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A hybrid continuum and molecular mechanics model for the axial buckling of chiral single-walled carbon nanotubes

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A B S T R A C T

The purpose of this study is to describe the axial buckling behavior of chiral single-walled carbon nanotubes (SWCNTs) using a combined continuum-atomistic approach. To this end, the nonlocal Flugge shell theory is implemented into which the nonlocal elasticity of Eringen incorporated. Molecular mechanics is used in conjunction with density functional theory (DFT) to precisely extract the effective in-plane and bending stiffnesses and Poisson's ratio used in the developed nonlocal Flugge shell model. The Rayleigh-Ritz procedure is employed to analytically solve the problem in the context of calculus of variation. The results generated from the present hybrid model are compared with those from molecular dynamics simulations as a benchmark of good accuracy and excellent agreement is achieved. The influences of small scale factor, commonly used boundary conditions and chirality on the critical buckling load are fully explored. It is indicated that the importance of the small length scale is affected by the type of boundary conditions considered.

1. Introduction

The past two decades have witnessed tremendous advances in the nano-science and -technology, as reflected by considerable research effort directed towards fundamentals, synthesis and applications of nanostructured materials. Despite publication of the first report on the tubular nature of carbon filaments in 1952 [1], the 1991 Iijima paper on carbon nanotubes (CNTs) [2] regenerated intense interest in the nano-community. Having superior mechanical properties such as high elastic modulus, high strengths, high thermal conductivity and low weight makes CNTs distinguished from other materials ever discovered.

Owing to technological complexities and also high costs of handling, experimental methods cannot be considered as efficient approaches to investigate the behavior of nanostructures. Therefore, theoretical approaches have still been the foremost tool for modeling of systems at the nanometer scale. There are different ways for theoretical modeling of nanostructures such as continuum mechanics, molecular mechanics and also molecular dynamics (MD). The MD simulations are computationally expensive so that they are limited to small time and length scale problems due to the limitation of computer speed, while the theoretical predictive models based on the continuum mechanics are computationally efficient and are gaining more popularity in recent years [3–13]. However, the negative aspect of classical continuum models is that they are scale free. Hence, modified continuum theories such as gradient elasticity theories have been suggested to accommodate the size dependence of nanostructures [14,15]. One of the well-known size-dependant continuum models is on the basis of the nonlocal elasticity theory initiated by the works of Eringen [16,17]. A review of the literature reveals that the nonlocal continuum models have been extensively applied by researchers to study different problems of nanostructures [18–37]. Molecular mechanics models have also attracted great research attentions as a result of their computationally efficiency and ability of capturing the effect of chirality. Molecular mechanics is a non-quantum mechanical method which can be applied to obtain some properties of molecules. Molecular mechanics has been widely used to analytically study mechanical behavior of CNTs [38–41].

In spite of their computational efficiency as well as reasonable accuracy, the continuum models have some drawbacks. At first, there is not any consensus on the accurate value of effective thickness used in the calculations. Yakobson et al. [3] extracted the effective thickness of CNTs equal to 0.066 nm through comparison of the MD simulation results with those of

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continuum model. Vodenitcharova and Zhang [42] proposed an effective thickness of 0.0617 nm using the ring theory of continuum mechanics. Additionally, in many researches the value of spacing of graphite (0.34 nm) has been utilized in the analyses. On the other hand, the results of continuum models depend on the applied values of mechanical properties such as Young's modulus and Poisson's ratio. In this respect, Ansari and Rouhi [33] via a nonlocal Flugge shell model revealed that the varying Young's modulus and thickness of SWCNTs significantly affects the value of nonlocal parameter with the aim of get close fit to the MD results.

In the present work, in order to predict the stability characteristics of SWCNTs under the action of axial load in a more accurate way, a hybrid of continuum and molecular mechanics is implemented. To this end, first, within the framework of nonlocal continuum mechanics, Eringen's nonlocal constitutive equation is incorporated into the Flugge-type shell equations and the coupled field governing equations are derived. Then, by employing the molecular mechanics method and using DFT calculations, the accurate values for in-plane and bending stiffnesses and Poisson's ratio of SWCNTs with different chiralities are obtained. Hence, the proposed hybrid model takes the advantages of continuum and molecular mechanics approaches. In other words, the presented model has the computational efficiency of a continuum model whose input material properties are determined using the molecular mechanics which is an accurate chirality-dependent atomistic approach. Finally, to analytically solve the problem, the Rayleigh-Ritz technique in company with the beam mode shapes are applied to the variational statement derived from the Flugge-type buckling equations. Also, due to the vagueness that is present in defining nanotube wall thickness in the literature, the idea of in-plane stiffness (i.e. classical Young's modulus multiplied by the nanotube thickness) is adopted in this work to avoid this ambiguity. Accordingly, by applying the present hybrid model, the need for thickness of nanotube disappears. Furthermore, MD simulations are conducted to assess the validity of the present analysis. Selected numerical results are also given to investigate the effects of different parameters on the axial buckling of SWCNTs.

2. Analytical buckling solution for nonlocal Flugge shell model

According to Eringen [16,17], in the theory of nonlocal continuum mechanics which contains information about the long-range forces between atoms, the stress tensor at a reference point is considered to be a functional of the strain tensor at all the points of the body. Therefore, Hooke's law for the stress and strain relation is given by.

$$\begin{Bmatrix} \sigma_{xx} \\ \sigma_{\theta\theta} \\ \sigma_{x\theta} \end{Bmatrix} - (e_0 a)^2 \nabla^2 \begin{Bmatrix} \sigma_{xx} \\ \sigma_{\theta\theta} \\ \sigma_{x\theta} \end{Bmatrix} = \begin{bmatrix} \dfrac{E}{1-\nu^2} & \dfrac{\nu E}{1-\nu^2} & 0 \\ \dfrac{\nu E}{1-\nu^2} & \dfrac{E}{1-\nu^2} & 0 \\ 0 & 0 & \dfrac{E}{2(1+\nu)} \end{bmatrix} \times \begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{\theta\theta} \\ \gamma_{x\theta} \end{Bmatrix}, \tag{1}$$

where E is Young's modulus, ν is Poisson's ratio and $e_0 a$ denotes the nonlocal parameter which leads to consider the small scale effect.

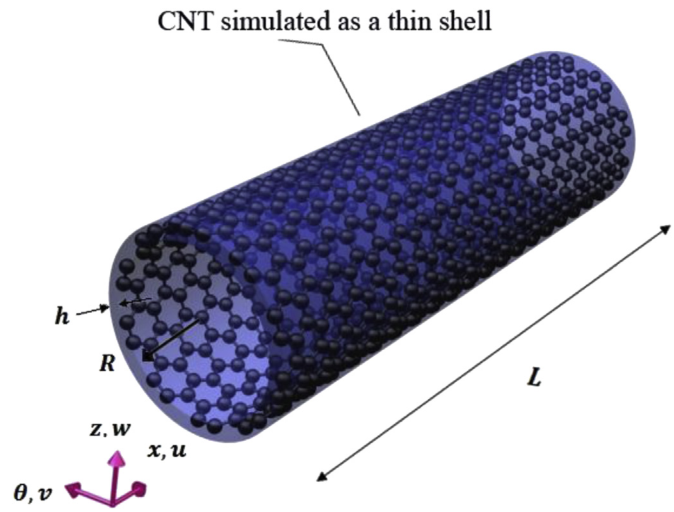

Fig. 1. Schematic of an SWCNT treated as an elastic shell.

To model the SWCNTs, consider an elastic cylindrical shell with radius R and thickness h as illustrated in Fig. 1.

Based on the classical shell theory, the displacement components u_x, u_θ and u_z in the x, θ and z directions, respectively, are expressed as.

$$\begin{aligned} u_x(x,\theta,z) &= u(x,\theta) - z\frac{\partial w}{\partial x}(x,\theta) \\ u_\theta(x,\theta,z) &= v(x,\theta) - z\frac{\partial w}{\partial \theta}(x,\theta) \\ u_z(x,\theta,z) &= w(x,\theta,z), \end{aligned} \tag{2}$$

where u, v, w are the reference surface displacements. The kinematic relations are also given by

$$\begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{\theta\theta} \\ \gamma_{x\theta} \end{Bmatrix} = \begin{Bmatrix} \dfrac{\partial u}{\partial x} \\ \dfrac{1}{R}\dfrac{\partial v}{\partial \theta} + \dfrac{w}{R} \\ \dfrac{\partial v}{\partial x} + \dfrac{1}{R}\dfrac{\partial u}{\partial \theta} \end{Bmatrix} + z \begin{Bmatrix} -\dfrac{\partial^2 w}{\partial x^2} \\ -\dfrac{1}{R^2}\left(\dfrac{\partial^2 w}{\partial \theta^2} + w\right) \\ -\dfrac{2}{R}\dfrac{\partial^2 w}{\partial x \partial \theta} + \dfrac{1}{R}\dfrac{\partial v}{\partial x} - \dfrac{1}{R^2}\dfrac{\partial u}{\partial \theta} \end{Bmatrix}. \tag{3}$$

The force and moment resultants in terms of stresses are formulated as.

$$\begin{aligned} N &= (N_{xx}, N_{\theta\theta}, N_{x\theta})^T \mathrm{d}z = \int_{-h/2}^{h/2} (\sigma_{xx}, \sigma_{\theta\theta}, \sigma_{x\theta})^T \mathrm{d}z M \\ &= (M_{xx}, M_{\theta\theta}, M_{x\theta})^T \mathrm{d}z = \int_{-h/2}^{h/2} (\sigma_{xx}, \sigma_{\theta\theta}, \sigma_{x\theta})^T z \mathrm{d}z. \end{aligned} \tag{4}$$

According to the nonlocal shell theory, the force and moment resultants are defined based on the stress components in Eq. (4). Thus, they can be expressed as follows by referencing the kinematic relations in the Flugge shell theory [43].