SEMINAIRE ISMO

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Investigating the structure-property relationship of disordered carbons with atomistic simulations

Owing to recent theoretical developments and to the increasing capabilities of modern computers, computer simulations are on the ways of becoming routine tools for the investigation of structure-property relationships in solid state and materials science. Unlike other materials like minerals, which are generally either found under crystalline or amorphous (glass) states, the versatility of the C-C bond (sp, sp^2, sp^3, aromatic, aliphatic, etc...) implies that a lot of carbonaceous materials are found in partially (dis-)ordered states. This is particularly the case of industrially relevant carbons, like carbon-fibers, carbon/carbon (C/C) composites, nuclear graphite or even some synthetic graphene. Using atomistic simulations to investigate such materials requires (i) some accurate reactive interatomic potentials able to deal with large systems (> 10^4 atoms), (ii) a reconstruction procedure able to determine structural models based on experimental input, and (iii) a suited simulation strategy to determine the properties of interest.

In this talk I will present a reconstruction strategy that we have proposed some years ago to build structural models of anisotropic (i.e. disordered graphitic) carbons based on information collected from high-resolution transmission electron microscopy. This image guided atomistic reconstruction (IGAR) method has been used to investigate the structural features of some pyrocarbon matrices (constituents of C/C composites), of irradiated graphite and polycrystalline graphene. I will then discuss the relationships between the nanoscale structure of these materials and their corresponding mechanical (elasticity and fracture) and thermal properties as well as the behavior of graphite under irradiation.

Mardi 19 juin 2018 à 11 h
Amphithéâtre du bât 520 (3ème étage)
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