NANOMECHANICS OF GRAPHENE AND ITS CHEMICAL DERIVATIVES

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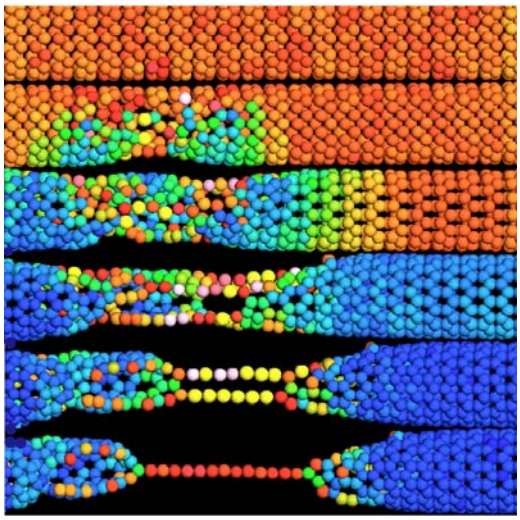
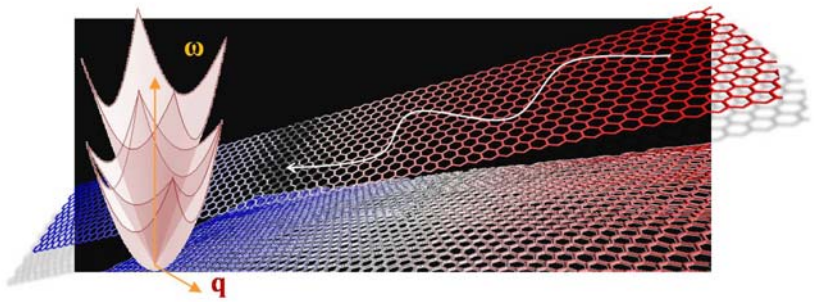
Introduction

A honeycomb lattice of covalently bonded carbon atoms in sp^2-states was called *graphene* because it was initially obtained by peeling of a mono-atomic layer of common graphite—of of the basic carbon allotropes. Graphene emerged initially due to its unique physical properties: as ideal material carrier of 2-dimensional electron gas, with zero band-gap and a particular linear dispersion characteristic for relativistic electrons. Its mechanical properties, initially secondary, now attract growing attention as well. Carbon lattice is known for its strength, especially from the studies of nanotubes: it can sustain ~20% strain before failure, which is accompanied by fascinating pullout of mono-atomic chains of the so called *carbynes*, $[\ldots\text{-C}\equiv\text{C-}\ldots]_n$., as in the early simulations [1], figure 1. Here we discuss mechanics at three levels: low-energy elastic deformations where the shell-models are applicable; mid-energy defects and grain boundaries, and the "higher-energy" chemical modifications when a covalent component is added to form graphane CH, graphene-oxide $C_{1-x}O_x$, fluorinated graphene CF, or even chemically different but structurally similar "white graphene" BN.



Elastic mechanics

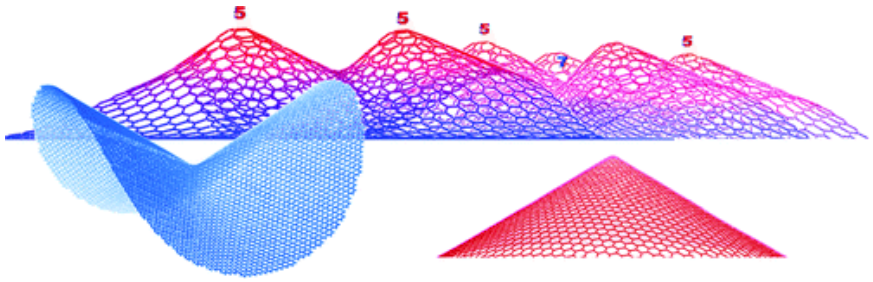
Hexagonal 2D-crystal must be isotropic in linear elastic behavior, and characterized by two basic parameters, in-plane rigidity C and bending stiffness D. In case of graphene, C = 350 N/m can be obtained by *ab initio* methods, and agrees with the graphite Young's modulus, while D = 1.4 eV can also be obtained from the first-principles (e.g. DFT-based) computations and is on accord with the speed of sound values [2]. More special calculations (due to lack of experimental data) should be performed for other compositions and yield the values C = 245 N/m and D = 2.2 eV for graphane CH, and C = 228 N/m and D = 6.3 eV for fluorinated CF. One can also list the values for BN-sheet, C = 270 N/m and D = 3.6 eV. General trend can be easily seen that the functionalization reduces the in-plane rigidity but increases the bending stiffness. In other words, it "softens" the constituent material but increases the effective thickness. In spite of great interest to graphene-oxides [3], we cannot presently quantify this material due to lack of unique composition and certainly variable morphology of oxygen-groups attachments. Besides the infinite sheet basics, the edge warping and twist instabilities caused by the stress from the dangling bonds have also been explored [4].



One interesting extension of the elastic nanomechanics is the ability to quantitatively model *thermal transport* [5]. The underlying reason for that is simple: all these lattices are rigid and therefore thermal motion essentially does not agitate any optical phonons (where neighboring atoms would move out

of phase, which costs high energy), but all are limited to the long-wave acoustic phonons, and can be described by continuum shell model with just two parameters, C and D. As a result, we could recently calculate the dispersion laws for all four branches of sound in graphene ribbons, as shown in the figure 2. Following this, quantization of the eigenmodes-oscillators leads to rather accurate theory of ballistic thermal conductivity (that is with no scattering accounted for).

Inelastic structural defects



Next level of deformations must include formation of irreversible defects, and here of particular interest are the *disclinations* such as pentagons "5" or heptagons "7", or their combinations as dislocation cores "5/7". Furthermore, in recent work [6] we have explored how these constituent defects define the morphology and energy of the natural *grain boundaries* in graphene (lines separating the domains of different lattice orientations). Analysis shows that 5-pentagon induces a cone in the lattice, 7-heptagon induces a pringle-shaped buckling, while their distribution in the lattice and especially near the grain boundaries can cause stable intricate landscapes, one computed example shown in the figure 3.

2D-composites electronics

Beyond mechanical properties, functionalization of graphene changes its electronic properties, generally from metallic to insulating. This leads to the tantalizing possibilities of pattern-engineering where linear (interconnects) or confined islands (quantum dots) can be built into the same 2D-material and together form a circuit of useful functionality. In particular, we have recent demonstrated possibility of such nanoroads and quantum dots [7], well defined domains of pure graphene inclusions into the insulating host material (CH, CF, or BN), as figure 4 illustrates for a graphene quantum dot (QD).

References

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