Séminaire de Francesca BOIOLI

Laboratoire d'Étude des Microstructures (CNRS-ONERA)

Lundi 18 février 2019 à 14h

Salle 4-014 (zone A), Institut Jean Lamour, Campus Artem

Defects and plasticity across the scales

Bridging the gap between atomic scale properties and macroscopic behavior

Plasticity in crystals, as well as in amorphous solids, is a complex phenomenon involving several physical mechanisms emerging at different scales. A multiscale modeling approach is thus highly desirable to capture such complexity. In this respect, I will present few examples of simulations aiming at bridging the gap between atomic scale properties and macroscopic plastic behavior.

In the case of crystalline solids, particular interest has been dedicated to dislocations, because these defects govern the crystal ability to flow and yield under stress, as well as many other mechanical, optical and electrical properties. The development of Dislocation Dynamics (DD) at the mesoscale, technique designed to bridge the gap between atomic scale dislocation properties and continuum models of plasticity, has been a major step forward in the development of such multiscale strategies. To demonstrate the strength of this approach, we show how, by using atomically informed DD simulations, it is possible to predict, for example, dislocation patterning in semiconductors and creep behavior of relevant mineral phases, in agreement with experimental observation. We present also a more recent development of DD coupled with a Fast-Fourier-Transform elastic solver, which represent a very promising technique to increase the length and time scale reached by DD simulations.

The deformation of amorphous solids involves instead, local rearrangements of small clusters of atoms. The occurrence and organization of these plastic events, called Shear Transformations (STs) has a strong impact on strain localization and, as a consequence, on the mechanical properties of this class of materials. Several mesoscale models based on STs have been proposed, still the fundamental mechanisms underlying ST occurrence and organization are not yet clear. To this aim, we characterize STs from the atomic scale and we address the effect of pressure on the ST characteristics, particularly their size and plastic strain. Furthermore, we investigate the dynamic process of ST formation, determining the characteristic time involved in the development of STs and the influence of the strain rate on the STs distribution and organization. The bottom-up approach presented gives access to relevant parameters employed in mesoscale models aimed at describing the mechanical properties of amorphous solids.

Séminaire organisé par le Département Science et Ingénierie des Matériaux et Métallurgie.