PAPER REF: 4032

MODELLING OF BUCKLING OF SINGLE-WALLED CARBON NANOTUBES BASED ON COSSERAT SURFACE THEORY

Yu Zhang[1(*)], Carlo Sansour[2], Chris Bingham[1]
[1]School of Engineeing, University of Lincoln, Lincoln, U.K.
[2]Department of Civil Engineering, University of Nottingham, Nottingham, U.K.
[(*)]*Email:* yzhang @lincoln.ac.uk

ABSTRACT

This paper studies the mechanical properties of single-walled carbon nanotubes (SWCNTs) under compression. The Cauchy-Born rule is applied to link the deformation of atom lattice vectors at the atomic level with the material deformation at a macro continuum level. SWCNTs are modelled as Cosserat surfaces, and modified shell theory is adopted where a displacement field-independent rotation tensor is introduced, which describes the micro-rotation. Empirical interatomic potentials are employed and a finite element approach is implemented. Results of simulations for SWCNTs under compression are presented. In addition, critical buckling strains for SWCNTs are predicted in this paper.

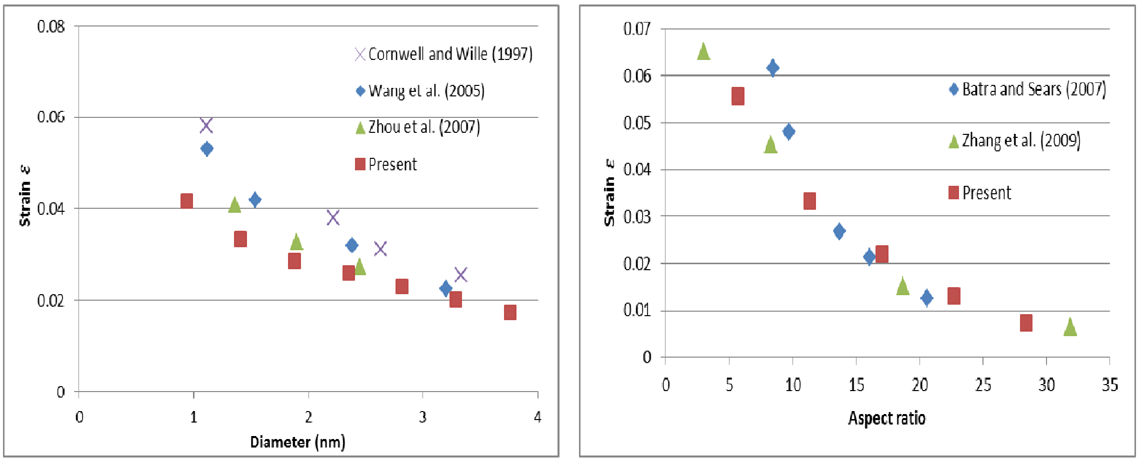
Keywords: single-walled carbon nanotube, Cauchy-Born rule, Cosserat surface theory, empirical interatomic potential, critical buckling strains.

INTRODUCTION

The mechanical properties of single-walled carbon nanotubes (SWCNTs) have been studied worldwide by scientists and engineers. However, a robust, theoretically precise and computationally efficient prediction method has not yet been found. Continuum shell theory has been applied extensively to model SWCNTs (Arroyo, 2004). They pointed out that a modification of the standard Cauchy-Born to applications for modelling CNTs as shells needs to be established. In this paper, an alternative way of modifying the standard Cauchy-Born rule is investigated. A shell theory based on two-dimensional Cosserat continua is presented to model SWCNTs following the work of (Sansour, 1995). A displacement field-independent rotation tensor is introduced to describe the micro-level rotation, which also makes up for the shortcomings of the standard Cauchy-Born rule, and can take size-effects into account. The main idea of the method is to consider SWCNT as a two-dimensional manifold and to solve it with the Cosserat surface theory. The deformation can be described by a stretch tensor and a rotation tensor. Responding to external force, the surface deforms providing a force stress field and a couple stress field. In order to solve for these four fields to describe the material mechanical properties, one needs to identify the right potential forms that are adequate at an atomistic level and applicable for continuum formulations. Empirical functions of potentials (Brenner, 2002) are adopted which are practical and appropriate to describe the total potential of SWCNTs relatively accurately. The finite element formulation is developed on the basis of variational principles. The stress fields and the modulus fields can thus be calculated via iteration procedures by updating displacement fields and rotation fields. By the cylinder shell model based on Cosserat surface theory, buckling patterns of SWCNTs are simulated, and the critical buckling strains are investigated.

RESULTS AND CONCLUSIONS

Through Cosserat surface theory, buckling of SWCNTs are simulated, and the critical buckling strains of SWCNTs are investigated. Variations of critical strain with respect to tube diameter are compared in Fig. 1(a) with results from three other authors all of which obtained from atomistic simulations. Fig. 1(b) demonstrates the critical buckling strain with respect to aspect ratio.



(a) (b)

Fig. 1 - Prediction of critical buckling strains of SWCNTs with respect to: (a) tube diameter; (b) aspect ratio.

The results obtained are in good agreement with the literature, and it is shown that shell model based on Cosserat Surface theory is capable of simulating the mechanical properties of SWCNTs.

REFERENCES

[1]-Arroyo, M., Belytschko, T. Finite element methods for the non-linear mechanics of crystalline sheets and nanotubes. International Journal for Numerical Methods in Engineering, 2004, 59, p.419-456.

[2]-Sansour, C., Bednarczyk, H. The Cosserat surface as a shell model, theory and finite-element formulation. Computer Methods in Applied Mechanics and Engineering, 1995, 120 (1-2), p.1-32.

[3]-Brenner, D.W., Shenderova, O.A., Harrison, J.A., Stuart, S.J., Ni, B., Sinnott, S.B. A second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons. Journal of Physics: Condensed Matter, 2002, 14, p.783-802.

[4]-Zhou, L., Zhu, B.E., Pan, Z.Y., Wang, Y.X., Zhu, J. Reduction of the buckling strength of carbon nanotubes resulting from encapsulation of C60 fullerenes. Nanotechnology, 2007, 18, p.27-35.

[5]-Zhang, Y.Y., Wang, C.M., Duan, W.H., Xiang, Y. Zong, Z. Assessment of continuum mechanics models in predicting buckling strains of single-walled carbon nanotubes. Nanotechnology, 2009, 20, p.707-714.