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Deformation Analysis of Single- Wall Carbon Nanotubes: a Shell theory Based on the Interatomic Potential

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ABSTRACT

The aim of current study is to present a finite deformation shell theory incorporating interatomic potentials for single-wall carbon nanotubes (CNTs). For this purpose, a linkage between the strain energy density, induced in the continuum, and the interatomic potential is established by the employment of the modified Cauchy-Born rule. This theory, which considers the nonlinear, multi-body atomistic coupling and the CNT chirality, incorporates the important effects of bending moment and curvature for a curved surface. The theory is applied to extract the constitutive relations, which bypass the use of nanotube thickness and Young's modulus, among stress, moment, strain, curvature and the interatomic potential. Through constitutive models, the interatomic potential and atomic structure of a material are directly incorporated into the continuum analysis of the solids. Numerical examples including rolling of a graphene to a CNT and tension of a CNT are carried out to examine the efficiency of the current model. It is found that the chirality affects the mechanical behavior of the nanotube in tension and bending and this effect is less profound for the CNTs with higher radius at vanishing strain and curvature.

KEYWORDS

Shell Theory, Interatomic Potential, Carbon Nanotube, Bending, Curvature, Constitutive Model.

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1- INTRODUCTION

Due to the superior mechanical and electrical properties of the carbon nanotubes, they have many potential applications in emerging fields of nanotechnology [1, 2]. In recent years, a lot of researchers studied the deformation of carbon nanotubes based on the continuum mechanics [3, 4]. In the continuum studies based on the shell theories, the multi-body coupling and the effect of the chirality are neglected. Further, these theories involve Young's modulus and wall thickness of the CNT whose values are scattered in the literature.
Motivated by these studies, an atomistic-based finite deformation shell theory is developed to study the behavior of single-wall CNTs under different deformations. In contrast to the conventional continuum-based models, the present model is independent of Young's modulus and thickness of the CNT. Further, it considers the important influences of the bending moment and curvature as well as the nonlinear, multi-body atomistic interactions and CNT chirality.

2- NONLINEAR FINITE DEFORMATION SHELL THEORY BASED ON INTERATOMIC POTENTIAL

1-2- INTERATOMIC POTENTIAL

Brenner et al. [2] proposed an interatomic potential for carbon as:

$$V(r_{ij}) = V_R(r_{ij}) - B_{ij} V_A(r_{ij}) \tag{1}$$

where r_{ij} denotes the distance between atoms i and j and V_R and V_A stand for the repulsive and attractive pair terms. Also, B_{ij} is the multi-body coupling which depends on the neighboring atoms of the atom i.

2-2- DEFORMATION OF A CURVED SURFACE

Assume $\mathbf{P}(\xi^1,\xi^2)$ to be a point on a curved surface deforming to the new point $\mathbf{p}(\xi^1,\xi^2)$. The covariant base vectors $\mathbf{a}_\alpha$, the unit normal to the surface $\mathbf{n}$, the coefficients of the first and second fundamental form for the deformed surface $a_{\alpha\beta}$, $b_{\alpha\beta}$ are given by:

$$\mathbf{a}_\alpha = \frac{\partial \mathbf{p}}{\partial \xi^\alpha},\ \mathbf{n} = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{|\mathbf{a}_1 \times \mathbf{a}_2|},$$
$$a_{\alpha\beta} = \mathbf{a}_\alpha \cdot \mathbf{a}_\beta,\ b_{\alpha\beta} = \mathbf{n} \cdot \frac{\partial^2 \mathbf{p}}{\partial \xi^\alpha \partial \xi^\beta} \tag{2}$$

Now, it is assumed that two points $\mathbf{P}(\xi^1,\xi^2)$ and $\mathbf{P}+\Delta\mathbf{P}(\xi^\alpha,\xi^\alpha+\Delta\xi^\alpha)$ on the initial surface deform to $\mathbf{p}$ and $\mathbf{p}+\Delta\mathbf{p}$, respectively. $\Delta\mathbf{p}$ can be calculated using the Taylor series as:

$$|\Delta\mathbf{p}|^2 = (A_{\alpha\beta}+2E_{\alpha\beta})\Delta\xi^\alpha\Delta\xi^\beta - \frac{1}{12}\left[(B_{\alpha\beta}+K_{\alpha\beta})\Delta\xi^\alpha\Delta\xi^\beta\right]^2 \tag{3}$$

where $E_{\alpha\beta}=1/2(a_{\alpha\beta}-A_{\alpha\beta})$ and $K_{\alpha\beta}=1/2(b_{\alpha\beta}-B_{\alpha\beta})$ separately indicate the components of the Green strain and the curvatures [5]. The hexagonal lattice of a graphite sheet can be decomposed to the two sub-lattices with triangular structure. Based on the Cauchy-Born rule [6], the strain energy density is given by:

$$w = w(E_{\alpha\beta},K_{\alpha\beta},\eta^\lambda(E_{\alpha\beta},K_{\alpha\beta})) = \sum_{j=1,2,3} V(r_{ij})/2S_0 \ ,\ (S_0 = 3\sqrt{3}/4r_{ij}^{(0)^2}) \tag{4}$$

where η^λ are the components of a shift vector between the two sub-lattices introduced to ensure the equilibrium of the atoms.

3-2- STRESS AND MOMENTS IN SINGLE-WALL CNTs

The strain and curvature tensors are $\mathbf{E}=E_{\alpha\beta}\mathbf{A}^\alpha\mathbf{A}^\beta$ and $\mathbf{K}=K_{\alpha\beta}\mathbf{A}^\alpha\mathbf{A}^\beta$, respectively where $\mathbf{A}^\alpha$ represents the contravariant base vector. The second Piola-Kirchhoff stress tensor $\mathbf{T}$ and the moment tensor $\mathbf{M}$ are obtained by:

$$\mathbf{T} = \frac{Dw}{D\mathbf{E}} = \frac{\partial w}{\partial \mathbf{E}} + \frac{\partial w}{\partial \boldsymbol{\eta}} \cdot \frac{\partial \boldsymbol{\eta}}{\partial \mathbf{E}} = \frac{\partial w}{\partial \mathbf{E}} \tag{5}$$

$$\mathbf{M} = \frac{Dw}{D\mathbf{K}} = \frac{\partial w}{\partial \mathbf{K}} + \frac{\partial w}{\partial \boldsymbol{\eta}} \cdot \frac{\partial \boldsymbol{\eta}}{\partial \mathbf{K}} = \frac{\partial w}{\partial \mathbf{K}} \tag{6}$$

3- PROBLEMS

1-3- ROLLING OF A GRAPHENE TO A CNT

Let ε_1 and ε_2 be the circumferential and axial strains, respectively. The strains can be computed by minimizing the strain energy. Figure (1) shows the variations of ε_1 and ε_2 versus the CNT radius R. For small CNTs, the circumferential strain achieves a value of 5% while, the axial strain is very low. At large radiuses, the difference between the strains are reduced because the curvature of CNT diminishes and the nanotube becomes close to a graphene.

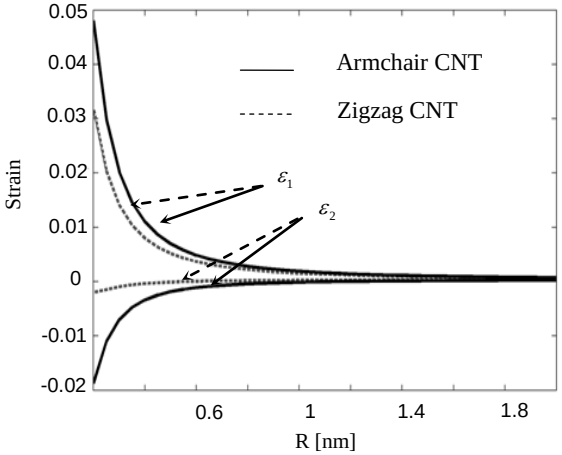

Figure (1): Strain versus the CNT radius during rolling a graphene to nanotube

Figure (2) shows the strain energy against the radius. The result of the molecular dynamics simulation is given [7]. The present results agree well with the ones obtained by $\Delta U = EIS_0 / 2R^2$. It is seen that with an increase in the radius, the curvature and then the energy decrease.

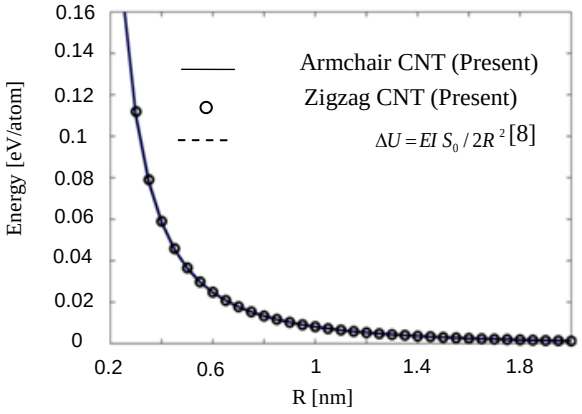

Figure (2): Variation of energy versus CNT radius

2-3- CNT UNDER TENSION

Using the equilibrium equations, the axial force can be evaluated as $P = 2\pi R\sqrt{1+2E_{ZZ}}T_{ZZ}$. Depicted in figure (3) is the axial force to the nanotube circumference ratio versus the axial strain. At $\varepsilon_{axial} = 2\%$, the value of the force for the CNT (12,12) is equal to 33.6 N/m which is in agreement with that of Ref. [8] as 34.17 N/m.

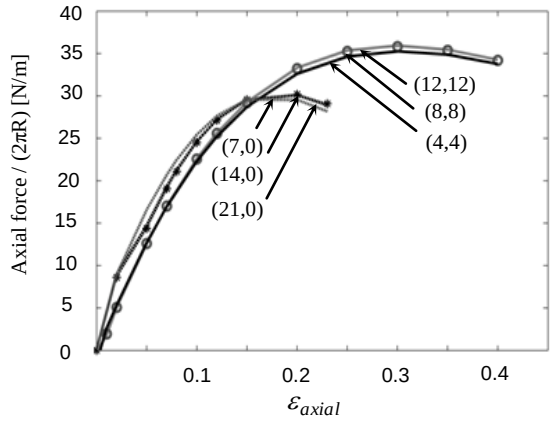

Figure (3): Axial force to the CNT circumference ratio versus axial strain

4- CONCLUSION

Described in the current study was the behavior of a single-wall CNT under various deformations based on a finite-deformation shell theory. The proposed model incorporates the interatomic potential into the membrane theories and takes the influence of bending moment and curvature into account. It was discerned that the chirality has effect on the behavior of a nanotube and the dependence of the tensile force on the chirality is much higher than the one on the radius.

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