Deformation of Ductile Materials (cont'd) Fracture of brittle materials

Lecture 5

Department of
Civil & Environmental Engineering
Massachusetts Institute of Technology

Markus J. Buehler

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. **The Cauchy-Born rule**
   Calculation of elastic properties of atomic lattices
   Friday Jan 19, 09-10:30am

5. **Dynamic Fracture of Brittle Materials**
   Nonlinear elasticity in dynamic fracture, geometric confinement, interfaces
   Wednesday Jan 17, 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

- **Topic:** Fracture mechanisms in ductile materials.

- **Examples:** Large-scale simulation of a copper nanocrystal – analysis of dislocation mechanisms

- **Material covered:** Metallic bonding, EAM potentials, energy approach to elasticity, Cauchy-Borne rule; basics in fracture mechanics – prediction of dislocation nucleation and crack extension

- **Important lesson:** Dislocation as fundamental carrier of plasticity, driving force for fracture processes, competition between ductile and brittle processes

- **Historical perspective:** Origin of Griffith's fracture theory
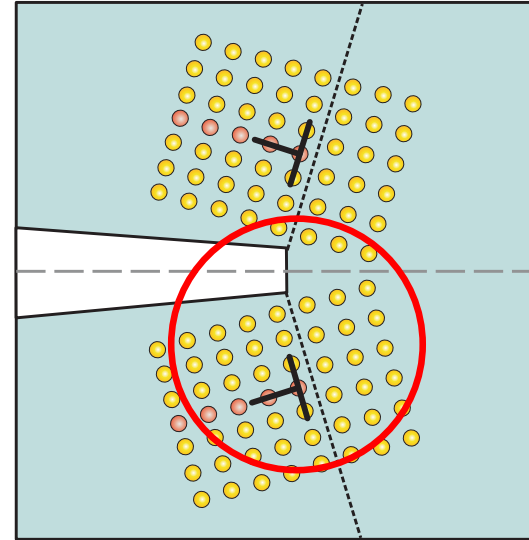
Ductile versus brittle materials

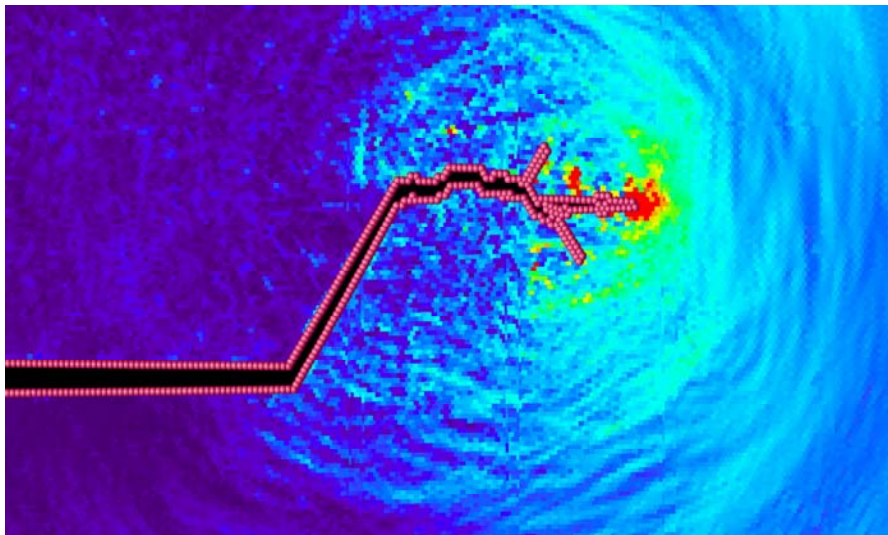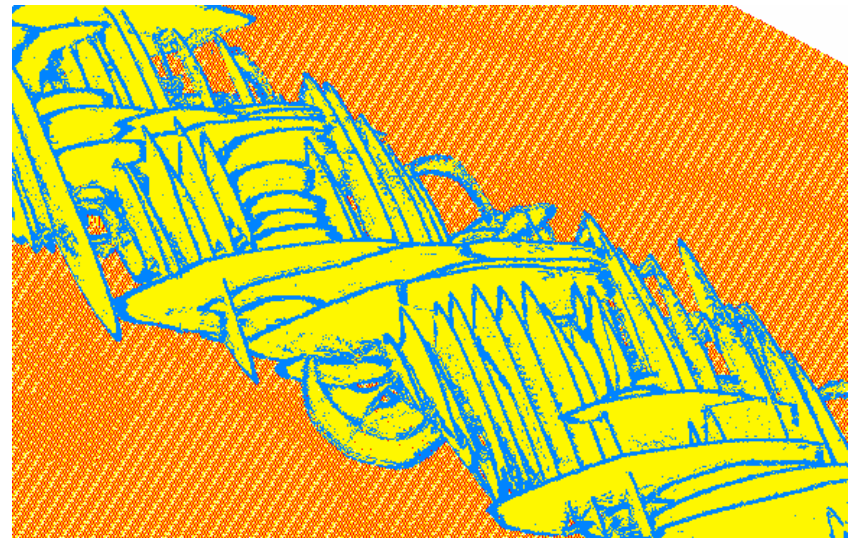brittle

ductile

Glass,
Polymers,
Ice…

Surface
energy!
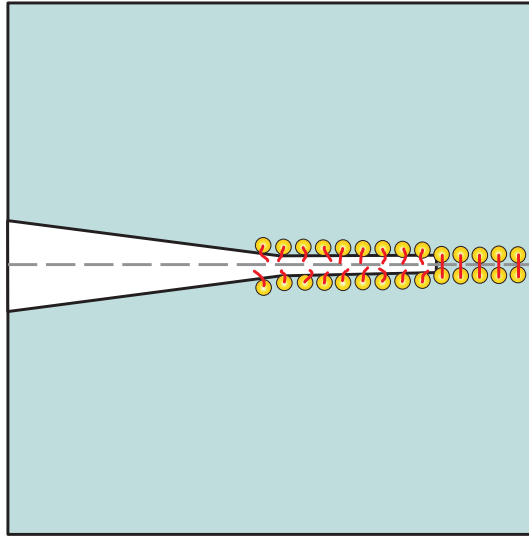
Copper,
Gold,
…

shear load

(a)
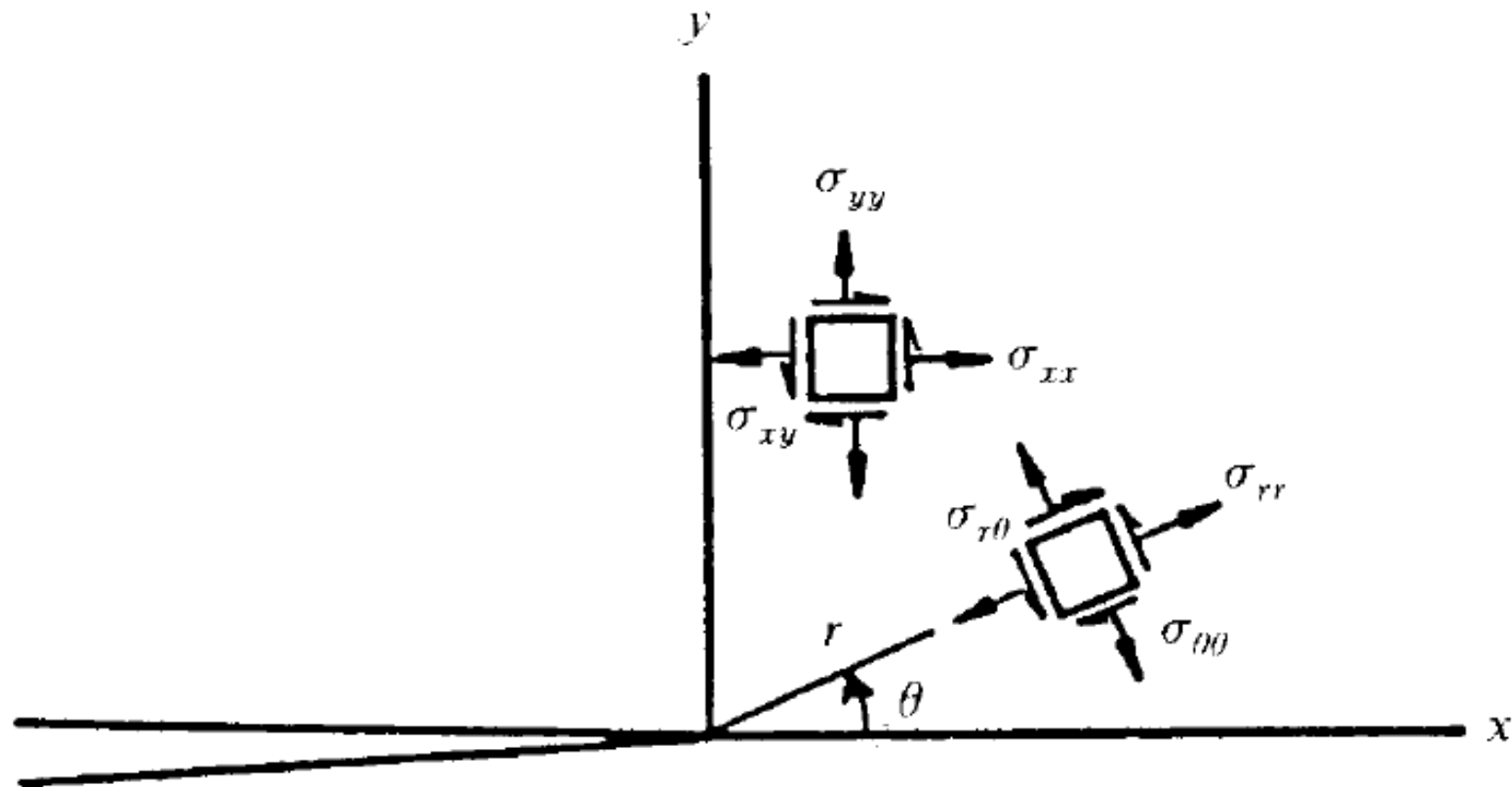
(b)

■ **Derivation stress field around crack tip**

See lecture notes

Asymptotic stress field

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0,$$

$$\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{2\sigma_{r\theta}}{r} = 0.$$

EQ eq.

$$\frac{\partial^2 \epsilon_{\theta\theta}}{\partial r^2} + \frac{2}{r} \frac{\partial \epsilon_{\theta\theta}}{\partial r} - \frac{1}{r} \frac{\partial^2 \epsilon_{r\theta}}{\partial r \partial \theta} - \frac{1}{r^2} \frac{\partial \epsilon_{r\theta}}{\partial \theta} + \frac{1}{r^2} \frac{\partial \epsilon_{rr}^2}{\partial \theta^2} - \frac{1}{r} \frac{\partial \epsilon_{rr}}{\partial r} = 0.$$

Compat. cond.

$$\sigma_{rr} = \frac{1}{r} \frac{\partial \chi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \chi}{\partial \theta^2}, \qquad \sigma_{\theta\theta} = \frac{\partial^2 \chi}{\partial r^2}, \qquad \sigma_{r\theta} = -\frac{\partial}{\partial r}\left(\frac{1}{r} \frac{\partial \chi}{\partial \theta}\right)$$

$$\chi = r^{(\lambda+2)} \left[A_1 \cos \lambda\theta + B_1 \cos(\lambda+2)\theta\right]$$

$$+ r^{(\lambda+2)}\left[A_2 \sin \lambda\theta + B_2 \sin(\lambda+2)\theta\right]$$

Airy stress function: Ansatz

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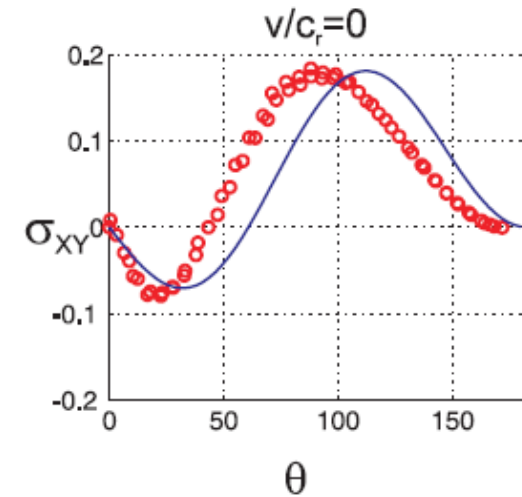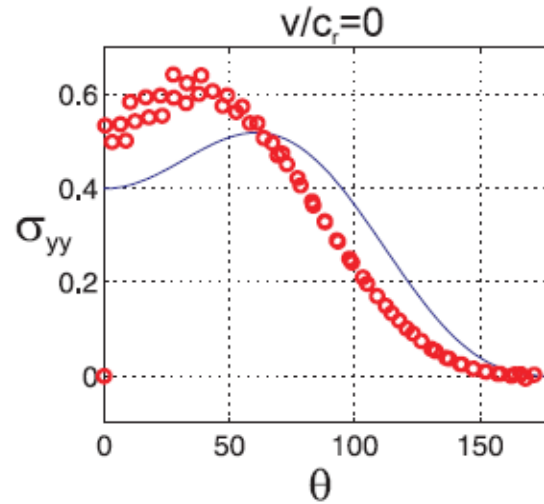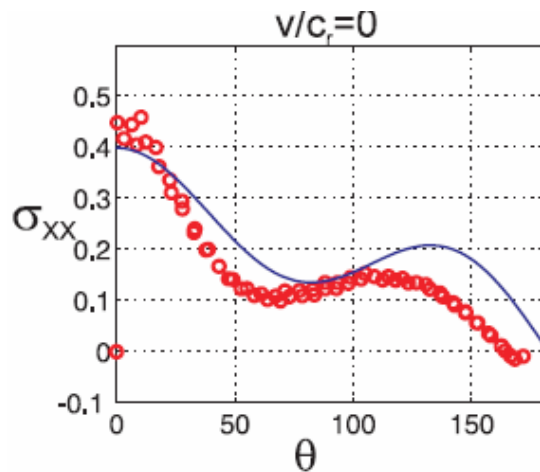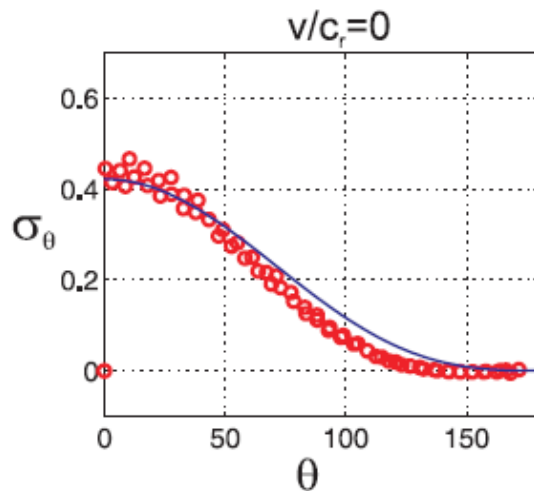
$$\begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{r\theta} \end{Bmatrix} = \frac{K_I}{\sqrt{2\pi r}} \cos\frac{\theta}{2} \begin{Bmatrix} 1 + \sin^2\frac{\theta}{2} \\ \cos^2\frac{\theta}{2} \\ \sin\frac{\theta}{2}\cos\frac{\theta}{2} \end{Bmatrix}$$

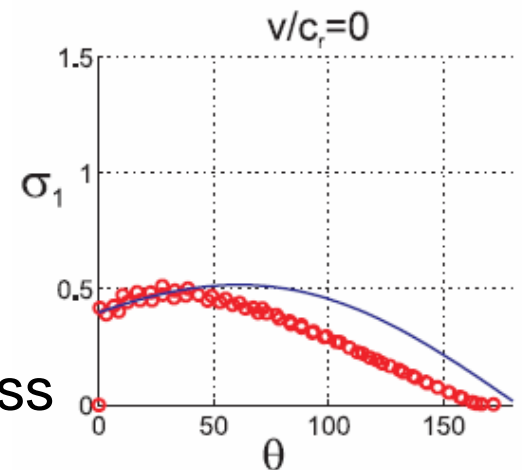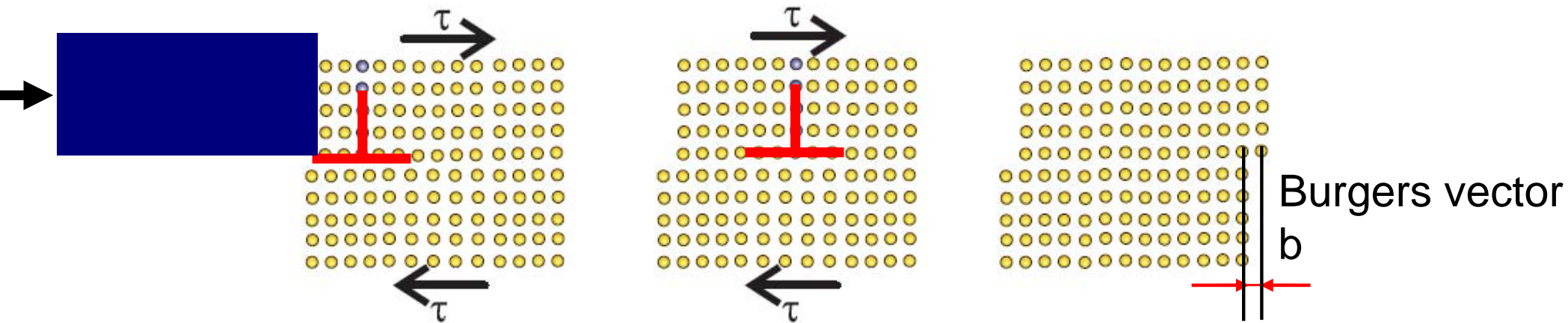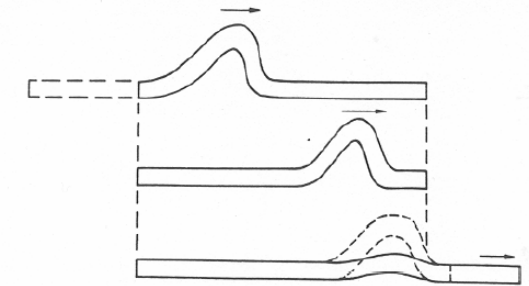# Stress field around a (static) crack
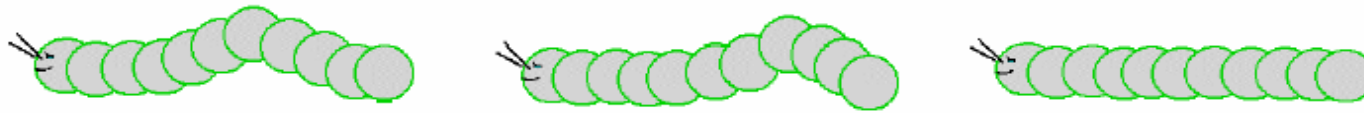

Hoop or opening stress

Maximum principal stress

Continuum theory
○ MD modeling

Burgers vector b

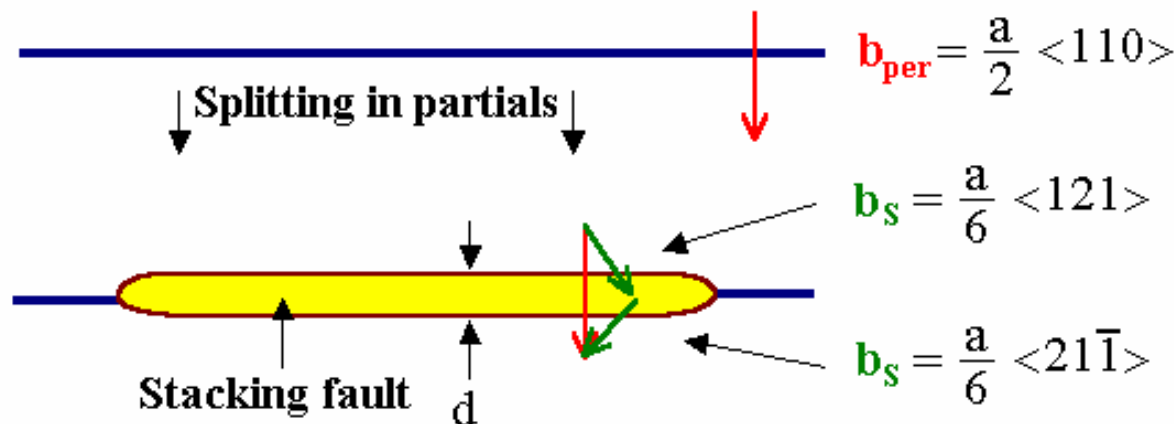Dislocations are the <u>discrete</u> entities that carry plastic (permanent) deformation; measured by "Burgers vector"

Partial dislocations

- In FCC, dislocations with Burgers vector [110] split up into two "partial dislocations" with Burgers vector 1/6[112]

Energy of the perfect dislocation $= G \cdot b^2 = G \cdot (a/2 <110>)^2 = \dfrac{G \cdot a^2}{2}$

Energy of the two partial dislocations $= 2G \cdot (a/6 <112>)^2 = 2G \cdot a^2/36 \cdot (1^2 + 1^2 + 2^2) = \dfrac{G \cdot a^2}{3}$

$b_{per} = \dfrac{a}{2} <110>$

$b_S = \dfrac{a}{6} <121>$

$b_S = \dfrac{a}{6} <21\bar{1}>$

Metals with low SFE and materials under geometric confinement often have large stacking faults
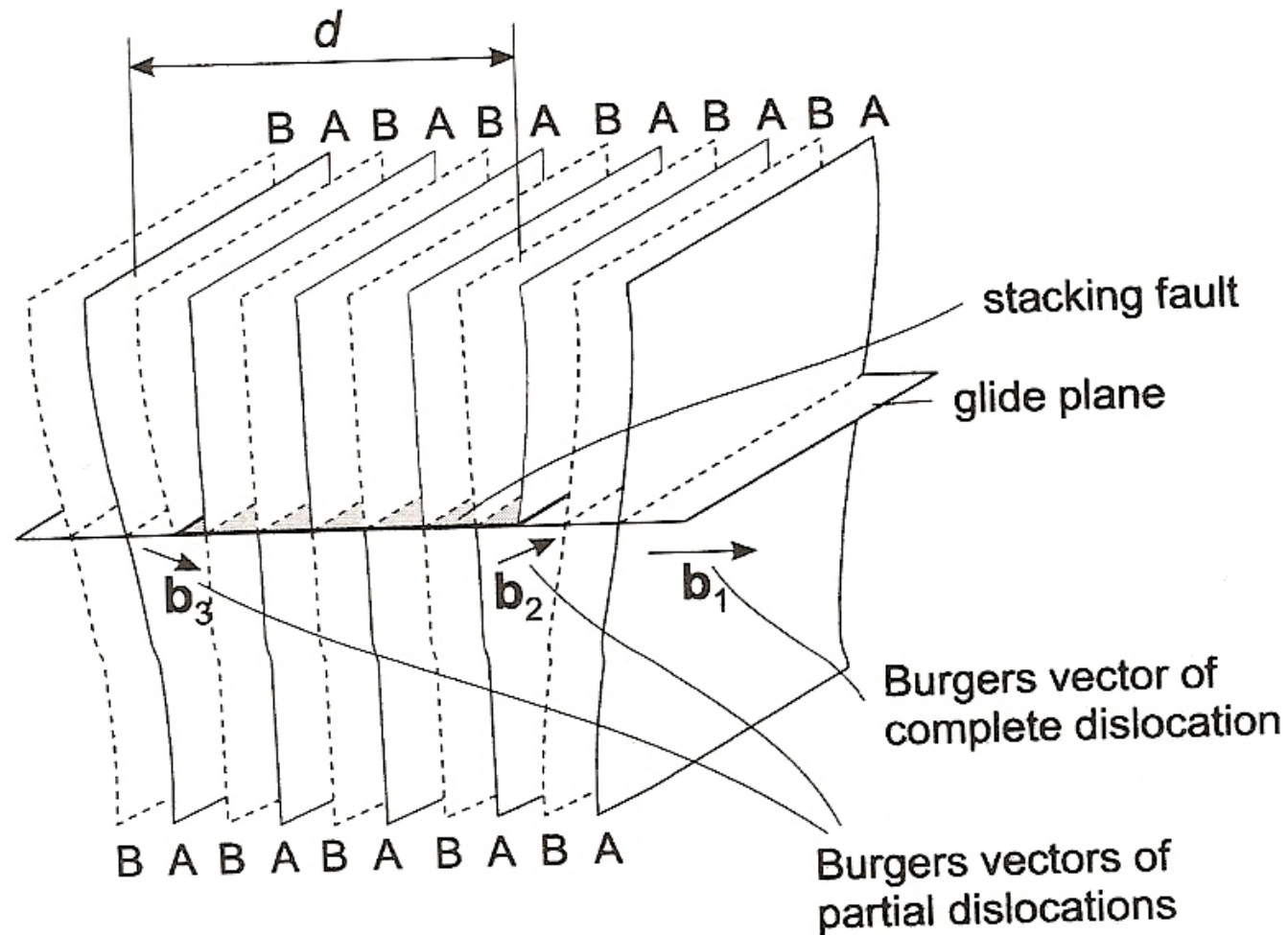
Stacking fault: Long range atomic order distorted → HCP vs. FCC

Dislocation nucleation from a crack tip
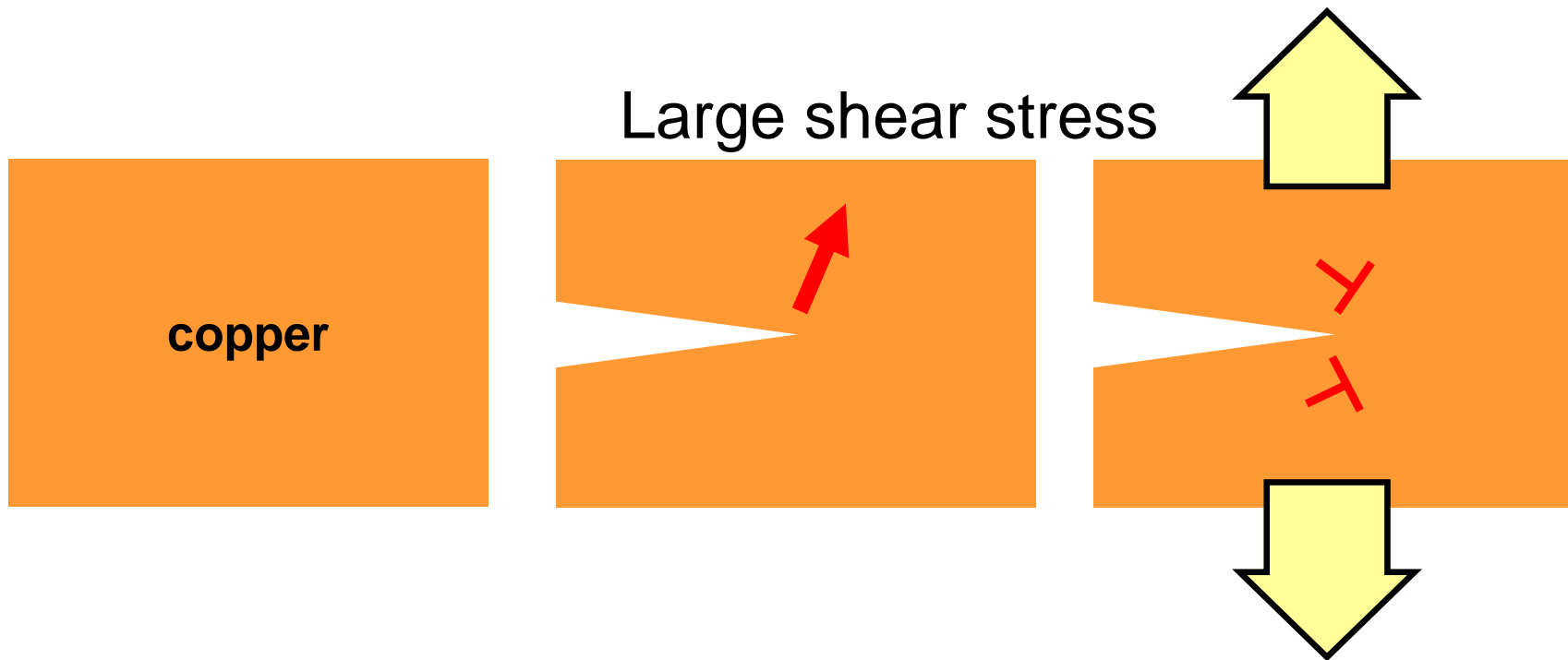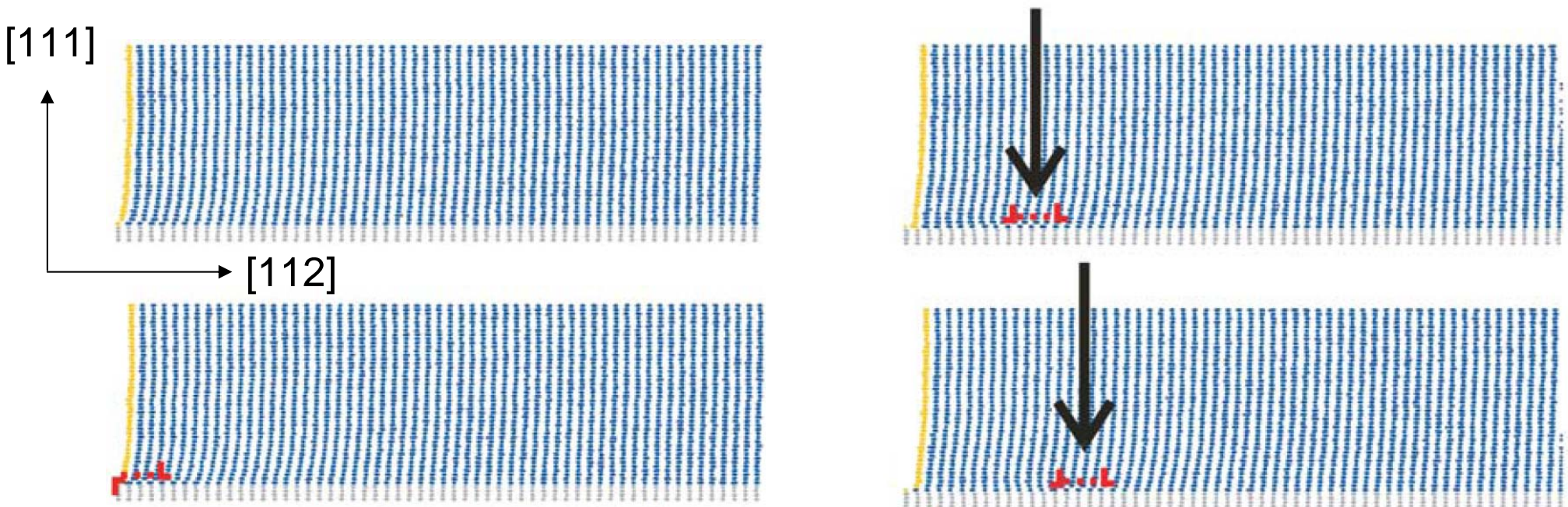

Large shear stress

copper

- Critical load for cracking
- What happens when the load becomes large?
- How to analyze the complex data?
- Limitations of modeling…

Atomistic details of dislocation nucleation

- Dislocation nucleation from a traction-free grain boundary in an ultra thin copper film

- Atomistic results depict mechanism of nucleation of partial dislocation

Chemical bonding in metals
## "metallic bonding"

- Bonding between atoms with low electronegativity 1,2 or 3 valence electrons, therefore there are many vacancies in valence shell.
- When electron clouds overlap, electrons can move into electron cloud of adjoining atoms.
- Each atom becomes surrounded by a number of others in a three-dimensional lattice, where valence electrons move freely from one valence shell to another.
- Delocalized valence electrons moving between nuclei generate a binding force to hold the atoms together

positive ions in a sea of electrons

Thus:

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

•   Electron (q=-1)
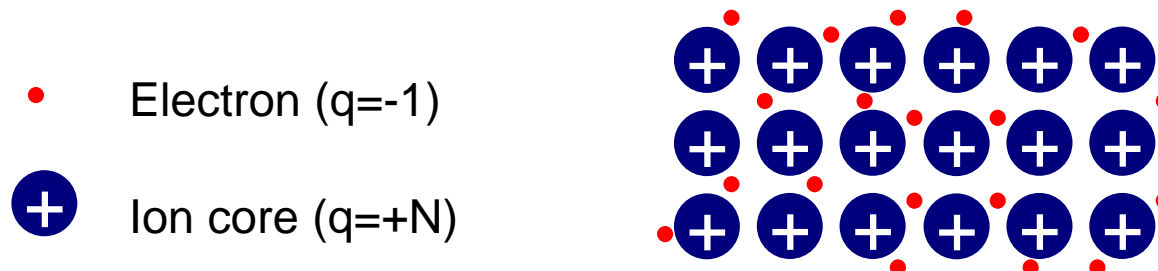
⊕   Ion core (q=+N)

Properties of metals

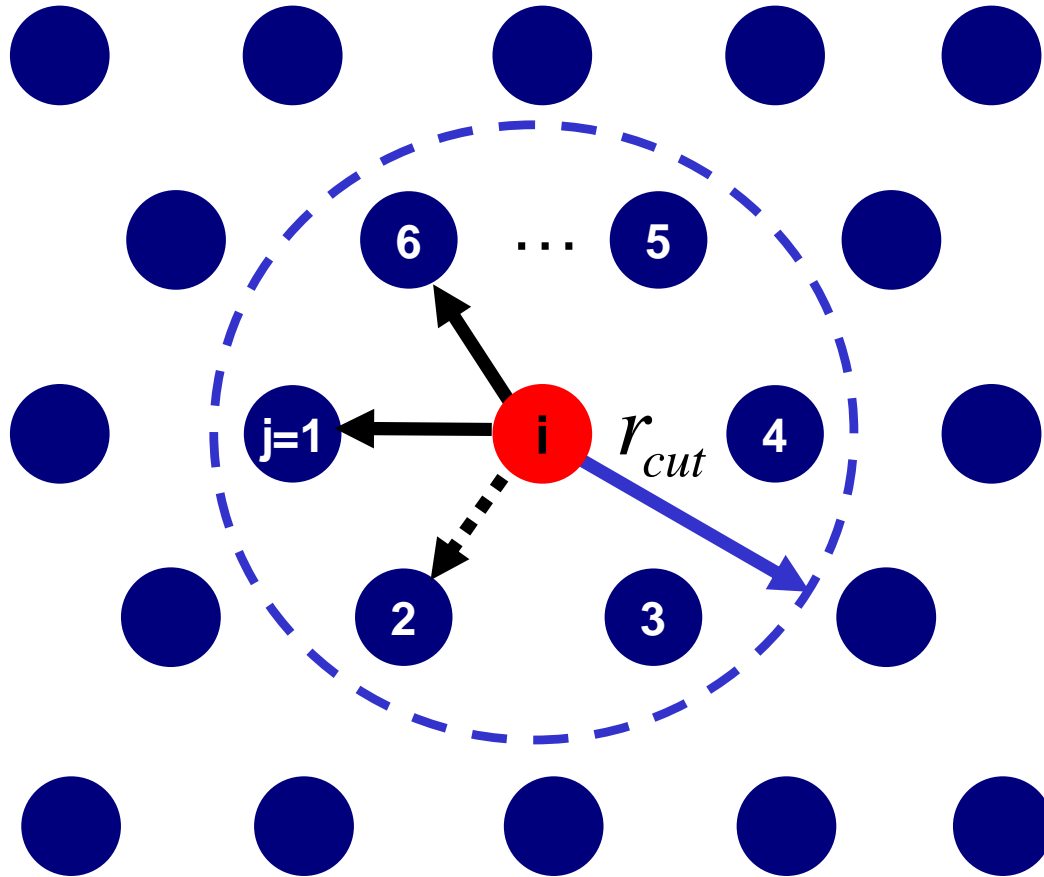| Property	Physical/atomic reason
High density	Tightly packed FCC, BCC, HCP
High melting temperature	Strong forces between ion core and delocalized electrons
Good conductors of heat	Vibration transport via delocalized electrons (+phonons)
Good electrical conductors	Delocalized electrons (flow in and out)
Many metals are ductile	Glide (and climb) of dislocations
Lustrous	Reflection of light by electron gas

Why pair potentials fail…

- In pair potentials, the strength of each bond is dependent only on the distance between the two atoms involved:
The positions of all the other atoms are not relevant
(works well e.g. for Ar where no electrons are available for bonding and atoms are attracted with each other only through the weak van der Waals forces)

- However: QM tells that the strength of the bond between two atoms **is affected by the environment** (other atoms in the proximity)

- As a site becomes more crowded, the bond strength will generally decrease as a result of Pauli repulsion between electrons.
The modeling of many important physical and chemical properties depends crucially on the ability of the potential to **"adapt to the environment"**

- Can not reproduce surface relaxation (change in electron density)

- First attempts using pair potentials

$$\phi_i = \sum_{j=1..N_{neigh}} \varphi(r_{ij})$$

Lennard-Jones 12:6

$$\varphi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$
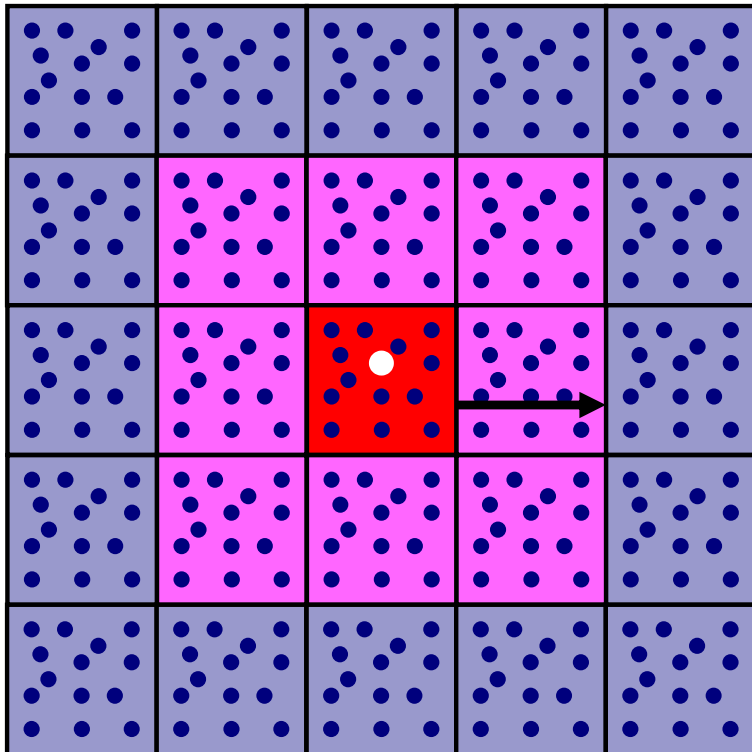
Morse

$$\varphi(r_{ij}) = D\{1 - \exp[-\beta(r_{ij} - r_0)]\}^2$$

Good for noble gas Ar
(FCC in 3D)

- Need nested loop to search for neighbors of atom *i:* Computational disaster

- Concept: Divide into computational cells ("bins", "containers", etc.)

- Cell radius $R > R_{cut}$ (cutoff)

- Search for neighbors within cell atom belongs to and neighboring cells (8+1 in 2D)

- Most classical MD potentials/force fields have finite range interactions

- Other approaches: Neighbor lists

- Bin re-distribution only necessary every 20..30 integration steps (parameter)

Modeling attempts: Multi-body potential

- Multi-body potential depend on more than pairs of atoms, but instead also on the environment of each atom
- Important for metals due to existence of "electron gas"

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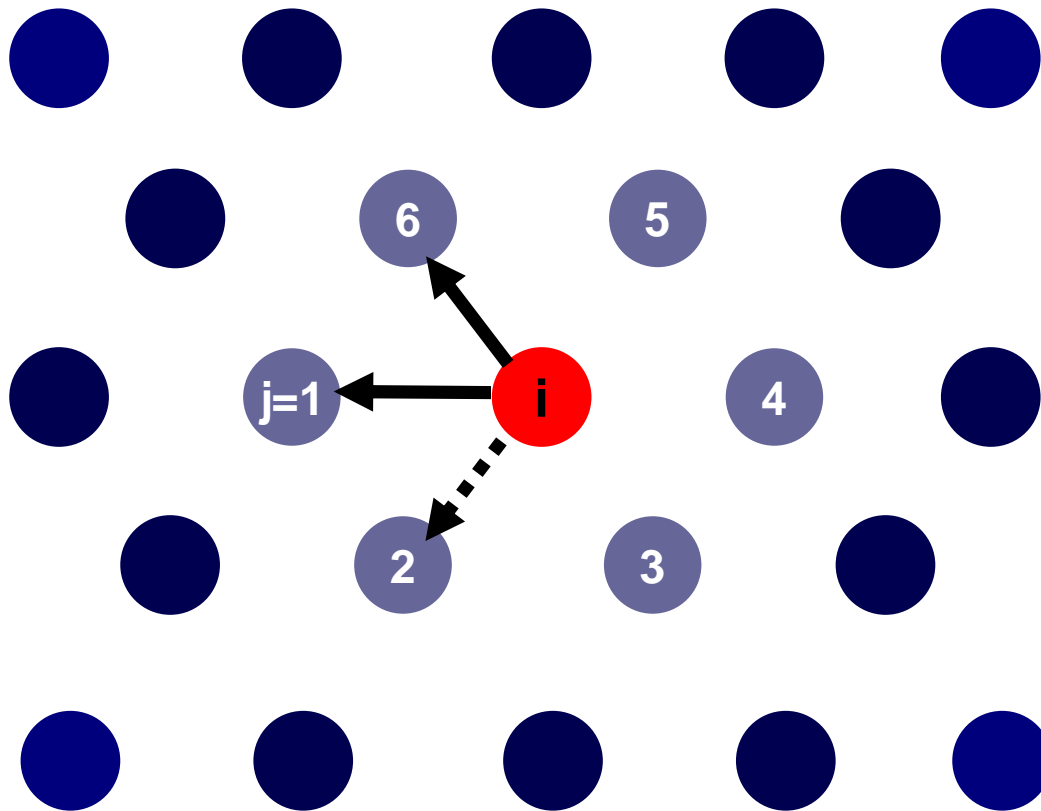
$$\phi_i = \underbrace{\sum_{j=1..N_{neigh}} \frac{1}{2} \varphi(r_{ij})}_{\text{Pair potential energy}} + \underbrace{F(\rho_i)}_{\substack{\text{Embedding} \\ \text{energy} \\ \text{as a function of} \\ \text{electron density}}}$$

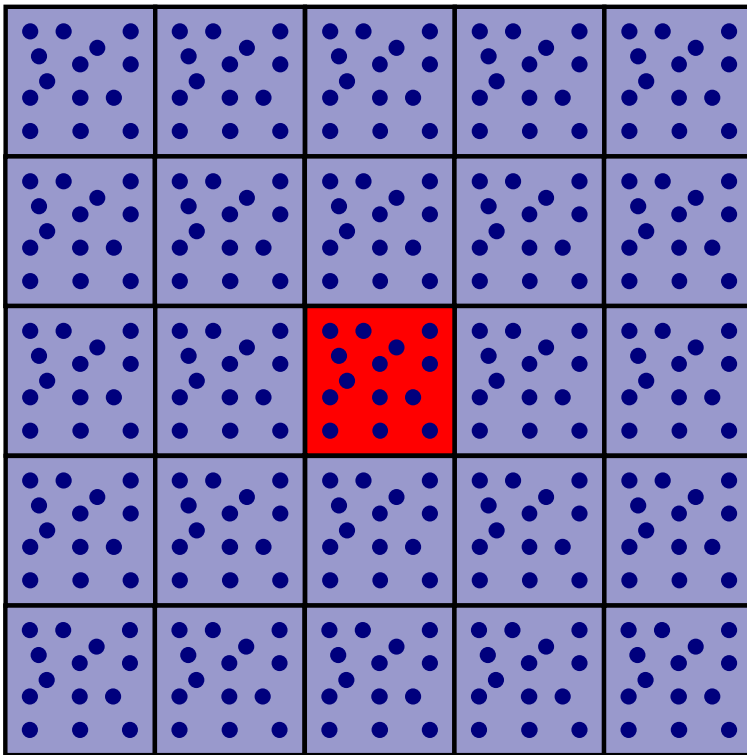ρ_i Electron density at atom *I* based on a pair potential:

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

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

- Requires two loops over atoms within each cell
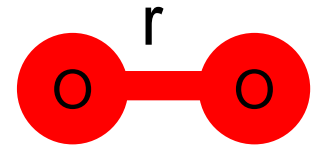
Loop 1:

(i) Pair contributions (derivatives and potential)
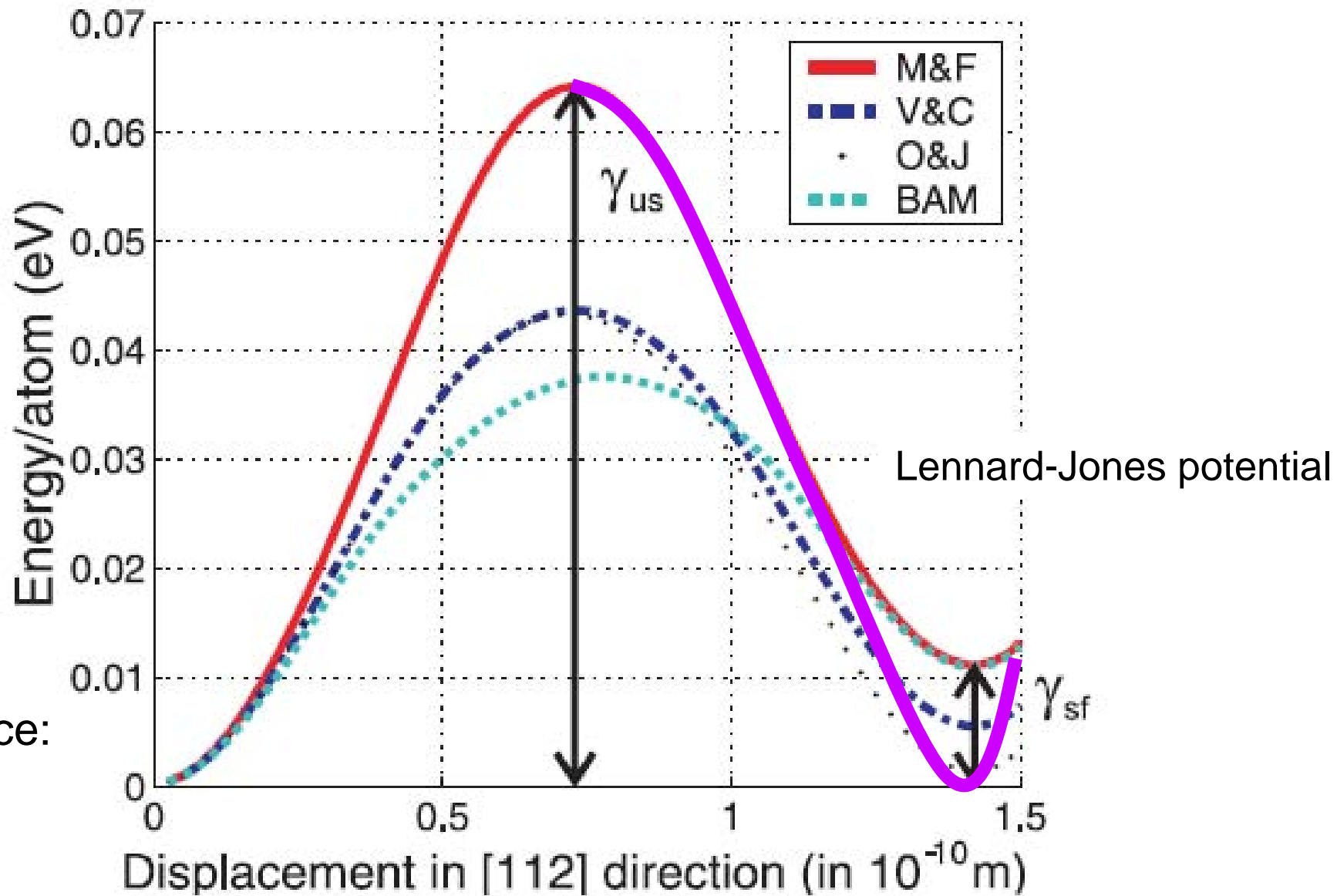
(ii) Calculate electron density

Loop 2:

(iii) Calculate embedding function and derivatives

$$\mathbf{F}_i = -\sum_{j \neq i} \Big(\phi'(r_{ij}) + [U'(n_i) + U'(n_j)]\rho'(r_{ij}) \Big) \frac{\mathbf{r}_{ij}}{r_{ij}}$$

Due to additional (i) calculation of electron density and (ii) embedding contribution EAM potentials are 2-3 times slower than pure pair potentials

Consequence:

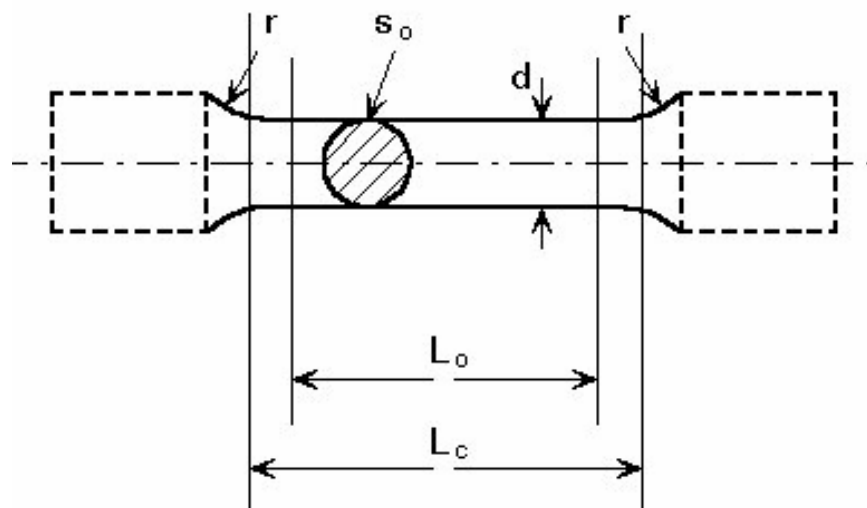Only partial dislocations expected

Lennard-Jones potential

(schematic)

Width of stacking fault

$$r_e = \frac{\mu b^2}{8\pi\gamma_{sf}} \frac{2-v}{1-v}\left(1 - \frac{2v\cos(2\beta)}{2-v}\right) \sim \frac{1}{\gamma_{sf}}$$

Approaches infinity for $\gamma_{sf} \rightarrow 0$

L_o = Gauge length
L_c = Parallel length
r = Transition radius
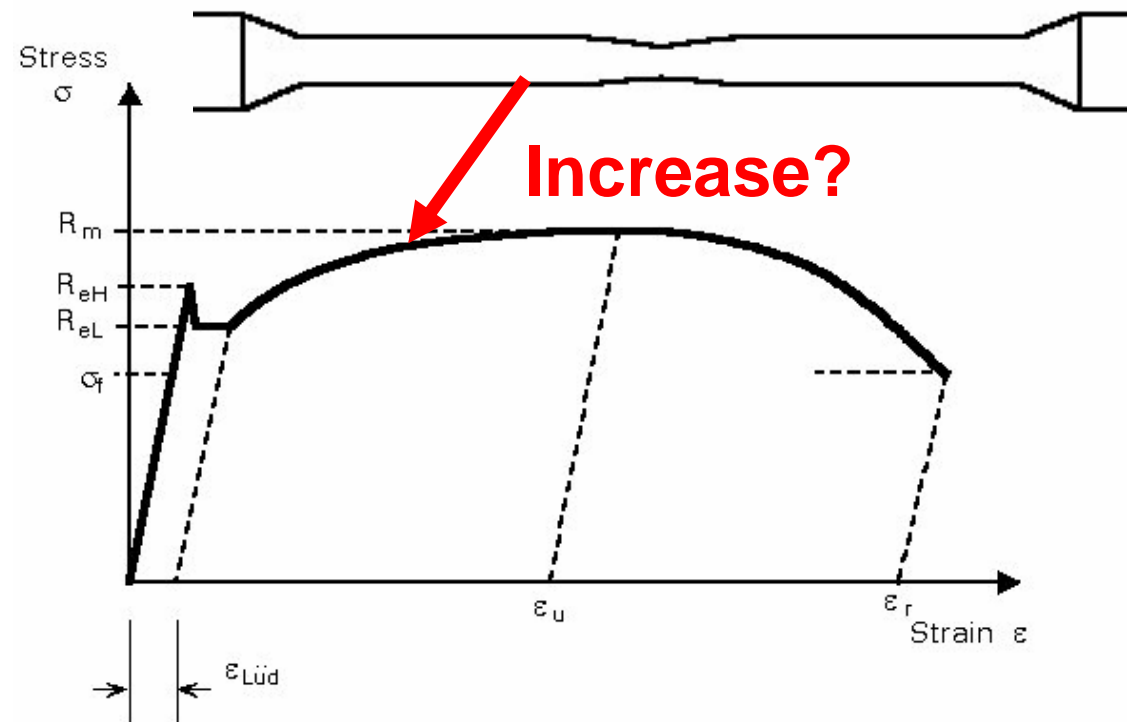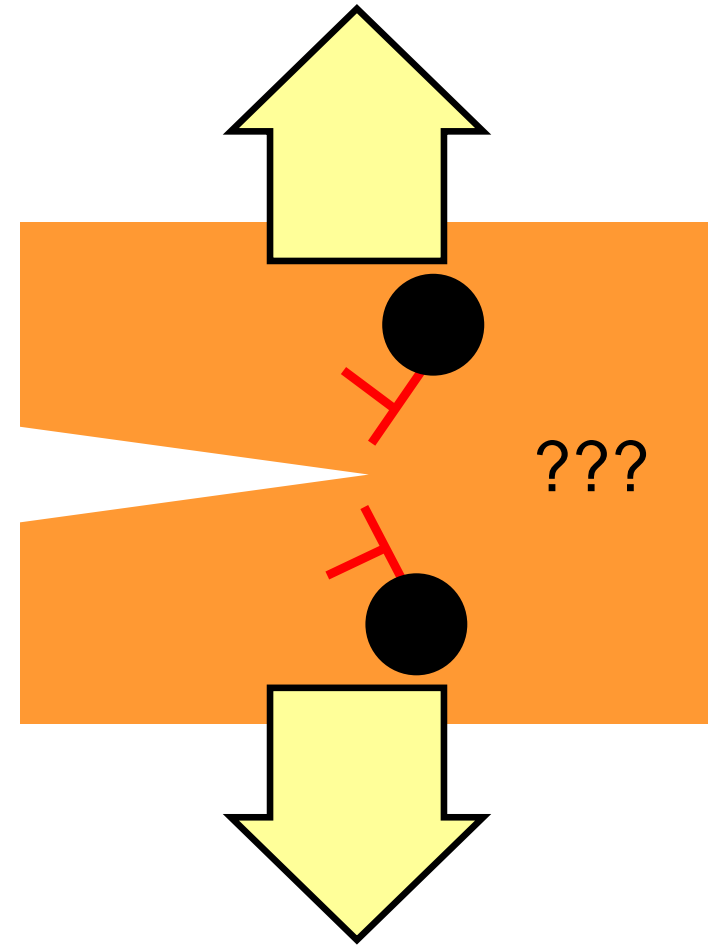s_o = Original cross-section area
d = Gauge length diameter

Increase?
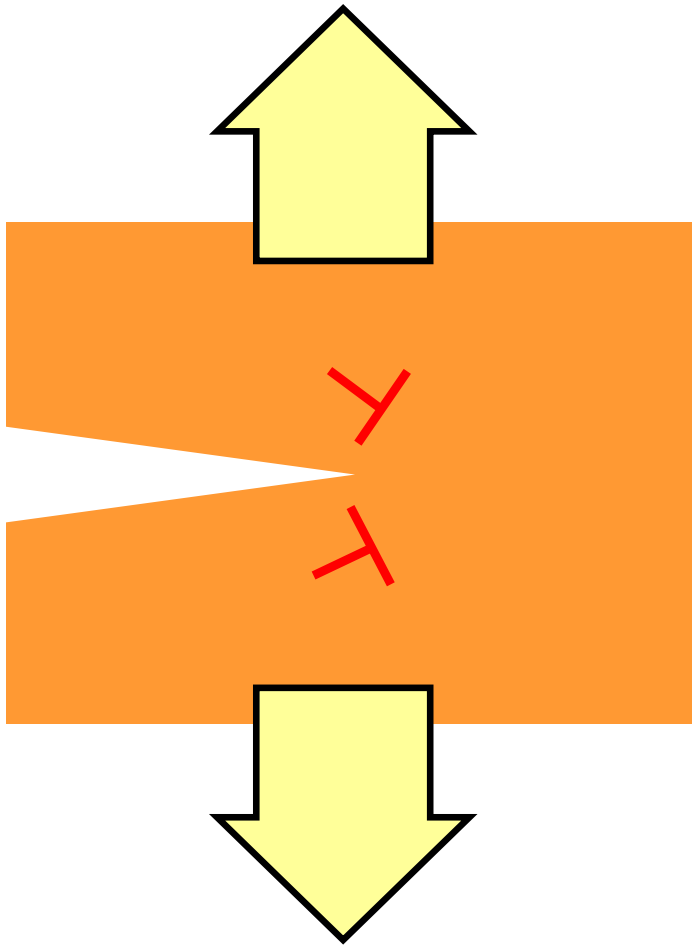
Figure 6 Engineering stress-strain curve of a metal,
e.g. mild steel, with a yield point

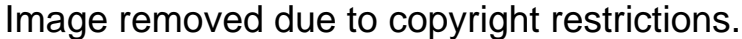http://www.kuleuven.ac.be/bwk/materials/Teaching/master/wg02/l0310.htm

Strengthening mechanisms
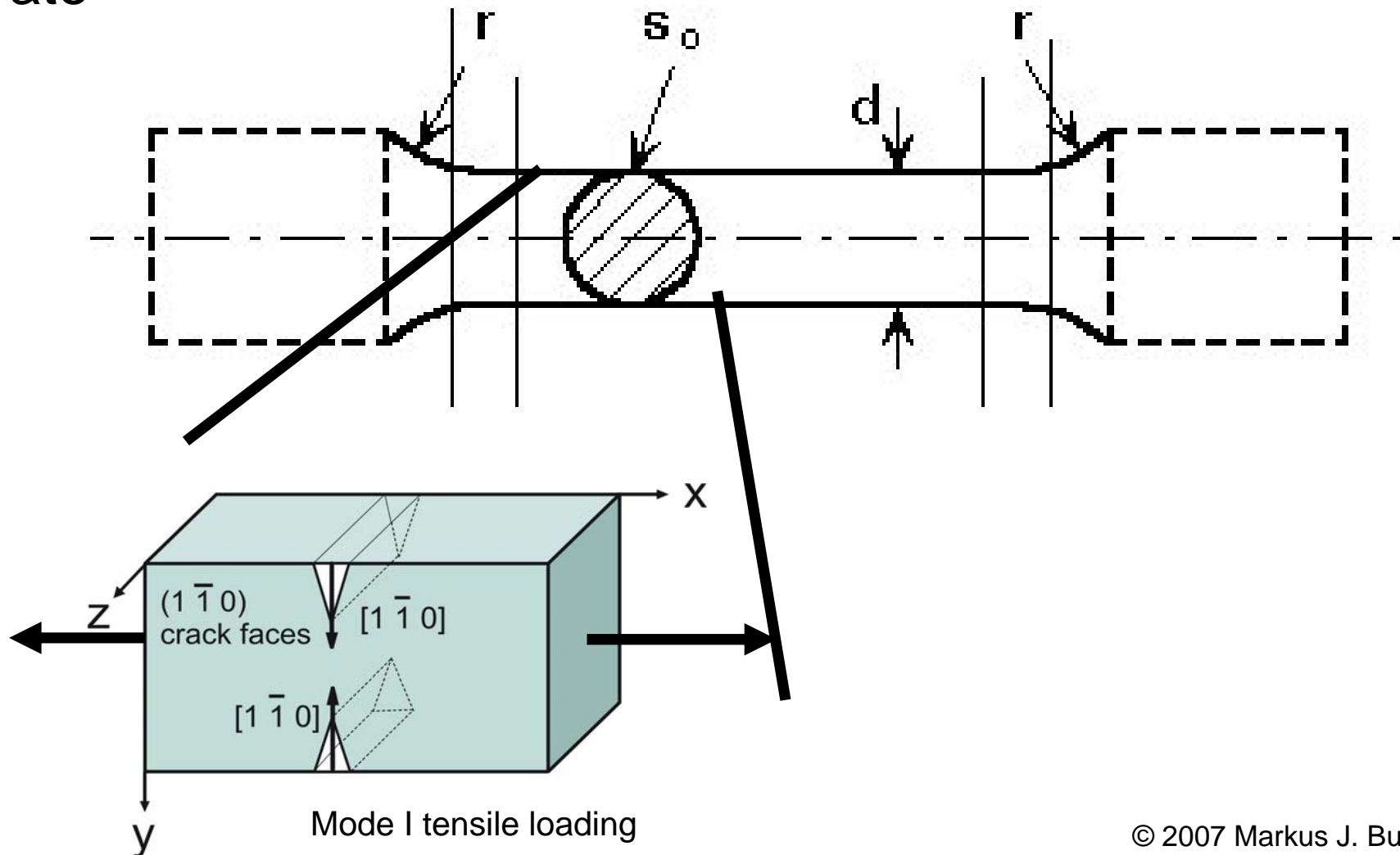
Strengthening mechanisms

- Remember: Theoretical shear strength of materials is not reached due to the existence of dislocations

- By hindering the motion or the possibility to create dislocations, the material becomes stronger, approaching the theoretical strength

- Mechanisms:

    ☐ Grain boundary strengthening

    Image removed due to copyright restrictions.

    ☐ Grain size reduction

    ☐ Introduction of foreign atoms that create strain field (solid-solution strengthening)

    ☐ Introduction of particles that pin/hinder dislocation motion

    Image removed due to copyright restrictions.

- Micrometer range of dislocation-dislocation interactions
- Thus: Need crystal with 100..200 nm side length – 1E9 atoms

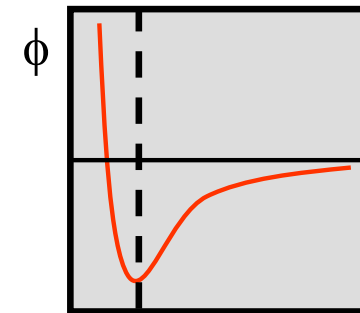$(1\,\bar{1}\,0)$ crack faces $[1\,\bar{1}\,0]$

$[1\,\bar{1}\,0]$

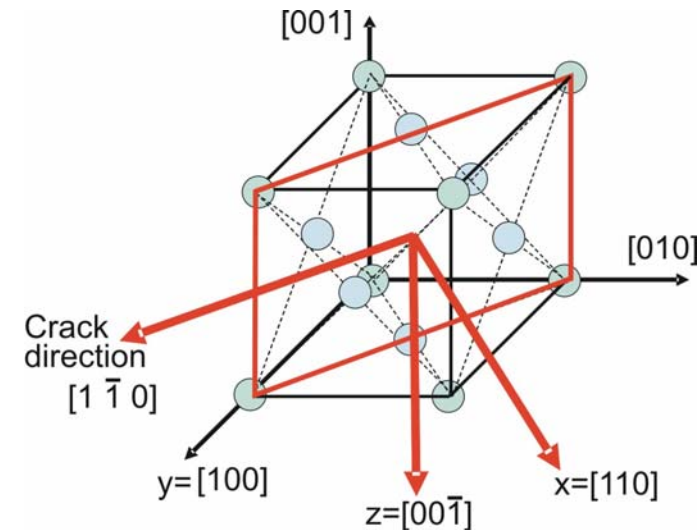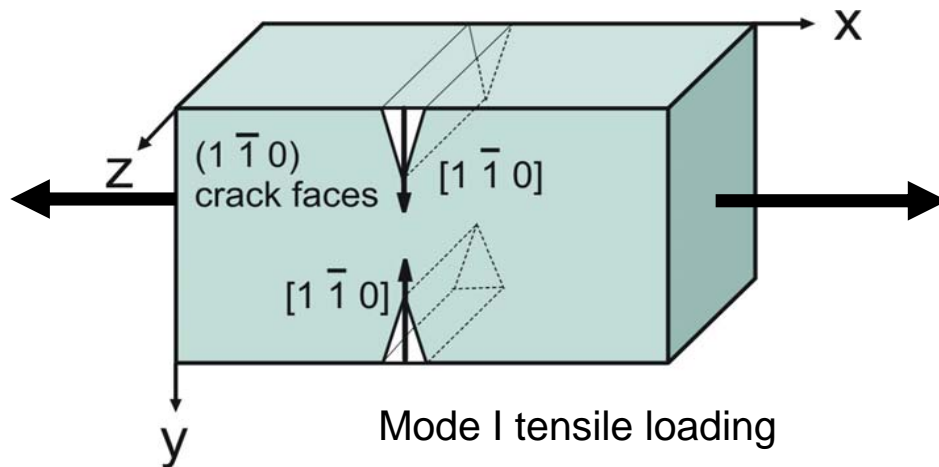Mode I tensile loading

© 2007 Markus J. Buehler, CEE/MIT

Simulation details

➢ 1,000,000,000 atom

➢ Lennard-Jones ductile "model material"

Generic features of atomic bonding: „repulsion vs. attraction"

Mode I tensile loading

"Petaflop" computers

Computer power

BlueGene/L (USA) 70 TFLOP
NASA Ames (USA) 50 TFLOP
Earth Simulator (Japan) 40 TFLOP
LINUX clusters

10^{11} atoms

Focus

10^9 atoms

"Teraflop"

IBM Almaden Spark

"Gigaflop"
10^8 atoms

10^6 atoms

10^2 atoms 10^5 atoms

Year

1965   1975   1985   1995   2005   2012

(Buehler *et al.*, to appear 2006)

© 2007 Markus J. Buehler, CEE/MIT
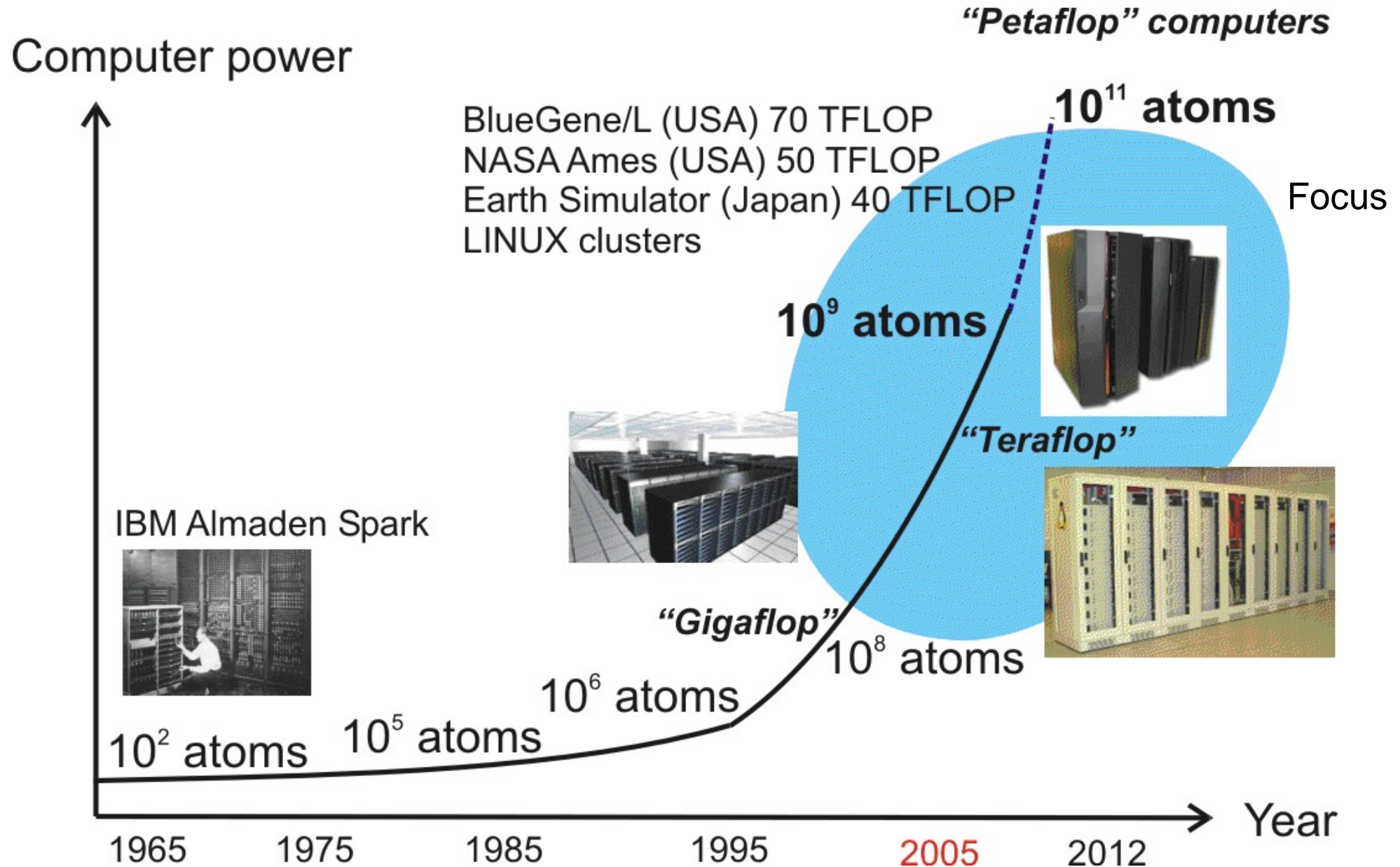
Parallel Molecular Dynamics

Zone of interest of CPU (i,j)

| CPU (i−1,j−1) | CPU (i−1,j) | CPU (i−1,j+1) |

| CPU (i,j−1) | **CPU (i,j)** | CPU (i,j+1) |

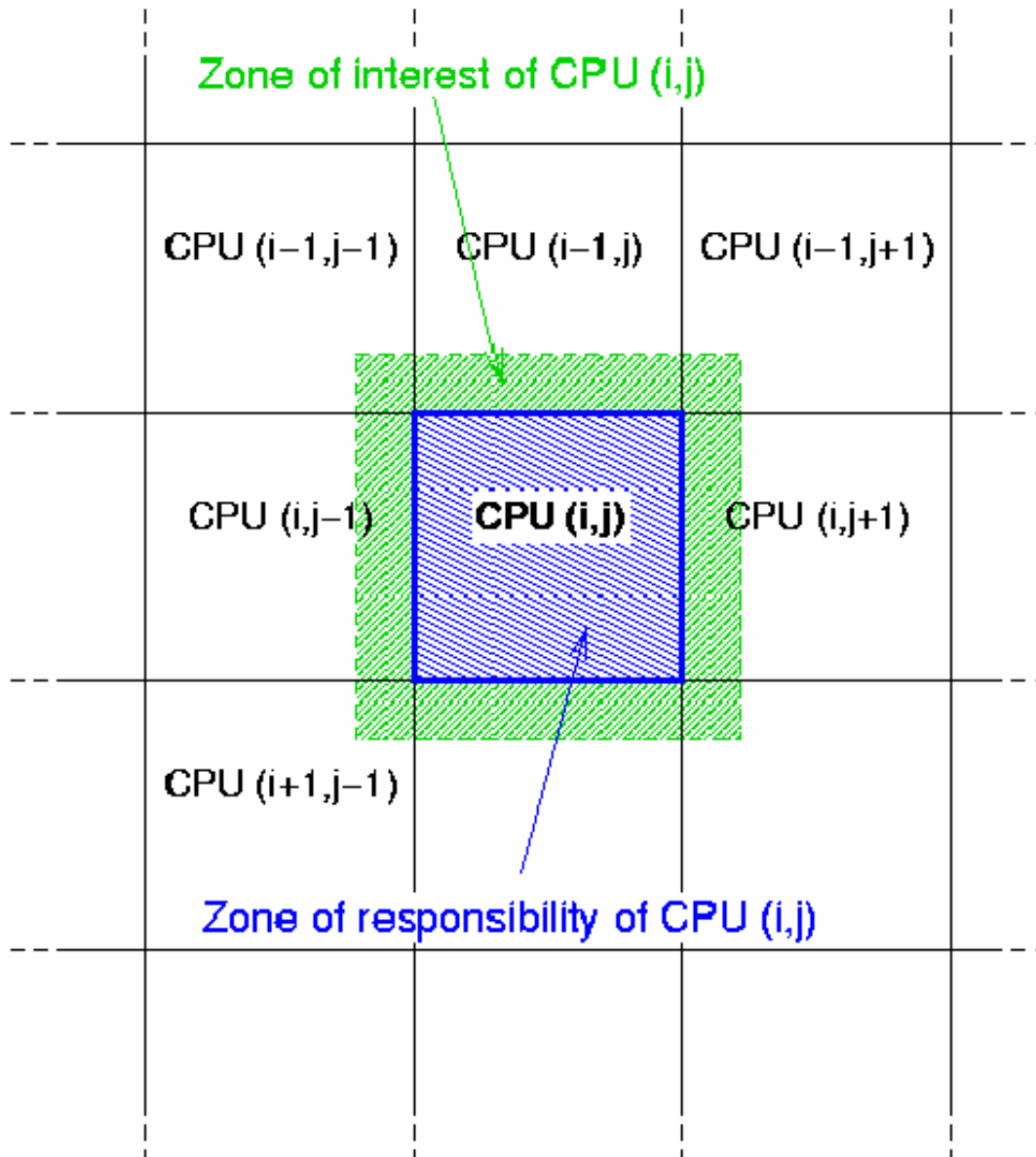CPU (i+1,j−1)

Zone of responsibility of CPU (i,j)

Concept:

Divide the workload

No (immediate) long range interaction (only via dynamics)

• Each CPU is responsible for part of the problem

• Atoms can move into other CPUs (migration)

• Need to know topology or the geometric environment on other CPUs (green region)

• 1,000,000,000 particles on 1,000 CPUs: Only 1,000,000 atoms/CPU

(after Schiotz)

Implementation of parallelization

- Shared memory systems (all CPUs "see" same memory)
  - ☐ OpenMP (easy to implement, allows incremental parallelization)
  - ☐ POSIX threads

- Distributed memory systems
  - ☐ MPI (=Message Passing Interface)
    Most widely accepted and used, very portable, but need to parallelize whole code at once

- Parallelization can be very tedious and time-consuming and may distract from solving the actual problem; debugging difficult

- **Challenges:** Load balancing, different platforms, input/output, compilers and libraries, modifications and updates to codes, "think parallel" as manager

- Strategy for your own code: Find similar code and implement your own problem

Why is large-scale modeling useful?

- Bridging length scales by direct numerical simulation (DNS)

- Understand the behavior of complex many-particle systems, without imposing constraints or boundary conditions

- Discover new physical phenomena, e.g. collective events that involve a large number of particles

Caution:
- Need to make sure that model produces useful results, *i.e.* includes new scientific content and discoveries
- Pictures may be pretty, but what do we learn?

Increase in computing power: Parallelization

Modeling of mechanical behavior of materials is highly demanding and requires models with millions and billions of atoms

2000
1,000,000,000 particles
10 TFLOP computers

0.3 µm

2005
70,000,000,000 particles
70 TFLOP computers

1.2 µm
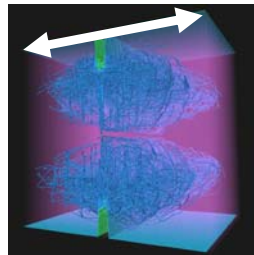
5 µm

2010
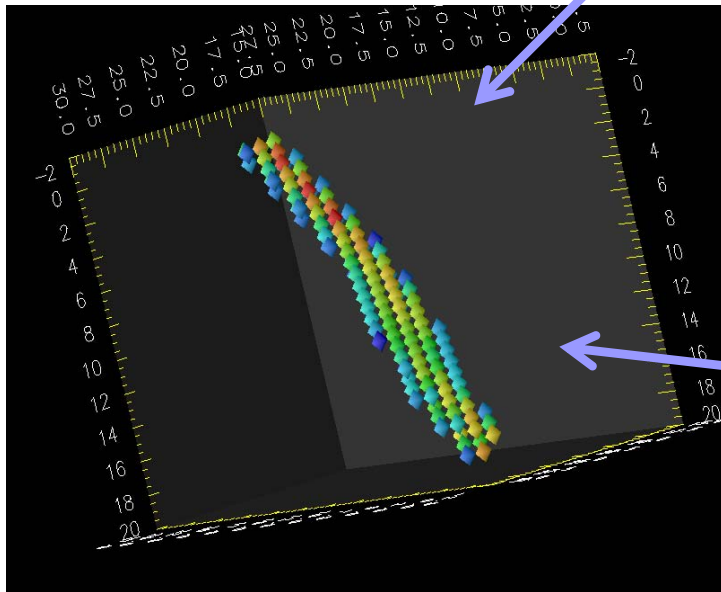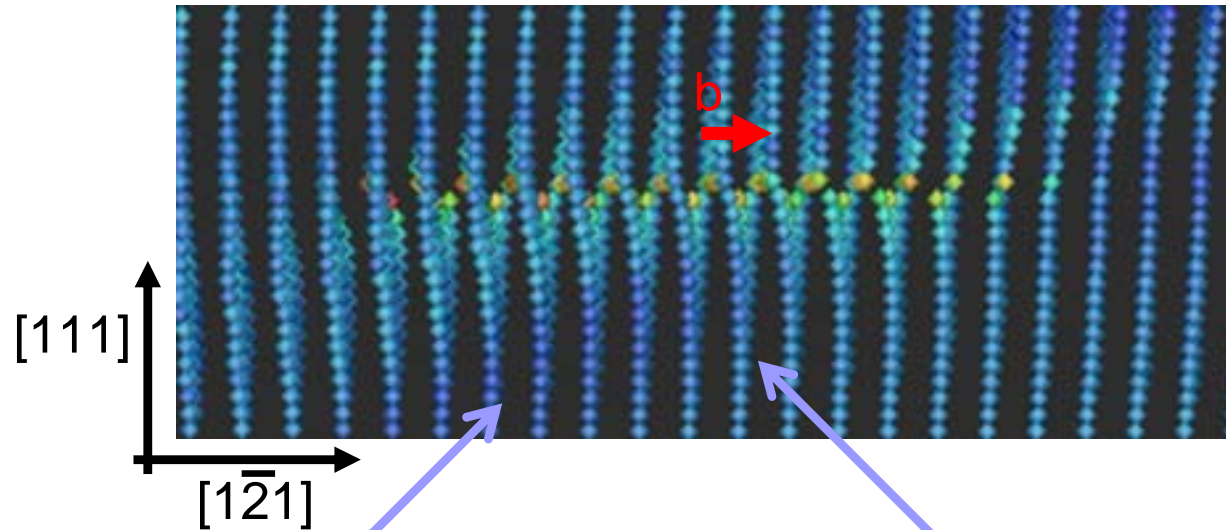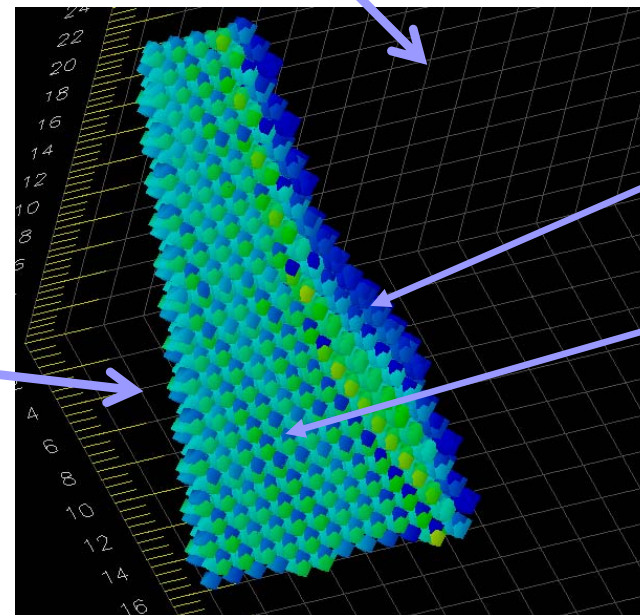7,000,000,000,000 particles
1,000 TFLOP computers
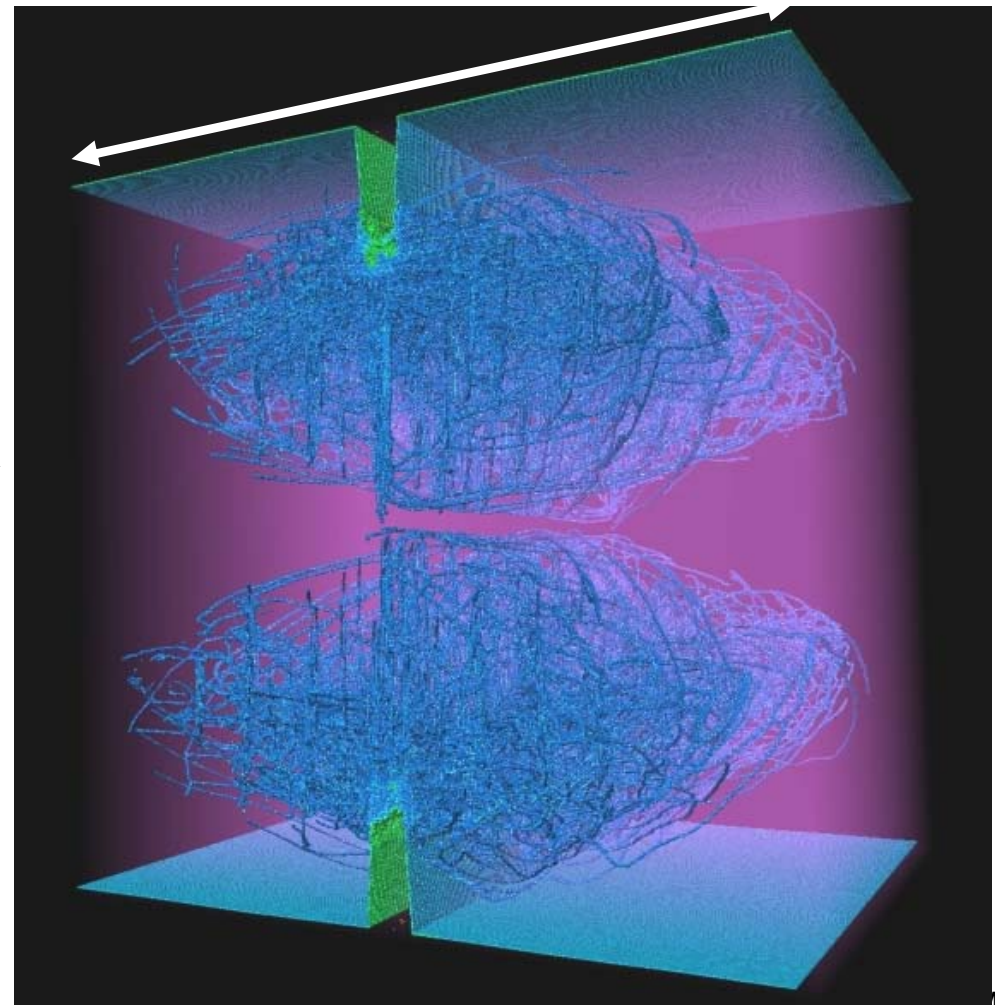
Analysis of glide plane and Burgers vector

Lattice around dislocation

[111]

[1$\bar{2}$1]

b

Atoms with higher energy than bulk are highlighted

Centrosymmetry method

partial dislocation

Stacking fault

1. Dislocation cutting processes: Intersection of dislocations leads to generation of trails of point defects (trails of partial point defects, vacancy tubes and interstitials): when two screw dislocations intersect, each acquires a jog with a direction and length equal to the Burgers vector of the other dislocation. Upon intersection, the dislocations cannot glide conservatively since each jog has a sessile edge segment.

- Energy required to create point defects
- **Therefore**: Pinning of dislocations – dragging force:

Images removed due to copyright restrictions.
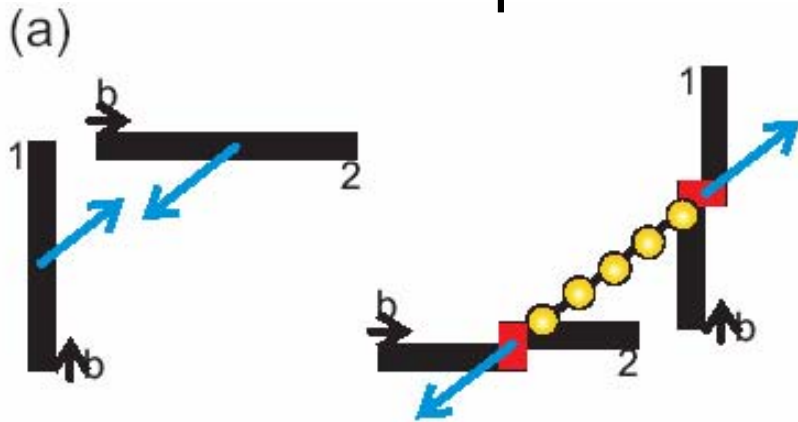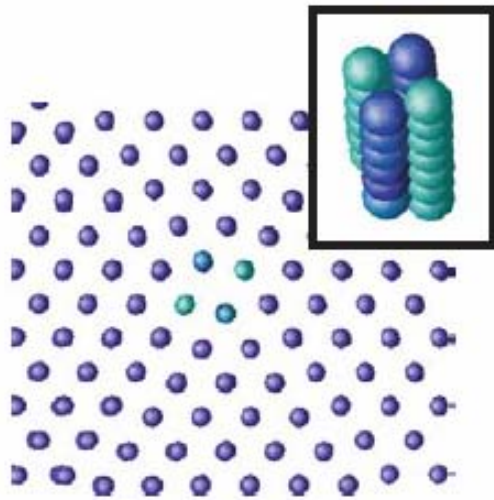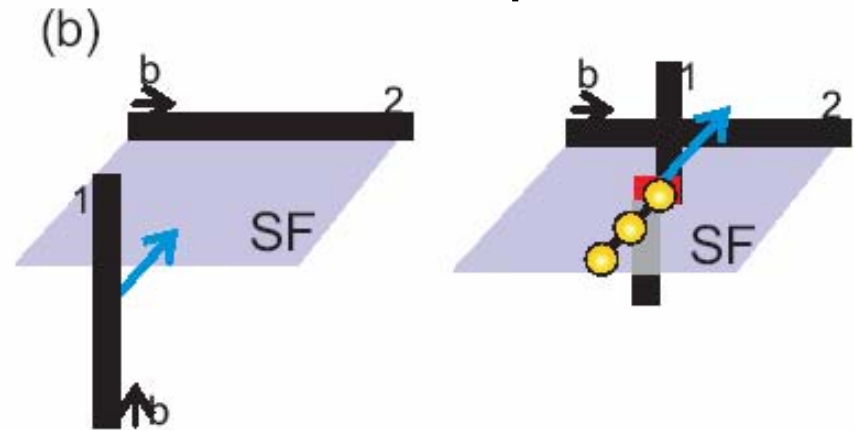
Different kinds of point defects

F_{drag}

Trail of partial point defects

Reduced dragging force (20% of vacancy tube)
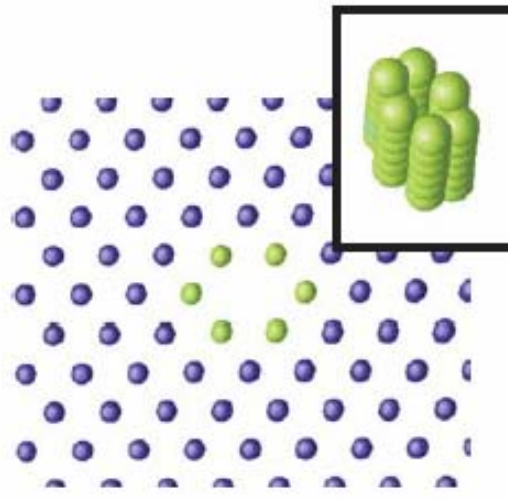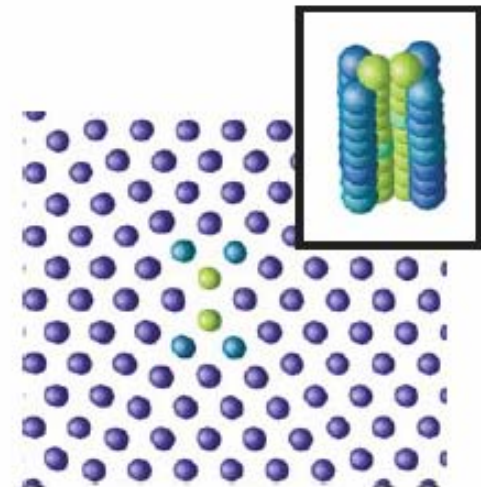
Vacancy tubes

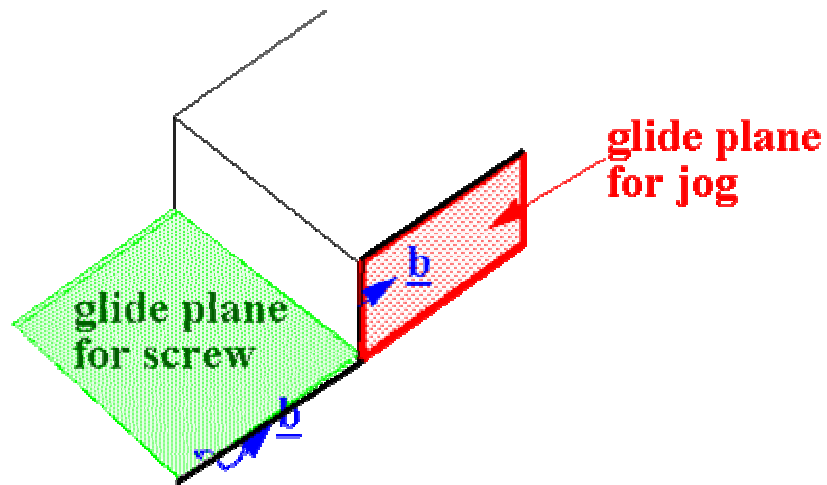Trail of interstitials
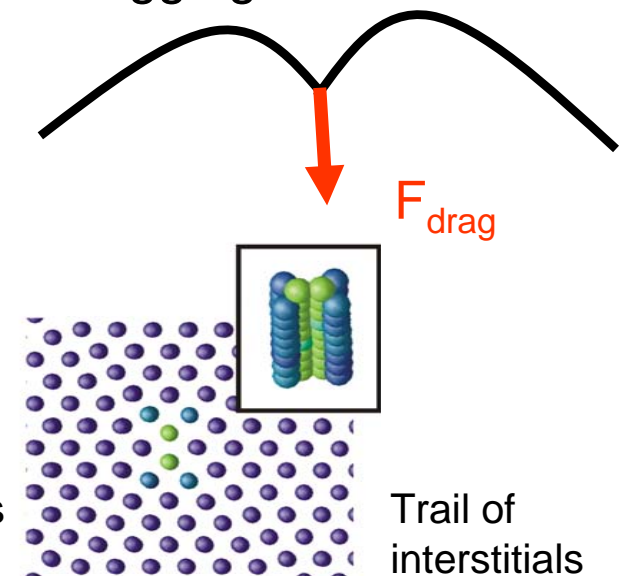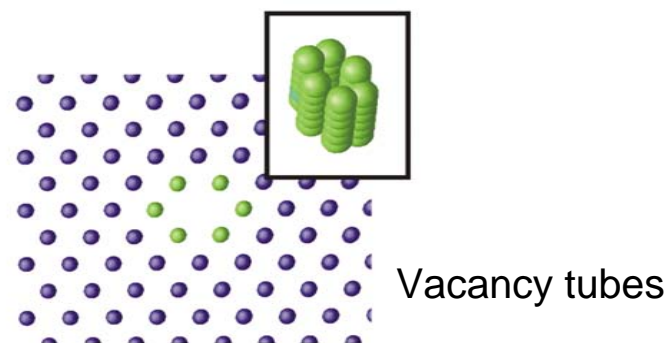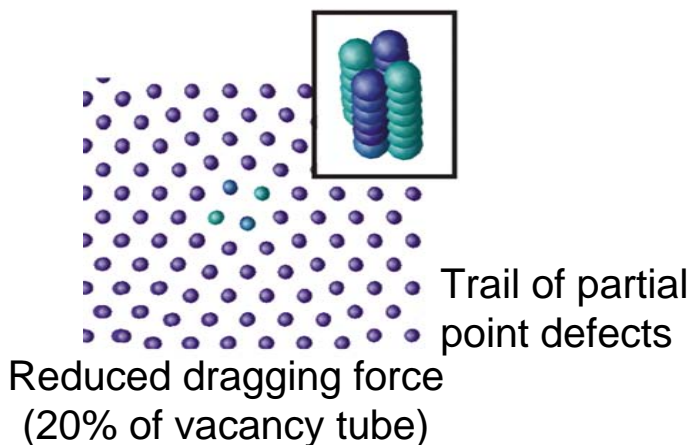
Reaction of two partials

Reaction of one partial w/ SF

1/3 vacancy defect, volume $a_0^3/12$ (vacancy: $a_0^3/4$)

glide plane for jog

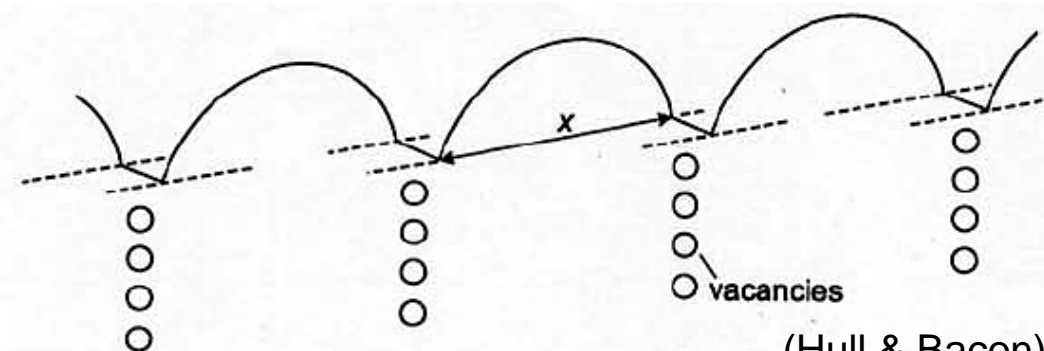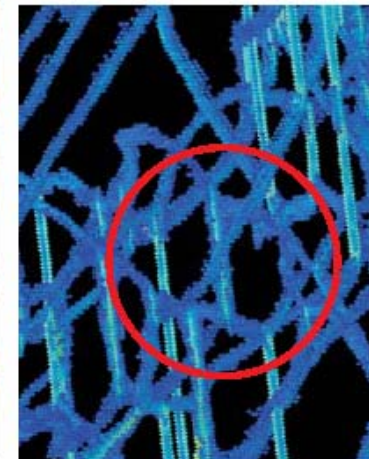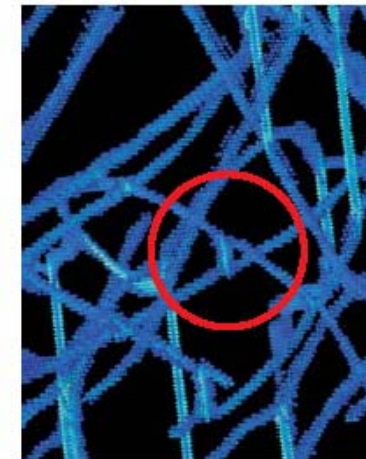glide plane for screw

b

Sessile segment
Pinning
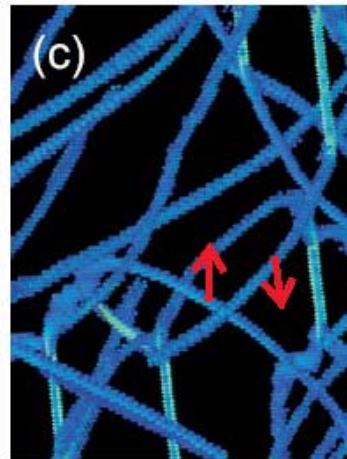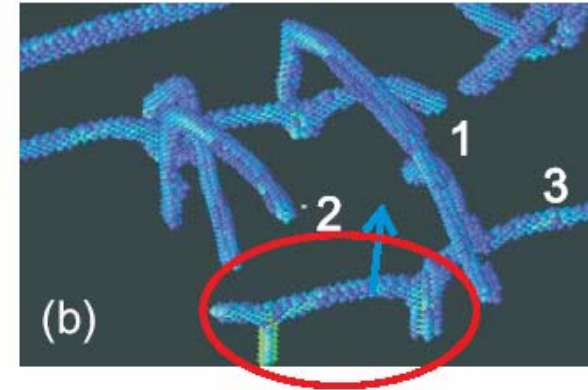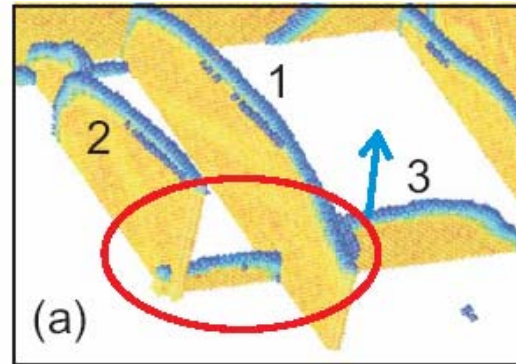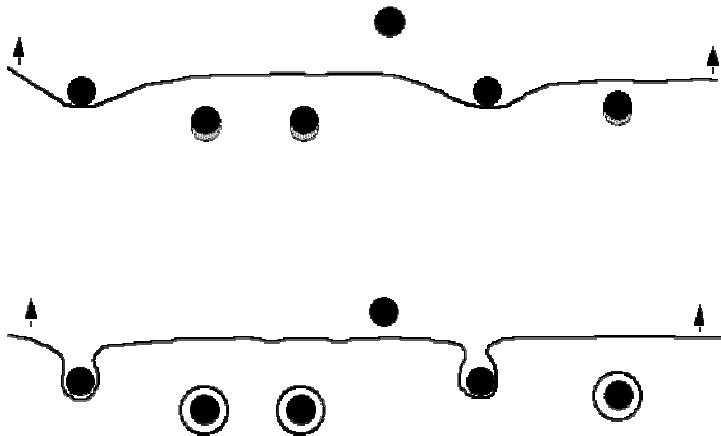
(a) (b)

(c)

vacancies

x

(Hull & Bacon)

Image removed due to copyright restrictions.

The plots show how two dislocations (denoted by "1" and "2") from opposite cracks intersect and create reaction products. When a second reaction takes place at dislocation "2" involving a third dislocation, the dislocation motion is severely hindered which is seen in the bowing out of the dislocations. Many of such reactions occur during the simulation causing the generation of a complex defect network.

Image removed due to copyright restrictions.

2. Cross-slip

Activation of secondary slip systems by cross-slip and Frank-Read mechanisms: At later stages of the simulation

• After activation of secondary slip systems: More dislocation reactions (e.g. cutting processes).

• **"Rediscovered" Fleischer's mechanism of cross-slip of partials that was proposed 1959**

Images removed due to copyright restrictions.

• At a critical dislocation density, secondary slip systems are activated

• This enables for additional plasticity to occur, but also further contributes to work-hardening as the dislocation density increases making it more difficult for dislocations to move

Images removed due to copyright restrictions.

3. Formation of Lomer-Cottrell locks

• Formation of sessile Lomer-Cottrell locks, with its typical shape of a straight sessile arm connected to two partial dislocations

• Sessile junctions provide a severe burden for further dislocation glide

Final sessile structure

Consists of…:
Vacancy tubes,
interstitials, partial
dislocations, and
sessile dislocations

Image removed due to copyright restrictions.

The characteristic structure of the network:

➢ All sessile defects (both trails of partial and complete point defects) as well as sessile dislocations are straight lines that lie on the edges of Thompson's tetrahedron (at intersections of stacking fault planes)

Final sessile structure

Image removed due to copyright restrictions.

See:

1. Buehler, M. J., et al. "The dynamical complexity of work-hardening: a large scale molecular dynamics situation." Acta Mechanica Sinica 21, no. 2 (2005): 103-111.

2. Buehler, M. J., et al. "Atomic plasticity: description and analysis of a one-billion atom simulation of ductile materials failure." Computer Methods in Applied Mechanics and Engineering 193, no. 48-51 (2004): 5257-5282.
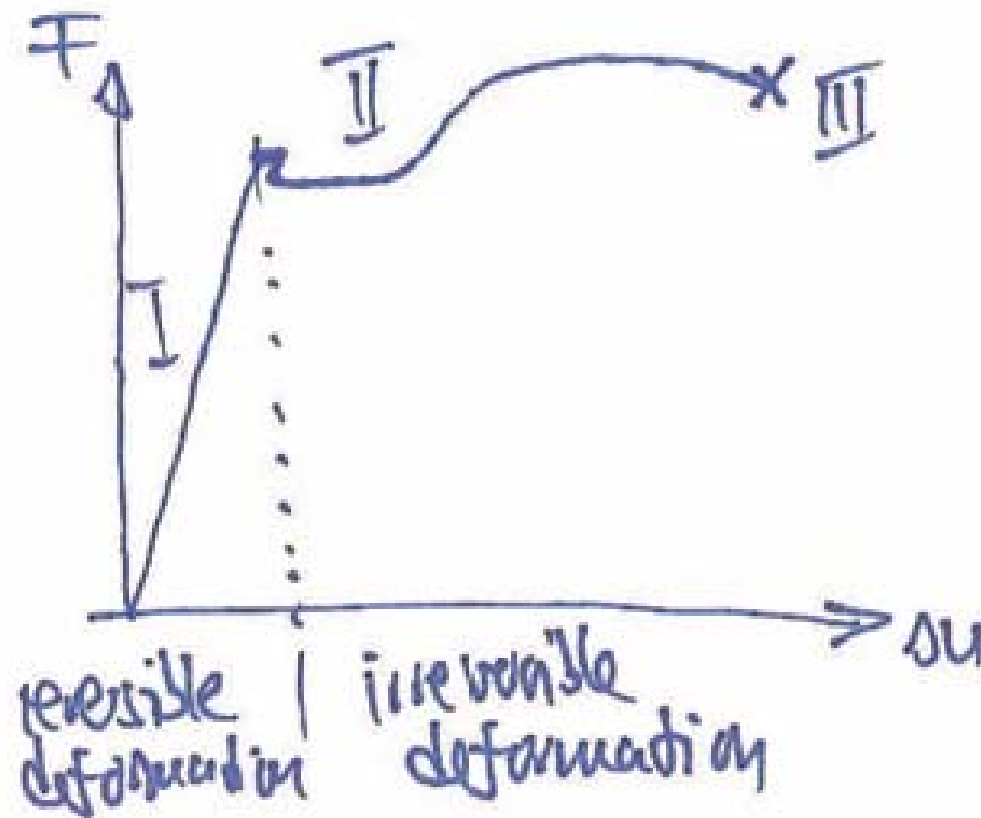
Case study:
Cracking of a copper crystal…

- Critical load for cracking
- What happens when the load becomes large?
- How to analyze the complex data?
- Limitations of modeling…

$$F = k_s \Delta u$$

Energy approach to elasticity

1st law of TD

$$\frac{dU}{dt} = \delta W + \delta Q.$$

External work rate

$$\delta W = \dot{x} F_e$$

Applied force

2nd law

$$\frac{dS}{dt} \geq \frac{\delta Q}{T}$$

Change in entropy is always greater or equal than the entropy supplied in form of heat; difference is due to internal dissipation

$$\frac{dD}{dt} = T\frac{dS}{dt} - \delta Q \geq 0 \qquad \delta Q = dU/dt - \delta W$$

Dissipation rate

Dissipation rate after consider 1st law of TD:

$$\frac{dD}{dt} = \delta W - \frac{d}{dt}(U - TS)$$

$F = U - TS$ is defined as free energy or Helmholtz energy,

Energy approach to elasticity

Elastic deformation:

$$\frac{\mathrm{d}D}{\mathrm{d}t} = 0$$

$$\delta W - \frac{\mathrm{d}F}{\mathrm{d}t} = 0$$

Assume only internal energy change (more general: $\delta W - dF/dt = 0$)

$$\dot{x}\left(F_e - \frac{\mathrm{d}F}{\mathrm{d}x}\right) = 0.$$

Expand equation $dU/dt = dU/dx \; dx/dt$

$$\dot{x}F_e - \frac{\mathrm{d}F}{\mathrm{d}x}\frac{\mathrm{d}x}{\mathrm{d}t} = 0$$

Therefore:

$$F_e = \frac{\mathrm{d}F}{\mathrm{d}x} \qquad F_e = \frac{\mathrm{d}U}{\mathrm{d}x}$$

With strain energy density:

$$\Psi = F/V \qquad \Psi = U/V$$

$$\sigma_{ij} = \frac{\mathrm{d}\Psi}{\mathrm{d}\varepsilon_{ij}} \qquad c_{ijkl} = \frac{\mathrm{d}^2\Psi}{\mathrm{d}\varepsilon_{ij}\mathrm{d}\varepsilon_{kl}}$$

Cauchy-Born rule

- Idea: Express elastic energy (strain energy density) for a atomistic representative volume element as a function of macroscopic applied strain

$$\Phi = \frac{1}{\Omega_0} \int_{\Omega_0^*} U(l)\, D_\Omega \, d\Omega$$

U(l) a function of deformation gradient

- D_Ω: Mapping function, e.g. $\quad D(l_0, \theta, \phi) = \delta_D(l_0 - l_0^*) D_{\theta\phi}(\theta, \phi)$

- Impose macroscopic deformation gradient on atomistic volume element, then calculate atomic stress – this corresponds to the macroscopic stress
- Strictly valid only far away from defects in periodic lattice (homogeneous deformation, perfect lattice, amorphous solid-average)

- Allows direct link of potential to macroscopic continuum elasticity

1D example: Cauchy-Born rule

- Impose homogeneous strain field on 1D string of atoms
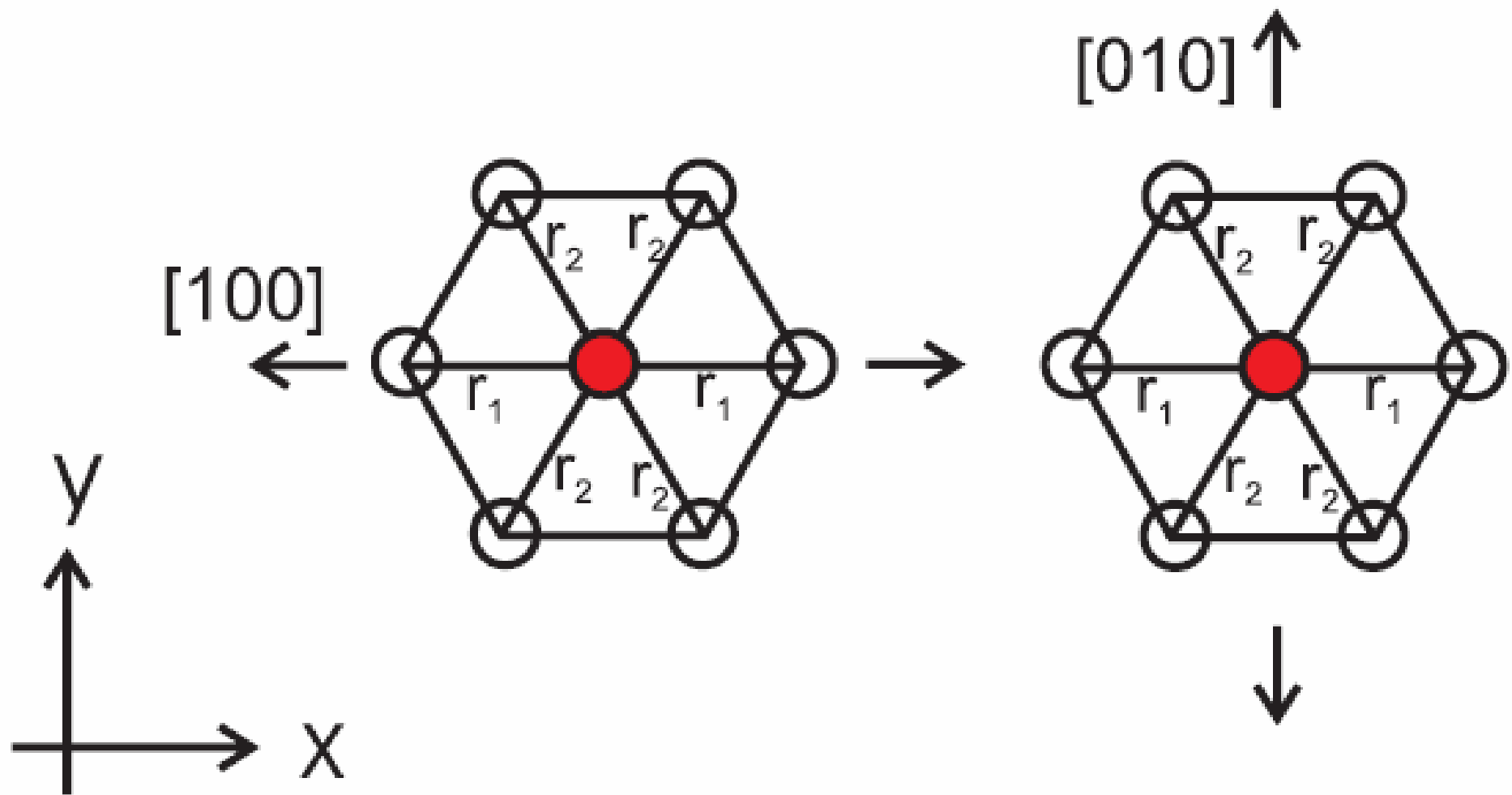- Then get $\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$

$(1+\varepsilon)\,r_0$ from that

r_0
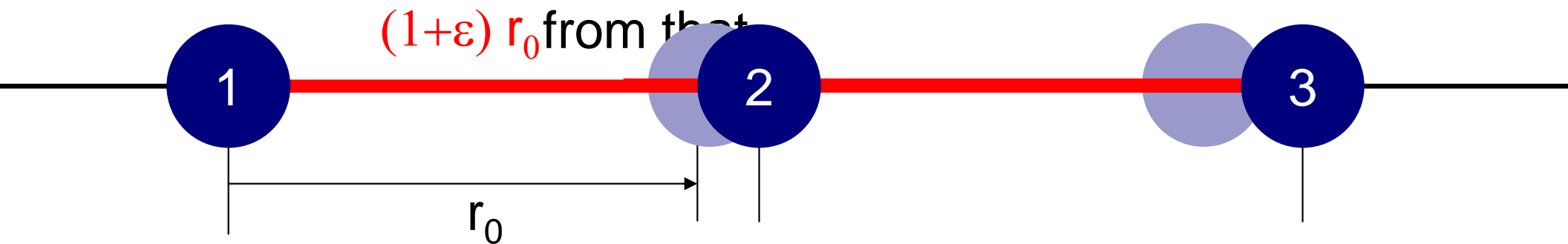
$$\Phi(\varepsilon) = \frac{1}{r_0 \cdot D}\phi(r) = \frac{1}{r_0 \cdot D}\phi((1+\varepsilon)\cdot r_0)$$

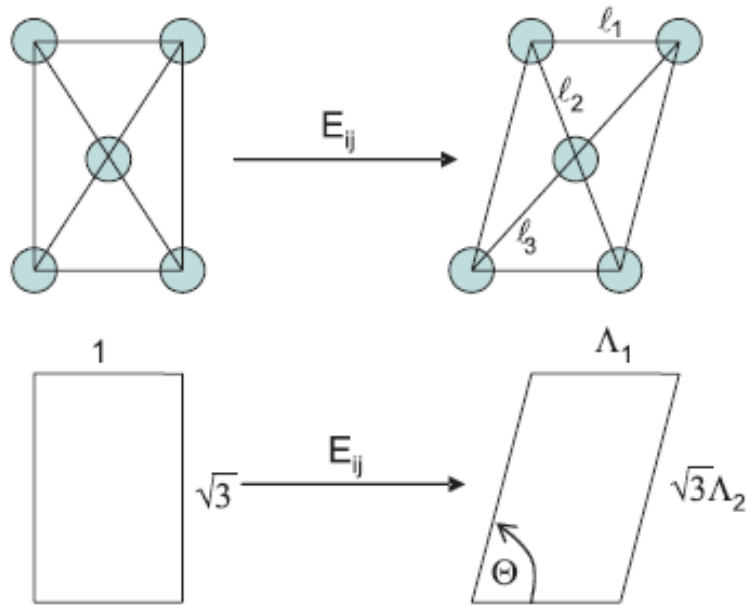Strain energy density function

$r_0 \cdot D$ Atomic volume

$$\Phi = \frac{2}{\sqrt{3}} \left(\phi(l_1) + \phi(l_2) + \phi(l_3) \right)$$

Small strains: $E_{ij} \rightarrow \varepsilon_{ij}$

(E_{ij} are Green-Lagrangian strain components from hyperelasticity)

$$E_{xx} = \left(\Lambda_1^2 - 1 \right)/2, \quad E_{yy} = \left(\Lambda_2^2 - 1 \right)/2, \quad E_{xy} = E_{yx} = \Lambda_1 \Lambda_2 \cos\left(\Theta/2 \right)$$

$$l_1 = \sqrt{1 + 2E_{xx}},$$

$$l_2 = \sqrt{1 + 1/2 E_{xx} + 3/2 E_{yy} - \sqrt{3}/2 (E_{xy} + E_{yx})}$$

$$l_3 = \sqrt{1 + 1/2 E_{xx} + 3/2 E_{yy} + \sqrt{3}/2 (E_{xy} + E_{yx})}$$

$$S_{ij} = \frac{\partial \Phi}{\partial E_{ij}}$$

Small strains: $S_{ij} \to \sigma_{ij}$

$$C_{ijkl} = \frac{\partial^2 \Phi}{\partial E_{ij} \partial E_{kl}}$$

$$C_{ijkl} \to c_{ijkl}$$

Small deformations (1st order elastic terms):

$$\Phi = \frac{\sqrt{3}}{8} \phi'' \left(3\varepsilon_{xx}^2 + 2\varepsilon_{xx}\varepsilon_{yy} + 3\varepsilon_{yy}^2 + (\varepsilon_{yx} + \varepsilon_{xy})^2 \right)$$

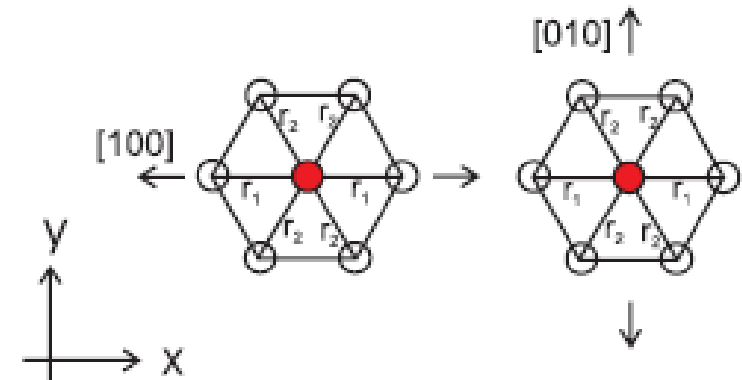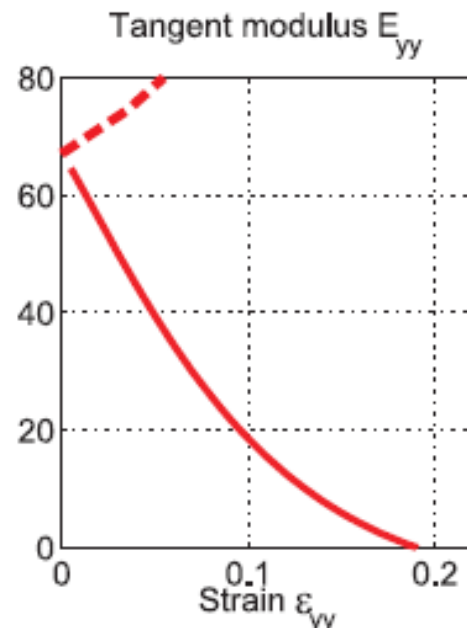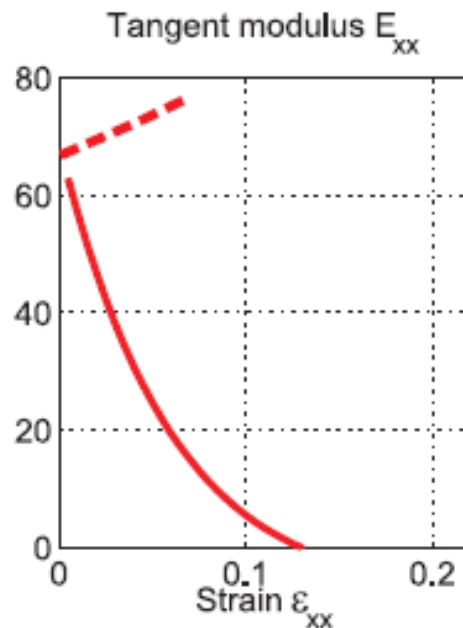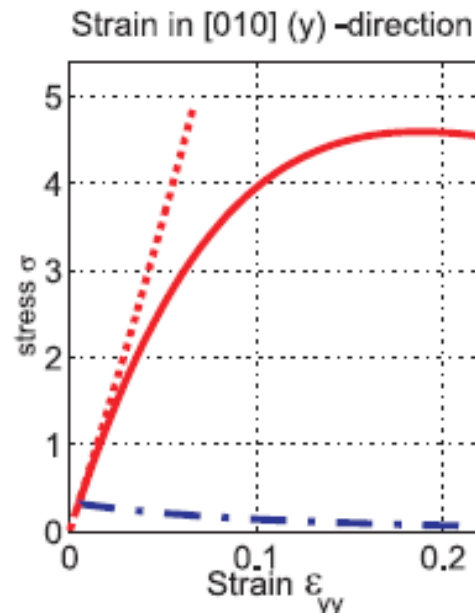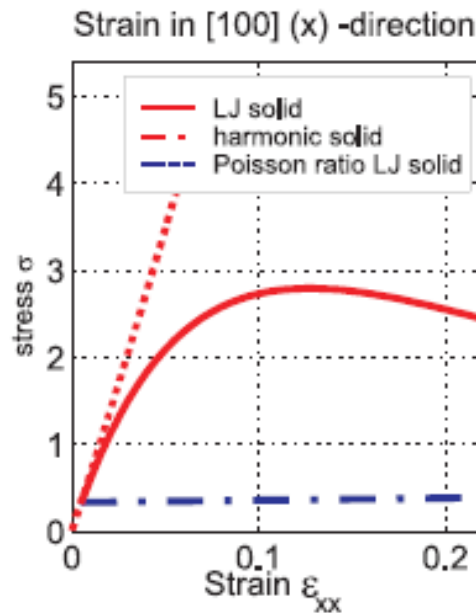$$\Phi = \frac{1}{\Omega_0} \int_{\Omega_0^*} U(l)\, D_\Omega\, d\Omega$$

This expression is obtained by expanding the potential energy (potential) up to second order terms

$$\sigma_{ij} = \frac{\partial \Phi}{\partial \varepsilon_{ij}}$$

$$\sigma_{yy} = \frac{\partial \Phi}{\partial \varepsilon_{yy}} = \frac{\sqrt{3}}{4} \phi''(r_0) \left(\varepsilon_{xx} + 3\varepsilon_{yy} \right)$$
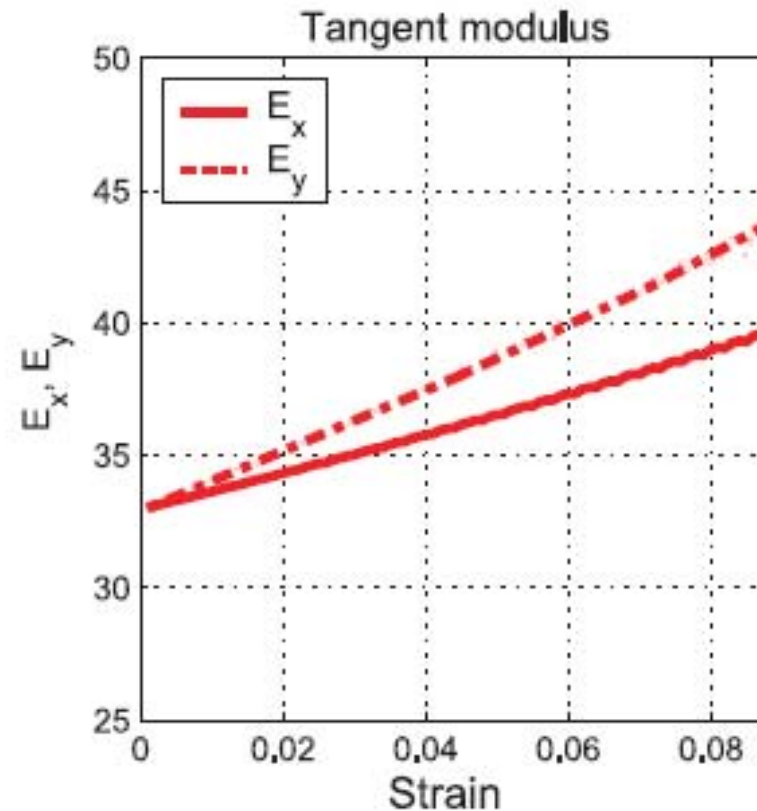
$\varepsilon=1$
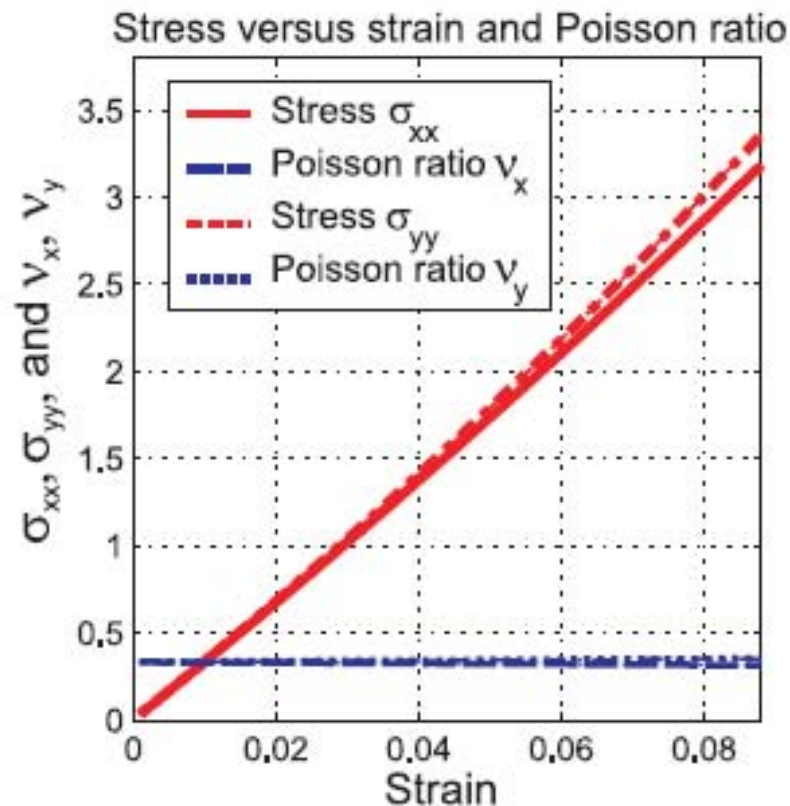
$\sigma=1$

12:6 LJ potential

Figure 5.5.: Elastic properties of the triangular lattice with harmonic interactions, stress versus strain (left) and tangent moduli E_x and E_y (right). The stress state is uniaxial tension, that is the stress in the direction orthogonal to the loading is relaxed and zero.

- **Dislocation nucleation and fracture condition**

  Ductile or brittle?