat{t}} \tag{2}$$

where σ_x^{nl} is the nonlocal axial stress, a is the internal characteristic length, e.g., lattice parameter or C–C bond length, and e_0 is a calibration constant. The value of e_0 should be obtained by using the molecular simulation results. This parameter is a function of the boundary conditions, length-to-diameter ratio, mode shape and molecular lattice [15–17]. In addition, η is the damping coefficient based on Kelvin–Voigt model and ε_x denotes the axial strain in the CNT. Resultant nonlocal bending moment and axial force can be expressed as:

$$M^{nl} = -\int_A z\sigma_x^{nl} dA_{nt} \tag{3}$$

$$N^{nl} = \int_A \sigma_x^{nl} dA_{nt} \tag{4}$$

In the above equations, A_{nt} shows the cross-sectional area of the CNT. The strain energy of the CNT is given by

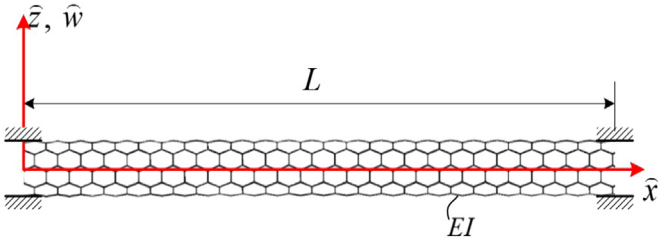

Fig. 1. Schematic of a CNT clamped at both ends.