HOMOGENIZED ELASTIC PROPERTIES OF GRAPHENE FOR LARGE DEFORMATIONS

Eduard Marenić[1*], Jurica Sorić[1] and Adnan Ibrahimbegovic[2]

[1] Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Ivana Lučića 5, 10000 Zagreb, Croatia, {eduard.marenic, jurica.soric}@fsb.hr
[2] Ecole Normale Supérieure de Cachan, Lab. of Mechanics and Technology, 61 avenue du Président Wilson, 94230 Cachan, France, adnan.ibrahimbegovic@ens-cachan.fr

Key words: *Graphene, molecular mechanics, atomistic-to-continuum modelling, Cauchy-Born rule.*

Graphene [1] is the name given to a flat monolayer of carbon atoms tightly packed into a two-dimensional honeycomb lattice, thus often abbreviated as Single Layer Graphene Sheet (SLGS). Its discovery started a real revolution related to the graphene-based materials and devices due to its remarkable properties [2]. However, prior to the practical usage of these novel materials, a good knowledge of their mechanical properties and ability to model their performance is needed. The main challenge is that parts of graphene-based devices modelled with discreet models such as molecular mechanics (MM) typically contain extremely large number of particles, even though the actual physical dimension may be quite small. Thus, we reach for a substitute, continuum model which simulates the average behaviour of atomic system. Equivalent continuum, *i.e.*, hierarchical atomistic-to-continuum modelling of large deformations of SLGS goes beyond what linear theory can handle [3]. We seek to adopt the nonlinear membrane theory which includes, as a special case, the hyperelastic model in terms of strain energy density (SED), W, as a function of principal stretches $W(\lambda_1, \lambda_2)$. This is an elegant alternative for the construction of the elastic constitutive response that satisfies the material indifference and isotropy restrictions, and which was often used to characterise rubberlike materials, see [4].

In order to construct SED potential $W_{\text{fit}}(\lambda_1, \lambda_2)$, we determine the equilibrium potential energy of atomistic system driven by modified Morse potential [5] for the series of biaxial loading cases. These loading cases are designed to form the uniform grid in the space of λ_1, λ_2 resulting with the cloud of points shown as dots in Fig. 1 (right). These results are further used to perform a polynomial surface fitting given as

$$W_{\text{fit}}(\lambda_1, \lambda_2) = \sum_{i}^{n} \sum_{j}^{n} a_{ij} \lambda_1^i \lambda_2^j, \tag{1}$$

where i and j are the the degree in λ_1 and in λ_2, respectively. With this result in hand, we can calculate the second Piola-Kirchhoff stress tensor ($\boldsymbol{S}$) and the elastic tangent modulus
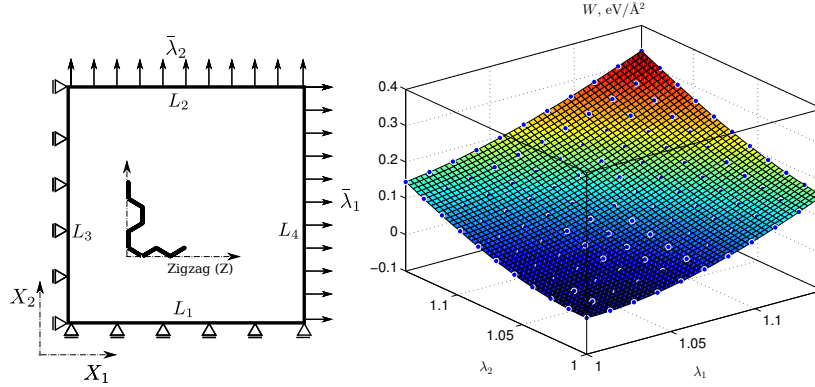
Figure 1: Scheme of the lattice sample with symmetry BCs used for biaxial tensile tests. The envelope of the sample is composed of lines L_1 to L_4 which coincides with boundary atoms (left). The polynomial surface fit W of SED obtained by series of biaxial tests performed by molecular mechanics simulation.

($\mathbb{C}$) in a closed form, see (2). Note that the matrix representations of these results can

$$\boldsymbol{S} := \sum_{i=1}^{2} \underbrace{\frac{1}{\lambda_i} \frac{\partial W(\lambda_1, \lambda_2)}{\partial \lambda_i}}_{s_i} \mathbf{n}_i \otimes \mathbf{n}_i \qquad \mathbb{C} := 2 \sum_{i=1}^{2} \frac{\partial s_i}{\partial \boldsymbol{C}} \mathbf{n}_i \otimes \mathbf{n}_i + 2 \sum_{i=1}^{2} s_i \frac{\partial}{\partial \boldsymbol{C}} (\mathbf{n}_i \otimes \mathbf{n}_i) \quad (2)$$

further be directly used for the calculation of the internal force vector and the element tangent stiffness matrix of the standard 2D large displacements elastic membrane finite element. Moreover, this procedure obviates the Cauchy-Born (CB) rule (common link between atomistic and continuum scales) to be valid, and we plan to confront this approach based on the numerical homogenization procedure with the CB based approach from [6].

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