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Torsional vibration of carbon nanotubes: Comparison of two nonlocal models and a semi-continuum model

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ABSTRACT

In recent years, people were puzzled about two reverse nonlocal models in studying transverse bending of nanobeams. Following the ideologies of both nonlocal models, two kinds of torsional models were constructed to investigate the nonlocal torsional vibration of carbon nanotubes, respectively. Just like the transverse bending of nanobeams, it is strange to observe two opposite size-dependent performances. The first nonlocal continuum model (weakened model) was based on equilibrium equations and nonlocal torsional shear stress relation. Natural frequency decreases with an increase in nonlocal nanoscale parameter, or it increases with increasing length of the carbon nanotube. Thus the torsional stiffness of carbon nanotubes is weakened. On the other hand, the second nonlocal model (enhanced model) was developed from the strain energy variational principle. Natural frequency increases (or decreases) with increasing nonlocal nanoscale parameter (or length of the carbon nanotube), or the nanostructural stiffness is strengthened. For judgment, a torsional semi-continuum model with discrete atomic layers in the cross section of a carbon nanotube was proposed. The relaxation effects on surface atoms were considered in the torsional semi-continuum model. It is concluded that the relaxation type (attractive or repulsive) of surface atoms results in two different nonlocal results. Consequently, both the existing reverse models are proved to be valid.

1. Introduction

Since the carbon nanotube was discovered by Iijima [1] in the year 1991, such nanostructure has attracted intensive attention, including studies of buckling, post-buckling, bending, wave propagation, transverse vibration and so on [2–5]. Due to some technical difficulties in experiments at such tiny scale, two main approaches available including atomic simulation and continuum modeling are applied to the analyses of carbon nanotubes currently. However, as the atomic modeling considers each individual atom and its multiple mechanical web-interactions, the utilization requires extremely fast computing facilities and hence it is largely confined to relatively restricted systems with a limited number of atoms. Consequently, this is why so many researchers have resorted to some new modified continuum models.

Of all the new continuum models, Eringen's nonlocal theory [6,7] has been extensively applied to exhibit the mechanical properties and application potential in nanomechanics [3–5,8–22]. The common nonlocal theory contains integral and differential nonlocal constitutive [23,24], respectively. The integral nonlocal constitutive assumes that the nonlocal stress at a point is a function of strains at all points in the domain, while the differential nonlocal constitutive regards the stress at a reference point is not only dependent on the strain at that point, but also related to the gradient of strain at the same point. Despite the integral and differential nonlocal constitutive, it is found that the nonlocal theory is much different from the most classical continuum models because the latter are based on elastic constitutive relation and it assumes that the stress at a point is a function of strain at only that particular point. On the other hand, the classical continuum models have been proved to fail in nanomechanics. For example, according to the classical continuum theory, the stress is singular at a crack tip despite how weak the external load is. However, it is no doubt that each material has limited fatigue strength and in fact, both atomic simulation and experiment proved its nonsingularity at the crack tip. Similarly, such nonsingularity was also observed since the nonlocal theory was utilized to reveal the stress concentration at the tip of crack [25]. This is because the nonlocal continuum theory contains information about the forces between atoms, and the internal length scale is introduced into the constitutive equation as a material parameter. Therefore, the nonlocal theory has been one of the most popular approaches to investigate the mechanical features of nanomaterials or nanostructures during the past decades. For instance, based on the Eringen's nonlocal theory, Aydogdu [11] presented a generalized nonlocal beam theory to investigate

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the nanobeam bending, buckling and free vibration. Various beam theories including those of Euler-Bernoulli, Timoshenko, Reddy, Levinson and Aydogdu were considered as some special cases. It was concluded that the bending deflection increases, while the critical buckling load and vibration frequency decrease with increasing the nonlocal effects. Consequently, nanobeam stiffness is lower than that predicted by classical continuum mechanics [11]. Yu and Lim [22] studied the axisymmetric bending of annular nanoplates which may model the graphene sheets based on the nonlocal elasticity theory and developed a new nonlinear nonlocal constitutive relation in polar coordinates. They introduced an iterative procedure to solve the coupled nonlinear constitutive and expressed the nonlocal stress asymptotically in stress gradients. It was indicated that the deflection decreases with increasing nonlocal effects. Similar stiffness enhancement effects were also observed clearly in some other literatures (see e.g. [13,14]).

Although the nonlocal elasticity theory has been applied to some research topics on carbon nanotubes (e.g. see [3–5,10,13–15,17–19]), only a few of them are focused on torsional vibration of such common nanostructure [15,18,19]. As we know, torsional deformation and vibration are very common for carbon nanotubes subjected to external forces in some new nanoscale devices such as nano-electromechanical system (NEMS). Even in the existing fewer literatures, the torsional conclusions are quite different [15,19]. Hao et al. [15] presented the torsional thermal buckling behaviors of multi-walled carbon nanotubes by nonlocal theory. The critical buckling strain was found to be smaller than the ones from the classical theory and hence the nonlocal stiffness softening effects were concluded. However, Li et al. [19] studied the torsional statics and dynamics of circular nanosolids (e.g. nanorods/nanotubes) based on the enhanced nonlocal model and they concluded the angular displacement decreases while the natural frequency increases with an increase in nonlocal nanoscale effects. Due to the inconsistency in current nonlocal nanostructural studies, two nonlocal continuum models for torsional vibration of carbon nanotubes are constructed in this work, respectively, and the nonlocal effects on size-dependent natural frequency are taken into account in each model. Surprisingly, the two nonlocal models (i.e. the weakened and enhanced models) derive some opposite size-dependent phenomena, just like the reports in [15] and [19]. Actually, similar reverse conclusions have been reported on the bending behaviors of nanobeams or wave propagation of carbon nanotubes, e.g. weakened model [3,8,15], enhanced model [13,14,16]. Hence, people are really confused with these different predictions because each model has been investigated and published extensively [3,8,11–16,18–22]. Subsequently, a semi-continuum model with relaxation phenomenon for torsional vibration is proposed to judge which nonlocal model is correct. It is found that relaxation coefficient in semi-continuum model is a critical factor in nanoscale materials and structures, and the two kinds of nonlocal size-dependent predictions are related to such relaxation coefficient. When the relaxation coefficient is larger than 1.0, the semi-continuum torsional model degenerates to the weakened nonlocal model, while when the relaxation coefficient is less than 1.0, the semi-continuum model degenerates to the enhanced nonlocal counterpart. Therefore, both of the two nonlocal models are proved to be reasonable and they depend on the specific surface properties and atomic relaxation type of the nanomaterial.

The content of the present work is structured as follows: in Section 2 we developed two different nonlocal elasticity models for torsional vibration analyses according to the weakened model and enhanced model, respectively. Natural frequencies were determined and the effects of nonlocal nanoscale were observed. Section 3 was devoted to construct a semi-continuum torsional model for carbon nanotubes, and the nonlocal nanoscale effects were also taken into account for comparisons. Finally, the main conclusions were summarized in Section 4. The results reported in this research could be useful for understanding the nonlocal effects and further optimizing some new nanostructures in NEMS.

2. Two nonlocal models

In this section, two kinds of nonlocal models for torsion vibration are constructed, respectively. Nonlocal torsional natural frequencies are determined and some comparisons of nonlocal and classical solutions are illustrated. Our particular attention is paid to the nonlocal size-dependence of natural frequency.

2.1. The weakened model

Nonlocal elasticity is a long-range force theory, of which the differential nonlocal constitutive relation regards the stress at a reference point depends on the classical stress and its gradients at that point, given by [7]

$$[1-(e_0a)^2\nabla^2]t_{kl}=\lambda\varepsilon_{rr}\delta_{kl}+2\mu\varepsilon_{kl} \tag{1}$$

where t_{kl} is nonlocal stress tensor, ε_{kl} is strain tensor, δ_{kl} is Kronecker operator, λ and μ are Lame constants of materials, e_0 is a constant dependent on each material, a is an internal characteristic scale. For cylindrical nanostructures, length scale is much larger than cross sectional scale. Therefore, nonlocal constitutive relation expressed in Eq. (1) can be simplified as a one-dimensional form. Since the object of this work is to research torsional vibration, the nonlocal torsional relation between shear stress and shear strain can be written as

$$s_r-(e_0a)^2\frac{\partial^2 s_r}{\partial x^2}=G\gamma_r \tag{2}$$

where s_r and γ_r are shear stress and strain at the point with a distance r from center of the circular section, respectively, G is shear modulus and x is the axial coordinate. Here the classical shear strain satisfies

$$\gamma_r=r\frac{\partial\theta}{\partial x} \tag{3}$$

where θ is relative angular rotation between two sections.

Subsequently, the relation between torsion moment and relative angular rotation is thus determined from Eqs. (2) and (3), as

$$T-(e_0a)^2\frac{\partial^2 T}{\partial x^2}=GI_P\frac{\partial\theta}{\partial x} \tag{4}$$

where $T=\iint_A rs_r dA$ is the torsion moment, and $I_P=\iint_A r^2 dA$ is the polar moment of inertia with respect to the center of circular section.

On the other hand, force analysis is applied to the element dx, and the equilibrium equation is derived based on D′ Alembert principle as

$$\rho I_P\frac{\partial^2\theta}{\partial t^2}dx=\frac{\partial T}{\partial x}dx \tag{5}$$

where ρ is mass density of material, t is time. Consequently, nonlocal governing equation of torsional vibration is obtained from Eqs. (4) and (5), given by

$$\rho\frac{\partial^2\theta}{\partial t^2}-(e_0a)^2\rho\frac{\partial^4\theta}{\partial x^2\partial t^2}=G\frac{\partial^2\theta}{\partial x^2} \tag{6}$$

For a macroscale structure, the external characteristic scale is far more than internal characteristic scale, e.g. $L\gg a$ (L is length of the carbon nanotube), hence the governing equation of torsional vibration based on the classical continuum mechanics can be recovered from Eq. (6) since e_0a approaches zero.