Annie Raoult

A discrete homogenization technique for graphene sheets

This is joint work with Denis Caillerie and Ayman Mourad.

Graphene sheets are made of carbon atoms that remain located at the vertices of hexagonal rings. The hexagons generated by a deformation are neither necessarily planar, nor isometric to one another. But all atoms can be identified with the vertices of a planar network of regular hexagons with equal side length. The smallness of the length at rest - 0.14 nm - leads us to use a discrete homogenization technique in order to replace the lattice by an equivalent continuous medium.

It is easily seen that a hexagonal lattice can be covered by translating an elementary Y-shaped pattern made of three segments (or atomic bonds) and of two nodes (or carbon atoms). For modeling the whole of this discrete structure, we use in this talk a simple energetic model (more complicated energies such as the Tersoff-Brenner functional can be used as well). The internal energy contains a term that accounts for the changes of length between adjacent atoms and another term that accounts for angle variations between adjacent bonds. The equilibrium is modelized by a minimization problem in terms of the deformed positions of all carbon atoms.

The Euler-Lagrange equation of this problem is equivalent to the equilibrium system in a large deformation framework of a set of elastic bars that interact by means of moments. This is an algebraic system, not a differential system. By using the homogenization technique that we set up for the modeling of the myocardial tissue, we obtain the equilibrium equation of the equivalent continuous medium. This is a system of three partial differential equations that makes apparent what the equivalent macroscopic stress vectors are. Then we identify the macroscopic constitutive law that we are searching for: with any 3x2 matrix, that stands for the gradient of a macroscopic deformation, we have to associate two stress vectors. Obtaining this pair of vectors requires solving an implicit equation which is the so-called self-equilibrium equation of the reference pattern. This equation whose unknown is a vector can be seen as the Euler-Lagrange equation of an energy defined on the reference pattern and existence follows. The obtained model is a nonlinear membrane model.

Linearizing the above nonlinear membrane problem around a uniformly extended state gives rise, as in similar settings, to a linear membrane problem. The simple geometric structure of the lattice allows to compute explicitly all equivalent material constants in terms of microscopic data.

For a graphene sheet which undergoes deformations that remain planar, we obtain by linearizing around the identity a bidimensional elasticity model and we compare equivalent material constants (Young's modulus and Poisson's ratio) with experimental values.

[1] N.L. Allinger, Y.H. Yuh, J.H. Lii, Molecular mechanics. The MM3 force field for hydrocarbons, *J. Am. Chem. Soc.* **111** (1989), 8551-8566.

[2] D. Caillerie, A. Mourad, A. Raoult, Cell-to-muscle homogenization. Application to a constitutive law for the myocardium, *M2AN Math. Model. Numer. Anal.* **37** (2003), 4, 681-698.

[3] B.I. Yakobson, C.J. Brabec, J. Bernholc, Nanomechanics of carbon tubes; Instabilities beyond linear response, *Phys. Rev. Lett.* **76** (1996), 2511-2514.

[4] X. Zhou, J. Zhou, Z. Ou-Yang, Strain energy and Young's modulus of single-wall carbon nanotubes calculated from electronic energy-band theory, *Phys. Rev. B* **62** (2000), 13692-13696.