A HYPOELASTIC CONSTITUTIVE MODEL FOR GRAPHENE AND CARBON NANOTUBES BASED ON INTERATOMIC INTERACTIONS

D. Jasińska

Institute of Structural Mechanics, Cracow University of Technology, Cracow, Poland

e-mail: djasinska@pk.edu.pl

1. Introduction

Several continuous hyperelastic theories have been proposed for the description of mechanical properties of graphene and carbon nanotubes, based on interatomic potentials [1], [2], [3] or calibrated from existing quantum data [4]. In the present paper the hypoelastic constititutive model is proposed for modeling of the mechanical behavior of graphene sheets and CNT under the assumption of large displacements but small strains. The model is based on the modified Cauchy-Borne rule with the introduction of inner relaxation, and directly incorporates potentials describing interatomic interactions accounting for the multi-body effects through terms depending on angles between bonds.

2. Materials and methods

Unlike the molecular dynamics simulations, where the motion of every atom is tracked, the continuum theories based on molecular statics represent the collective behavior of atoms through the constitutive model. Since graphene is a non-centrosymmetric atomic structure, the internal atom of the representative unit cell (Fig.1) doesn‘t follow the homogenous deformation of the cell edges. Hence the Cauchy_Borne hypothesis, bridging molecular and continuous scales, has to be augmented with an additional internal degree of freedom: the vector parameter describing this internal inhomogenity [1].

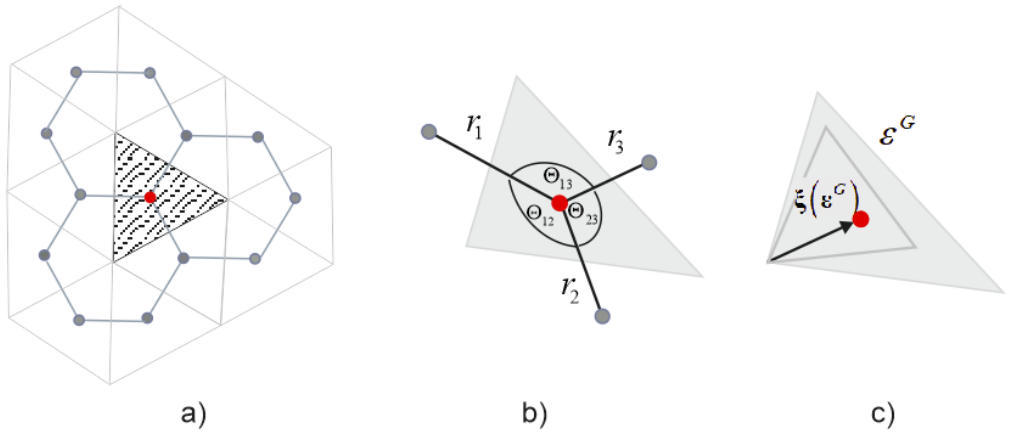

Fig.1 a) undeformed graphene lattice, b) deformed representative cell as function of intermolecular distances and angles, c) deformed representative cell as function of strain tensor and internal vector parameter

The internal energy of the representative cell U^a, depending on bond lengths and interbond angles, resulting from the applied atomistic multibody potential is equated to the strain energy of the equivalent hyperelastic continuum U^e depending on the Green strain tensor $\boldsymbol{\varepsilon}^G$ and the internal vector parameter $\boldsymbol{\xi}$.

(1) $$U^a\left(r_1, r_2, r_3, \Theta_{12}, \Theta_{13}, \Theta_{23}\right) = U^e(\boldsymbol{\varepsilon}^G, \boldsymbol{\xi})$$

For a given strain state, the internal degree of freedom is determined by minimizing the cell strain energy, which leads to a nonlinear implicit equation system which is solved numerically

(2) $$\frac{\partial U^e(\boldsymbol{\varepsilon}^G, \boldsymbol{\xi})}{\partial \boldsymbol{\xi}} = 0 \rightarrow \boldsymbol{\xi} = \boldsymbol{\xi}\left(\boldsymbol{\varepsilon}^G\right)$$

Restricting further analysis to small strains (while maintaining the large displacements assumption), allows for proposing the hypoelastic model, in which the rate of change of stress is defined as

$$d\sigma = D(\varepsilon) : d\varepsilon, \tag{3}$$

where $d\varepsilon$ is the rate of change of infinitesimal elastic strains and $D(\varepsilon)$ is the tangent stiffness matrix calculated as

$$D(\boldsymbol{\varepsilon}) = \frac{\partial^2 U^e(\boldsymbol{\varepsilon})}{\partial \boldsymbol{\varepsilon} \partial \boldsymbol{\varepsilon}} \tag{4}$$

The dependence of the elasticity tensor (4) on the deformation state is analyzed for two interatomic multibody potential types: Tersoff-Brenner and modified Morse.
The restriction placed upon the strain size, which obviously limits model applicability range, allows for proposing the hypoelastic orthotropic or even isotropic model. The elastic moduli can be expressed directly as functions of strain invariants in the tabular form. Such tables are compiled for both discussed interatomic potentials. The advantages of such a formulation are: the possibility of implementing this model in any advanced finite element code without the necessity of developing own numerical procedures describing material constitutive behavior, and a significant reduction of the computation time, since equation (2) can be approximated as the polynomial function of infinitesimal strains, and there is no need to solve it numerically for each consecutive deformation state in every finite element.

3. Results

The proposed hypoelastic model is applied to the FEM analysis of the behaviour of graphene sheets and CNT of different chiralities under stretching bending and torsion. The results are compared with those obtained by the atomic-scale finite element method [5] which is based directly on molecular mechanics, can handle discrete atoms and takes into account the multibody interactions. Calculations were performed by means of the FEM code Abaqus.

4. Conclusions

The results of numerical tests prove the effectiveness of the proposed model. The explicit tabular dependence of Young's modulus and Poisson's ratio on the strain invariants allows for its straightforward application in many standard FEM codes, for instance in numerical simulations of nanocomposites or multiscale analysis.

Acknowledgments The research was supported by Pl-grid Infrastructure.

References

[1] P.Zhang, H.Jiang,Y.Huang, P.H.Geubelle and K.C.Hwang. An atomistic-based continuum theory for carbon nanotubes: analysis of fracture nucleation. *J.Mech.Phys.Solids*, 52: 977,2004.
[2] M.Aroyo and T. Belytschko,, An atomistic-based finite deformation membrane for single layer crystalline films, *J.Mech.Phys.Solids*, 50:1941, 2002.
[3] Q. Dong, Z. Qingjin, R.S. Ruoff. Multiscale simulation of nanostructures based on spatial secant model: a discrete hyperelastic approach. Comput Mech, 42:557, 2008.
[4] R.Gharffari and R.A.Sauer. A new efficient hyperelastic finite element model for graphene and its application to carbon nanotubes and nanocones,arXiv:1802.09825v1, 2018
[5] B.Liu,Y.Huang,H. Jiang, S.Qu,K.C.Hwang. The Atomic Scale finite element method.*Comp.Methods App.Mech.Eng,* 193,17-20:1849, 2004.