Dislocation Dynamics (part 1)

Computational Material Science
Lecture 7

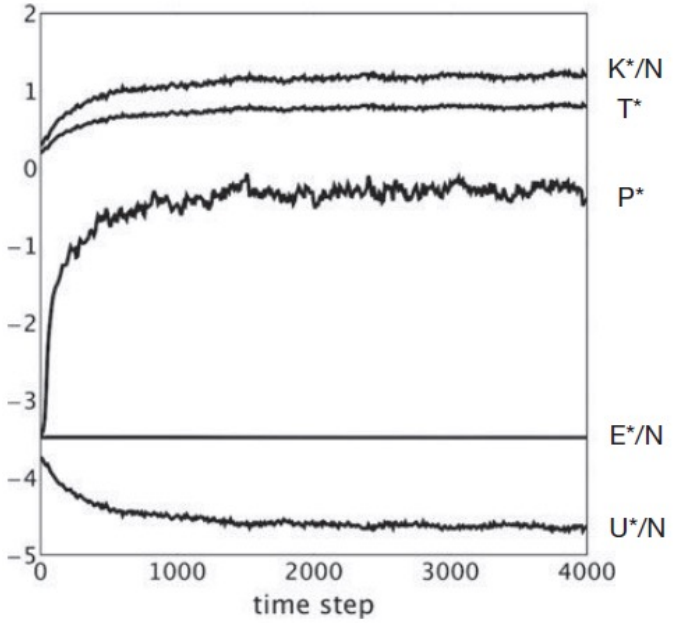
Last time

- Molecular dynamics simulations are used to reach a better understanding of nanoscale phenomena, examples discussed were indentation, contact, friction
- MD simulations describe bodies atomistically and they keep track of the individual position of each atom over time.
- Statistical mechanics provides us with a link between microscopic and macroscopic thermodynamics variables
- This allows us to calculate thermodynamic quantities in an MD simulation through averaging over time
- Averages should be taken after the simulation has equilibrated, i.e. when quantities fluctuate around a constant mean

Equilibration

We want to perform a simulation for a solid crystal, with given atomic positions, with a cubic shape and periodic boundary conditions, in an NVE ensamble. The atomic interactions are described by means of a LJ potential, and initial velocities are assigned that correspond to a reduced temperature 0.2.

864 atoms,
T*=0.2,
LJ, cutoff=5,
t*=0.005



How does the volume curve look like?

We run an equilibration and plot the macroscopic thermodynamics quantities K, T, E, U, P.
What do we notice?

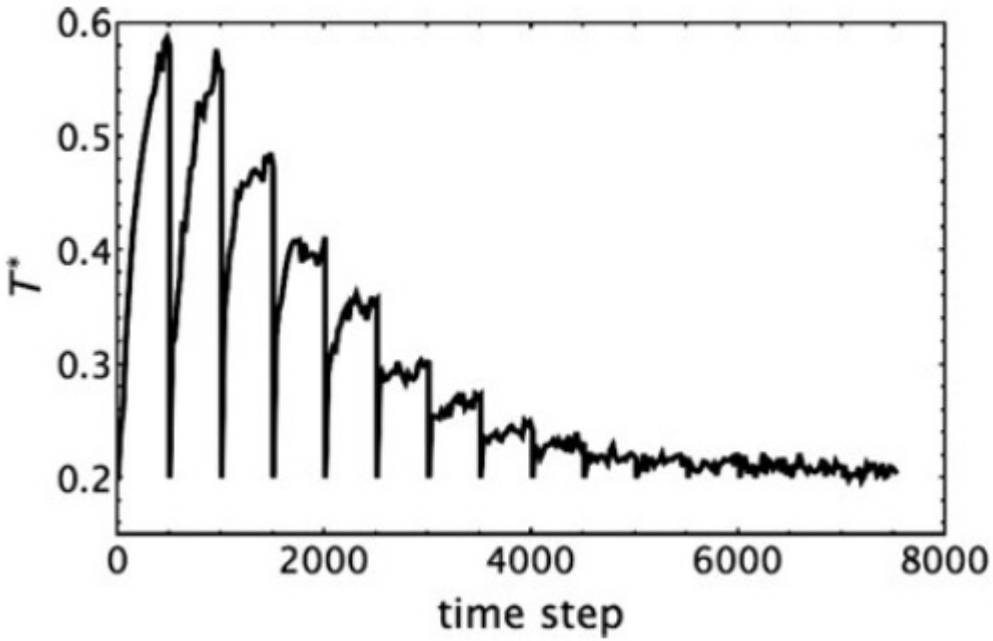
Velocity control

How do we fix the inability of setting a specific temperature?
Rescaling velocities!

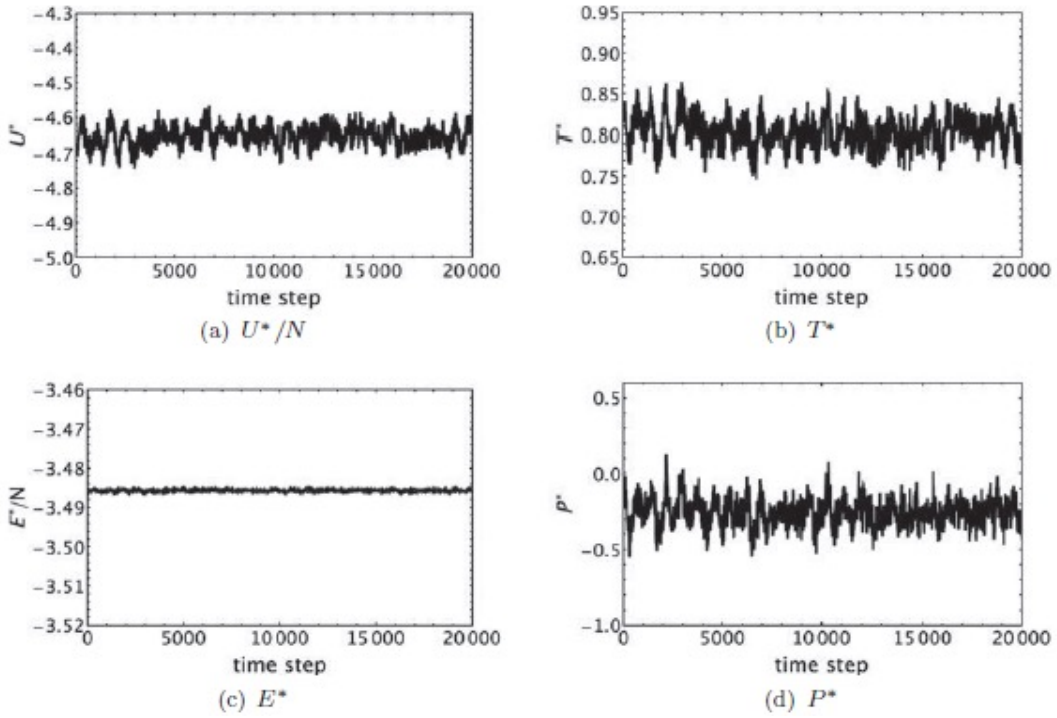
Desired temperature: T_s
Actual temperature: $T(t) = 2K(t)/(3Nk_B)$

$$v_{i\alpha}^{new} = \sqrt{\frac{T_s}{T}} v_{i\alpha}$$

Then equilibration, the ensemble is still NVE



At equilibrium



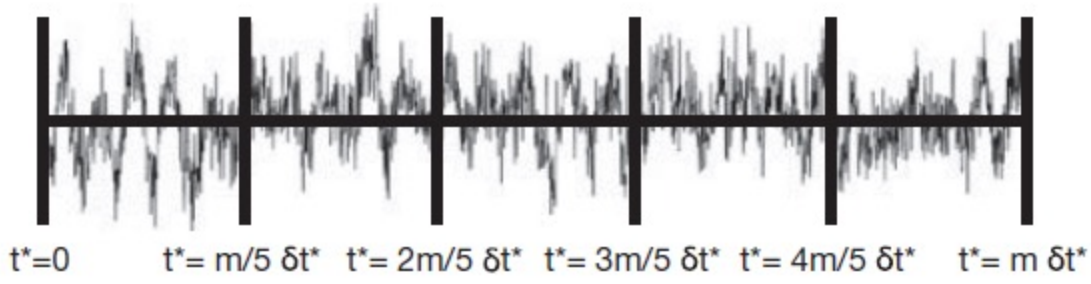
The averages of the quantities can be obtained by simple time averaging in a selected interval, over the time steps

$$\langle U \rangle = (1/\tau_{max}) \sum_{\tau=1}^{\tau_{max}} U(\tau)$$

The numerical data can be treated as experimental data, and one can calculate the variance to get a measure of the fluctuations of U around the average

$$\sigma_U^2 = (1/\tau_{max}) \sum_{\tau=1}^{\tau_{max}} (U(\tau) - \langle U \rangle)^2 = \langle (U(\tau) - \langle U \rangle)^2 \rangle = \langle U^2 \rangle - \langle U \rangle^2$$

Binning



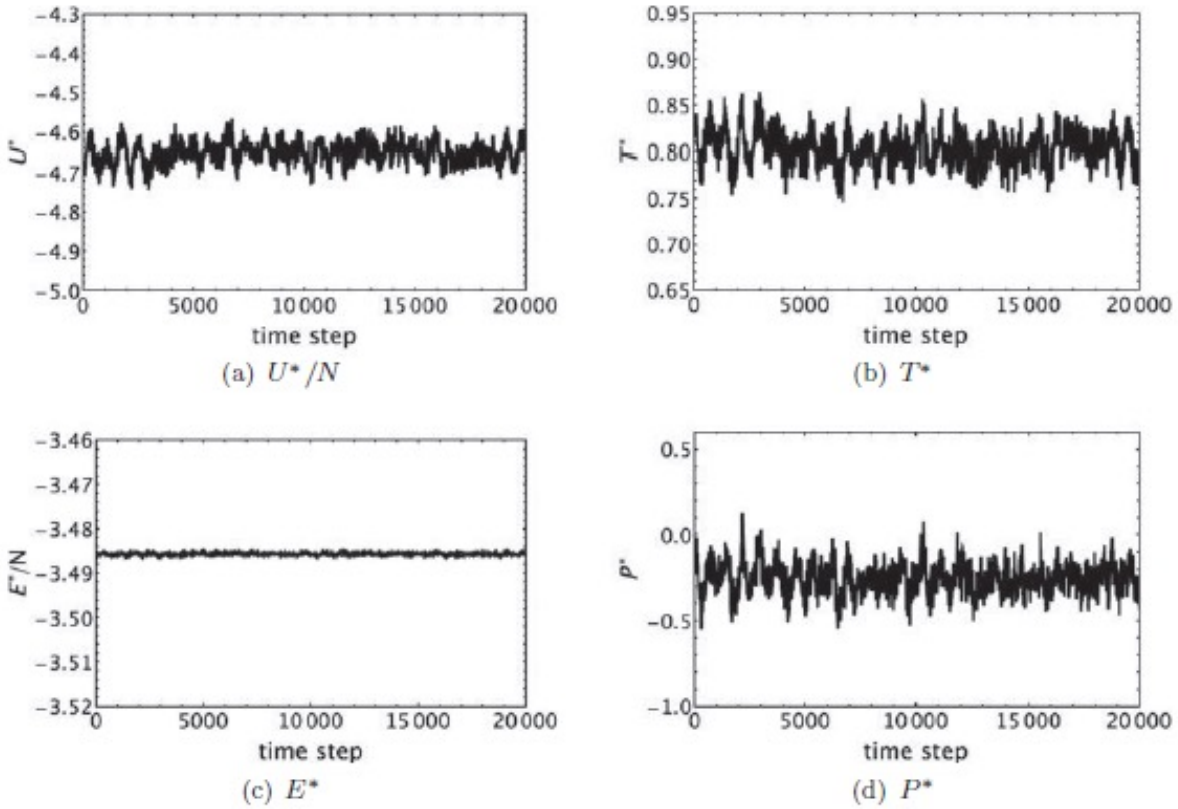
A measure of the statistical error in a simulation is given by the variance of the mean, which can be evaluated through the binning procedure. Average quantities are given by:

$$\langle U \rangle = (1/\tau_{max}) \sum_{\tau=1}^{\tau_{max}} U(\tau)$$

$$\langle U \rangle_i = \frac{1}{\tau_b} \sum_{\tau=\tau_o}^{\tau_o+\tau_b} U(\tau)$$

The variance of the bin energy is a measure of the quality of the data,

Averages after equilibration



(a) U^*/N (b) T^*

(c) E^* (d) P^*

Also one can measure the standard deviation, the square root of the variance, and obtain for this data set:

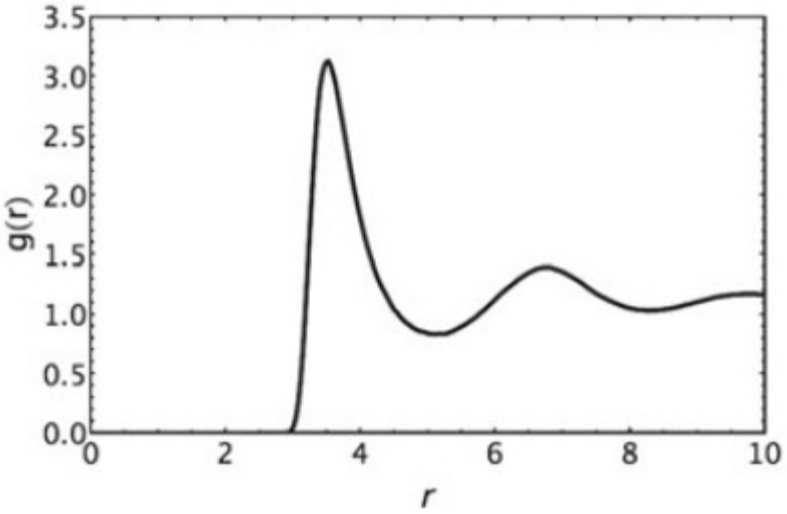
$$\langle U^* \rangle = -4.651 \pm 0.005 \qquad \langle P^* \rangle = -0.25 \pm 0.02$$

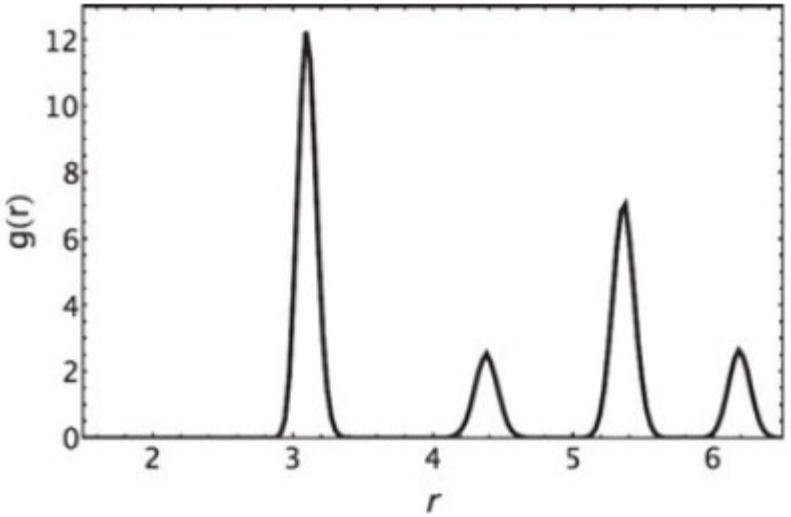
$$\langle T^* \rangle = 0.804 \pm 0.003 \qquad \langle E^* \rangle = -3.486 \pm 3 \times 10^{-5}$$

Spatial correlation functions

In addition to info about T, K, U, MD simulations gives info on structure

The pair distribution function g(r), gives the probability of finding two atoms at distance r. Does not depend on direction





Integration of the function over a range gives the number of atoms in that range

Spatial correlation functions

The **pair distribution function**

$$g(r) = \frac{V}{4\pi r^2 N^2}\left\langle \sum_i \sum_{j \neq i} \delta(r - r_{ij}) \right\rangle$$

is the probability density of finding a particle at a given distance r_{ij} when another particle i is at the origin

1) The calculation goes from 0 to r_max (which cannot exceed L/2)
   The range should be divided into n_b intervals, such that $\Delta r = r_{max}/n_b$
2) Determine distance between each pair and calculate $k = \mathrm{int}(r_{ij}/\Delta r)$
3) g(k) is a count of how many times r_ij falls between $k\,\Delta r$ and $(k+1)\Delta r$

Graded assignment 2

Use your MD code to model the melting of a solid FCC Cu crystal described through the LJ potential.

1. Check that you take a sufficiently small time step and that you do not have other mistakes in the code by making sure the total energy is conserved.
2. Plot how temperature, density, pressure change during the simulation.
3. Plot the atomic structure in the initial solid phase (after equilibration) and in the final liquid phase (after melting and equilibration).
4. As an additional check, plot also the radial distribution function for the solid and the liquid:

$$g(r) = \frac{V}{4\pi r^2 N^2}\left\langle \sum_i \sum_{j \neq i} \delta(r - r_{ij}) \right\rangle$$

This is the probability density of finding a particle at rij given that another particle i is at the origin

Compare the results of your code with the ones you obtain when doing the same simulation using LAMMPS (same number of atoms, same potential, same materials…same everything).

Today

- Recap: what are dislocations?
- Continuum representation of dislocation fields
- Dislocation structures

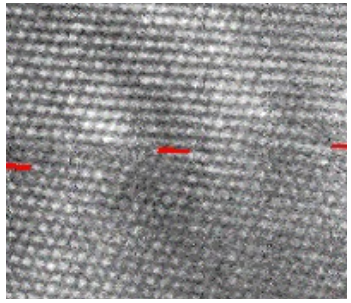
Learning goals:

- Capability to describe dislocations in a continuum framework through continuum fields

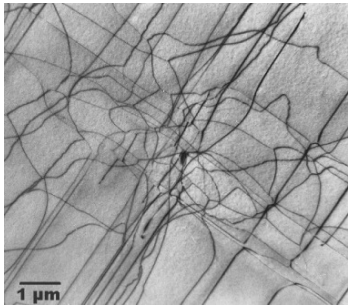
- Programming:

  first DD simulation

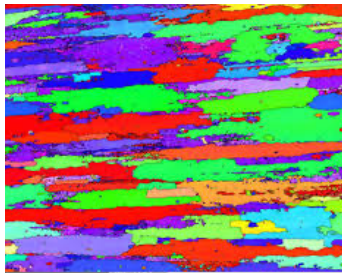
observing plasticity at different scales



high resolution TEM



TEM



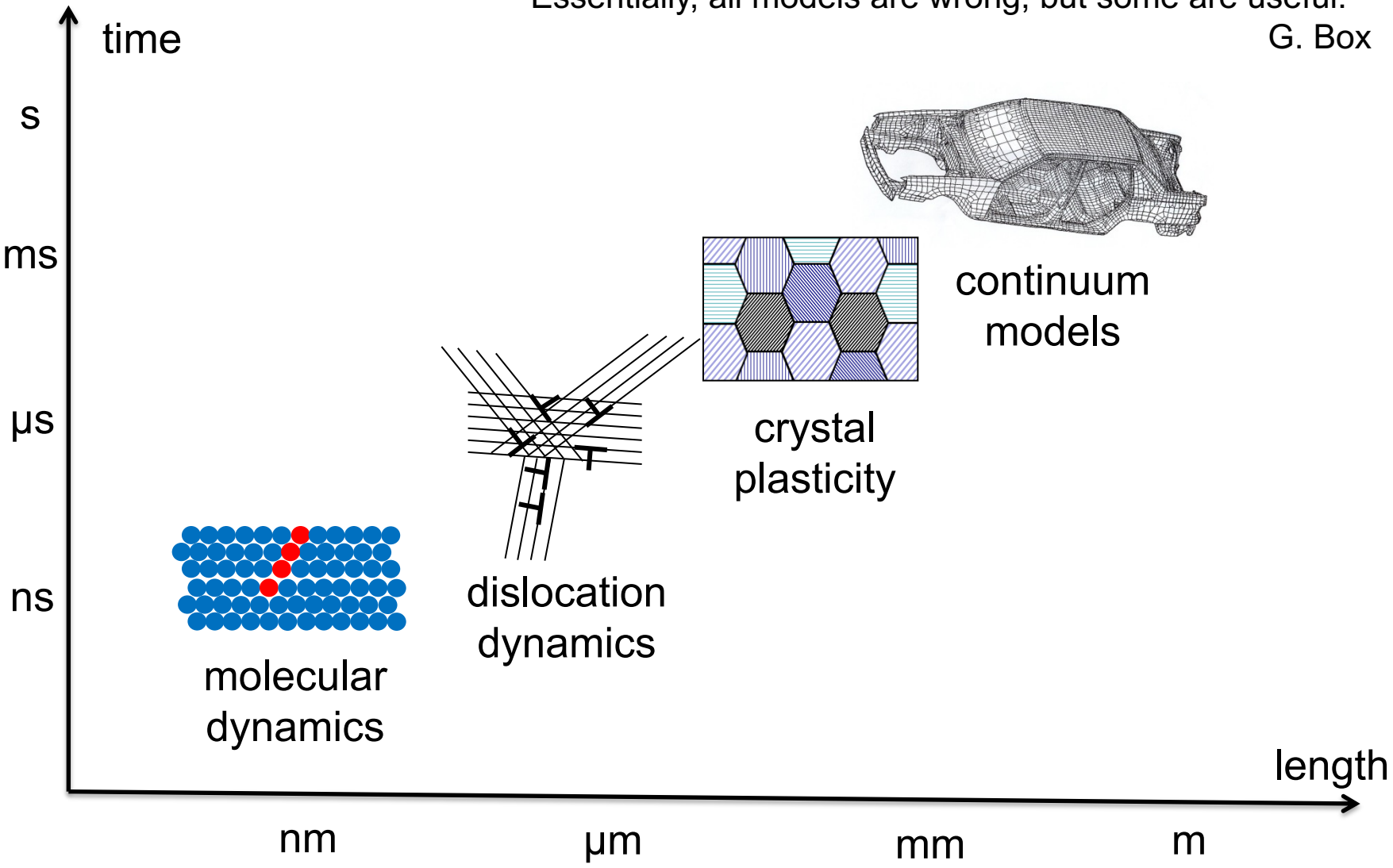
EBSD

length

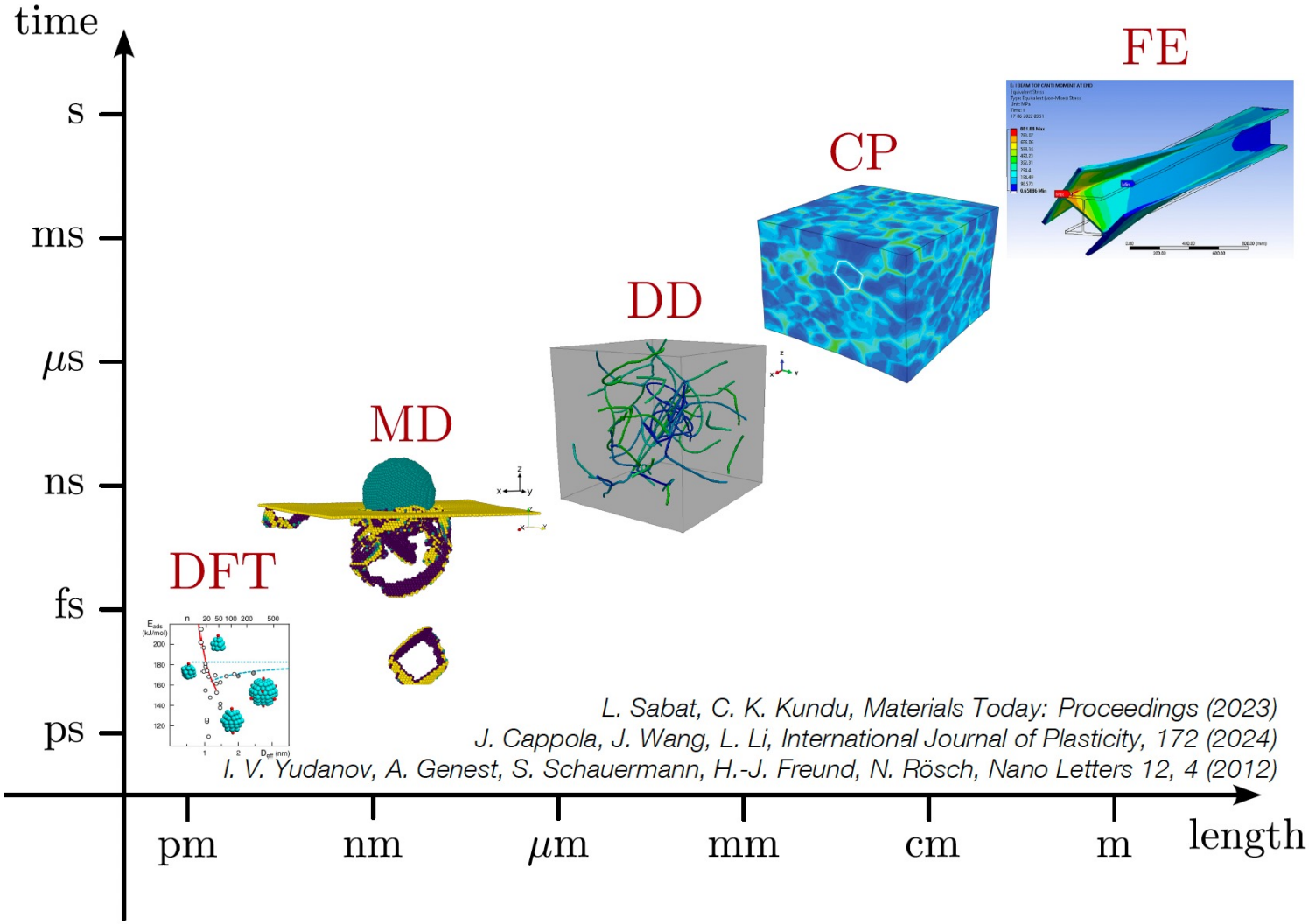
nm µm mm

modeling plasticity at different scales

Essentially, all models are wrong, but some are useful.
G. Box



modeling plasticity at different scales



L. Sabat, C. K. Kundu, Materials Today: Proceedings (2023)
J. Cappola, J. Wang, L. Li, International Journal of Plasticity, 172 (2024)
I. V. Yudanov, A. Genest, S. Schauermann, H.-J. Freund, N. Rösch, Nano Letters 12, 4 (2012)

what is a dislocation?

Solid crystals are characterized by various types of defect, introduced during production and/or manufacturing

Defects are classified based on their dimensionality: vacancies and impurities are point defects (0D), dislocations are line defects (1D), grain boundaries are surface defects (2D), voids are volume defects (3D).

Dislocations are line defects that have the important characteristic of carrying plastic deformation in metallic solids.

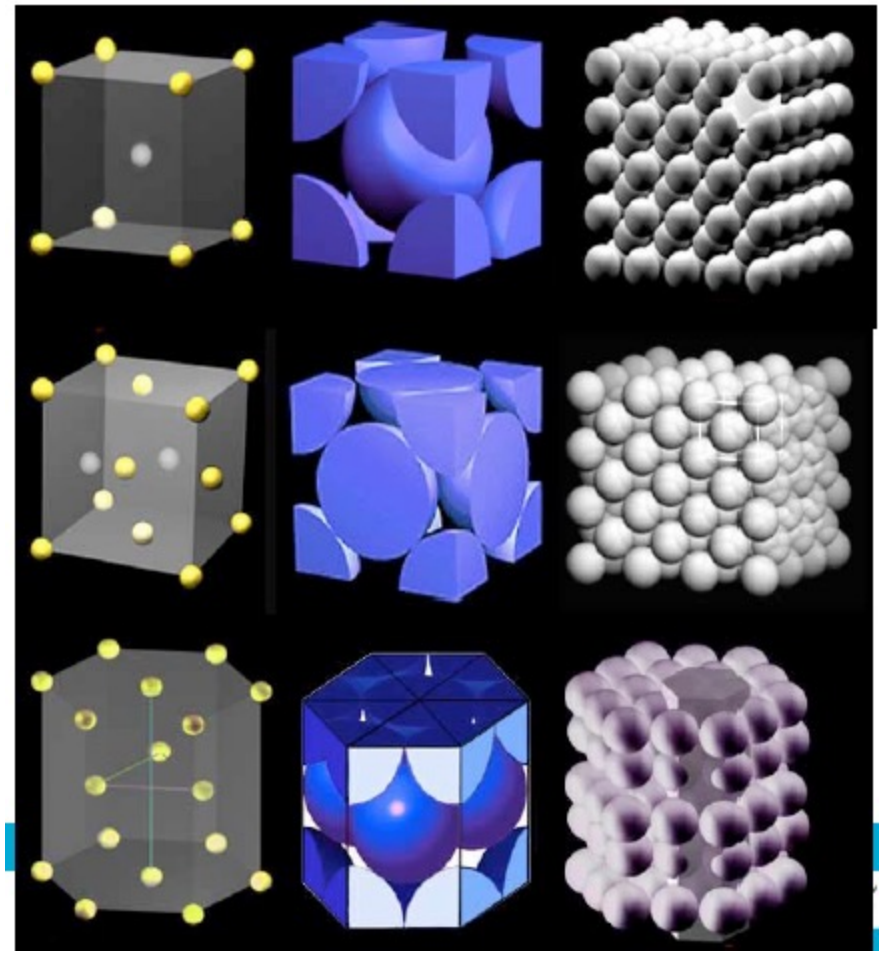
Dislocations are classified based on their character: edge, screw, and mixed dislocations. In a continuum they are fully described by their Burgers vector, dislocation line and slip plane.

crystalline metals

BCC

FCC

HCP



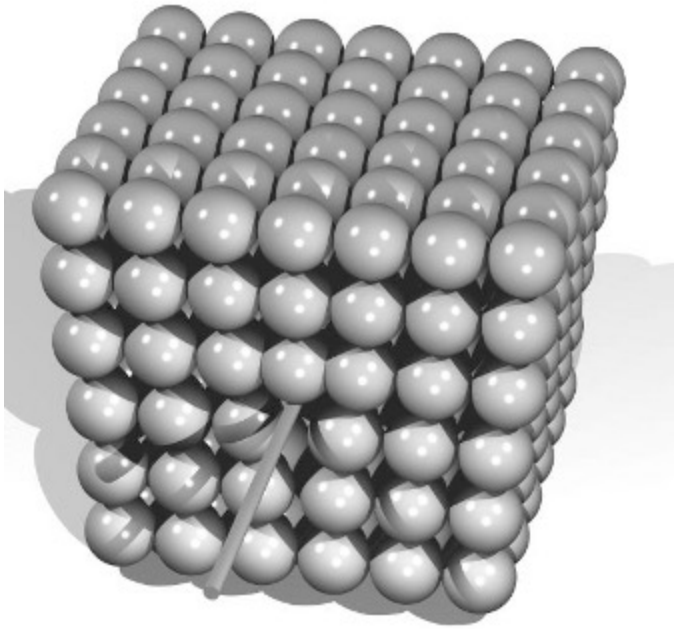
Fe, W, Mo

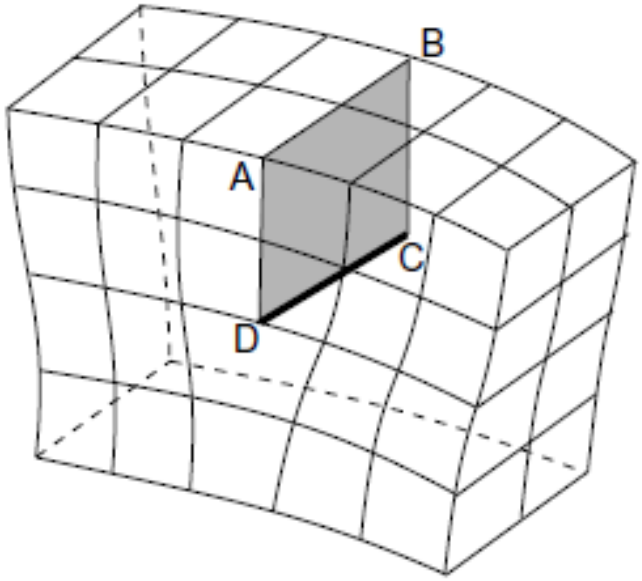
Cu, Al, Ni

Mg, Ti, Zn

Why metals and not semiconductors?

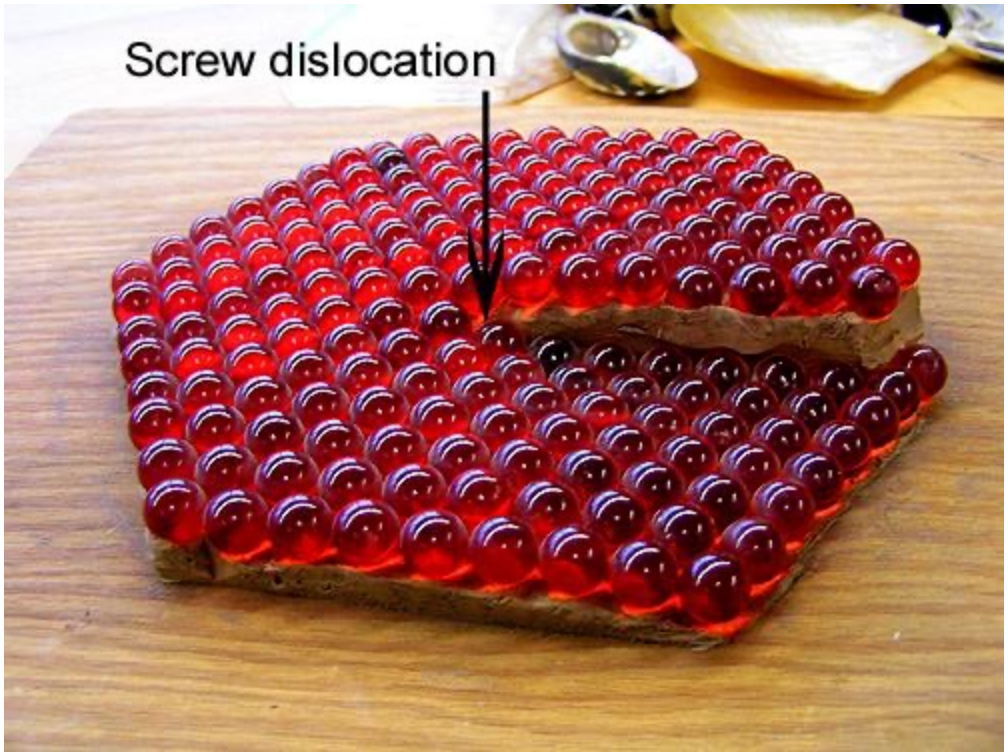
edge dislocation





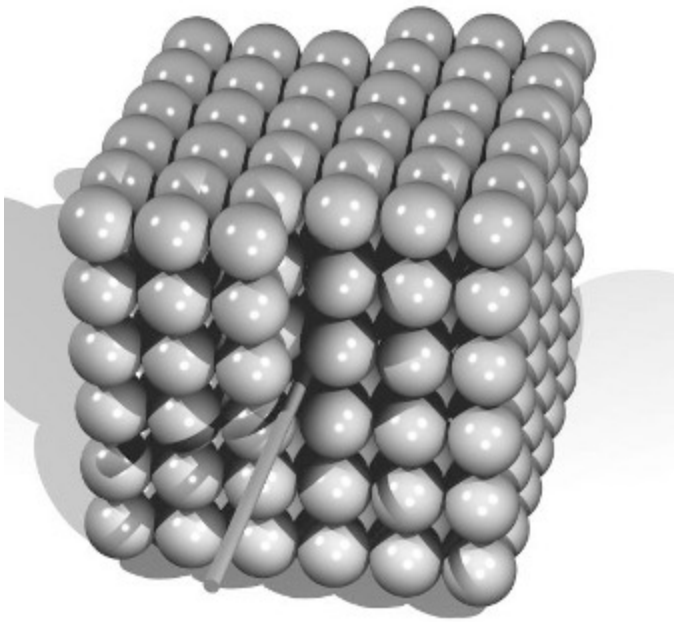
DC is the dislocation line

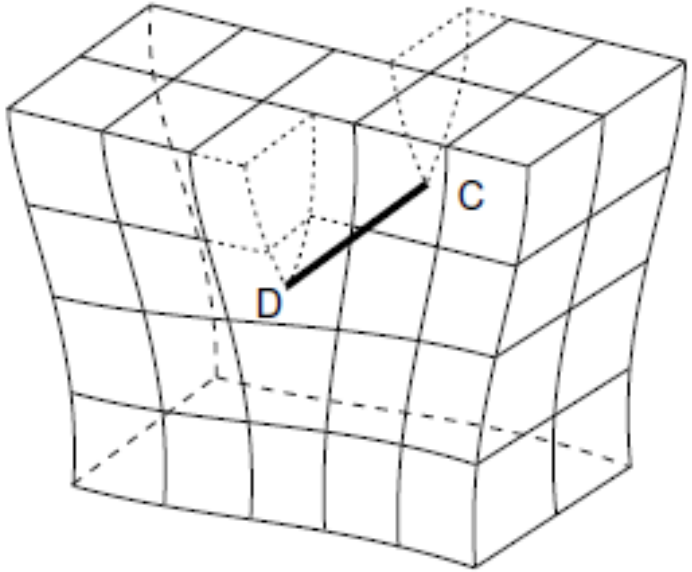
screw dislocation



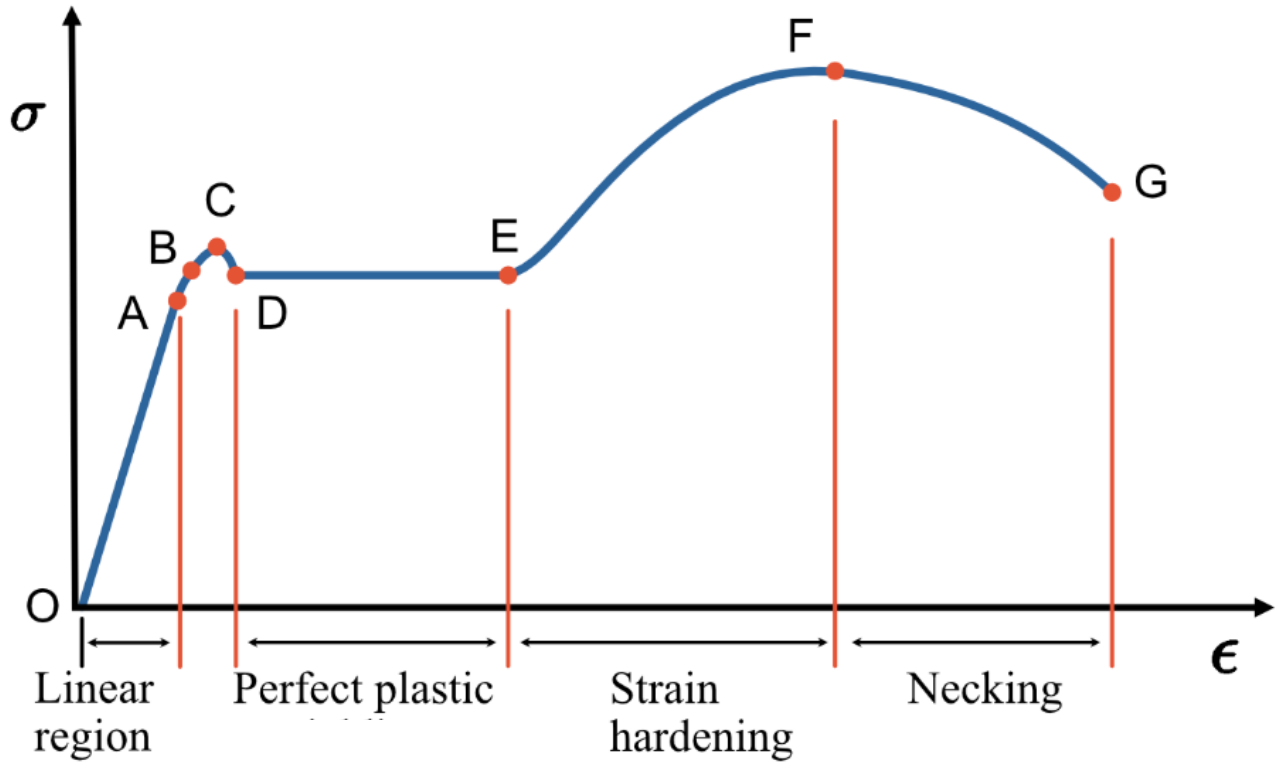
Friends of the minerals forum

screw dislocation





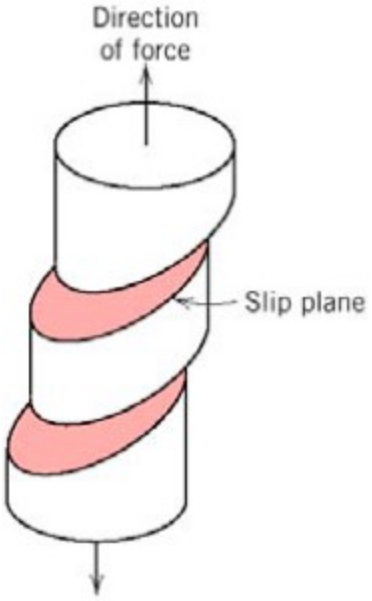
Stress strain curve in a mild steel



experimental observations

- evidence of slip on preferential planes
- shear strength much smaller than theoretical strength

observation of slip



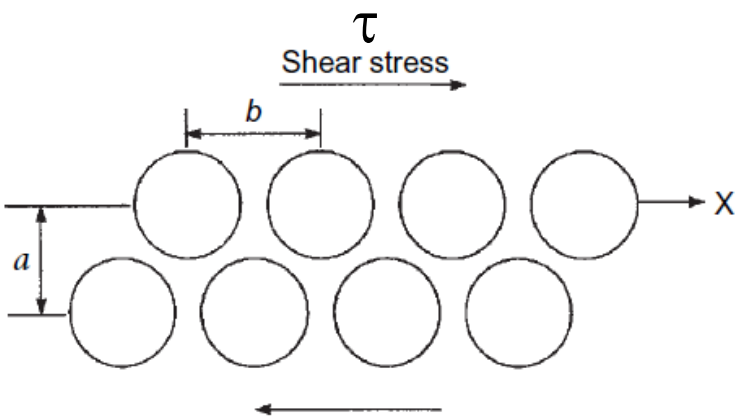
Deformation occurs by slip along specific lattice planes

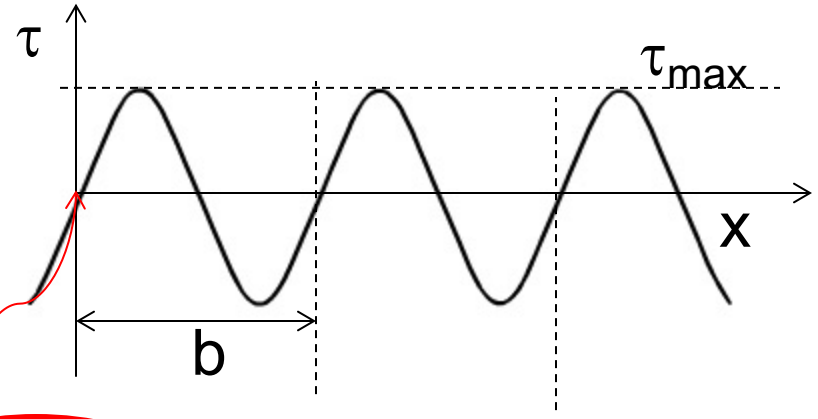
Frenkel model

1924 discrepancy between theoretical and measured shear strength

Existence of dislocations already inferred before they could be seen (1934 by Polanyi, Taylor and Orowan)

late 1950 observation of dislocation by TEM





$$\tau = \tau_{\max} \sin\left(\frac{2\pi x}{b}\right) \approx \tau_{\max} \frac{2\pi x}{b};$$

$$\tau = \gamma G = \frac{x}{a} G$$

$$\tau_{\max} \approx \frac{G}{2\pi}\frac{b}{a} \approx \frac{G}{2\pi} \approx \frac{G}{10}$$

Frenkel model

Existence of dislocations already inferred before they could be seen (1934 by Polanyi, Taylor and Orowan)

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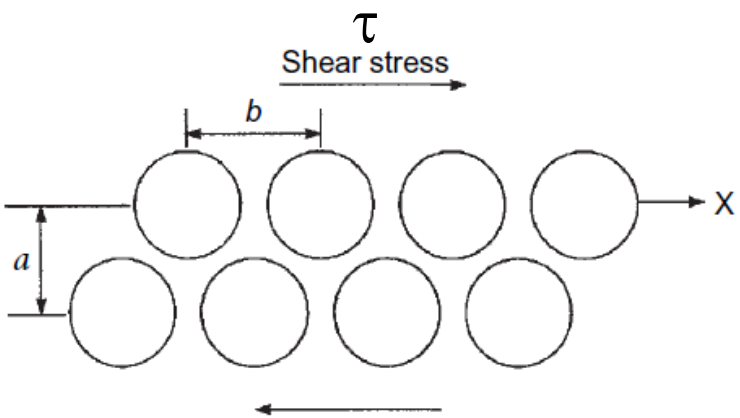
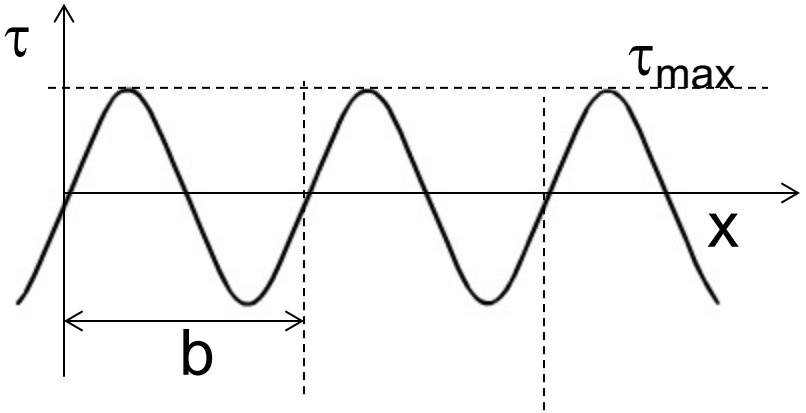
late 1950 observation of dislocation by TEM





theoretical

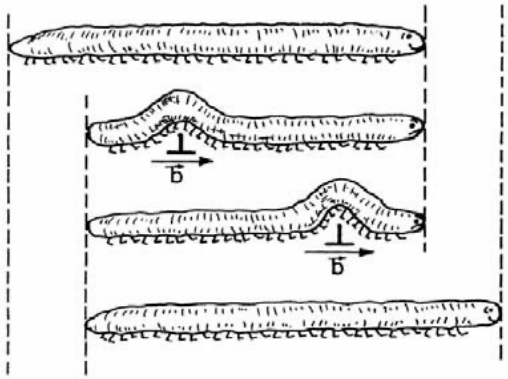
G=10-250 GPa

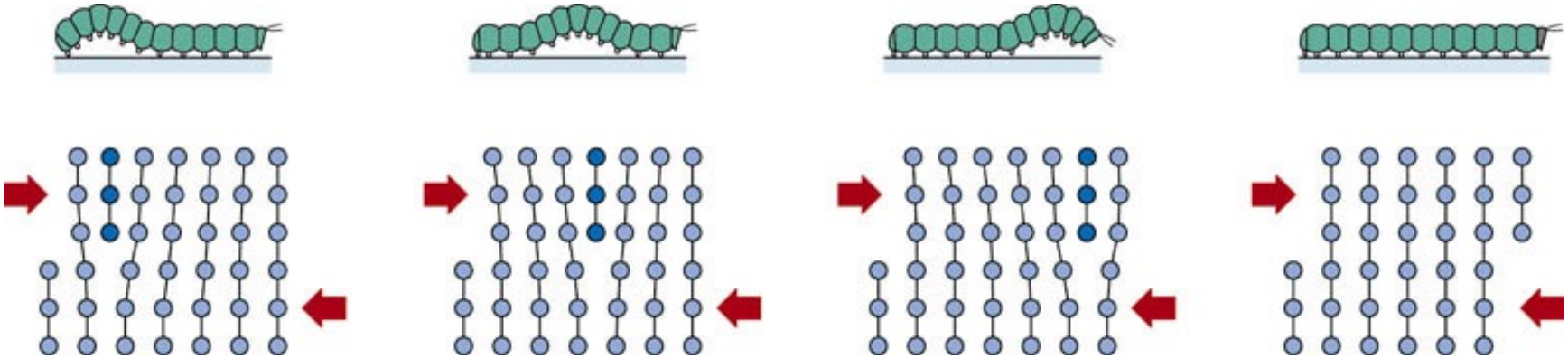
measured!!!

tau=0.5-10 MPa

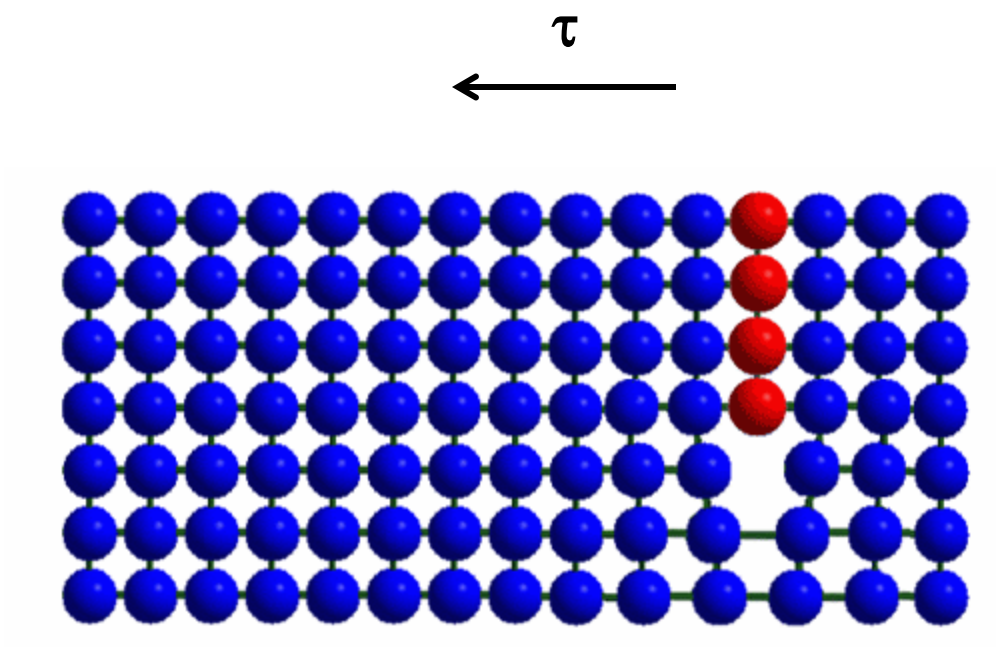
$$\tau_{max} \approx \frac{G}{2\pi}\frac{b}{a} \approx \frac{G}{2\pi} \approx \frac{G}{10}$$

dislocation motion

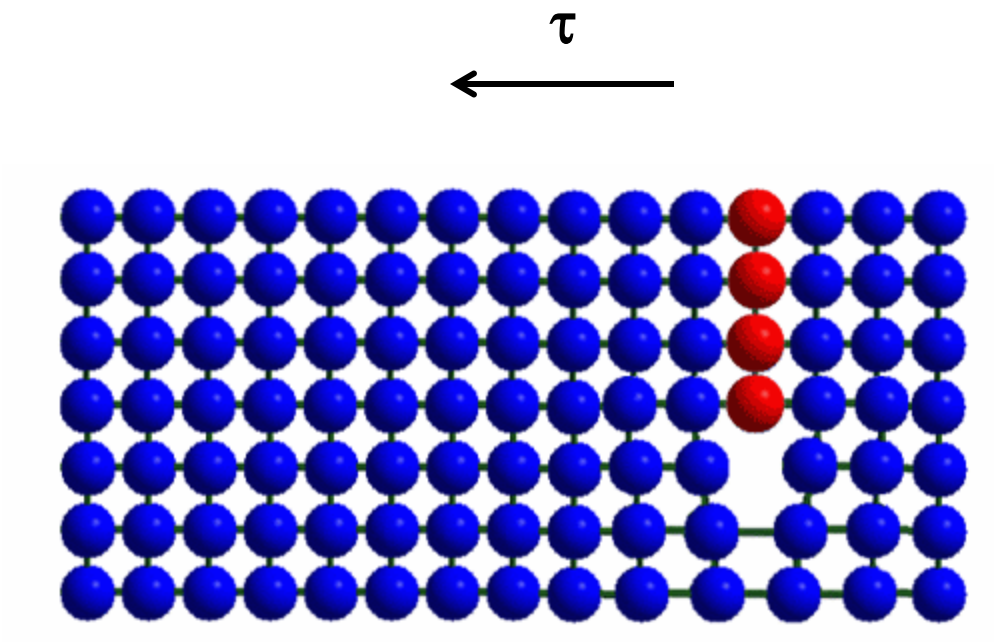




dislocation motion



dislocation motion

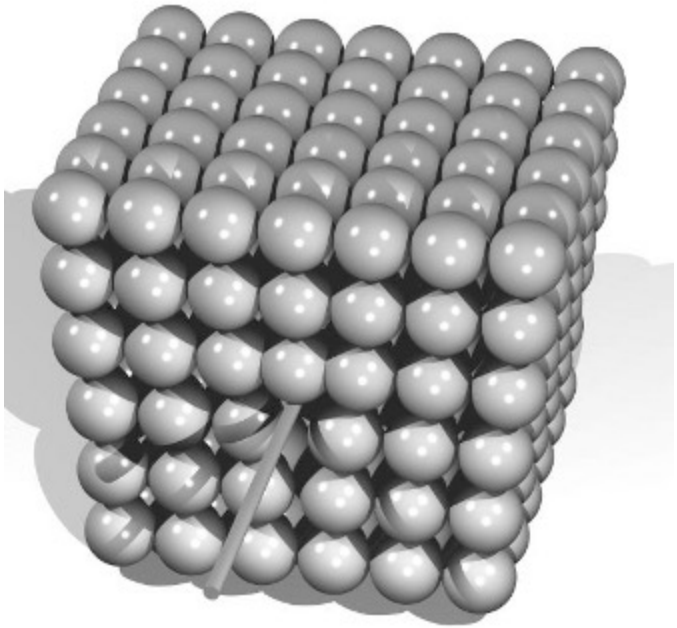


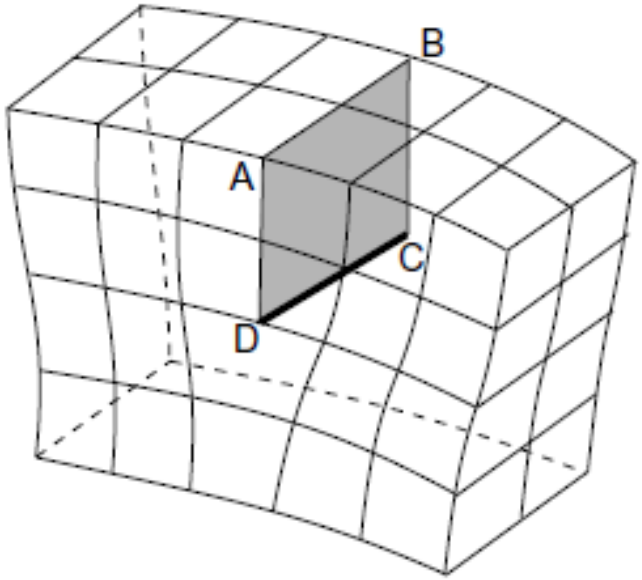
The crystal lattice is not deformed: both the lattice parameter and the volume remain constant

→implication for continuum theories and models: plasticity conserves volume

edge dislocation

DC is the dislocation line



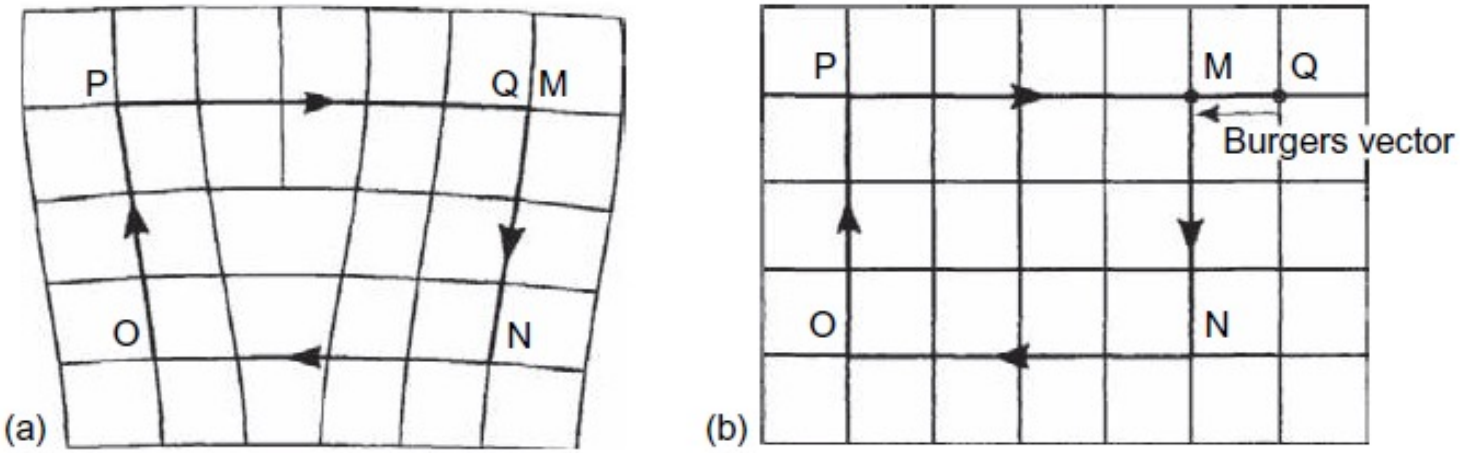


We seek a model for the micro-scale where the solid crystal can be approximated as a continuum body, so that we do not need to store and keep track of all atomic positions,

but we need to preserve the information on the dislocation

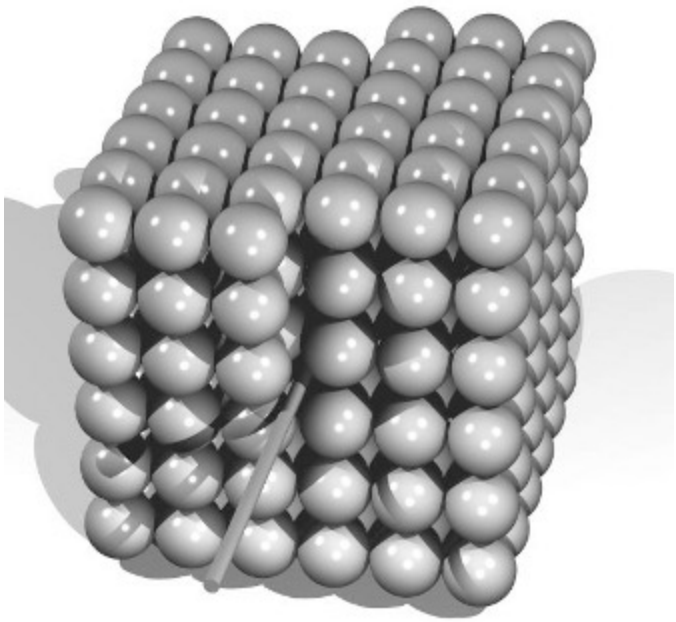
Burgers circuit

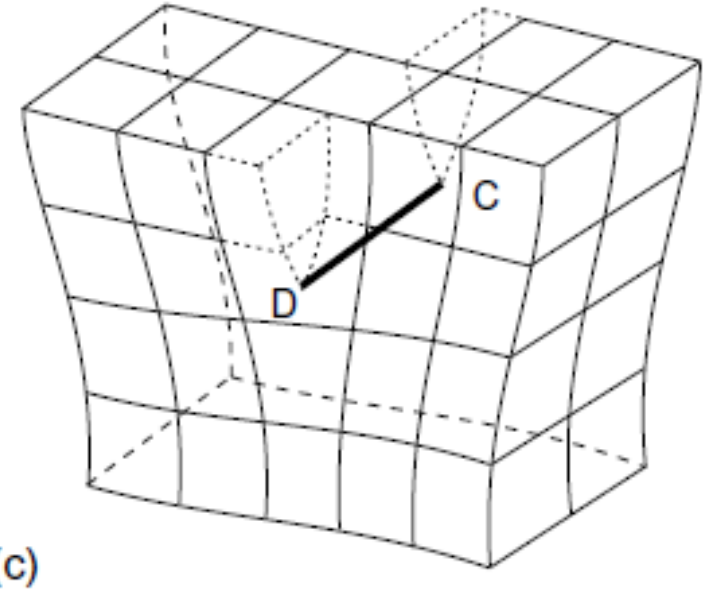
There is no extra plane, the circuit does not close at the same point



1) the dislocation line has positive direction into the plane
2) the Burgers circuit is drawn in clockwise direction
3) the Burgers vector is drawn from finish to start (FS)

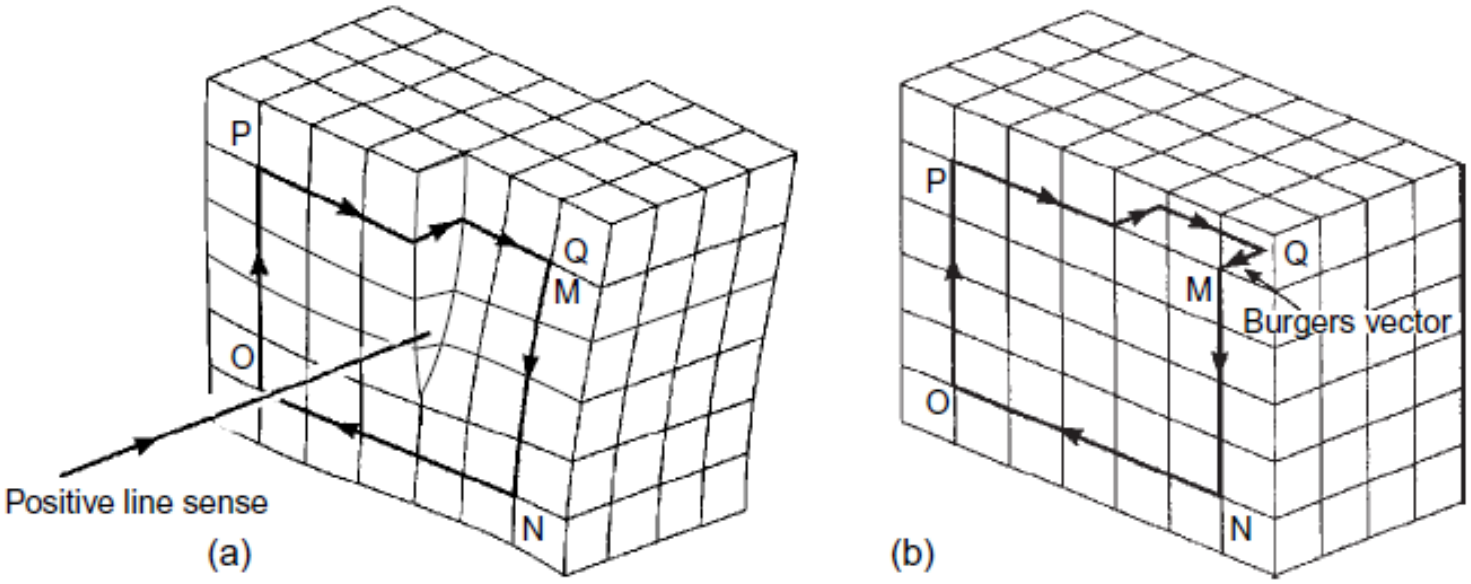
screw dislocation



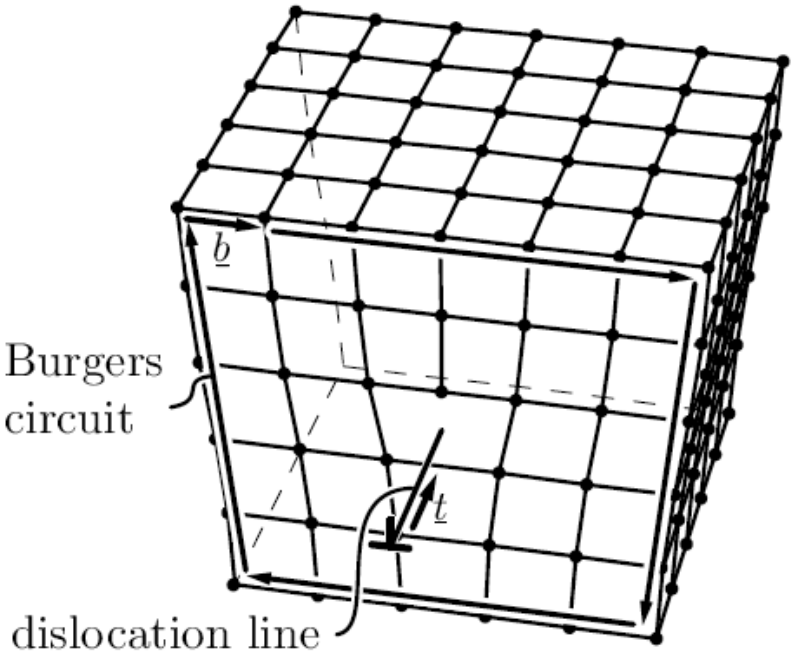


(c)

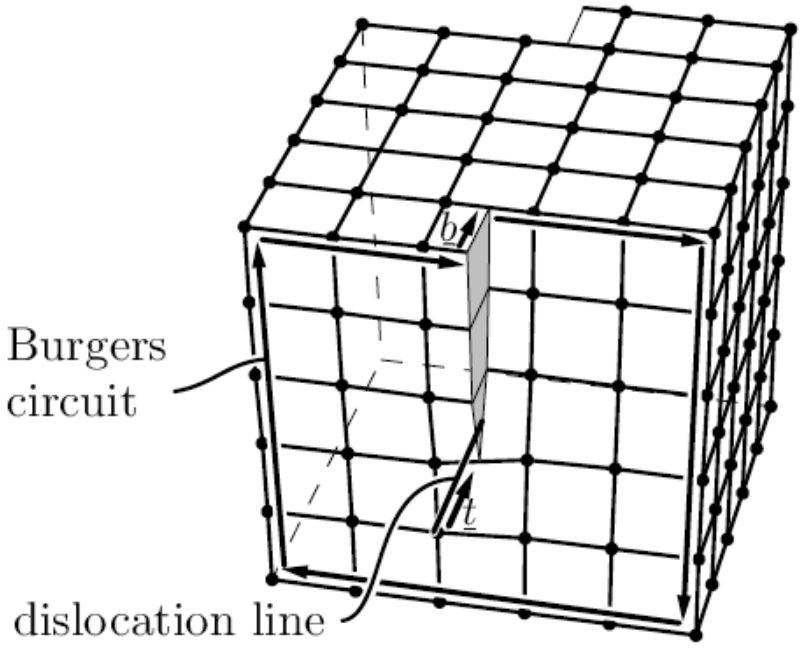
Burgers circuit



edge and screw dislocations



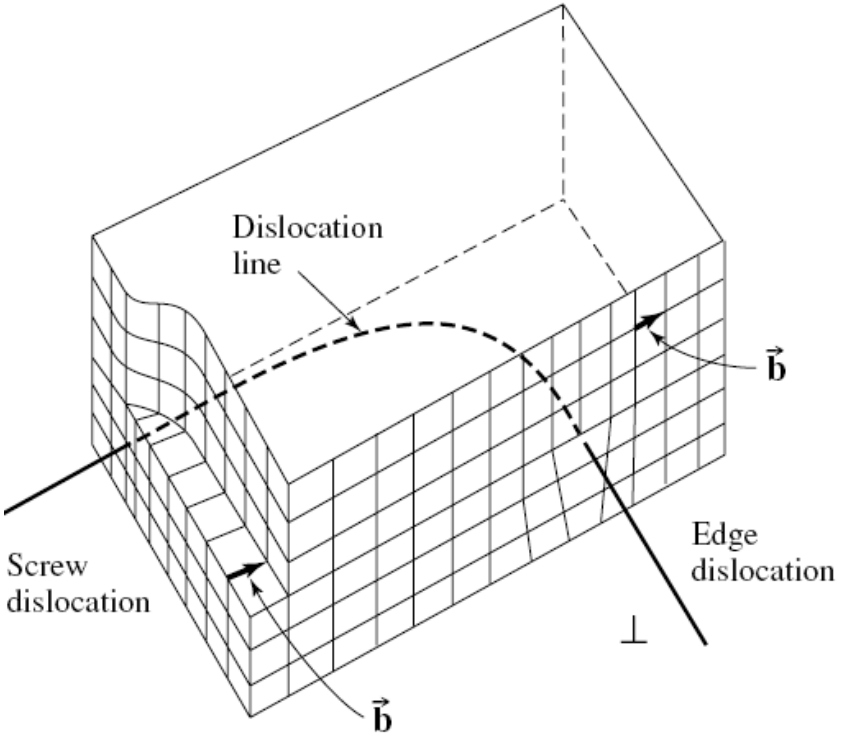
b is normal to the dislocation line **t**

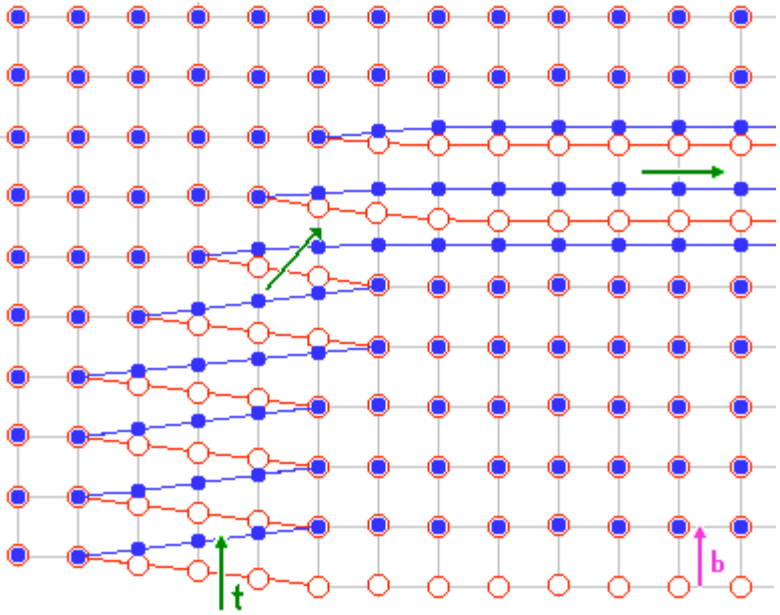


b is parallel to the dislocation line **t**

mixed dislocation

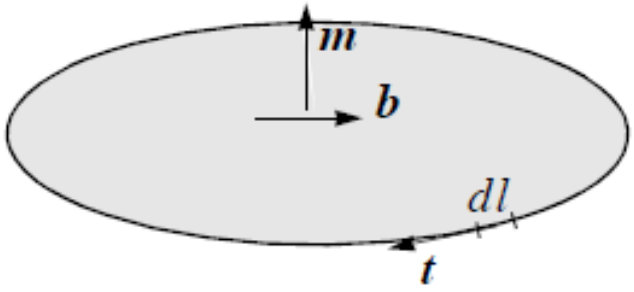
mixed dislocation if **b** is neither parallel nor normal to the dislocation line





The Burgers vector is always the same, while dislocation line vector changes while the dislocation changes character

dislocation loop in continuum theory



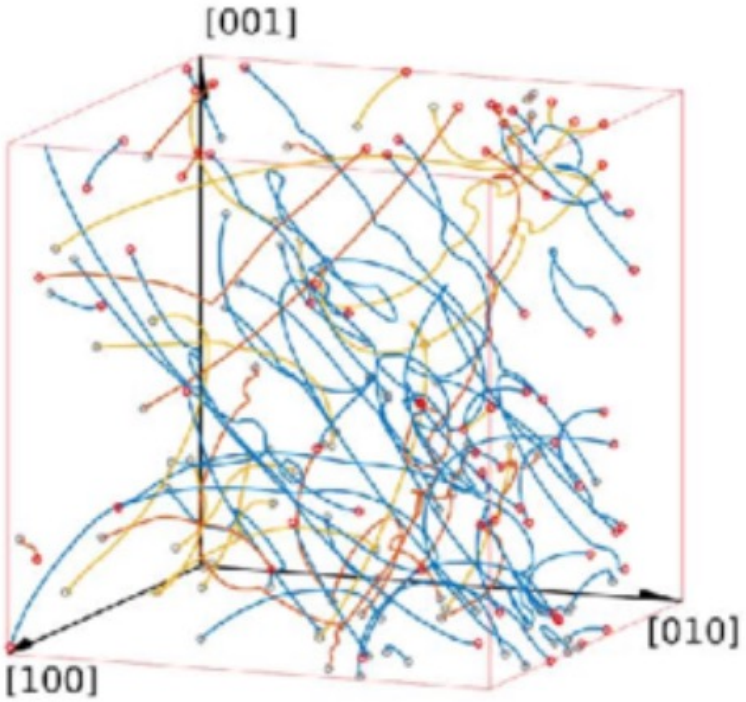
edge: $\boldsymbol{b}\cdot\boldsymbol{t}=0$;

screw: $\boldsymbol{b}\cdot\boldsymbol{t}=\pm b$

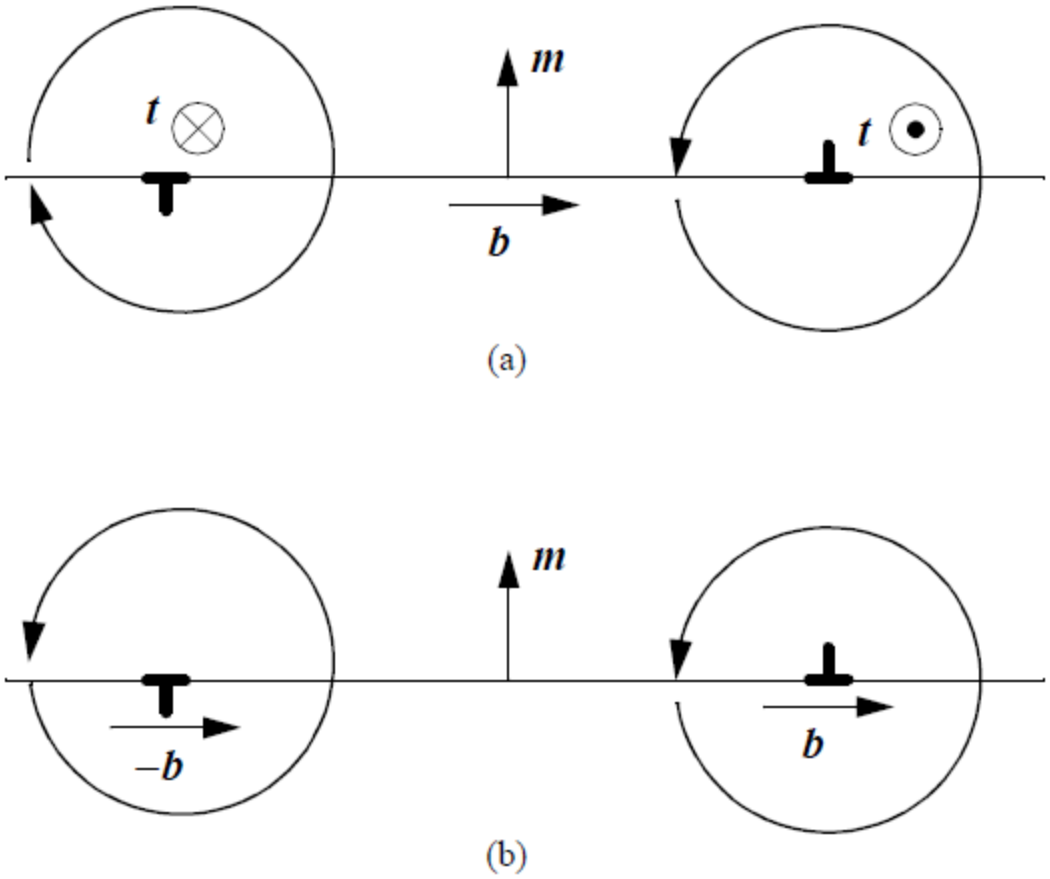
- the slip plane with its unit normal vector $\boldsymbol{m}$;
- the dislocation line as a parameterized line on this plane and with a local tangent vector $\boldsymbol{t}$;
- the Burgers vector $\boldsymbol{b}$.

We now have only three parameters that define the dislocation in a continuum

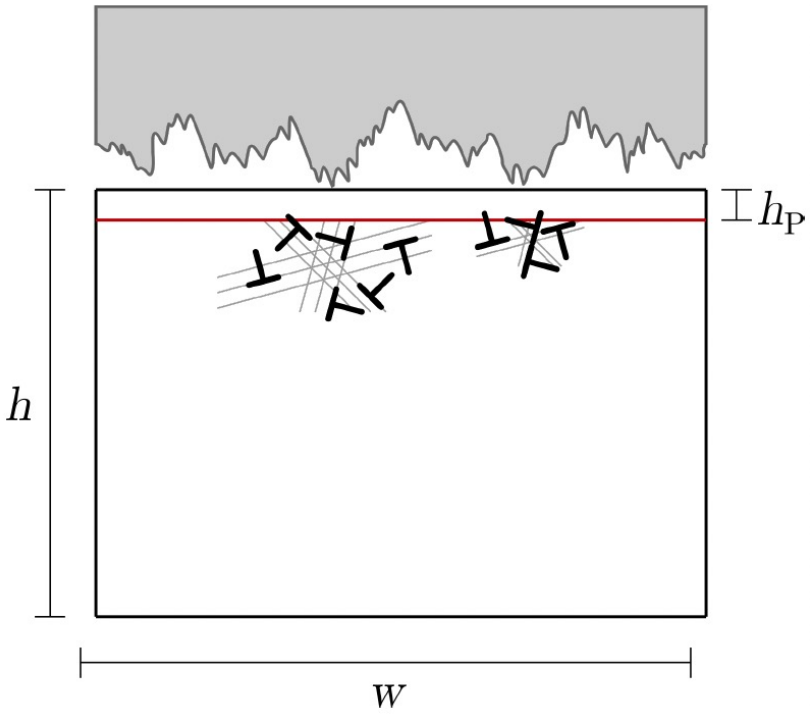
dislocations in a 3D DD simulation

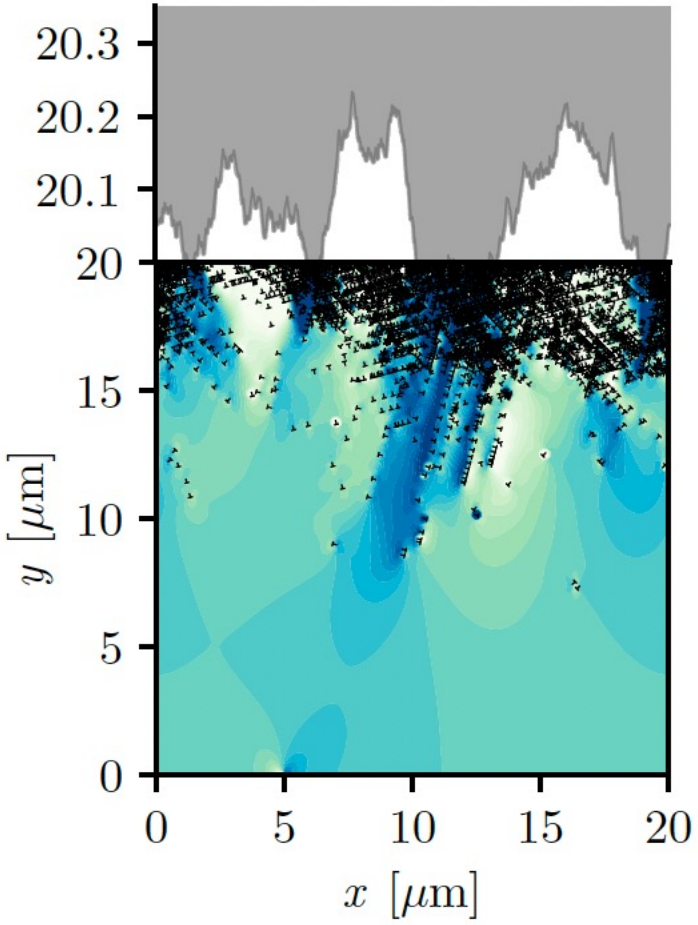


dislocation loop in 2-D



dislocations in a 2D DD simulation





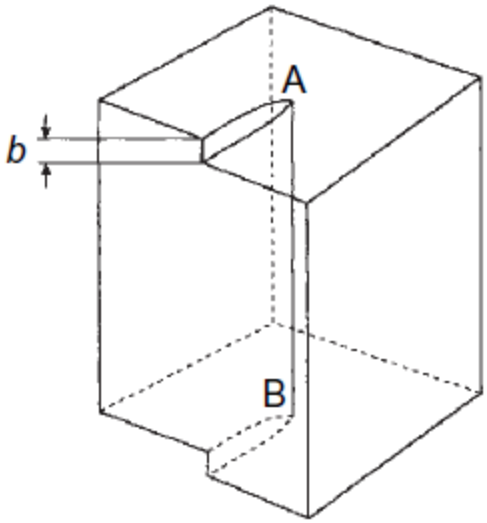
Dislocation dynamics uses linear elasticity

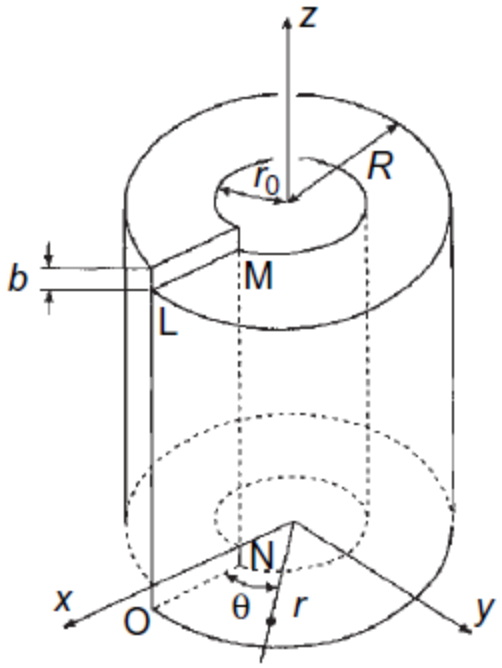
$$\begin{aligned} \text{equilibrium} &: \sigma_{ij,j} = 0 \\ \text{elasticity} &: \sigma_{ij} = \mathcal{L}_{ijkl}\varepsilon_{kl} \\ \text{strains} &: \varepsilon_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}) \end{aligned}$$

Here, for simplicity: isotropic elasticity (shear modulus μ, Poisson ratio ν):

$$\mathcal{L}_{ijkl} = 2\mu \left[\tfrac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + \frac{\nu}{1-2\nu}\delta_{ij}\delta_{kl} \right] .$$

fields of screw dislocation

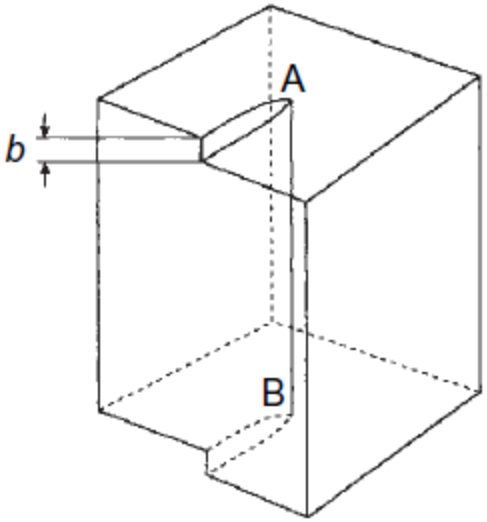


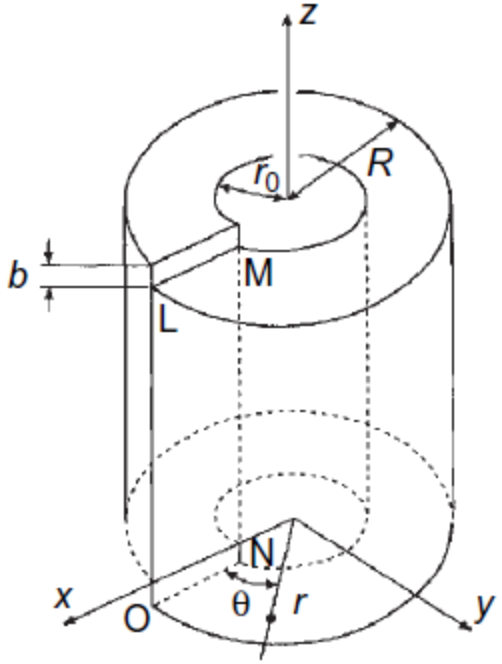


Volterra dislocation

fields of screw dislocation

What is the displacement field of a screw dislocation?





Volterra dislocation

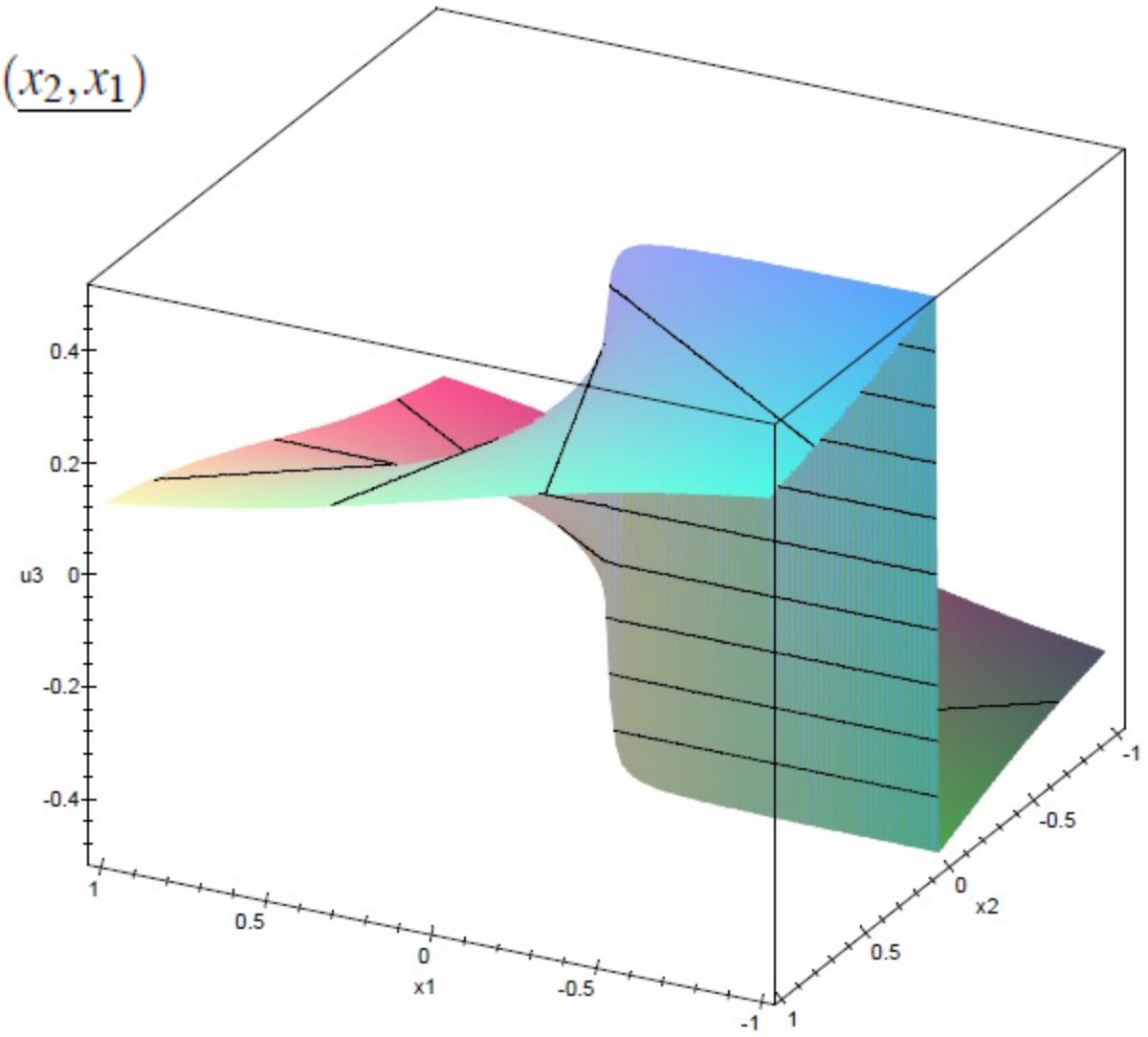
2D anti-plane shear problem: $\nabla^2 u_3 = 0$

$$u_1 = u_2 = 0, \quad u_3 = u_3(x_1, x_2)$$

$$u_3(x_1, 0^+) - u_3(x_1, 0^-) = b$$

displacement field screw dislocation

$$u_3 = \frac{b}{2\pi}\arctan(x_2, x_1)$$



stress field of screw dislocation

$$u_3 = \frac{b}{2\pi} \arctan\left(\frac{x_2}{x_1}\right)$$

$$\sigma_{13} = -\frac{\mu b}{2\pi} \frac{x_2}{{x_1}^2 + {x_2}^2}, \quad \sigma_{23} = \frac{\mu b}{2\pi} \frac{x_1}{{x_1}^2 + {x_2}^2}$$

or in terms of polar coordinates $(r, \theta, z = x_3)$

$$\sigma_{\theta z} = \frac{\mu b}{2\pi r}$$

stress field of screw dislocation

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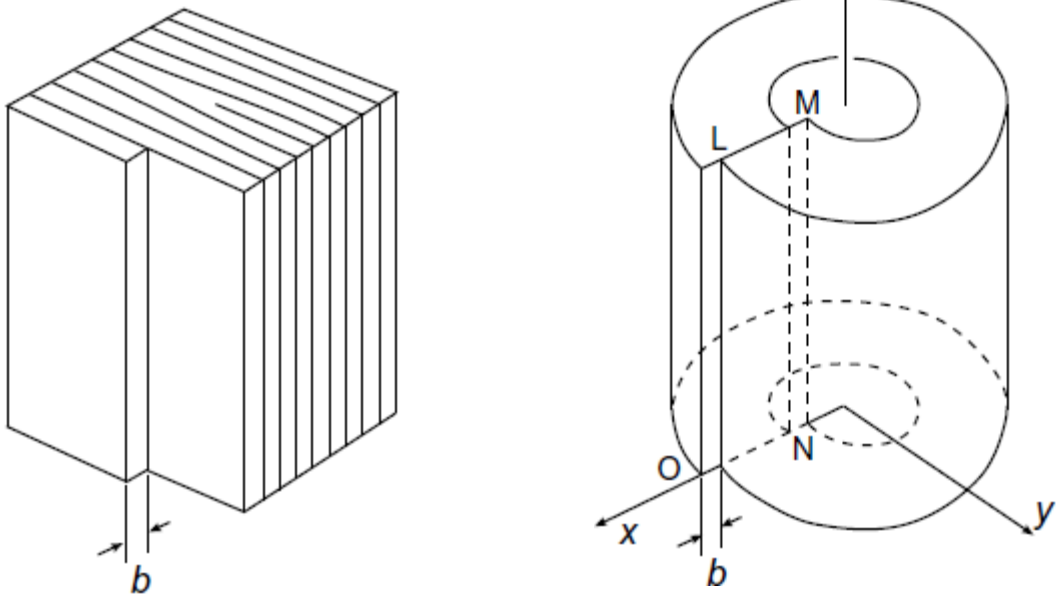
or in terms of polar coordinates $(r, \theta, z = x_3)$

$$\sigma_{\theta z} = \frac{\mu b}{2\pi r}$$

Hence, dislocations have a *long-range effect*.

This means that we cannot cut-off dislocation fields without doing a significant mistake.

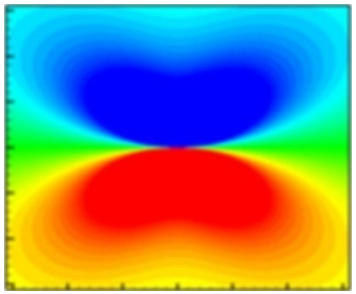
fields of edge dislocation



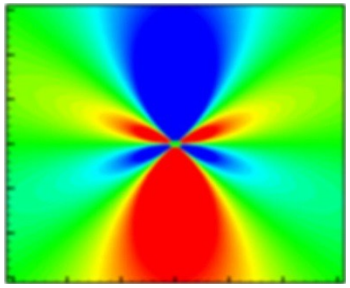
plane strain problem: u=u(x,y), u_z=0

stress field edge dislocation

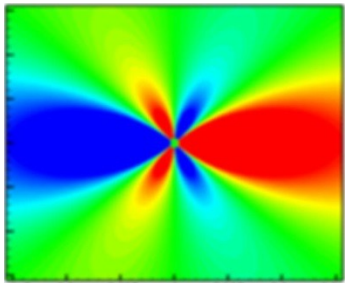
$$\sigma_{xx} = \frac{-\mu b}{2\pi(1-\upsilon)} \frac{y(3x^2+y^2)}{(x^2+y^2)^2}$$



$$\sigma_{yy} = \frac{\mu b}{2\pi(1-\upsilon)} \frac{y(x^2-y^2)}{(x^2+y^2)^2}$$

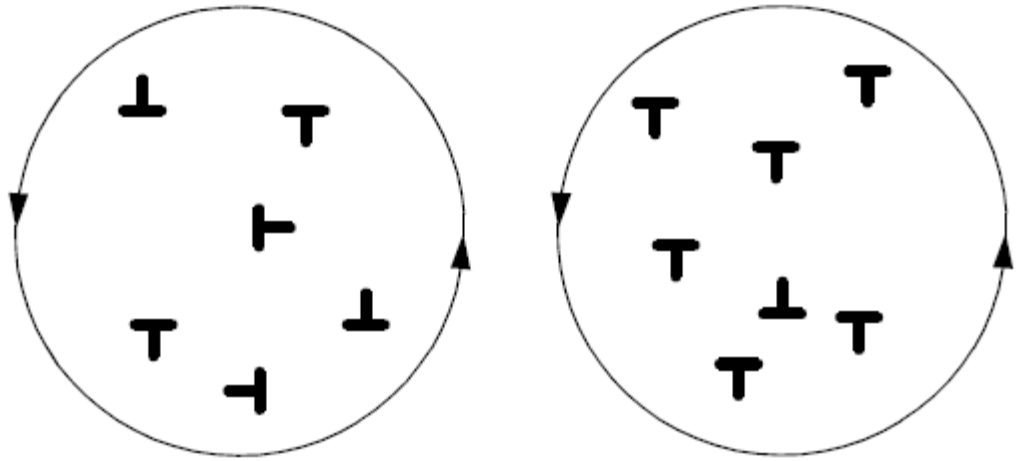


$$\sigma_{xy} = \frac{\mu b}{2\pi(1-\upsilon)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}$$



dislocation interaction

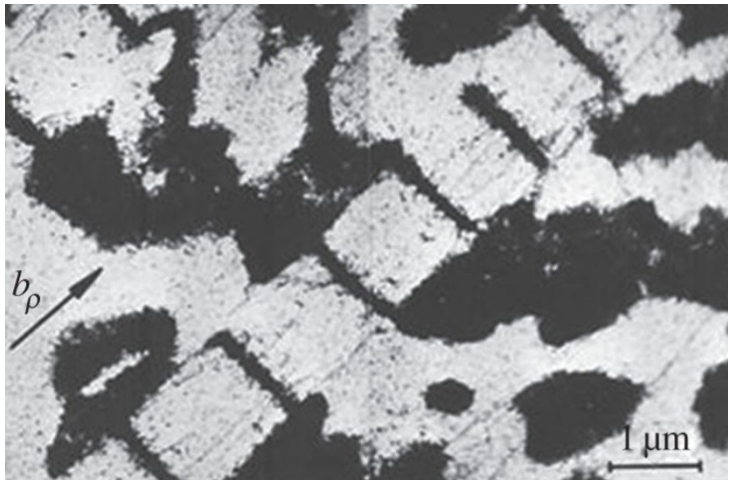
- Stress $\propto$ distance^{-1}
- Because of long-range effects, dislocations can interact to form structures
- Characterisation of structures by means of *net Burgers vector*



(a) (b)

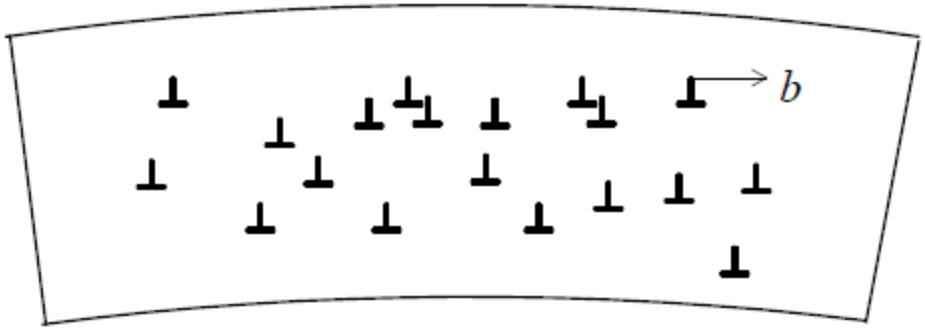
net $b = 0$ net $b = \top$

ladder structure

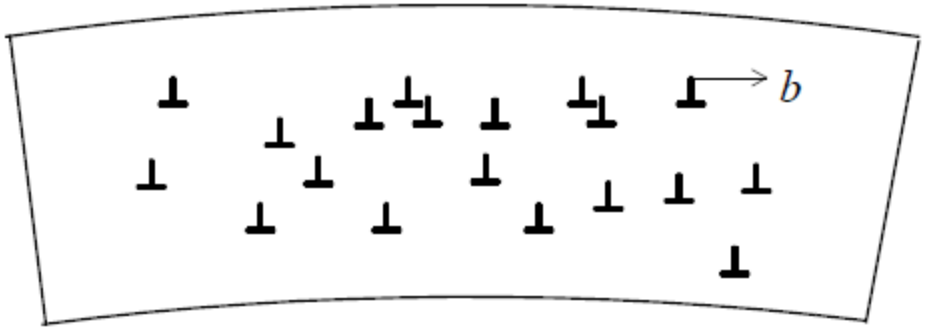


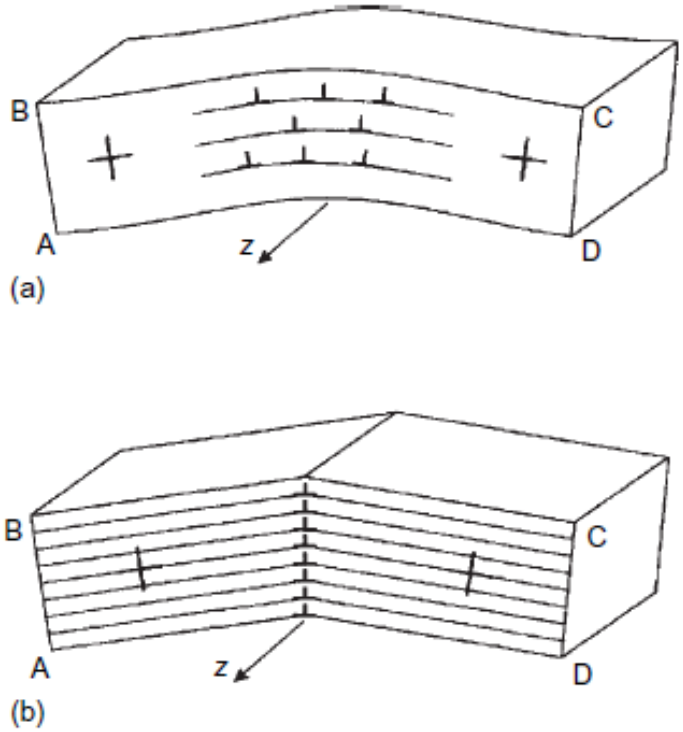
Muhgrabi, *Acta Metall 1983*

geometrically necessary dislocations

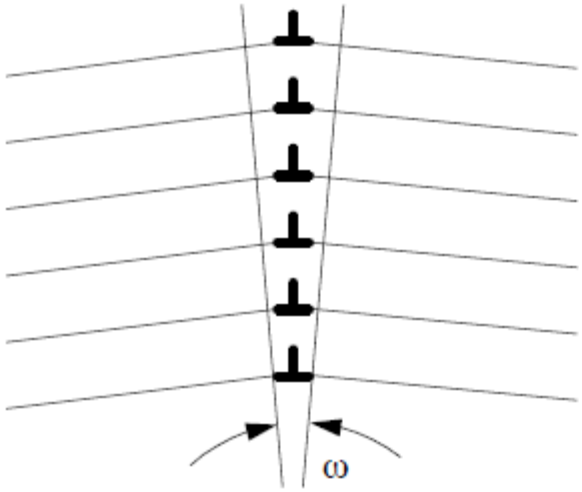


formation of a low angle grain boundary





dislocation wall, tilt grain boundary



$$\omega = b/h$$

$$\sigma_{12} = \frac{\mu b}{2\pi(1-\nu)} \sum_{n=-\infty}^{\infty} \frac{x_1(x_1^2 - (x_2 - nh)^2)}{(x_1^2 + (x_2 - nh)^2)^2}$$

$$= \frac{\mu b}{2\pi(1-\nu)} \frac{2\pi^2 \xi(\cosh 2\pi\xi \cos 2\pi\eta - 1)}{(\cosh 2\pi\xi - \cos 2\pi\eta)^2}, \quad \xi = x_1/h, \eta = x_2/h$$

Exponential decay away from the wall

This is a short-range field, which means that we can cut-off the fields produced by a dislocation wall without doing a significant mistake.

One versus two dislocations

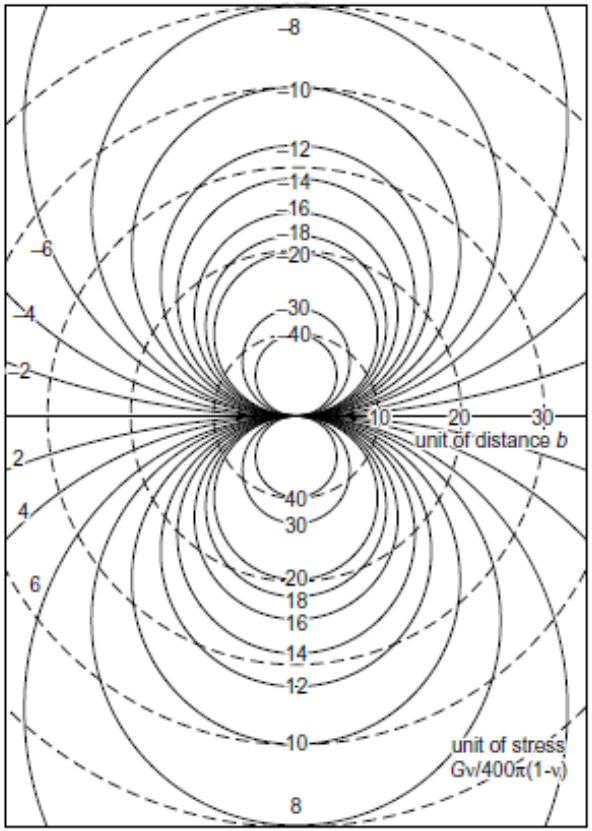


FIGURE 9.10
Constant value contours of the stress field σ_{zz} of a single edge dislocation. Dashed circles show distance from the origins. *(From Li (1963),* Electron Microscopy and Strength of Crystals, *p. 713.*

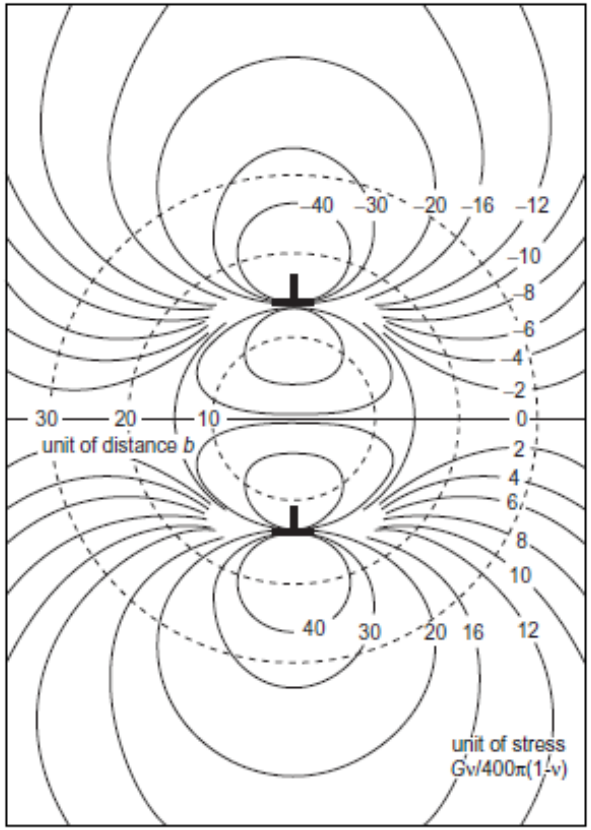


FIGURE 9.11
The stress field σ_{zz} of a vertical wall of two edge dislocations spaced 28*b* apart. *(From Li (1963),* Electron Microscopy and Strength of Crystals, *p. 173. Interscience.)*

infinite array

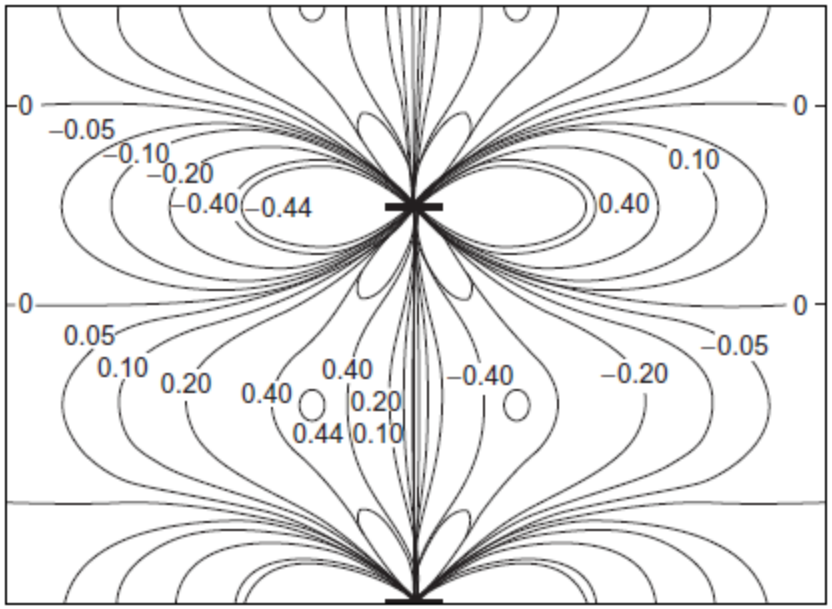
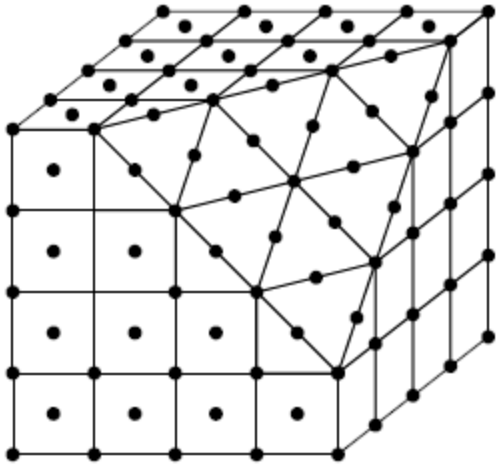
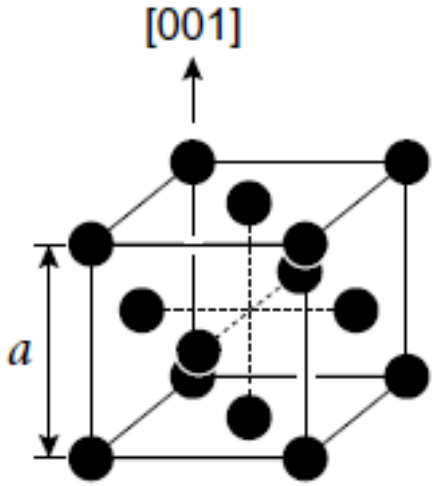


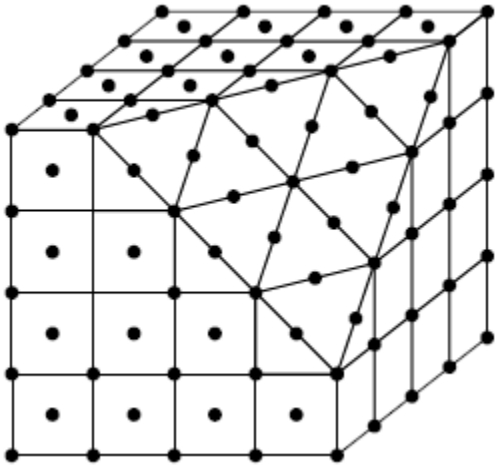
FIGURE 9.12
The shear stress field σ_{xy} of an infinite array of edge dislocations. Unit of stress $Gb/2(1-\nu)D$. *(From Li,* Acta Metall. *8, 296, 1960.)*

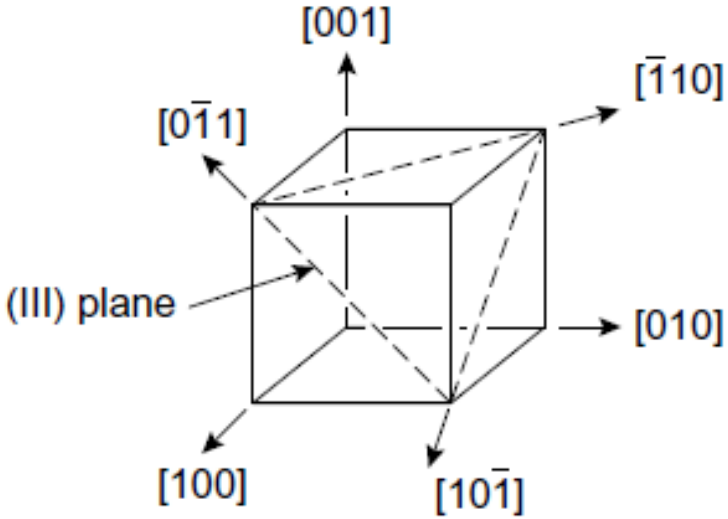
where do dislocations move?



FCC structure







Dislocations move on the mostly packed plane in the mostly packed direction

slip systems

Metals	*Slip Plane*	*Slip Direction*	*Number of Slip Systems*
	Face-Centered Cubic		
Cu, Al, Ni, Ag, Au	{111}	$\langle 1\bar{1}0 \rangle$	12
	Body-Centered Cubic		
α-Fe, W, Mo	{110}	$\langle \bar{1}11 \rangle$	12
α-Fe, W	{211}	$\langle \bar{1}11 \rangle$	12
α-Fe, K	{321}	$\langle \bar{1}11 \rangle$	24
	Hexagonal Close-Packed		
Cd, Zn, Mg, Ti, Be	{0001}	$\langle 11\bar{2}0 \rangle$	3
Ti, Mg, Zr	$\{10\bar{1}0\}$	$\langle 11\bar{2}0 \rangle$	3
Ti, Mg	$\{10\bar{1}1\}$	$\langle 11\bar{2}0 \rangle$	6

slip plane = a densely packed plane

slip direction = most densely packed direction

The slip direction corresponds with the direction of the Burger vector, i.e. the shortest translation vector

critical resolved shear stress

Dislocations move in response to the shear stress acting on the slip plane, the resolved shear stress.

The resolved shear stress that acts on the slip plane due to force F equals:

$$\tau_{rs} = \frac{F}{A}\cos\phi.\cos\lambda$$

When the resolved shear stress becomes sufficiently large, the crystal will start to yield. Dislocations start to move along the most favourably slip system. The minimum shear stress to initiate slip is termed "critical resolved shear stress":

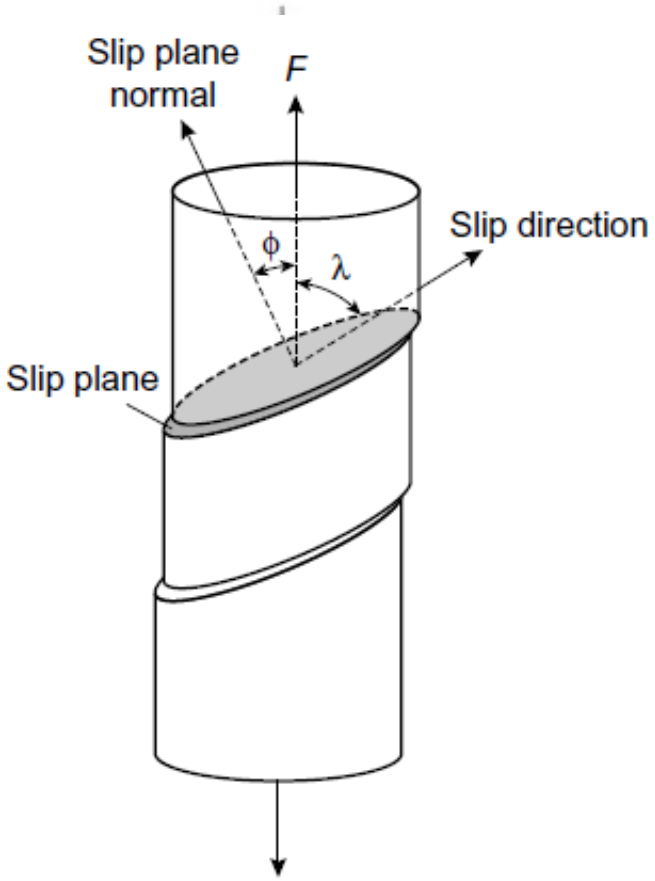
$$\tau_{crss} = \sigma_y(\cos\phi.\cos\lambda)_{\max}$$

The onset of yielding corresponds with the yield stress

$$\sigma_y = \frac{\tau_{crss}}{(\cos\phi.\cos\lambda)_{\max}}$$

The minimum stress for yielding, if $\phi=\lambda=45^o$,then:

$$\sigma_y = 2\tau_{crss}$$



dislocation glide in thin films

Courtesy of Gehrard Dehm

Take home messages

- Dislocations are lattice defects in crystalline solids that can be represented in a continuum framework by their slip plane, line direction and Burgers vector
- The dislocations can be represented, outside of their core, as the elastic distortion of an elastic continuum
- Dislocations fields have a long range effect, and therefore dislocations attract or repel each other forming structures
- Since the fields are long-ranged they cannot be cut-off without an error
- Dislocations glide on highly packed slip planes and directions

Dislocation dynamics

Let's write a very simple DD code in 2 dimensions. Dislocations of edge character can glide only along horizontal planes. A density of randomly positioned dislocations are the starting point of the simulations.
There are no external fields, so that the dislocations move only due to the interaction between their stress fields.
The section of the crystal is represented by a square.

Dislocation dynamics

Let's write a very simple DD code in 2 dimensions. Dislocations of edge character can glide only along horizontal planes. A density of randomly positioned dislocations are the starting point of the simulations.
There are no external fields, so that the dislocations move only due to the interaction between their stress fields.
The section of the crystal is represented by a square.

```
% create initial positions
%
% input: n = number of dislocations  (assumed to be even)
%        a = size of dislocation cell
%
% output: (x,y) coordinates and Burgers vector b for each dislocation
%
%
function[x,y,b] = initDD(n,a)
```

initDD.m

```
% create initial positions
%
% input: n = number of dislocations  (assumed to be even)
%        a = size of dislocation cell
%
% output: (x,y) coordinates and Burgers vector b for each dislocation
%
%
function[x,y,b] = initDD(n,a)
%  created scaled coordinates in an fcc lattice
x = rand(n,1)*a;
y = rand(n,1)*a;
% assign b
b = zeros(n,1);

for i=1:n/2
   b(i) = 1;
end

for i=n/2+1:n
   b(i) =-1;
end
scatter(x,y,50,b,'d'); axis square;
```

sumDD.m

Now sum over the forces that dislocations exchange with each other.
This is similar to the force calculation we did for the atoms in the MD code.

In the absence of external loading the dislocations glide due to the Peach-Koehler force induced by the other dislocations.
The force that one dislocation exerts on the other is:

$$F_x(i) = bb_i\sigma_{xy}(j)$$

$$F_x(i) = \frac{Gb^2 b_j b_i}{2\pi(1-\nu)} \frac{x_{ji}\left(x_{ji}^2 - y_{ji}^2\right)}{\left(x_{ji}^2 + y_{ji}^2\right)^2} \quad \Rightarrow \quad F_x(i) = b_j b_i \frac{x_{ji}\left(x_{ji}^2 - y_{ji}^2\right)}{\left(x_{ji}^2 + y_{ji}^2\right)^2}$$

```
function[fx,fmax]= sumDD(n,a,rc,x,y,b)
```