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 $\lambda_1, \lambda_2$ 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

$$W_{\text{fit}}(\lambda_1, \lambda_2) = \sum_i \sum_j a_{ij} \lambda_1^i \lambda_2^j,$$

where $i$ and $j$ are the the degree in $\lambda_1$ and in $\lambda_2$, respectively. With this result in hand, we can calculate the second Piola-Kirchhoff stress tensor ($\mathbf{S}$) 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.

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

$$S := \sum_{i=1}^{2} \frac{1}{\lambda_i} \frac{\partial W(\lambda_1, \lambda_2)}{\partial \lambda_i} n_i \otimes n_i$$

$$C := 2 \sum_{i=1}^{2} \frac{\partial s_i}{\partial C} n_i \otimes n_i + 2 \sum_{i=1}^{2} s_i \frac{\partial}{\partial C} (n_i \otimes n_i)$$

(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].

REFERENCES


