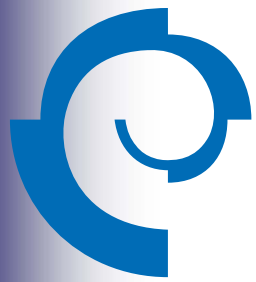
Mechanics of Ductile Materials

Lecture 4



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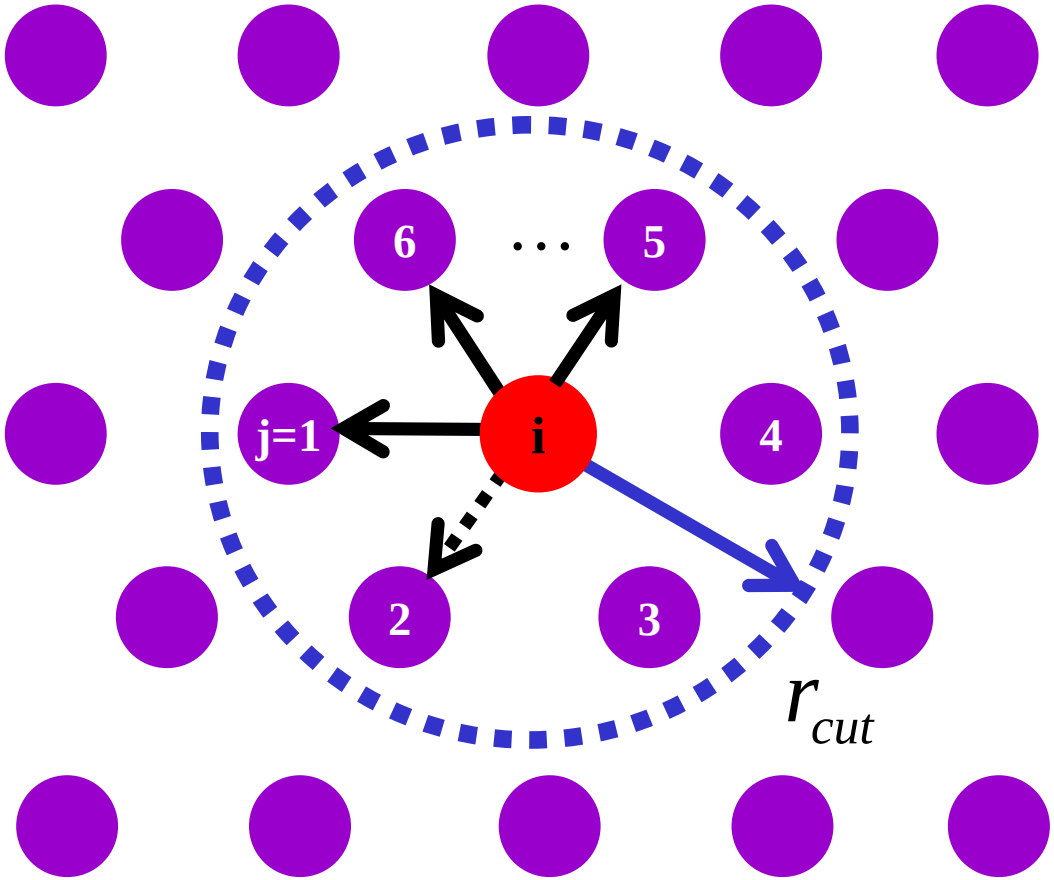
Markus J. Buehler

Pair potentials



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

Lennard-Jones 12:6

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

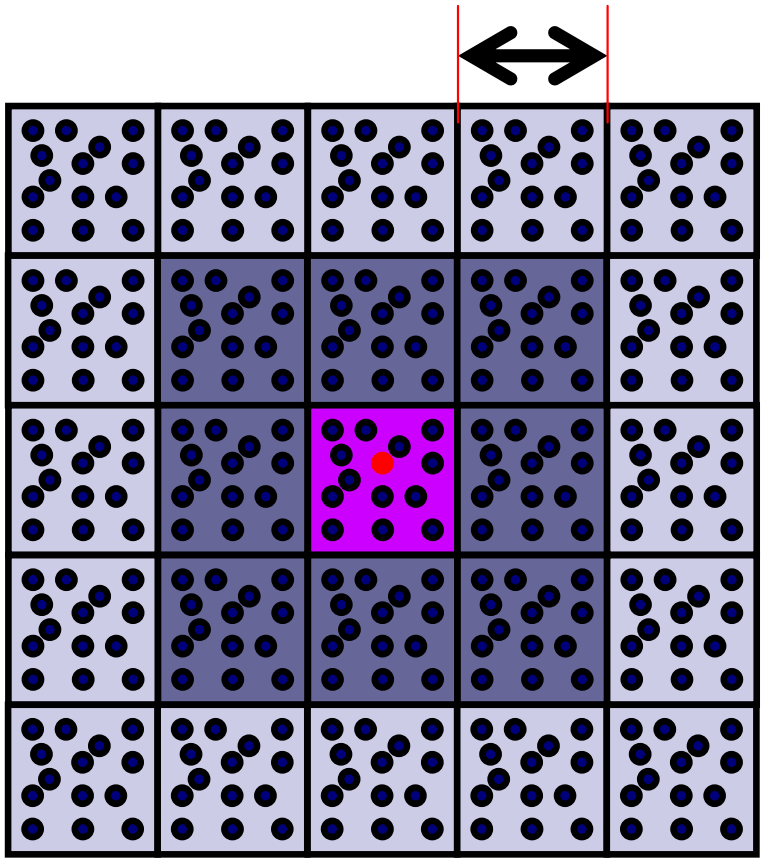
Morse

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

Reasonable model for noble gas Ar (FCC in 3D)

Numerical implementation of neighbor search: Reduction of N^2 problem to N problem

- 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)

The atomic viewpoint…

"If in some cataclysm all scientific knowledge were to be destroyed and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words? I believe it is the atomic hypothesis that all things are made of atoms - little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another. In that one sentence, you will see there is an enormous amount of information about the world, if just a little imagination and thinking are applied."

--Richard Feynman

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

Historical references

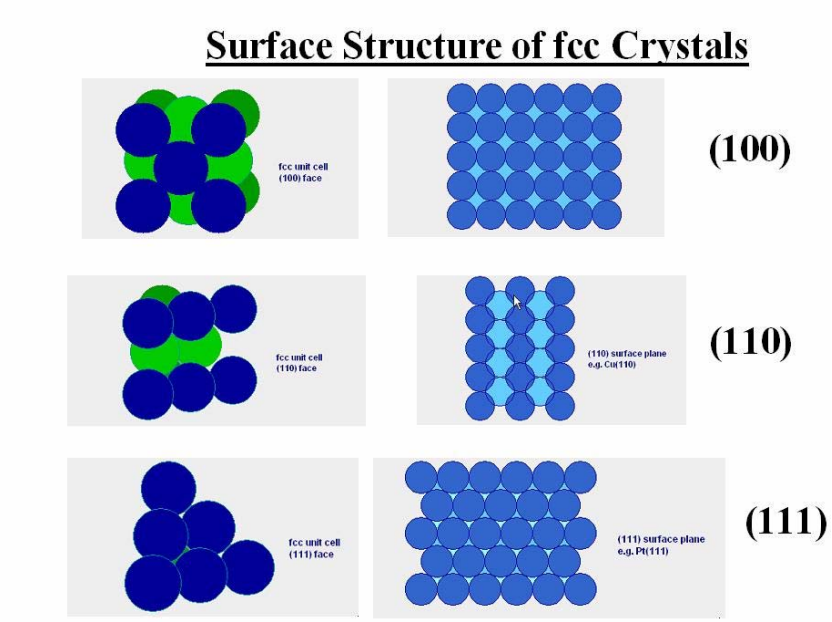
- Alder, B. J. and Wainwright, T. E. *J. Chem. Phys.* **27**, 1208 (1957)
- Alder, B. J. and Wainwright, T. E. *J. Chem. Phys.* **31**, 459 (1959)
- Rahman, A. *Phys. Rev.* **A136**, 405 (1964)
- Stillinger, F. H. and Rahman, A. *J. Chem. Phys.* **60**, 1545 (1974)
- McCammon, J. A., Gelin, B. R., and Karplus, M. *Nature (Lond.)* **267**, 585 (1977)

Outline and content (Lecture 4)

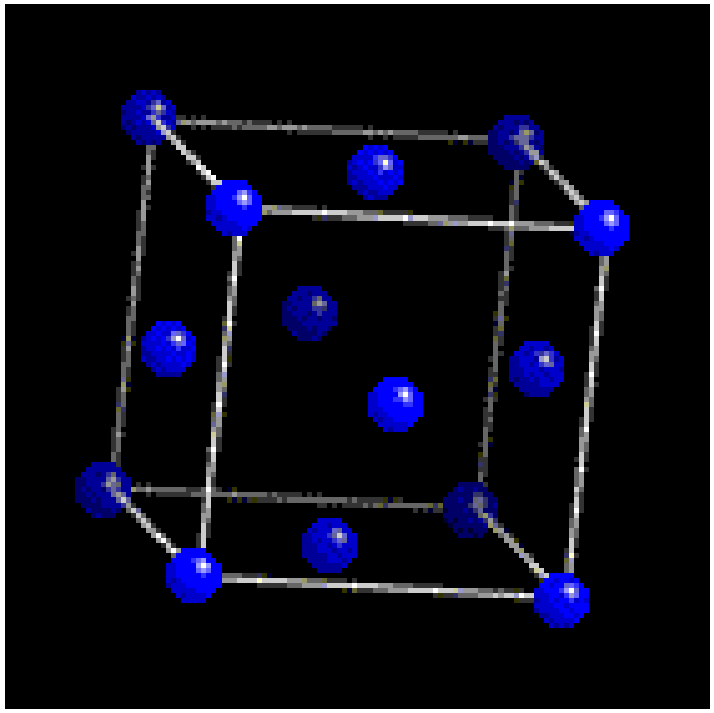
- **Topic:** Fracture and deformation – particularly of crystalline materials (metals, ceramics,..)
- **Examples:** Some MD studies of copper nanocrystals
- **Material covered:** Fundamental dislocation mechanics, energetics of dislocations, stress field around crack, dislocation interactions, basis for MD modeling of metals – EAM potentials
- **Important lesson:** Dislocation as fundamental carrier of plasticity, what goes into MD modeling
- **Historical perspective:** Discovery of dislocations in 1930s and understanding of “strength” of materials

Crystal structures: FCC

- Different crystal symmetries exist, depending on the material considered.
- For example, many metals have a cubical structure, such as FCC=face centered cubic
- http://home3.netcarrier.com/~chan/SOLIDSTATE/CRYSTAL/fcc.html



http://www.bss.phy.cam.ac.uk/~amd3/teaching/A_Donald/Crystalline_Solids_1.htm

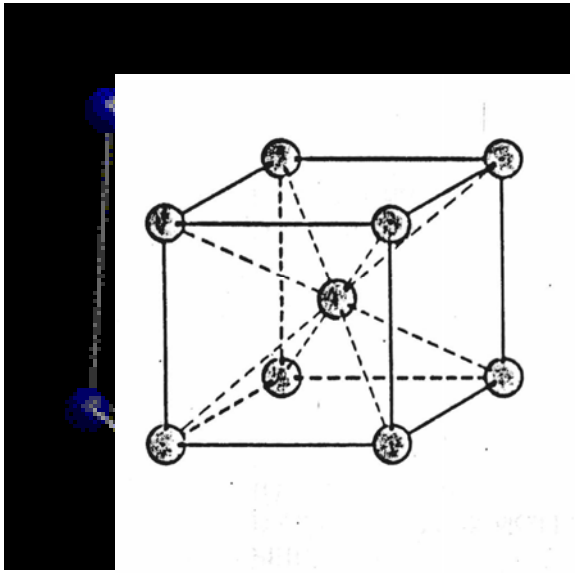


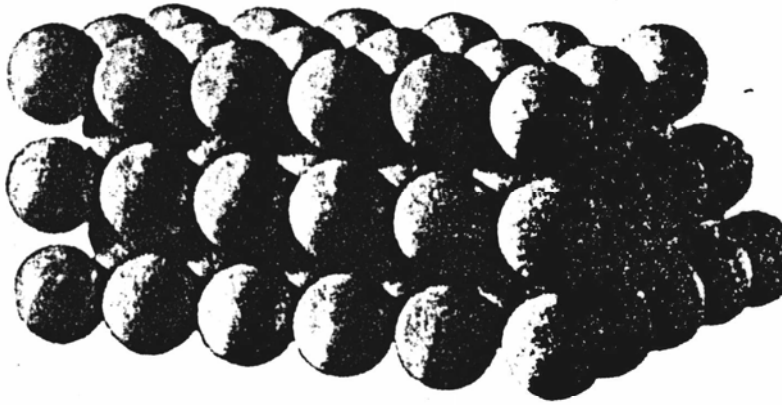
FCC

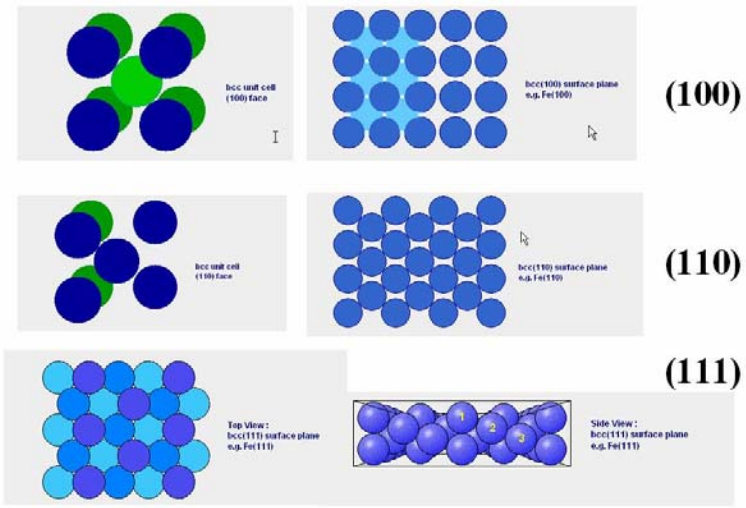
Crystal structure: BCC

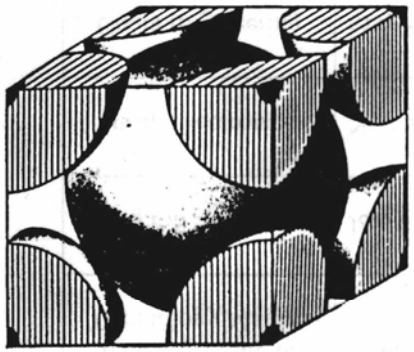
BCC

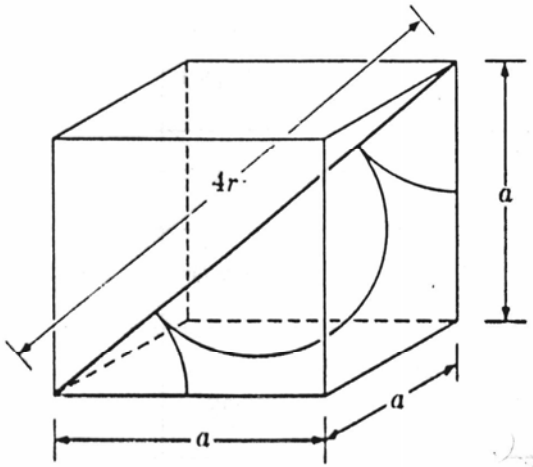
Iron (BCC)







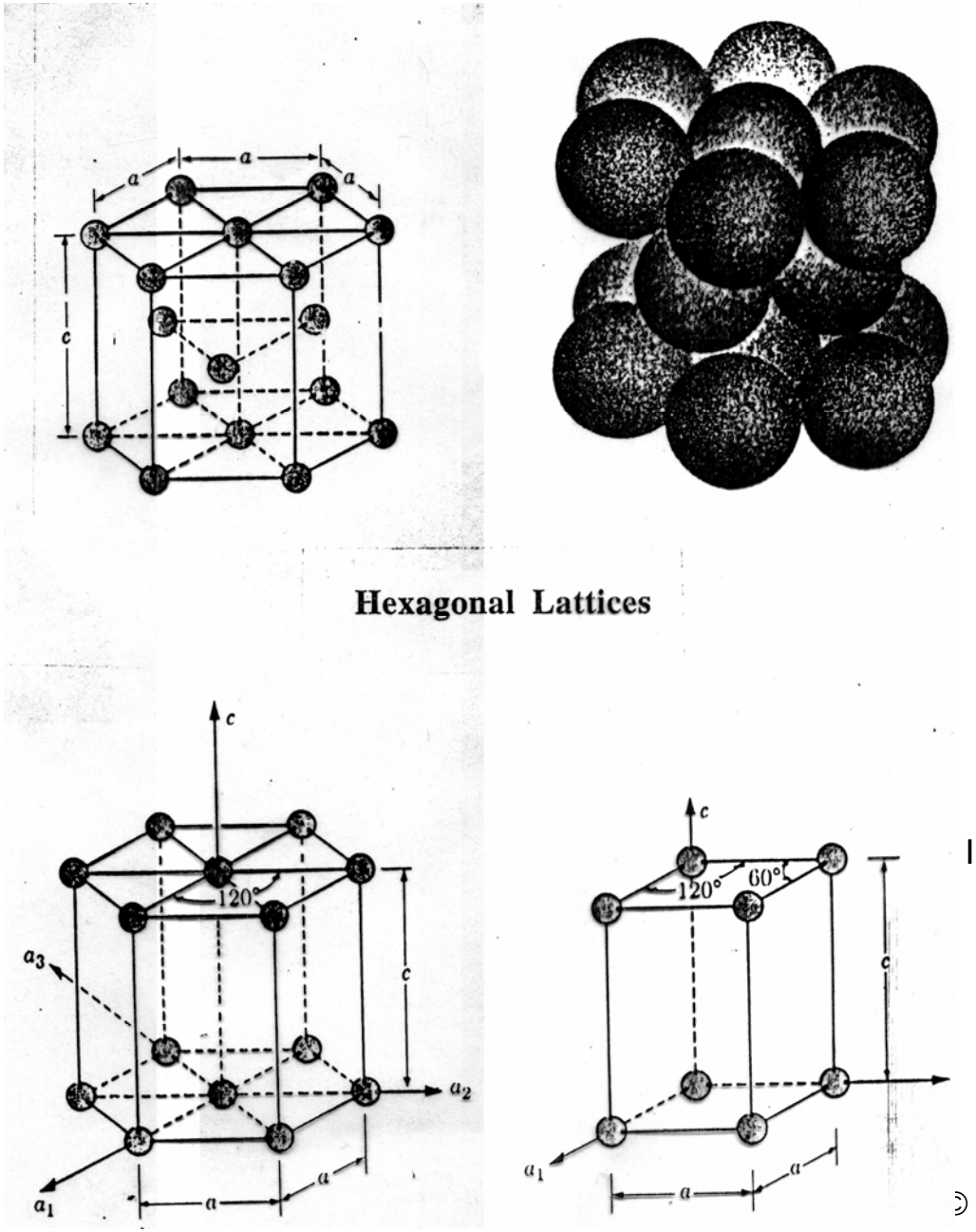




Crystal structure: HCP

HCP

Zink



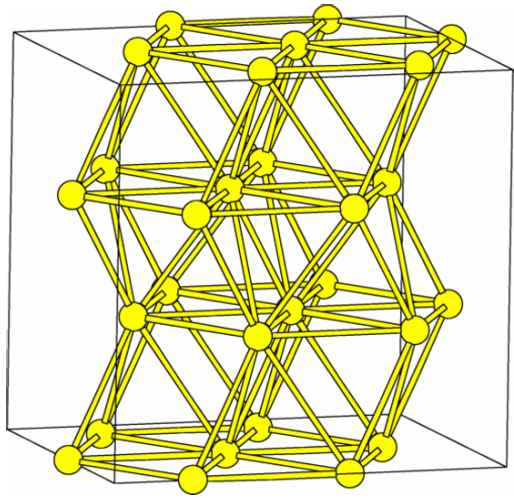
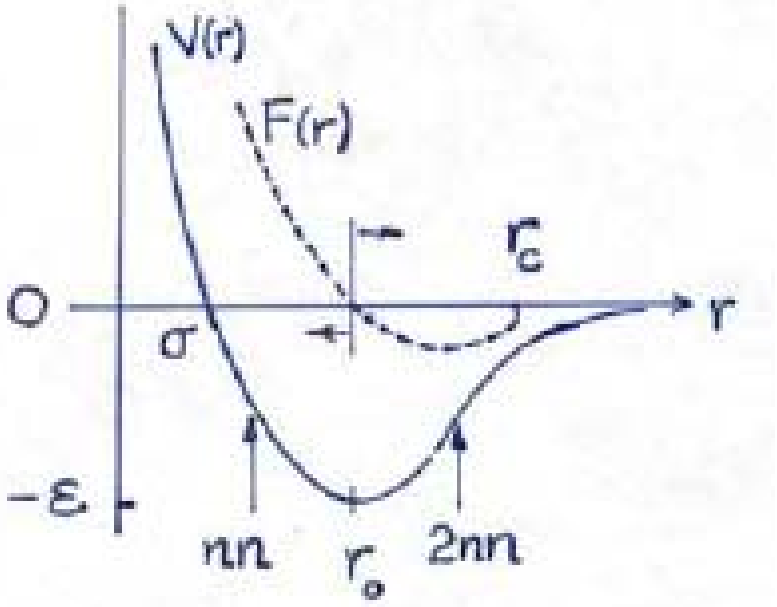
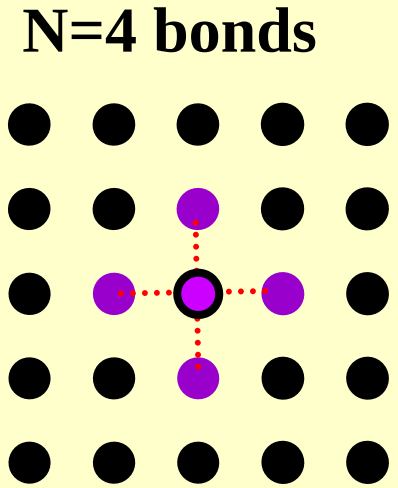


Image courtesy of the U.S. Navy.

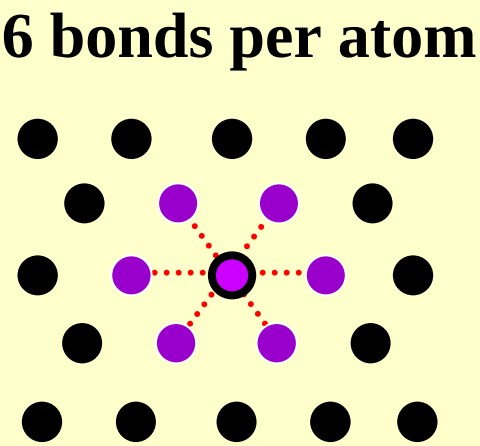
Crystal structure and potential

- The regular packing (ordering) of atoms into crystals is closely related to the potential details
- Several local minima for crystal structures exist, but materials tend to go to the structure that minimizes the energy; often this can be understood in terms of the energy per atomic bond and the equilibrium distance (at which a bond features the most potential energy)





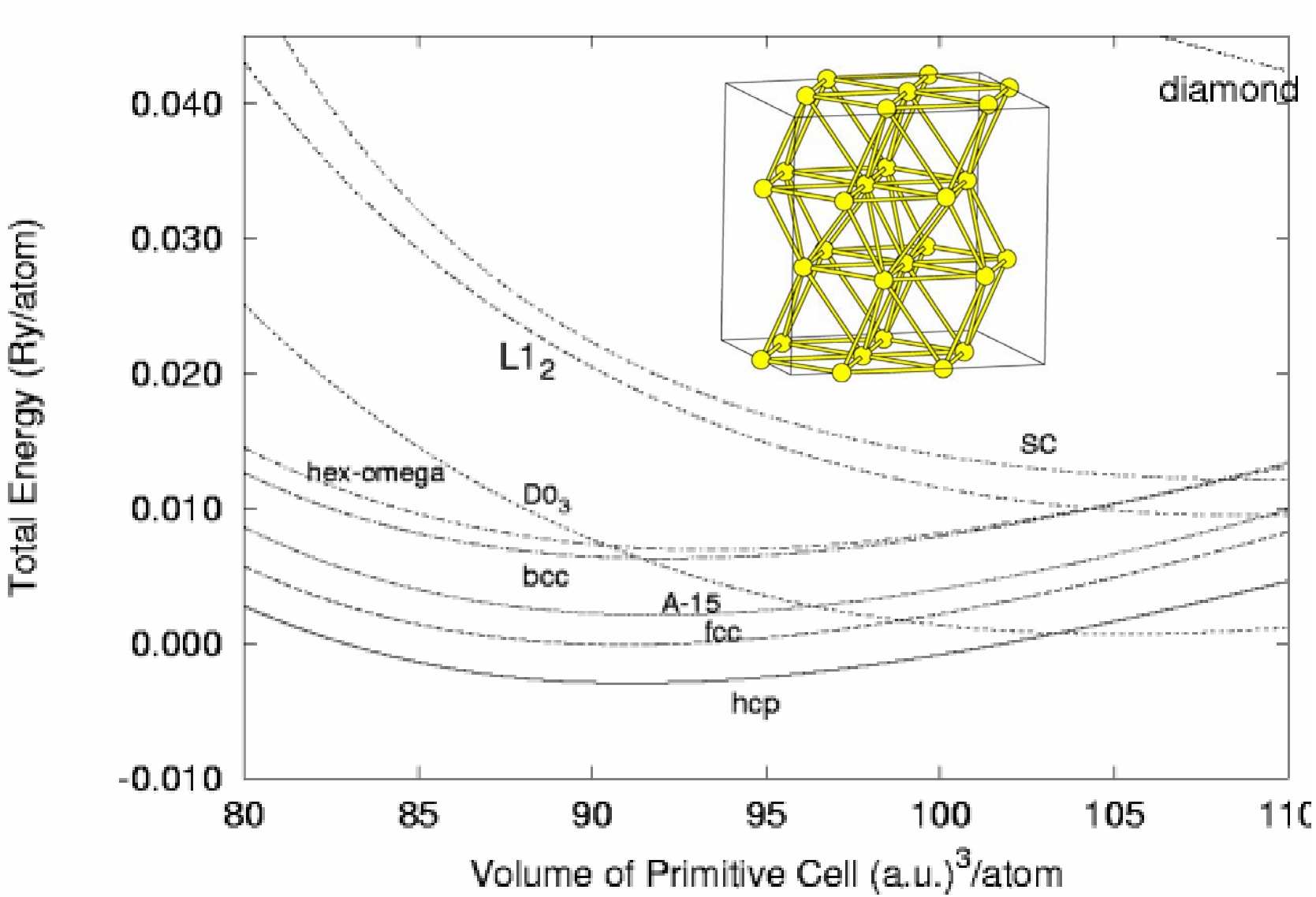
Square lattice



Hexagonal lattice

Equation of state

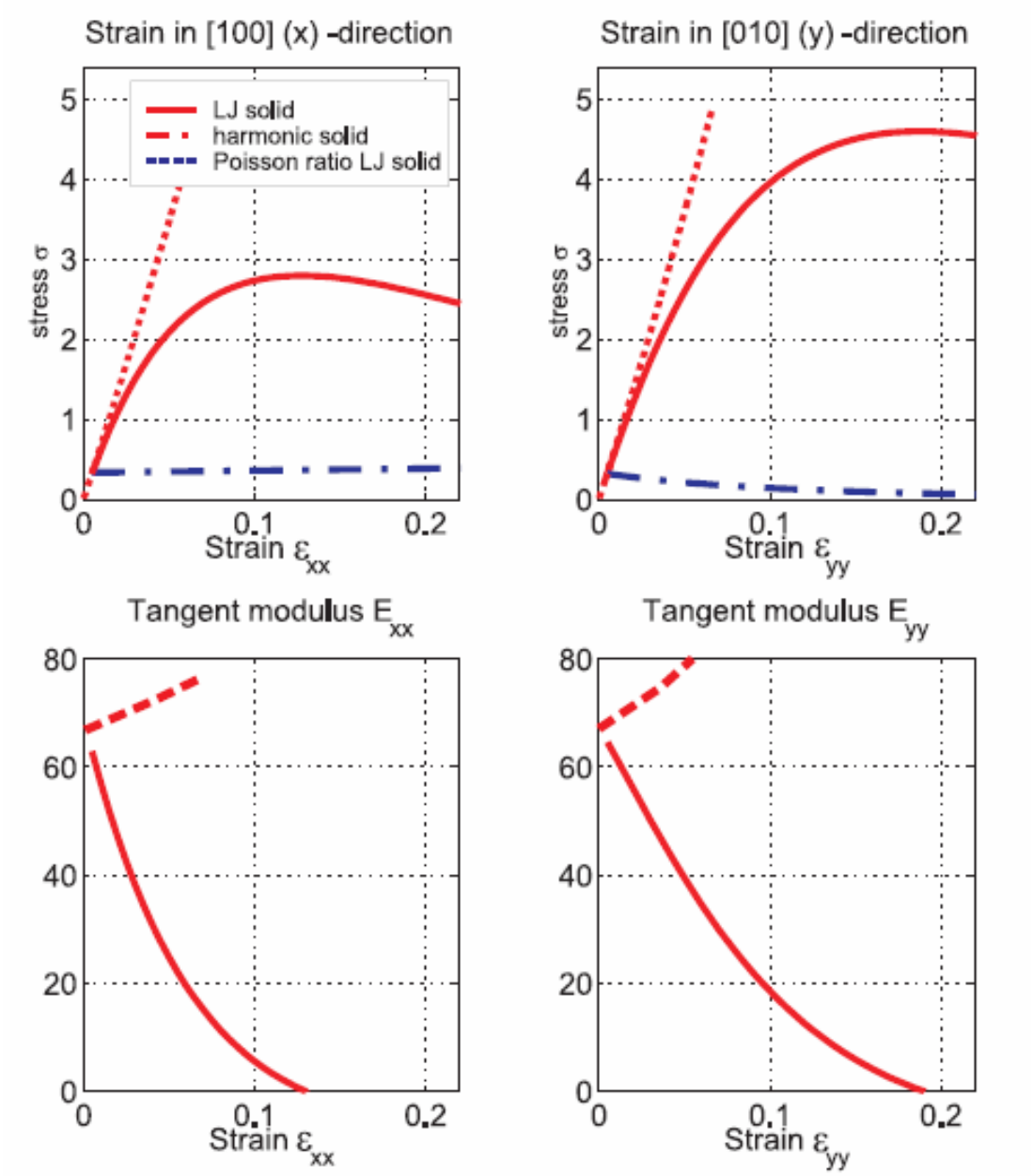
Zinc



Images courtesy of the U.S. Navy.

http://cst-www.nrl.navy.mil/~richards/projects/slr.html

Stress versus strain properties: 2D



Stress-strain response

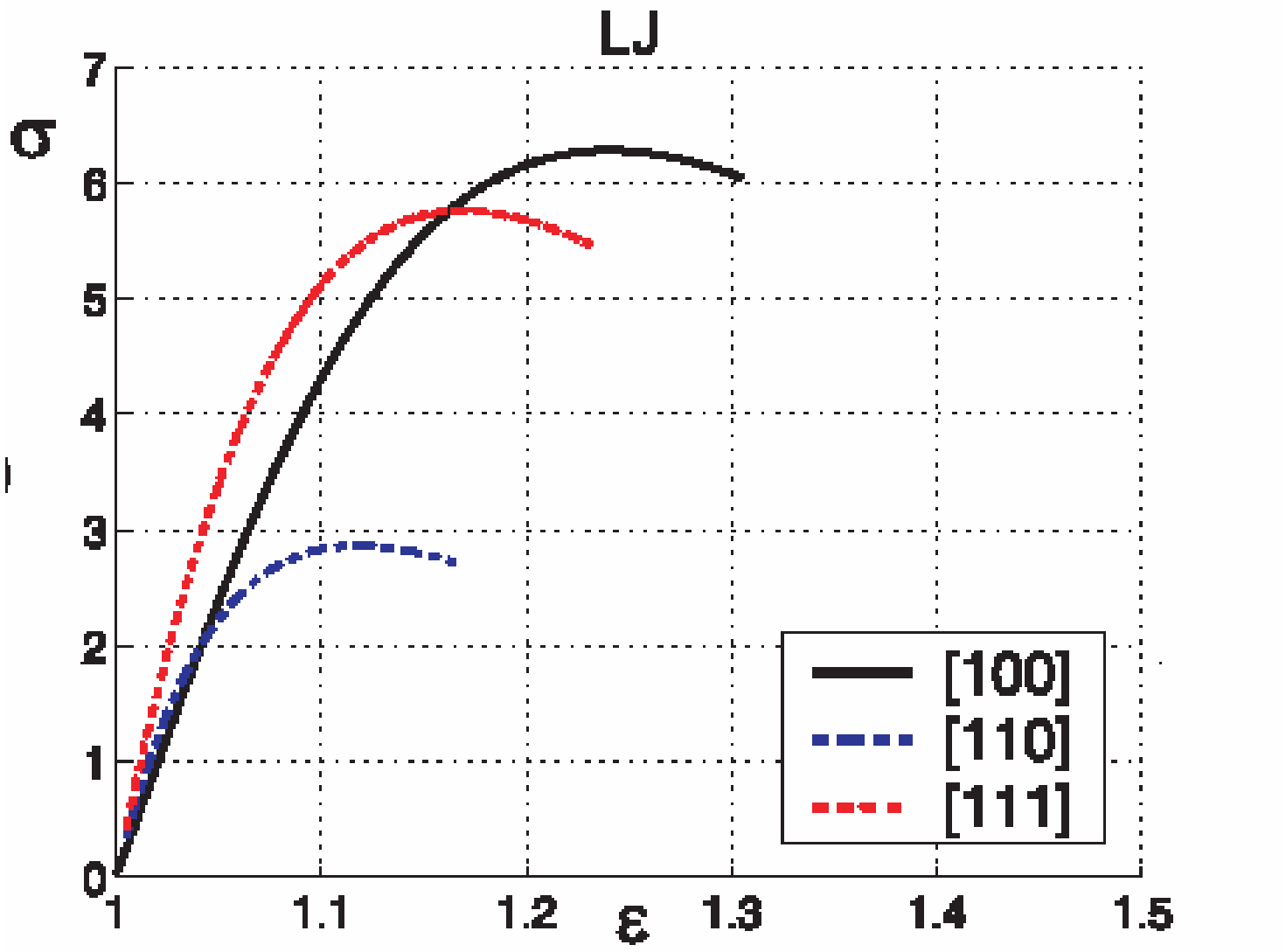
Apply uniaxial strain

Change strain in orthogonal direction so that stress is zero (Poisson effect)

Measure stress vs. strain based on virial stress

Obtain derivatives – E, c_{ijkl}

Stress versus strain properties: 3D



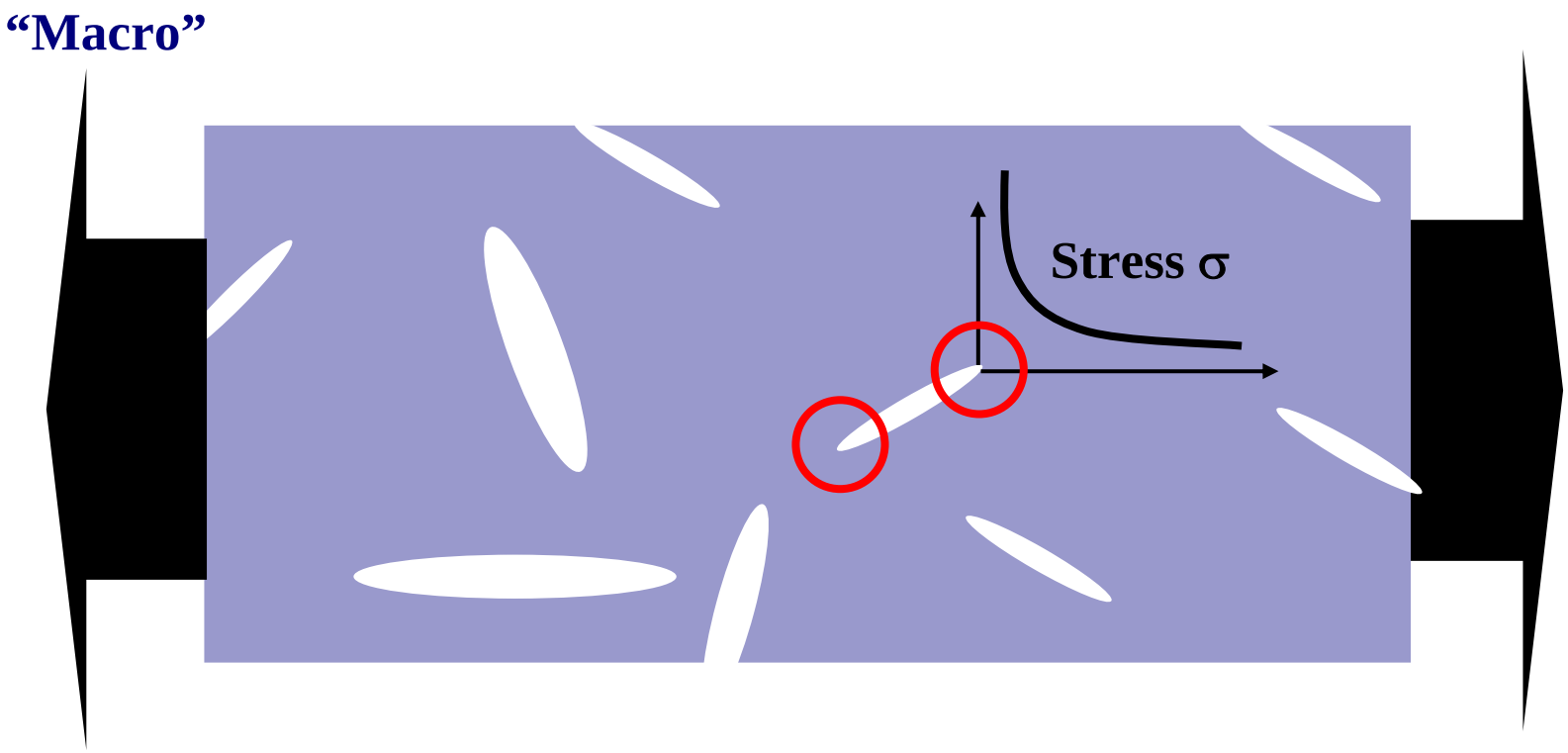
What controls the strength of materials?

- Puzzled and still puzzles scientists…
- Strength not controlled by single unit cell
- Inhomogeneities are crucial:

  Flaws, defects…
- Goal: Summarize important crystal defects and their role in deformation

  Atomistic modeling?

Deformation of materials: 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

Inglis' solution: Elliptical hole and hole

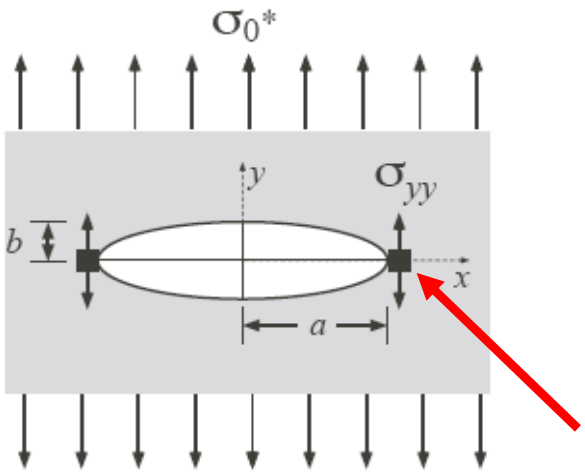


Fig. 10.7. Model setup for the Inglis/ Kolosov problem.

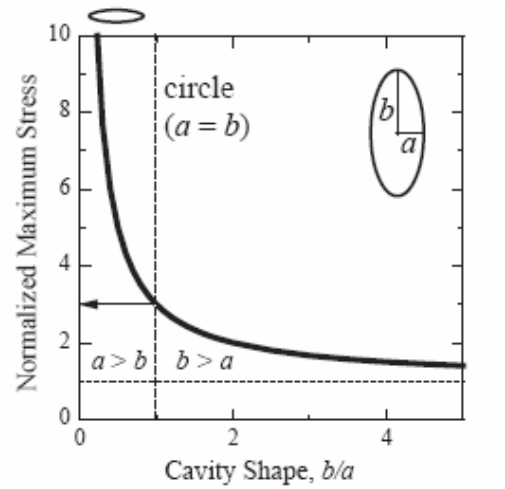


Fig. 10.8. Plot of stress changes at the edge of elliptical cavities; data from Table 10.2. Normalized maximum stress is σ_{yy}/σ_0^*; insets at top show ellipse orientations. The dashed horizontal line shows the level of stress change in the plate without a cavity present. Arrow shows stress concentration (3.0) for the circular hole ($a = b$).

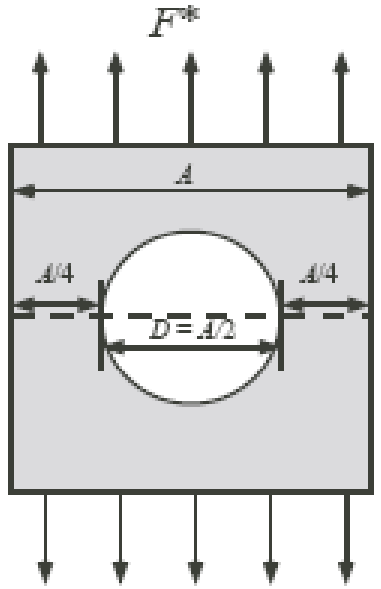


Fig. 10.5. Geometry for calculating stress in a plate with a circular hole.

$$\sigma_{yy} = \sigma_0^* \left(1 + 2\frac{a}{b}\right)$$

$$\sigma_{yy} = \sigma_0^* \left(1 + 2\sqrt{\frac{a}{\rho}}\right)$$

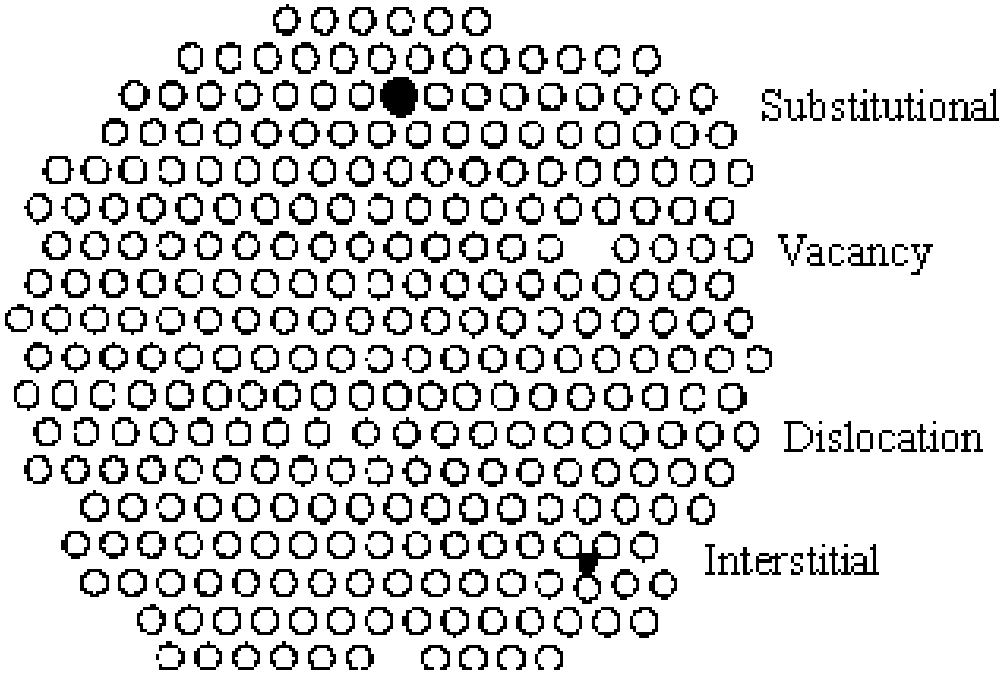
Stress magnification

Other crystallographic defects

- Point defects: Vacancies and interstitials
- (Can be produced by plastic deformation)

• Vacancy formation energy ca. E_v~1-3 eV/atom, scale with melting temperature T_m: $E_v \sim 8kT_m$

• Impurity either substitutional (other atom species on lattice site) or interstitial (non-lattice site)



http://chemed.chem.purdue.edu/genchem/topicreview/bp/materials/defects3.html

Grain boundaries

Image removed due to copyright restrictions.

Grain boundary misfit dislocations

Dieter, G. E. (1988) *Mechanical Metallurgy* ISBN 0071004068
Honeycombe, R.W.K. (1984) *The Plastic Deformation of Metals* ISBN 0713121815
Hull, D. & Bacon, D. J. (1984) *Introduction to Dislocations* ISBN 0080287204
Read, W. T. Jr. (1953) *Dislocations in Crystals* ISBN 1114490660

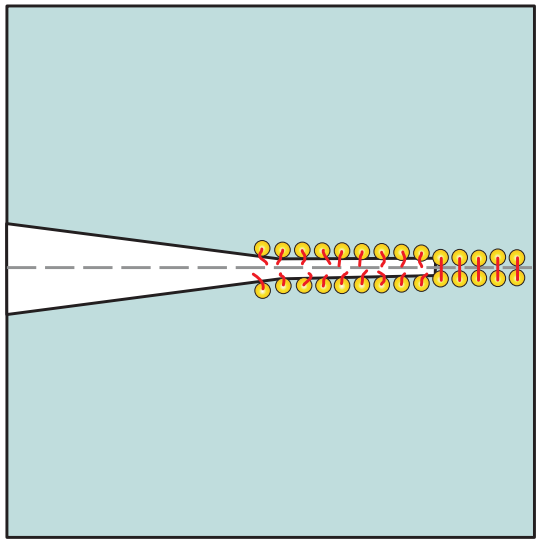
Ductile versus brittle materials

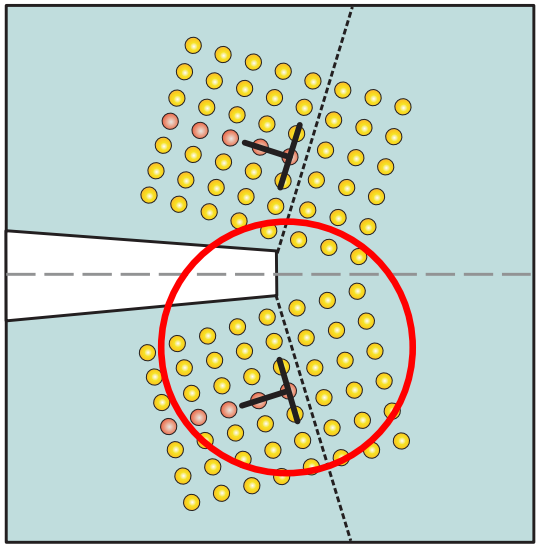
brittle

ductile

Glass,
Polymers,
Ice…

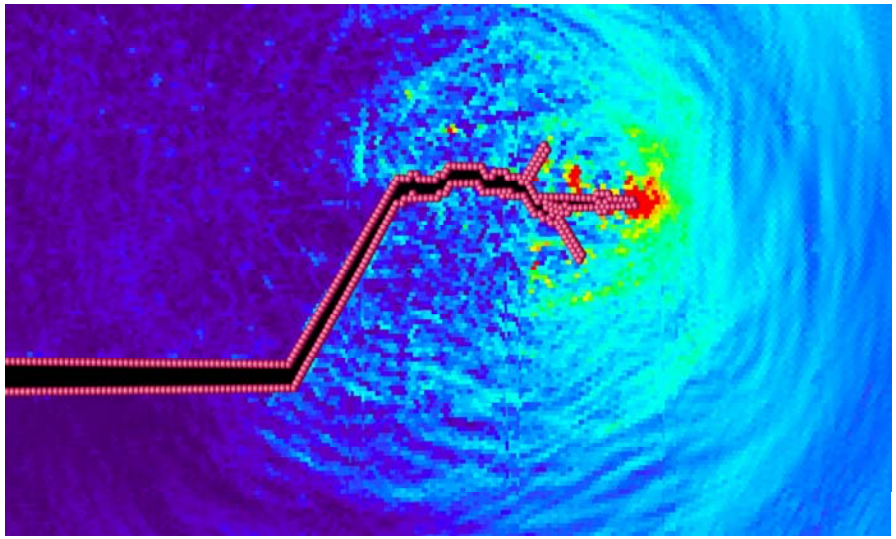
Surface energy!



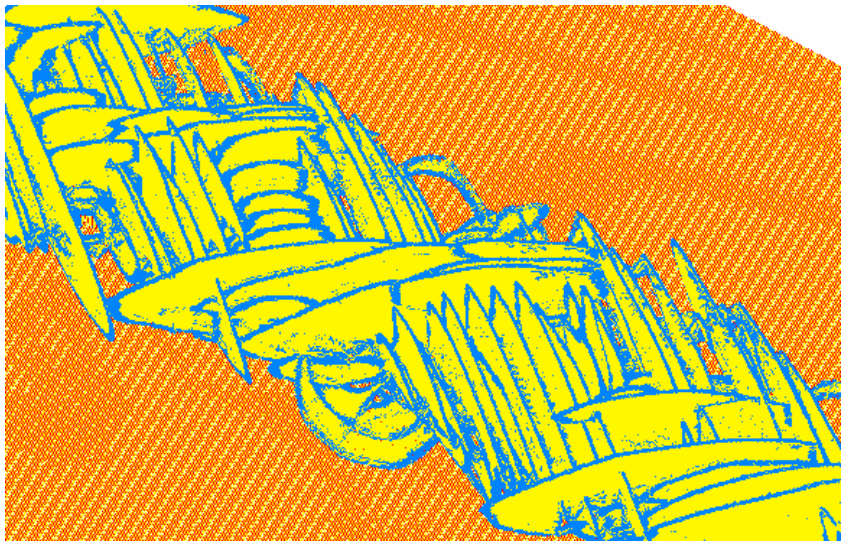


Copper,
Gold,
…

shear load



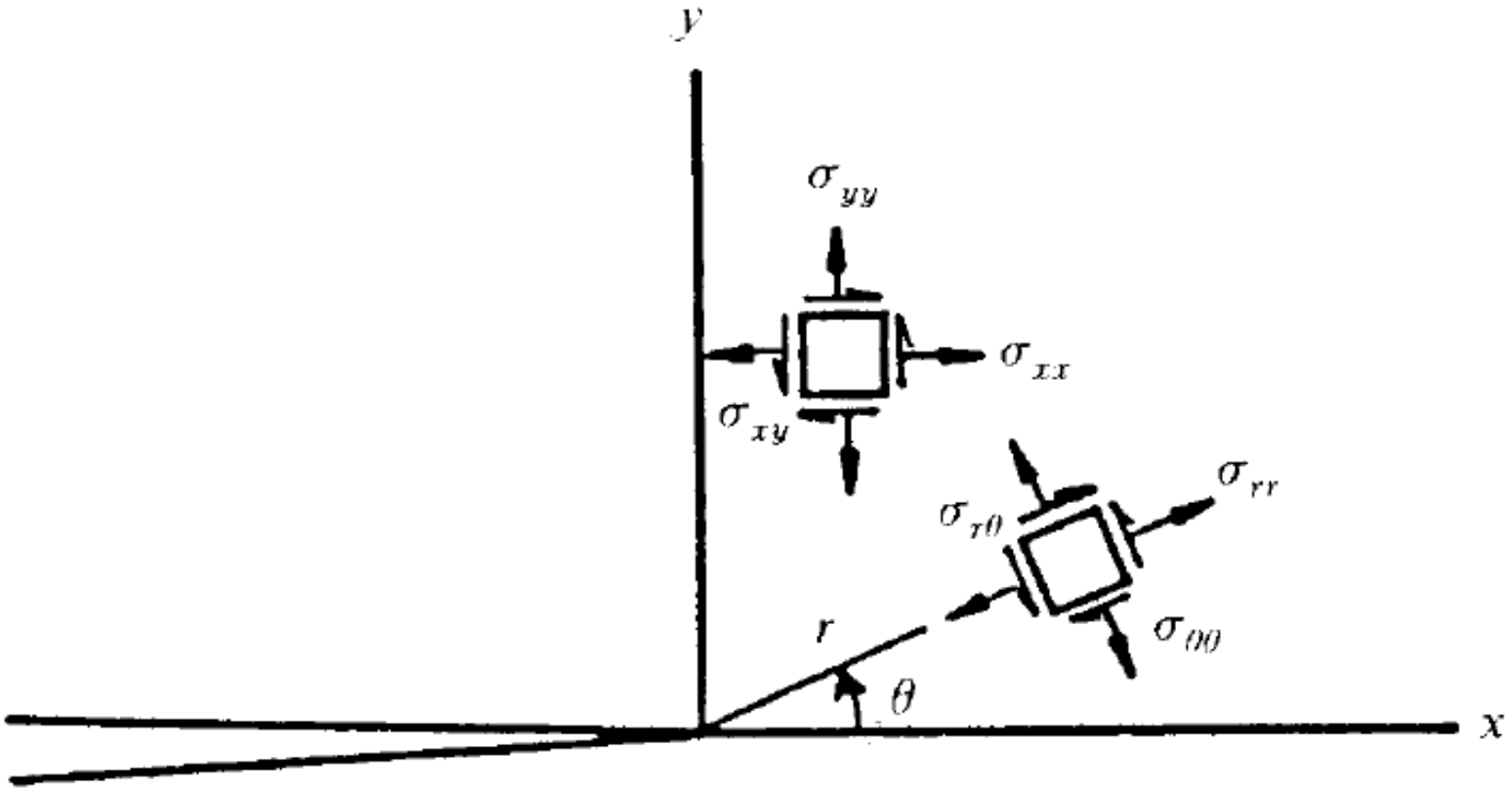
(a)



(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.

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

$$\chi = r^{(\lambda+2)}\left[A_1 \cos \lambda\theta + B_1 \cos (\lambda + 2)\theta\right] + r^{(\lambda+2)}\left[A_2 \sin \lambda\theta + B_2 \sin (\lambda + 2)\theta\right]$$

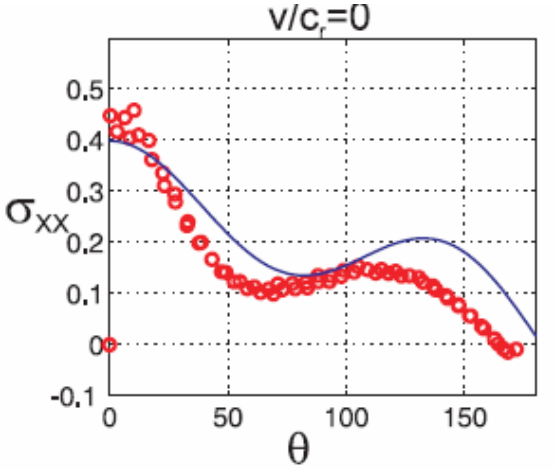
Airy stress function: Ansatz

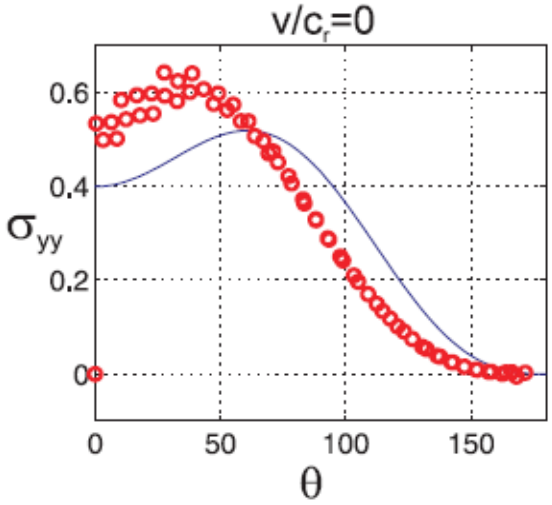
Asymptotic stress field

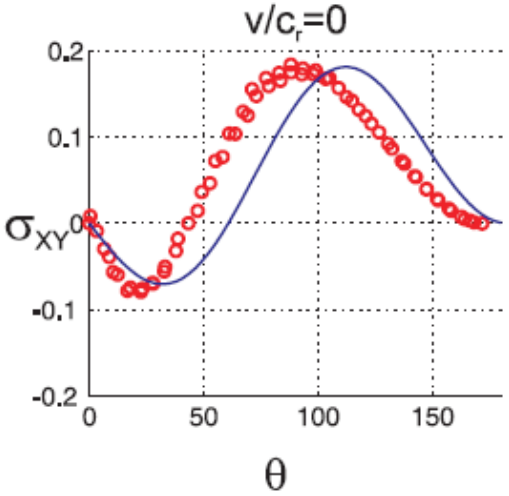
$$\begin{Bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{Bmatrix} = \frac{K_I}{\sqrt{2\pi r}} \cos\frac{\theta}{2} \begin{Bmatrix} 1 - \sin\frac{\theta}{2}\sin\frac{3\theta}{2} \\ 1 + \sin\frac{\theta}{2}\sin\frac{3\theta}{2} \\ \sin\frac{\theta}{2}\cos\frac{3\theta}{2} \end{Bmatrix}$$

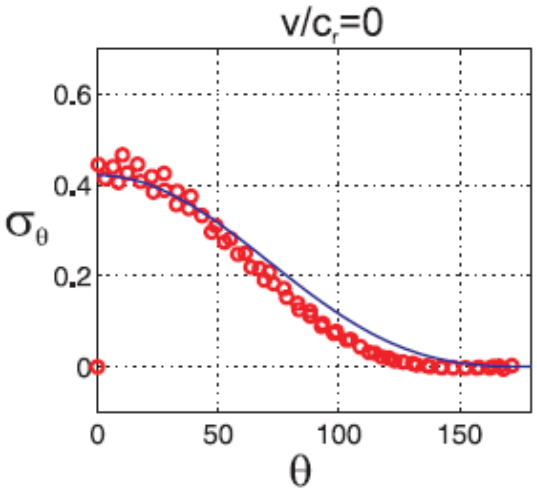
$$\begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{r\theta} \end{Bmatrix} = \frac{K_I}{\sqrt{2\pi r}} \cos\frac{\theta}{2} \begin{Bmatrix} 1 + \sin^2\frac{\theta}{2} \\ \cos^2\frac{\theta}{2} \\ \sin\frac{\theta}{2}\cos\frac{\theta}{2} \end{Bmatrix}$$

Stress field around a (static) crack



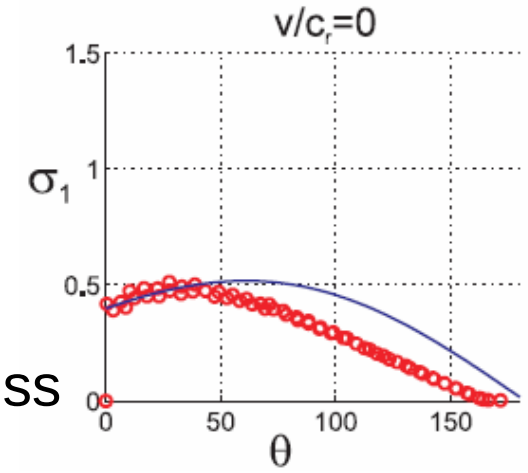






Hoop or opening stress

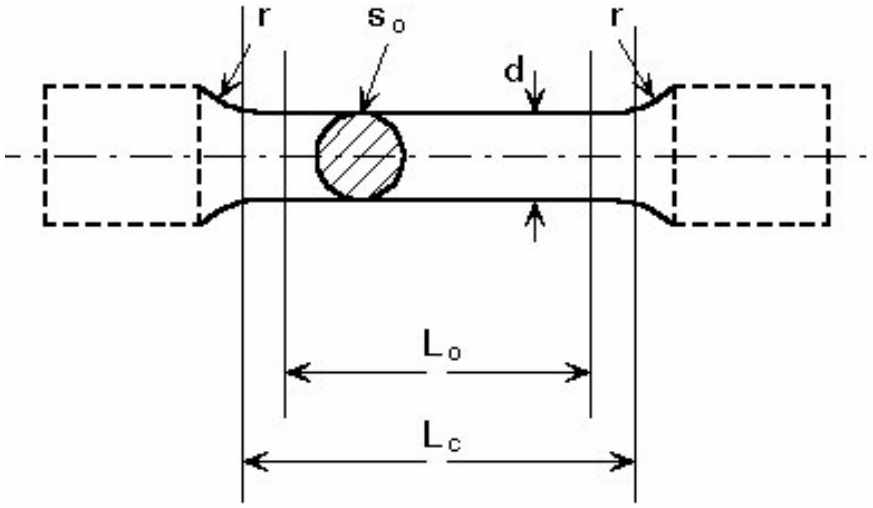
Maximum principal stress



Continuum theory

MD modeling

Deformation of metals: Example



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

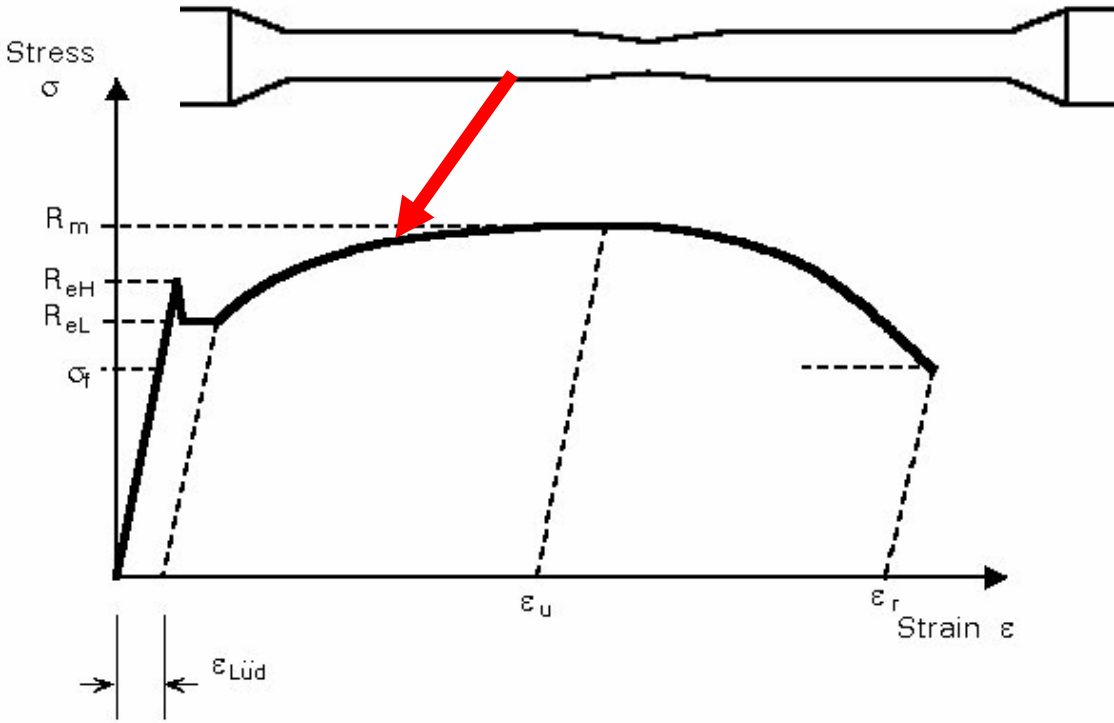


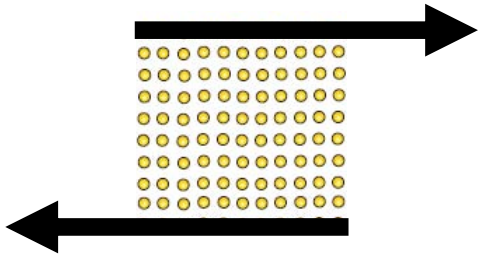
Figure 6 Engineering stress-strain curve of a metal, e.g. mild steel, with a yield point

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

Theoretical shear strength

- Perfect crystal: Deformation needs to be cooperative movement of all atoms; the critical shear stress for this mechanism was calculated by Frenkel (1926):

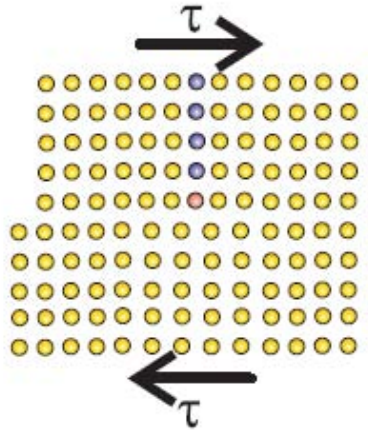
$$\tau_{th} = \frac{b}{a}\frac{G}{2\pi} \approx \frac{G}{30}$$



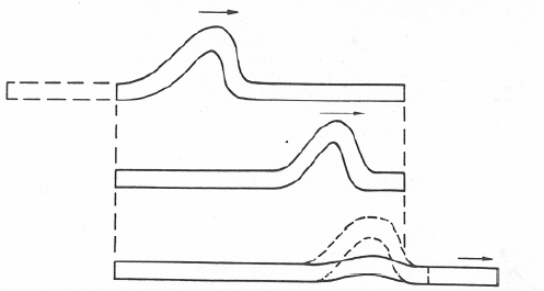
- Although this is an approximation, the shear strength measured in experiment is much lower:

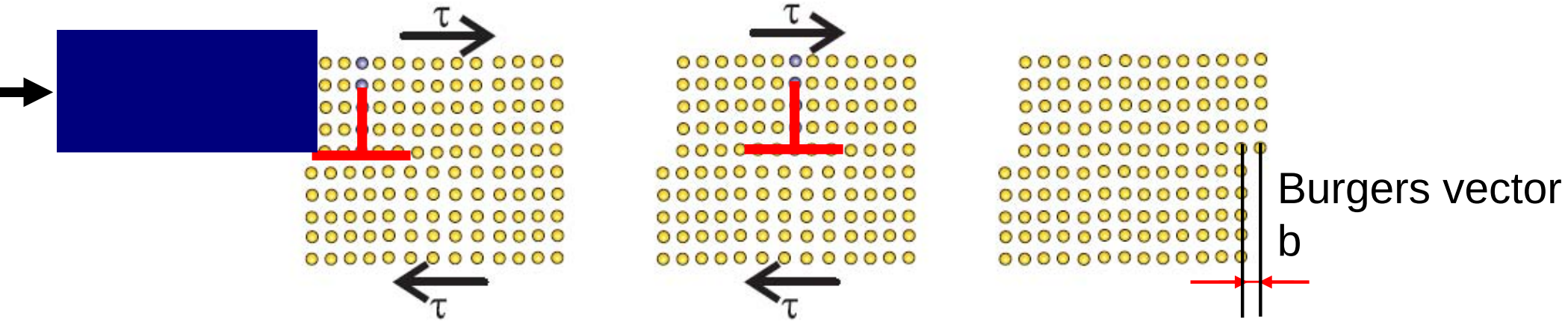
$$\tau_{\exp} = \frac{G}{10{,}000...100{,}000{,}000}$$

- Difference explained by existence of dislocations by Orowan, Polanyi and Taylor in 1934
- Confirmed by experiments with whiskers (dislocation free crystals)



Ductile materials are governed by the motion of dislocations: Introduction





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

http://www.people.virginia.edu/~lz2n/mse209/Chapter7.pdf

Deformation of crystals

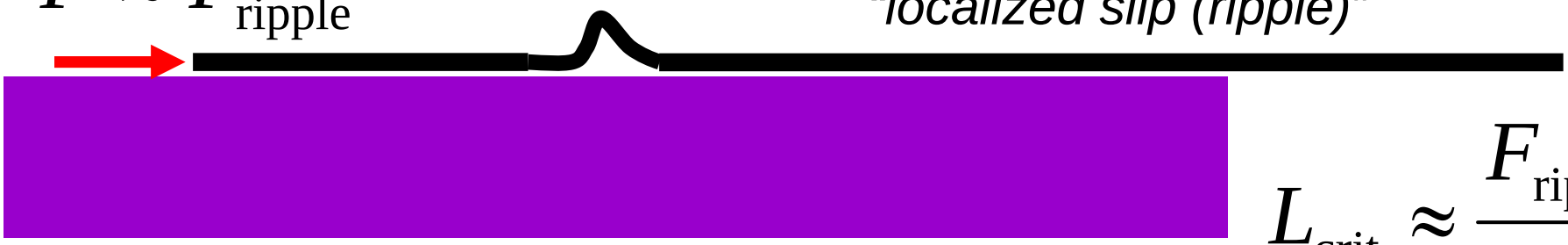
- Deformation of a crystal is similar to pushing a sticky tape across a surface:

$$F \sim \tau \cdot L$$

"homogeneous shear"

$$F \approx F_{\text{ripple}}$$

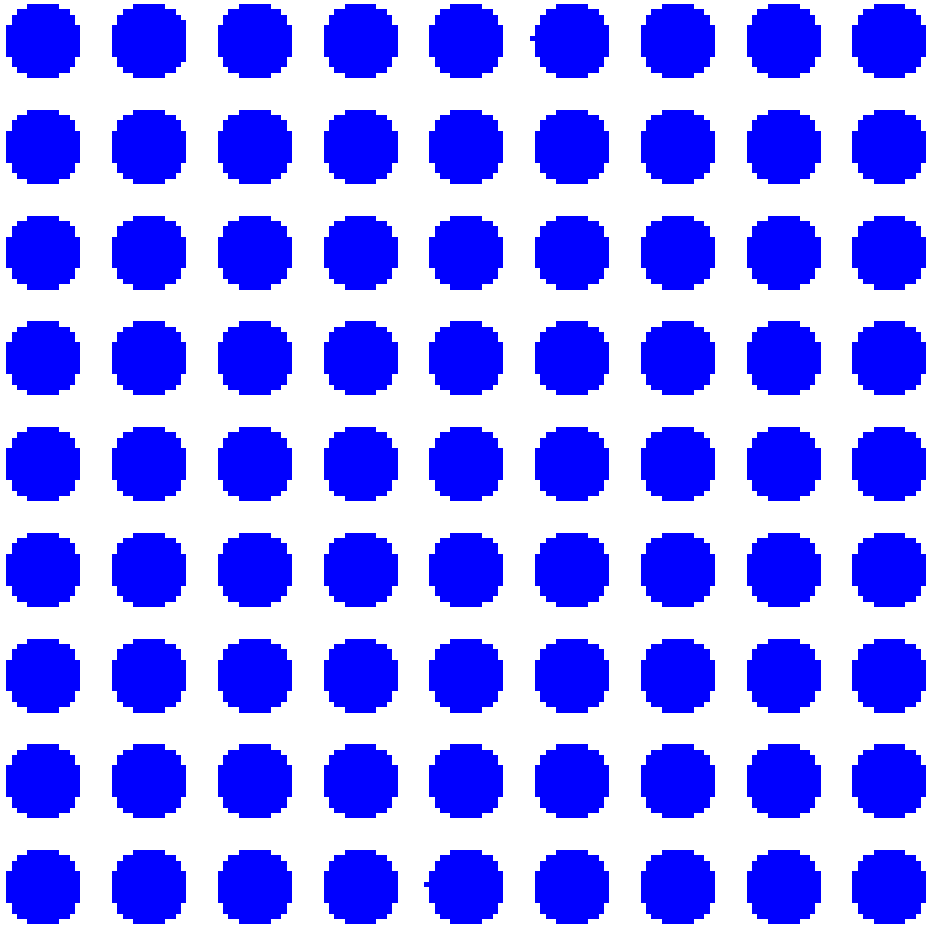
"localized slip (ripple)"



$$L_{\text{crit}} \approx \frac{F_{\text{ripple}}}{\tau}$$

Beyond critical length *L* it is easer to have a localized ripple…

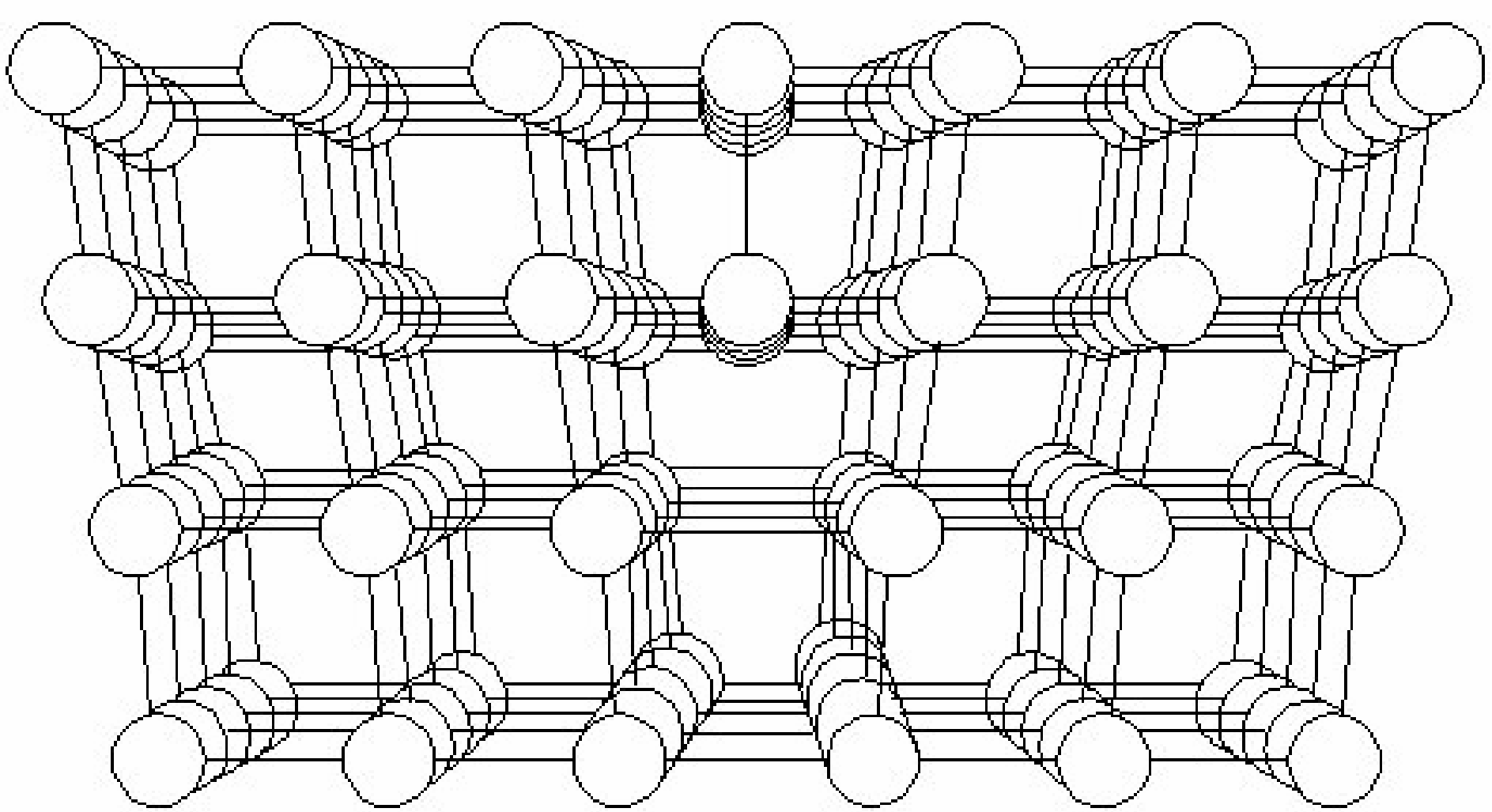
Animation: Dislocation motion



Animation online:

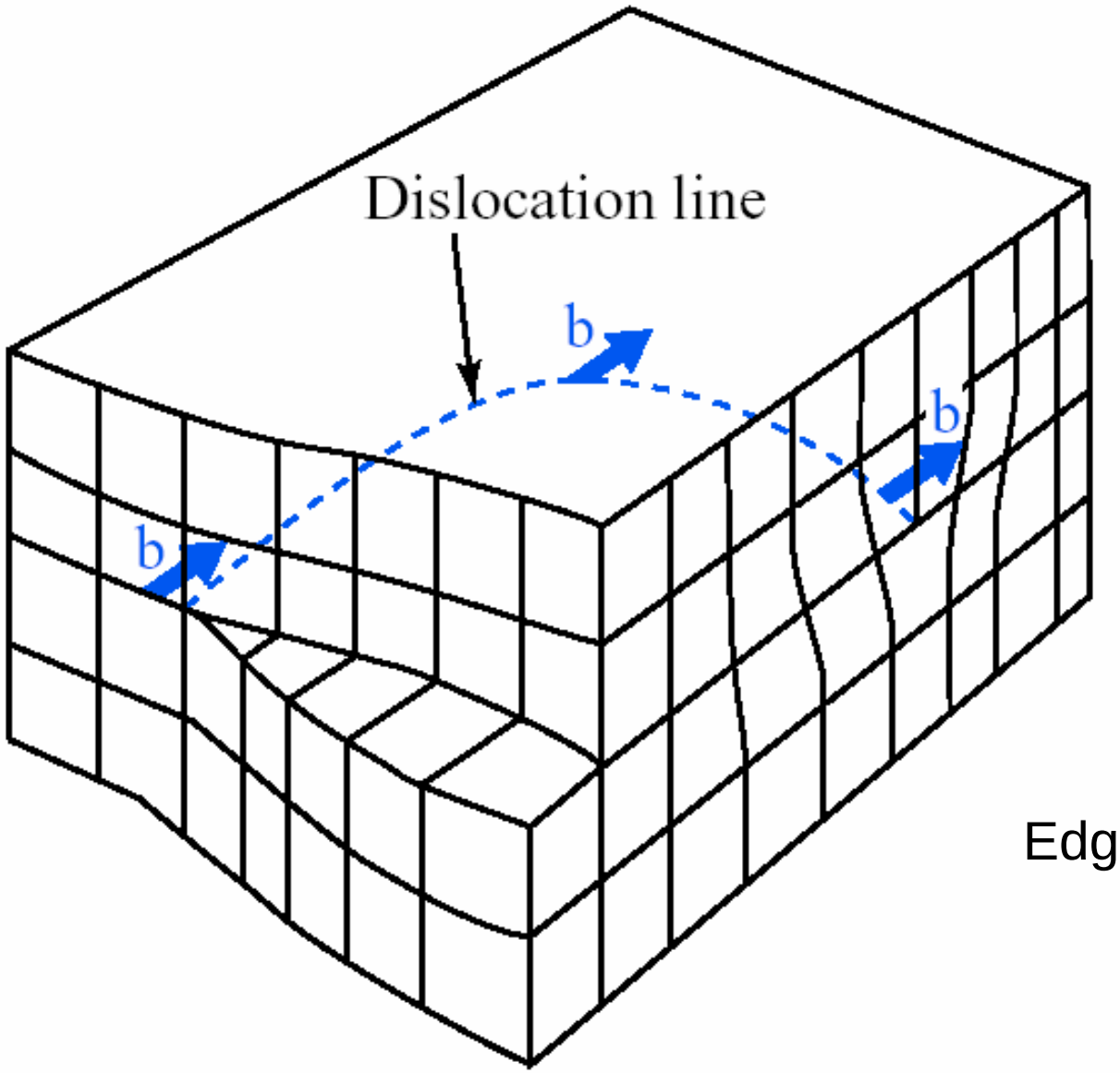
http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/illustr/a5_1_1.html

Geometry of a dislocation (3D view)



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

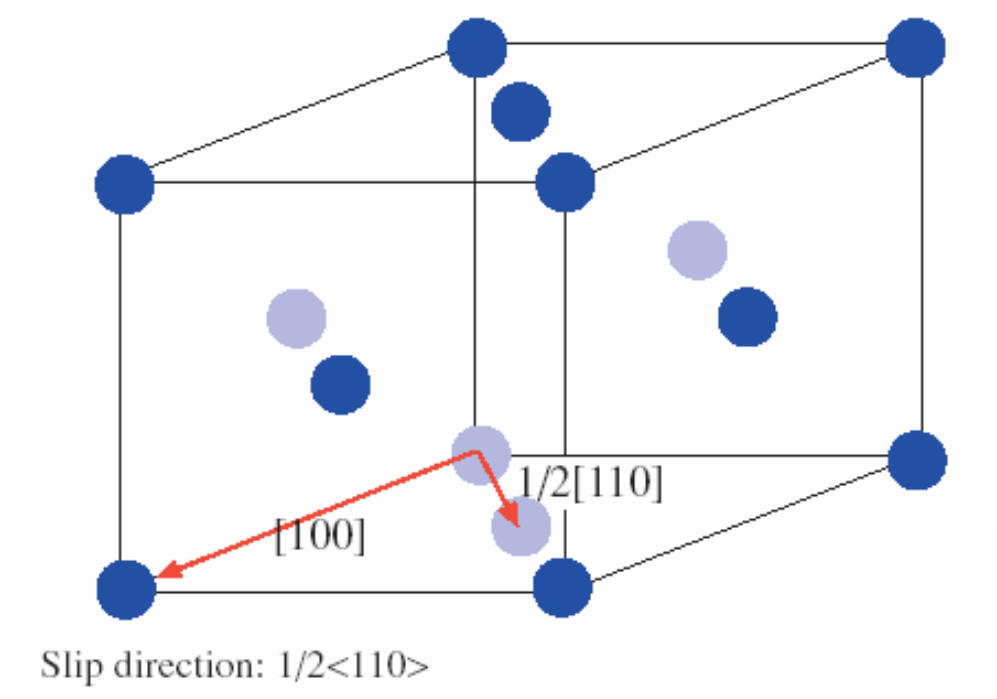
Edge and screw dislocations



Screw

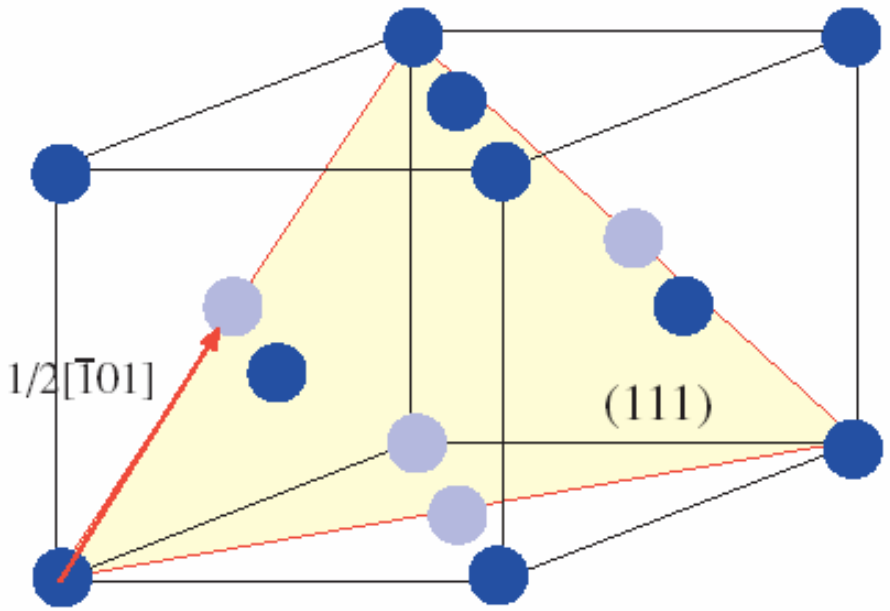
Edge

Slip direction and plane in FCC



Slip direction: 1/2<110>

For specific crystals, there are certain directions of Burgers vectors and slip planes that are energetically favored



Slip plane: {111}

FCC:

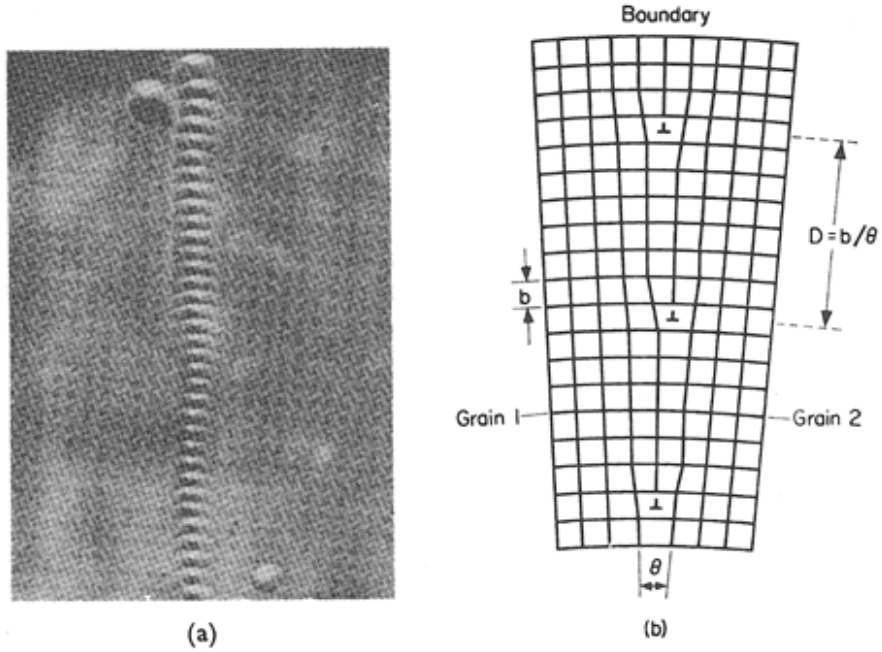
Slip directions are ½<110>

Glide planes are {111}

The slip planes and directions are those of highest packing density

Experimental observation

Transmission Electron Micrograph of Dislocations



Grain boundary misfit dislocations

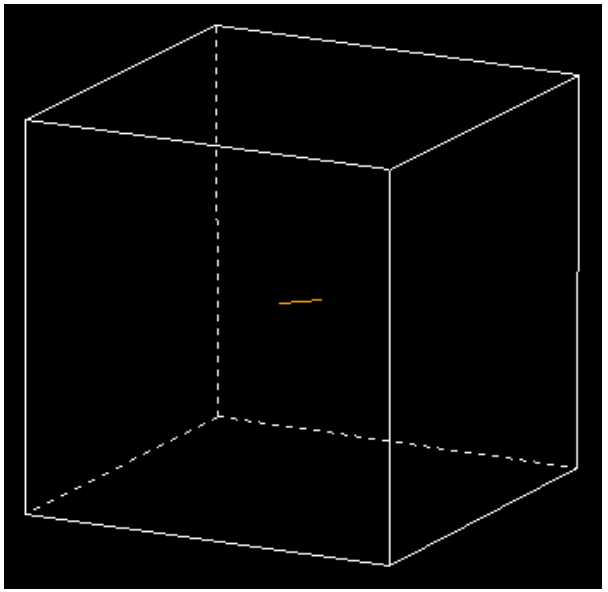
Dieter, G. E. (1988) *Mechanical Metallurgy* ISBN 0071004068
Honeycombe, R.W.K. (1984) *The Plastic Deformation of Metals* ISBN 0713121815
Hull, D. & Bacon, D. J. (1984) *Introduction to Dislocations* ISBN 0080287204
Read, W. T. Jr. (1953) *Dislocations in Crystals* ISBN 1114490660

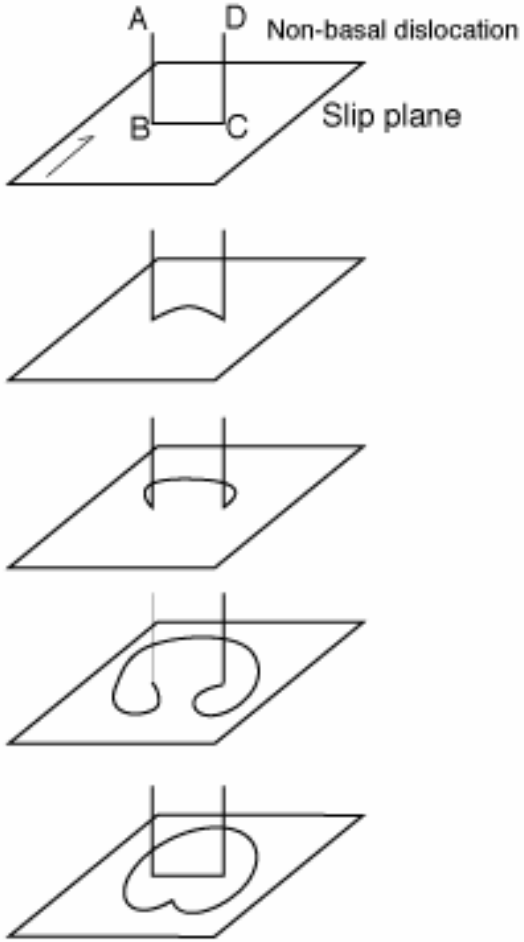
Geometry of a dislocation (3D view)

- How to model nucleation, propagation of dislocations?
- Particularities in different crystal structures
- Energetics?
- Motion of a dislocation? Eq. of motion? Newton's laws?
- Interactions?
- …

Sources of dislocations

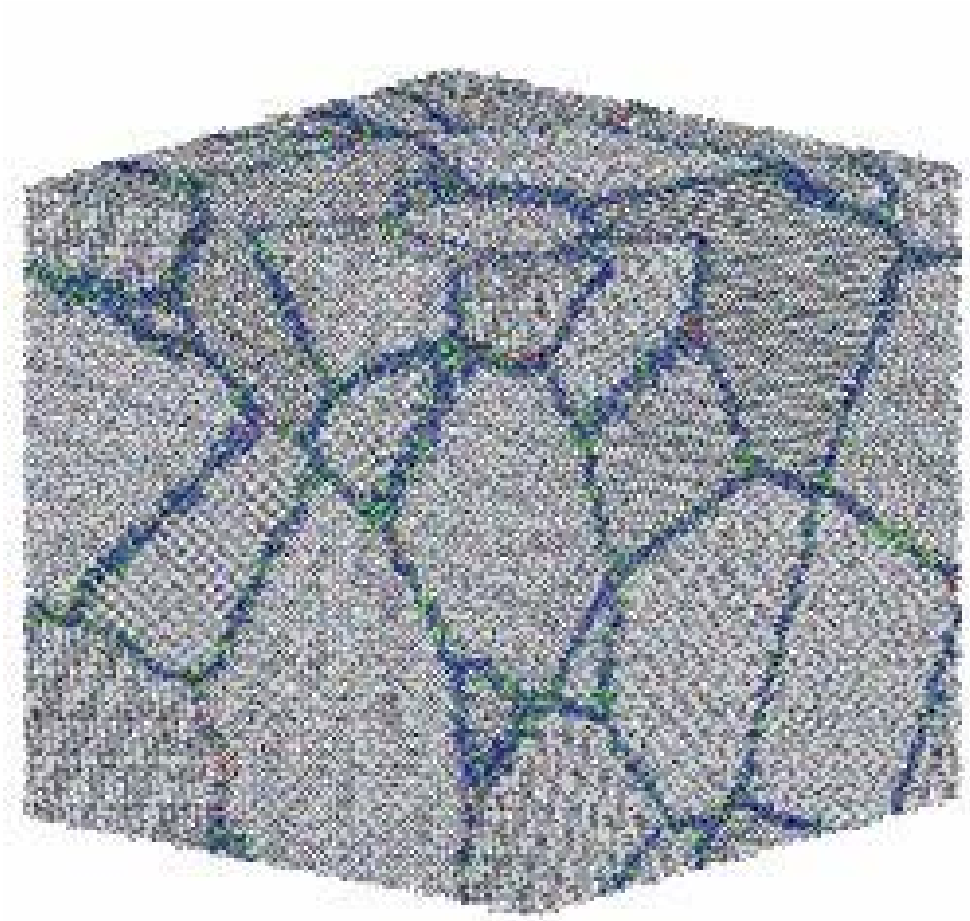
- Dislocation densities can vary from 10^5 cm^{-2} in carefully solidified metal crystals to 10^{12} cm^{-2} in heavily deformed metals
- Most metals have dislocations intrinsically present (statistical dislocations), e.g. due to deformation or manufacturing history
- During deformation, dislocations are nucleated from cracks (see earlier slides), grain boundaries, other dislocations, or surface defects/surfaces
- Frank-Read sources

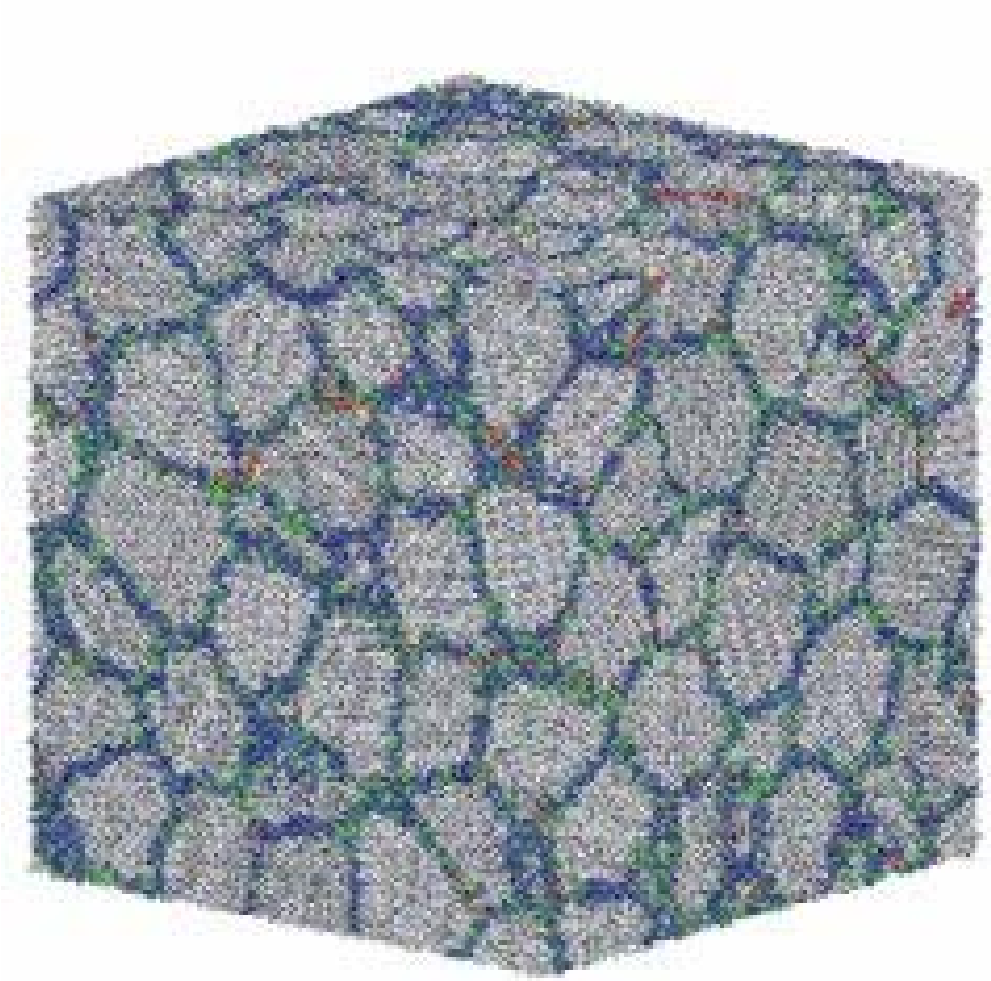




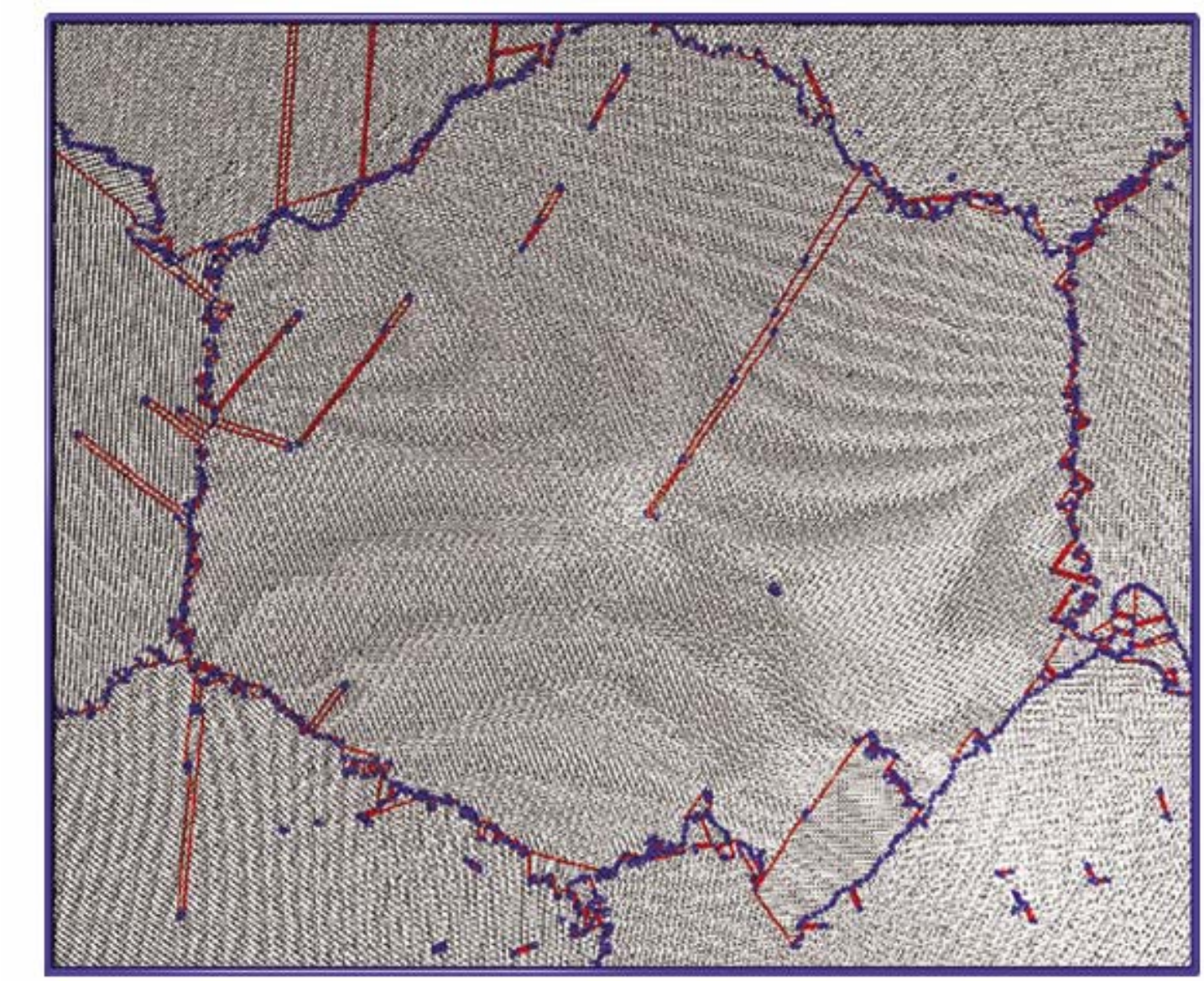
http://web.earthsci.unimelb.edu.au/wilson/ice1/generations.html
http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/backbone/r5_3_2.html

Polycrystals



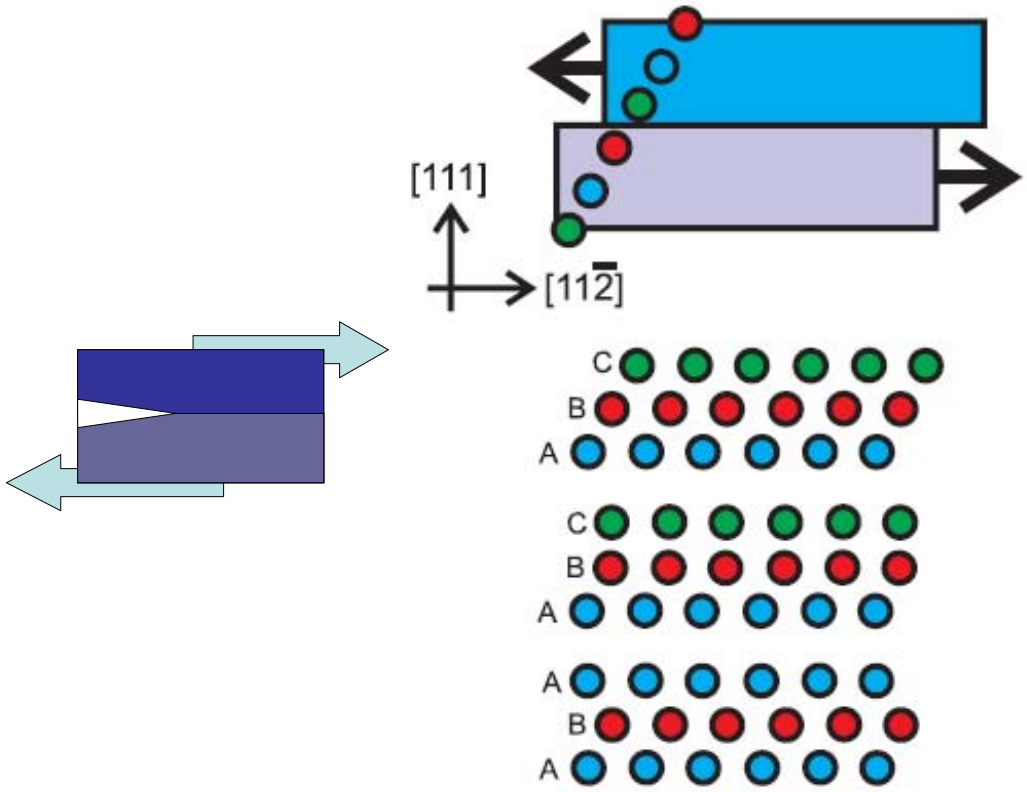


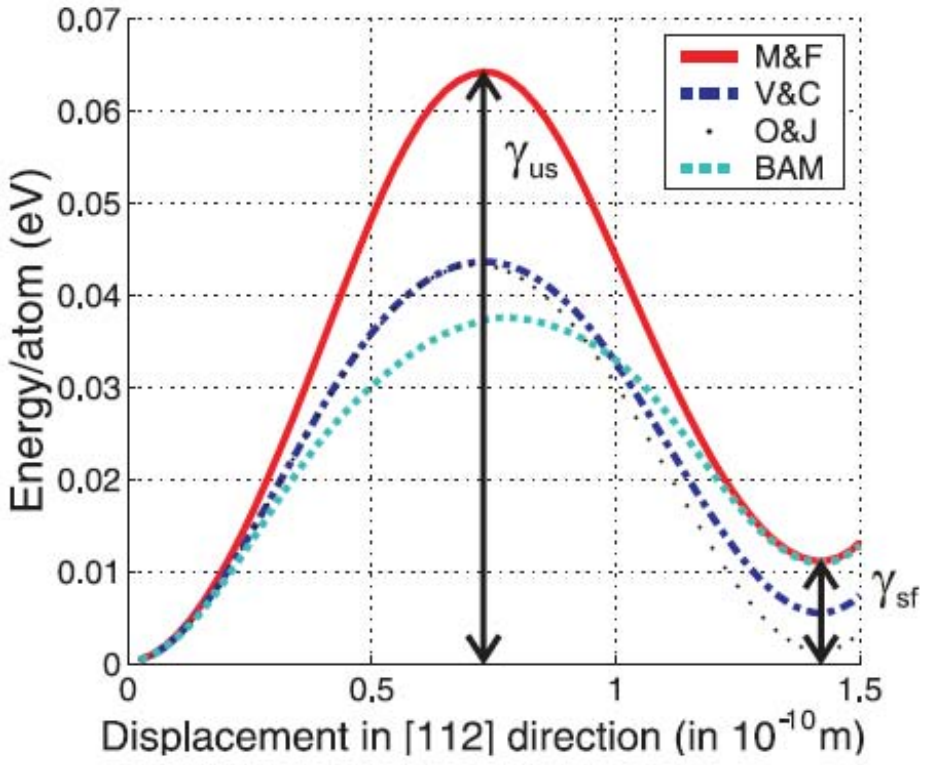
Deformation mechanisms



Stacking fault energy

Difficulty of creating a dislocation (γ_{us}) and moving a dislocation through the crystal (γ_{sf})





(Buehler, 2006)

Calculation of stacking fault energy for different interatomic potentials

Short-range pair potentials have zero SFE!

Partial dislocations

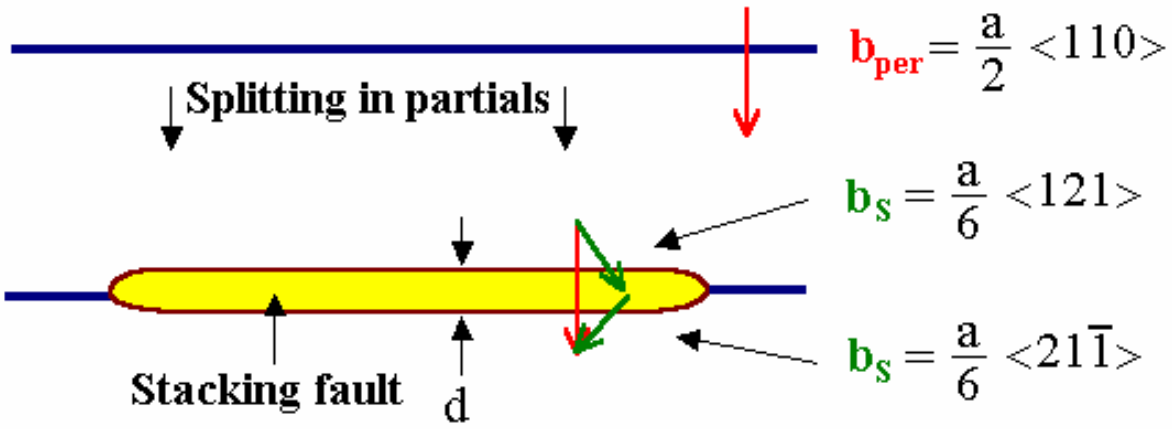
- In FCC, dislocations with Burgers vector [110] split up into two "partial dislocations" with Burgers vector 1/6[112]

Energy of the perfect dislocation

$$= G \cdot b^2 = G \cdot (a/2\langle 110\rangle)^2 = \frac{G \cdot a^2}{2}$$

Energy of the two partial dislocations

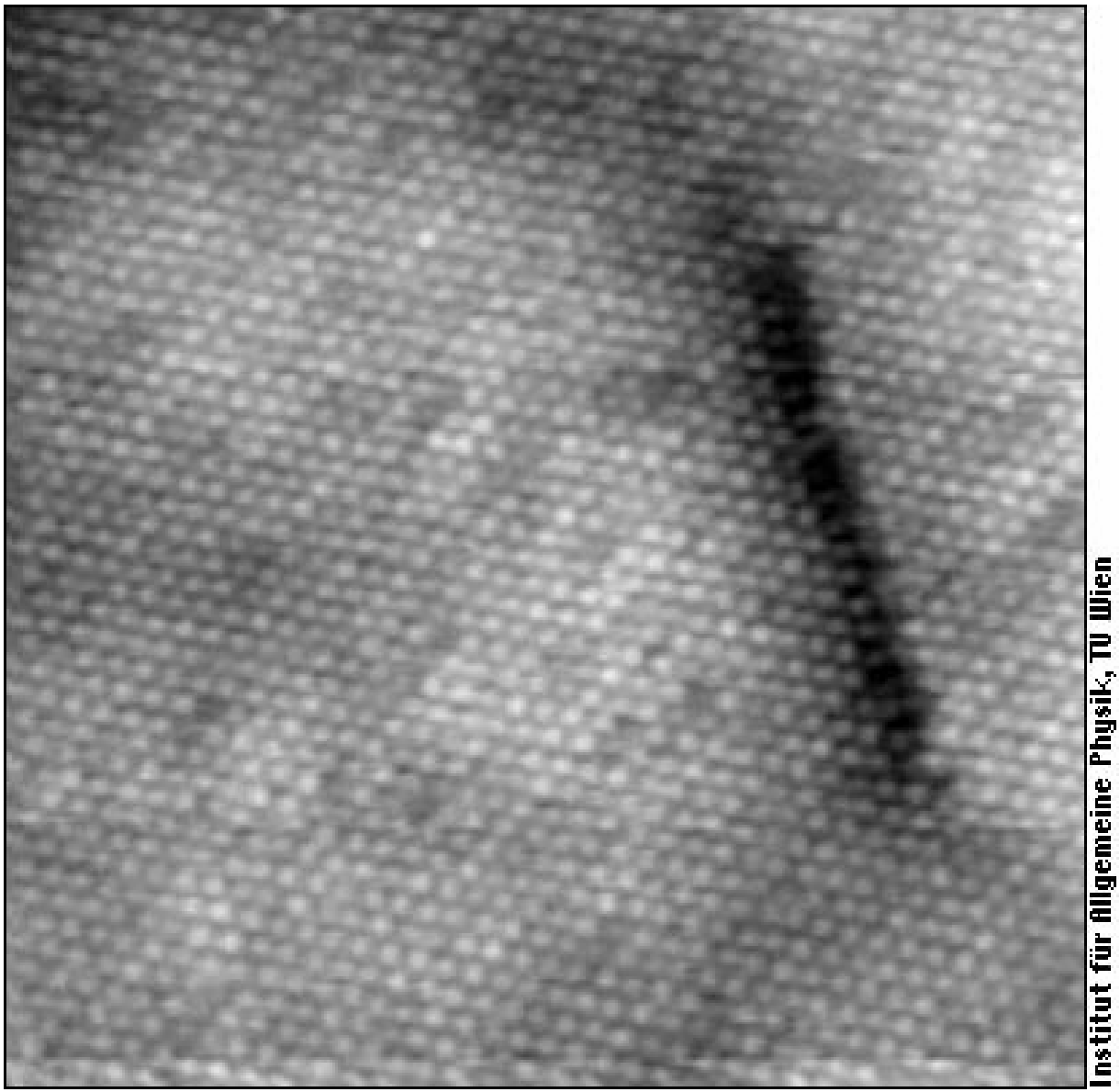
$$= 2G \cdot (a/6\langle 112\rangle)^2 = 2G \cdot a^2/36 \cdot (1^2 + 1^2 + 2^2) = \frac{G \cdot a^2}{3}$$



Metals with low SFE and materials under geometric confinement often have large stacking faults

http://www.tf.uni-kiel.de/matwis/amat/def_en/kap_5/backbone/r5_4_2.html

Partial dislocations



Separation of partial dislocations

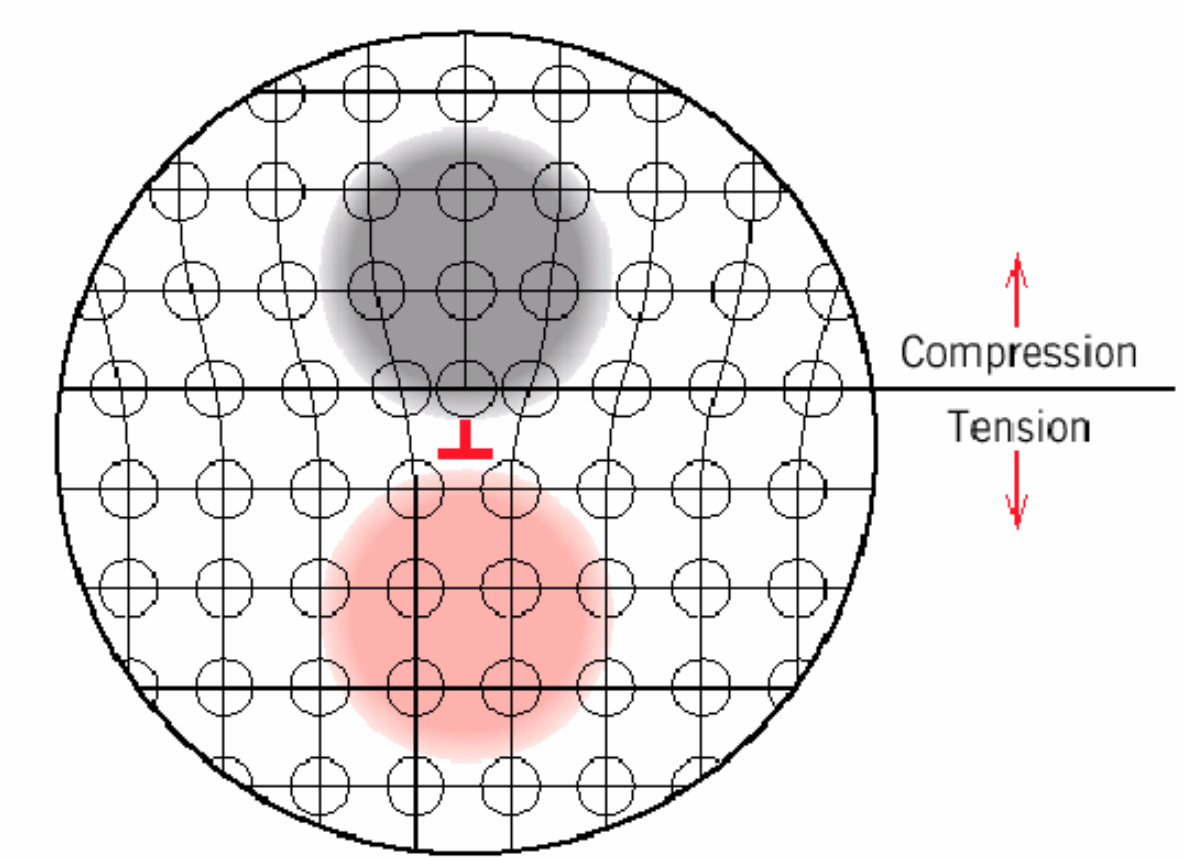
Width of stacking fault

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

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

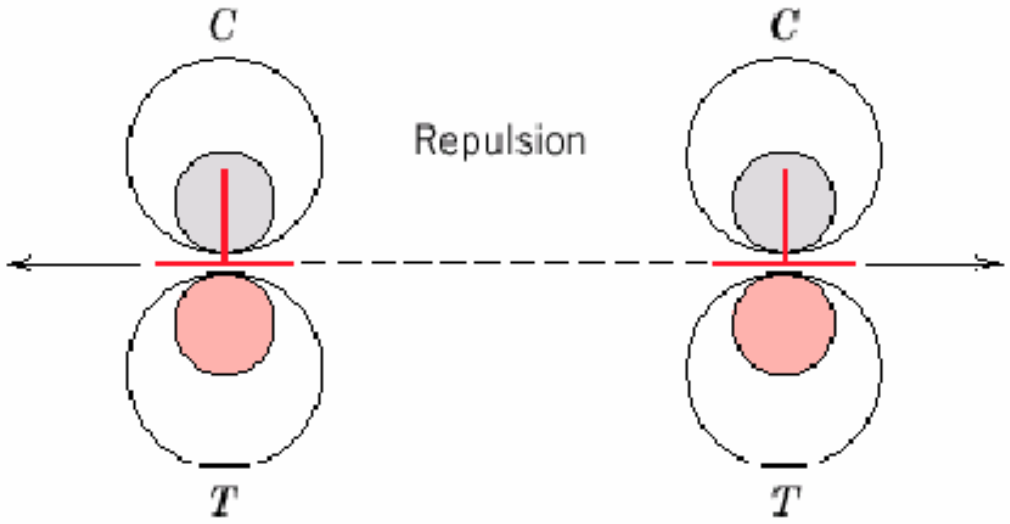
Stress field around a dislocation

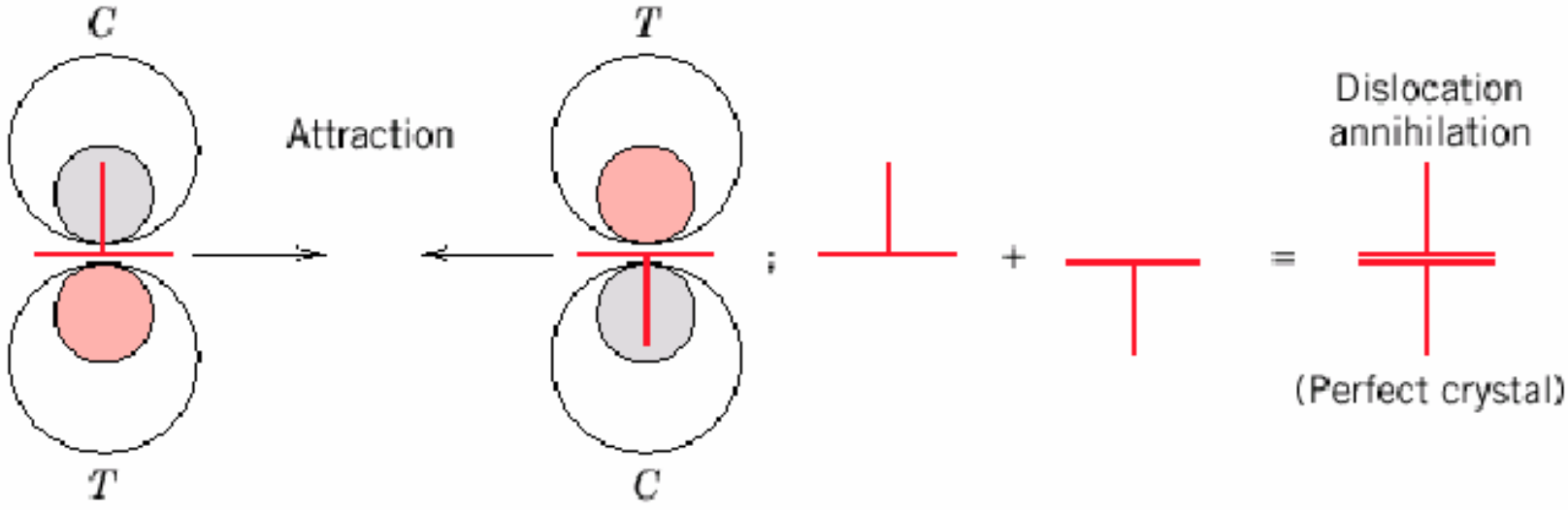
- Each dislocation induces a long-range stress field in the crystal
- Around the dislocation core:



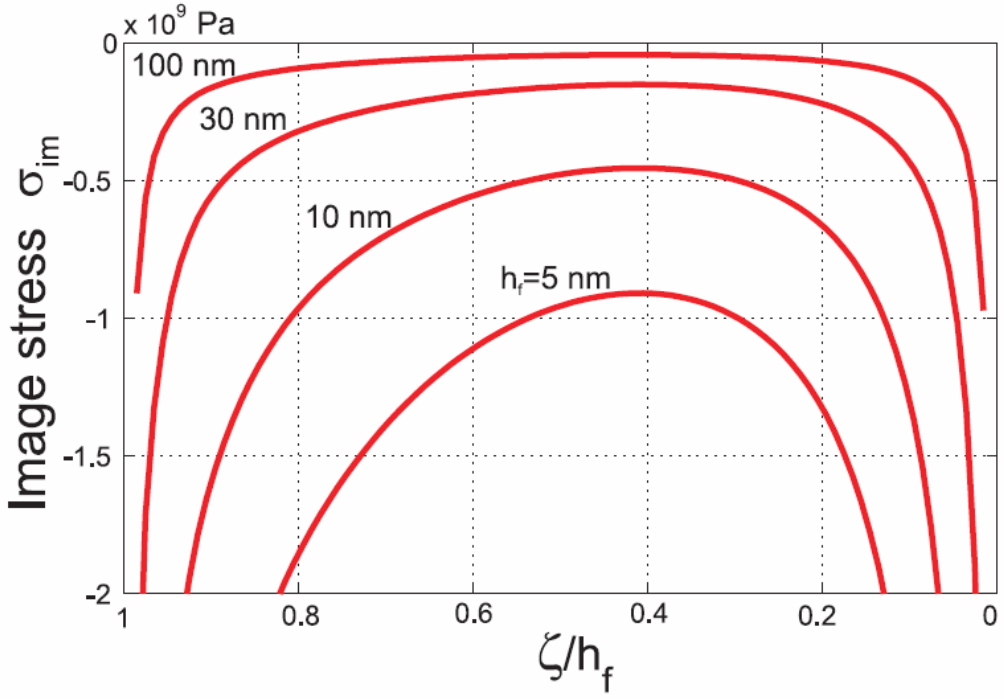
Dislocations: Interaction

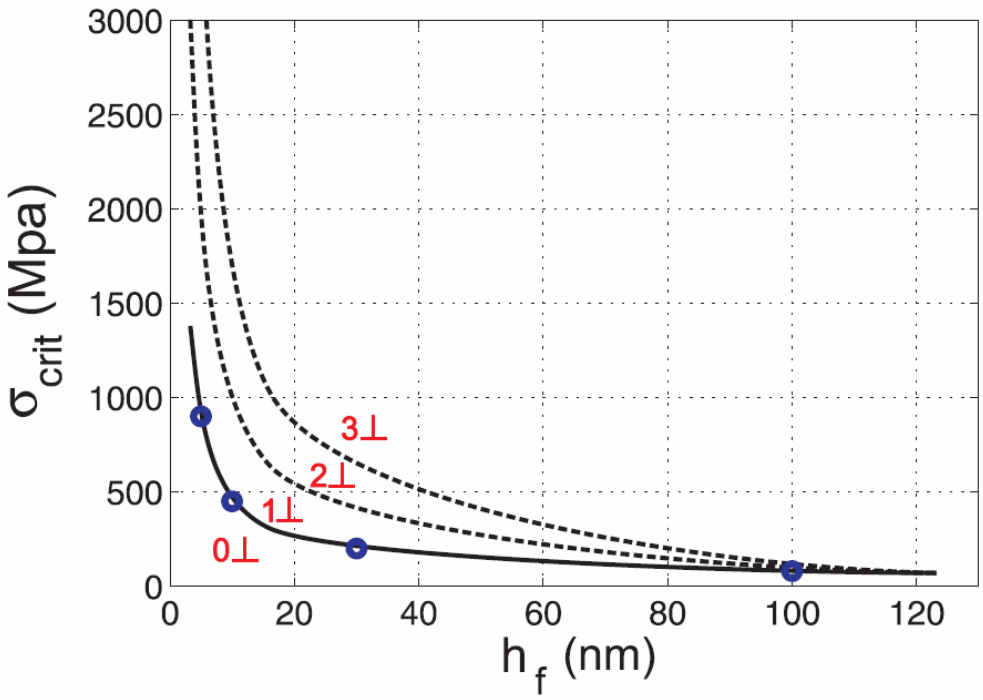
Important to understand how materials deform

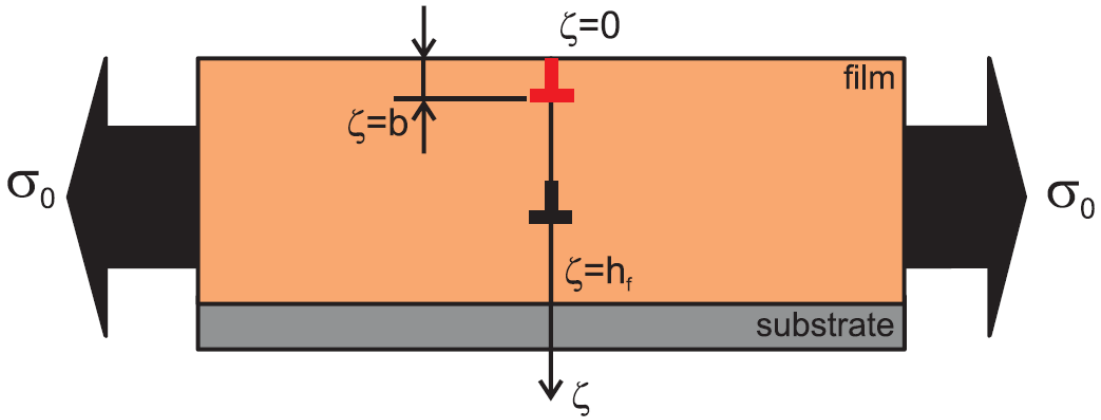




Nano-confinement of dislocations in ultra thin films on substrates





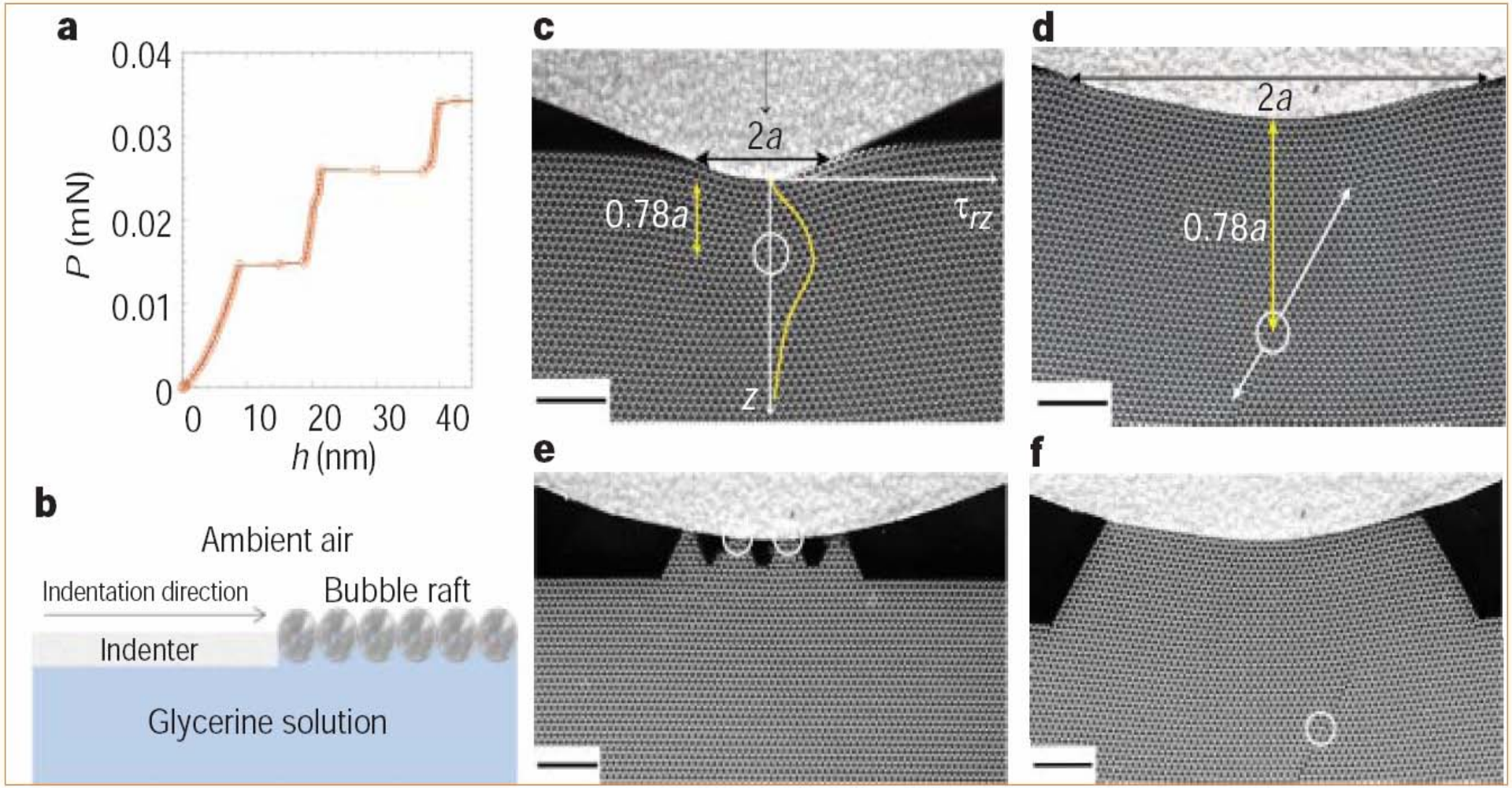


(Buehler *et al*., 2006)

Summary: The nature of dislocations

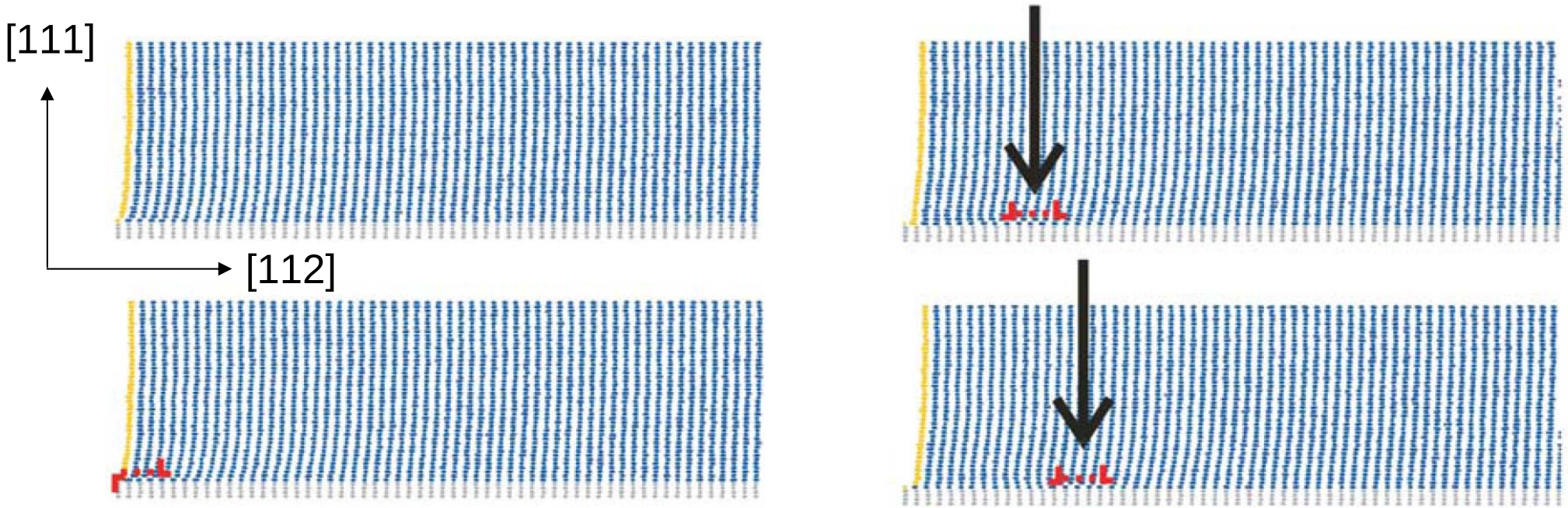
- Dislocations are complex line defects with complicated interaction with each other and other defects and the crystal lattice
- They are made up out of atoms, but all atoms are not necessary to describe their behavior unless they undergo reactions; long-range interactions
- Dislocations are critical to understand the behavior of many materials, in particular metals
- Modeling of atomistic dislocations with realistic material dimensions of micrometers and beyond has so far been elusive
- Current research efforts are geared towards developing models that describe deformation of materials based on fundamental principles
- Dislocations also appear in molecular crystals; but their role remains unclear

Bubble raft models

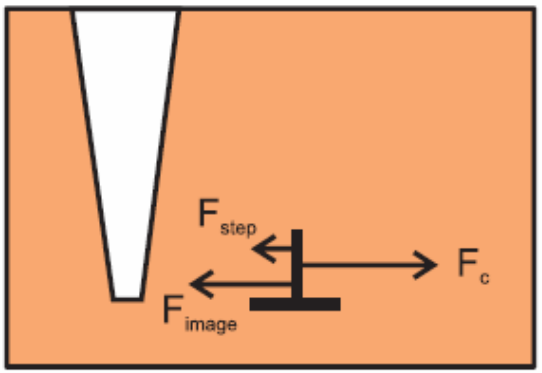


Van Vliet, Suresh, Nature, 2001

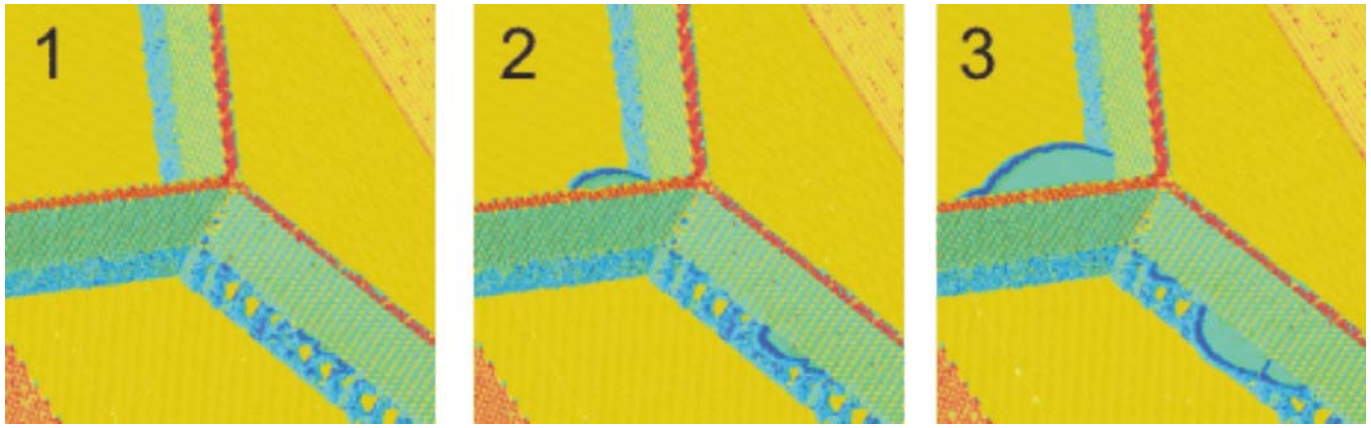
Atomistic details of dislocation nucleation



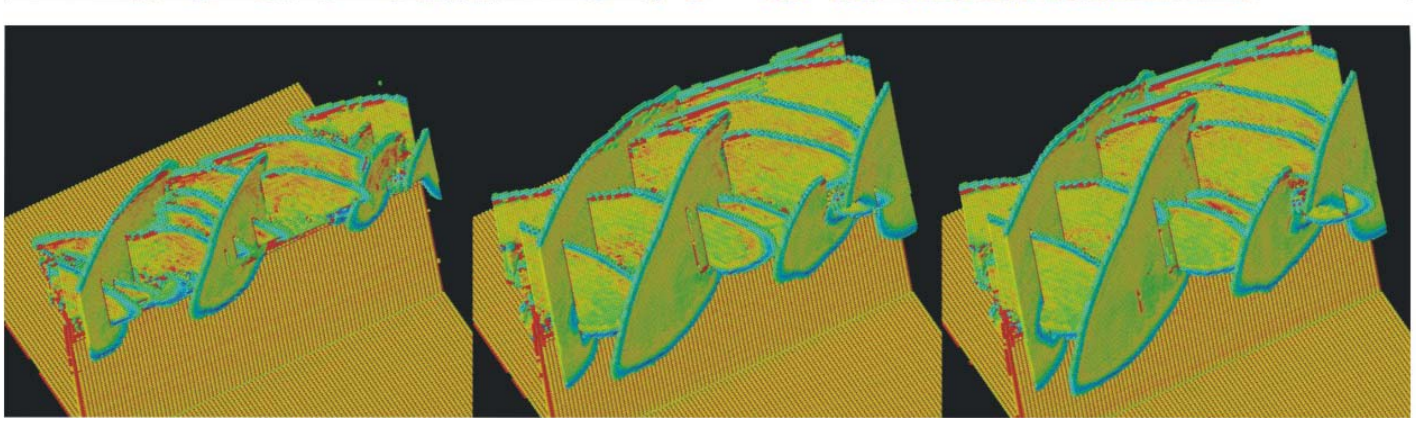
- Dislocation nucleation from a traction-free grain boundary in an ultra thin copper film
- Atomistic results depict mechanism of nucleation of partial dislocation



… more dislocations



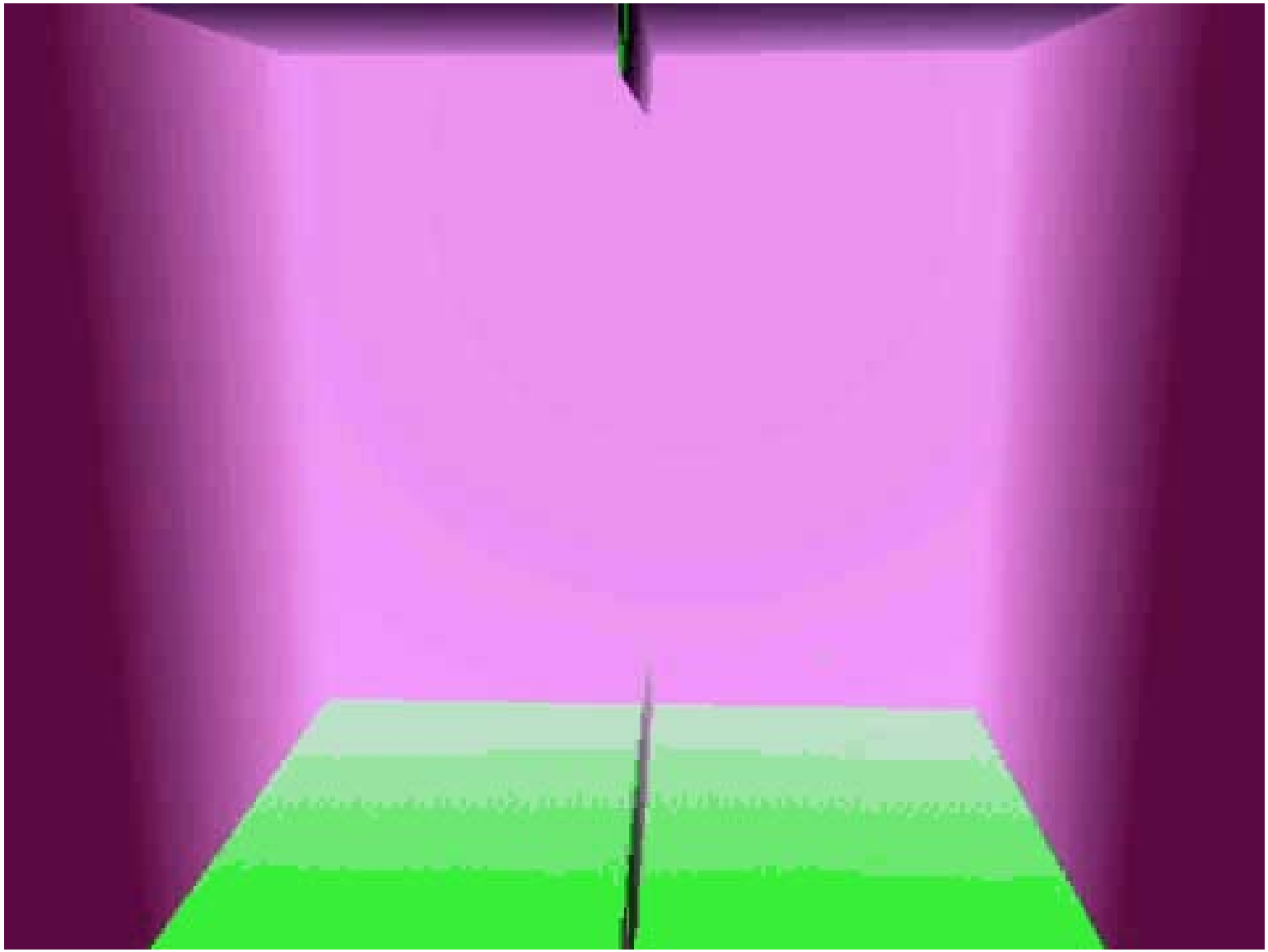
Dislocation nucleation at grain triple junction



Single crack

(Buehler, CEE/MIT)

A simulation with 1,000,000,000 particles



(F. Abraham, *et al*.)

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

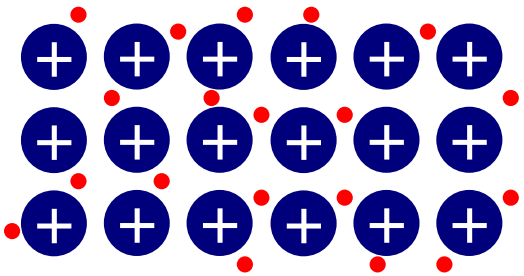
positive ions in a sea of electrons

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

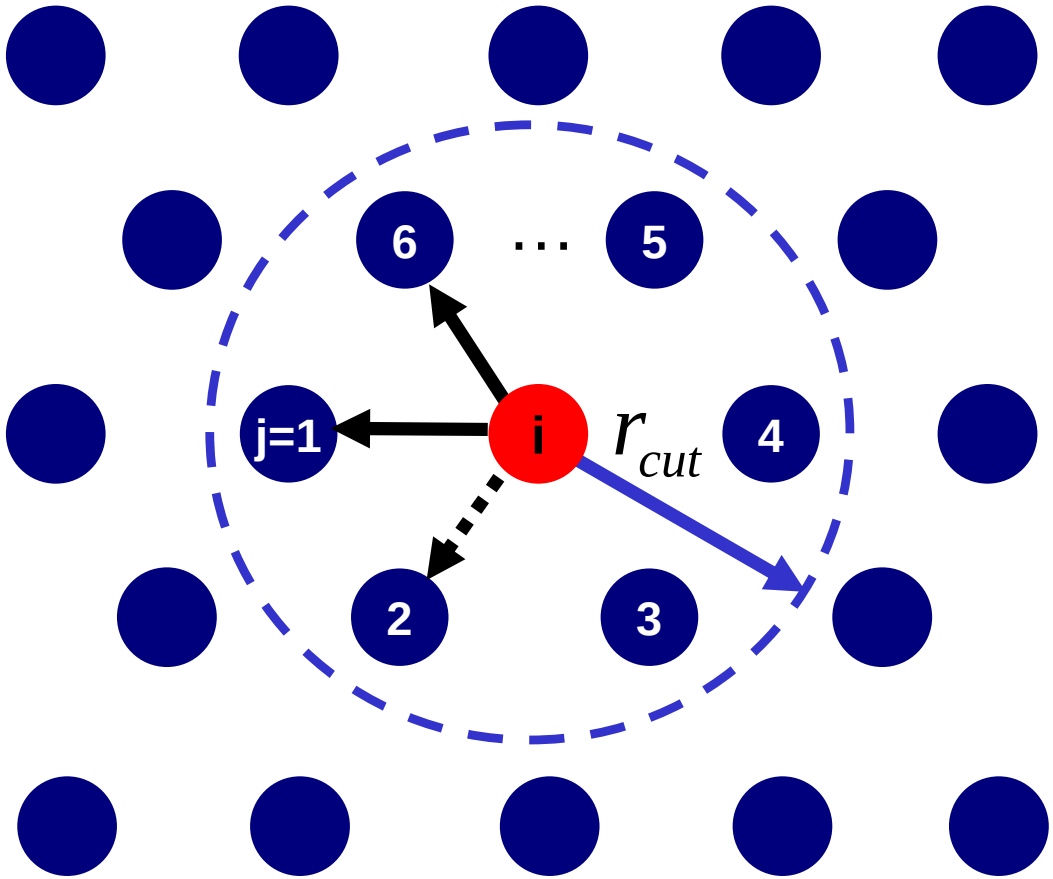
Property	Physical/atomic reason
High density	Tightly packed FCC, BCC, HCP
High melting temperature	Strong forces between ion core and delocalized electrons
Good conductors of heat	Vibration transport via delocalized electrons (+phonons)
Good electrical conductors	Delocalized electrons (flow in and out)
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)

Modeling attempts: Pair potential

- First attempts using pair potentials



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

Lennard-Jones 12:6

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

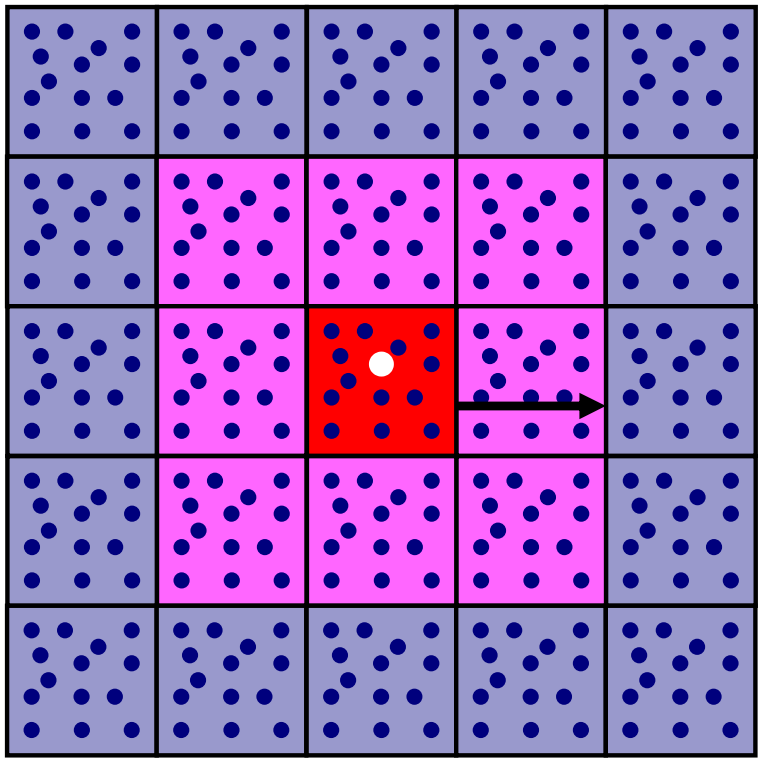
Morse

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

Good for noble gas Ar
(FCC in 3D)

Numerical implementation of neighbor search: Reduction of N^2 problem to N problem

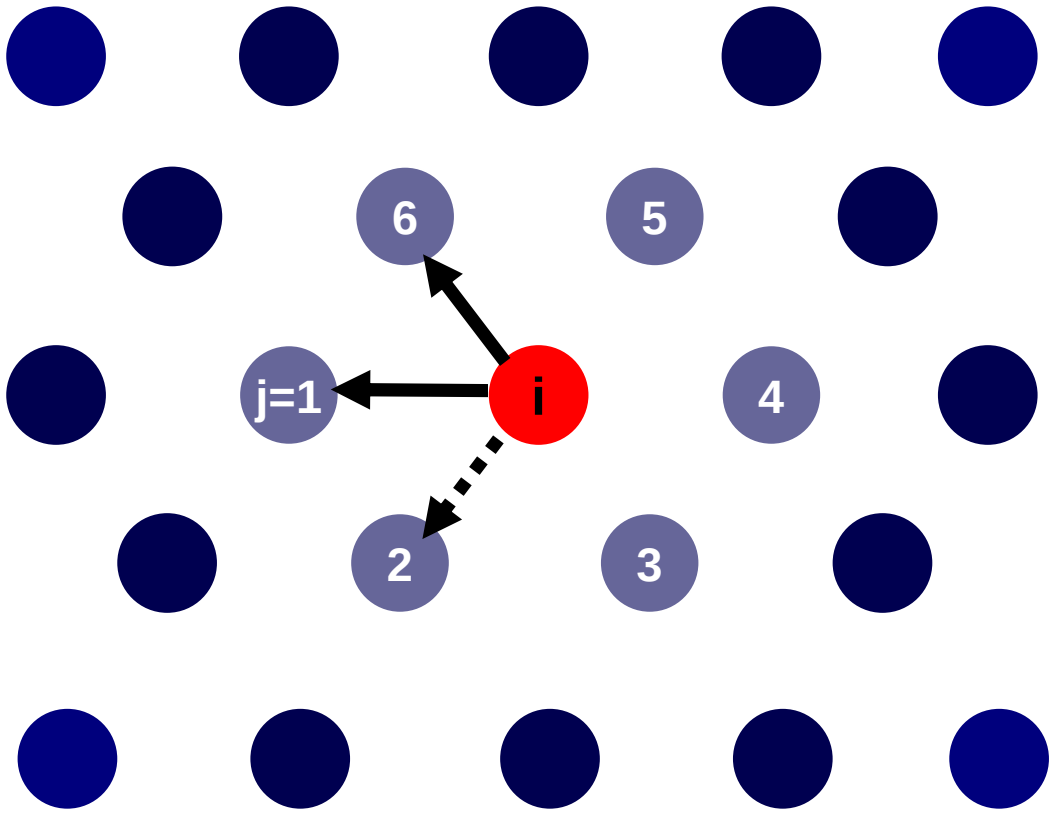
- Need nested loop to search for neighbors of atom *i:* Computational disaster
- Concept: Divide into computational cells ("bins", "containers", etc.)
- Cell radius $R>R_{cut}$ (cutoff)



- 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

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

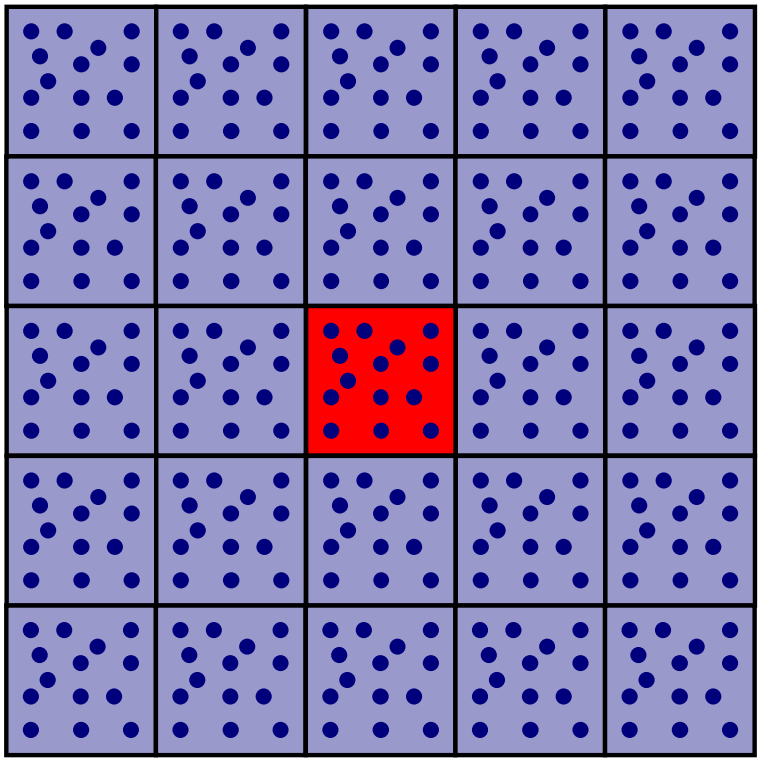
ρ_i Electron density at atom *I* based on a pair potential:

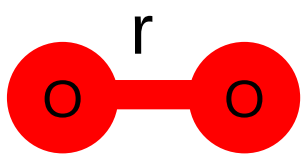
$$\rho_i = \sum_{j=1..N_{neigh}} \pi(r_{ij})$$

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

Numerical implementation of multi-body EAM potential

- Requires two loops over atoms within each cell





Loop 1:

(i) Pair contributions (derivatives and potential)

(ii) Calculate electron density

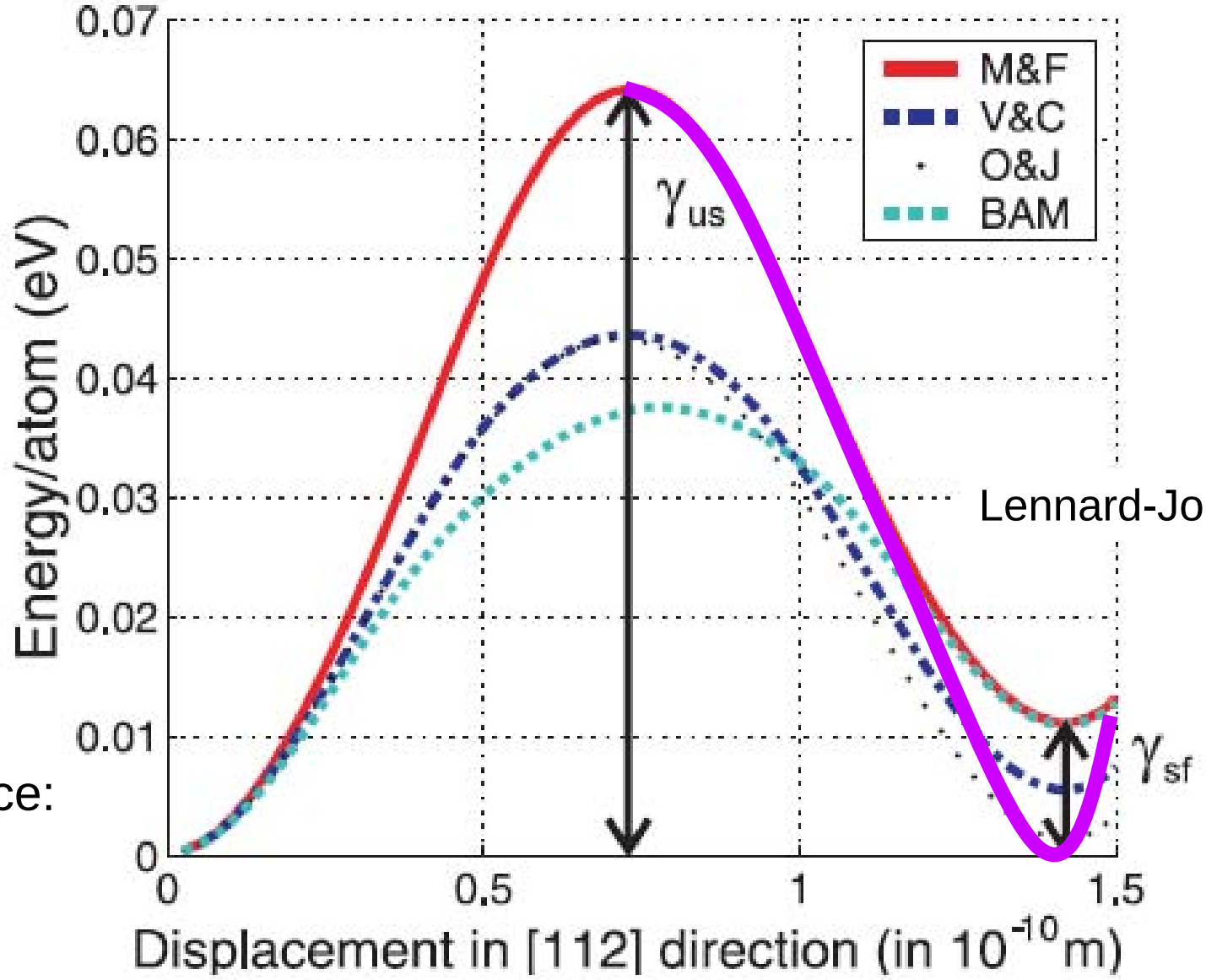
Loop 2:

(iii) Calculate embedding function and derivatives

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

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

Stacking fault energy: LJ potential vs. EAM potential



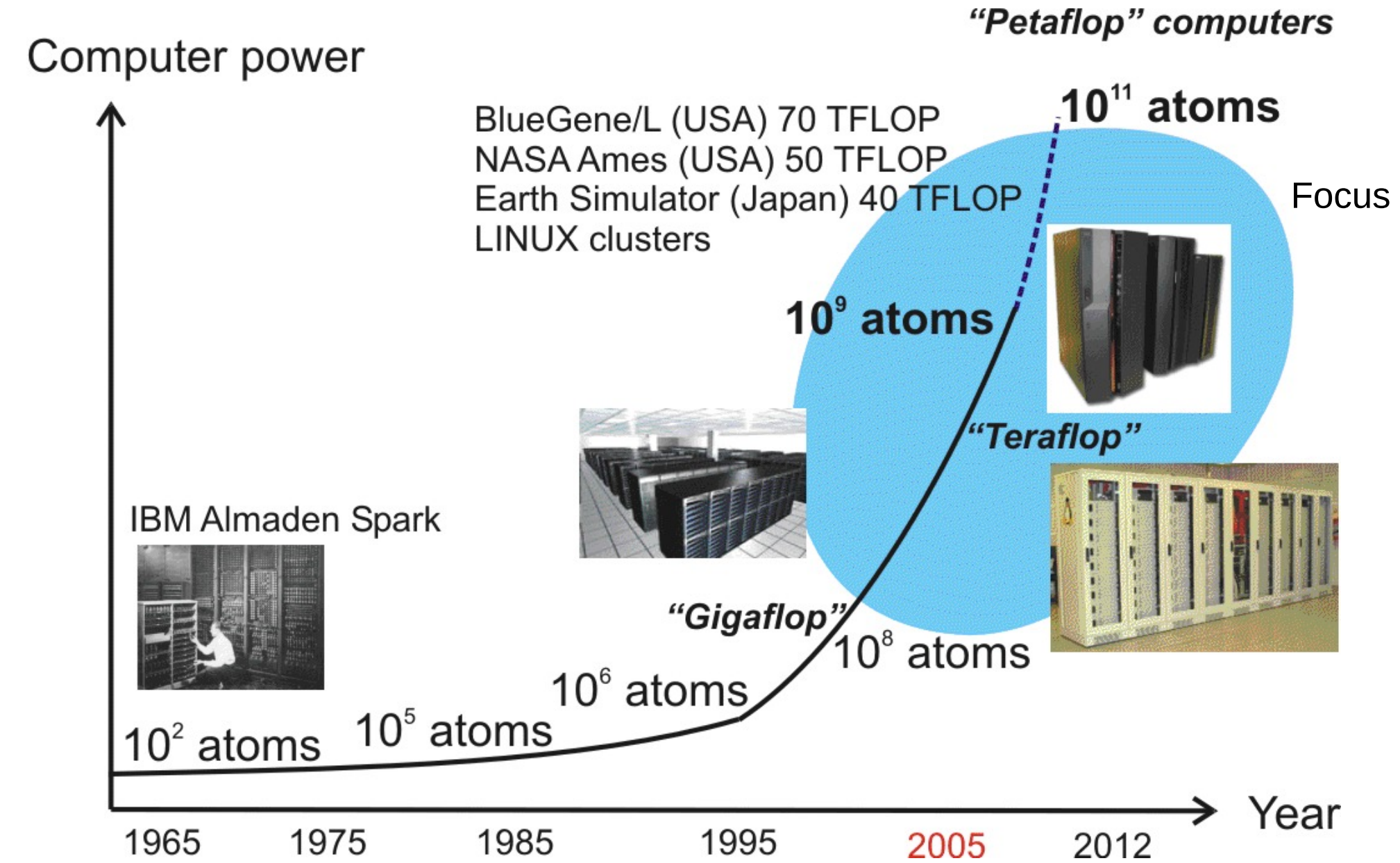
Lennard-Jones potential

(schematic)

Consequence:

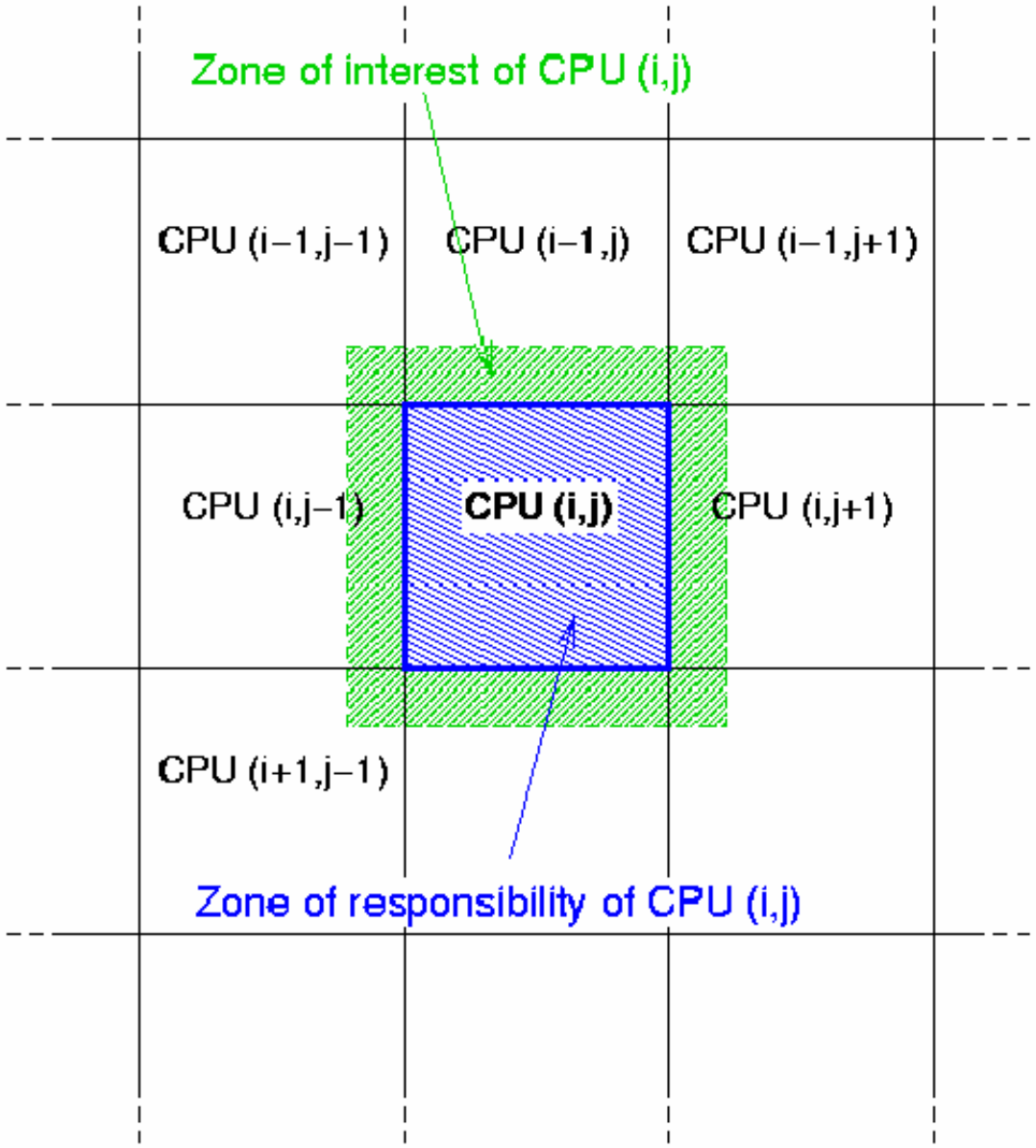
Only partial dislocations expected

Increase in computing power
Classical molecular dynamics



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

Parallel Molecular Dynamics



(after Schiotz)

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

Implementation of parallelization

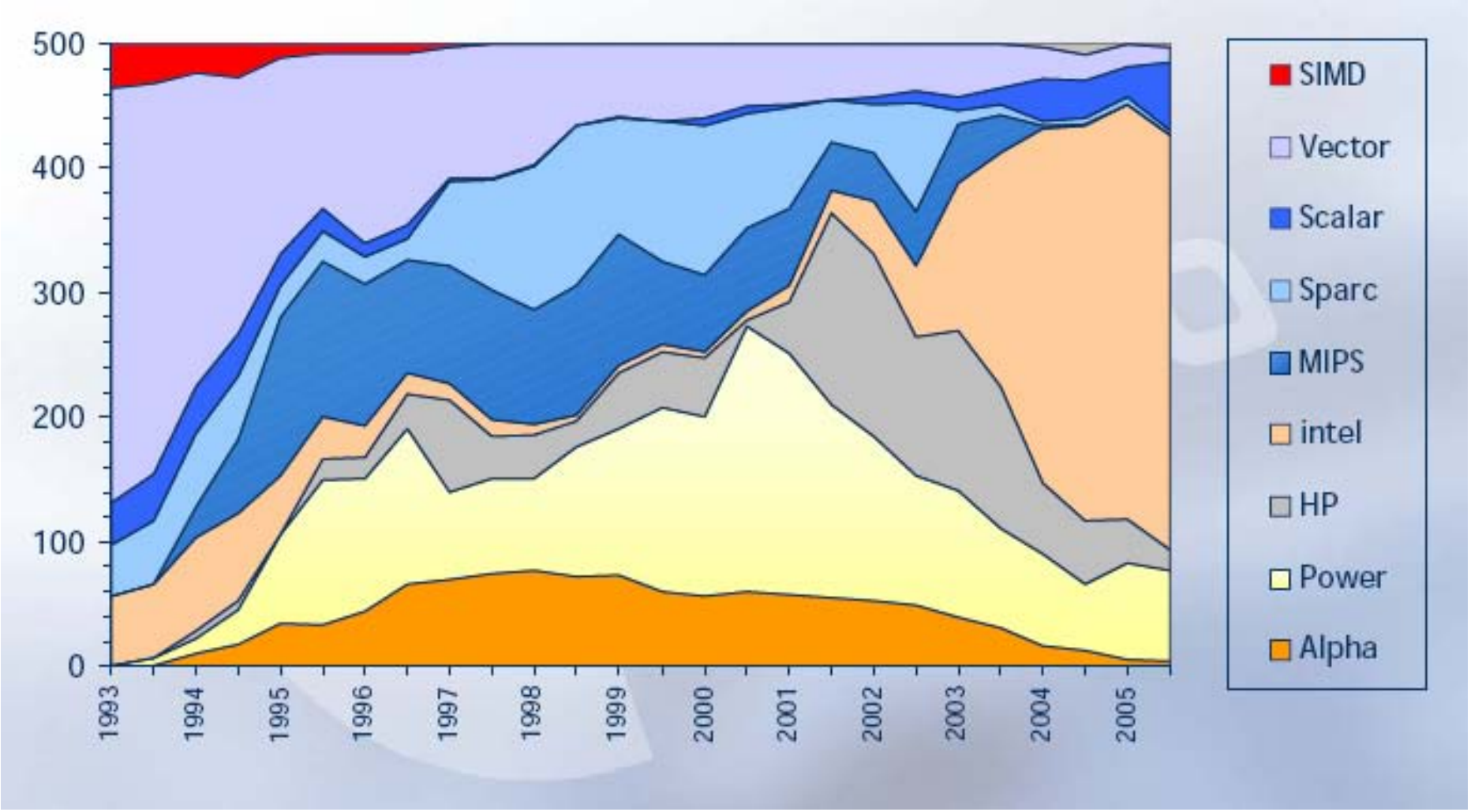
- Shared memory systems (all CPUs “see” same memory)
  - OpenMP (easy to implement, allows incremental parallelization)
  - POSIX threads
- Distributed memory systems
  - MPI (=Message Passing Interface)
    Most widely accepted and used, very portable, but need to parallelize whole code at once
- Parallelization 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

http://nf.apac.edu.au/training/MPIProg/slides/index.html, http://www.openmp.org/, http://www.eecs.umich.edu/~qstout/parallel.html

Performance history

http://www.top500.org/lists/2005/11/TOP500_Nov2005_Highlights.pdf

Architecture distribution



Dominance of LINUX clusters

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?

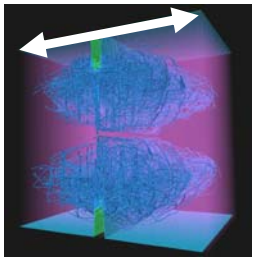
Increase in computing power: Parallelization

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

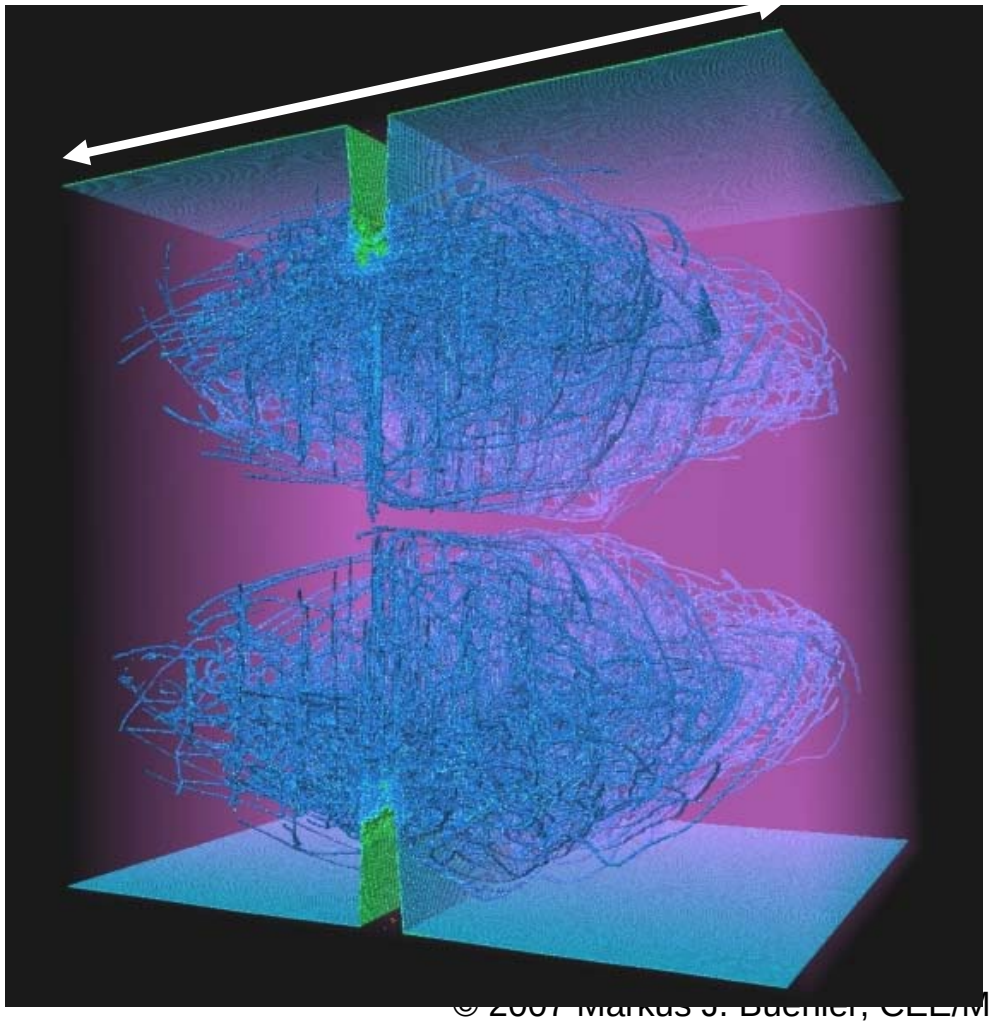
0.3 µm

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



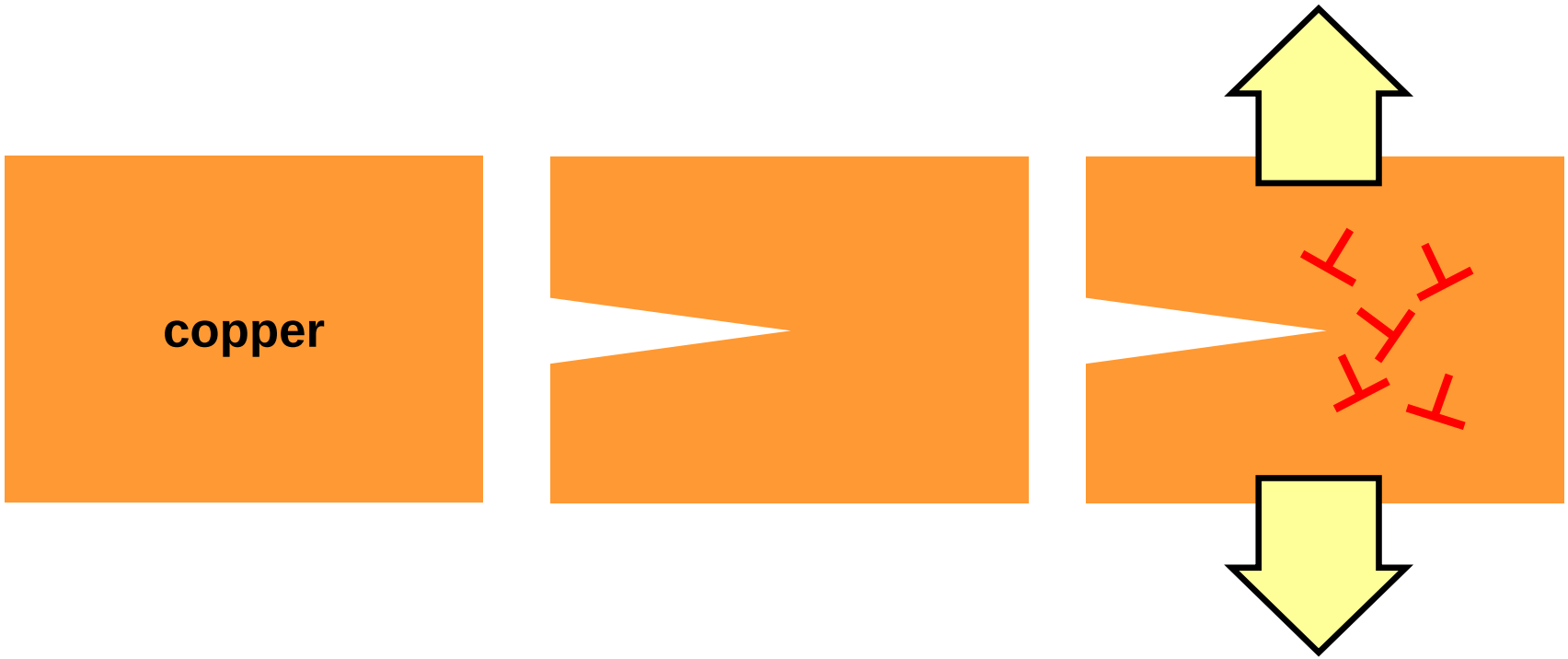
1.2 µm

5 µm



2010
7,000,000,000,000 particles
1,000 TFLOP computers

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…