Axial compression based hyper elastic modeling of buckling response in single wall carbon nanotubes

K. Sunil Babu[1], K.S.R. Murthy[1], E. Kiran Kumar[2]

[1]Department of Physics, Miracle Educational Society Group of Institutions, India
[2]Department of Electronics & Communication Engineering, Miracle Educational Society Group of Institutions, India

ABSTRACT *: This paper presents a hyper elastic finite element-based lattice access for the illustration of post-buckling reaction in single wall carbon nanotubes (SWCNTs). A one-term incompressible Ogden-type hyper elastic model is taken in under axial compression to describe mechanical response of SWCNTs. Numerical experiments are transferred and the results are juxtapose to finite atomistic simulations, indicating the forecasting capabilities of the present model in seizing buckling manner and the main deformation mechanisms under huge thorough deformations.*
Keywords - *Buckling; single wall carbon nanotube; Atomistic Finite element method; hyper elastic*

I. INTRODUCTION

In the recent past, the research for carbon nanotubes by means of computational simulations has come to significant development, specifically in connection to the understanding of their mechanical actions [1]. In the context of numerical models, two main classifications can be traced considerably in the current literature. The first classification correlate to the atomistic approach[2], in which classical molecular dynamics and tight-binding molecular dynamics consists of the most popular techniques. Though these classifications have been proved to be fruitful in holding complex deformation mechanisms in atomistic systems, they are affected by the drawback of excessive computing costs. Their usage has been bounded to the analysis of small to moderate size problems.

The second classification is indicated by finite elements simulations [4]. Distinctly in this classification, the lattice approach [5] has been proved to be an appropriate technique for the analysis of carbon nanotubes. This access establishes bondage between structural and molecular mechanics at the C-C bond level, and supplies a way to model the deformation of carbon nanotubes by means of accurate finite element analyses using classical beam elements. Interestingly, In spite of the extensive work performed in this context, a reassessment of the current literature on the finite element-based lattice indicates that the endorsement of a hyper elastic framework to illustrate the atomic covalent bonds in SWCNTs at large strains continues to be extensively neglected. Furthermore, the little research published in this context [6] has been limited wholly to the study of carbon nanotubes under axial tension.

In order to inspire others researchers in this realm to utilize such concepts our main aim in this paper is to taken in a hyper elastic framework in the constitutive modeling of C-C bonds in order to seize the main characteristics of buckling behavior in SWCNTs under axial compression. We expect here that with the use of such a hyper elastic model, the forecasting of the main mechanisms of deformation and the buckling reaction under huge strains is performed swimmingly.

The paper is fabricated as follows. Section II gives the composed description of SWCNTs by means of a hyper elastic framework. The conformation of the present model is given in Section III. Finally, Section IV outlines our resolution.

II.   HYPER ELASTIC DESCRIPTION

A common finite hyper elastic model is typified by the survival of a strain energy density function, which illustrates the progress of the Kirchhoff stress tensor, τ, in terms of the current Eulerian logarithmic strain tensor, ε. The constitutive equation for the Kirchhoff stress tensor is given by [7]

$$\tau = \frac{\partial \Psi}{\partial \varepsilon} \tag{1}$$

The strain tensor ε can be represented as a function of the left stretch tensor, *V*, by means of the term $\varepsilon = \ln V$. Moreover, if the strain energy function Ψ is assumed to be isotropic, it is possible to approve a representation for *V* in terms of the principal stretches, λ_i, i=1...3. Hence, we can write the constitutive equation for the eigenvalues τ_i of the Kirchhoff stress tensor as

$$\tau_i = \frac{\partial \Psi}{\partial \ln(\lambda_i)} \tag{2}$$

The exact choice of the strain energy density Ψ is commonly considered to be a matter of mathematical or experimental convenience. Here, due to its simplicity and analytical accuracy for huge deformations in conventional materials, an Ogden hyper elastic isotropic material model [9] is chosen for the mechanical modeling of C-C bonds. A one-term incompressible version of the Ogden strain energy density function is accepted, whose expression is given by

$$\Psi = \frac{2\chi}{\alpha^2} \{(\lambda_1)^{\alpha} + (\lambda_2)^{\alpha} + (\lambda_3)^{\alpha} - 3\} \tag{3}$$

where χ and α are material parameters. These are χ = 3.93 TPa and α = 2.0, along with a C-C bond equivalent diameter d = 0.10 nm and an actual shear stiffness is GAs = 141.24 nN. Additional details about the determination of these values can be found in Saavedra Flores et al. [10]. With the choice of the these values for the material constants, we enable the present hyper elastic model to get better the AMBER bond stretching, angle bending and torsional force constants, in the infinitesimal strains regime. The length of the equilibrium bond length among carbon atoms is considered here as 0.142 nm.

III.   VALIDATION OF THE MODEL

Main reason in this section is to confirm the present hyper elastic model with published data. The commercial software ABAQUS [11] is used in all our computational simulations. Because of the improvement of local instabilities during the non-linear deformation process, we adopt the automatic stabilization method provided by ABAQUS in order to capture buckling and post-buckling response. In all the subsequent analyses presented in this paper, we select the two-noded hybrid beam element, type B31H, which includes transverse shear strains (Timoshenko beam theory) in its formulation. In the cases analyzed in this section, the Z axis corresponds to the axial (longitudinal) direction of the tube, whereas X and Y correspond to the transverse directions. Zero approved displacements are forced on all the degrees of freedom of the nodes located at one of the ends of the tube, at Z = 0. On the opposite end, we apply incremental compressive displacements in the axial.

Figure 1 illustrates the variation of the strain energy per atom and the deformation mechanisms from our atomistic finite element simulations during the compression of a (7, 7) SWCNT of 6 nm length. Moreover, the strain energy reported by [12], using Brenner's first and second [13] generation potential, and also the strain energy designed by [3] for the same geometry, are also presented here. The atomistic finite element mesh consists of 686 nodes and 1015 beam elements.

In a first nearly quadratic regime, the consequences obtained with our simulation and those obtained from [3] and [12], using Brenner's second generation potential, show identical, up to 0.03 strain. Here, the deformation is uniform as shown in inset (a).

As the compressive buckle progresses these curves tend to diverge up to 0.05 strain in which the molecular dynamics simulation from [3] and the atomic-scale finite element model from [12] using Brenner's second generation potential reach the first instant of buckling. In this stage, Yakobson's simulation displays (though not shown here) two identical flattening perpendicular to each other, non-symmetrically located along the tube axis. The first buckling mechanism in our simulation is found at a later stage, at 0.072 strain, coinciding closely with the second buckling strain reported by Yakobson, at 0.076. At this point, if we evaluate the morphological patterns in both cases we will view that they match perfectly. Inset (b) shows two orthogonal views of the first buckling deformation mechanism predicted by our numerical simulation, characterized by a three axial half-wave symmetric configuration with a still straight axis. Moreover, we observe that even though the little difference detected at about 0.05 strains between the amount of energy reported by Yakobson and our model, at a strain about 0.07 the results predicted by both simulations tend to converge into the same amount of stored energy. On the contrary, despite the fact that Leung's simulations seem to show a similar deformation mechanism (not shown here), the amount of energy reported in both cases, with Brenner's first and second generation potential, is substantially lower.
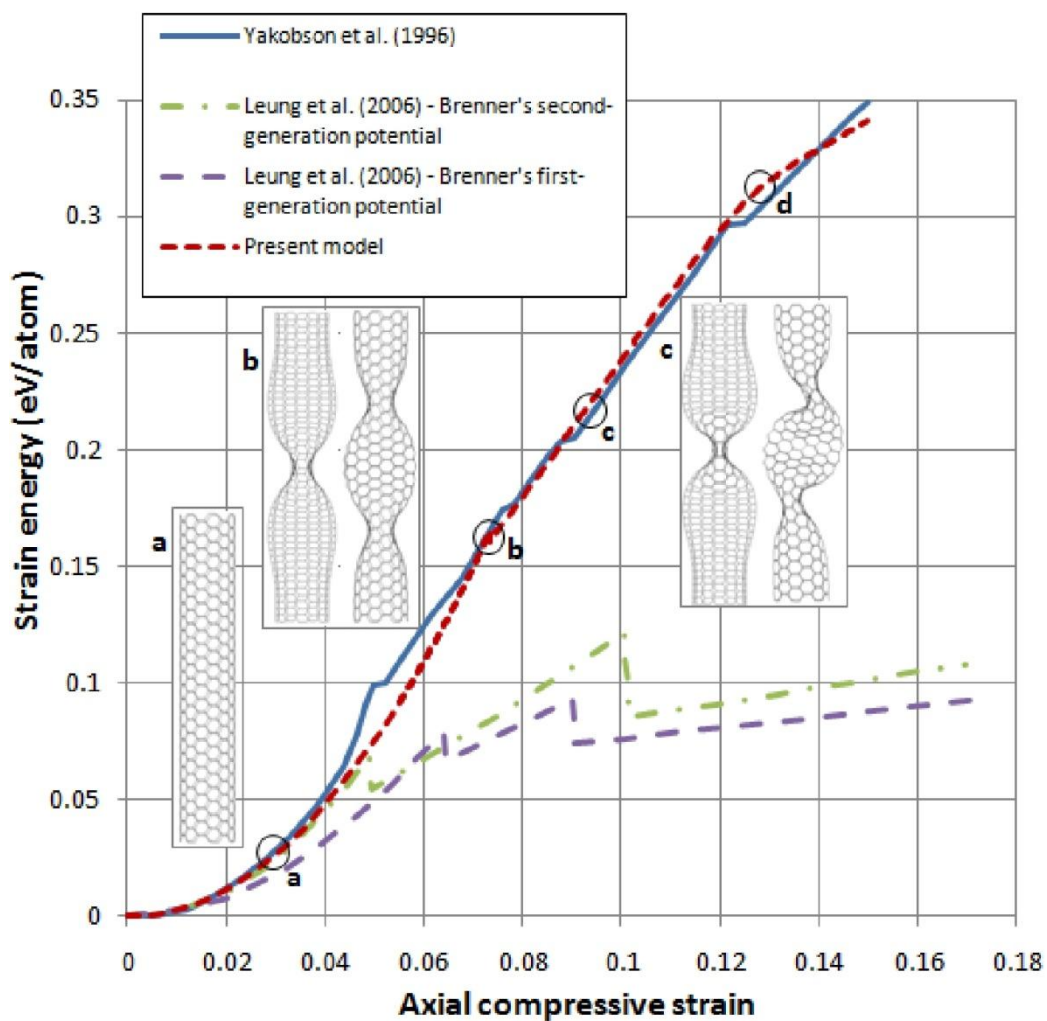

Fig.1. Strain energy for a (7, 7) SWCNT under axial compression

Further increase of the compressive deformation results in a new mechanism of deformation, represented by a buckling sideways in which the corresponding flattening serve as hinges. Inset (c) plots this stage (with two perpendicular views) in our finite element simulation, revealing the preservation of only one plane of symmetry after buckling. Yakobson's simulation predicts this critical strain at 0.09. However, our numerical model varies gradually (discontinuity not visible in the curve) but during a transition which occurs at about this level of strain. In any case, we find again a morphological agreement connecting both methodologies.

Moreover, the amount of energy calculated in these two simulations shows almost a perfect match to over 0.12 strain, where a new buckling mechanism is triggered. Yakobson reported over this level of deformation an entirely squashed asymmetric configuration. Our numerical model predicts after 0.125 strain (refer to Figure 1, circle labeled with letter **d**) a morphological pattern (not shown here) similar to that shown in inset (c) but much more distorted. Beyond this point, a gradual transition in the slope of our curve is observed, enlightening a slightly lower slope when compared to Yakobson's results. Here, the van der Waals interactions and other different atomic energy terms are crucial in order to describe accurately the mechanical response of carbon nanotubes for even advance levels of deformations.

IV.   CONCLUSION

The buckling behavior of single wall carbon nanotubes (SWCNTs) has been investigated by means of atomistic finite element-based lattice approach. A one-term incompressible Ogden-type hyper elastic model has been chosen to describe the mechanical response of SWCNTs under axial compression.

Finite element simulations have been carried out on SWCNT models and the results have been compared to published data, representing the predictive capability of the present hyper elastic model. The projected description has been able to capture the main deformation mechanisms and buckling behavior under large deformations, revealing the potential applications of our approach on the study of fullerenes.

REFERENCES

[1].   S. Iijima, C. Brabec, A. Maiti, J. Bernholc, "*Structural exibility of carbon nanotubes*",. *Journal of Chemical Physics 104 (1996)* 2089-2092.
[2].   C. Li, T. W. Chou, "*A structural mechanics approach for the analysis of carbon nanotubes*",. *International Journal of Solids and Structures 40 (2003) 2487-2499.*
[3].   B. Yakobson, C. Brabec, J. Bernholc, "*Nano-mechanics of carbon tubes: Instabilities beyond linear response*", *Physical Review Letters 76 (1996) 2511-2514.*
[4].   X. Chen, C. Cao, "*A structural mechanics study of single-walled carbon nanotubes generalized from atomistic simulation*", *Nanotechnology 17 (2006) 1004-1015.*
[5].   F. Scarpa, S. Adhikari, C. Remillat, "*The bending of single layer graphene sheets: the lattice versus continuum approach*", *Nanotechnology 21 (2010) 125702.*
[6].   E. I. Saavedra Flores, S. Adhikari, M. I. Friswell, F. Scarpa, "*Hyper elastic finite element model for single wall carbon nanotubes in tension*", *Computational Materials Science 50 (2011) 1083-1087.*
[7].   E. A. de Souza Neto, D. Peric, D. R. J. Owen, "*Computational Methods for Plasticity: Theory and Applications*", Wiley: Chichester, 2008.
[8].   J. Lemaitre, J. L. Chaboche, "*Mechanics of Solid Materials*", Cambridge University Press, Cambrige, 1990.
[9].   R. W. Ogden, "*Non-linear elastic deformations*", Chichester: Ellis Horwood, 1984.
[10].   E. I. Saavedra Flores, S. Adhikari, M. I. Friswell, F. Scarpa, "*Lattice hyper elastic finite element approach for axial buckling of single wall carbon nanotubes*", *Submitted for publication.*
[11].   ABAQUS, Theory manual. Version 6.4, Hibbitt, Karlsson and Sorensen, Inc., Rhode-Island. USA, 2002.
[12].   A. Leung, X. Guo, X. He, H. Jiang, Y. Huang, "*Post buckling of carbon nanotubes by atomic-scale finite element*", *Journal of Applied Physics 99 (2006) 124308.*
[13].   D. Brenner, O. Shenderova, J. Harrison, S. Stuart, B. Ni, S. Sinnott, "*A second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons*", *Journal of Physics: Condensed Matter 14 (2002) 783.*