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Sanders shell model for buckling of single-walled carbon nanotubes with small aspect ratio

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ABSTRACT

In this paper, the buckling behaviour of single-walled carbon nanotubes (CNTs) is revisited by resorting to Donnell and Sanders shell models, which are put in parallel and shown to lead to very distinct results for CNTs with small aspect ratio (length-to-diameter). This paper demonstrates inability of the widely used Donnell shell theory while it shows the validity and accuracy of the Sanders shell theory in reproducing buckling strains and mode shapes of axially compressed CNTs with small aspect ratios. The results obtained by the later shell theory are close to molecular dynamics simulation results.The Sanders shell theory could capture correctly the length-dependent buckling strains of CNTs which the Donnell shell theory fails to achieve. In view of this study, researchers should adopt the Sanders thin shell theory from hereon instead of the Donnell theory when analyzing CNTs with small aspect ratios.

1. Introduction

It is generally accepted that molecular dynamics (MD) simulations provide good predictions of the mechanical behaviour of carbon nanotubes (CNTs) under external forces. However, MD simulations take an awfully long time to produce the results, especially when dealing with long and multiple walled CNTs incorporating a large number of atoms. This spurred researchers to explore the use of continuum beam and shell theories to model CNTs as an alternative tool. Many papers on this topic have since been published over the last decade (see a literature survey paper by Wang et al. [1]). Regarding shell theories for CNTs, the great majority of the works published in the past (e.g., [2]) and recently (e.g., [3]) were based on the Donnell shell theory due to its inherent simplicity and ability to accommodate new constitutive relations (non-local) and the influence of several parameters (van der Waals forces, elastic media).

Recently, Zhang et al. [4] performed a rigorous assessment exercise on the validity and accuracy of the Euler Bernoulli beam model and Donnell cylindrical shell model and their non-local counterparts in predicting the buckling strains of single-walled CNTs. By comparing with MD simulation results conducted at room temperature, they concluded that

- The simple Euler–Bernoulli beam model is sufficient for predicting the buckling strains of CNTs with large aspect ratios (i.e. length to diameter ratio $L/d > 10$).
- The more refined Timoshenko beam model or non-local beam theory is needed for CNTs with intermediate aspect ratios (i.e. $8 < L/d < 10$).
- The Donnell thin shell theory is unable to capture the length-dependent critical strains obtained by MD simulations for CNTs with small aspect ratios (i.e. $L/d < 8$) and hence this simple shell theory is unsatisfactory in modelling small aspect ratio CNTs.

In view of the last conclusion, many researchers tried to improve the Donnell thin shell theory for the buckling analysis of short CNTs. The great majority of works attributed this lack of accuracy to the inadequate modelling of CNT constitutive relations. At atomic length scale the material microstructure becomes increasingly important and small scale effects cannot be ignored. In order to improve the CNT constitutive relations, many authors [5–8] adopted Eringen's equations of non-local elasticity and incorporated them into several continuum models. The use of non-local elasticity relations in either Euler–Bernoulli or Timoshenko beam models were shown to be accurate for long CNTs [9]. However, the incorporation of non-local elasticity relations into the Donnell shell model was shown to provide more accurate results [6,8], but unexpected discrepancies between the results and MD simulations still remain due to the unknown (and widely scattered) values of non-local constant e_0. As it will be explained in this paper, the main reason for the inaccuracy of Donnell shell model is the inadequate

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kinematic hypotheses underlying it, either using the model with local or non-local elasticity relations. In this paper, we show that the inaccuracy of Donnell shell model is mostly due to the inadequacy of kinematic simplifying assumptions. We investigate the use of the more refined Sanders cylindrical thin shell theory for modelling the buckling behaviour of CNTs with small aspect ratios. The Sanders thin shell model results are compared with the Donnell shell model results and validated against MD simulations results. It will be shown herein how surprising well the Sanders shell theory is able to reproduce buckling strains of CNTs that are length dependent as well as mode shapes that are relatively close to those predicted by MD simulations.

2. Revisiting Donnell and Sanders shell theories

Let us consider a circular cylindrical shell (see Fig. 1) of radius R with the cylindrical coordinate system (x, z, θ), having the origin O at the centre of one end of the shell – longitudinal coordinate $x \in [0; L]$, circumferential coordinate $\theta \in [0; 2\pi]$, radial coordinate $z \in [-h/2; +h/2]$. The displacements of an arbitrary point of coordinates (x, θ) on the mid-surface of the shell are denoted by u, v and w, in the longitudinal, circumferential and radial directions, respectively.

In order to compare the results obtained from continuum mechanics and MD simulations, two different strain–displacement relationships for thin shells are used in the present study. These two different strain–displacement relationships are associated with the Donnell [10] and Sanders [11] theories of thin shells [12–15]. Both are based on Love's first approximation assumptions: (i) the shell thickness h is small with respect to the radius of curvature R of the mid-plane, (ii) strains are small, (iii) transverse normal stress is small and (iv) the Kirchhoff–Love kinematic hypothesis, in which it is assumed that the normal to the undeformed middle surface remains straight and normal to the mid-surface after deformation, and undergoes no thickness stretching. For both Donnell and Sanders theories, the effect of transverse shear deformations are neglected. According to these shell theories, the strain components ε_x, ε_θ and $\gamma_{x\theta}$ at an arbitrary point of the shell are given by

$$\varepsilon_x = u_{,x} + \frac{1}{2}(w_{,x})^2 + \frac{1}{2}\beta^2 - z w_{,xx} \tag{1}$$

$$\varepsilon_\theta = \frac{v_{,\theta} + w}{R} + \frac{1}{2}\beta_\theta^2 + \frac{1}{2}\beta^2 + z\left(\frac{1}{R}\beta_{\theta,\theta}\right) \tag{2}$$

$$\gamma_{x\theta} = \frac{u_{,\theta}}{R} + v_{,x} - w_{,x}\beta_\theta + z\left(-\frac{w_{,x\theta}}{R} + \beta_{\theta,x} + \frac{1}{R}\beta\right) \tag{3}$$

where z is the distance of the arbitrary point of the shell from the mid-surface, β_θ is the rotation in the direction perpendicular to the $R\theta$–z plane (about x-axis) and β is the rotation in the direction perpendicular to the $R\theta$–x plane (about z-axis), that is the z-rotation of a fibre orthogonal to the shell mid-surface. These two terms (β_θ and β) play a crucial role in the results obtained from both theories.

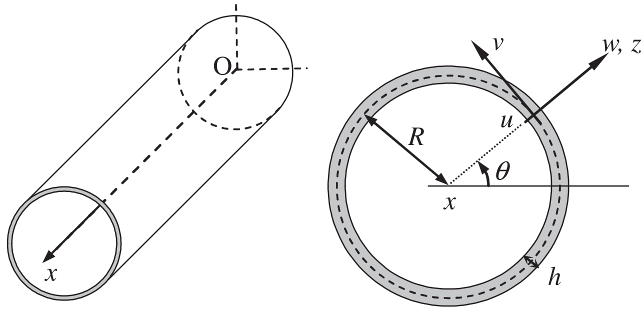

Fig. 1. Shell coordinate system and displacement components.

In the Donnell shell theory, these two rotations have the simplified form [10]

$$\beta_\theta = -\frac{w_{,\theta}}{R} \tag{4}$$

$$\beta = 0 \tag{5}$$

It is seen that (i) the rotation in the direction perpendicular to the $R\theta$–z plane (about x-axis) only depends on w and (ii) the rotation in the direction perpendicular to the $R\theta$–x plane (about z-axis) is deemed null. This last assumption considers that the rotation of a fibre orthogonal to the shell mid-surface about itself is null.

By introducing the expressions (4) and (5) into the strain–displacement relationships (1)–(3), it is shown that both curvatures (linear terms multiplied by z) and non-linear terms only depend on the radial w-displacement. Since the u and v displacements only appear in the membrane strain components (linear terms not multiplied by z), these displacements are assumed to be infinitesimal. The trademark of Donnell's theory is that (i) the shell non-linear behaviour (geometric stiffness) and (ii) bending behaviour only depend on the displacement of w, which leads to that Donnell's theory is designated for shallow shells. It is well known (e.g., [13]) that the set of differential equations of Donnell's theory for shallow shells under uniform compression is given by

$$R^2 u_{,xx} + \frac{1-\nu}{2}u_{,\theta\theta} + \frac{1+\nu}{2}R v_{,x\theta} + \nu R w_{,x} = 0 \tag{6}$$

$$\frac{1+\nu}{2}R u_{,x\theta} + \frac{1-\nu}{2}R^2 v_{,xx} + v_{,\theta\theta} + w_{,\theta} = 0 \tag{7}$$

$$D\nabla^4 w + \frac{C}{R^2}(v_{,\theta} + w + R\nu u_{,x}) - \sigma_x h w_{,xx} = 0 \tag{8}$$

where $D = Eh^3/12(1-\nu^2)$ is the shell flexural rigidity, $C = Eh/(1-\nu^2)$ the shell membrane rigidity, E the Young's modulus, ν the Poisson ratio, h the shell thickness, R the shell radius and σ_x the applied compressive stress, respectively. It is also known that the coupled system of Eqs. (6)–(8) can easily be transformed into the following set of three uncoupled equations [13],

$$\nabla^4 u = -\frac{\nu}{R}w_{,xxx} + \frac{1}{R^3}w_{,x\theta\theta} \tag{9}$$

$$\nabla^4 v = -\frac{\nu+2}{R^2}w_{,xx\theta} - \frac{1}{R^4}w_{,\theta\theta\theta} \tag{10}$$

$$D\nabla^8 w + \frac{1-\nu^2}{R^2}C w_{,xxxx} - \nabla^4(\sigma_x h w_{,xx}) = 0 \tag{11}$$

The well-known Eq. (11) is seen to be an homogeneous linear equation of w alone. After solving Eq. (11) for w, the membrane displacements u and v can be determined from Eqs. (9) and (10). This is the major advantage of Donnell's theory of shells, whose equations can be easily solved and exact analytical solutions can be obtained. This is the main reason why Donnell shell theory has been extensively used for CNT analysis.

In the Sanders shell theory, these two rotations have the exact and complete form [11]

$$\beta_\theta = \frac{v}{R} - \frac{w_{,\theta}}{R} \tag{12}$$

$$\beta = \frac{1}{2}\left(v_{,x} - \frac{u_{,\theta}}{R}\right) \tag{13}$$