1.978 From Nano to Macro: Introduction to Atomistic Modeling Techniques and Application in a Case Study of Modeling Fracture of Copper

IAP 2006

Lecturer

Markus J. Buehler
Department of Civil and Environmental Engineering, MIT
Tel: (617)452-2750
Fax: (617)258-6775
E-mail: mbuehler@MIT.EDU
Website: http://web.mit.edu/mbuehler/www/

Subject Summary

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.
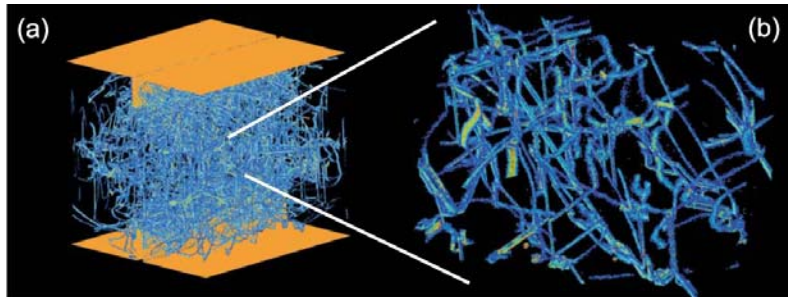
We offer lectures covering the theoretical and numerical basics associated with failure of materials. After the lectures, students will work on modeling fracture of a copper nano-crystal using atomistic simulation. Participants will learn the basics of atomistic modeling, including setting up the problem, 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.

Schedule

Jan. 9 (Monday): Introduction to classical molecular dynamics: Brittle versus ductile materials behavior *(basic concepts of MC/MD, interatomic potentials, failure dynamics of materials and brittle versus ductile behavior)*

Jan. 11 (Wednesday): Deformation of ductile materials like metals using billion-atom simulations with massively parallelized computing techniques *(geometry of dislocations,*

plasticity, dislocation nucleation and propagation, stacking fault, dislocation reactions, work hardening mechanisms, ultra-large scale computing)

Jan. 13 (Friday): Dynamic fracture of brittle materials: How nonlinear elasticity and geometric confinement governs crack dynamics *(dynamic fracture in brittle materials and the role of hyperelasticity, crack limiting speed, instability dynamics, cracks at interfaces)*

Jan. 16 (Monday): Size effects in deformation of materials: Smaller is stronger *(size effects in materials, Griffith criterion of fracture initiation, adhesion and size effects, shape optimization, fracture of protein crystals)*

Jan. 18 (Wednesday): Introduction to the problem set: Atomistic modeling of fracture of copper *(code compilation and usage, commands, pre- and post-processing)*

Course reference material

Research articles and additional lecture notes

- http://web.mit.edu/mbuehler/www/Teaching/IAP2006/intro.htm

Modeling and Simulation

- *Allen, M. P. and Tildesley, D. J., Computer Simulation of Liquids* (Oxford University Press, 1989)
- *Frenkel, D., Smit, B.* Understanding Molecular Simulation: From Algorithms to Applications

Mechanics of materials - Introductory

- *Courtney, T.H.* Mechanical Behavior of Materials, 2nd edition, McGraw Hill, 2000
- *Hull, D.* and Bacon D.J., Introduction to Dislocations, Butterworth Heinemann, 4th edition, 2001
- *Anderson, T. L.,* Fracture mechanics: Fundamentals and applications (CRC Press, 1991)

Advanced

- *Hirth J.P. and Lothe J.* Theory of dislocations, New York: McGraw-Hill.
- *Broberg, K.B.* Cracks and Fracture (Academic Press, 1990)
- *Ashby, M. F. and D. R. H. Jones.* Engineering Materials, An Introduction to their Properties and Application*s*. 2nd ed. Butterworth Heinemann, 1996

Grading

Project: 100% (PDF)