IAP 2006: From nano to macro: Introduction to atomistic modeling techniques and application in a case study of modeling fracture of copper

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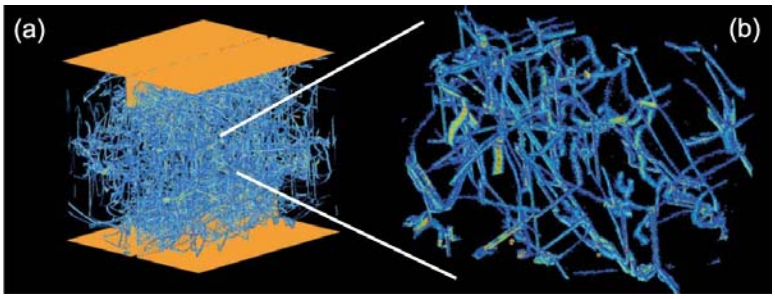
The objective is to introduce large-scale atomistic modeling techniques and motivate its importance for solving problems in modern engineering sciences. We demonstrate how atomistic modeling can be successfully applied to understand how materials fail under extreme loading, emphasizing on the competition between ductile and brittle materials failure. We will demonstrate the techniques in describing failure of a copper nano-crystal.



We offer lectures covering the theoretical and numerical basics associated with failure of materials. After the lectures, students will work on modeling fracture of a copper nano-crystal using atomistic simulation. Participants will learn the basics of atomistic modeling, including setting up the problem, choosing and using interatomic potentials, analysis and visualization of results. We will link our modeling results to continuum mechanics theories of fracture and dislocation plasticity. Animations of the failure processes will be generated. We will discuss limitations and potentials of atomistic modeling of fracture of materials.

All simulation codes and numerical tools will be explained in detail. The codes will be provided to participants. Both undergraduate and graduate students are encouraged to participate.

Course Schedule

Jan. 9 (Monday): Introduction to classical molecular dynamics: Brittle versus ductile materials behavior
Jan. 11 (Wednesday): Deformation of ductile ma terials like metals using billion-atom simulations with massively parallelized computing techniques
Jan. 13 (Friday): Dynamic fracture of brittle materials: How nonlinear elasticity and geometric confinement governs crack dynamics
Jan. 16 (Monday): Size effects in deformation of materials: Smaller is stronger
Jan. 18 (Wednesday): Introduction to the problem set: Atomistic modeling of fracture of copper
Jan. 18-Jan. 31: Lab assignment

The IAP activity can be taken for credit. Details will be posted on the IAP website (http://web.mit.edu/iap/). This course corresponds to 3 units.