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Circumferential nonlocal effect on vibrating nanotubules

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ABSTRACT

In this paper the nonlocal shell and beam theories are used to study the transverse vibration of slender *NTs*. The agreement between the shell model and molecular dynamics simulations shows that the nonlocal effect originates predominantly from the atom-atom interaction in circumferential direction. It thus does not decrease with rising axial wavelength. In this case, a nearly constant nonlocal coefficient e_0 can be achieved for vibrating *NTs*. These behaviors however cannot be captured by the widely used nonlocal beam theory where only the axial nonlocal effect is included. Thus, caution must be taken when the one-dimensional nonlocal model is applied to slender *NTs*.

1. Introduction

In 2003 nonlocal elasticity [1,2] was incorporated into continuum mechanics theory to capture the unique features of cylindrical nanotubes (*NTs*) [3,4]. The nonlocal beam [3–12] and shell [13–19] models were developed by using the gradient theory based on a special kernel function. Unique bending, vibration, wave propagation and buckling responses were achieved for carbon nanotubes (*CNTs*) [3–11,13–15,17–20] and microtubules (*MTs*) [12,16] showing significant difference between *NTs* and their macroscopic counterparts. It is now widely accepted that the nonlocal continuum models considering the new physics emerging at the nanoscale can play an important role in characterizing the mechanical responses of *NTs*, such as *CNTs*, zinc oxide *NTs* (*ZONTs*) [21], boron nitride *NTs* (*BNNTs*) [22] and their biological counterparts *MTs*. These *NTs* are fundamental building blocks in a nanoscale world.

In an effort to develop the nonlocal theory, researchers [6,8,13,15,17,18,20] have fitted the nonlocal continuum models based on the gradient theory to molecular dynamics simulations (MDS). The objective is to extract the value of nonlocal coefficient e_0 assumed to be appropriate for each material, i.e., a material constant. The obtained values of e_0 for *CNTs* however depend significantly on the boundary conditions, the geometric size and the mechanics problems discussed [6,8,13,15,20]. Also while the gradient models with selected e_0 matched some MDS [6,13,15,17,18], they led to significant errors in other mechanics problems of *NTs* [20]. Moreover, it is noted in the literature that the transverse vibration of *NTs* has been studied extensively based on the nonlocal beam theories [5,8–11]. This one dimensional model however only considers the nonlocal effect in axial direction. The effect in circumferential direction was tacitly ignored. Therefore, as will be shown later, for slender *NTs* significant discrepancy can be found between the nonlocal beam model and the nonlocal shell model where the nonlocal effect in both circumferential and axial directions is considered. These observations indeed have raised some fundamental issues in the nonlocal mechanics theory.

This paper aims to examine these fundamental issues in the nonlocal mechanics theory when it is applied to study the transverse vibration of *NTs*. In doing this, the nonlocal shell model [11–14] accounting for both axial and circumferential nonlocal effect is employed and compared with the nonlocal beam model [8–11] and existing MDS [8]. In Section 2 the nonlocal shell and beam models are presented and the method of vibration analysis is introduced briefly. Then, in Section 3 the nonlocal shell and beam models are compared with each other and also with MDS for the first four modes of transverse vibration. The discussions about aforementioned issues are given afterwards. The conclusions are drawn in Section 4.

2. Methodology

In nonlocal elasticity, the stress at one reference point is a function of strain at all points inside the domain [1,2]. This is in

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accordance with the atomic theory of lattice dynamics and experimental observations on phonon dispersion. For single-atom layer *NT*s, e.g., *CNT*s, *ZONT*s and *BNNT*s, such a theory reflects the prominent effect of the atom-atom interactions between a reference point and all other atoms in the nanostructures. The corresponding constitutive equations read

$$\sigma_{ij} = \int \alpha(|\chi-\chi'|,\tau) C_{ijkl}\varepsilon_{ij}\, dV(\chi') \quad \forall \chi \in V, \tag{1}$$

Here σ_{ij} is the stress tensors at reference point χ, C_{ijkl} is elastic modulus tensor and ε_{ij} is the strain tensor at point χ'. $\alpha(|\chi-\chi'|,\tau)$ is the nonlocal kernel function which measures the nonlocal effects at the reference point. $|\chi-\chi'|$ is the Euclidean distance. In $\alpha(|\chi-\chi'|,\tau)$, $\tau=e_0a/l$ where e_0 is assumed to be a constant appropriate to each material, a is an internal characteristic length (e.g., the length of the *C*–*C* bond, lattice parameter, granular distance), and l is an external characteristic length (e.g., crack length, wavelength). Selecting a special class of physically admissible kernel for α one can reduce the integral–partial differential equations of linear nonlocal elasticity (i.e., Eq. (1)) to a singular partial differential equation [2]

$$(1-(e_0a)^2\nabla^2)\sigma_{ij} = s_{ij} \tag{2}$$

where $s_{ij}=C_{ijkl}\varepsilon_{ij}$ is classical stress tensor. For two dimensional shell model the Laplace operator is $\nabla^2=(\partial^2/\partial x^2)+(\partial^2/r^2\partial\theta^2)$ where x is the axial coordinate, θ is circumferential angular coordinate and r is the radius of *NT*s. When one dimensional beam model is used the Laplace operator reduces to $\partial^2/\partial x^2$. Replacing the classical constitutive equations with the gradient theory (Eq. (2)) obtained based on the selected form of α in Timoshenko beam and Flugge thin shell theories leads to the nonlocal beam and shell models for *NT*s.

The dynamic equations for *NT*s as nonlocal Timoshenko beams were derived in Refs. [8–11].

$$\frac{\partial}{\partial x}\left[GAK_s\left(\frac{\partial w_b}{\partial x}-\phi\right)\right] = \rho A\left(1-(e_0a)^2\frac{\partial^2}{\partial x^2}\right)\frac{\partial w_b}{\partial t^2}$$

$$EI\frac{\partial^2\phi}{\partial x^2}+GAK_s\left(\frac{\partial w_b}{\partial x}-\phi\right) = \rho I(1-(e_0a)^2\nabla^2)\frac{\partial\phi}{\partial t^2} \tag{3}$$

Here w_b and ϕ are transverse displacement and rotation angle; t is time; E and G are Young's modulus and shear modulus; A and I are the area of cross-section and the second moment of area; ρ is mass density and K_s denotes the shear correction coefficient. A singular equation in terms of w_b can be obtained based on Eq. (3). The general solution to this singular equation takes the form [8–10].

$$w_b = [C_1\cosh(\beta x)+C_2\sinh(\beta x)+C_3\cos(\delta x)+C_4\sin(\delta x)]e^{-i\omega t} \tag{4}$$

Here ω is angular frequency (frequency $f=\omega/2\pi$); β and δ are the functions of E, G, A, I, Ks; C_1 to C_4 are some real numbers and $i=\sqrt{-1}$. In addition, ϕ can be expressed in terms of w_b. For clamped *NT*s of length L we have $w_b=0$ and $\phi(w_b)=0$ at $x=0$ and L. Substituting Eq.(4) into the boundary conditions yields $M_1[C_1,C_2,C_3,C_4]^T=0$. Here M_1 is the coefficient matrix. The condition for nonzero solution of C_1 to C_4 is $\det M_1=0$, which gives the vibration frequency of *NT*s. For more details on the method the reader may refer to Refs. [8–11].

The nonlocal shell equations for *NT* vibration were obtained in Refs. [13–15]

$$r^2\frac{\partial^2 u}{\partial x^2}+\frac{1}{2}(1-\nu)\frac{\partial^2 u}{\partial\theta^2}+\frac{r}{2}(1+\nu)\frac{\partial^2 v}{\partial x\partial\theta}-\nu r\frac{\partial w}{\partial x}$$
$$+\frac{D}{Kr^2}\begin{bmatrix}\frac{1}{2}(1-\nu)\frac{\partial^2 u}{\partial\theta^2}\\ +r^3\frac{\partial^3 w}{\partial x^3}\\ -\frac{r}{2}(1-\nu)\frac{\partial^3 w}{\partial x\partial\theta^2}\end{bmatrix} = \frac{\rho h}{K}r^2(1-(e_0a)^2\nabla^2)\frac{\partial^2 u}{\partial t^2},$$

$$\frac{r}{2}(1+\nu)\frac{\partial^2 u}{\partial x\partial\theta}+\frac{r^2}{2}(1-\nu)\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial\theta^2}-\frac{\partial w}{\partial\theta}$$
$$+\frac{D}{Kr^2}\begin{bmatrix}\frac{3r^2}{2}(1-\nu)\frac{\partial^2 v}{\partial x^2}\\ +\frac{r^2}{2}(3-\nu)\frac{\partial^3 w}{\partial x^2\partial\theta}\end{bmatrix} = \frac{\rho h}{K}r^2(1-(e_0a)^2\nabla^2)\frac{\partial^2 v}{\partial t^2},$$

$$\nu r\frac{\partial u}{\partial x}+\frac{\partial v}{\partial\theta}+w+\frac{D}{Kr^2}\begin{bmatrix}-r^4\nabla^4 w-r^3\frac{\partial^3 u}{\partial x^3}+\frac{r}{2}(1-\nu)\frac{\partial^3 u}{\partial x\partial\theta^2}\\ -\frac{r^2}{2}(3-\nu)\frac{\partial^3 v}{\partial x^2\partial\theta}-w-2\frac{\partial^2 w}{\partial\theta^2}\end{bmatrix}$$
$$=\frac{\rho h}{K}r^2(1-(e_0a)^2\nabla^2)\frac{\partial^2 w}{\partial t^2} \tag{5}$$

Here u, v and w are longitudinal, circumferential and radial displacements of *NT*s, D is effective bending stiffness; K is in-plane stiffness; ρh is mass density per unit lateral area on the surface of *NT*s. The solutions satisfying the clamped end condition are as follows [23]

$$u = U\left[-\sin\frac{\mu}{r}\left(\frac{L}{2}-x\right)+k\sinh\frac{\mu}{r}\left(\frac{L}{2}-x\right)\right]\cos(n\theta)e^{-i\omega t}$$
$$v = V\left[\cos\frac{\mu}{r}\left(\frac{L}{2}-x\right)+k\cosh\frac{\mu}{r}\left(\frac{L}{2}-x\right)\right]\sin(n\theta)e^{-i\omega t}$$
$$w = W\left[\cos\frac{\mu}{r}\left(\frac{L}{2}-x\right)+k\cosh\frac{\mu}{r}\left(\frac{L}{2}-x\right)\right]\cos(n\theta)e^{-i\omega t} \tag{6}$$

where U, V and W denote the longitudinal, circumferential and radial displacement amplitudes; n is circumferential wave number and $\mu L/r\equiv c=1.506\pi$, 2.5π, 3.5π, 4.5π, 5.5π and 6.5π corresponding to half axial wave number $m=1$ 2, 3, 4, 5, 6… Thus we have $\mu L/r\equiv c\approx(m+0.5)\pi$. Substituting Eq. (6) into (5) leads to the equations $M_2[U,V,W]^T=0$, where M_2 is a coefficient matrix. For the nonzero solutions of U, V and W we have $\det M_2=0$. The frequency can then be obtained by solving the equation.

In Flugge [24] and Timoshenko's books [25] it was shown that when circumferential wave number n is equal to one, the thin shell model is in perfect match with the Euler beam model in the buckling analysis of a long cylindrical thin shell. As explained by Flugge [24], in this particular case (i.e., $n=1$ and a sufficiently large length-to-aspect ratio), the thin shell model predicts a circular cross-section for a deformed cylindrical shell, which is exactly the same as assumed in the beam model. Recently, this conclusion has been further confirmed for the axial buckling [26] and transverse (or beam-like) vibration [26–29] of CNTs at the nanoscale. This reveals the fact that at a large axial wavelength the lowest frequency with $n=1$ given by the shell model corresponds to the transverse or beam-like vibration of *NT*s.

3. Results and discussions

In this Section the transverse vibration of *NT*s will be studied based on the classical (i.e., $e_0=0$) and nonlocal Timoshenko beam [8–11] and Flugge shell models with $n=1$ [14,15]. Single-walled carbon nanotubes (SWCNTs) having chirality (5, 5) with clamped ends are selected as a typical example of *NT*s (Fig. 1). The effective values of material properties used for SWCNTs as two dimensional shells are $D=2$ eV, $K=360$ J/m^2 and $\rho h=(2.27$ g/cm$^3)\times 0.34$ nm [28,29]. These values correspond to the effective thickness $h=0.1$ *nm* and equivalent Young's modulus $E=3.5$*TPa* [29,30] which are used here for SWCNTs as Timoshenko beams.