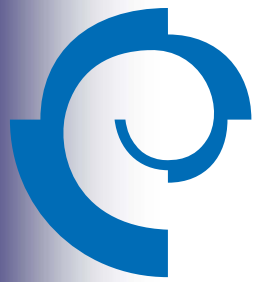
From nano to macro: Introduction to atomistic modeling techniques

IAP 2007

Introduction to Mechanics of Materials

Lecture 1



Department of
Civil & Environmental Engineering
Massachusetts Institute of Technology

Markus J. Buehler

Introduction – IAP Course

- Introduce large-scale atomistic modeling techniques and motivate its importance for solving problems in modern engineering sciences.
- Demonstrate how atomistic modeling can be successfully applied to understand dynamical materials failure of
  - Ductile materials
  - Brittle materials
  - Small-scale (“nano”-) materials – biological materials
- Focus on brittle and ductile materials behavior as well as mechanics of biological materials; provide introduction to hands-on procedure of atomistic modeling of fracture
- **Target group:** Undergraduate and graduate students

- **Goal:** After the class, students should have a basic understanding about the fundamentals, application areas and potential of classical molecular dynamics for problems in mechanics of materials. Particular emphasis is on developing a sensitivity for the significance of mechanics in different areas, and how atomistic and continuum viewpoints can be coupled.

Format

- Ca. 8 lectures ~90 minutes each, with time for discussion and questions
- Several smaller problem sets
- One lecture: Introduction to problem set
- Hands-on problem set (last part, project), introducing typical tasks in molecular modeling of fracture and deformation
  - Nanocrystal with crack under tension
  - Tensile test of a nanowire
  - Unfolding of a protein

Outline

1. **Introduction to Mechanics of Materials**
   Basic concepts of mechanics, stress and strain, deformation, strength and fracture
   Monday Jan 8, 09-10:30am
2. **Introduction to Classical Molecular Dynamics**
   Introduction into the molecular dynamics simulation; numerical techniques
   Tuesday Jan 9, 09-10:30am
3. **Mechanics of Ductile Materials**
   Dislocations; crystal structures; deformation of metals
   Tuesday Jan 16, 09-10:30am
4. **Dynamic Fracture of Brittle Materials**
   Nonlinear elasticity in dynamic fracture, geometric confinement, interfaces
   Wednesday Jan 17, 09-10:30am
5. **The Cauchy-Born rule**
   Calculation of elastic properties of atomic lattices
   Friday Jan 19, 09-10:30am
6. **Mechanics of biological materials**
   Monday Jan. 22, 09-10:30am
7. **Introduction to The Problem Set**
   Atomistic modeling of fracture of a nanocrystal of copper.
   Wednesday Jan 22, 09-10:30am
8. **Size Effects in Deformation of Materials**
   Size effects in deformation of materials: Is smaller stronger?
   Friday Jan 26, 09-10:30am

Course reference material

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)

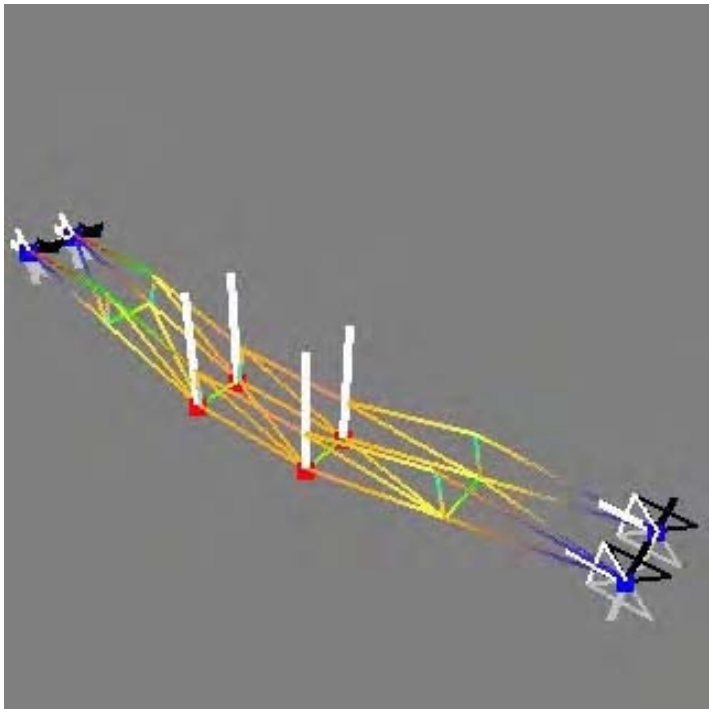
Advanced

- *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

Outline and content (Lecture 1)

- **Topic:** Introduction into basic concepts of mechanics; theoretical concepts of continuum theory
- **Examples:** Significance of mechanics of materials (deformation of membrane, car chassis, bridge,…)
- **Material covered:** Definition of elasticity, elastic response, energetic versus entropic elasticity, Young's modulus, stress and strain tensor, mechanics of a beam, nanomechanics
- **Important lesson:** The big challenge to couple atomistic, molecular or nano-scale with macro, as well as understanding the scales between "mesoscale"
- **Historical perspective:** The behavior of materials – theory, modeling and simulation as well as experiment

Mechanics of bridges



Courtesy of San Le. Used with permission.

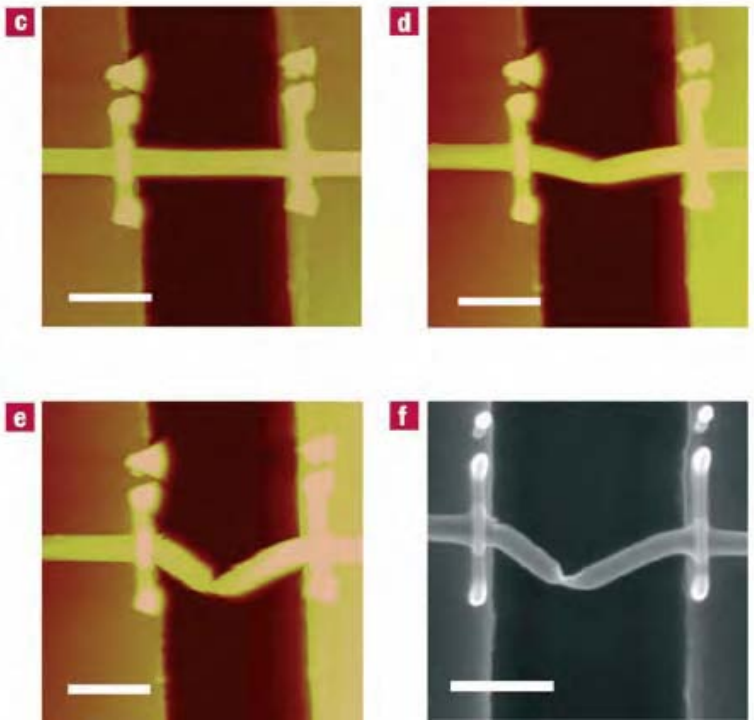
Courtesy of Pedro Albrecht. Used with permission.

http://www.geocities.com/Athens/2099/bridge.jpg
http://www.engr.umd.edu/~pedroalb/images/bridge_small.jpg

Deformation of materials: Significance of mechanics

Image removed due to copyright restrictions.
See http://www.gsi.gov.in/images/ex1.gif

Larger scale "earth" or soil mechanics



Small scale "nano"

Image removed due to copyright restrictions.
See http://www.arasvo.com/comp_figures/fig_wf3.htm

Bin Wu *et al.*, Nature Materials, 2005

Fig. 2 in Bin Wu, et al. "Mechanical properties of gold nanowires." Nature Materials 4 (2005): 525-529.
http://www.nature.com/nmat/journal/v4/n7/images/nmat1403-f2.jpg

Deformation of red blood cells

Image removed due to copyright restrictions.

See Fig. 5 in M. Dao et al. "Mechanics of the human red blood cell deformed by optical tweezers."

J. Mech. Phys. Solids 51 (2003): 2259 –2280.

http://www.mit.edu/~mingdao/movies/

Deformation of red blood cells

Image removed due to copyright restrictions.

See M. Dao et al. "Mechanics of the human red blood cell deformed by optical tweezers."

J. Mech. Phys. Solids 51 (2003): 2259 –2280.

http://www.mit.edu/~mingdao/movies/

Deformation of red blood cells

Image removed due to copyright restrictions.

See http://www.mit.edu/~mingdao/movies/

Single molecule mechanics

Image removed due to copyright restrictions.

See Fig. 1(f) in Tshkovrebova, L., et al.
"Elasticity and unfolding of single molecules of the giant muscle protein titin."
Nature 387 (1997): 308-312.

Image removed due to copyright restrictions

See Fig. 2 in Tshkovrebova, L., et al.
"Elasticity and unfolding of single molecules of the giant muscle protein titin."
Nature 387 (1997): 308-312.

Image removed due to copyright restrictions.

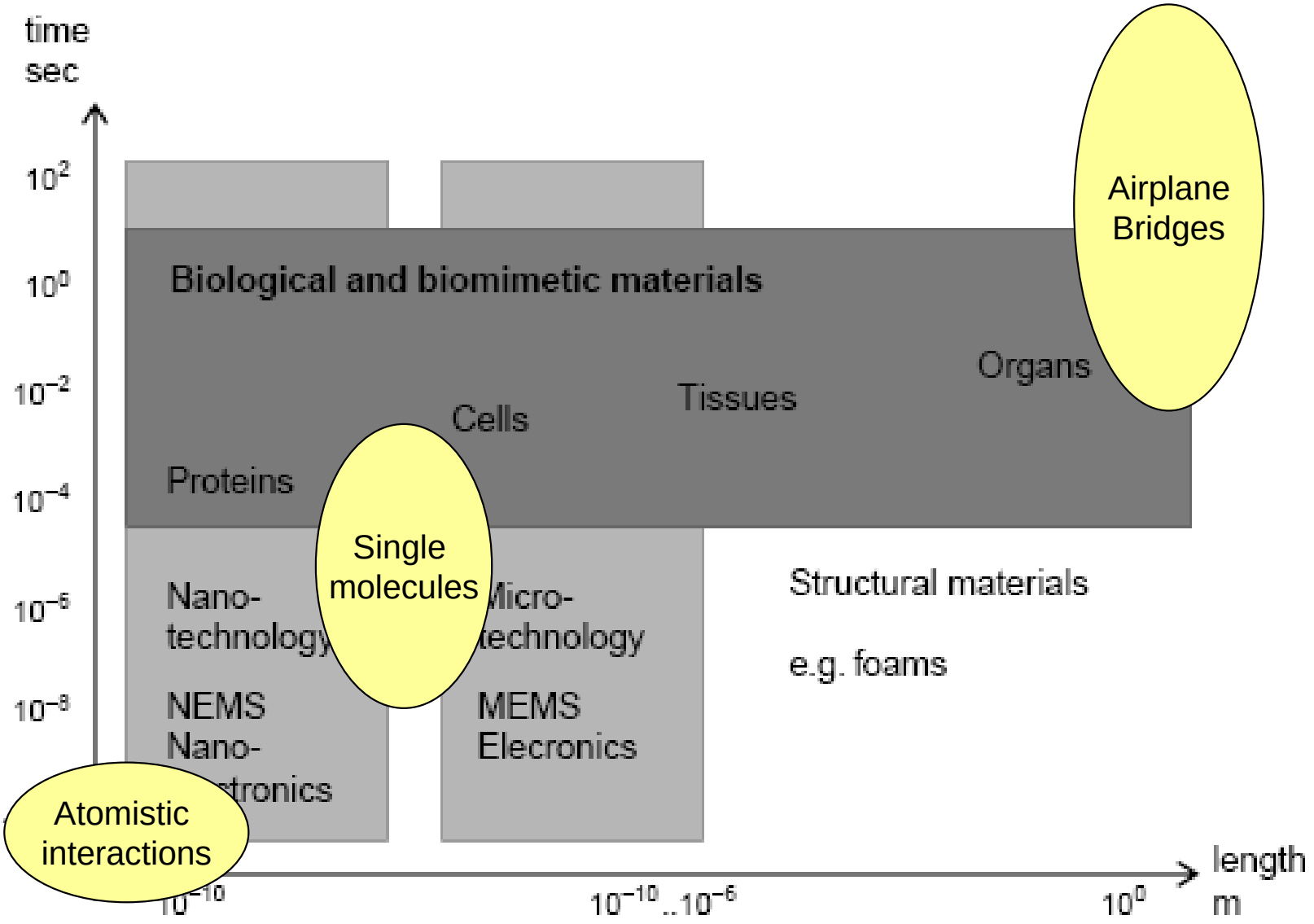
See Fig. 3(a) in Marszalek, Piotr E. et al.
"Mechanical unfolding intermediates in titin modules."
Nature 402 (1999): 100-103.

Image removed due to copyright restrictions

See Fig. 1 in Marszalek, Piotr E. et al.
"Mechanical unfolding intermediates in titin modules."
Nature 402 (1999): 100-103.

http://www.nature.com/nature/journal/v387/n6630/pdf/387308a0.pdf
http://www.nature.com/nature/journal/v402/n6757/pdf/402100a0.pdf

Scales in time and length…



Buehler and Gao, 2006

Scale coupling

Continuum mechanics

Images removed due to copyright restrictions.

Adhesion (does it stick)?

Interfaces?

Measure how soft/stiff it is

Images removed due to copyright restrictions.

Fracture?

Change at one scale-
influence on large scale properties?

Change of properties across scales

Images removed due to copyright restrictions.

Images removed due to copyright restrictions.

Chemistry

Physics

Challenges…

- Mechanics problems cover wide range of time and length scales (fs-hours, Angstrom to meters…)

- **Questions:** What methods can we use to measure properties at various scales, in an integrative way (i.e. connect different scales)?
  How can we model phenomena at different scales (physics based models, engineering models)?

  Further: How can we control structures or materials at each of these scales?
  What are the limitations today (e.g. can easily control micrometer, meter etc., but still in infancy is how to control atomic structure)

Historical perspective: Modeling of mechanics (behavior) of materials

- 1500-1600s: L. da Vinci, Galileo Galilei
  1700-1800: Euler, Bernoulli
  Beam theories, rods (partial differential equations, continuum theories)
- Continuum mechanics theories
- Development of theories of fracture mechanics, theory of dislocations (1930s)
- 1960..70s: Development of FE theories and methods (engineers)
- 1990s: Marriage of MD and FE via Quasicontinuum Method (Ortiz, Tadmor, Phillips) and others

Continuum

Atomistic

- 20th century: Atoms discovered (Jean Perrin)
- MD: First introduced by Alder and Wainwright in the late 1950's (interactions of hard spheres). Many important insights concerning the behavior of simple liquids emerged from their studies.
- 1964, when Rahman carried out the first simulation using a realistic potential for liquid argon (Rahman, 1964).
- Numerical methods like DFT (Kohn-Sham, 1960s-80s)
- First molecular dynamics simulation of a realistic system was done by Rahman and Stillinger in their simulation of liquid water in 1974 (Stillinger and Rahman, 1974).
- First fracture / crack simulations in the 1980s by Yip and others, 1990s Abraham and coworkers (large-scale MD)

- Now: MD simulations of biophysics problems, fracture, deformation are routine
- The number of simulation techniques has greatly expanded: Many specialized techniques for particular problems, including mixed quantum mechanical - classical simulations, that are being employed to study enzymatic reactions ("QM-MM") or fracture simulations (Kaxiras and others, Buehler and Goddard).

Outline

- Newton's laws: Basics for mechanics
- Elastic (reversible) and plastic (permanent) deformation of materials
- Stress and strain, Hooke's law
- Energy approach to elastic deformation
- Example: Beam bending
- Outlook: Permanent deformation

Newton's laws

- **First law**: An object in a state of rest or uniform motion tends to remain in that state of motion unless an external force is applied to it. That is, as long as the sum of forces acting it is zero

$$\mathbf{F} = \sum \mathbf{F}_i = 0, \tag{2.1}$$

the direction and magnitude of velocity of it does not change.

- **Second law**: The change of motion is proportional to the applied force to an object. That is,

$$\frac{\mathrm{d}(m\mathbf{v})}{\mathrm{d}t} = \mathbf{F}. \qquad \frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=1}^{N}(\mathbf{x}_i \times m_i\mathbf{v}_i) = \sum_{i=1}^{N}(\mathbf{x}_i \times \mathbf{F}_i) = \sum_{i=1}^{N}\mathbf{M}_i$$

For constant mass m, this law simplifies to

$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = m\mathbf{a} = \mathbf{F}, \tag{2.3}$$

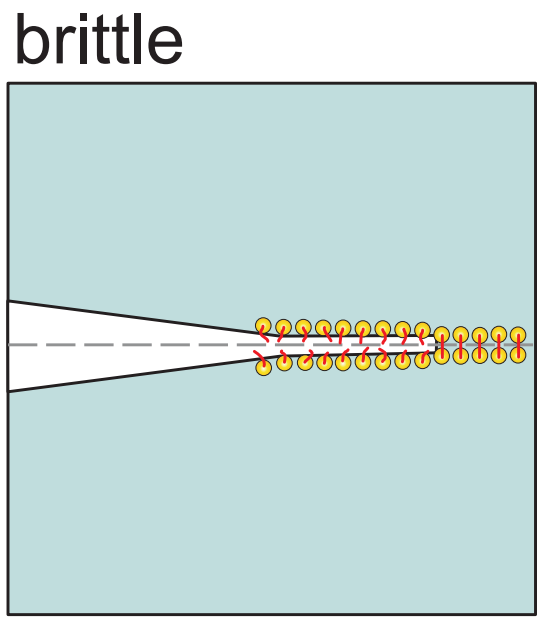
where $\mathbf{a}$ is the acceleration.

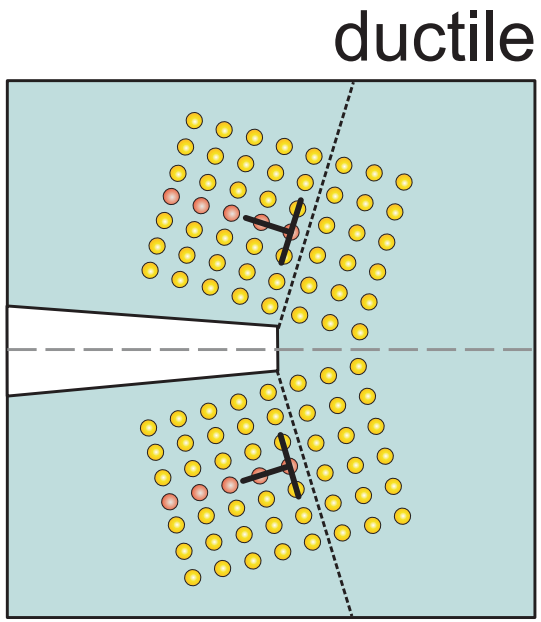
- **Third law**: To every action there is always a reaction with opposed direction. In other words, the mutual interaction of two bodies are always equal in magnitude, and directed contrary to each other. For two interacting particles, this implies that the mangitude of interaction $F_{ij} = F_{ji}$, and for the vectors

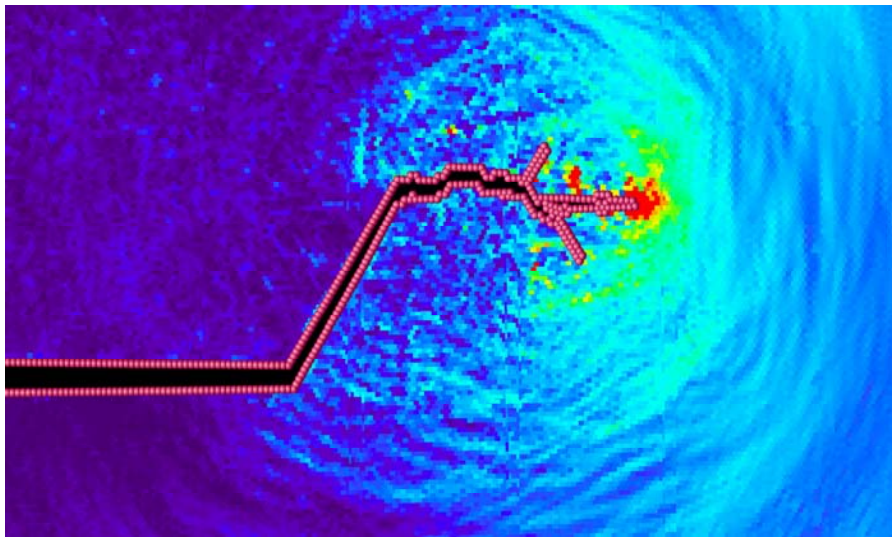
$$\mathbf{F}_{ij} = -\mathbf{F}_{ji}. \tag{2.4}$$

- See lecture notes

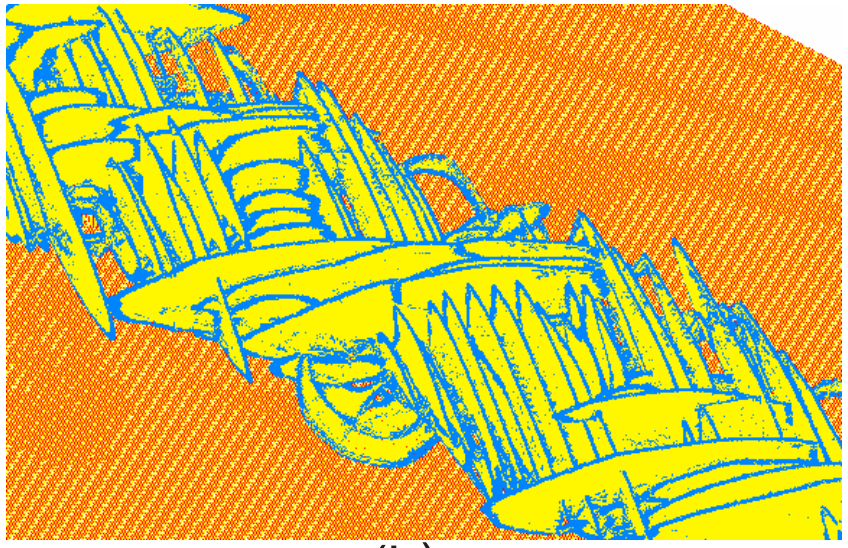
Ductile versus brittle materials







(a)



(b)

(Buehler, 2004)

Ductile versus brittle materials: Experiment

Images removed due to copyright restrictions.

Images removed due to copyright restrictions.

“brittle”
Separation long grain boundaries, Cleavage

“ductile”
Dislocations, material deformation (microscopic)

Ductile versus brittle materials: Experiment

Image removed due to copyright restrictions.

Image removed due to copyright restrictions.

See pp. 3-4 of http://people.virginia.edu/~lz2n/mse209/Chapter8.pdf

A. Very ductile, soft metals (e.g. Pb, Au) at room temperature, other metals, polymers, glasses at high temperature.
B. Moderately ductile fracture, typical for ductile metals
C. Brittle fracture, cold metals, ceramics.

Ductile fracture

(a) Necking,
(b) Cavity Formation,
(c) Cavity coalescence to form a crack,
(d) Crack propagation,
(e) Fracture

Image removed due to copyright restrictions.

See p. 5 of http://people.virginia.edu/~lz2n/mse209/Chapter8.pdf

Brittle fracture

- No appreciable plastic deformation

- Crack propagation is very fast
- Crack propagates nearly perpendicular to the direction of the applied stress

- Crack often propagates by cleavage – breaking of atomic bonds along specific crystallographic planes (cleavage planes).

Image removed due to copyright restrictions.

Image removed due to copyright restrictions.

See p. 7 of of http://people.virginia.edu/~lz2n/mse209/Chapter8.pdf

References

- http://www.ch.embnet.org/MD_tutorial/pages/MD.Part1.html
- Alder, B. J. and Wainwright, T. E. J. Chem. Phys. 27, 1208 (1957)
- Alder, B. J. and Wainwright, T. E. J. Chem. Phys. 31, 459 (1959)
- Rahman, A. Phys. Rev. A136, 405 (1964)
- Stillinger, F. H. and Rahman, A. J. Chem. Phys. 60, 1545 (1974)
- McCammon, J. A., Gelin, B. R., and Karplus, M. Nature (Lond.) 267, 585 (1977)
- D. Frenkel and B. Smit Understanding Molecular Simulations: from Algorithms to Applications, Academic Press, San Diego, 2nd edition (2002).
- M.J. Buehler, A. Hartmaier, M. Duchaineau, F.F. Abraham and H. Gao, “The dynamical complexity of work-hardening: A large-scale molecular dynamics simulation”, under submission to Nature.
- M.J. Buehler, A. Hartmaier, M. Duchaineau, F.F. Abraham and H. Gao, “The dynamical complexity of work-hardening: A large-scale molecular dynamics simulation”, MRS Proceedings, Spring meeting 2004, San Francisco.
- M.J. Buehler, A. Hartmaier, H. Gao, M. Duchaineau, and F.F. Abraham, “Atomic Plasticity: Description and Analysis of a One-Billion Atom Simulation of Ductile Materials Failure.” In the press: Computer Methods in Applied Mechanics and Engineering (to appear 2004).
- B. deCelis, A.S. Argon, and S. Yip. Molecular-dynamics simulation of crack tip processes in alpha-iron and copper. J. Appl. Phys., 54(9):4864–4878, 1983.

- See additional references & material on the website: http://web.mit.edu/mbuehler/www/Teaching/LS/lecture-1-supp.htm
- http://www.people.virginia.edu/~lz2n/mse209/