1.021, 3.021, 10.333, 22.00 Introduction to Modeling and Simulation
Spring 2011

Part I – Continuum and particle methods

How to model chemical interactions II

Lecture 6

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Content overview

I. Particle and continuum methods

Lectures 2-13

1. Atoms, molecules, chemistry
2. Continuum modeling approaches and solution approaches
3. Statistical mechanics
4. Molecular dynamics, Monte Carlo
5. Visualization and data analysis
6. Mechanical properties – application: how things fail (and how to prevent it)
7. Multi-scale modeling paradigm
8. Biological systems (simulation in biophysics) – how proteins work and how to model them

II. Quantum mechanical methods

Lectures 14-26

1. It's A Quantum World: The Theory of Quantum Mechanics
2. Quantum Mechanics: Practice Makes Perfect
3. The Many-Body Problem: From Many-Body to Single-Particle
4. Quantum modeling of materials
5. From Atoms to Solids
6. Basic properties of materials
7. Advanced properties of materials
8. What else can we do?

Overview: Material covered so far…

- **Lecture 1: Broad introduction to IM/S**
- **Lecture 2**: **Introduction to atomistic and continuum modeling** (multi-scale modeling paradigm, difference between continuum and atomistic approach, case study: diffusion)
- **Lecture 3**: **Basic statistical mechanics – property calculation I** (property calculation: microscopic states vs. macroscopic properties, ensembles, probability density and partition function)
- **Lecture 4**: **Property calculation II** (Monte Carlo, advanced property calculation, introduction to chemical interactions)
- **Lecture 5: How to model chemical interactions I** (example: movie of copper deformation/dislocations, etc.)
- **Lecture 6: How to model chemical interactions II**

Lecture 6: How to model chemical interactions II

Outline:

1. Case study: Deformation of copper wire (cont'd)
2. How to model metals: Multi-body potentials
3. Brittle versus ductile materials
4. Basic deformation mechanism in brittle materials - crack extension

Goal of today's lecture:

- Complete example of copper deformation
- Learn how to build a model to describe brittle fracture (from scratch)
- Learn basics in fracture of brittle materials
- Apply our tools to model a particular material phenomena – brittle fracture (useful for pset #2)

1. Case study: Deformation of copper wire (cont’d)

A simulation with 1,000,000,000 particles Lennard-Jones - copper

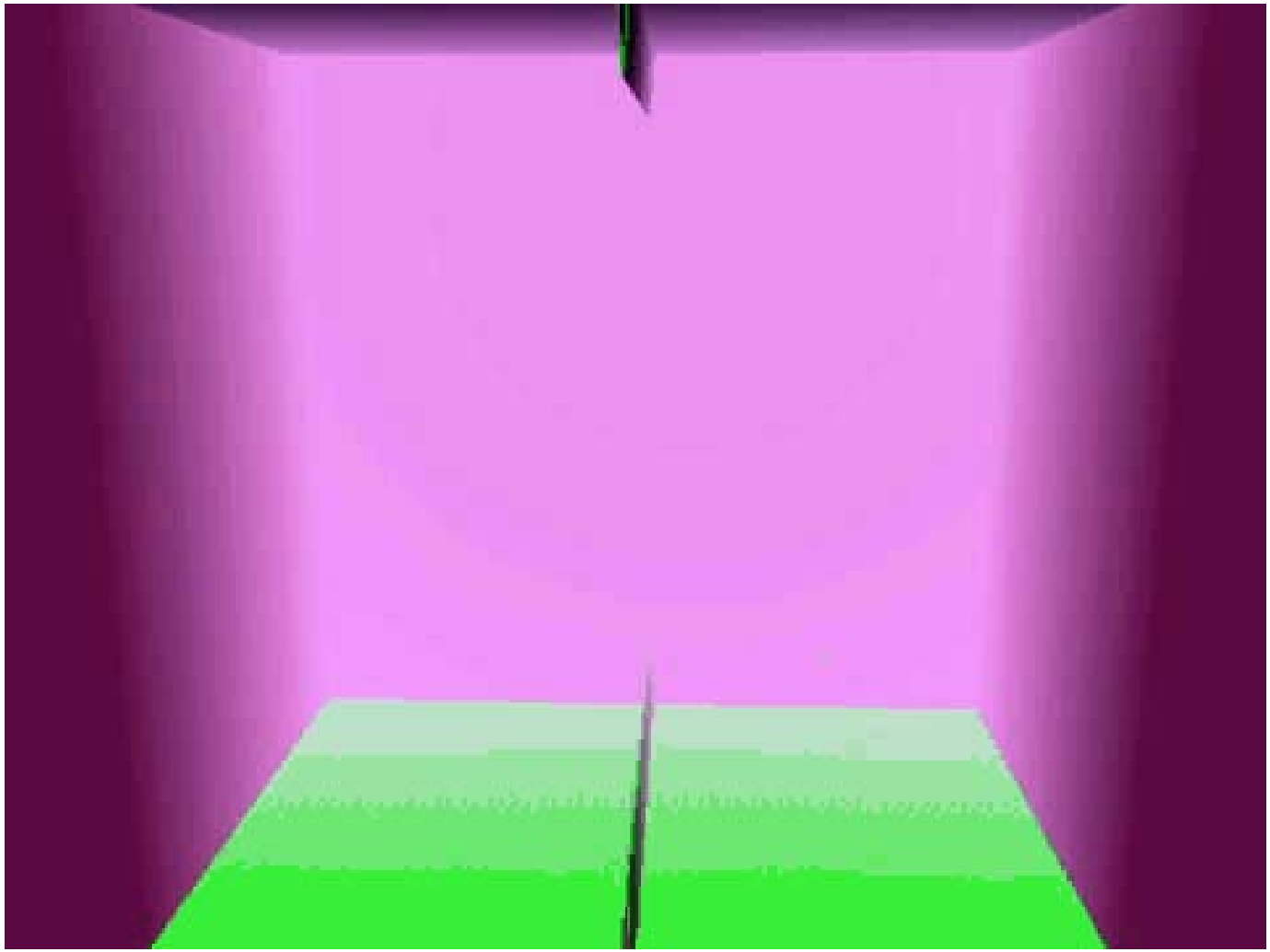
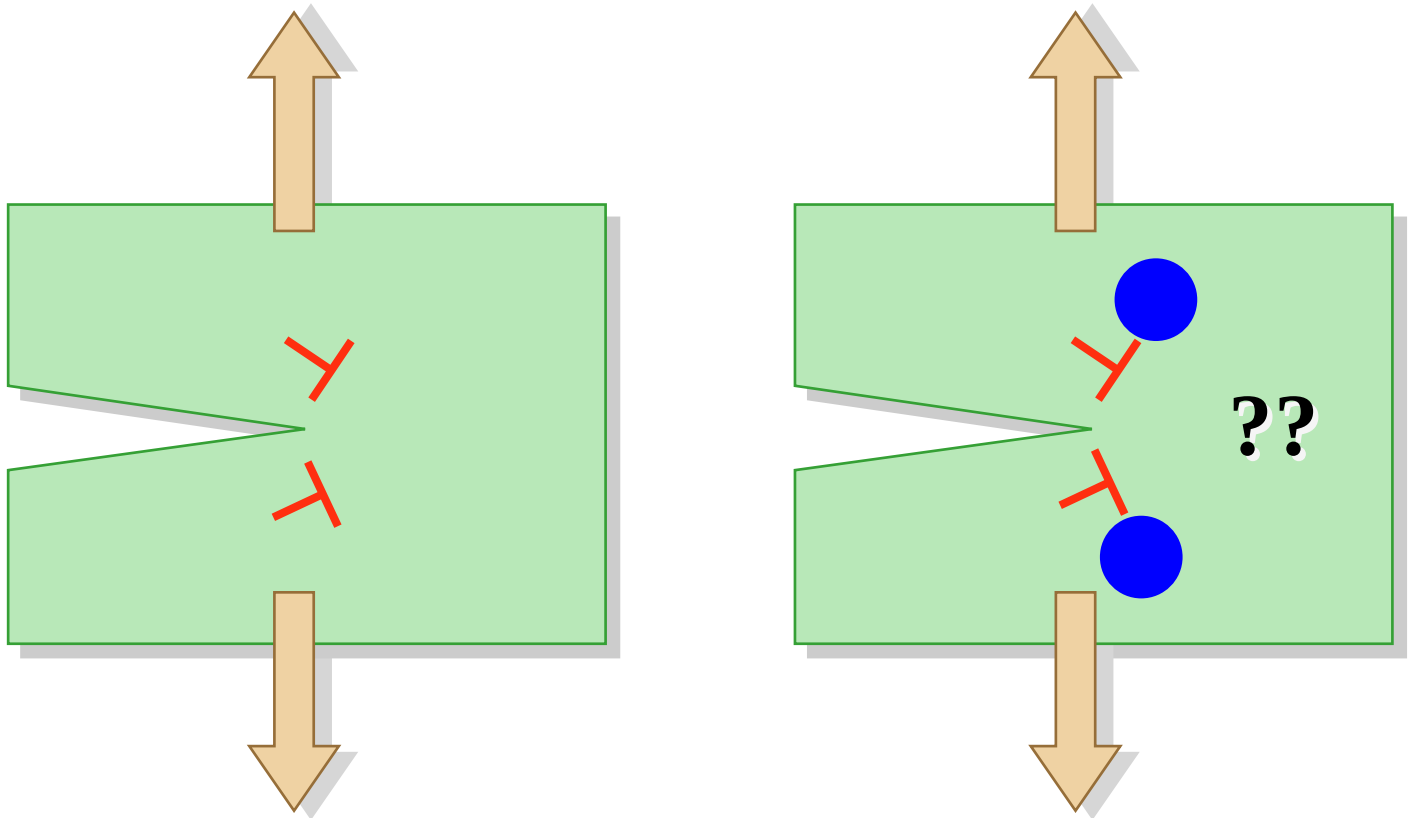
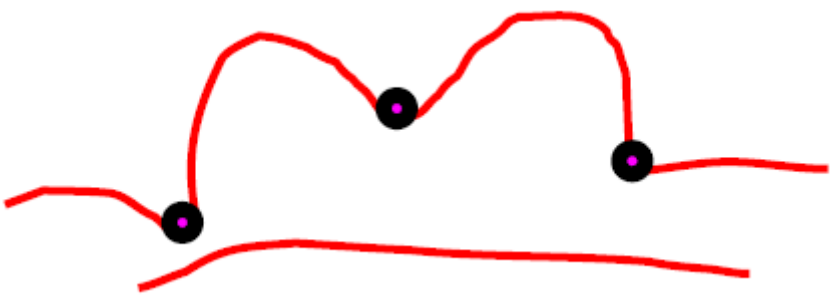


Fig. 1 c from Buehler, M., et al. "The Dynamical Complexity of Work-Hardening: A Large-Scale Molecular Dynamics Simulation." *Acta Mech Sinica* 21 (2005): 103-11.

Strengthening mechanisms





Strengthening caused by hindering dislocation motion

If too difficult, ductile modes break down and material becomes brittle

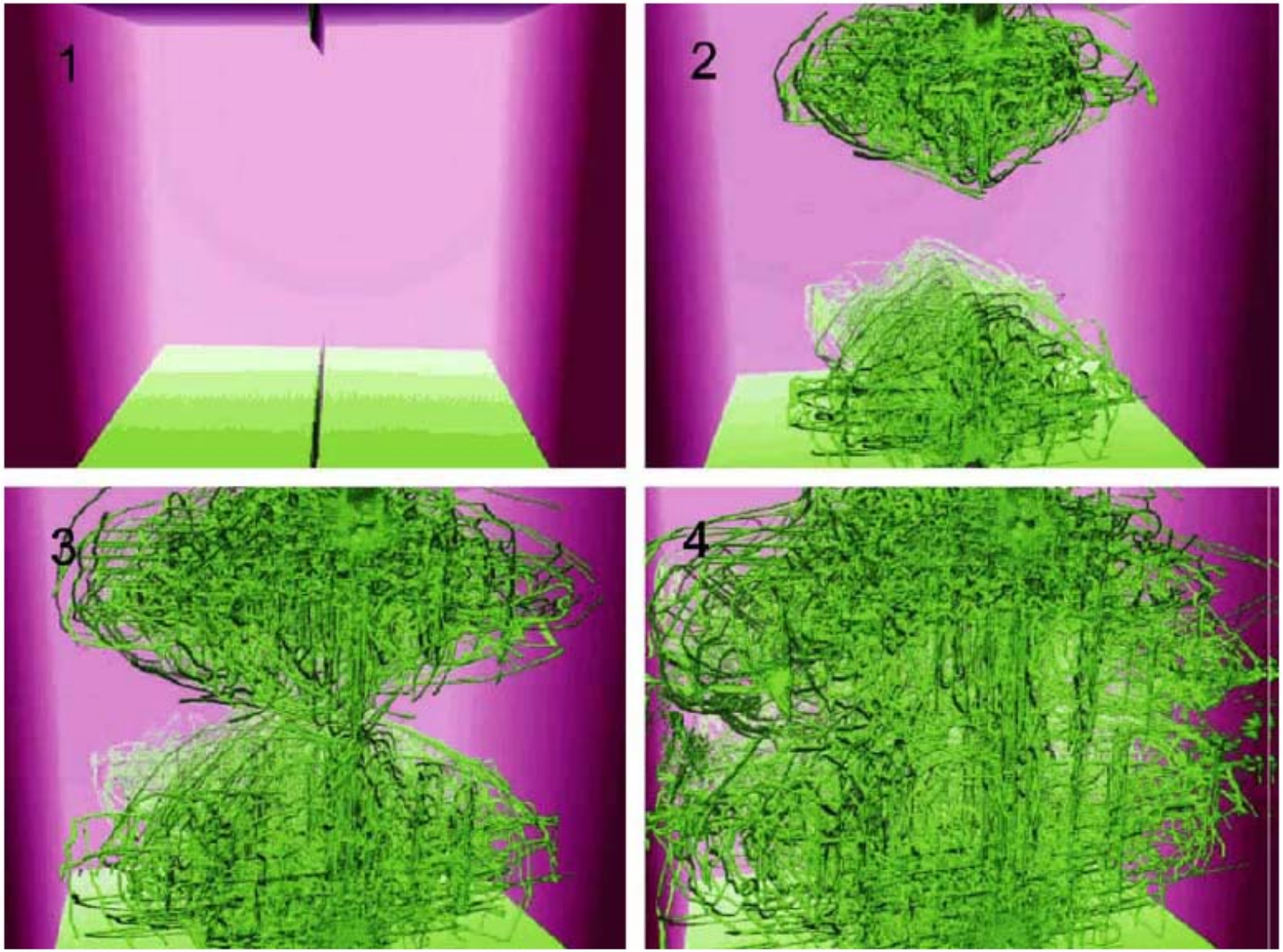


Fig. 1 c from Buehler, M. et al. "The Dynamical Complexity of Work-Hardening: A Large-Scale Molecular Dynamics Simulation." Acta Mech Sinica 21 (2005): 103-111.

Parameters for Morse potential

(for reference)

Morse potential parameters for various metals

Morse Potential Parameters for 16 Metals

Metal	αa_0	β	L x 10^{-22} (eV)	α (A^{-1})	r_0 (A)	D (eV)
Pb	2.921	83.02	7.073	1.1836	3.733	0.2348
Ag	2.788	71.17	10.012	1.3690	3.115	0.3323
Ni	2.500	51.78	12.667	1.4199	2.780	0.4205
Cu	2.450	49.11	10.330	1.3588	2.866	0.3429
Al	2.347	44.17	8.144	1.1646	3.253	0.2703
Ca	2.238	39.63	4.888	0.80535	4.569	0.1623
Sr	2.238	39.63	4.557	0.73776	4.988	0.1513
Mo	2.368	88.91	24.197	1.5079	2.976	0.8032
W	2.225	72.19	29.843	1.4116	3.032	0.9906
Cr	2.260	75.92	13.297	1.5721	2.754	0.4414
Fe	1.988	51.97	12.573	1.3885	2.845	0.4174
Ba	1.650	34.12	4.266	0.65698	5.373	0.1416
K	1.293	23.80	1.634	0.49767	6.369	0.05424
Na	1.267	23.28	1.908	0.58993	5.336	0.06334
Cs	1.260	23.14	1.351	0.41569	7.557	0.04485
Rb	1.206	22.15	1.399	0.42981	7.207	0.04644

Adapted from Table I in Girifalco, L. A., and V. G. Weizer. "Application of the Morse Potential Function to Cubic Metals." *Physical Review* 114 (May 1, 1959): 687-690.

$$\phi(r_{ij}) = D\exp\left(-2\alpha(r_{ij}-r_0)\right) - 2D\exp\left(-\alpha(r_{ij}-r_0)\right)$$

Morse potential: application example (nanowire)

See: Komanduri, R., et al. "Molecular Dynamics (MD) Simulation of Uniaxial Tension of Some Single-Crystal Cubic Metals at Nanolevel." *International Journal of Mechanical Sciences* 43, no. 10 (2001): 2237-60.

Further Morse potential parameters:

Table 3
Morse potential parameters used in MD simulation of uniaxial tensile loading [24]

Material	Crystal structure	Dissociation energy, D (eV)	Equilibrium radius, r_o (Å)	α-parameter ($Å^{-1}$)	Lattice constant (Å)
Aluminium	FCC	0.2703	3.253	1.1650	4.05
Copper	FCC	0.3429	2.866	1.3590	3.62
Nickel	FCC	0.4205	2.780	1.4199	3.52
Iron	BCC	0.4172	2.845	1.3890	2.87
Chromium	BCC	0.4414	2.754	1.5721	2.89
Tungsten	BCC	0.9906	3.032	1.4116	3.17

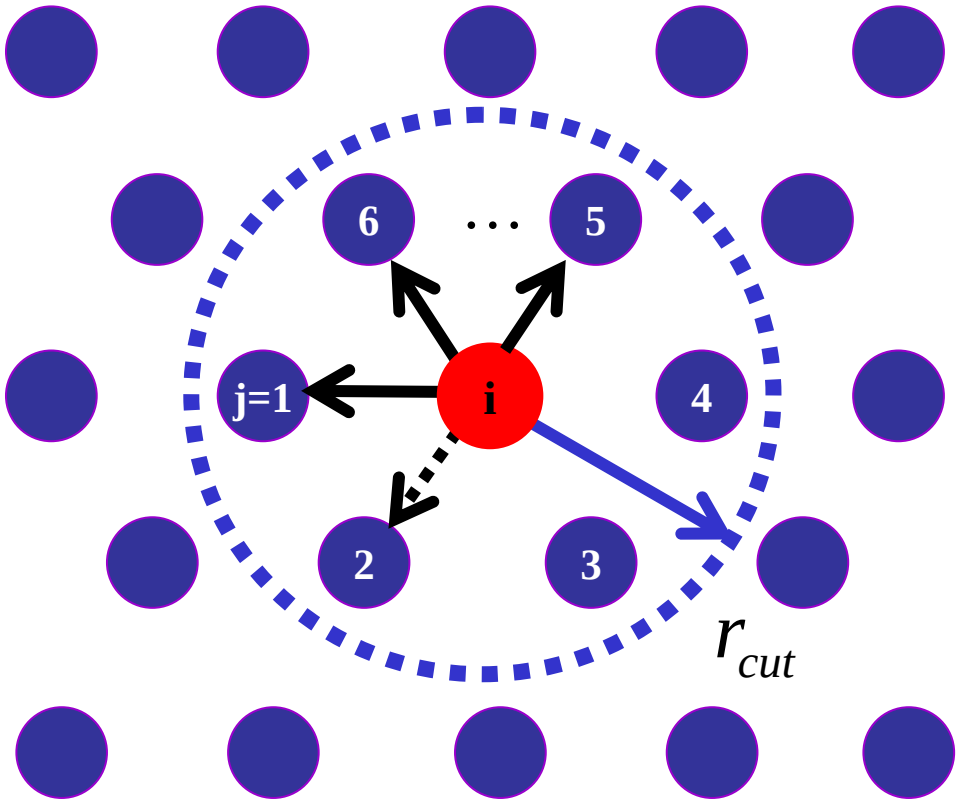
Cutoff-radius: saving time

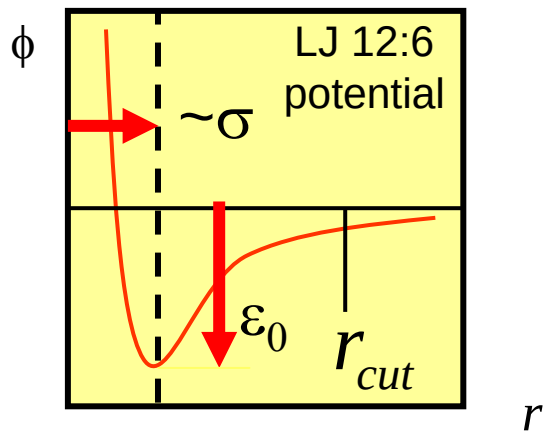
Cutoff radius

$$U_i = \sum_{j=1}^{N} \phi(r_{ij})$$

$$\downarrow$$

$$U_i = \sum_{j=1..N_{neigh}} \phi(r_{ij})$$





Cutoff radius = considering interactions only to a certain distance
Basis: Force contribution negligible (slope)

Derivative of LJ potential ~ force

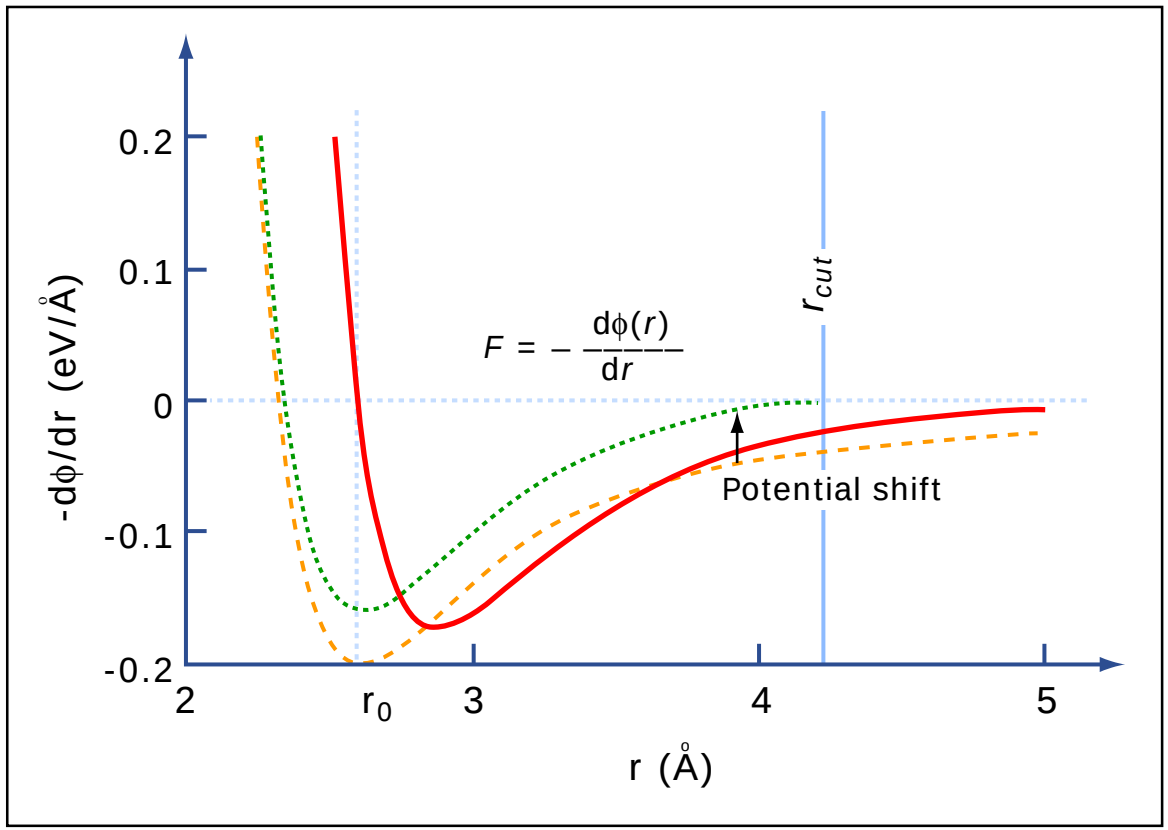


Image by MIT OpenCourseWare.

Beyond cutoff: *Changes in energy (and thus forces) small*

Putting it all together…

MD updating scheme: Complete

(1) Updating method (integration scheme)

$$r_i(t_0+\Delta t) = -r_i(t_0-\Delta t) + 2r_i(t_0)\Delta t + a_i(t_0)(\Delta t)^2 + \ldots$$

Positions at t_0-Δt | Positions at t_0 | Accelerations at t_0

(2) Obtain accelerations from forces

$$f_i = ma_i \qquad a_i = f_i / m$$

(3) Obtain forces from potential

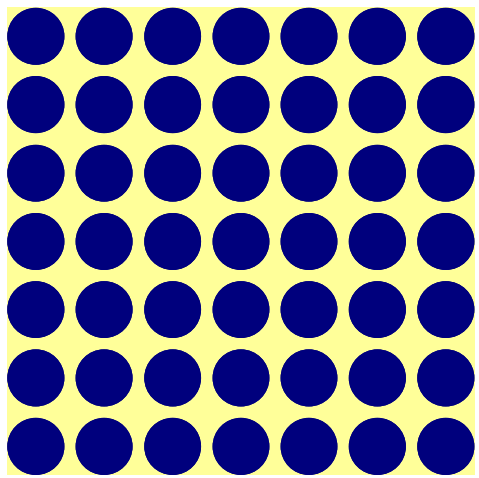
$$F = -\frac{\mathrm{d}\,\phi(r)}{\mathrm{d}\,r} \qquad f_i = F\frac{x_i}{r}$$

Potential

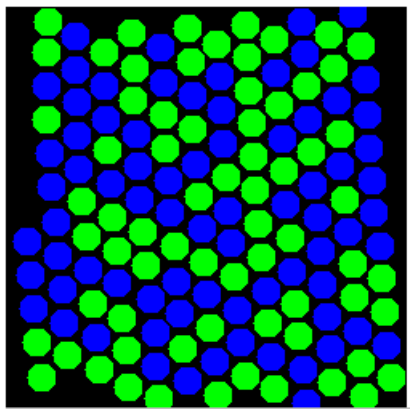
$$\phi(r) = 4\varepsilon\left(\left[\frac{\sigma}{r}\right]^{12} - \left[\frac{\sigma}{r}\right]^{6}\right)$$

(4) Crystal (initial conditions)

Positions at t_0



2.2 How to model metals: Multi-body potentials



Courtesy of the Center for Polymer Studies at Boston University. Used with permission.

Pair potential: Total energy sum of all pairs of bonds

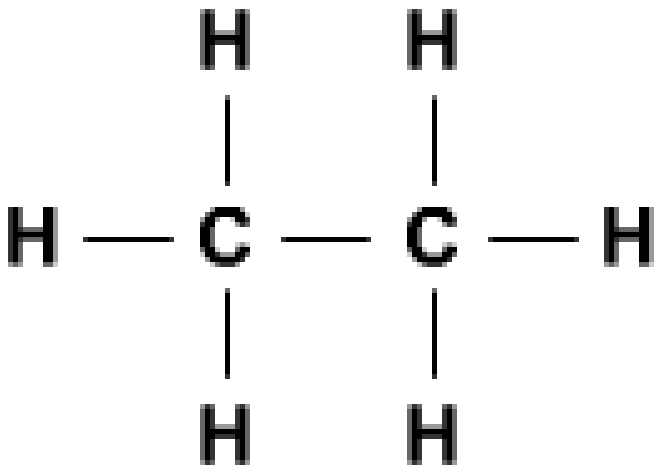
Individual bond contribution does not depend on other atoms

"all bonds are the same"

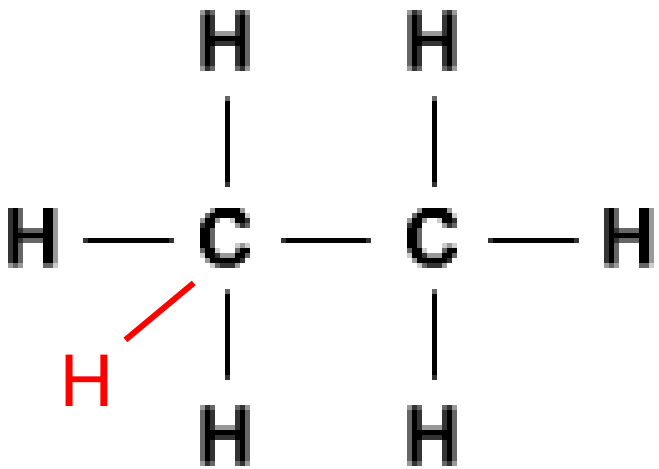
$$U_{total} = \frac{1}{2} \sum_{i=1, i \neq j}^{N} \sum_{j=1}^{N} \phi(r_{ij})$$

Is this a good assumption?

Are all bonds the same? - valency in hydrocarbons



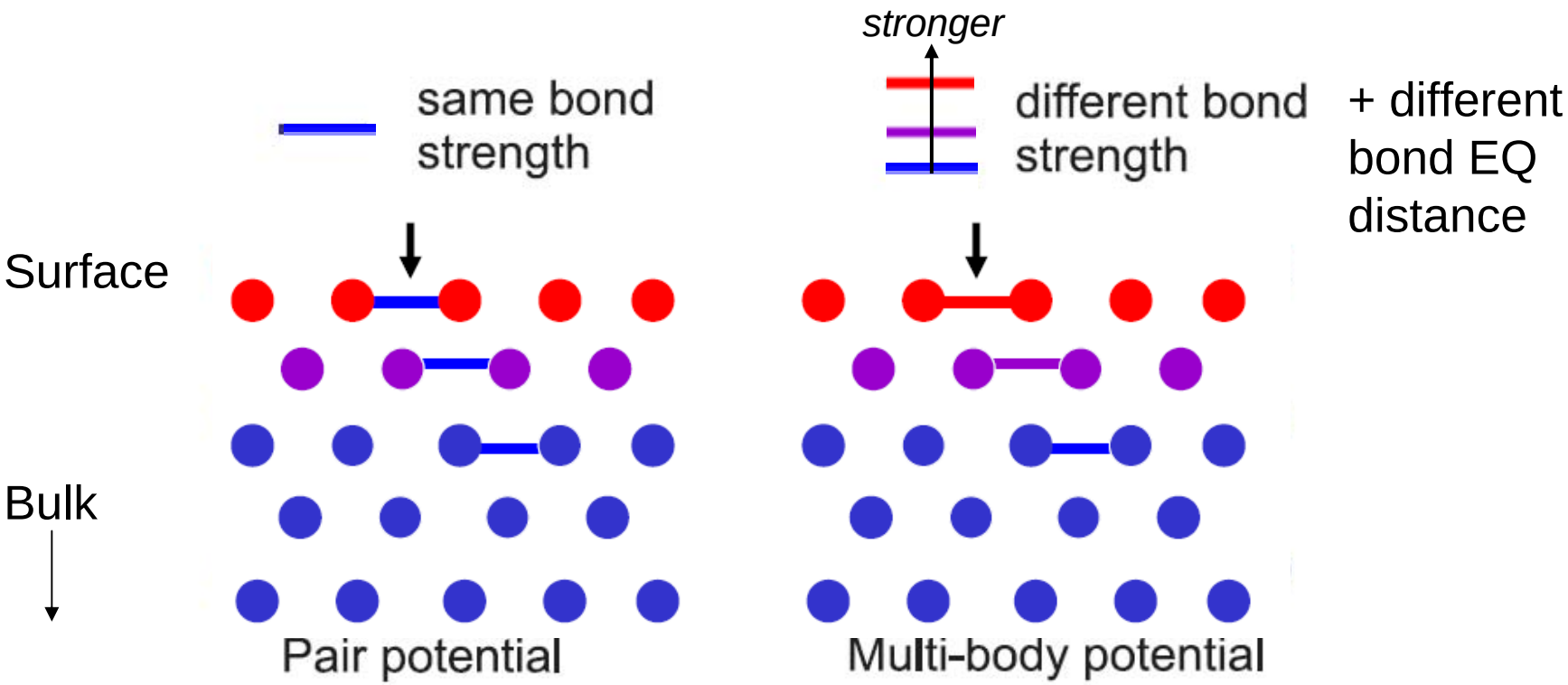
Ethane C_2H_6
(stable configuration)



All bonds are not the same!

Adding another H is not favored

Are all bonds the same? – metallic systems

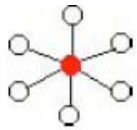


Pair potentials: All bonds are equal!

Reality: Have environment effects; it matter that there is a free surface!

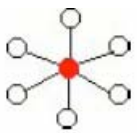
Bonds depend on the environment!

Are all bonds the same?

Bonding energy of red atom in  is six times bonding energy in 

This is in contradiction with both experiments and more accurate quantum mechanical calculations on many materials

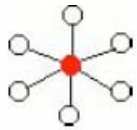
Bonding energy of atom i $$U_i = \sum_{j=1}^{N} \phi(r_{ij})$$



$$U_i = \sum_{j=1}^{6} \phi(r_{ij}) \quad \longleftrightarrow \quad U_i = \phi(r_{ij})$$

After: G. Ceder

Are all bonds the same?

Bonding energy of red atom in  is six times bonding energy in 

This is in contradiction with both experiments and more accurate quantum mechanical calculations on many materials

For pair potentials $\sim Z$

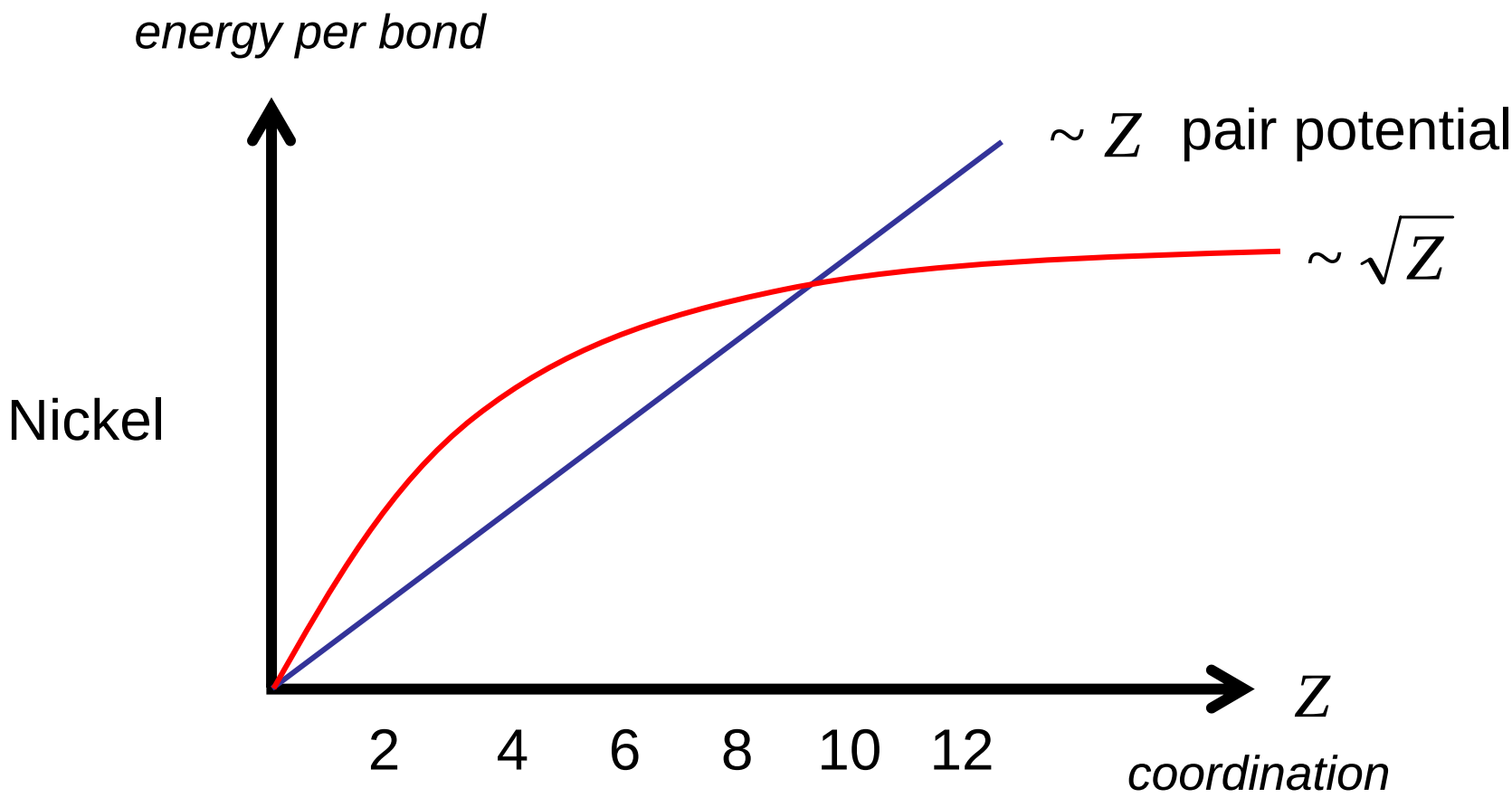
For metals $\sim \sqrt{Z}$

Z : Coordination = how many immediate neighbors an atom has

Bonds get "weaker" as more atoms are added to central atom

After: G. Ceder

Bond strength depends on coordination



Daw, Foiles, Baskes, *Mat. Science Reports*, 1993

Transferability of pair potentials

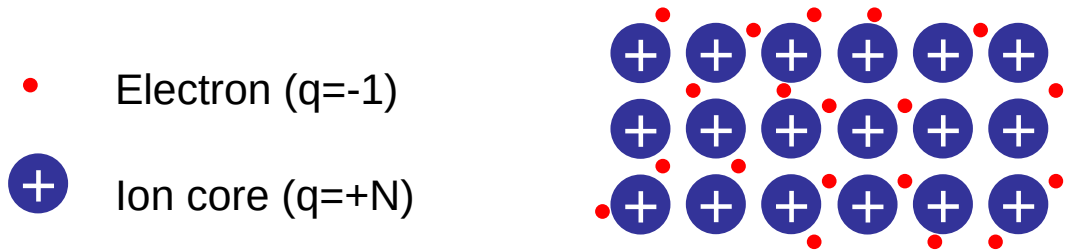
- Pair potentials have limited **transferability:**

  Parameters determined for molecules can not be used for crystals, parameters for specific types of crystals can not be used to describe range of crystal structures

- E.g. difference between FCC and BCC can not be captured using a pair potential

Metallic bonding: multi-body effects

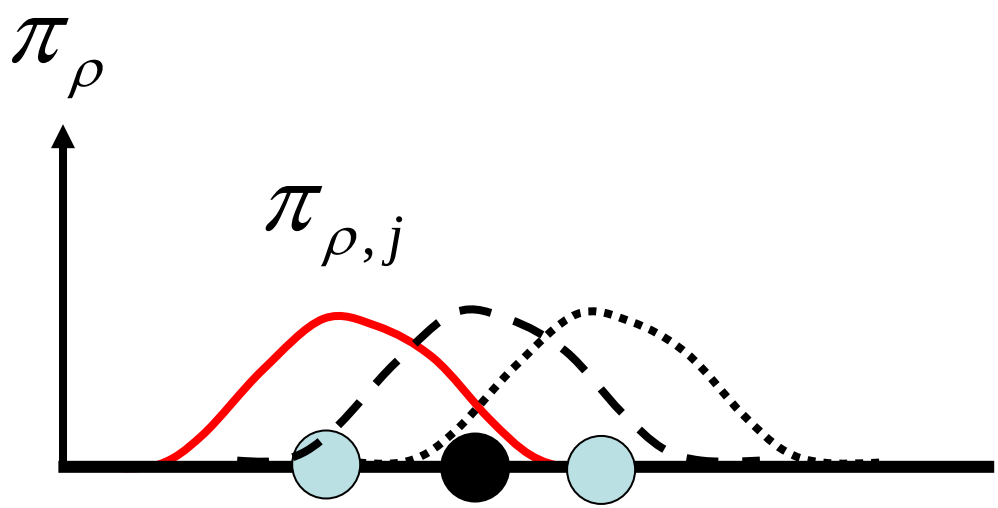
- Need to consider more details of chemical bonding to understand environmental effects



Delocalized valence electrons moving between nuclei generate a binding force to hold the atoms together: **Electron gas model (*positive ions in a sea of electrons*)**

Mostly non-directional bonding, but the bond strength indeed depends on the environment of an atom, precisely the electron density imposed by other atoms

Concept: include electron density effects

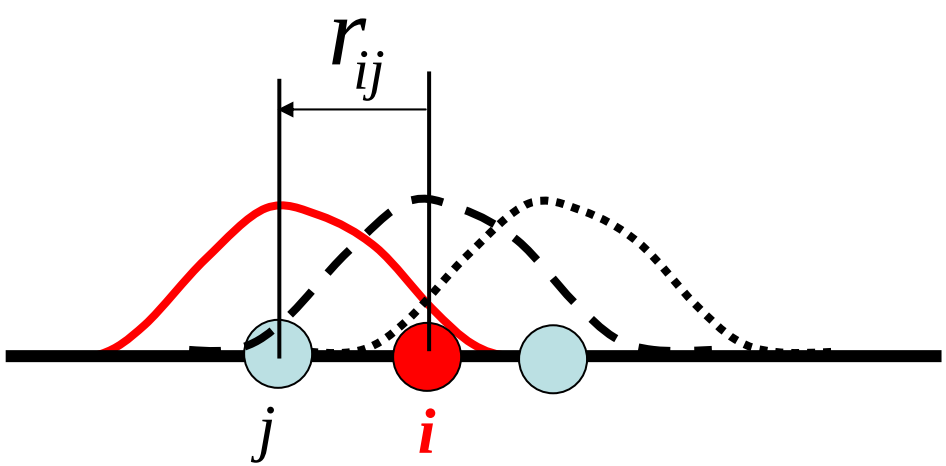


Each atom features a particular distribution of electron density

Concept: include electron density effects

Electron density at atom i

$$\rho_i = \sum_{j=1..N_{neigh}} \pi_{\rho,j}(r_{ij}) \qquad r_{ij} = x_j - x_i$$



$$\pi_{\rho,j}(r_{ij})$$

Atomic electron density contribution of atom j to atom i

Contribution to electron density at site i due to electron density of atom j evaluated at distance r_{ij}

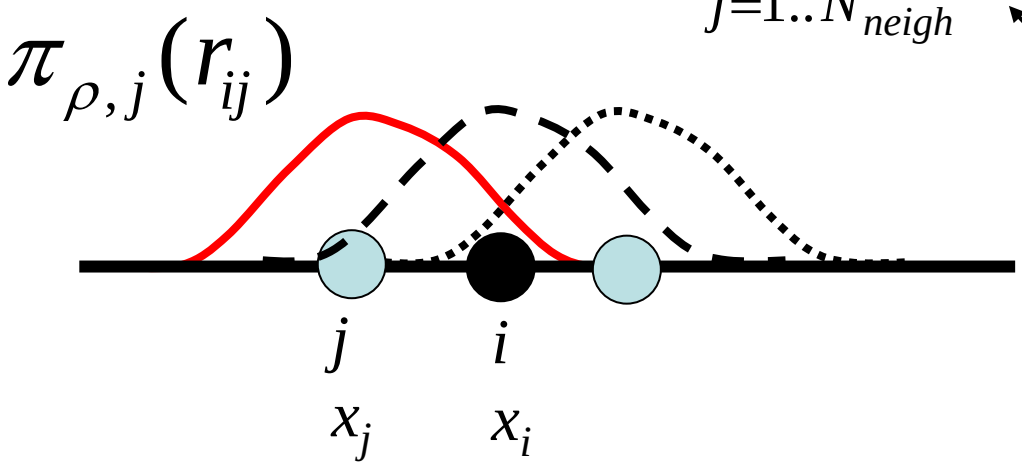
Concept: include electron density effects

$$\phi_i = \frac{1}{2} \sum_{j=1..N_{neigh}} \phi(r_{ij}) + F(\rho_i)$$

embedding term F (how local electron density contributes to potential energy)

Electron density at atom i

$$\rho_i = \sum_{j=1..N_{neigh}} \pi_{\rho,j}(r_{ij}) \qquad r_{ij} = x_j - x_i$$



Atomic electron density contribution of atom j to atom i

Embedded-atom method (EAM)

Atomic energy

new

$$\phi_i = \underbrace{\frac{1}{2}\sum_{j=1..N_{neigh}} \phi(r_{ij})}_{\text{Pair potential energy}} + \underbrace{F(\rho_i)}_{\text{Embedding energy as a function of electron density}}$$

Total energy

$$U_{total} = \sum_{i=1}^{N} \phi_i$$

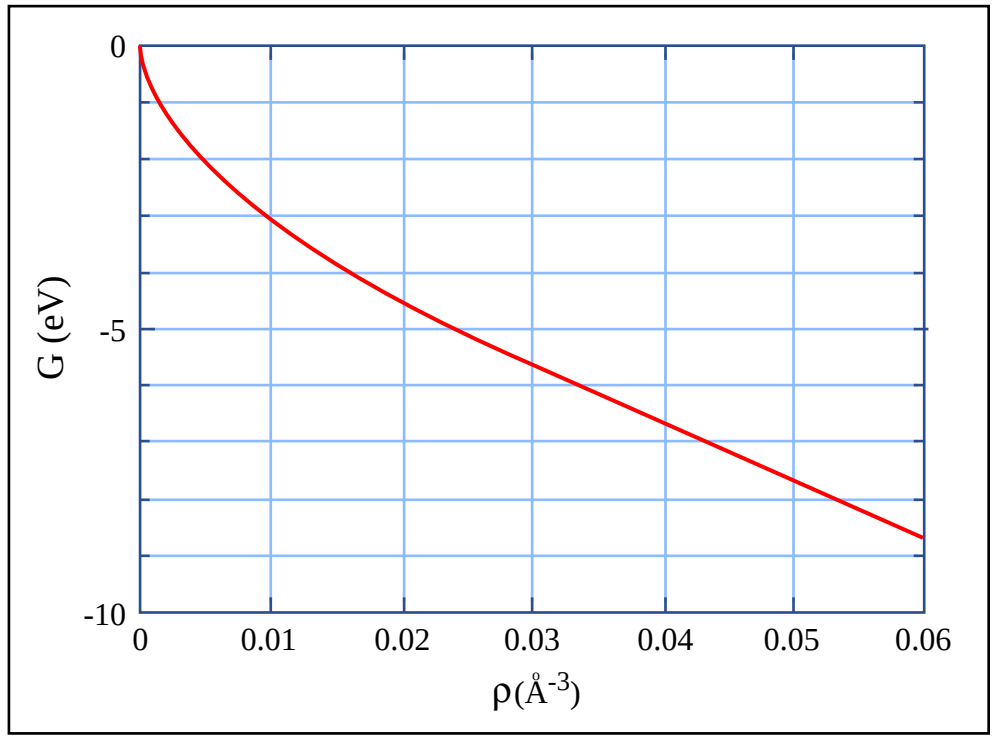
ρ_i Electron density at atom i based on a "pair potential":

$$\rho_i = \sum_{j=1..N_{neigh}} \pi_{\rho,j}(r_{ij})$$

First proposed by Finnis, Sinclair, Daw, Baskes *et al.* (1980s)

Embedding term: example

Embedding energy



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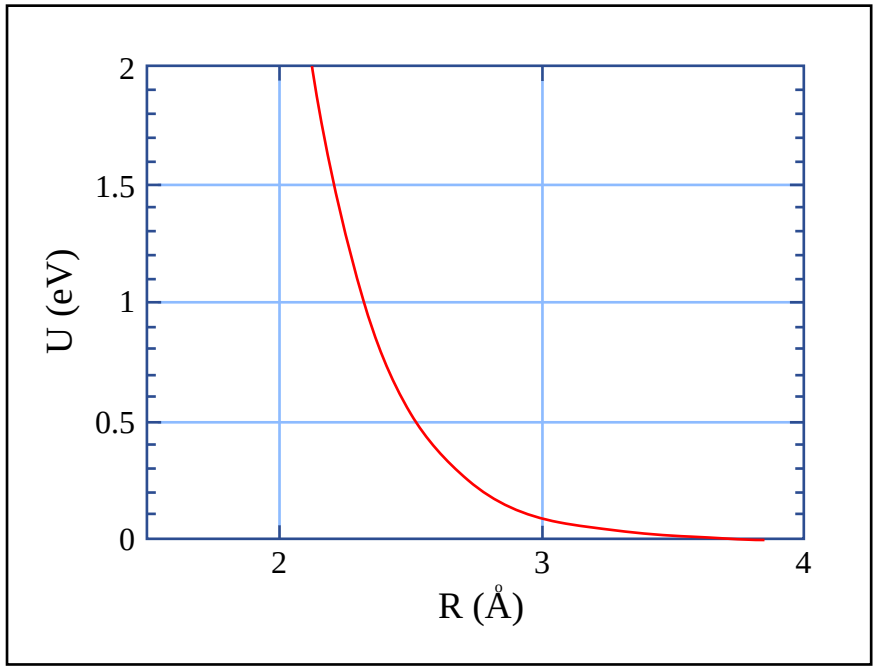
Electron density

$$\phi_i = \sum_{j=1..N_{neigh}} \left(\underbrace{\frac{1}{2}\phi(r_{ij})}_{\text{Pair potential energy}} + \underbrace{F(\rho_i)}_{\text{Embedding energy as a function of electron density}} \right)$$

Pair potential term: example

Pair contribution

$$\phi(r_{ij})$$



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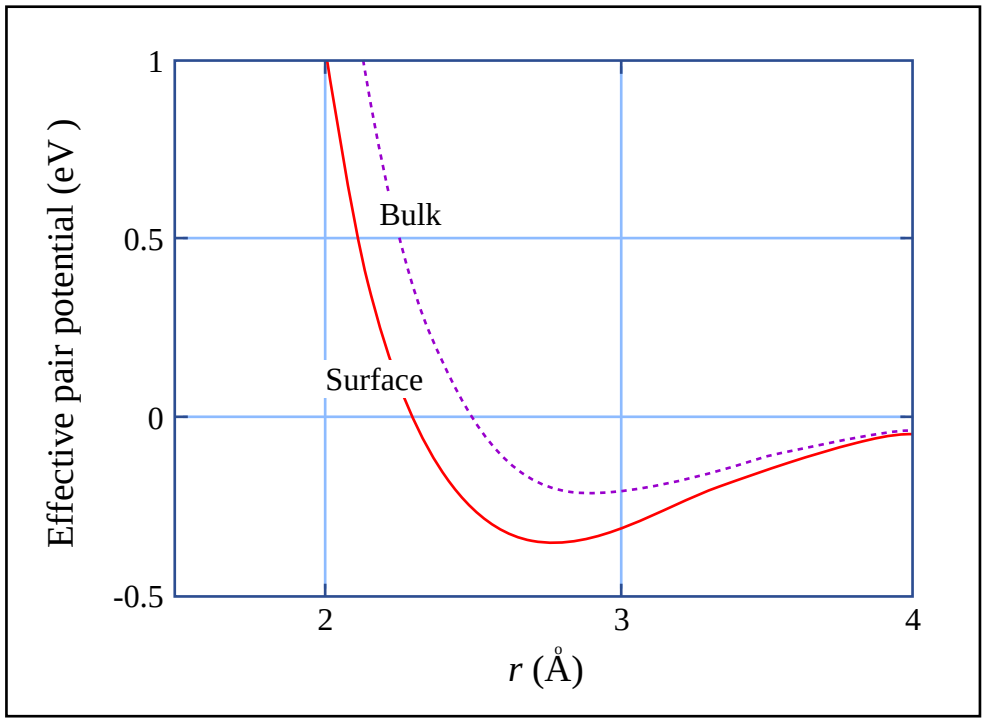
Distance r_{ij}

$$\phi_i = \sum_{j=1..N_{neigh}} \left(\underbrace{\frac{1}{2}\phi(r_{ij})}_{\text{Pair potential energy}} + \underbrace{F(\rho_i)}_{\text{Embedding energy as a function of electron density}} \right)$$

Effective pair interactions



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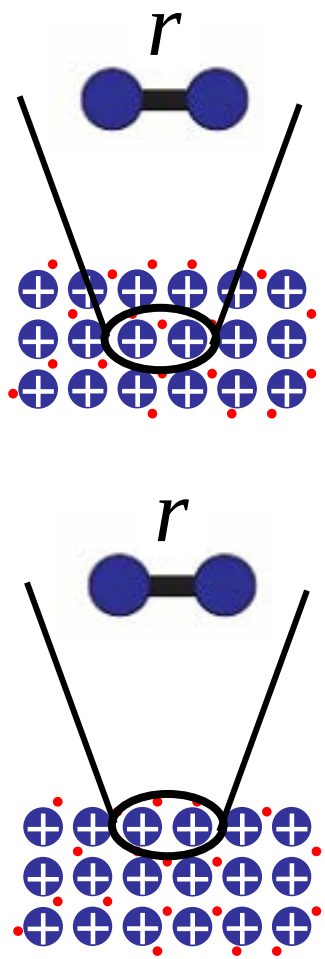


Can describe differences between bulk and surface

See also: Daw, Foiles, Baskes, *Mat. Science Reports*, 1993

Comparison with experiment

Diffusion: Activation energies

System	EAM	Exp.
Ag in Cu	2.05	2.02
Au in Cu	1.88	1.98
Ni in Cu	2.37	2.46
Pd in Cu	2.06	2.36
Pt in Cu	2.20	2.42
Cu in Ag	1.92	2.00
Au in Ag	2.04	2.06
Pd in Ag	2.19	2.46
Pt in Ag	2.33	2.44
Ag in Au	1.80	1.75
Cu in Au	1.82	1.76
Ni in Au	1.90	1.95
Pt in Au	2.07	2.09
Pd in Au	1.93	2.02
Ag in Ni	2.68	2.89
Cu in Ni	2.76	2.64
Au in Pt	2.49	2.61
Ag in Pt	2.71	2.68

(in eV)

Comparison EAM model vs. experiment

Element	EAM	Experiment
Cu	1340	1358
Ag	1170	1234
Au	1090	1338
Ni	1740	1726
Pd	1390	1825
Pt	1480	2045

Melting temperature (in K)

data from Elsevier from Daw, M. S., Foiles, S. M. & Baskes, M. I. The embedded-atom method: a review of theory and applications. *Materials Science Reports* **9**, 251 (1993).

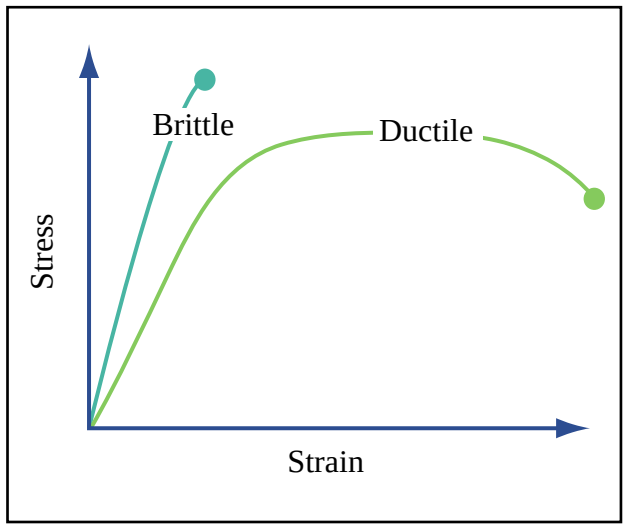
Summary: EAM method

- State of the art approach to model metals
- Very good potentials available for Ni, Cu, Al since late 1990s, 2000s
- Numerically efficient, can treat billions of particles
- Not much more expensive than pair potential (approximately three times), but describes physics much better

- ***Strongly recommended for use!***

3. Brittle versus ductile materials

Tensile test of a wire



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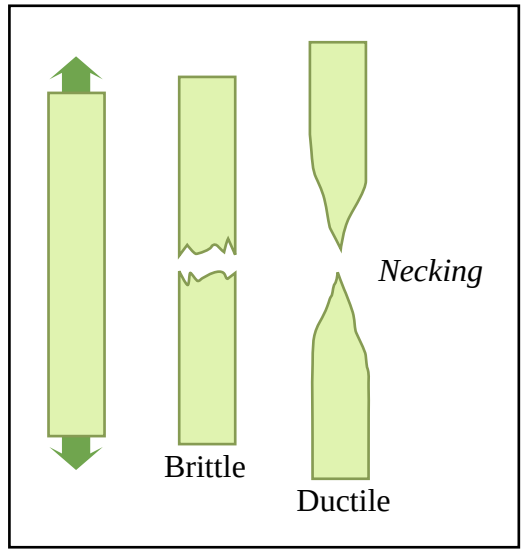

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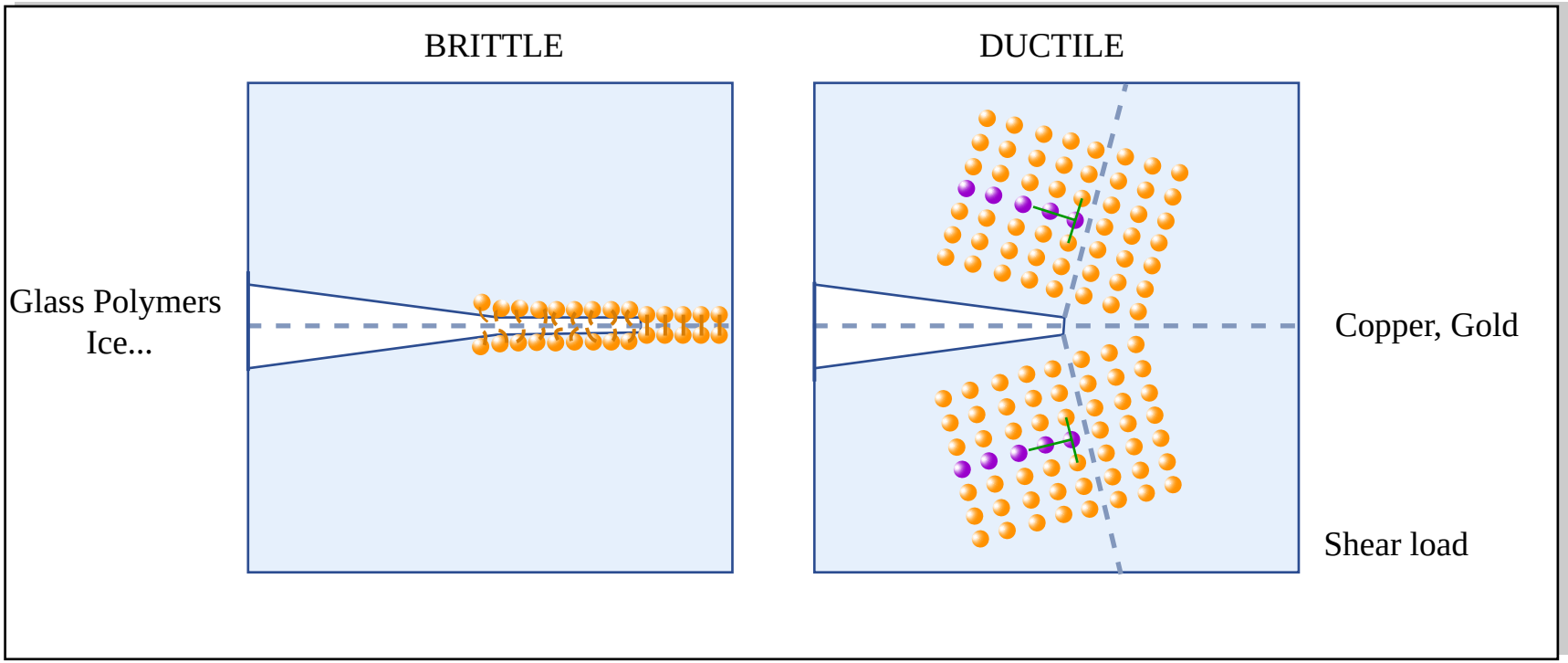
Ductile versus brittle materials



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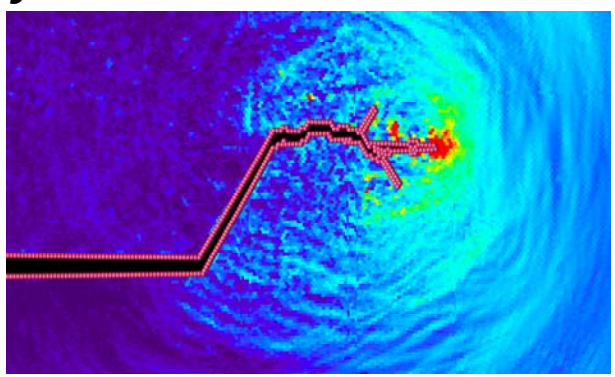
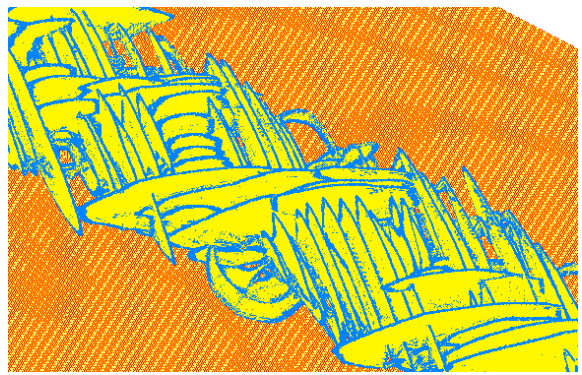
Difficult to deform, breaks easily



Easy to deform hard to break

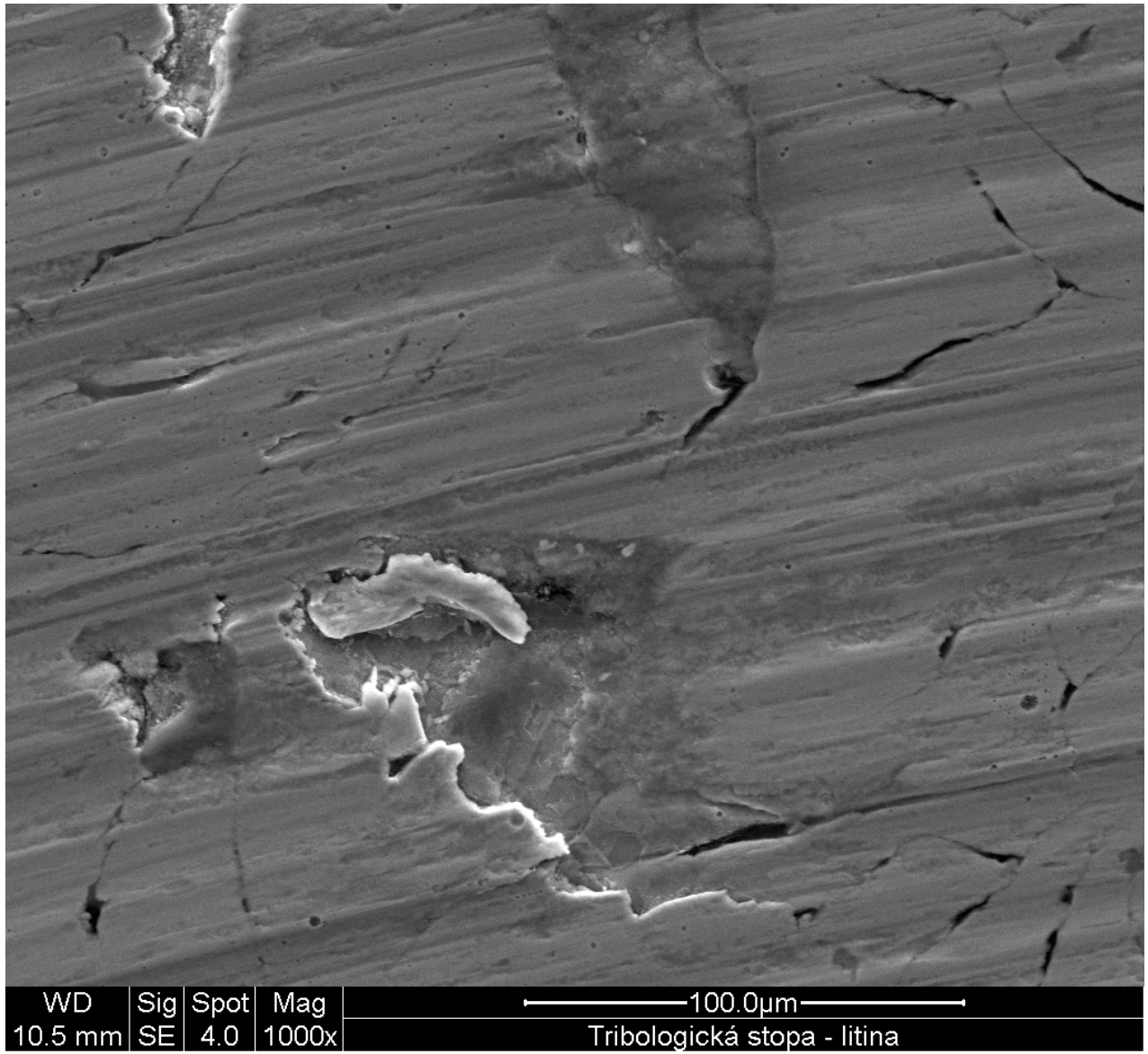


Deformation of materials:
Nothing is perfect, and flaws or cracks matter

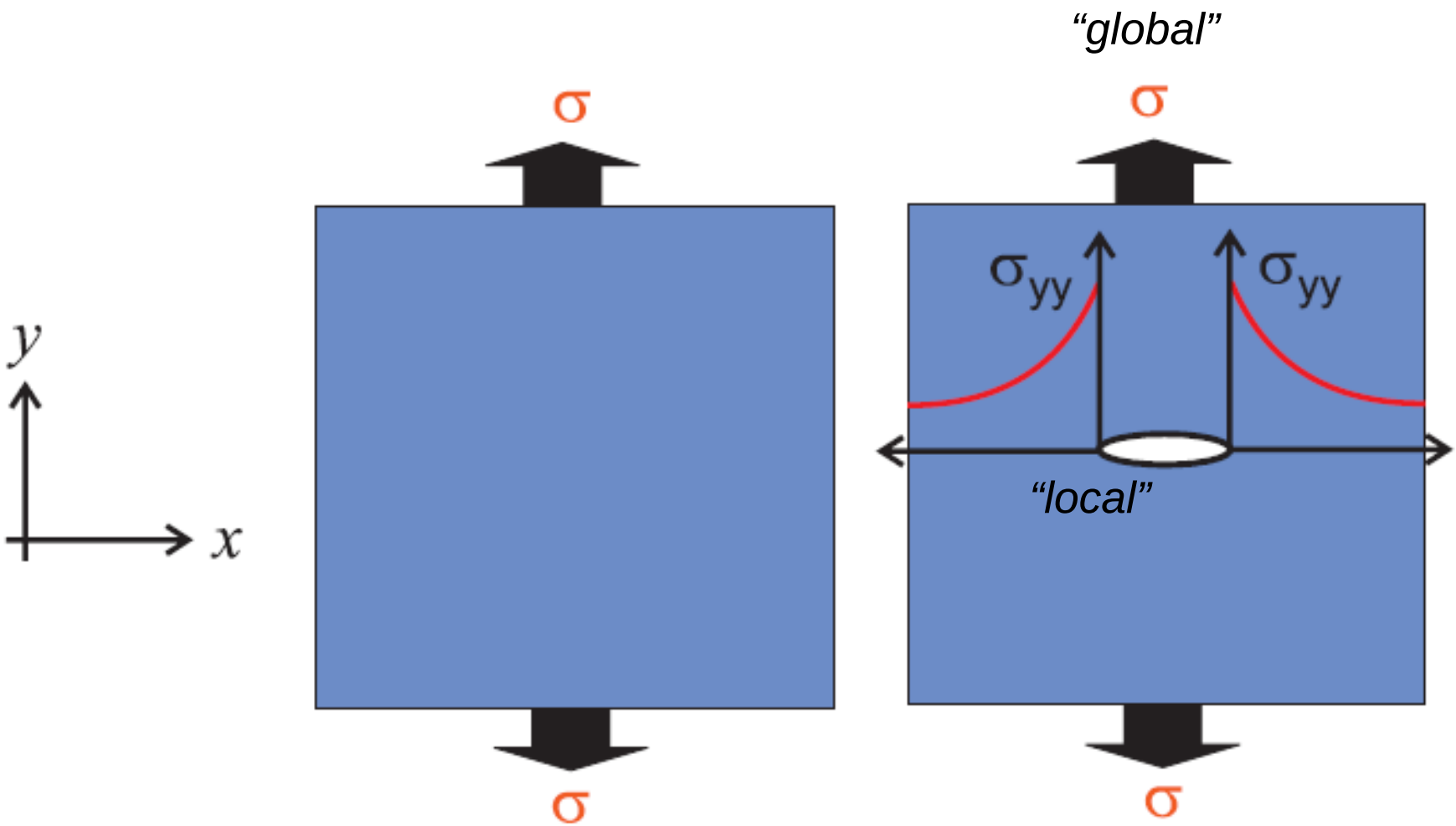
Failure of materials initiates at cracks

Griffith, Irwine and others: Failure initiates at defects, such as cracks, or grain boundaries with reduced traction, nano-voids, other imperfections

SEM picture of material: nothing is perfect

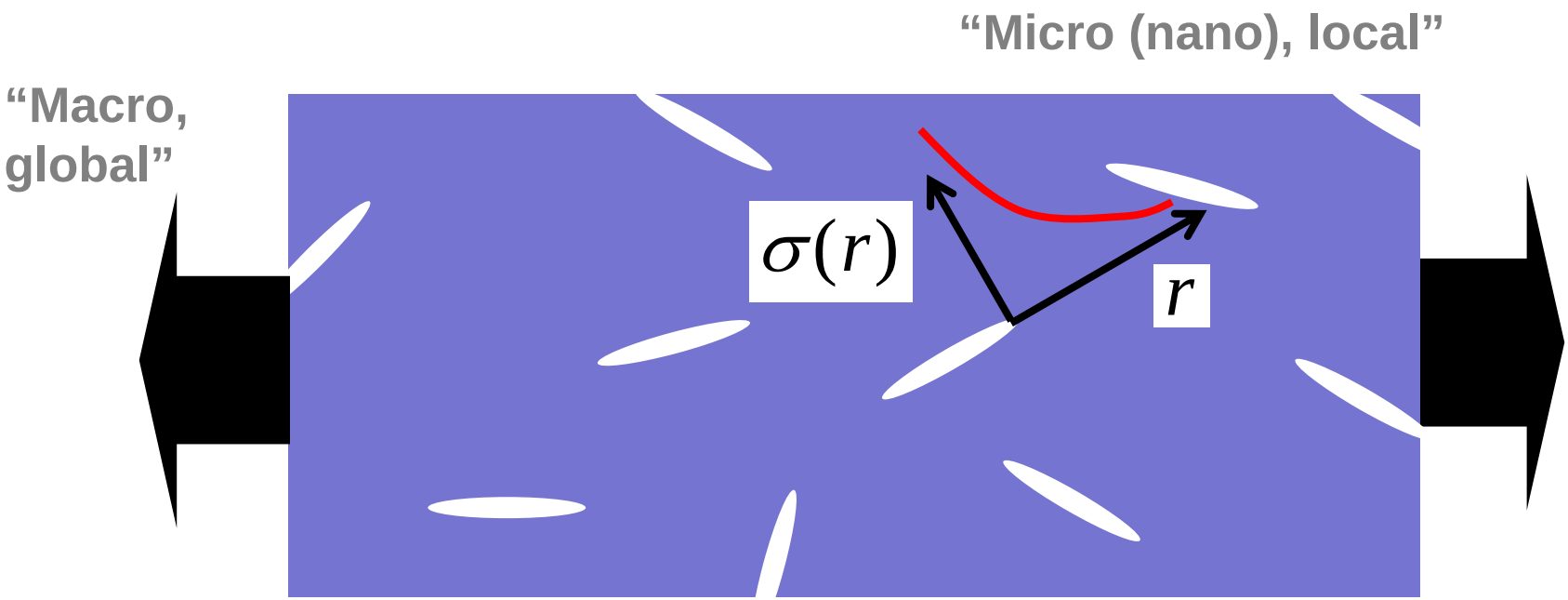


Significance of material flaws



Stress concentrators: ***local stress >> global stress***

Deformation of materials: Nothing is perfect, and flaws or cracks matter



Failure of materials initiates at cracks

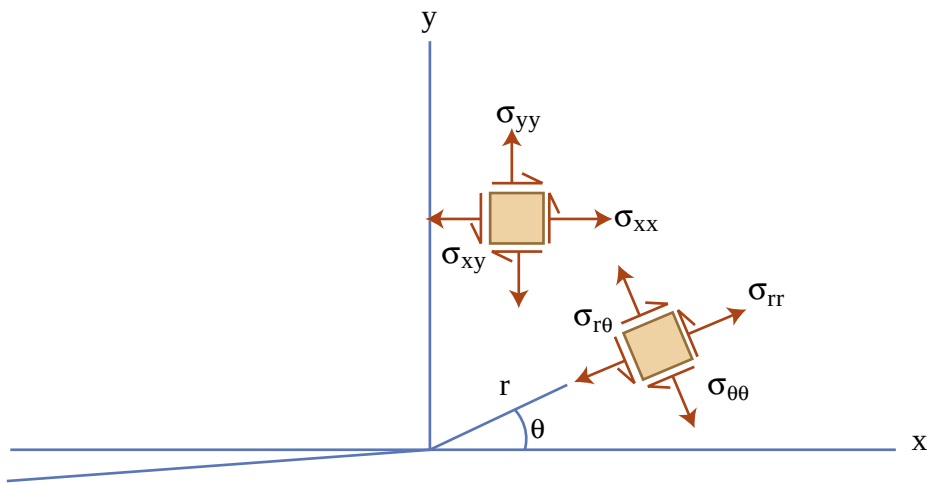
Griffith, Irwine and others: Failure initiates at defects, such as cracks, or grain boundaries with reduced traction, nano-voids, other imperfections

Cracks feature a singular stress field, with singularity at the tip of the crack

stress tensor

$$\begin{Bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{Bmatrix} = \frac{K_I}{\sqrt{2\pi r}} \cos\frac{\theta}{2} \begin{Bmatrix} 1 - \sin\frac{\theta}{2}\sin\frac{3\theta}{2} \\ 1 + \sin\frac{\theta}{2}\sin\frac{3\theta}{2} \\ \sin\frac{\theta}{2}\cos\frac{3\theta}{2} \end{Bmatrix}$$

$$\sigma(r) \sim \frac{1}{\sqrt{r}}$$



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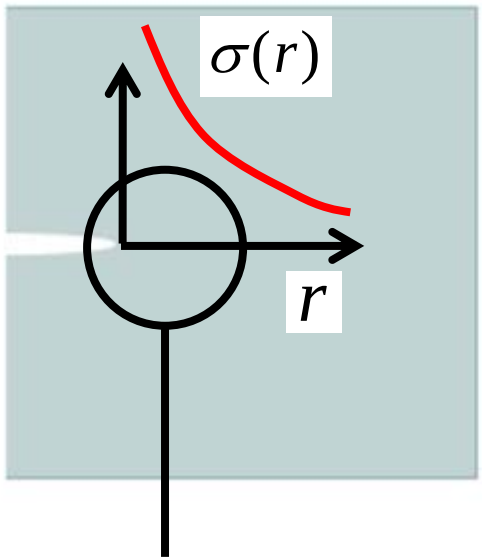
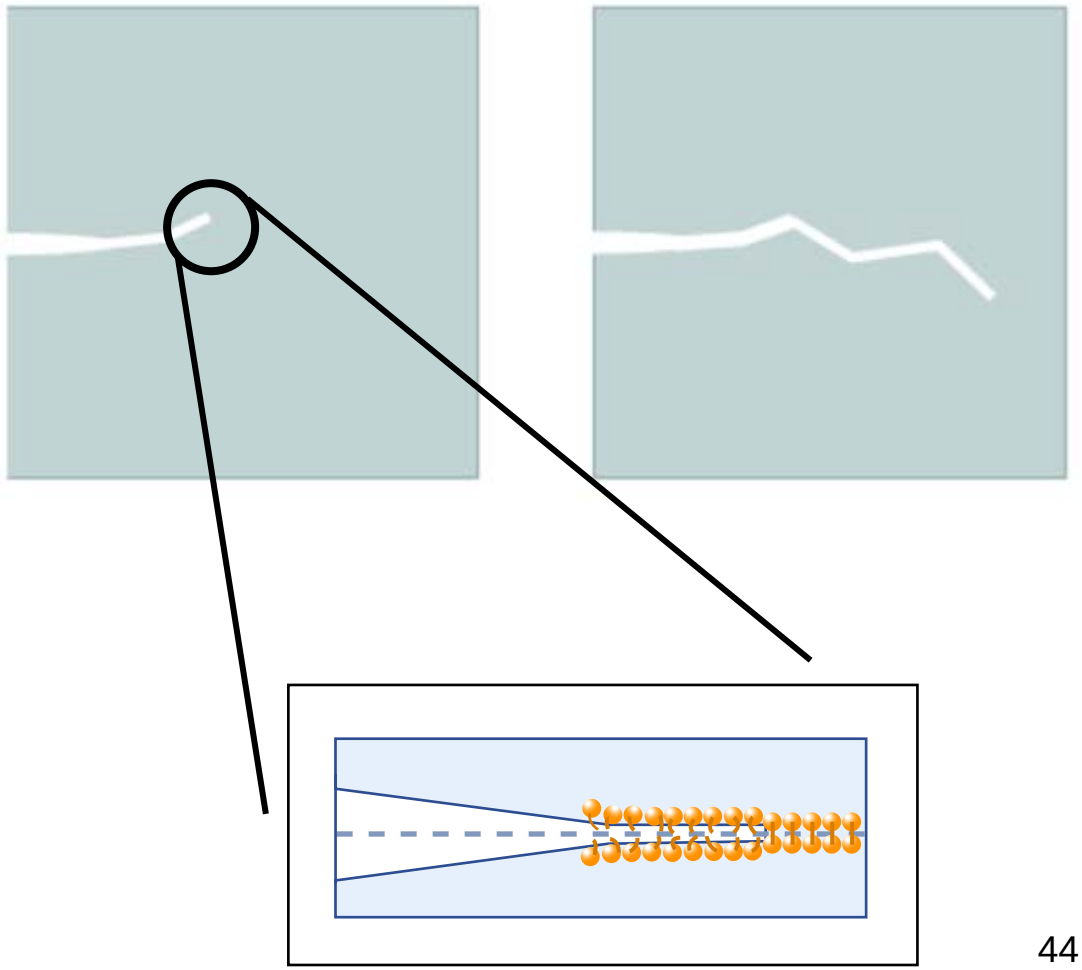
K_I : Stress intensity factor (function of geometry)

Crack extension: brittle response

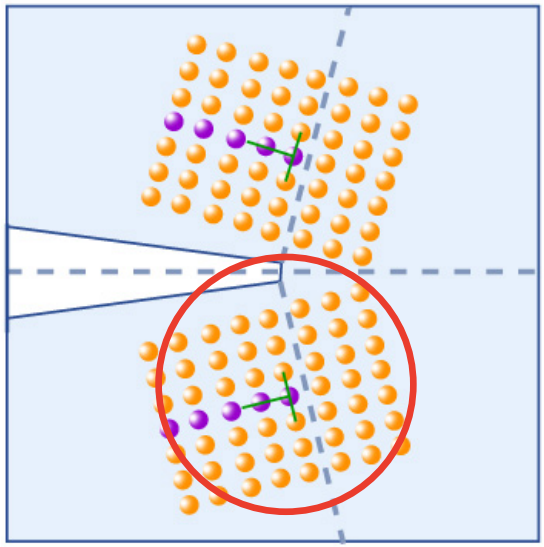




Large stresses lead to rupture of chemical bonds between atoms

Thus, crack extends

Lattice shearing: ductile response



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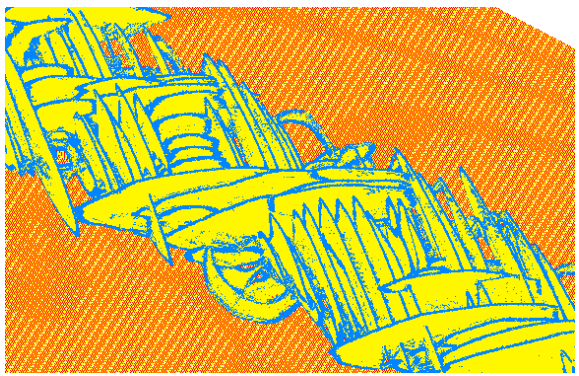
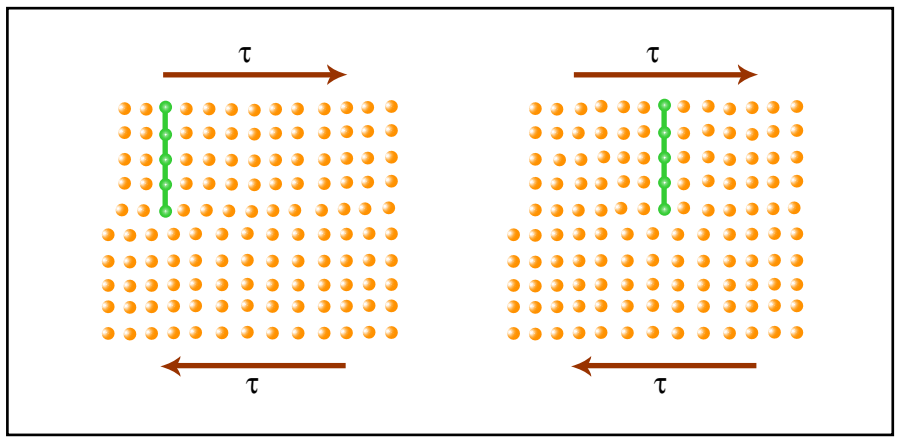
- Instead of crack extension, induce shearing of atomic lattice
- Due to large shear stresses at crack tip
- Lecture 5





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Brittle vs. ductile material behavior

- Whether a material is ductile or brittle depends on the material's propensity to undergo **shear at the crack tip**, or to **break atomic bonds that leads to crack extension**
- Intimately linked to the **atomic structure and atomic bonding**
- **Related to temperature (activated process)**; some mechanism are easier accessible under higher/lower temperature
- Many materials show a **propensity towards brittleness at low temperature**
- ***Molecular dynamics is a quite suitable tool to study these mechanisms, that is, to find out what makes materials brittle or ductile***

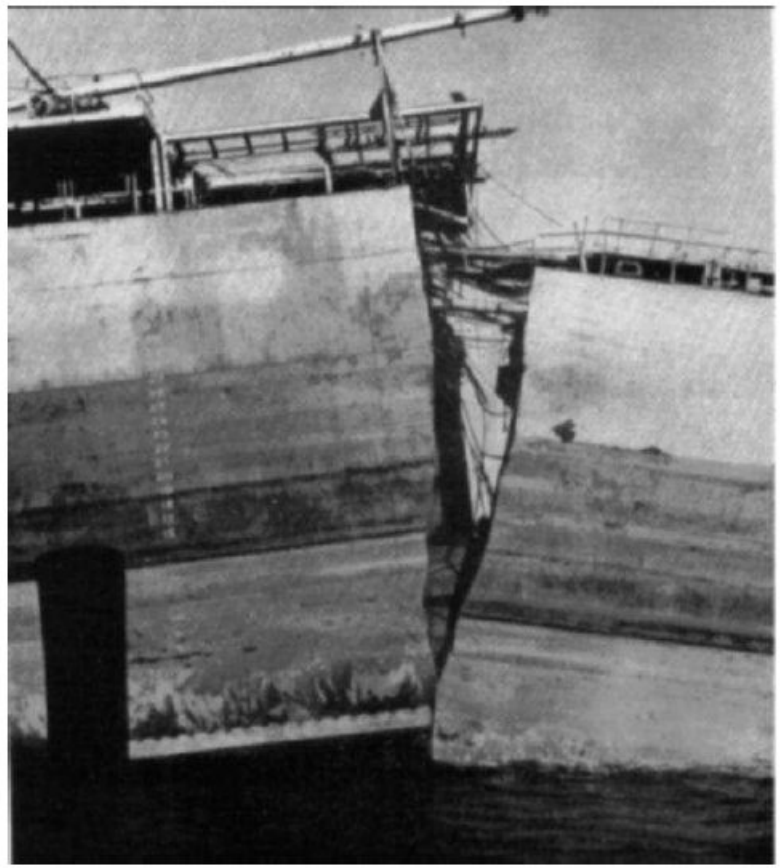
Historical example: significance of brittle vs. ductile fracture

- **Liberty ships**: cargo ships built in the U.S. during World War II (during 1930s and 40s)
- Eighteen U.S. shipyards built 2,751 Liberties between 1941 and 1945
- Early Liberty ships suffered hull and deck cracks, and several were lost to such structural defects

- Twelve ships, including three of the 2710 Liberties built, broke in half without warning, including the **SS John P. Gaines (sank 24 November 1943)**

- **Constance Tipper** of Cambridge University demonstrated that the fractures were initiated by the grade of steel used which suffered from **embrittlement**.
- She discovered that the ships in the North Atlantic were exposed to **temperatures** that could fall below a critical point when the **mechanism of failure changed from ductile to brittle**, and thus the hull could fracture relatively easily.

Liberty ships: brittle failure



Courtesy of the U.S. Navy.

4. Basic deformation mechanism in brittle materials - crack extension

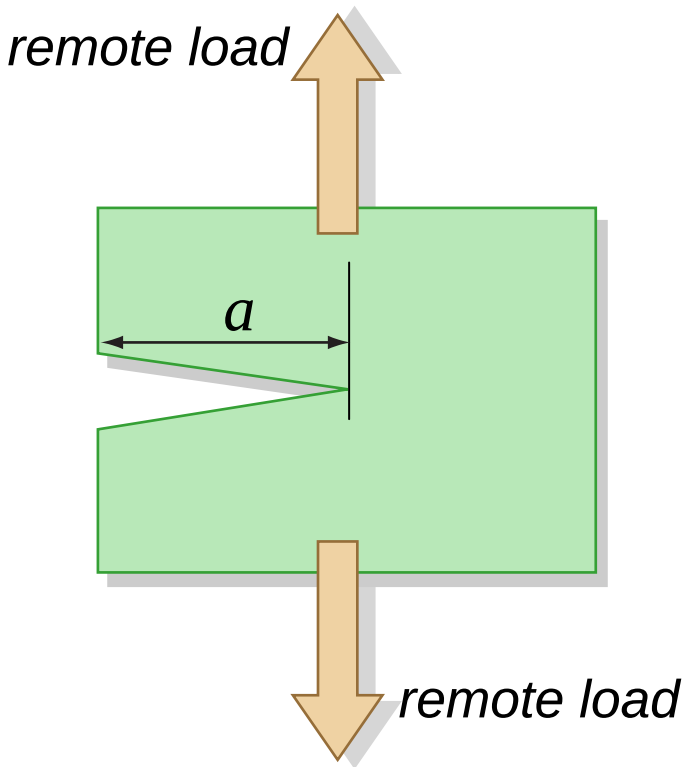
Introduction: brittle fracture

- Materials: **glass, silicon, many ceramics, rocks**

- At large loads, rather than accommodating a shape change, materials break

Science of fracture: model geometry

- Typically consider a single crack in a crystal
- Remotely applied mechanical load
- Following discussion focused on single cracks and their behavior



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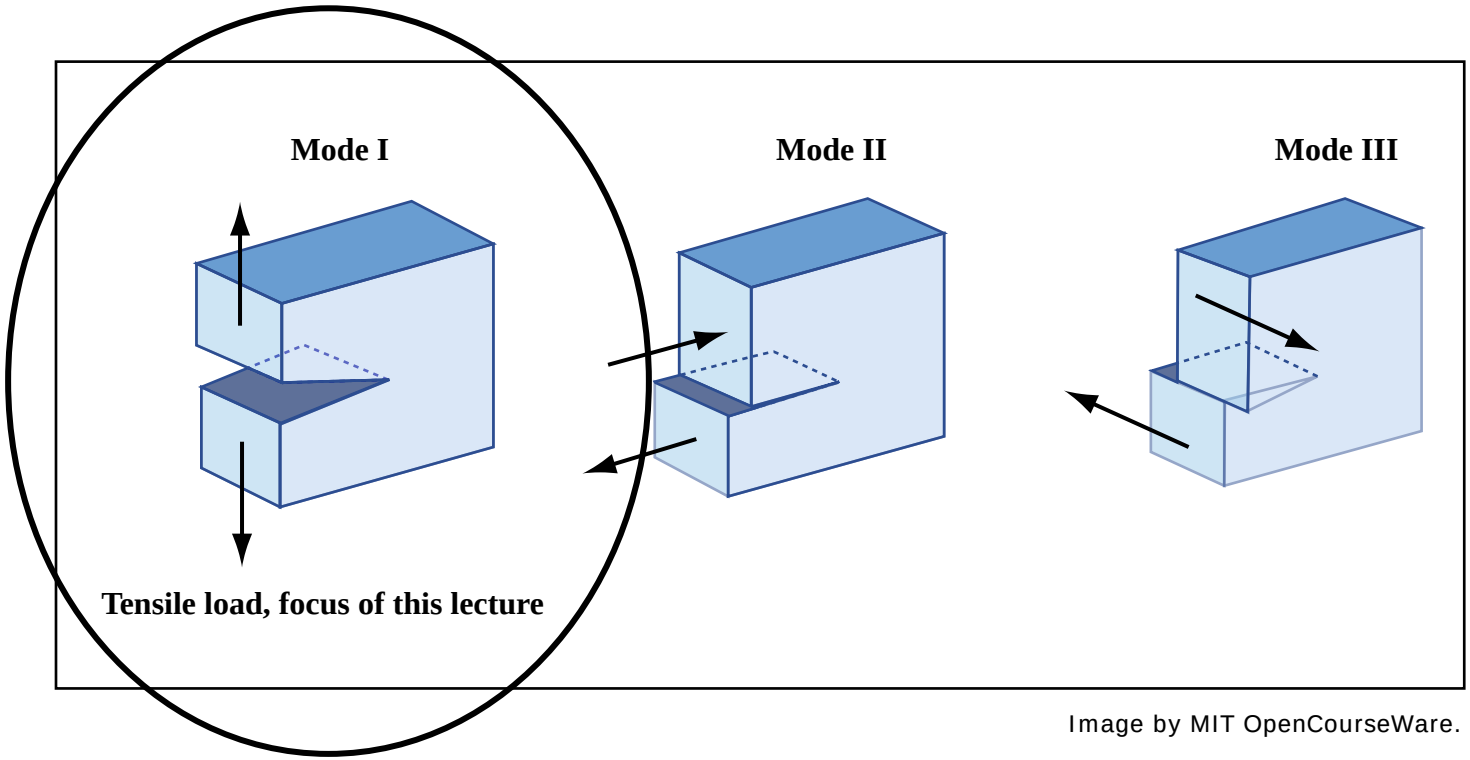
Brittle fracture loading conditions

- Commonly consider a single crack in a material geometry, under three types of loading: mode I, mode II and mode III



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Tensile load, focus of this lecture

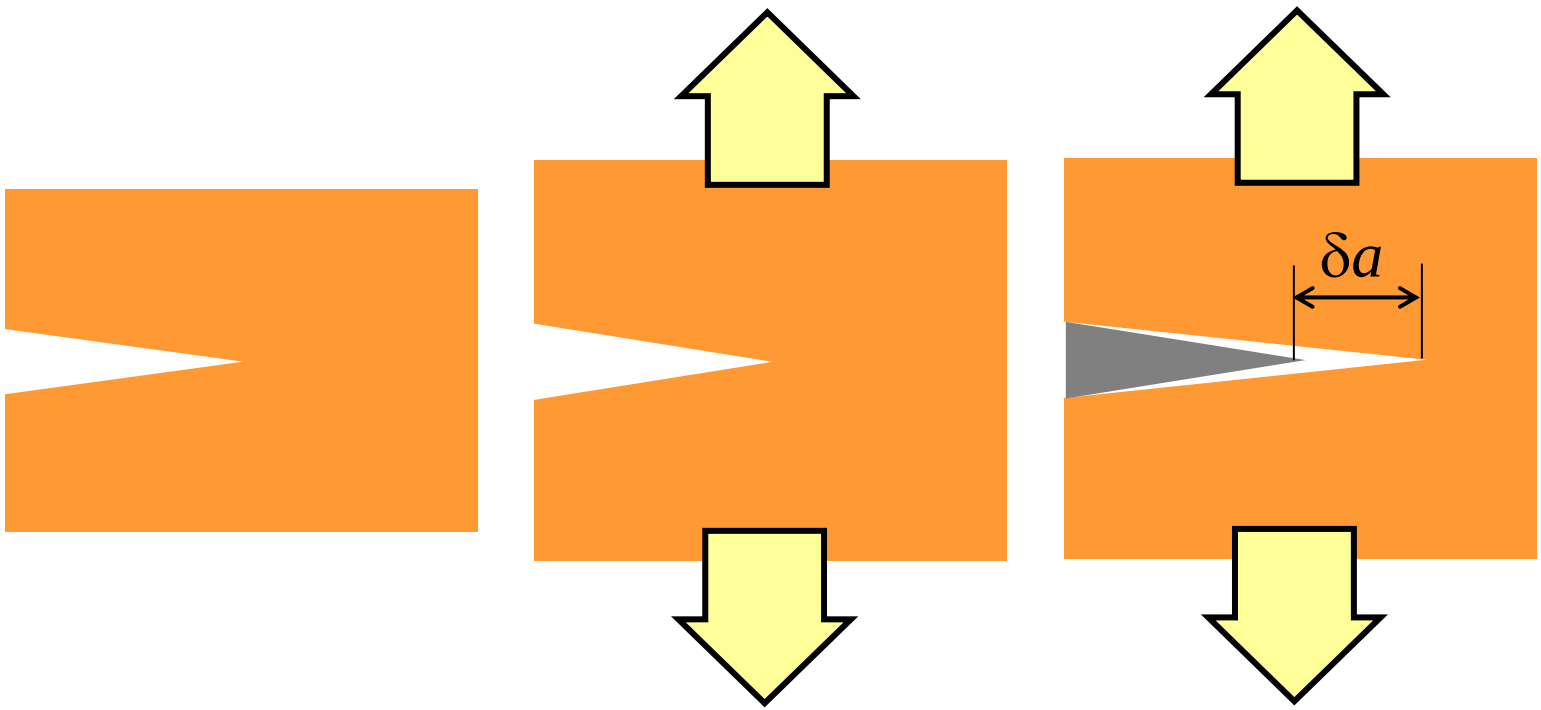
Brittle fracture mechanisms: fracture is a multi-scale phenomenon, from nano to macro

Image removed due to copyright restrictions. See Fig. 6.2 in Buehler, Markus J. *Atomistic Modeling of Materials Failure*. Springer, 2008.

Focus of this part

- **Basic fracture process**: dissipation of elastic energy
- **Fracture initiation**, that is, at what applied load to fractures initiate
- **Fracture dynamics**, that is, how fast can fracture propagate in material

Basic fracture process: dissipation of elastic energy

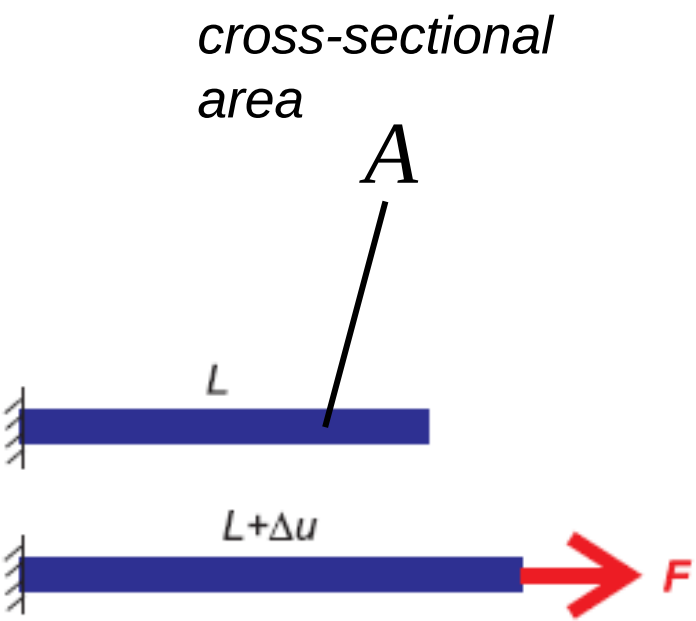


Undeformed

Stretching=store elastic energy

Release elastic energy dissipated into breaking chemical bonds

Elasticity = reversible deformation



Stress?

Force per unit area

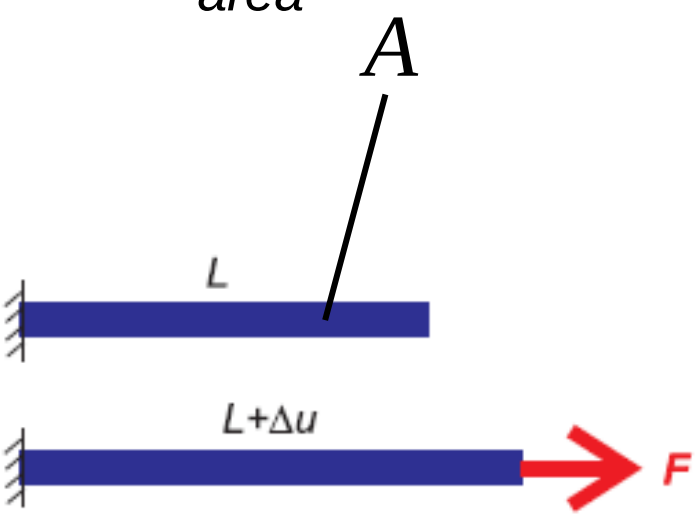
Elasticity = reversible deformation

cross-sectional area

$$\sigma = F / A$$

Stress?

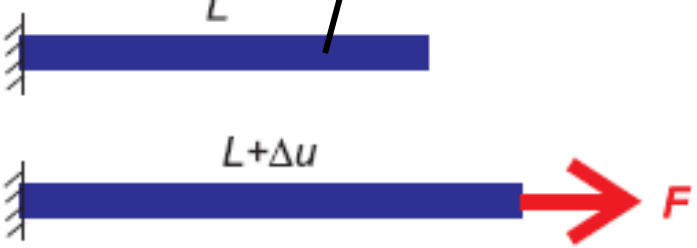
Force per unit area



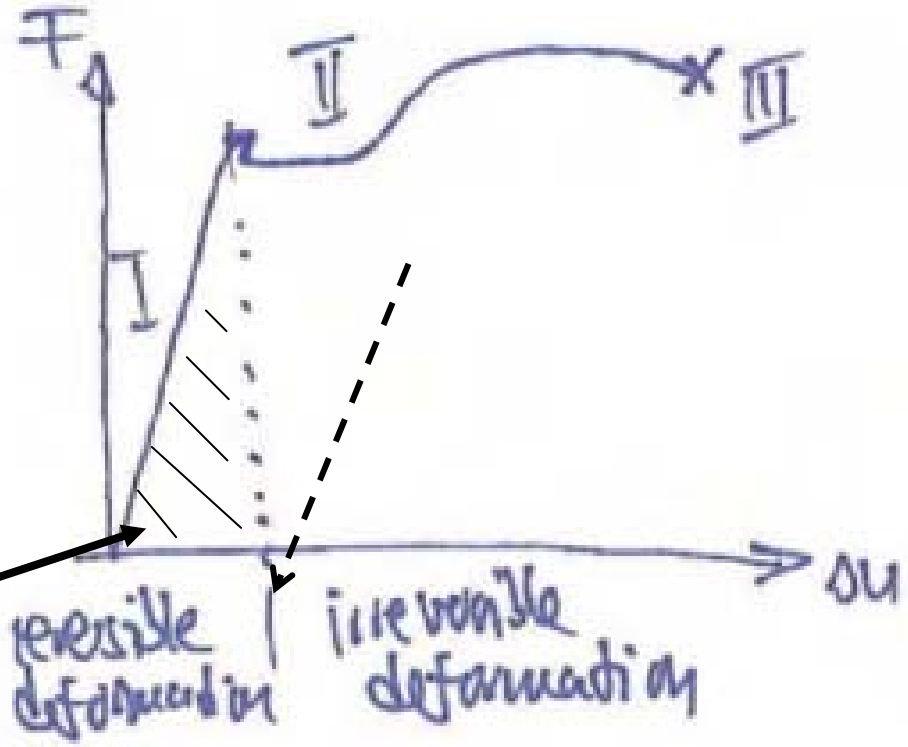
Elasticity = reversible deformation

cross-sectional area

A



$$\sigma = F / A$$



area under curve: stored energy

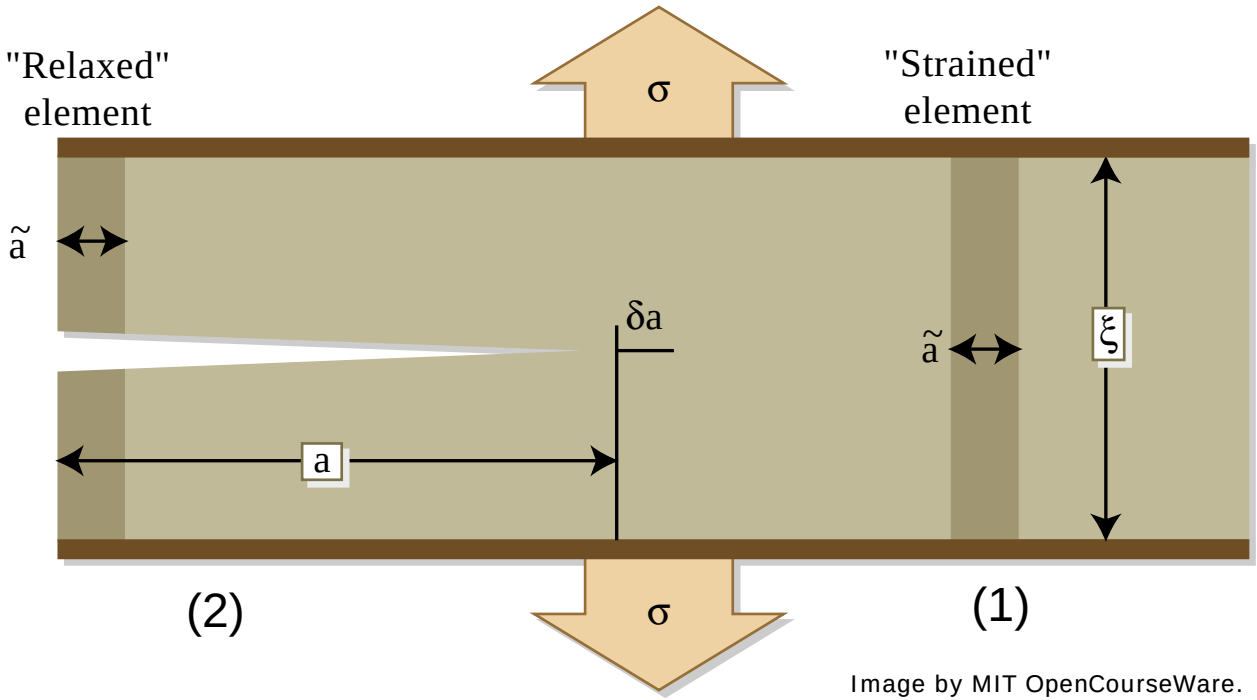
$$\varepsilon = \Delta u / L$$

$$\sigma = E\varepsilon$$

Young's modulus

Continuum description of fracture

- Fracture is a dissipative process in which elastic energy is dissipated to break bonds (and to heat at large crack speeds)
- Energy to break bonds = surface energy γ_s (energy necessary to create new surface, dimensions: energy/area, $\mathrm{Nm/m^2}$)



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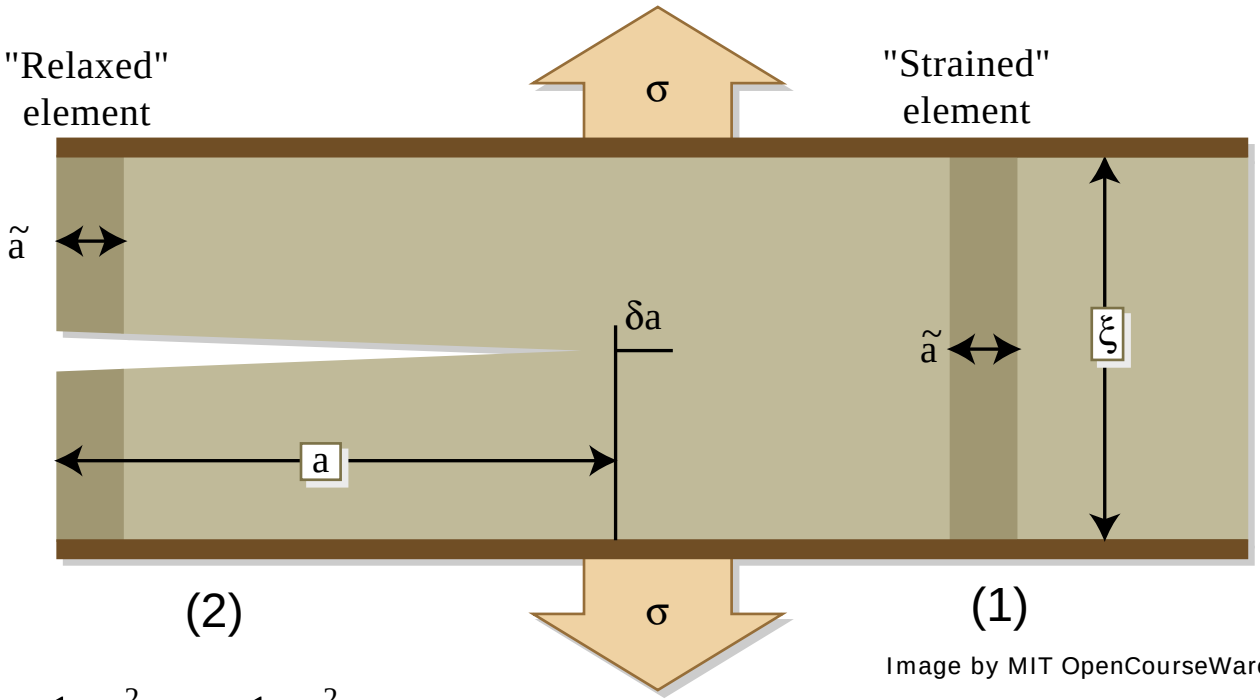

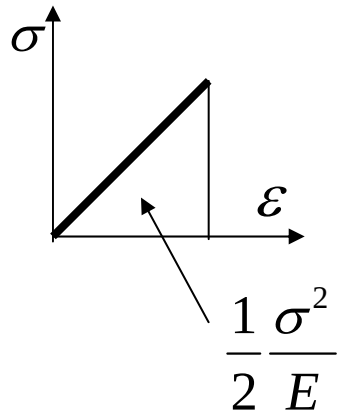

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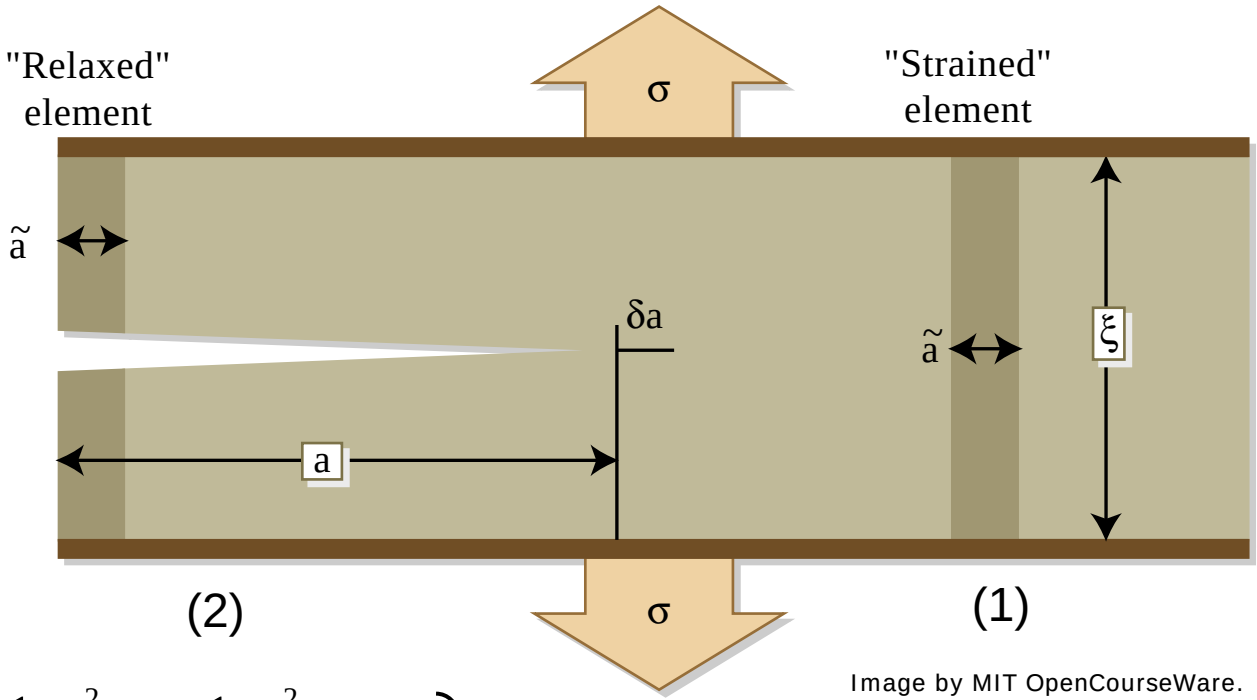
$$W_P(1) = \frac{1}{2}\frac{\sigma^2}{E}V = \frac{1}{2}\frac{\sigma^2}{E}\xi\tilde{a}B$$

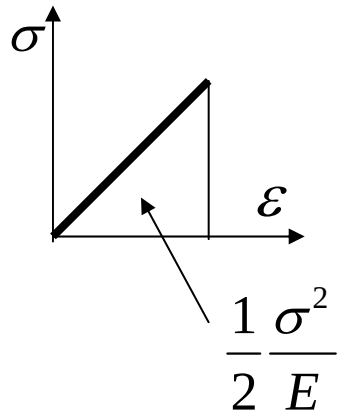
B out-of-plane thickness

$$W_P(2) = 0$$

Continuum description of fracture

- Fracture is a dissipative process in which elastic energy is dissipated to break bonds (and to heat at large crack speeds)
- Energy to break bonds = surface energy γ_s (energy necessary to create new surface, dimensions: energy/area, $\mathrm{Nm/m^2}$)





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$$W_P(1) = \frac{1}{2}\frac{\sigma^2}{E}V = \frac{1}{2}\frac{\sigma^2}{E}\xi\tilde{a}B$$

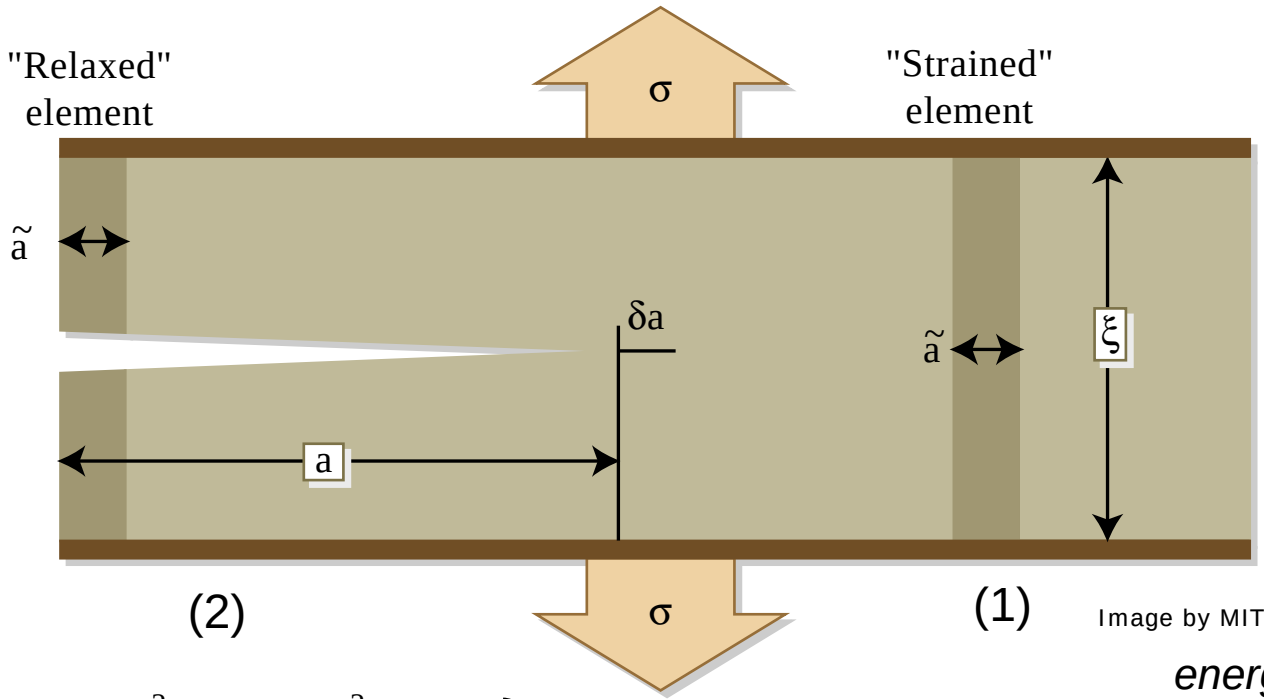
$$W_P(2) = 0$$

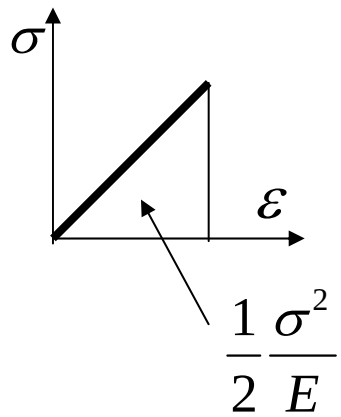
$$W_P(2) - W_P(1) = \underbrace{\frac{1}{2}\frac{\sigma^2}{E}\xi\tilde{a}B}$$

change of elastic (potential) energy

Continuum description of fracture

- Fracture is a dissipative process in which elastic energy is dissipated to break bonds (and to heat at large crack speeds)
- Energy to break bonds = surface energy γ_s (energy necessary to create new surface, dimensions: energy/area, $\mathrm{Nm/m^2}$)





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$$W_P(1) = \frac{1}{2}\frac{\sigma^2}{E}V = \frac{1}{2}\frac{\sigma^2}{E}\xi\tilde{a}B$$

$$W_P(2) = 0$$

$$W_P(2) - W_P(1) = \underbrace{\frac{1}{2}\frac{\sigma^2}{E}\xi\tilde{a}B}_{\text{change of elastic (potential) energy}} \overset{!}{=} \overbrace{2\gamma_s\tilde{a}B}^{\text{energy to create surfaces}}$$

Continuum description of fracture

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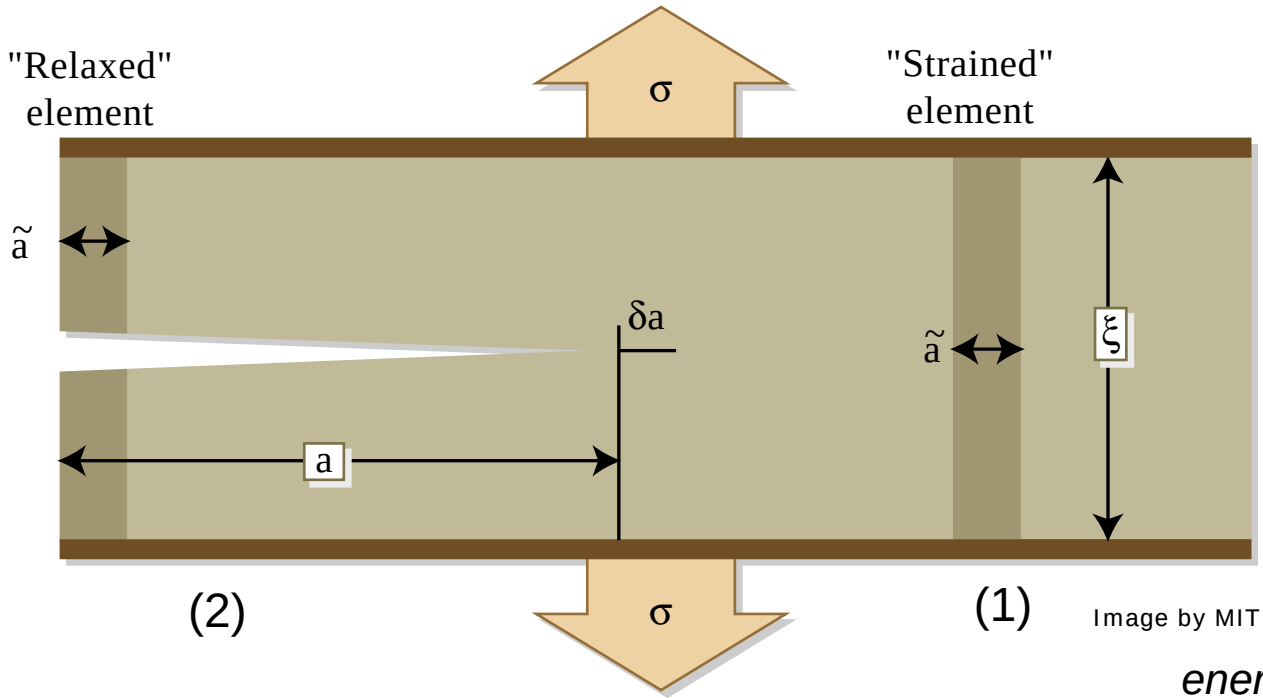

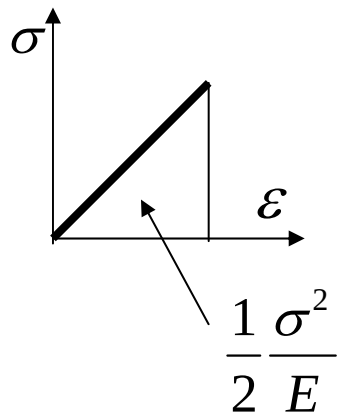

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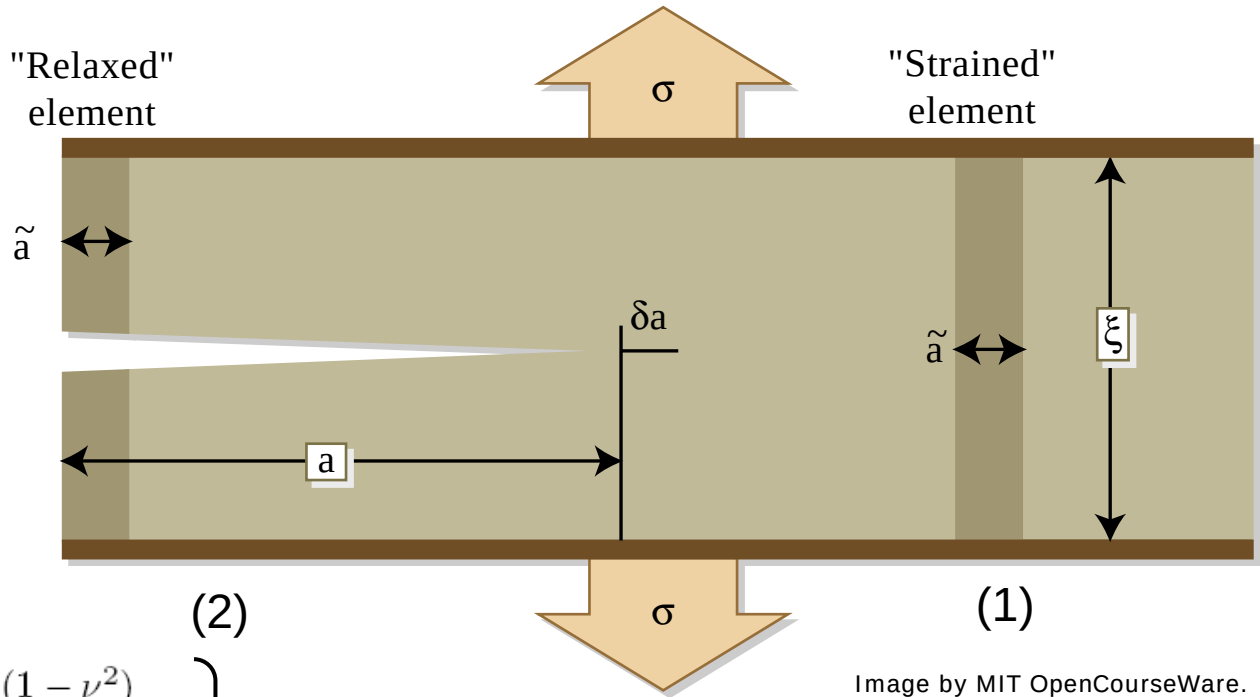
$$\sigma = \sqrt{\frac{4\gamma_s E}{\xi}}$$

Continuum description of fracture

- Fracture is a dissipative process in which elastic energy is dissipated to break bonds (and to heat at large crack speeds)
- Energy to break bonds = surface energy γ_s (energy necessary to create new surface, dimensions: energy/area, $\mathrm{Nm/m^2}$)



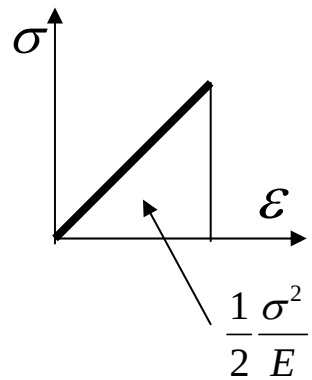


Image by MIT OpenCourseWare.

$$W_P^{(1)} = \frac{\sigma^2(1-\nu^2)}{2E}\xi\tilde{a}B$$

$$W_P^{(2)} = 0$$

$$W_P = W_P^{(2)} - W_P^{(1)} = \frac{1}{2}\frac{\sigma^2}{E}\xi\tilde{a}B \;!\; = 2\gamma_s B\tilde{a}$$

change of elastic (potential) energy = G

energy to create surfaces

$$\sigma = \sqrt{\frac{4\gamma_s E}{\xi}}$$

Griffith condition for fracture initiation

- **Energy release rate** G, that is, the elastic energy released per unit crack advance must be equal or larger than the energy necessary to create new surfaces

$$G := \frac{1}{2}\frac{\sigma^2}{E}\xi = 2y_s \qquad \boxed{G = 2\gamma_s}$$

- Provides **criterion to predict failure initiation**

- Calculation of G can be complex, but straightforward for thin strips as shown above

- Approach to calculate G based on "**stress intensity factor**" (see further literature, e.g. Broberg, Anderson, Freund, Tada)

Brittle fracture mechanisms

- Once nucleated, cracks in brittle materials spread rapidly, on the order of sound speeds

- Sound speeds in materials (=wave speeds):

  - Rayleigh-wave speed c_R (speed of surface waves)
  - shear wave speed c_s (speed of shear waves)
  - longitudinal wave speed c_l (speed of longitudinal waves)

- ***Maximum speeds of cracks is given by sound speeds, depending on mode of loading (mode I, II, III)***

  Linear elastic continuum theory

Sound speeds in materials: overview

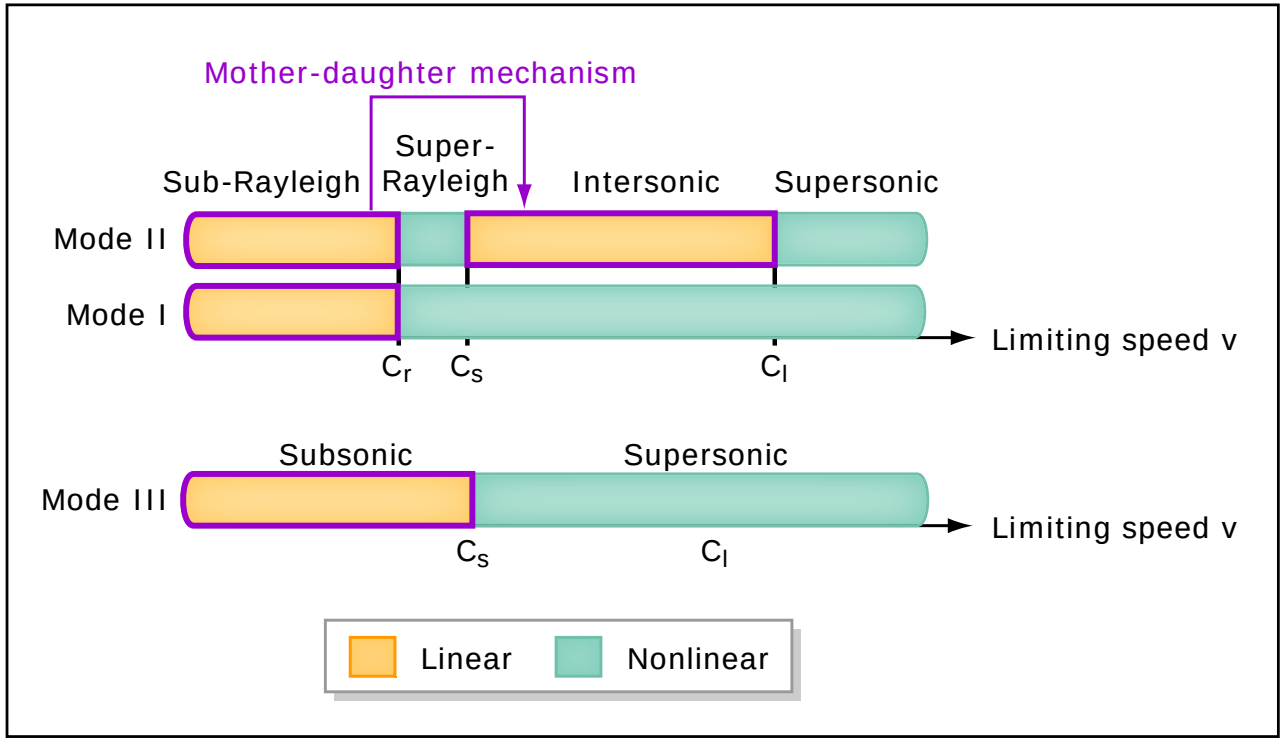
Material	c_R (in m/s)	c_s (in m/s)	c_l (in m/s)
Steel	2,940	3,200	6,000
Al	2,850	3,100	6,300
Glass	3,030	3,300	5,800
PMMA	920	1,000	2,400

Wave speeds are calculated based on elastic properties of material

$$c_l = \sqrt{\frac{3\mu}{\rho}} \qquad c_s = \sqrt{\frac{\mu}{\rho}} \qquad c_R \approx \beta c_s \qquad \beta \approx 0.923$$

μ = shear modulus $\qquad E = 8/3\mu \qquad \mu = 3/8E$

Limiting speeds of cracks: linear elastic continuum theory



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- Cracks **can not exceed** the limiting speed given by the corresponding wave speeds **unless material behavior is nonlinear**
- Cracks that exceed limiting speed would produce energy (physically impossible - ***linear elastic continuum theory***)

Physical reason for crack limiting speed

- Physical (mathematical) reason for the limiting speed is that it becomes increasingly difficult to increase the speed of the crack by adding a larger load
- When the crack approaches the limiting speed, the **resistance to fracture diverges to infinity (=dynamic fracture toughness)**

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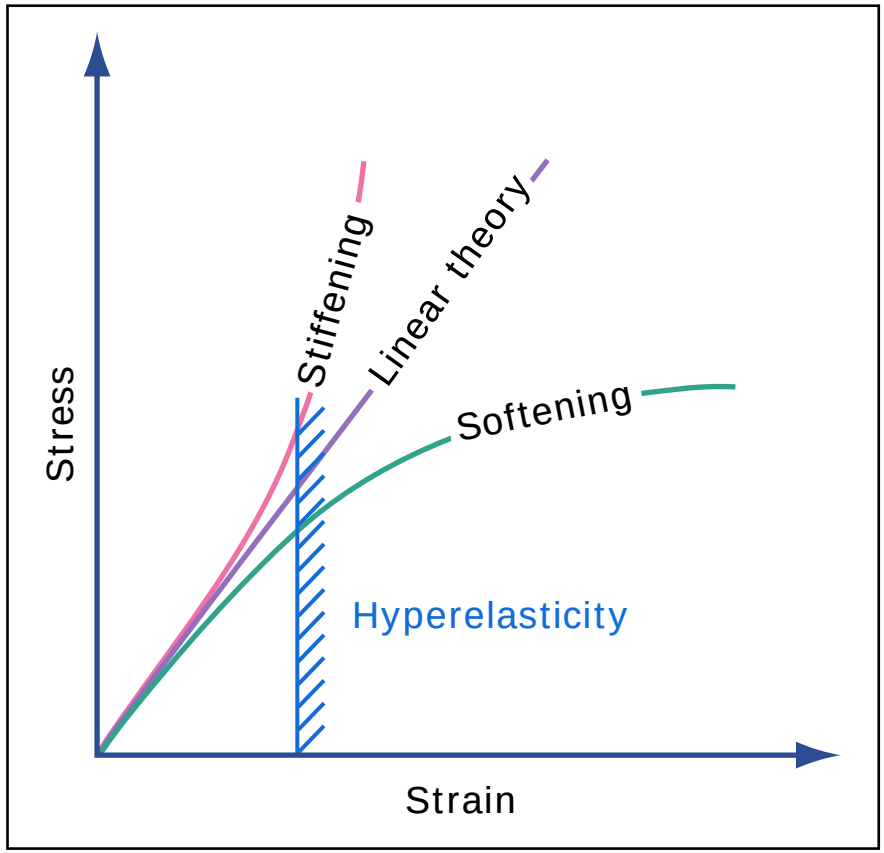
Please see: Fig. 6.15 in Buehler, Markus J. *Atomistic Modeling of Materials Failure*. Springer, 2008.

Linear versus nonlinear elasticity=hyperelasticity



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Linear elasticity: Young's modulus (stiffness) does not change with deformation

Nonlinear elasticity = hyperelasticity: Young's modulus (stiffness) changes with deformation

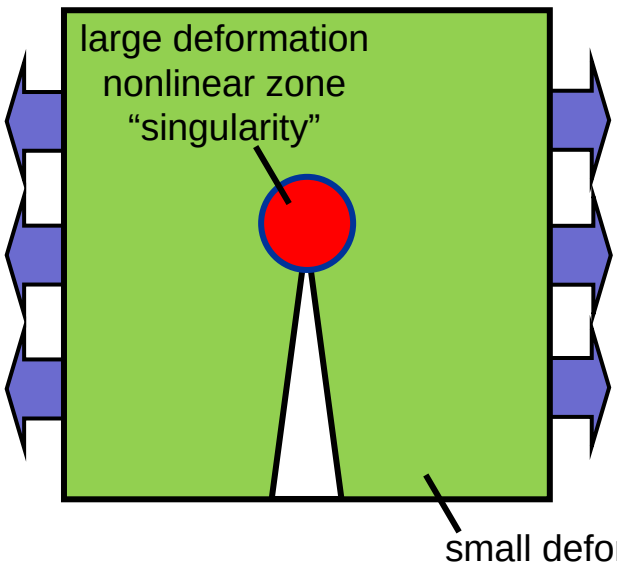
Subsonic and supersonic fracture

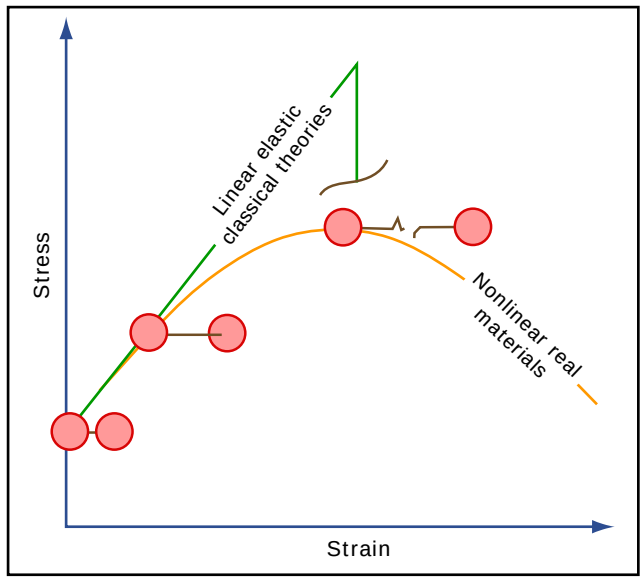
- Under certain conditions, material nonlinearities (that is, the behavior of materials under large deformation = hyperelasticity) becomes important

- This can lead to different limiting speeds than described by the model introduced above

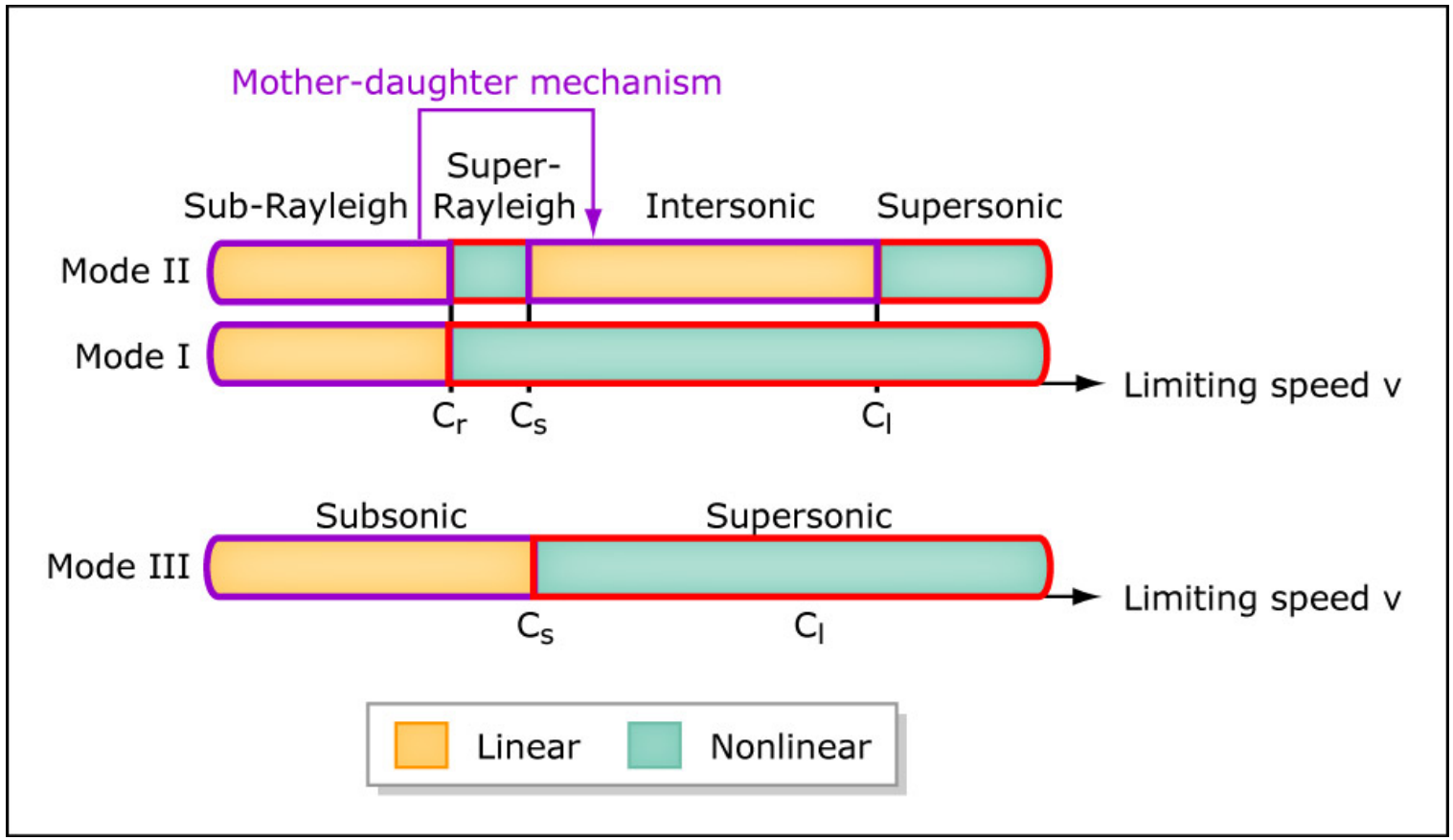
$$\sigma(r) \sim \frac{1}{\sqrt{r}}$$

Deformation field near a crack





Limiting speeds of cracks



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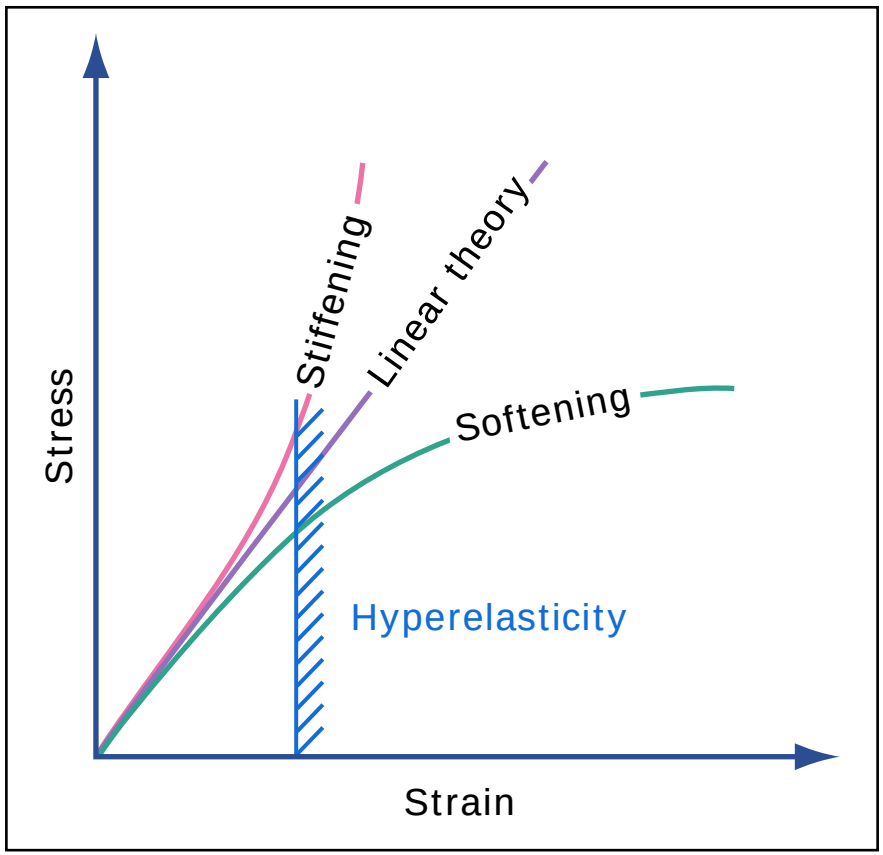
- Under presence of hyperelastic effects, cracks can exceed the conventional barrier given by the wave speeds
- This is a “local” effect due to enhancement of energy flux
- Subsonic fracture due to local softening, that is, reduction of energy flux

Stiffening vs. softening behavior

real materials



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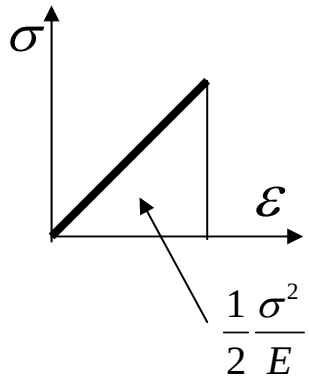
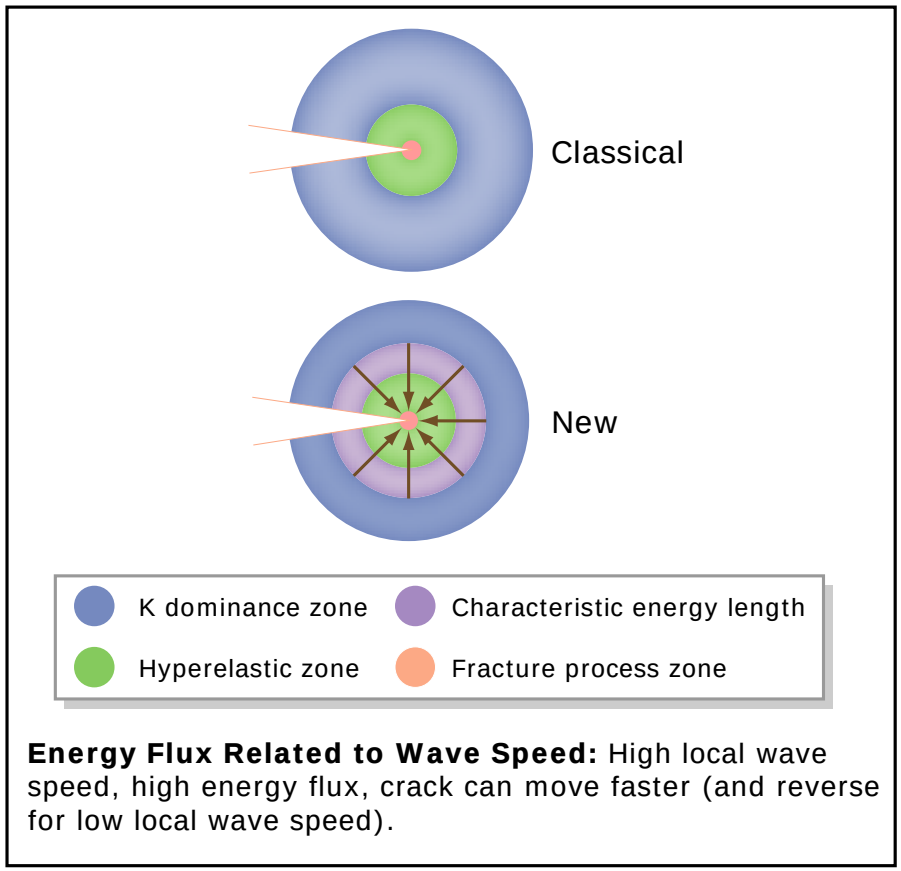
"linear elasticity"



Increased/decreased wave speed

$$c_l = \sqrt{\frac{3\mu}{\rho}} \qquad c_s = \sqrt{\frac{\mu}{\rho}} \qquad c_R \approx \beta c_s \qquad \beta \approx 0.923$$

Energy flux reduction/enhancement

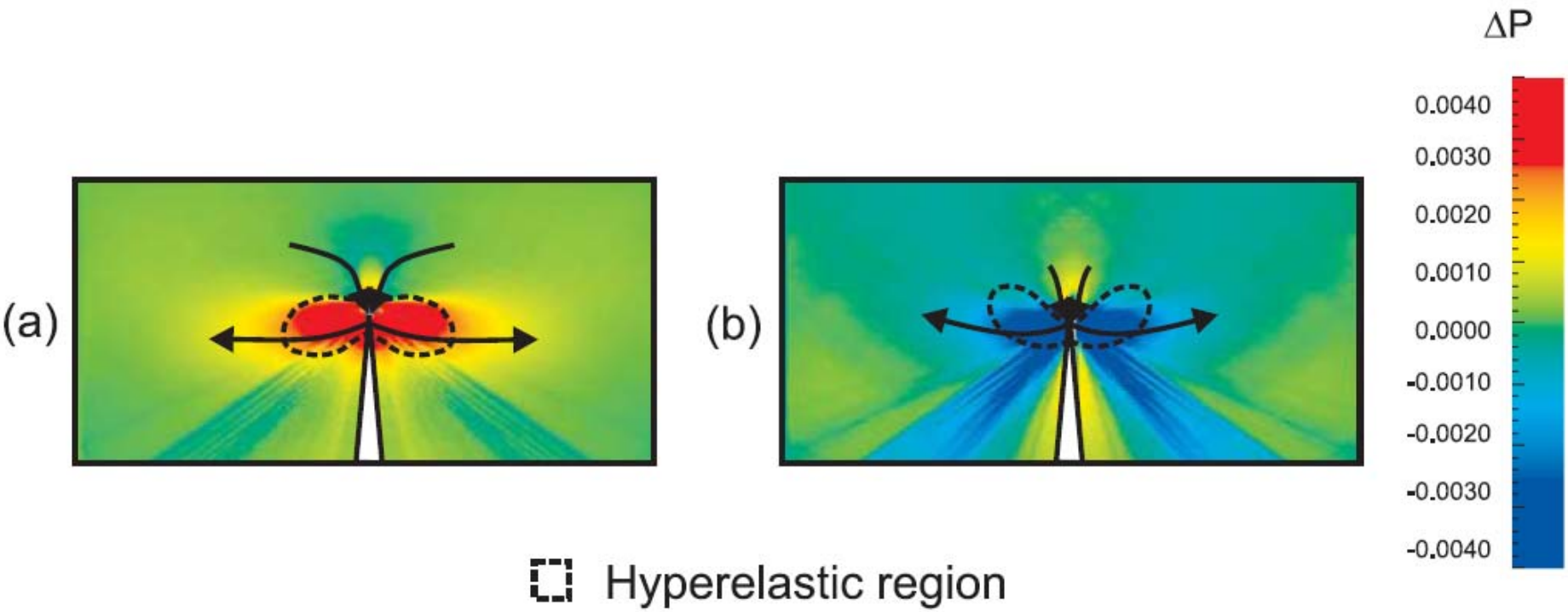


Energy Flux Related to Wave Speed: High local wave speed, high energy flux, crack can move faster (and reverse for low local wave speed).

Energy flux related to wave speed: high local wave speed, high energy flux, crack can move faster (and reverse for low local wave speed)

Physical basis for subsonic/supersonic fracture

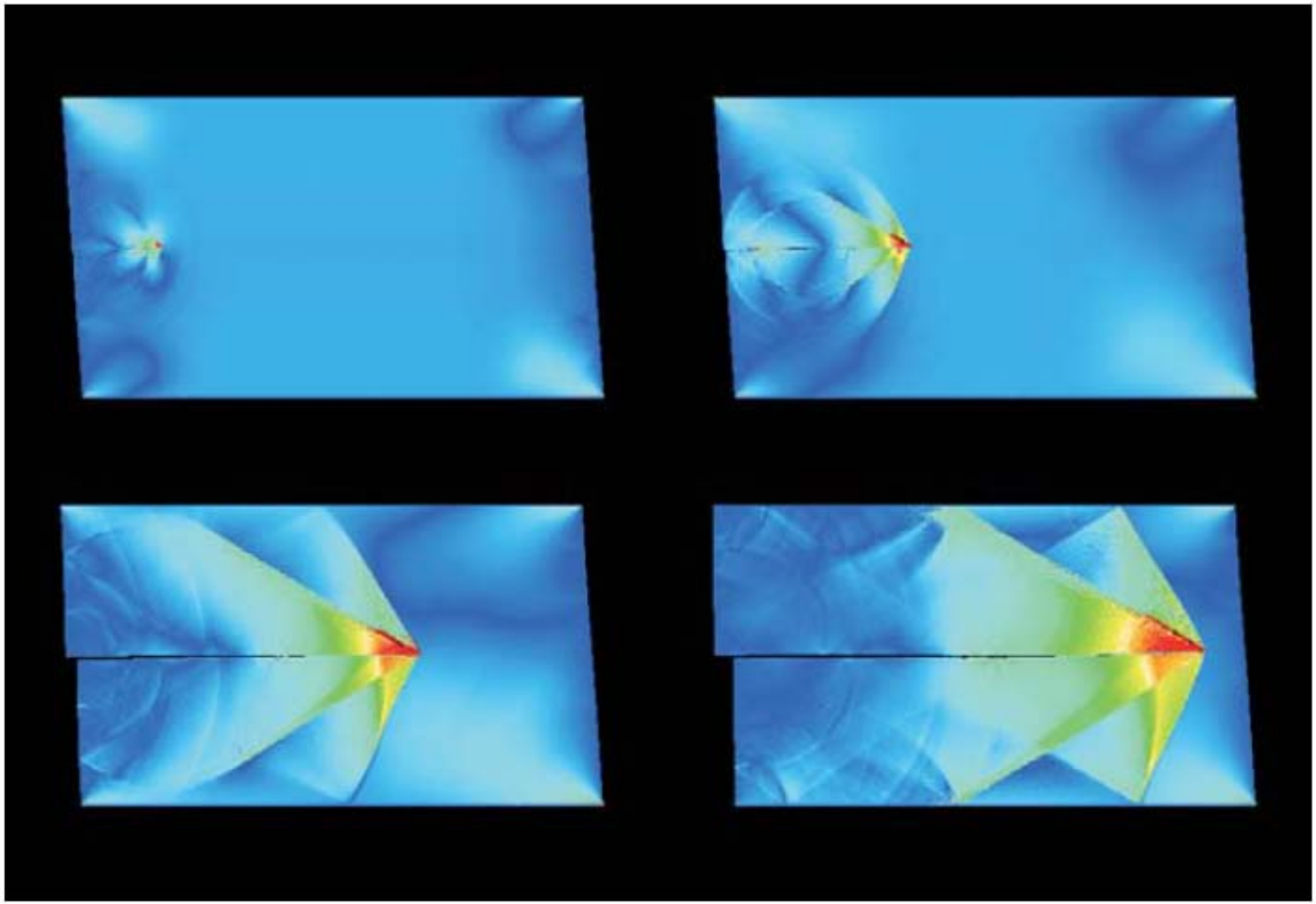
- Changes in energy flow at the crack tip due to changes in local wave speed (energy flux higher in materials with higher wave speed)
- Controlled by a characteristic length scale χ



Summary: atomistic mechanisms of brittle fracture

- Brittle fracture – **rapid spreading** of a small initial crack
- Cracks initiate based on **Griffith condition** $G = 2\gamma_s$
- Cracks spread on the order of **sound speeds** (km/sec for many brittle materials)
- Cracks have a **maximum speed**, which is given by characteristic sound speeds for different loading conditions)
- Maximum speed can be altered if material is strongly nonlinear, leading to **supersonic or subsonic fracture**

Supersonic fracture: mode II (shear)



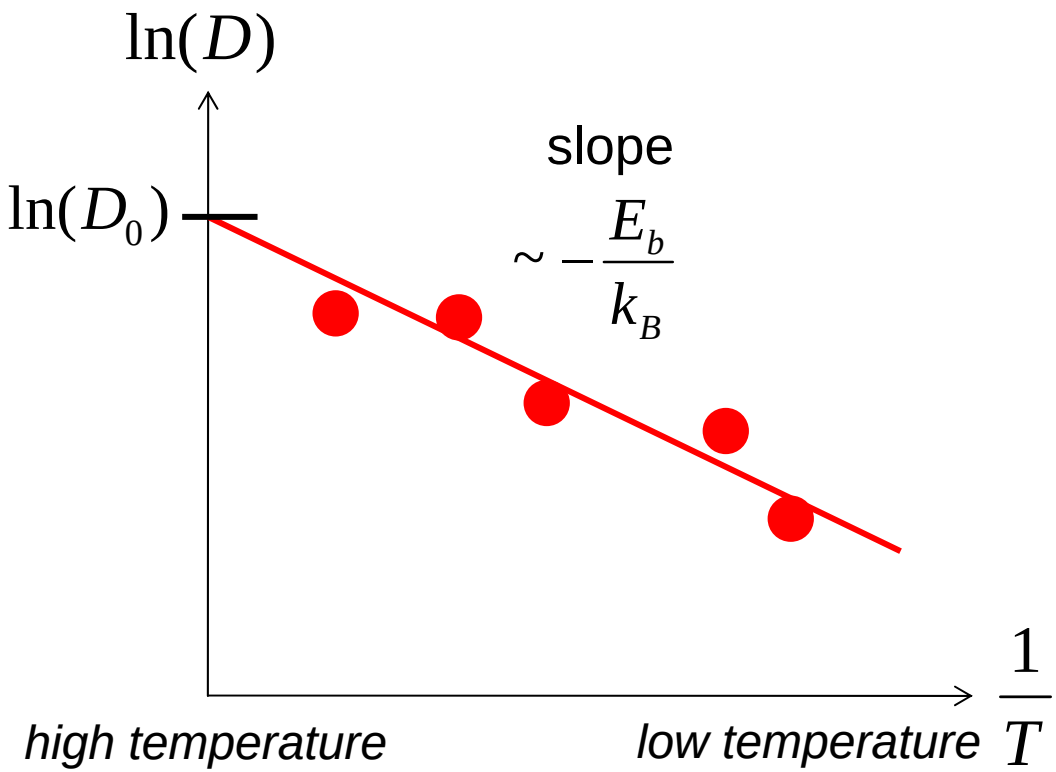
Please see: Buehler, Markus J., Farid F. Abraham, and Huajian Gao. "Hyperelasticity Governs Dynamic Fracture at a Critical Length Scale." *Nature* 426 (November 13, 2003): 141-146.

Appendix: Notes for pset #1

Notes regarding pset #1 (question 1.)

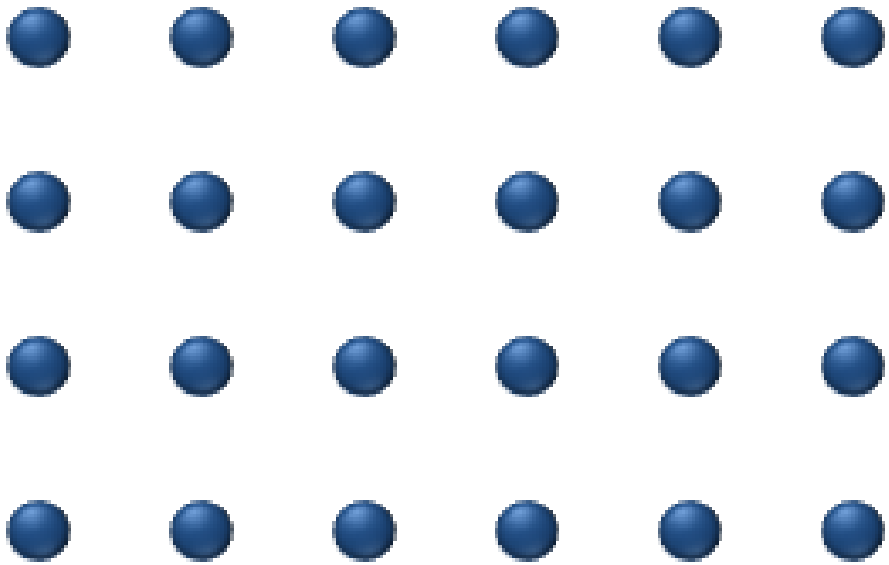
$$D = D_0 \exp\left(-\frac{E_b}{k_B T}\right)$$

$$\ln(D) = \ln(D_0) - \frac{E_b}{k_B T}$$



Plot data extracted from RMSD graph, then fit equation above and identify parameters

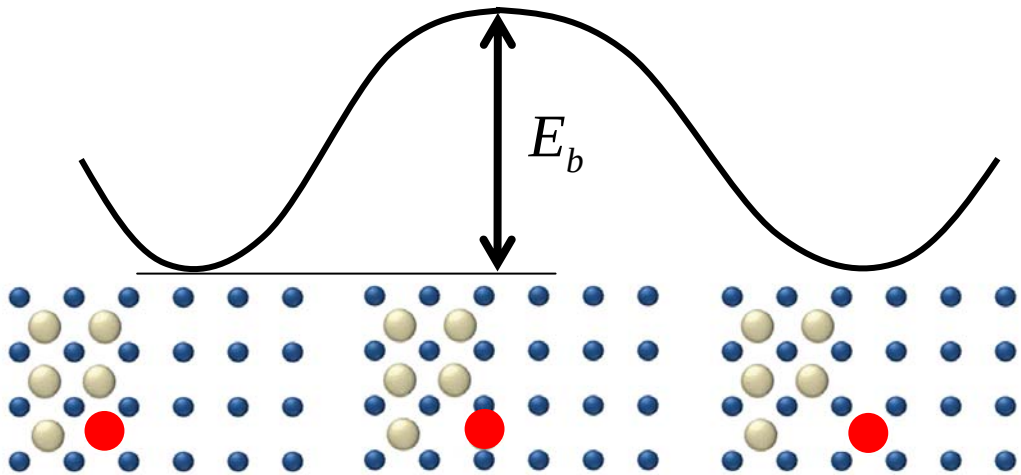
Mechanism and energy barrier



$$D = D_0 \exp\left(-\frac{E_b}{k_B T}\right)$$

D_0 : Rate of attempt

"transition state"



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