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A Timoshenko beam model for vibration analysis of chiral single-walled carbon nanotubes

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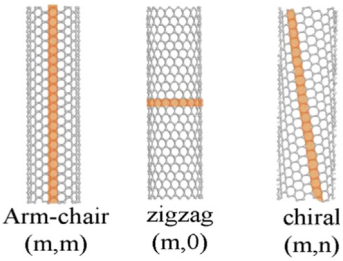
HIGHLIGHTS

- Dynamics of zigzag, armchair and chiral CNTs are studied.
- The governing equations are constructed based on the nonlocal Timoshenko beam theory.
- A significant dependence of natural frequencies on the chirality of a single-walled carbon is shown.
- Nonlocal effect on vibration characteristics of chiral CNTs is examined.

GRAPHICAL ABSTRACT

The dynamic properties of the single-walled carbon nanotube (SWCNT) with small scale effects are studied by using the nonlocal elasticity theory.



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ABSTRACT

In this paper, dynamic properties of a single-walled carbon nanotube (SWCNT) with small scale effects are studied. Based on the nonlocal continuum theory and the Timoshenko beam model, the equations of motion are derived. The influences of scale coefficients, the vibrational mode number, the chirality of carbon nanotube and the aspect ratio on the vibrational characteristics of the SWCNTs are discussed. Results indicate significant dependence of natural frequencies on the chirality of single-walled carbon, the small-scale parameter, the vibrational mode number and the aspect ratio. These findings are important in mechanical design considerations of devices that use carbon nanotubes.

1. Introduction

Since the discovery of carbon nanotubes by Iijima [1,2], nanostructures are being increasingly used due to their superior electronical, thermal and mechanical properties [3,4]. Others studies have shown that they have good properties so they can be used for nanoelectronics, nanodevices and nanocomposites [5,6].

Due to difficulties encountered in experimental methods to predict the responses of nanostructures under different loading conditions, the molecular dynamics (MD) simulations are used. This approach represents the dynamics of atoms or molecules of the materials by a discrete solution of Newton's classical equations of motion. But the computational problem here is that the time steps involved in the MD simulations are limited by the vibration modes of the atoms [7]. Jin and Yuan [8] used MD and force-constant approach and reported the Young's modulus of SWCNTs

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to be about 1236 ± 7 GPa. Cornwell and Wille [9] used the MD with the Tersoff–Brenner potential [10] to obtain Young's modulus of SWCNTs of about 0.8 TPa.

The continuum mechanics methods are often used to investigate some physical problems in the nanoscale [11,12]. Recently, the continuum mechanics approach has been widely and successfully used to study the responses of nanostructures, such as the static [13,14], the buckling [15–18], free vibration [19,20], wave propagation [21–27] and thermo-mechanical analysis of CNTs [28]. Yakobson et al. [29] utilize a continuum shell model to predict the buckling of a single-walled carbon nanotube and their results are compared with molecular dynamics simulations. Harik [30] reported ranges of applicability for the continuum beam model in the mechanics of carbon nanotubes and nanorods.

The majority of structural theories are derived using the constitutive assumptions that the stress at a point depends only on the strain at the point. On the other hand, nonlocal elasticity theory, advanced by Eringen [31,32], is based on the hypothesis that the stress at a point is a function of strains at all points in the continuum. Peddieson et al. [33], Zhang et al. [34], Wang [35], Wang et al. [36], Lu et al. [37,38] and Heireche et al. [25–27] have used the nonlocal elasticity constitutive equations to study vibration and buckling of CNTs.

In this paper, a nonlocal Timoshenko beam theory is proposed for the wave propagation in single-walled carbon nanotubes. Young's modulus of SWCNTs is predicted using MD simulation carried out by Bao et al. [39]. These results are in good agreement with the existing experimental results. The characteristic of transverse wave propagating in CNTs is investigated and the effects of both small scale parameter and chirality of carbon nanotube are discussed. The work should be useful in the design and application of nanoelectronics and nanoelectromechanical devices

2. Atomic structure of the single-walled carbon nanotube (SWCNT)

The single-walled carbon nanotube (SWCNT) is theoretically assumed to be made by rolling a graphene sheet (Fig. 1). The fundamental structure of carbon nanotubes can be classified into three categories as zigzag, armchair and chiral in terms of the chiral vector ($\vec{C_h}$) and the chiral angle (θ) shown in (Fig. 1).

The chiral vector can be expressed in terms of base vectors ($\vec{a_1}$) and ($\vec{a_2}$) (Fig. 1) as

$$\vec{C_h} = m\vec{a_1} + n\vec{a_2} \tag{1}$$

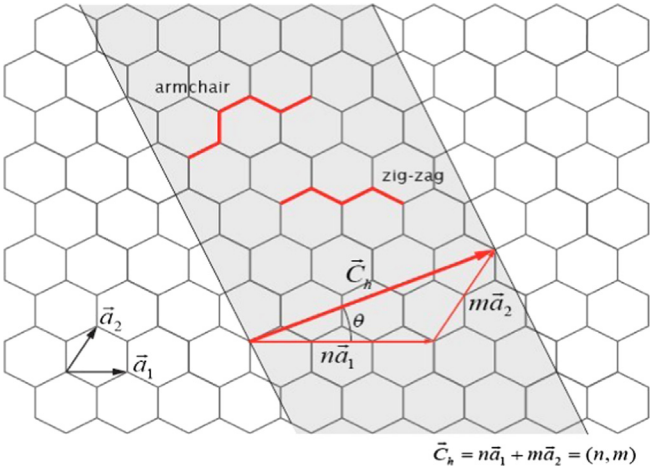

Fig. 1. Schematic diagram of the chiral vector and the chiral angle.

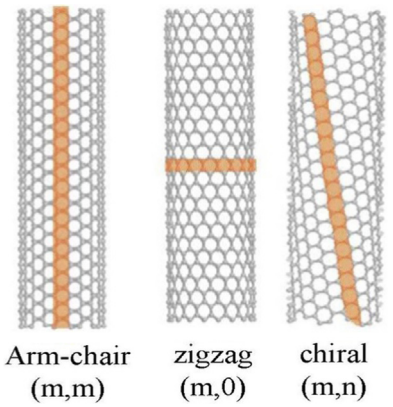

Fig. 2. Carbon nanotube: armchair, zigzag and chiral.

where the integer pair (n, m) are the indices of translation, which decide the structure around the circumference.

The relationship between the integers (n, m) and the chiral angle is given by [40]

$$\theta = \arccos\frac{2n+m}{2\sqrt{(m^2+n^2+mn)}} \tag{2}$$

According to different chiral angles, SWCNTs can be classified into zigzag ($\theta = 0^\circ$), armchair ($\theta = 30^\circ$) and chiral tubule ($0^\circ < \theta < 30^\circ$) (Fig. 2).

The relationship between the integers (n, m) and the diameter of SWCNTs is given by [41]

$$d = a\sqrt{3(n^2+m^2+nm)}/\pi \tag{3}$$

where a is the length of the carbon–carbon bond which is 1.42 Å.

3. Nonlocal Timoshenko elastic beam models of SWCNTs

The theory of nonlocal continuum elasticity proposed by Eringen [31,32] assumed that the stress at a reference point is considered to be a functional of the strain field at every point in the body. In the limit when the effects of strains at points other than x are neglected, one obtains classical or local theory of elasticity. For homogeneous and isotropic elastic solids, the constitutive equation of non-local elasticity can be given by Eringen [31,32]. Non-local stress tensor (t) at point (x') is defined by

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

$$\sigma_{ij}(x) = \int K(|x-x'|,\ \tau) C_{ijkl}\varepsilon_{kl}(x')dV(x'),\ \ \forall x \in V$$

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \tag{4}$$

where (C_{ijkl}) is the classical, macroscopic stress tensor at point x', σ_{ij} and ε_{ij} are stress and strain tensors respectively. $K(|x-x'|,\ \tau)$ is the kernel function and $\tau = e_0 a/l$ is a material constant that depends on internal and external characteristic length (such as the lattice spacing and wavelength), where e_0 is a constant appropriate to each material, a is an internal characteristic length, e.g., length of the C–C bond, lattice parameter, granular distance, and l is an external characteristic length.

Non-local constitutive relations for present nanobeams can be approximated to a one-dimensional form as

$$\left(1 - e_0 a^2 \frac{\partial^2}{\partial x^2}\right)\sigma_x = E\varepsilon_x \tag{5}$$

$$\left(1 - e_0 a^2 \frac{\partial^2}{\partial x^2}\right)\tau_{xz} = G\gamma_{xz} \tag{6}$$