From nano to macro: Introduction to atomistic modeling techniques

IAP 2007

Introduction to Mechanics of Materials

Lecture 1

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Civil & Environmental Engineering
Massachusetts Institute of Technology

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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
- Course material posted on the website (introductiory papers, books, etc.)

Check for updates and supplementary material

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

Research articles and additional lecture notes

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)

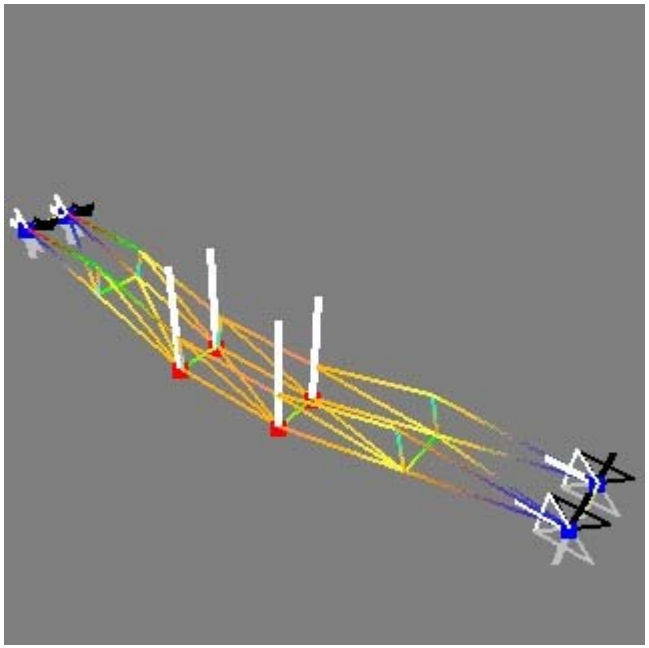
Advanced

- *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 Applications. 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.

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See http://www.engr.umd.edu/%7Epedroalb/images/bridge_small.jpg

http://www.geocities.com/Athens/2099/bridge.jpg

Deformation of materials: Significance of mechanics

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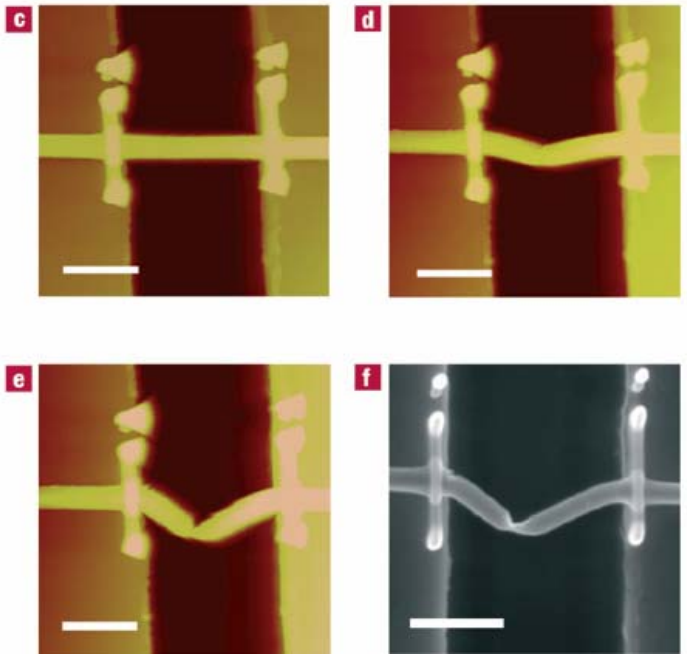
Larger scale
"earth" or soil
mechanics



Small scale
"nano"

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See http://www.arasvo.com/comp_figures/fig_wf3.htm

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

Image courtesy of Nature.
Fig. 2 in Bin Wu, et al. "Mechanical properties of ultrahigh-strength 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

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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/

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Deformation of red blood cells

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Single molecule mechanics

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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.

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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.

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

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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…

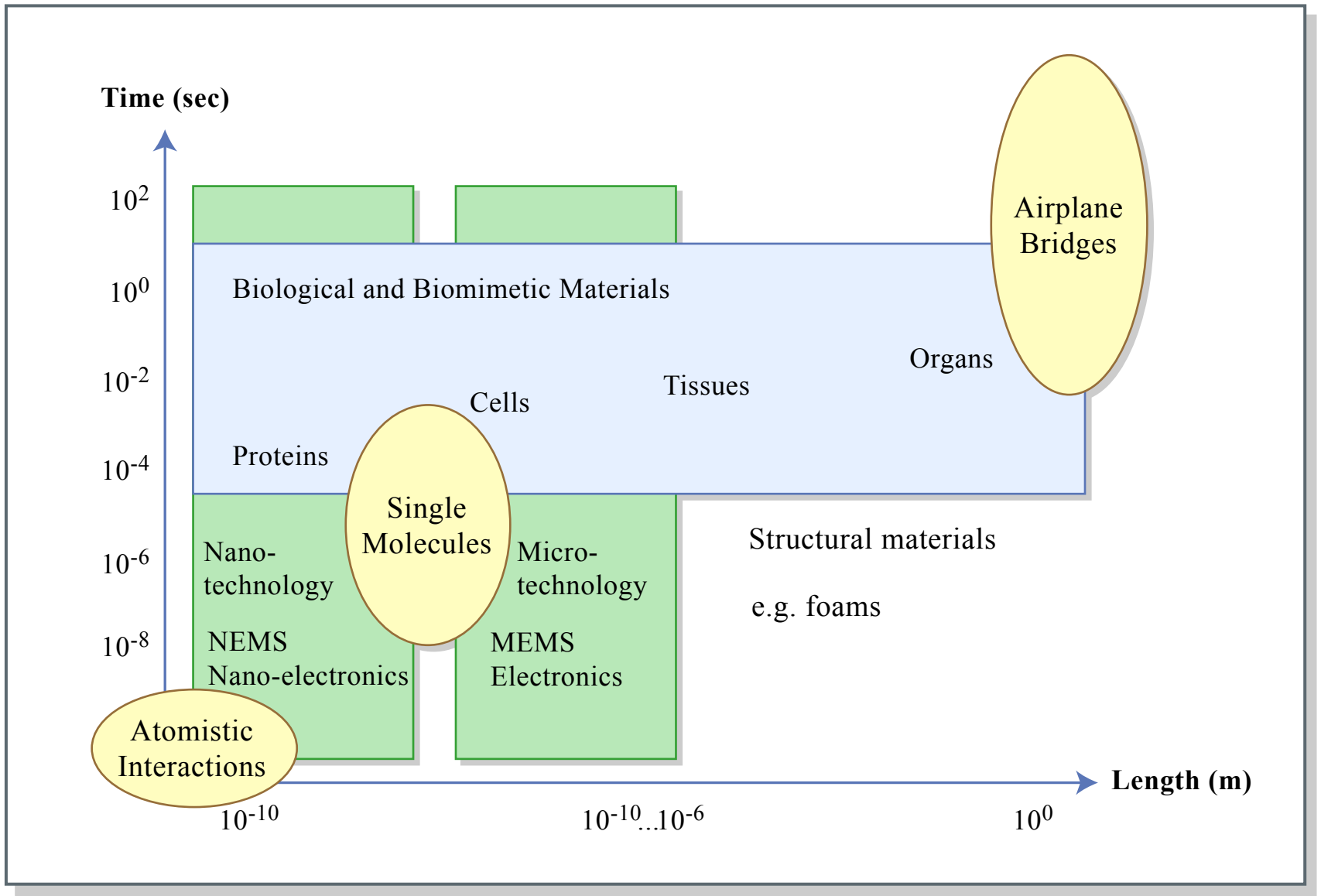

Figure by MIT OCW.

Buehler and Gao, 2006

Scale coupling

Adhesion (does it stick)?

Interfaces?

Measure how soft/stiff it is

Fracture?

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Change at one scale-
influence on large scale properties?

Change of properties across scales

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).

- **Note:** I plan to present the following material on the board, as far as possible.

- **Strategy:** First present some examples of deformation of materials (slides). Then draw a schematic that overlays different problems and what length-/ time-scales are covered. Then pose the question: How can we measure and model these properties? What kind of information can be obtain (i.e., scale-specific properties, cross-scale properties).
  First step now: Introduce the continuum scale (but note that during the lecture I will make remarks about the atomistic nature of the problem).
- **Continuum:** Then start off with introduction of elasticity; stress; and give rigorous derivation of the beam bending problem. This problem should include the free energy – from which we take derivatives; this will lay a natural foundation for the atomistic scale (I should point it out in the end).

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

What has the beam model shown?

- Can solve elasticity problem and obtain stresses and strains, by considering a relationship between stresses and strains

- Now: Brief outlook into deformation beyond the elastic regime (dissipation!);

  then next lecture fundamental means to calculate the properties of free energy

Ductile versus brittle materials

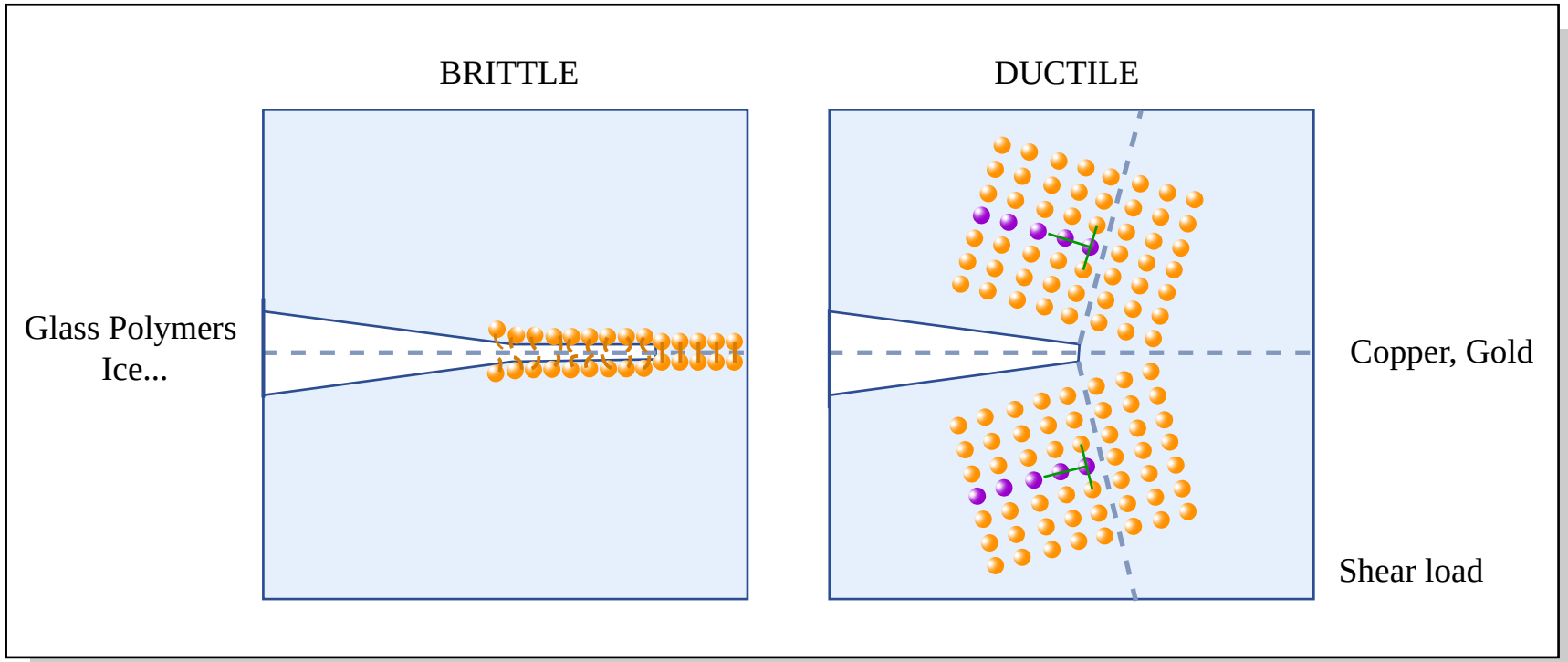
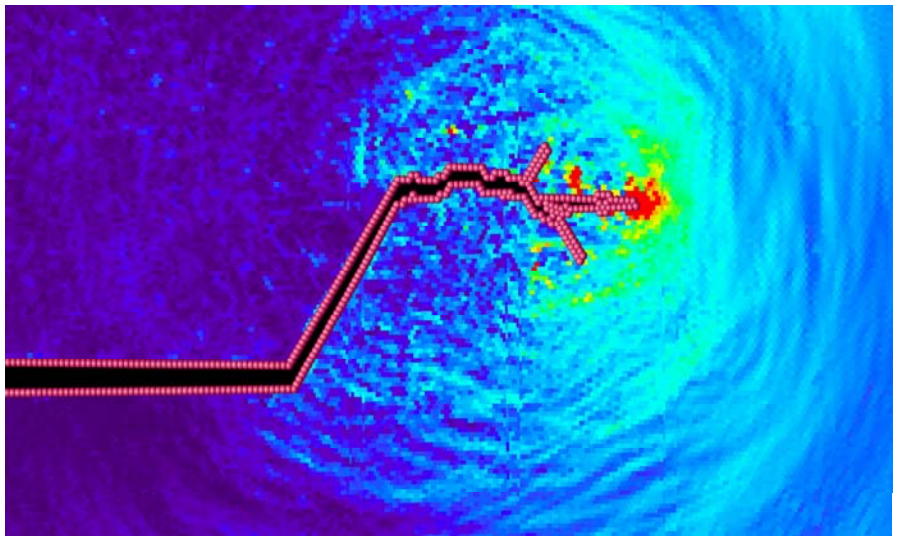
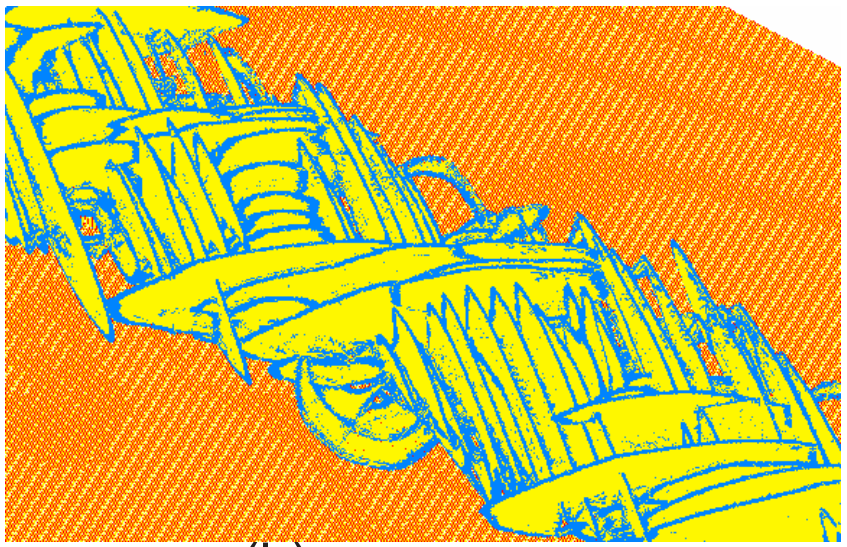


Figure by MIT OCW.



(a)



(b)

Ductile versus brittle materials: Experiment

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“brittle”
Separation long grain boundaries, Cleavage

“ductile”
Dislocations, material deformation (microscopic)

Ductile versus brittle materials: Experiment

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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

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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).

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

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- 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/