

Viscoelasticity of Planetary Interiors from Seismic to Convective Timescales

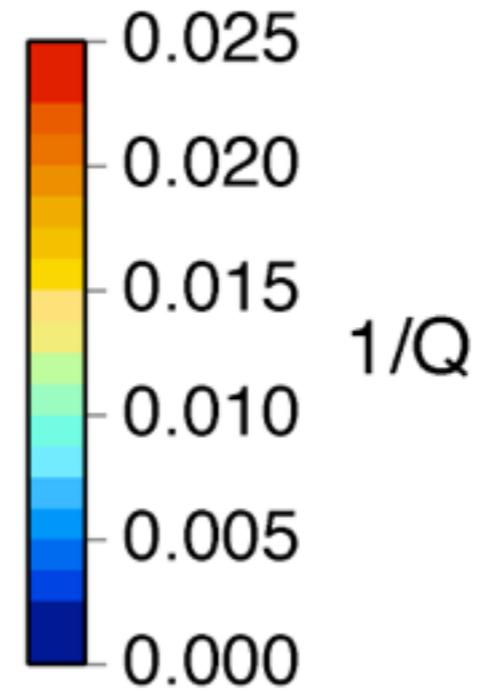
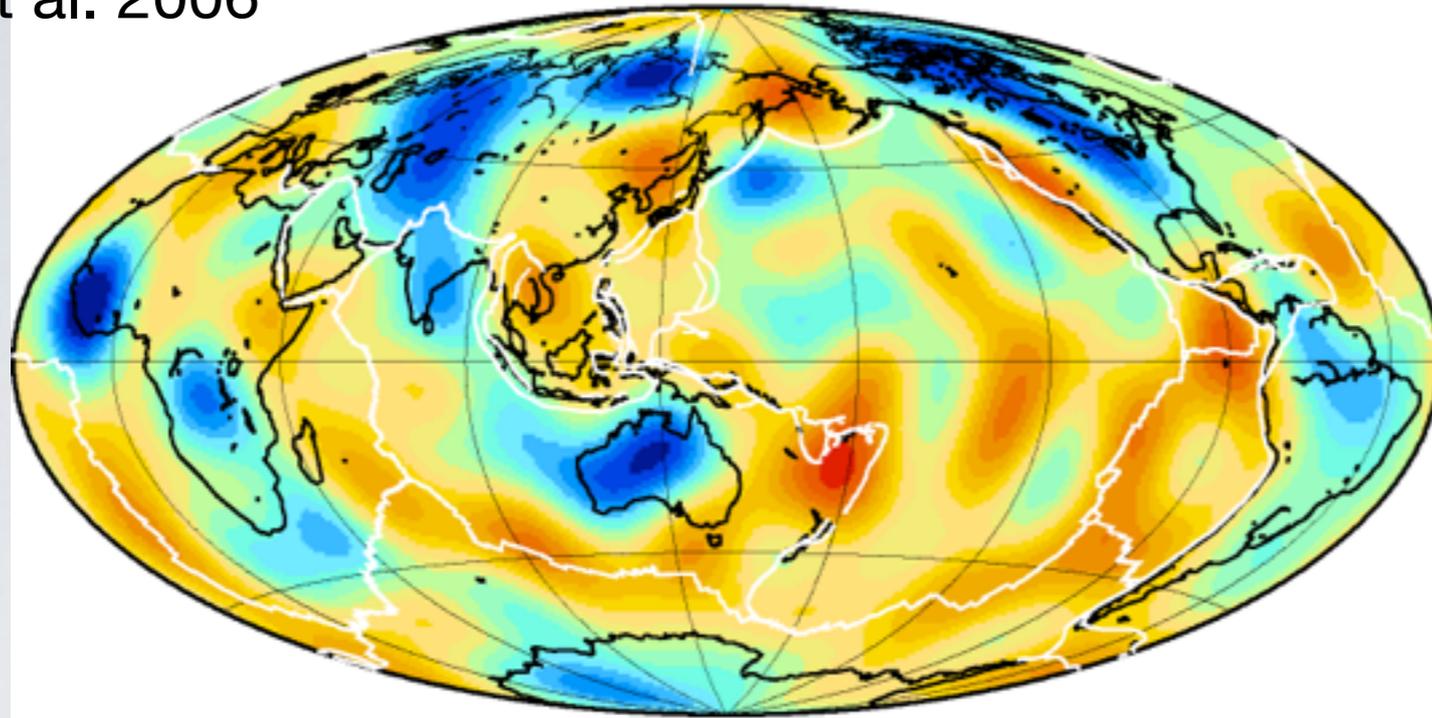
Uli Faul

EAPS

Massachusetts Institute of Technology

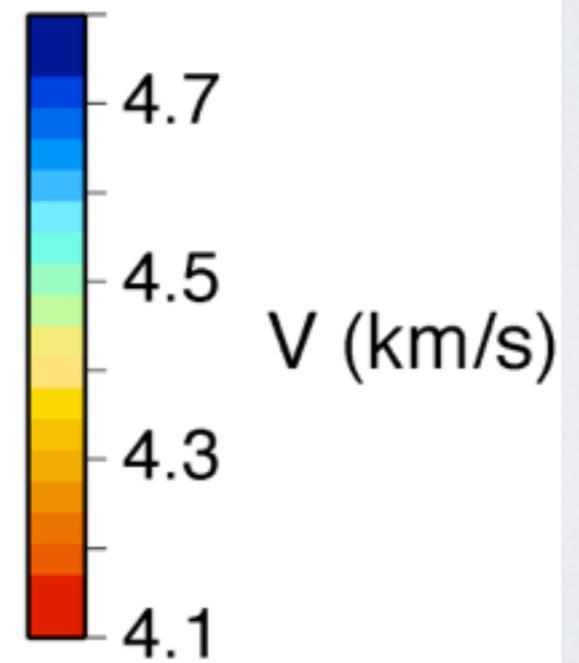
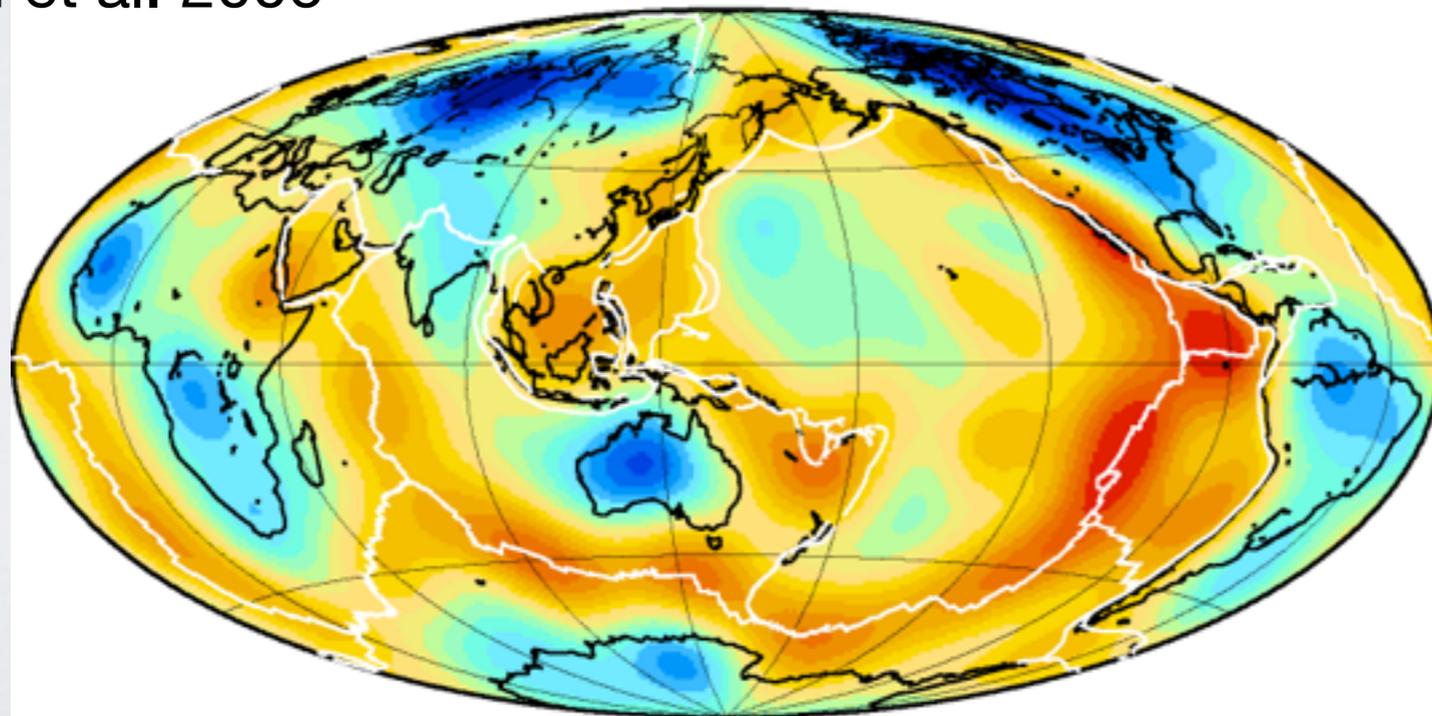
Dalton et al. 2006

Attenuation



Kustowski et al. 2006

Shear Velocity

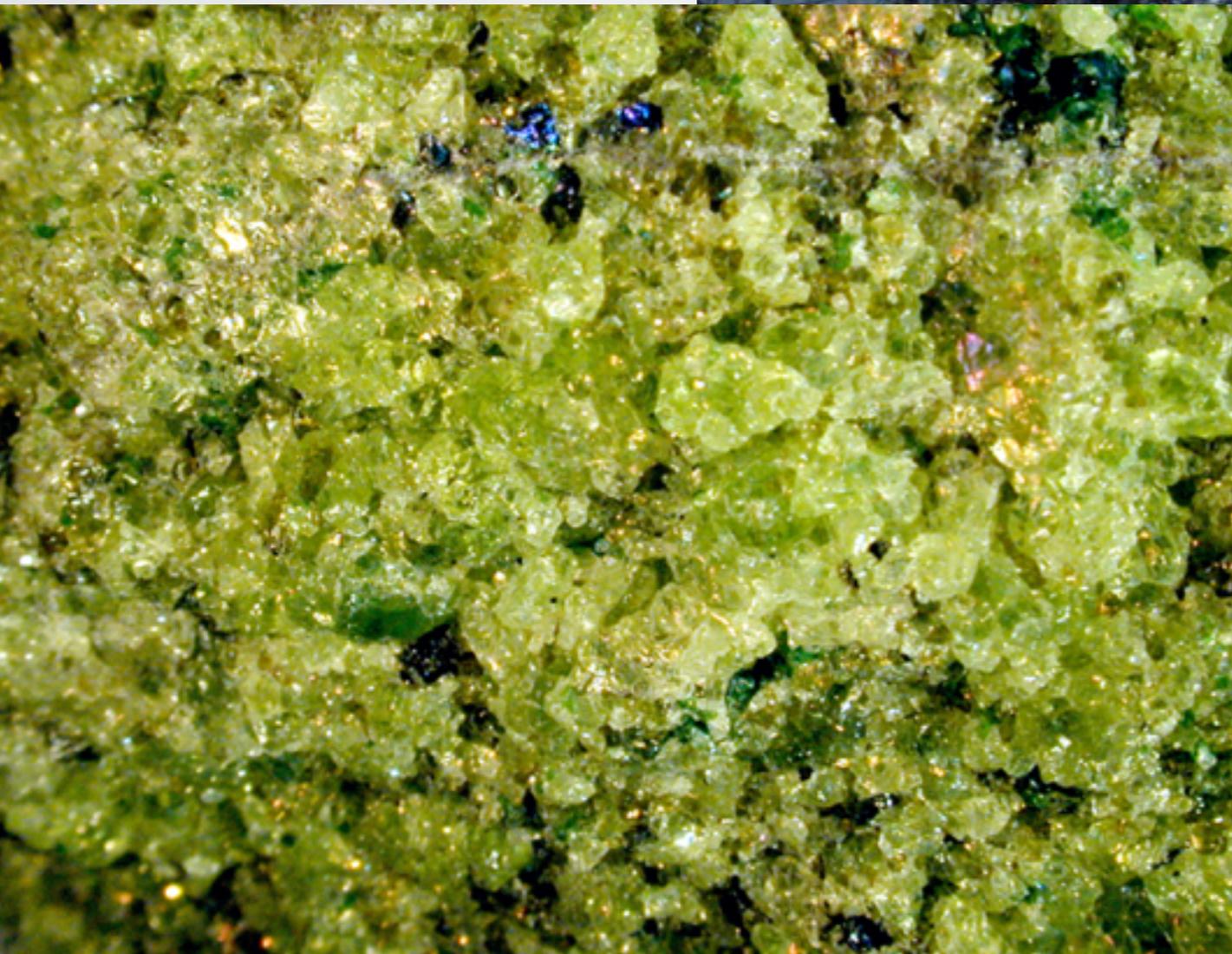
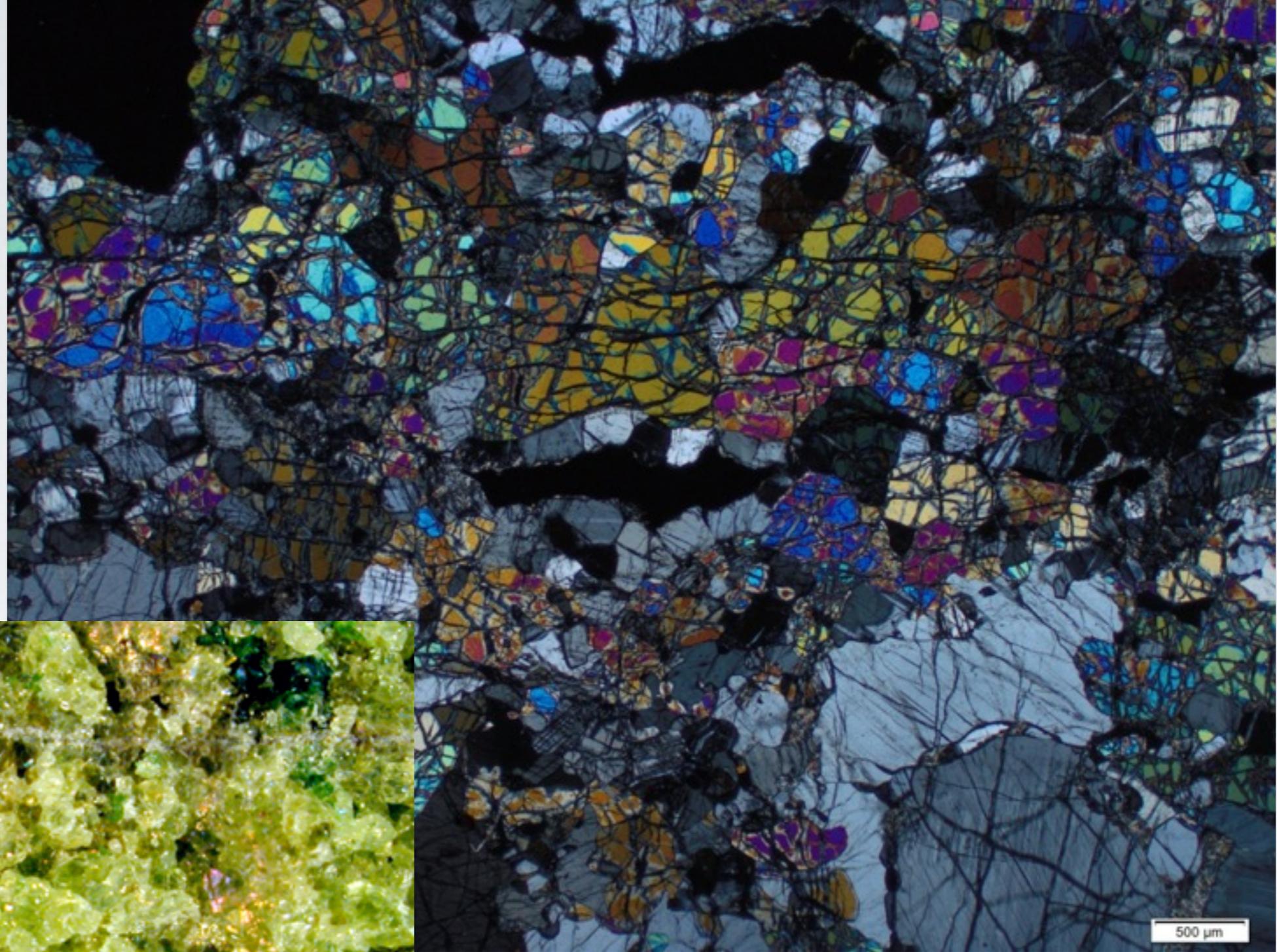


100 km depth

Today: fundamentals of defects , flow laws

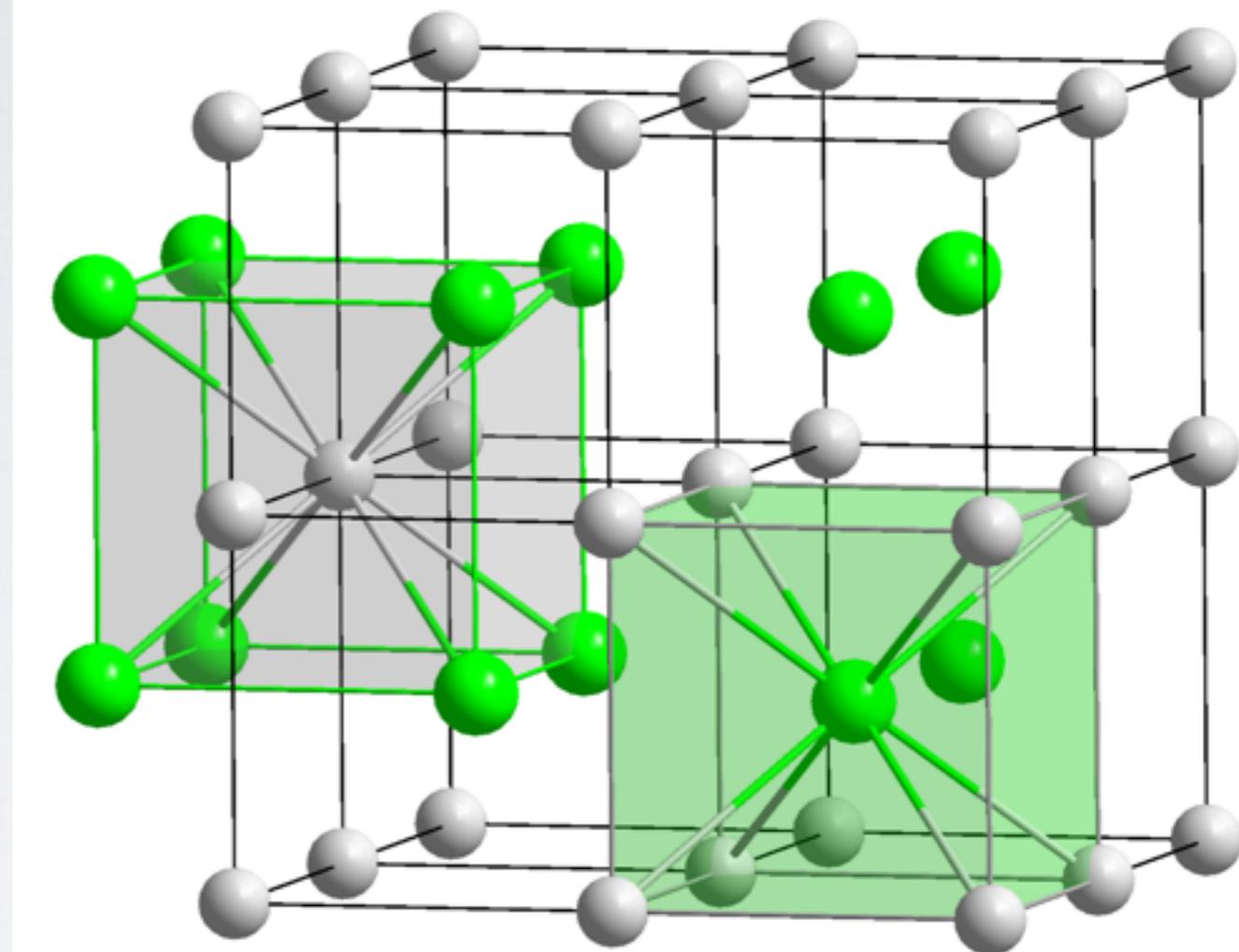
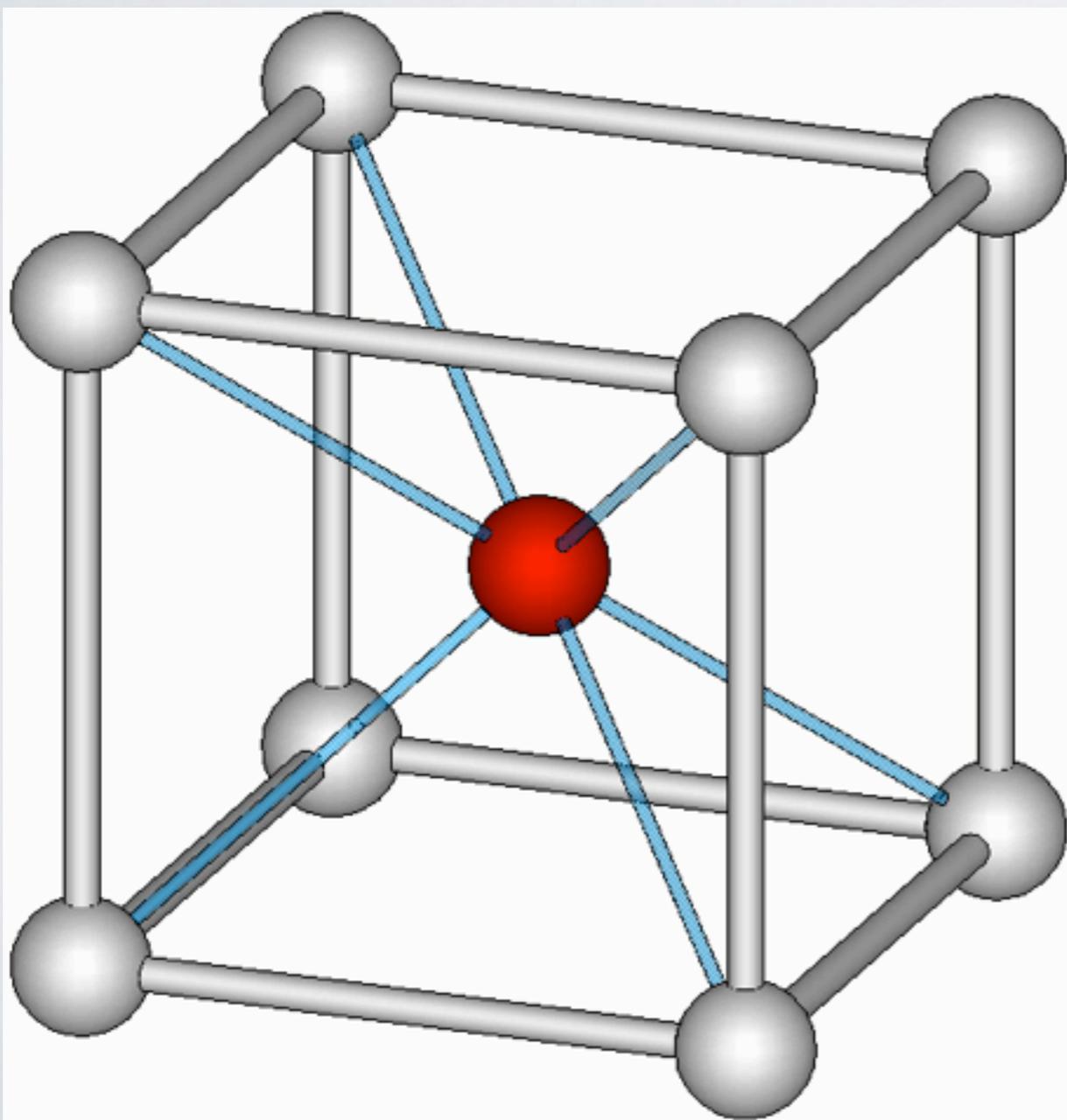
Friday: flow laws (cont.), transient creep, seismic properties & applications

cross-polarized
light image of a
peridotite

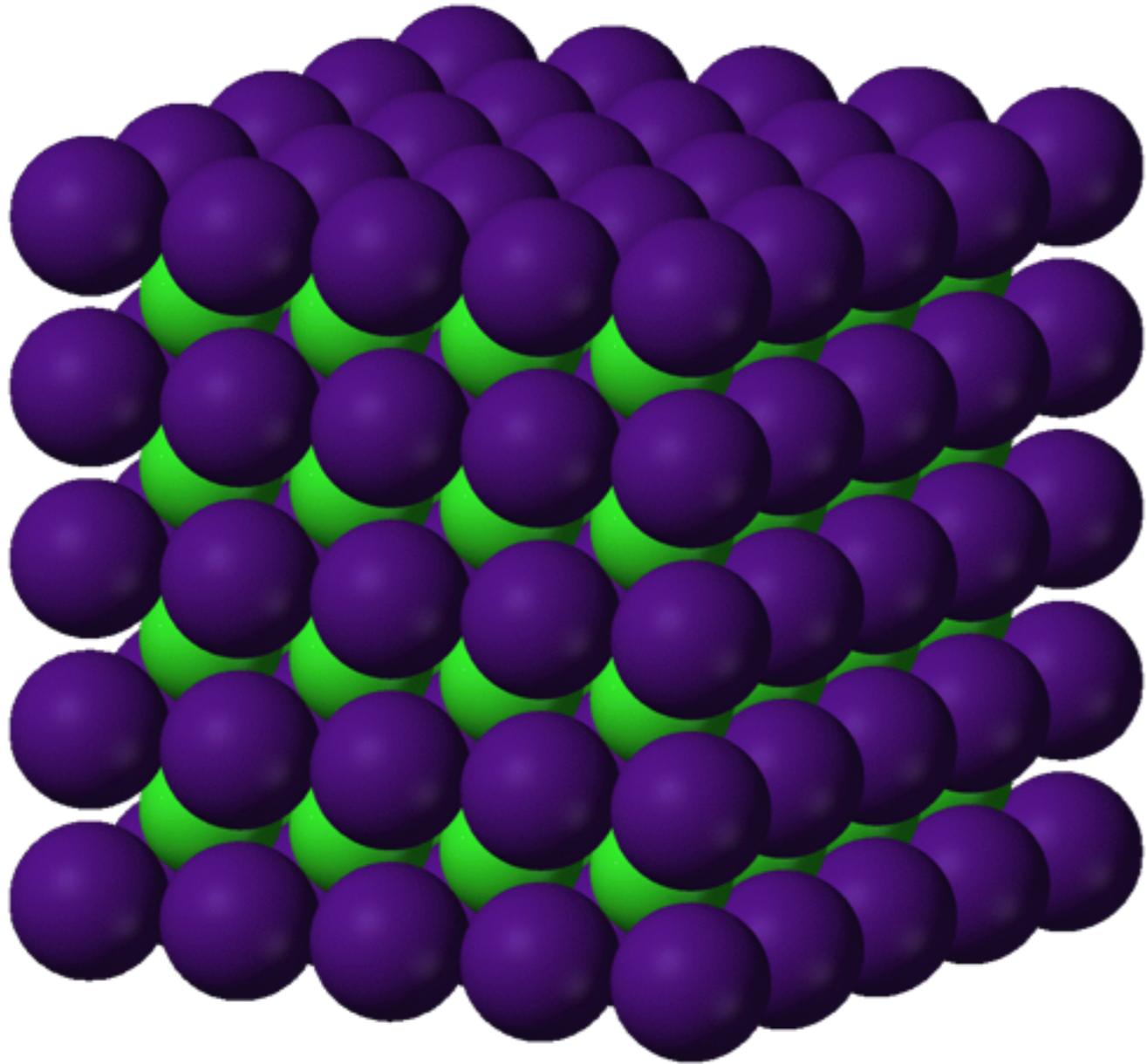


peridotite xenolith

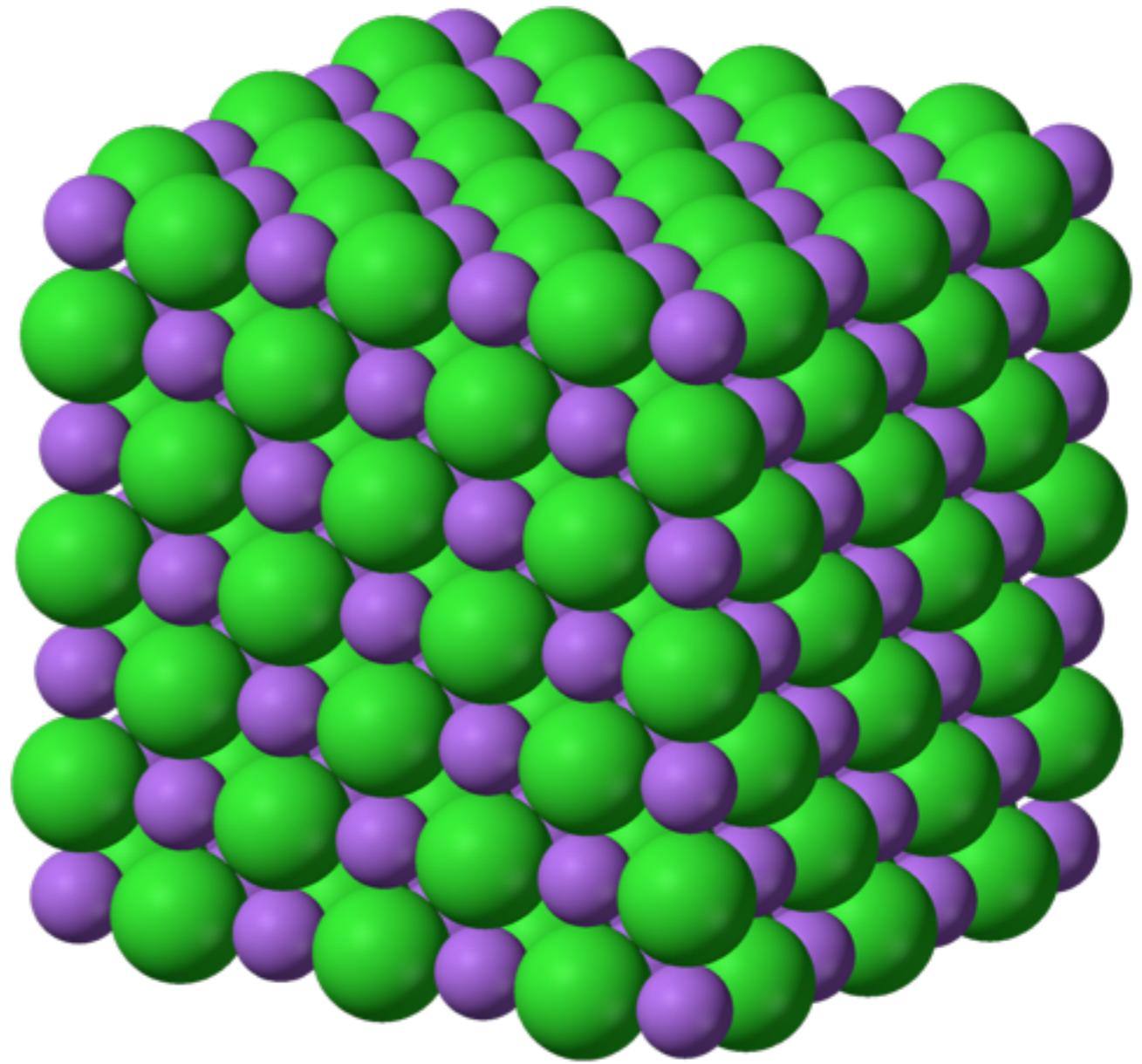
CsCl



Ionic bonding



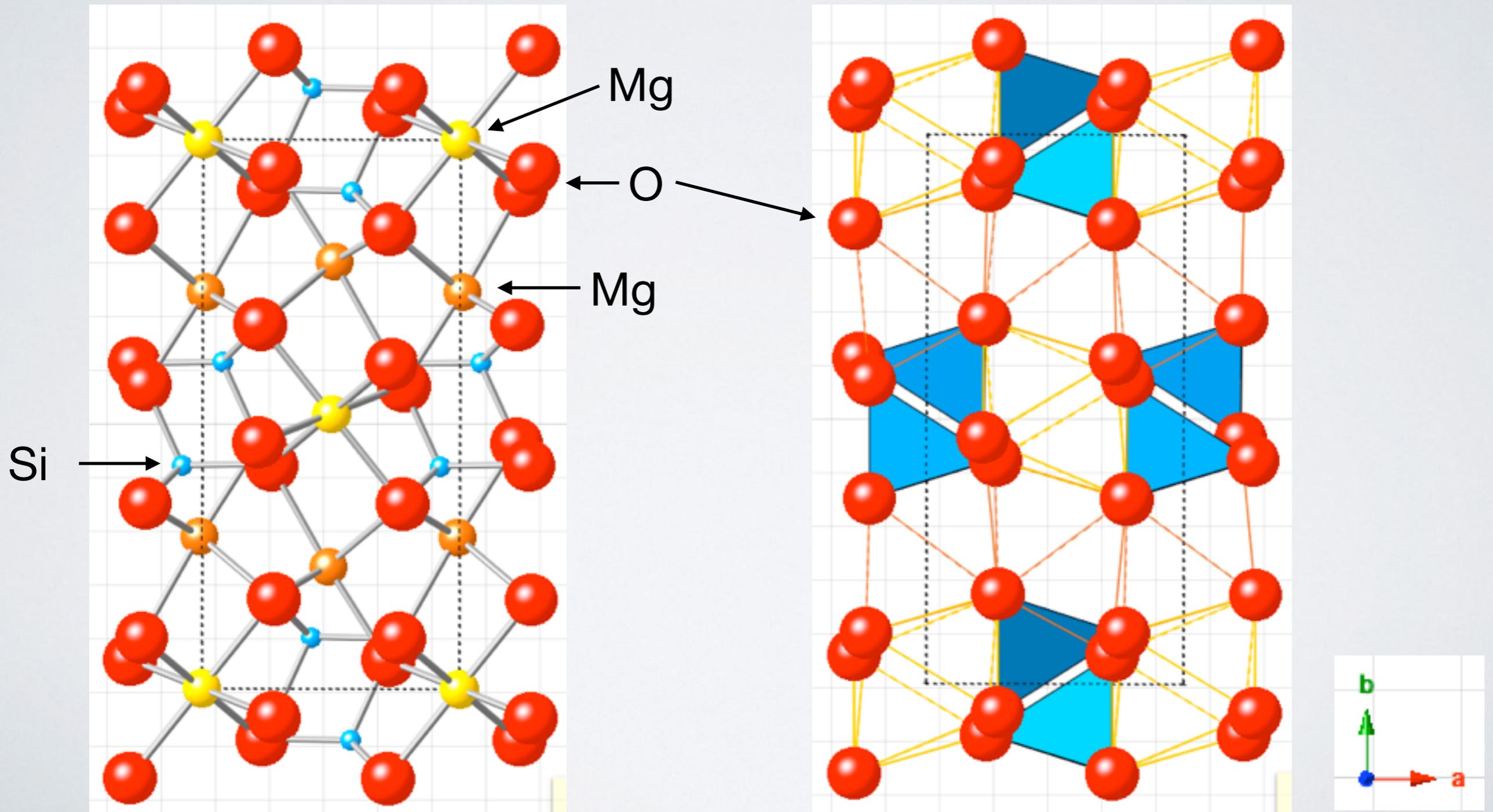
CsCl - simple cubic



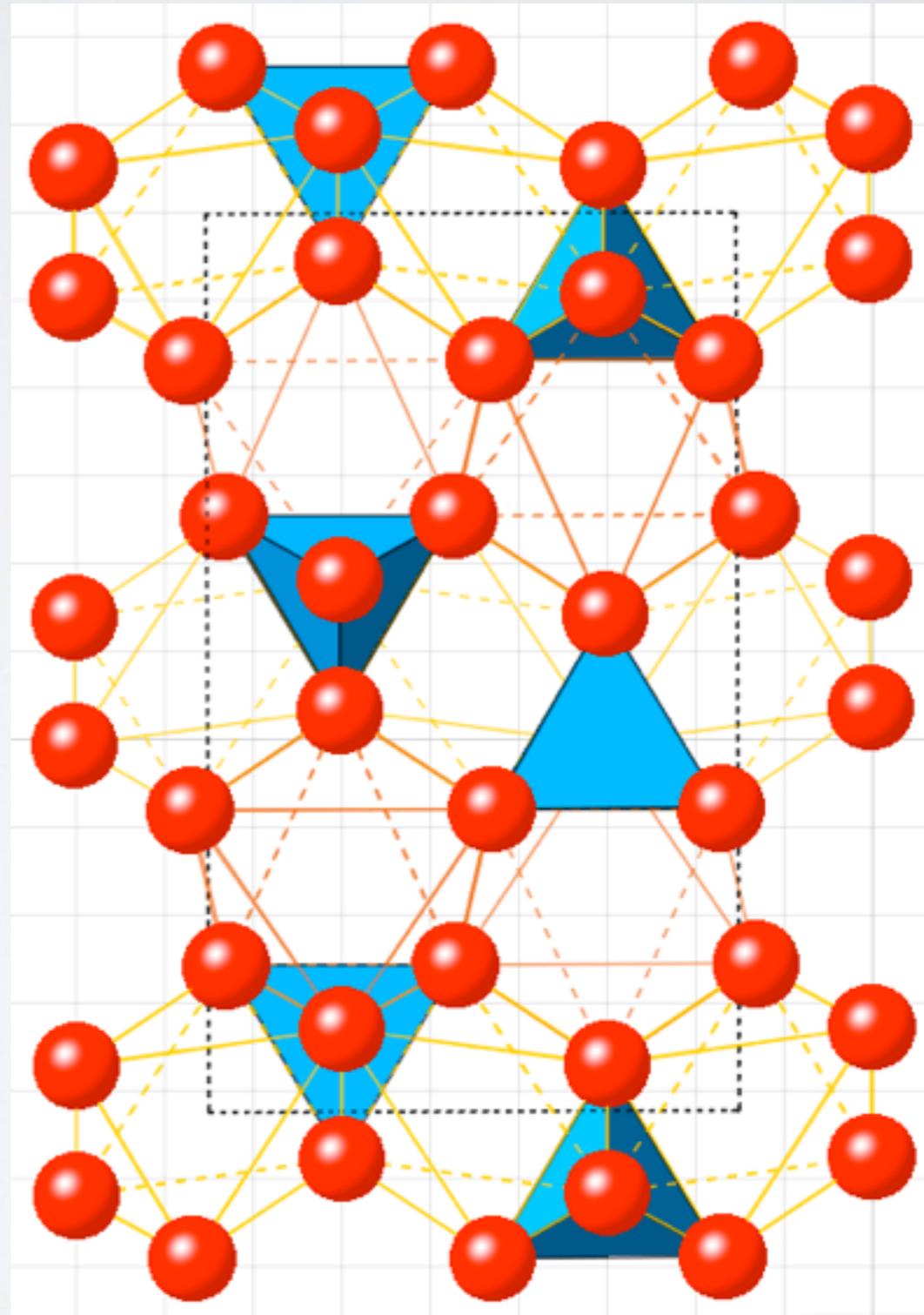
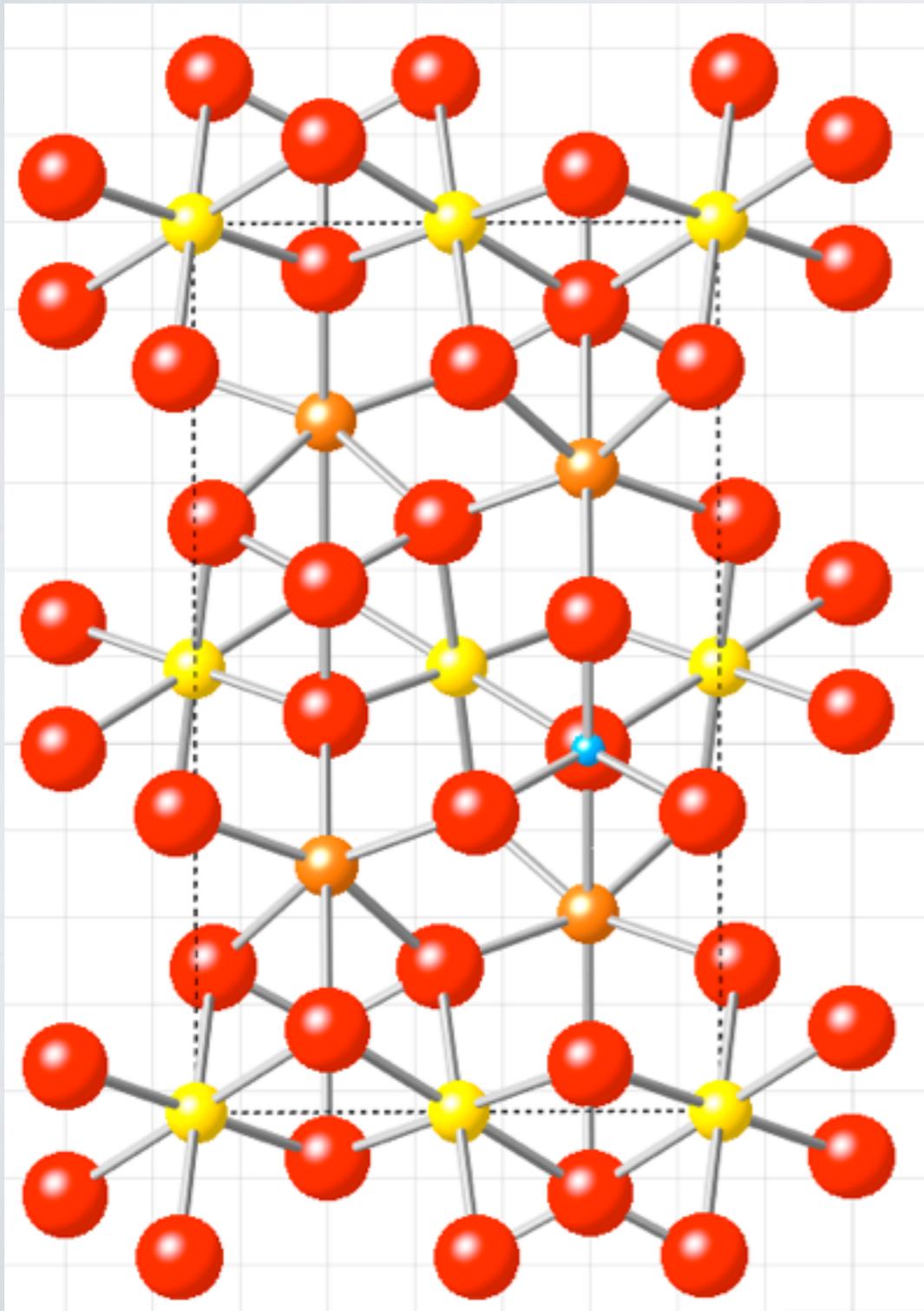
NaCl - face centered cubic

Olivine structure looking down on (001) plane.

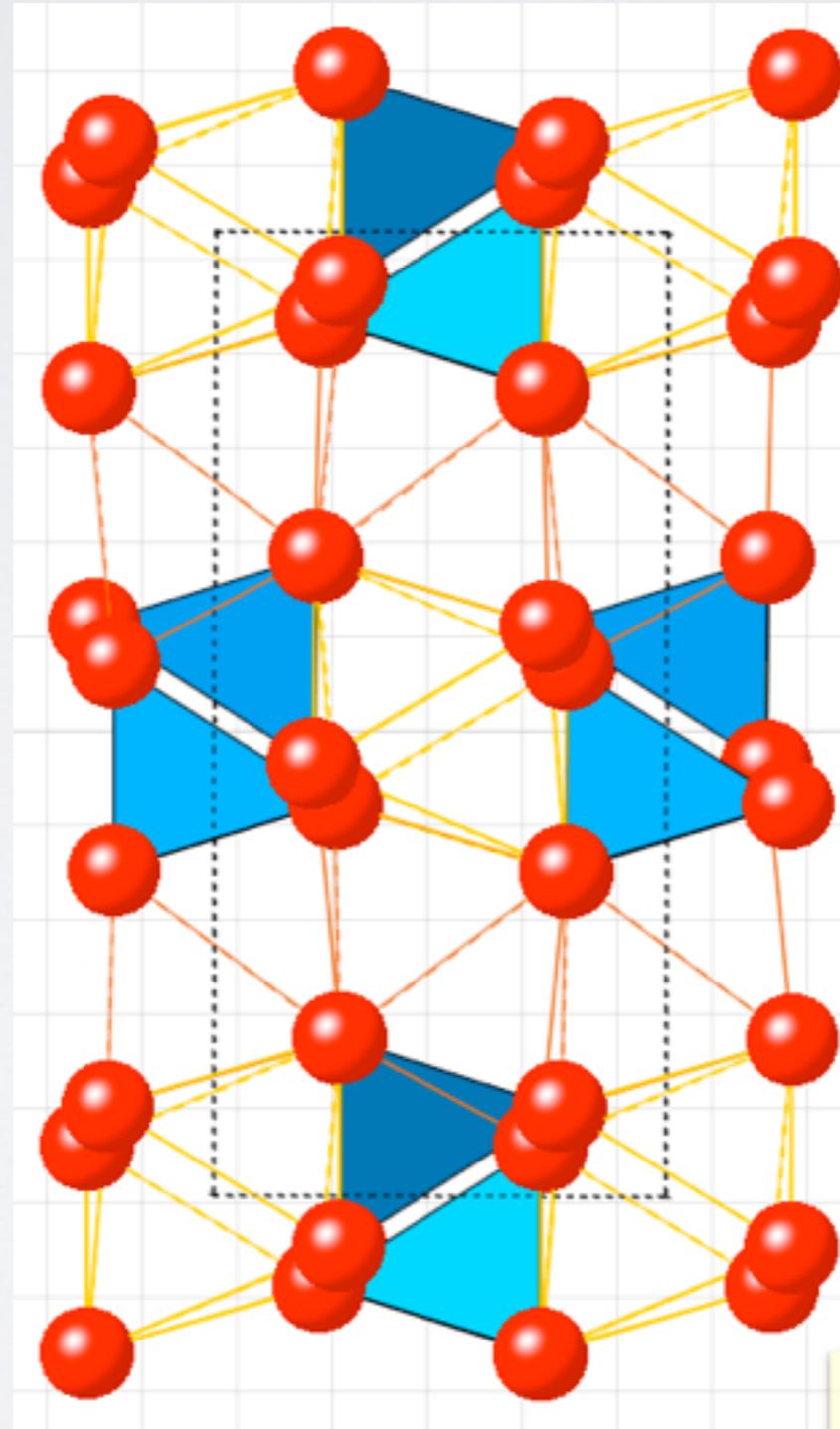
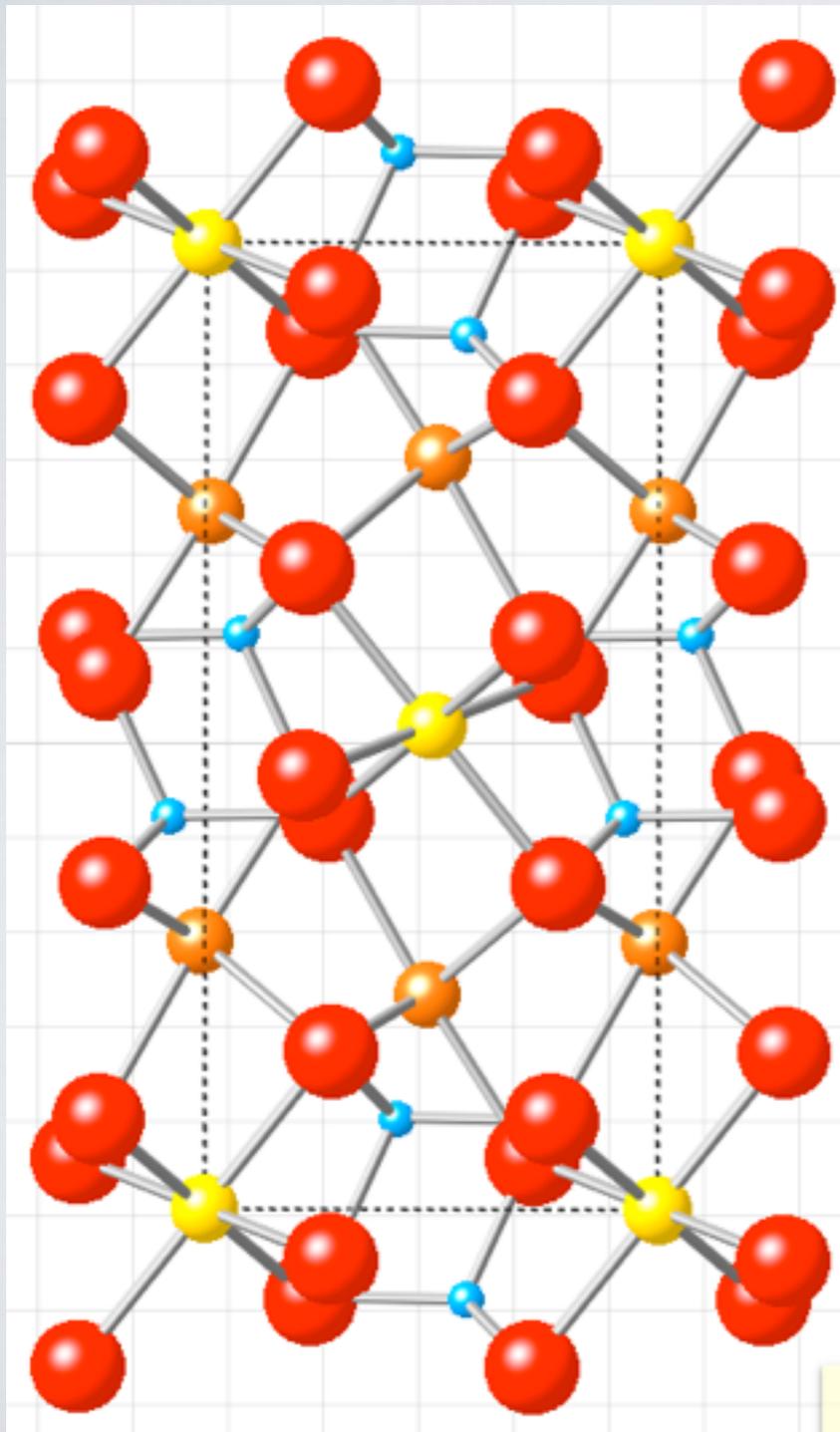
- Tetrahedrally coordinated Si, octahedrally coordinated M sites.
- Si-O bonds shortest and strongest.
- Large spacing of (010) planes and close spacing of (100) planes.



Olivine structure looking down on (100) plane.
Oxygen in (100) planes near hexagonal close-packed arrangement.



Anisotropy due to crystal structure

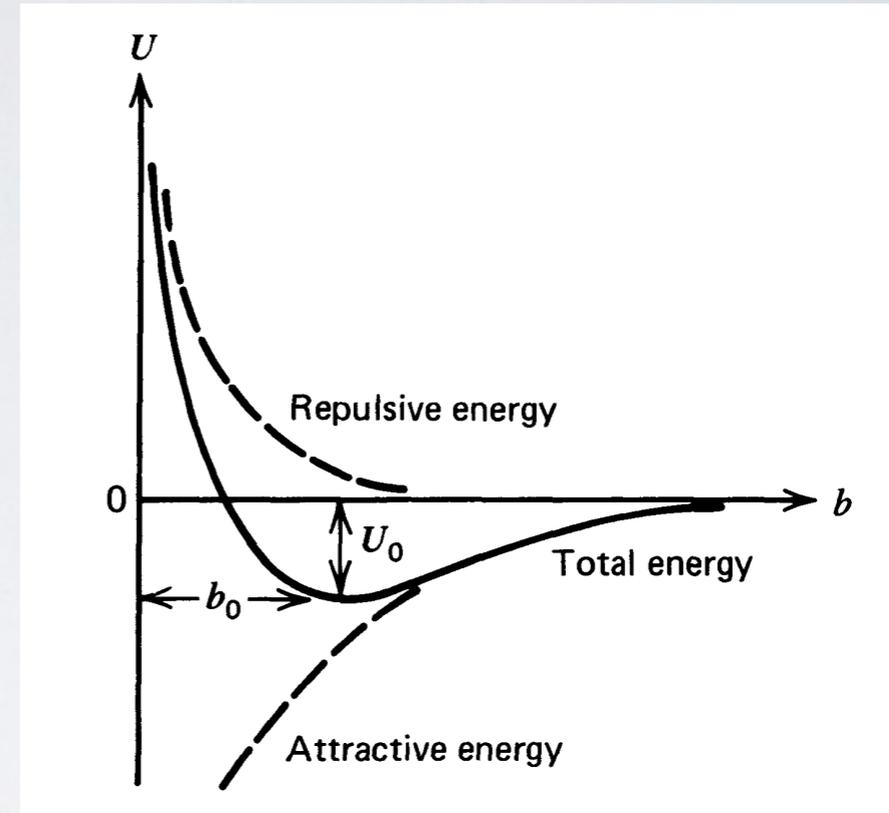
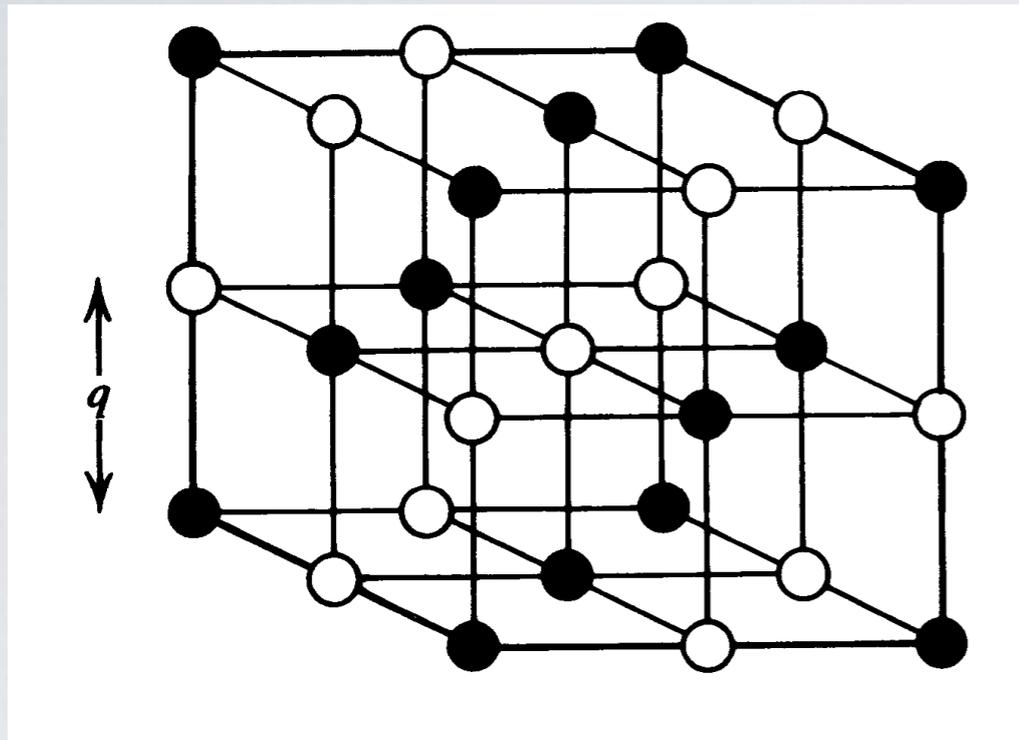


	a	b	c
unit cell dim. (Å)	4.78	10.25	6.3
V	9.89	7.72	8.43
V	4.89	4.42	4.87

$$V_s(\text{max}) = 5.53 \text{ km/s}$$



Elastic behavior: Solids



Unique equilibrium position of atoms in crystal lattice
displacement from that position requires force: elastic moduli

$$\text{e.g. } \sigma = E \varepsilon$$

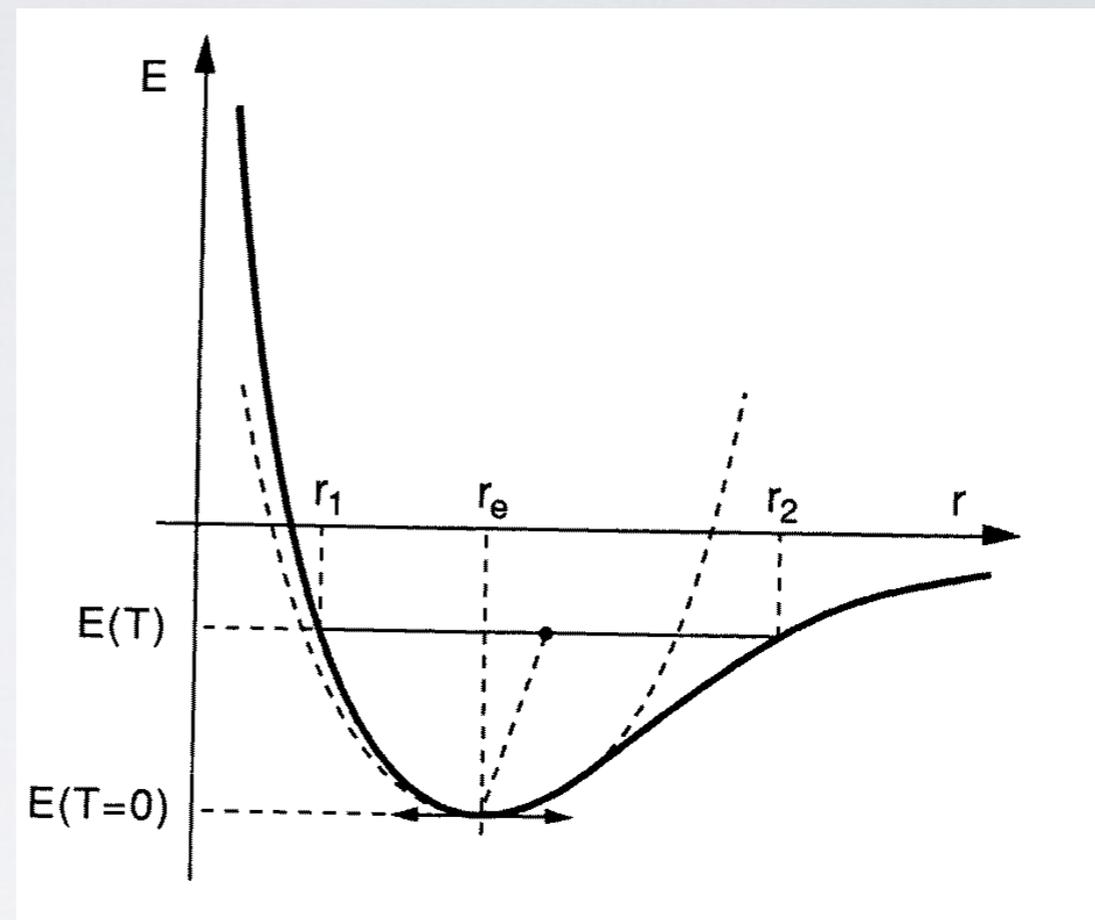
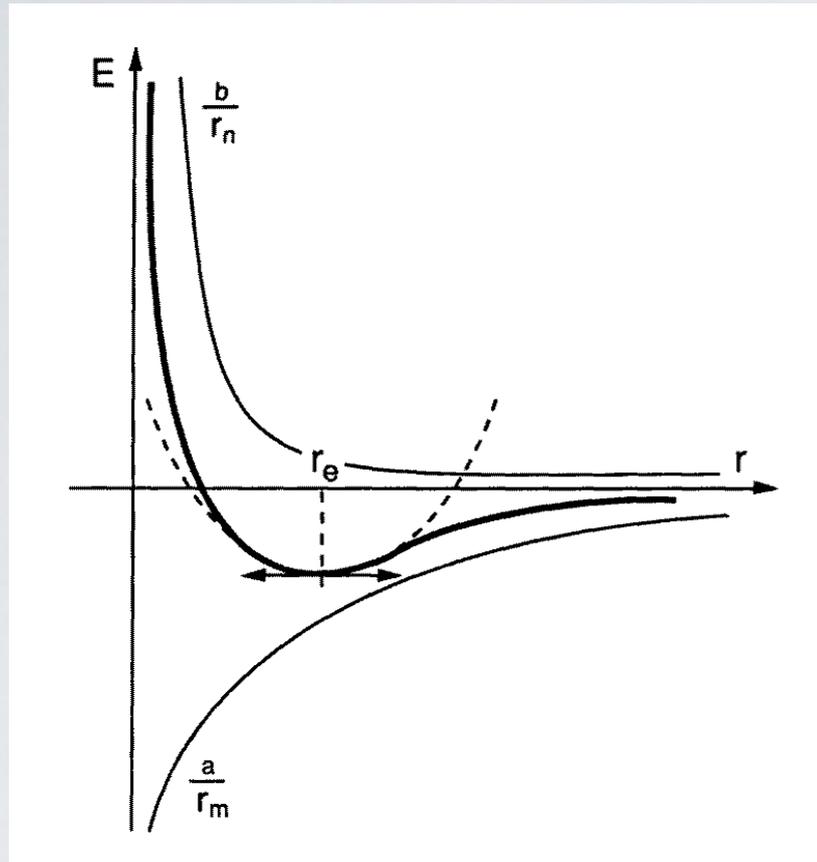
E Young's modulus (tensile deformation, linear strain)

K bulk modulus (uniform compression)

G shear modulus (rigidity, shear deformation)

Elastic moduli are of orders 10s of GPa

Harmonic vs anharmonic behavior



Finite T : thermal energy of atoms results in vibrations of atoms about equilibrium positions. This energy must be supplied as specific heat to raise the temperature.

Low T : vibrational amplitudes will be very small and approximately symmetric (sinusoidal) about the equilibrium positions (left).

High T : large asymmetric (i.e. non-sinusoidal or anharmonic) vibrations will be excited corresponding to states higher in the well (right).

Asymmetry of the vibration is such that the **bond length** averaged over one cycle of vibration is now greater than the equilibrium spacing.

This temperature-dependent increase in average bond length is **thermal expansion**.

Thermodynamics *(Fundamental state functions)*

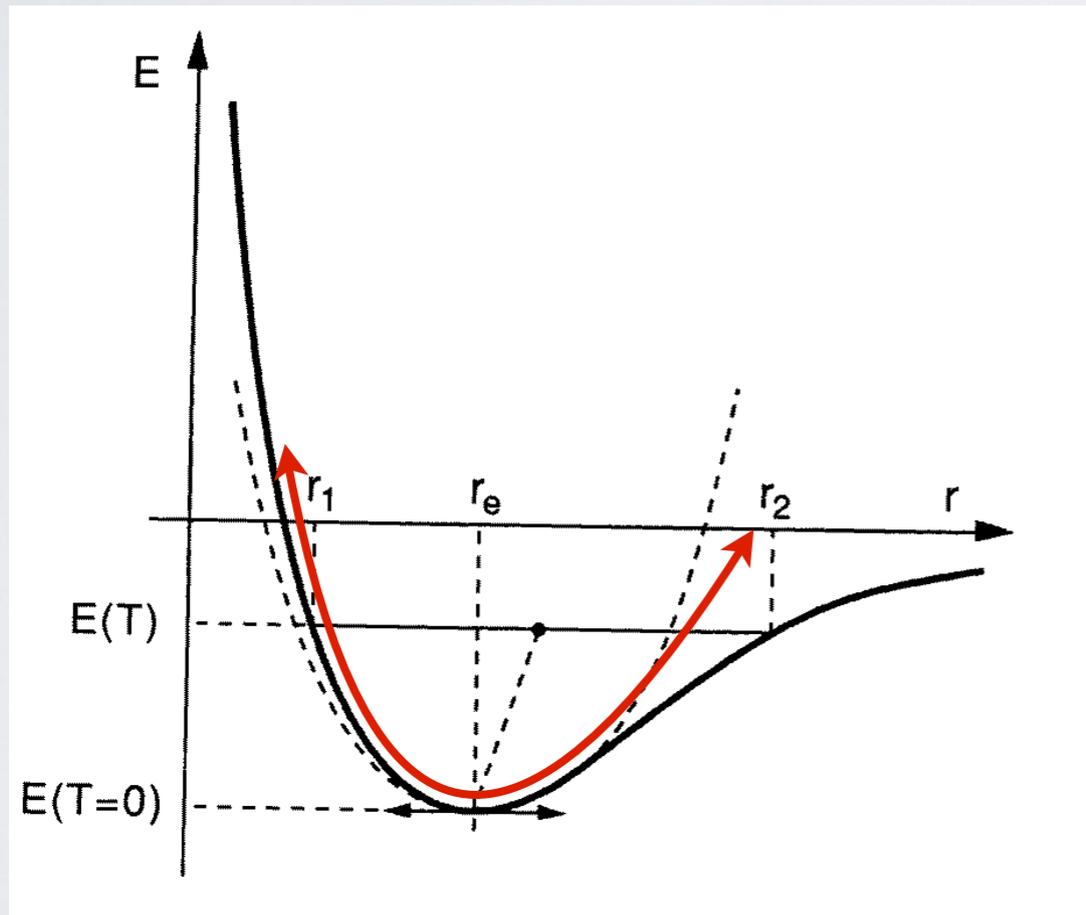
Internal energy U: Energy content of a system, the sum of the potential energy stored in interatomic bonding (electrostatic energy) plus the kinetic energy of atomic vibrations.



Temperature

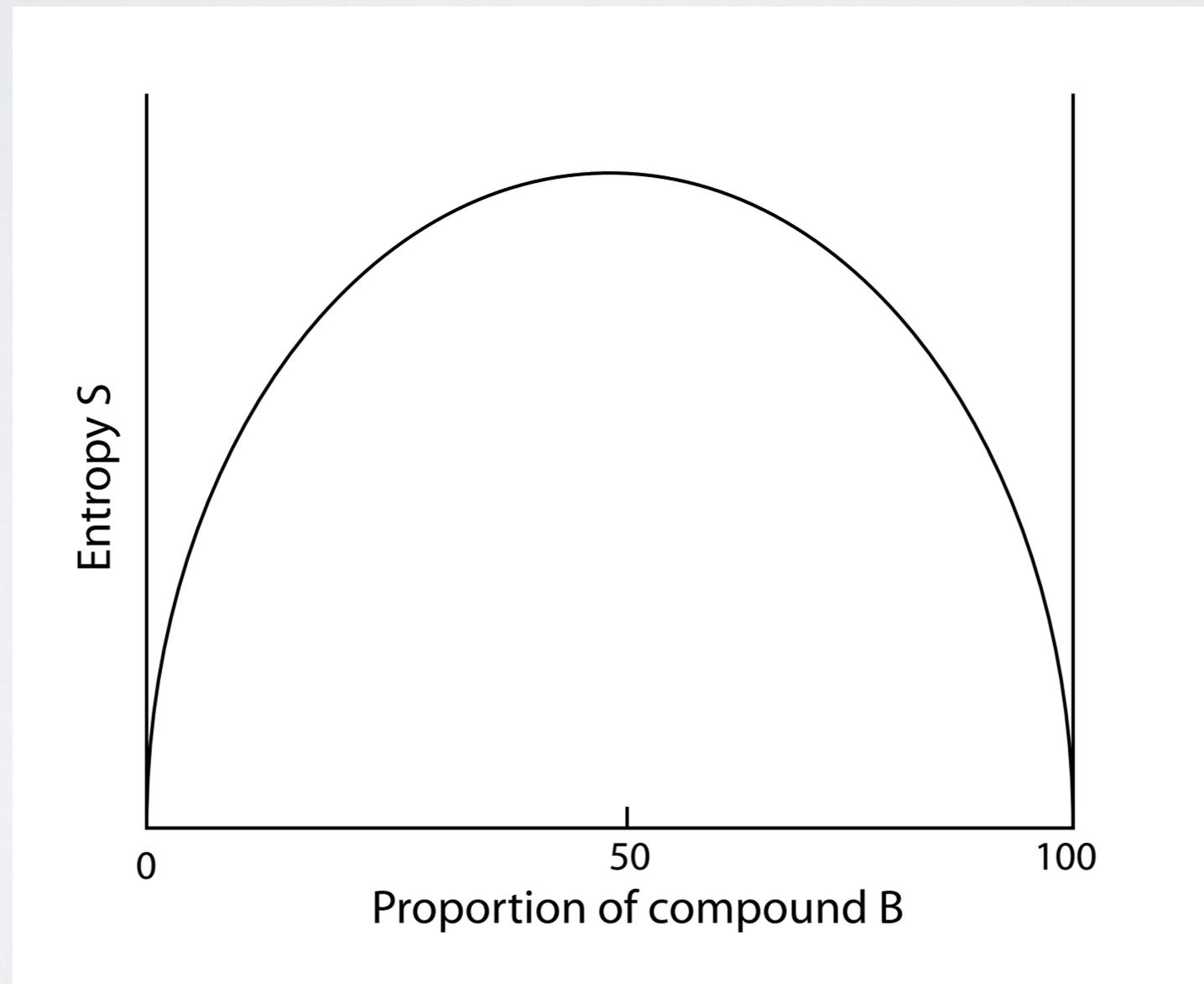
In the Earth need to account for pressure:

Enthalpy: $H = U + PV$



Entropy S: measure of the state of disorder in a system.

Example: Configurational entropy:
Entropy is at a maximum for $X_B = X_A$



Deformation:
stress = modulus x strain

$$\sigma = E \varepsilon$$

(Hooke's law)



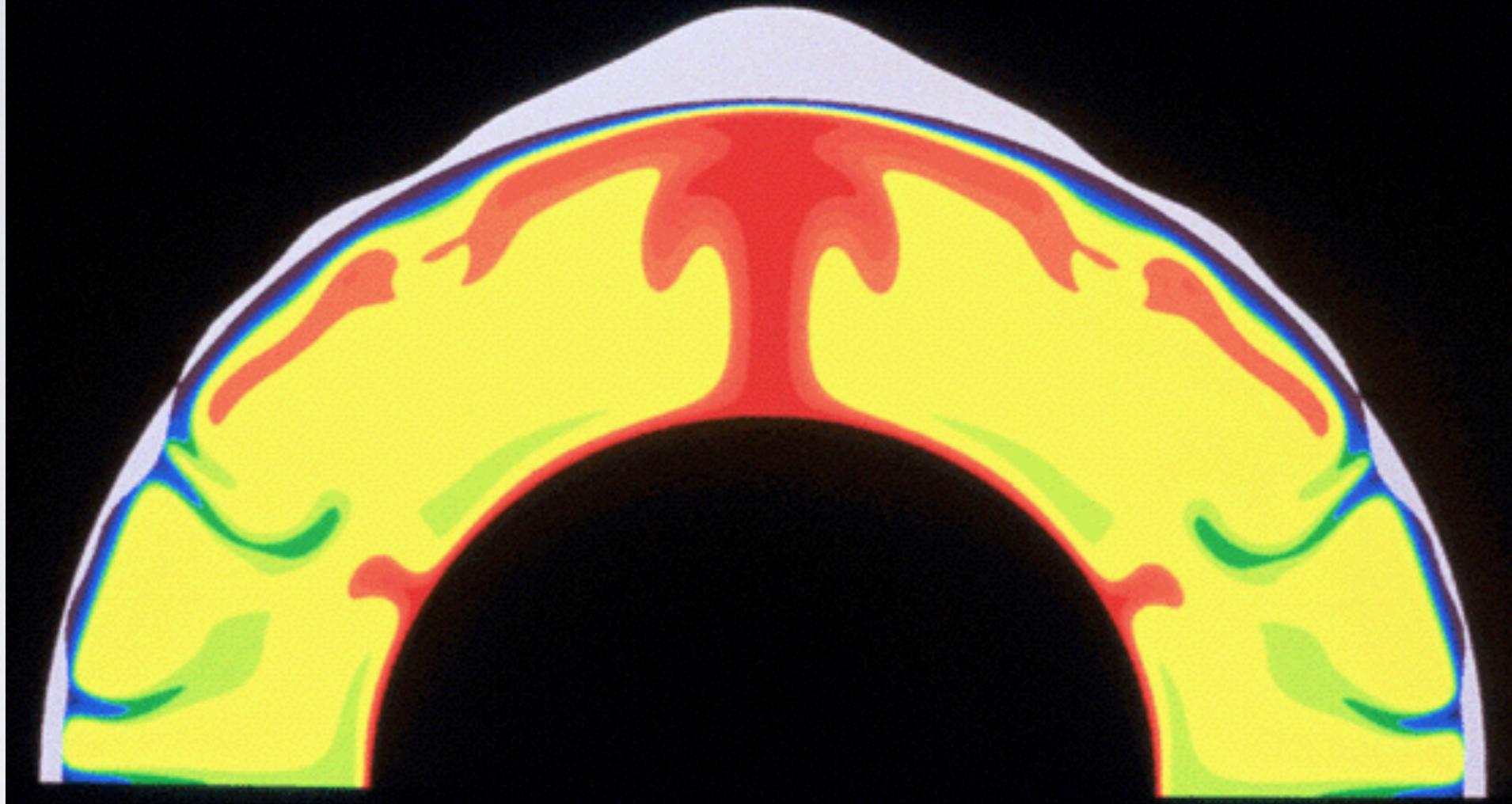
$$E \sim 10 \text{ GPa} = 10^{10} \text{ Pa (ice)},$$
$$\varepsilon \sim 1$$

flow of ice due to gravity:

$P = \text{density} \times g \times \text{thickness}$

$$= 1000 \text{ kg/m}^3 \times 10 \text{ m/s}^2 \times 1000 \text{ m} = 10^7 \text{ Pa}$$

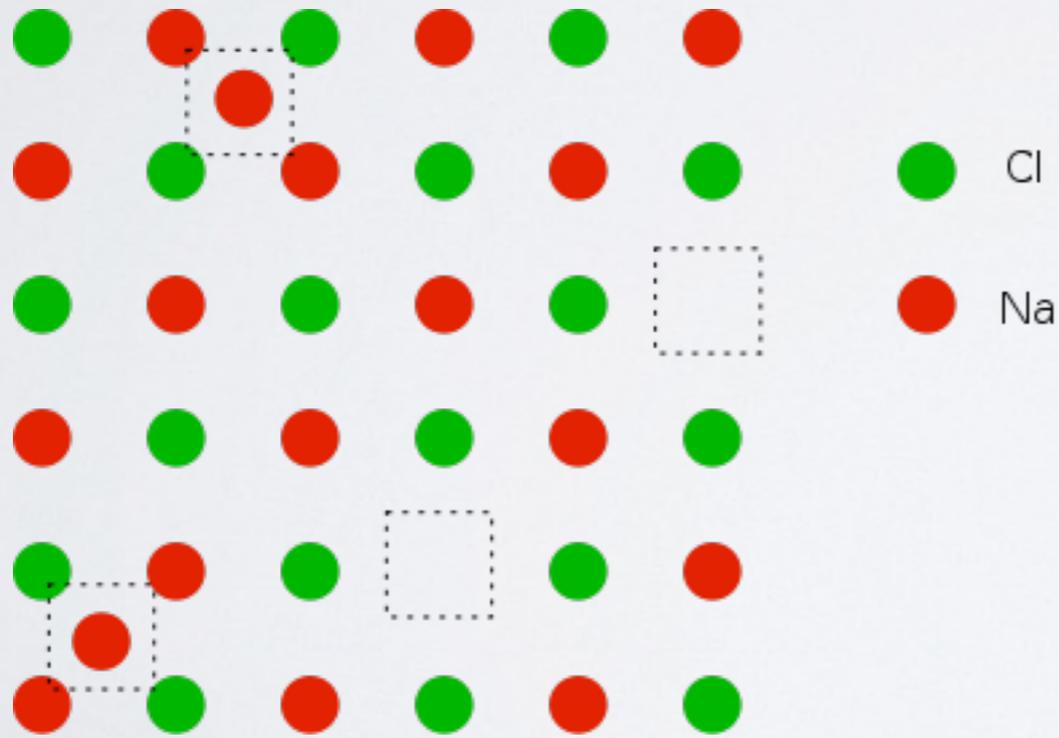
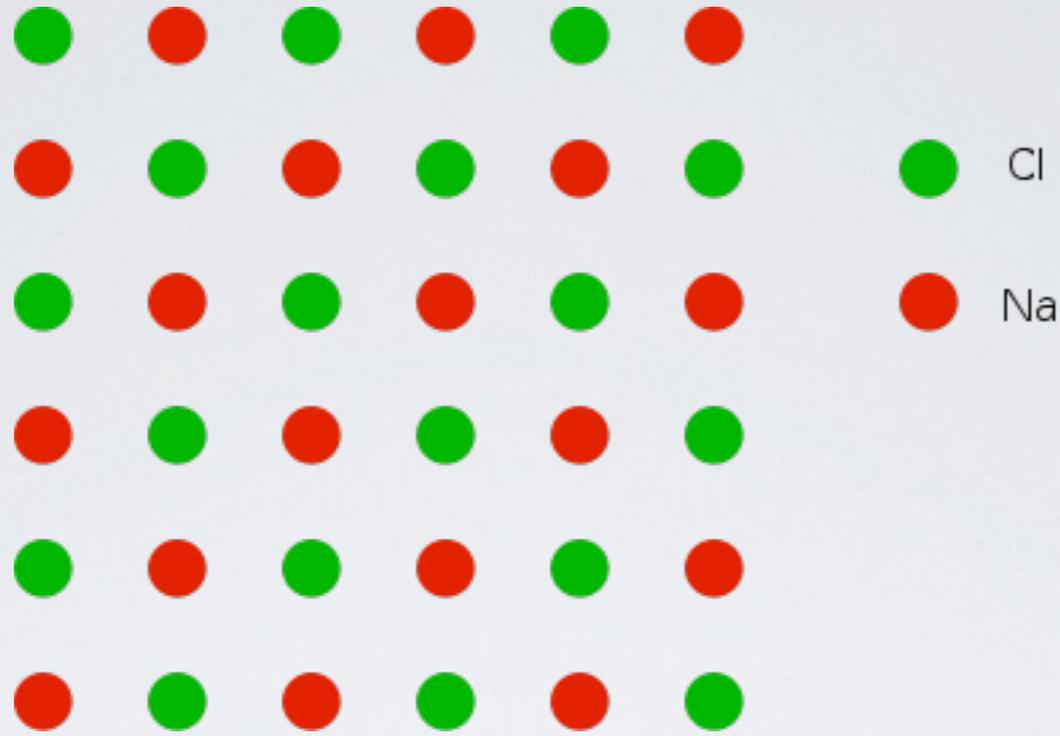
MANTLE CONVECTION SIMULATION



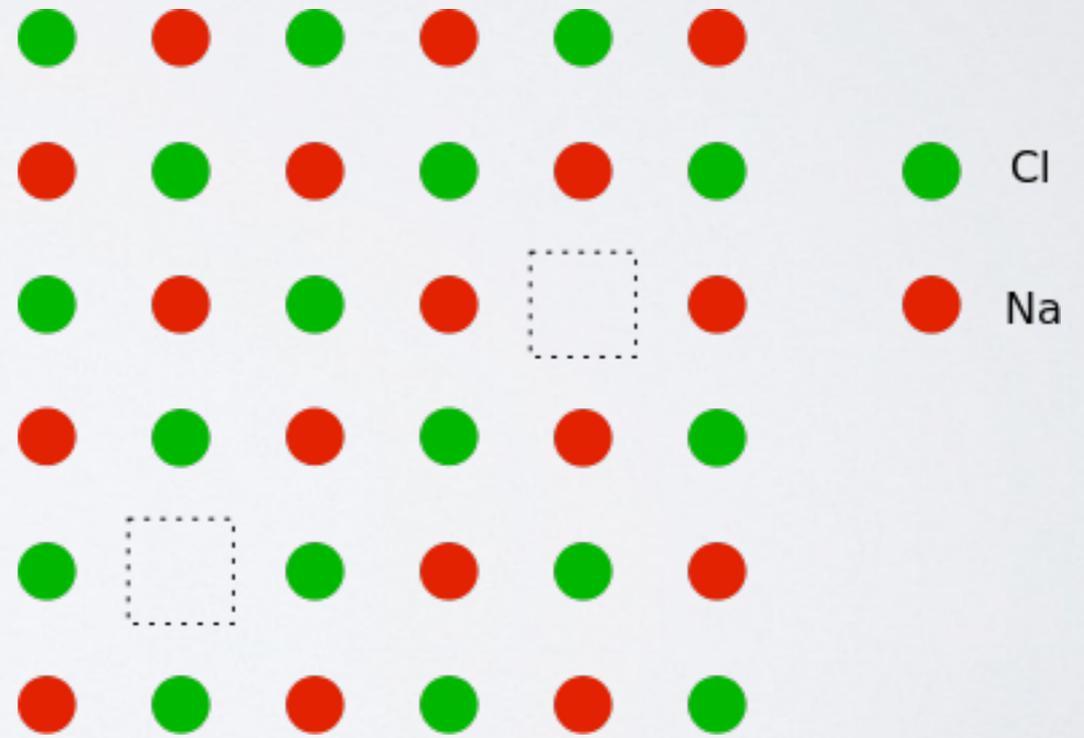
moduli of rock-forming minerals of order of 100 GPa
convective stresses ~ 0.1 MPa

Defects!

(point defects)

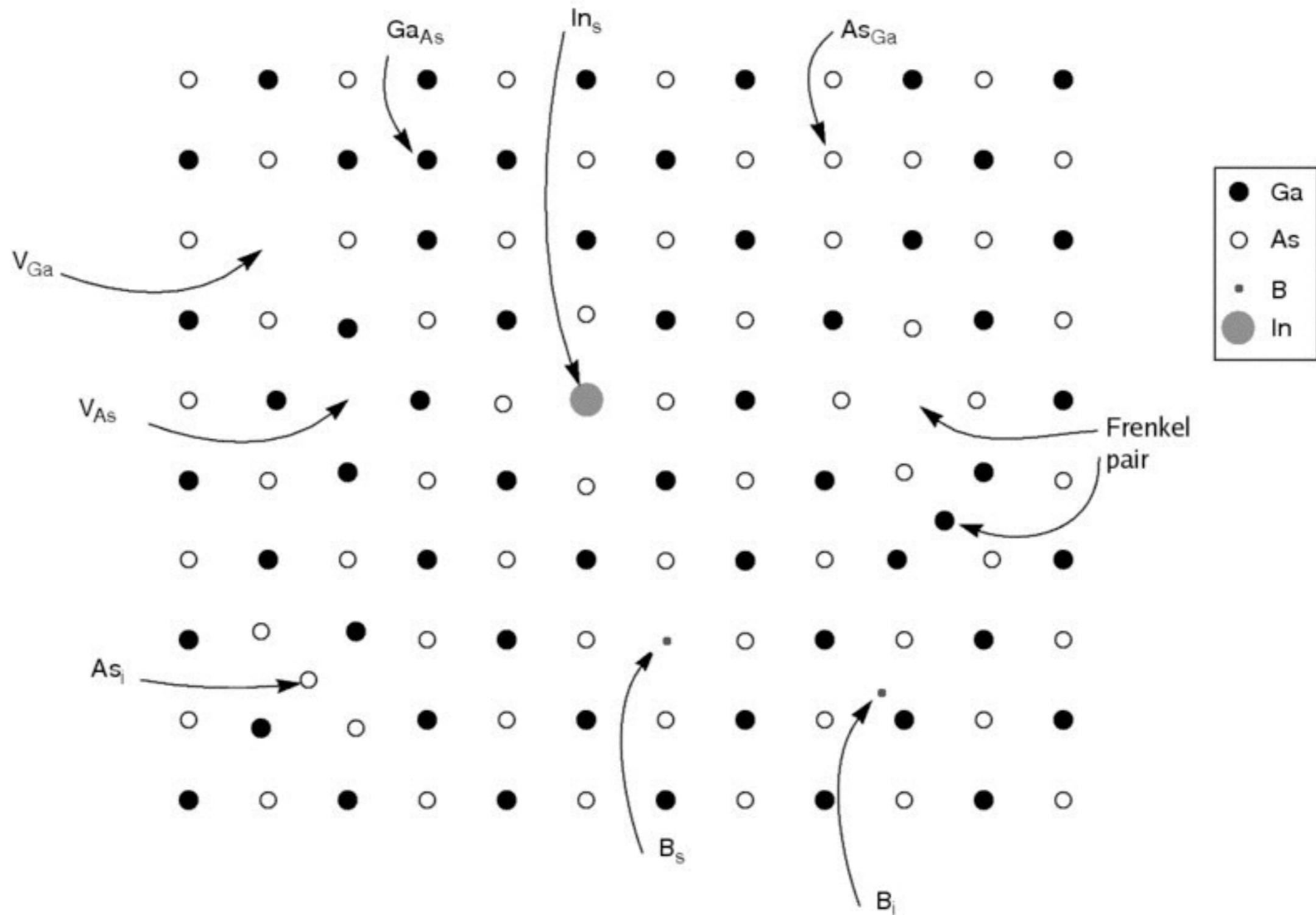


Frenkel



Schottky

defects can also be impurity atoms



Thermodynamically why do we have defects?

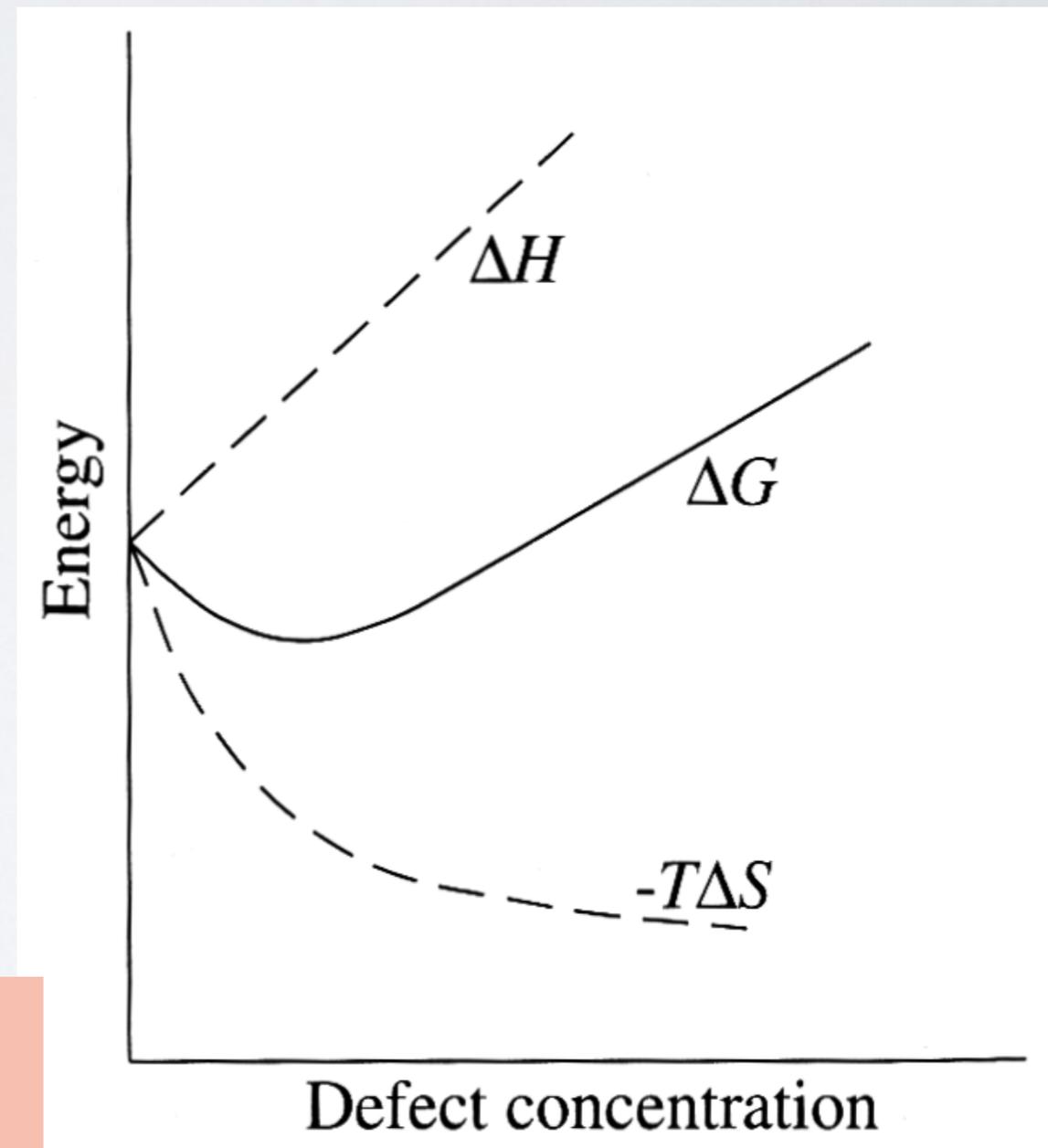
Creation of point defect requires energy:
local distortion of lattice + imperfect satisfaction of bonding
→ enthalpy H increases.

But: point defect increases disorder in
an otherwise perfect crystal:
entropy S increases.

(S is associated with the number of ways to
distribute defects within the crystal structure.)

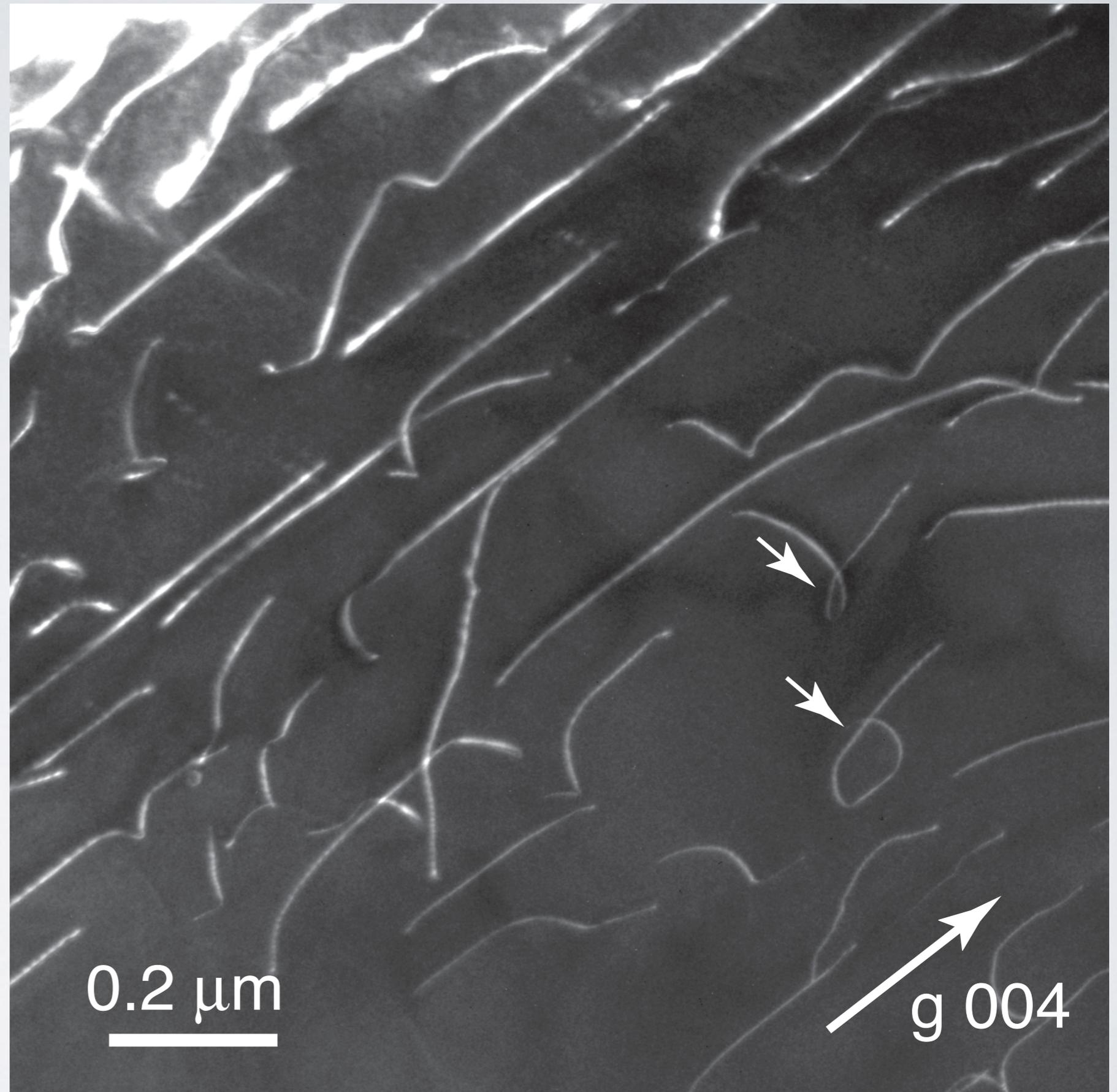
For small defect concentrations entropy
increase is *greater* than enthalpy
increase, for larger defect
concentrations enthalpy increase
dominates:

Minimum in Gibbs free energy at some
finite concentration of point defects!



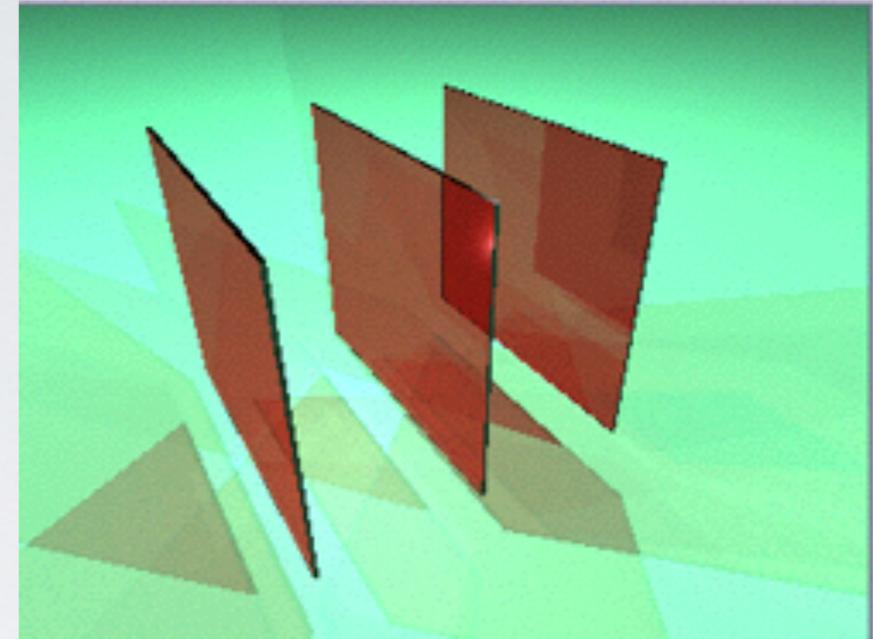
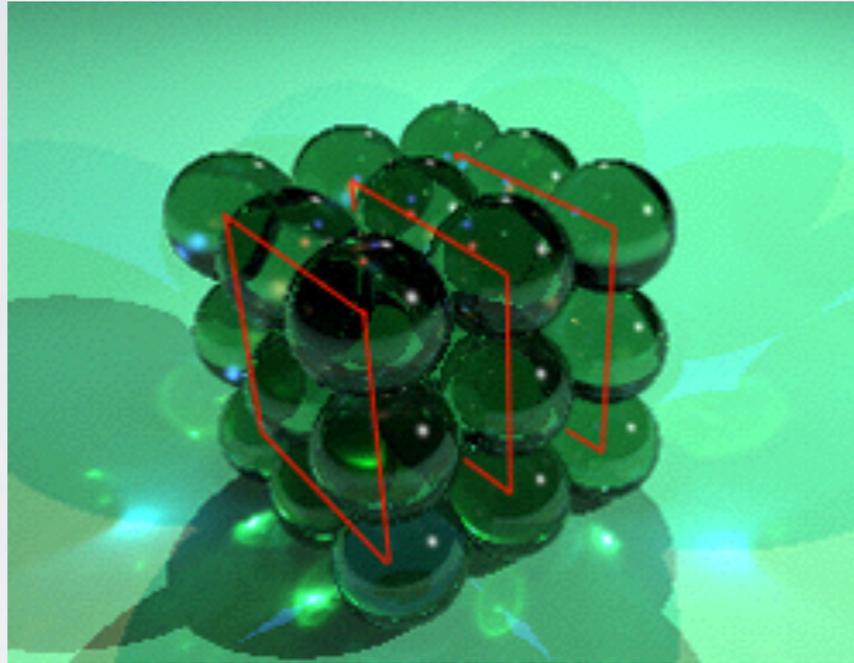
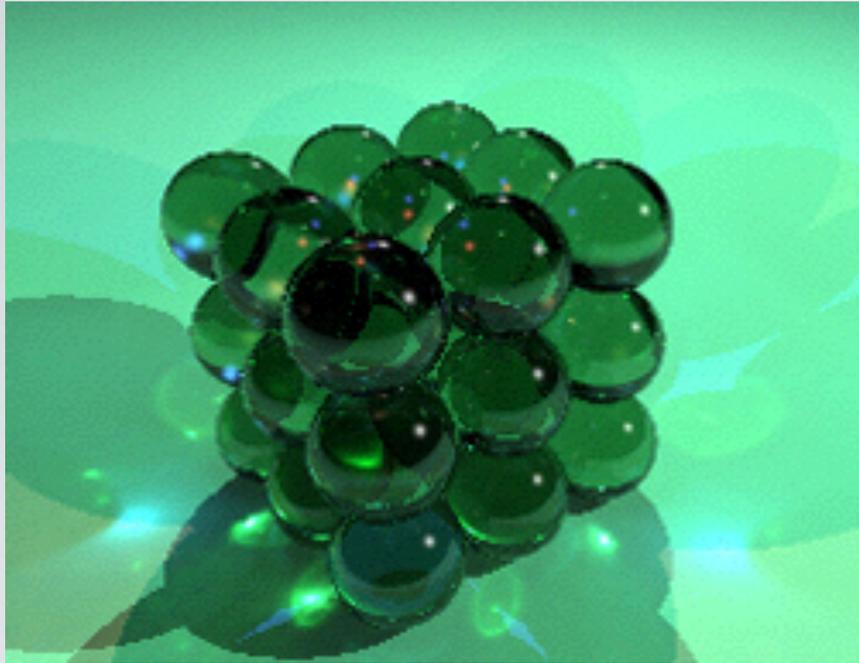


Dislocations
-line defects

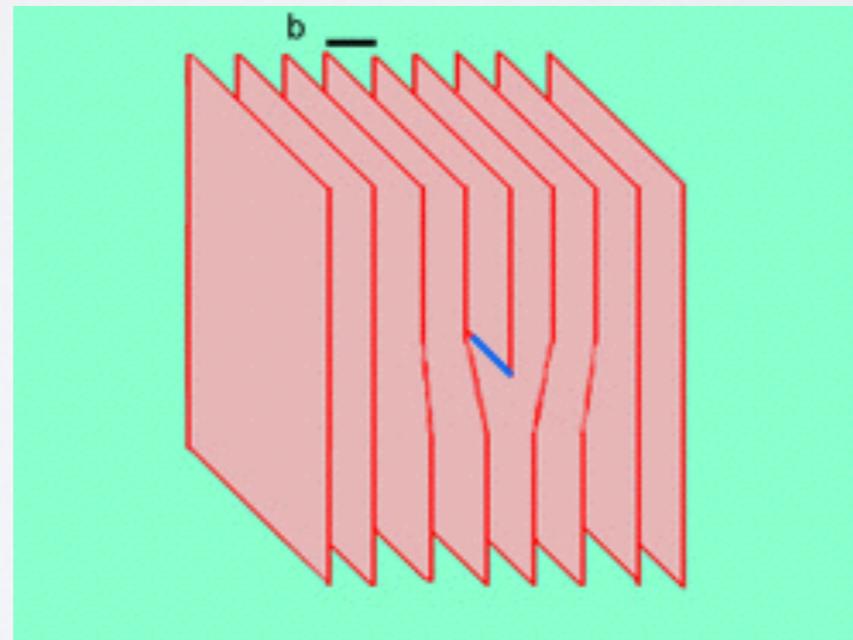


Transmission electron microscope image of screw dislocations in olivine

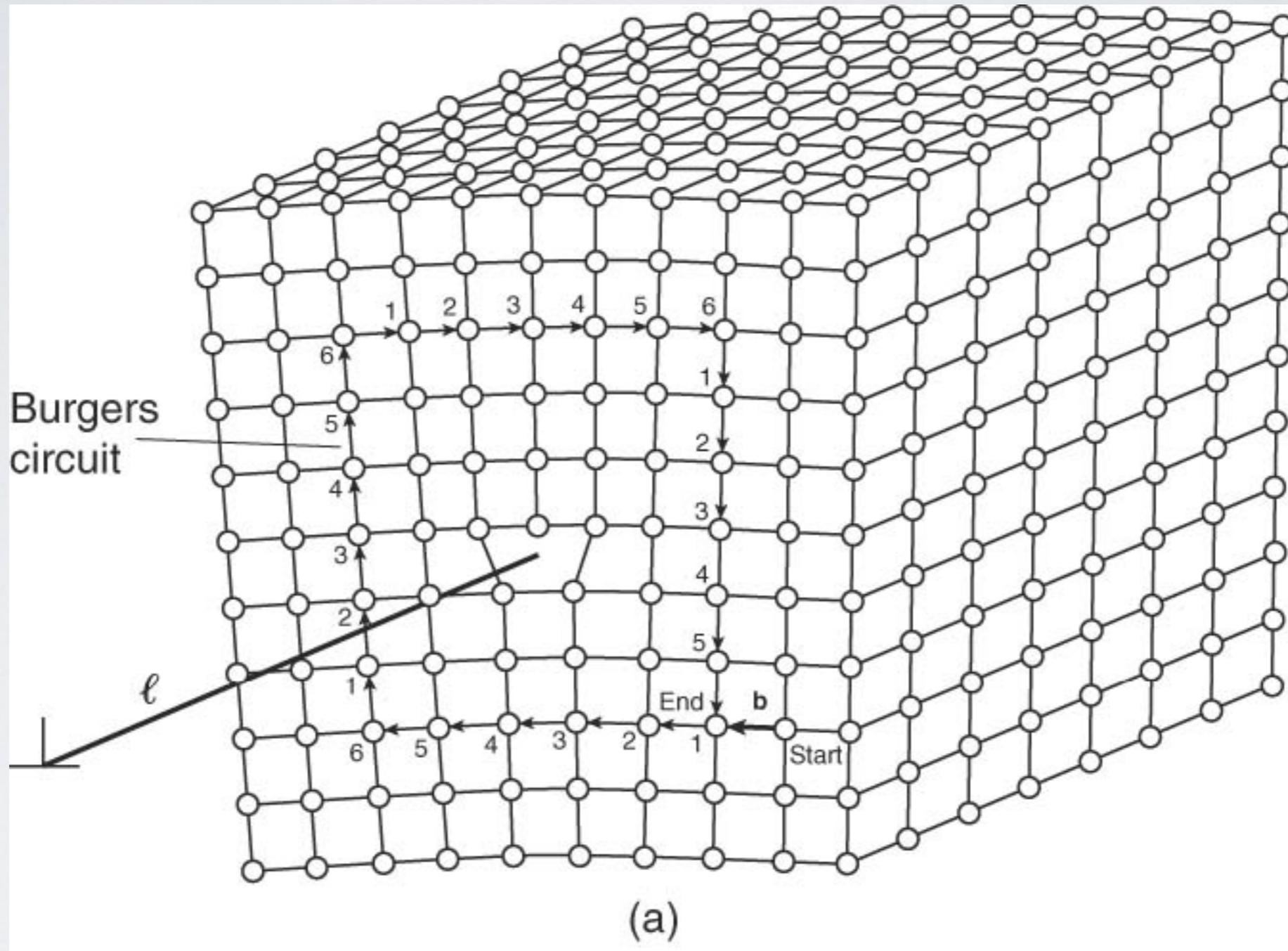
Lattice planes in a cubic crystal



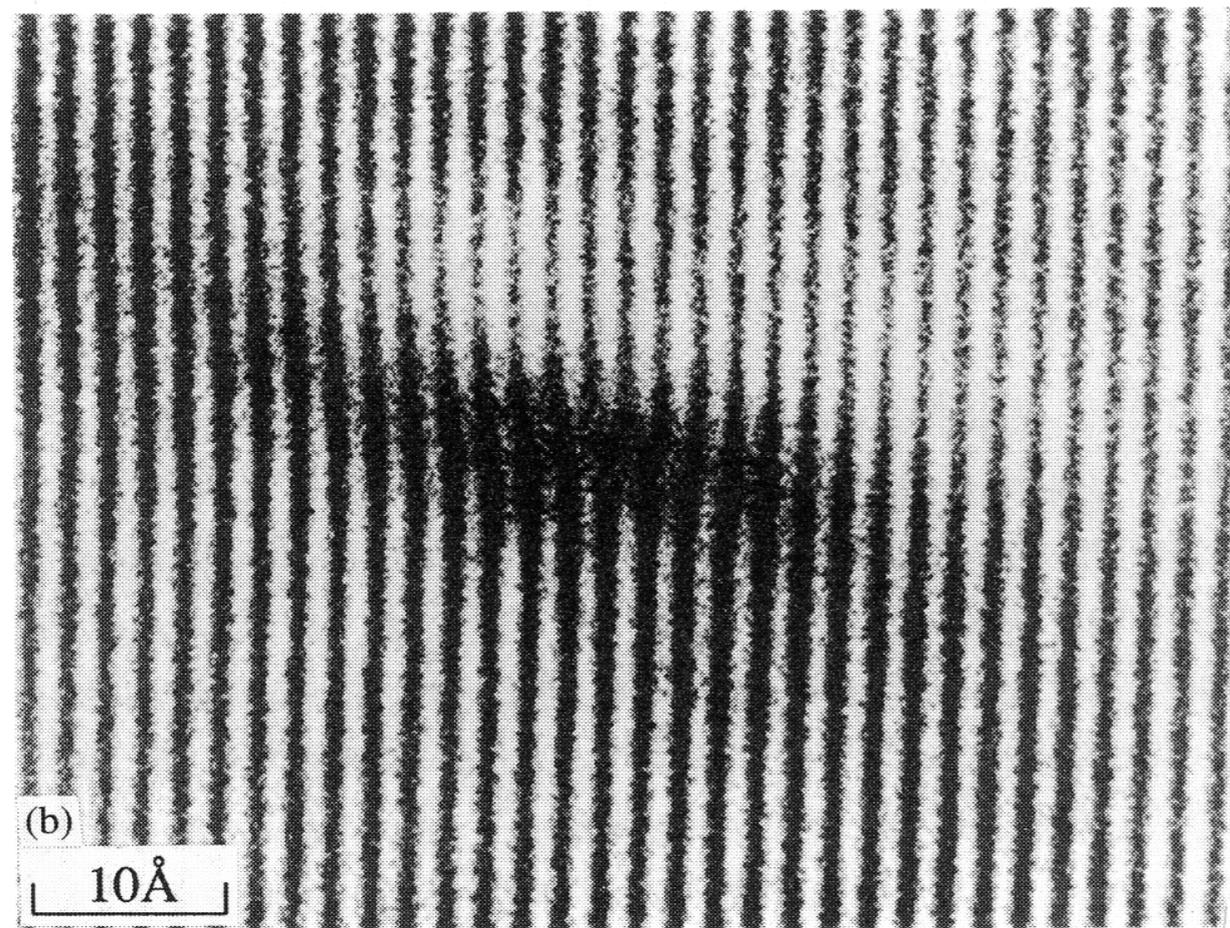
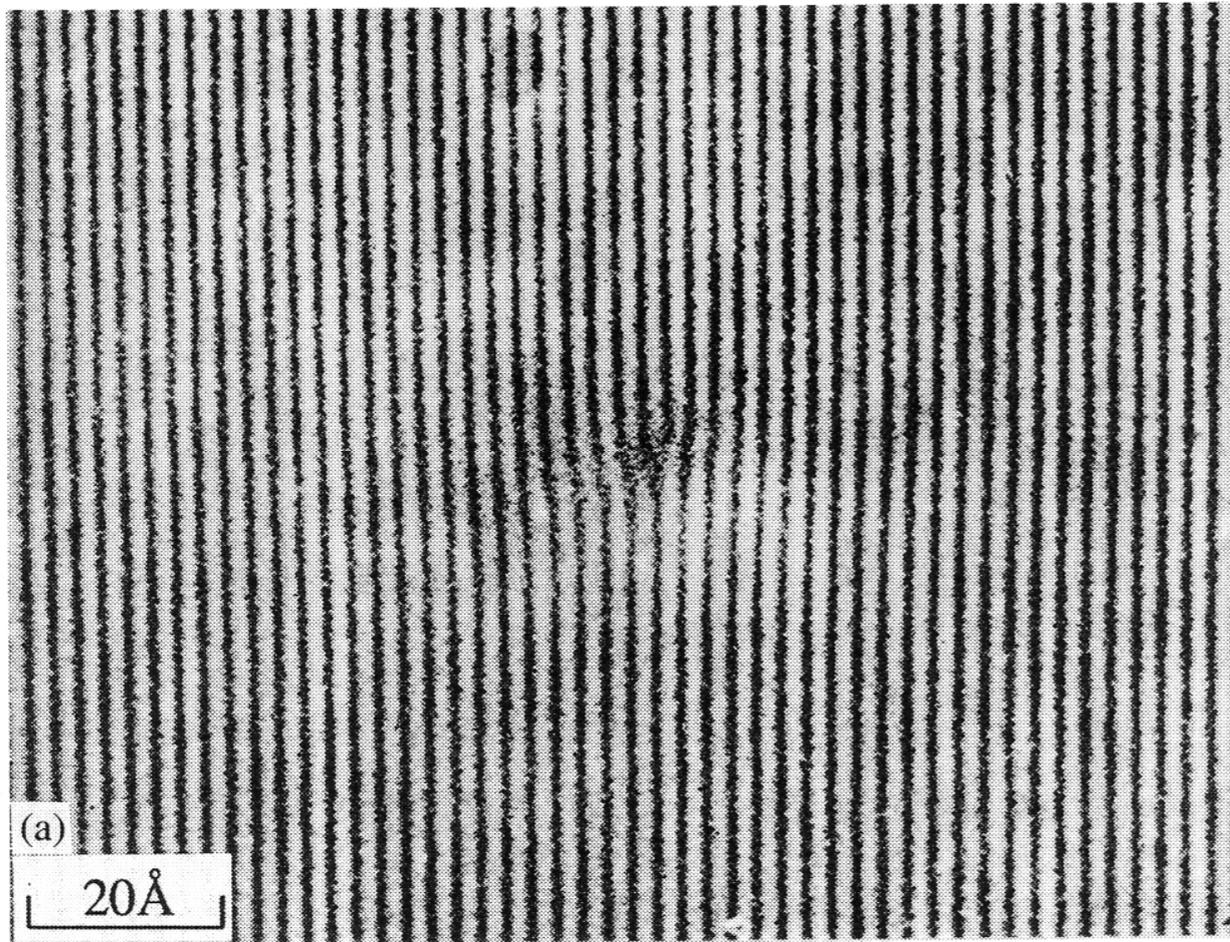
Insert an extra half plane



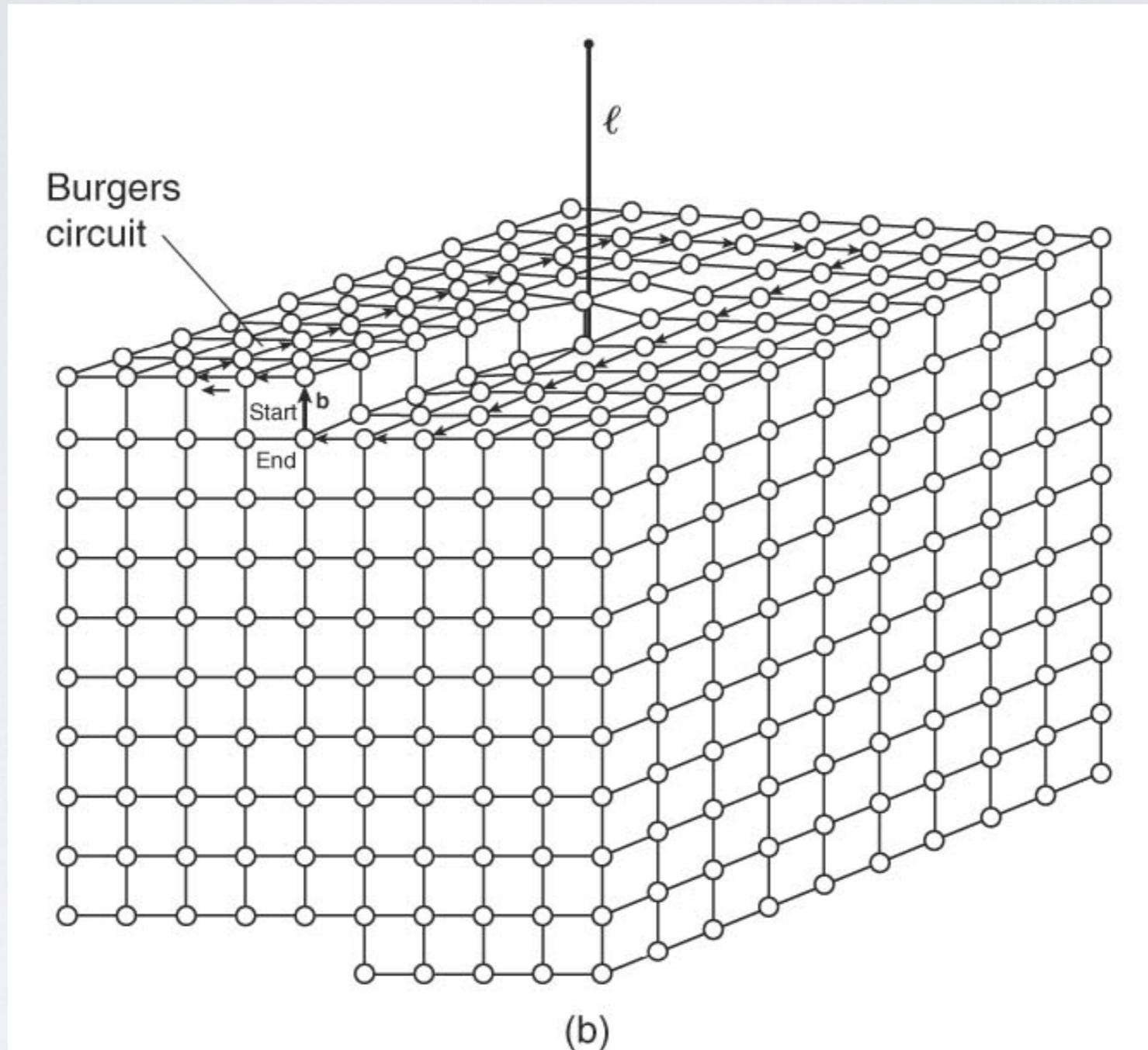
Edge dislocation



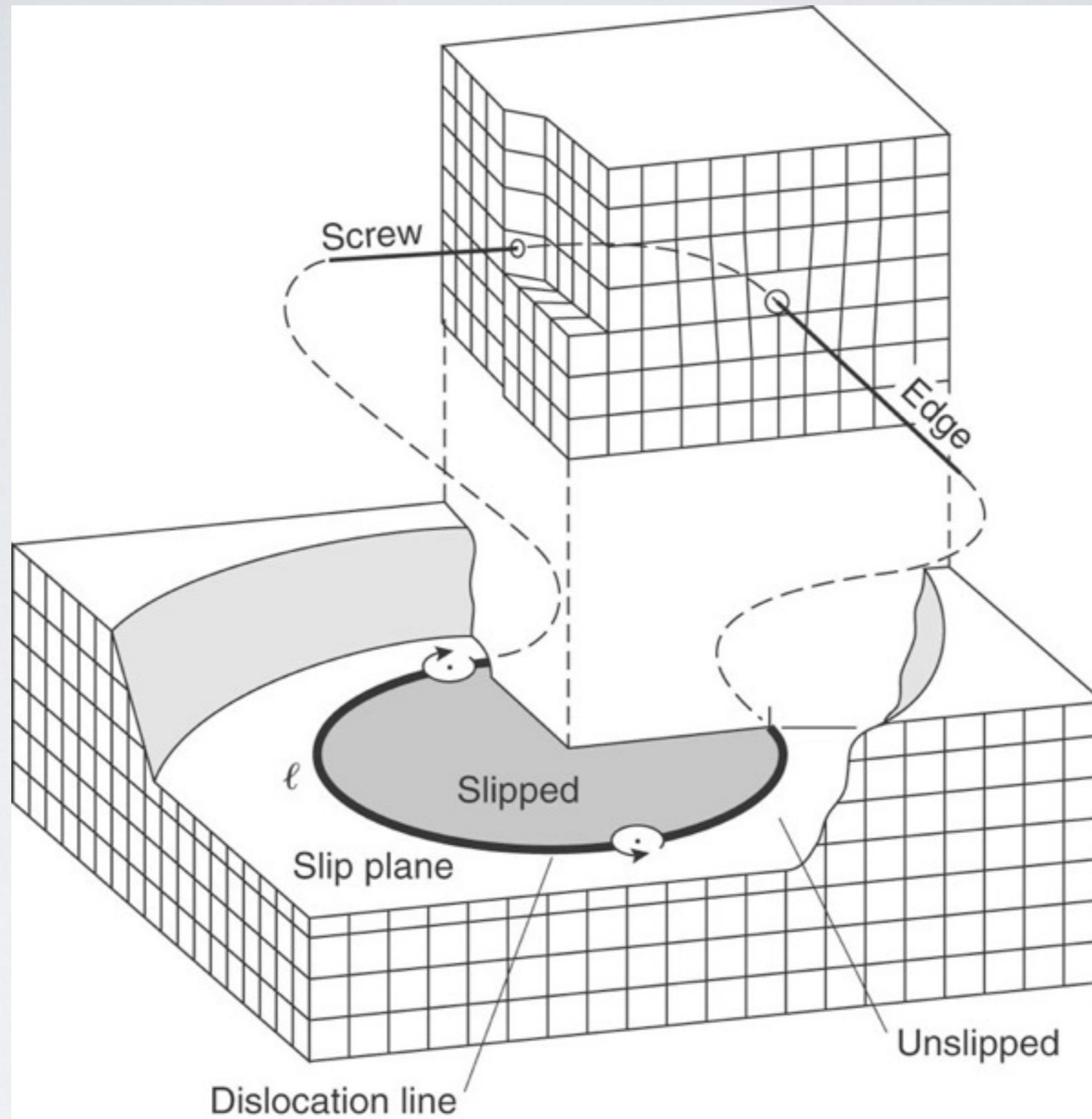
edge dislocation: Burgers vector perpendicular to dislocation line l



TEM lattice-fringe
images with electron
beam parallel to
dislocation line

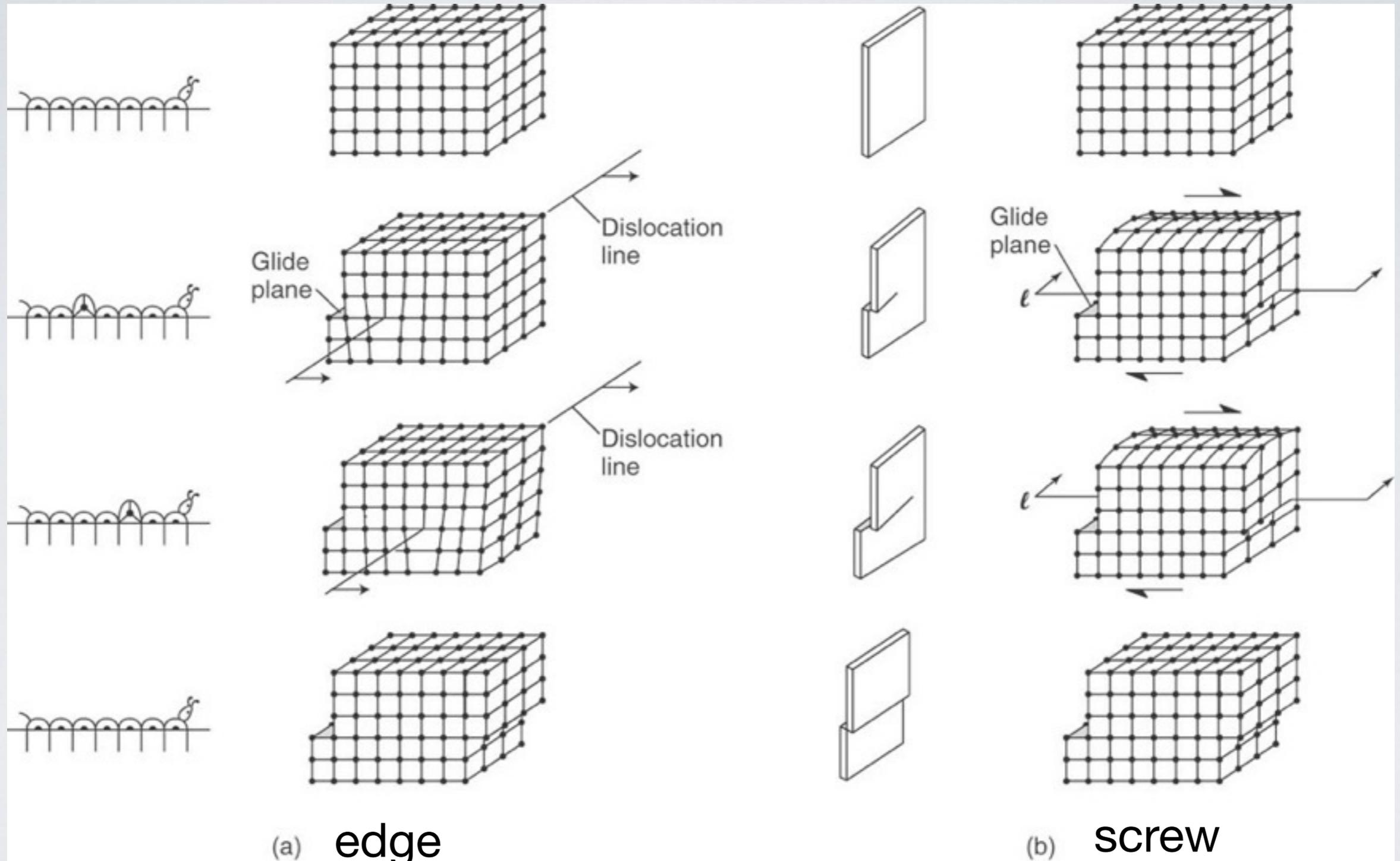


screw dislocation: Burgers vector parallel to dislocation line |

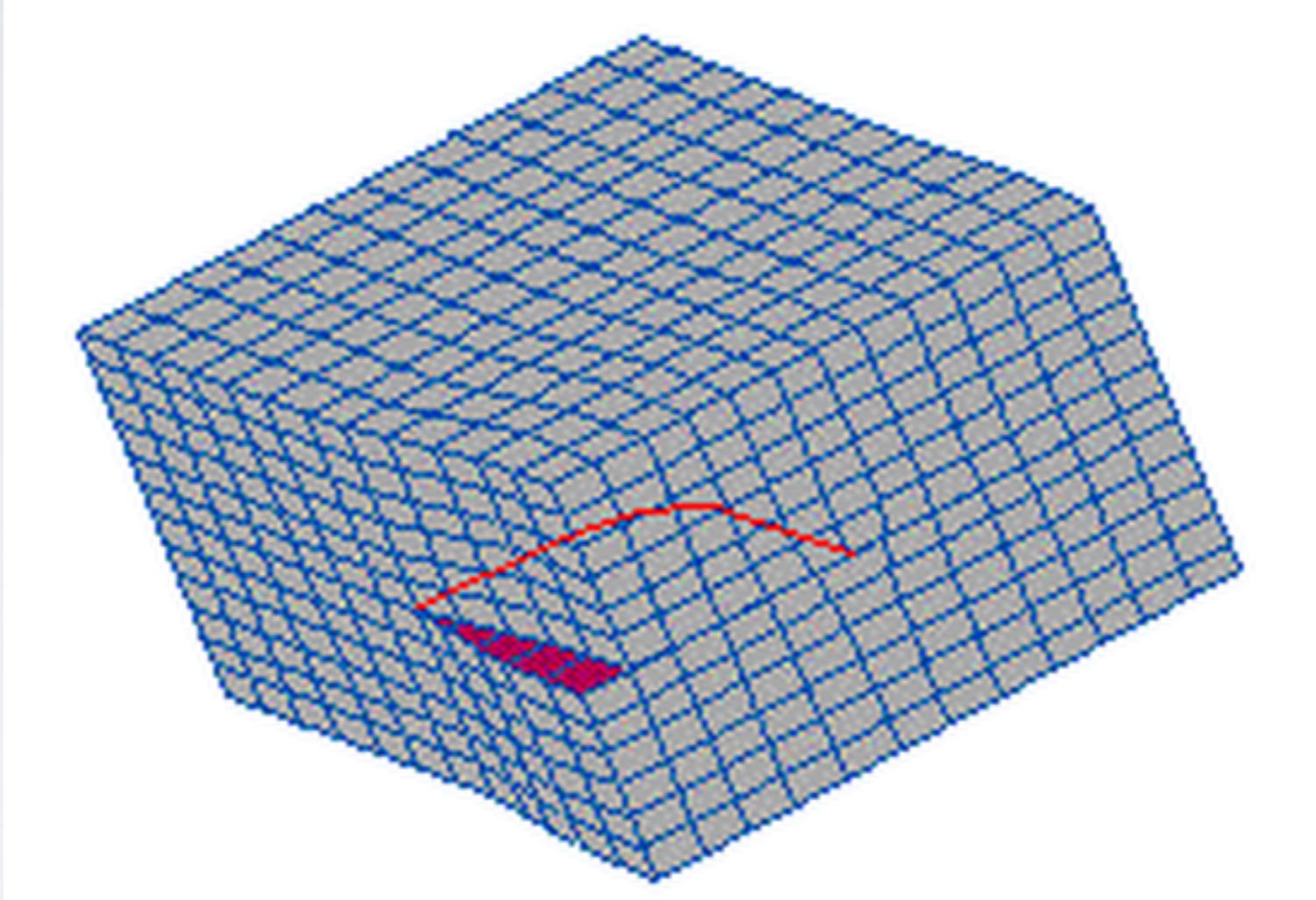


dislocations: mixed character

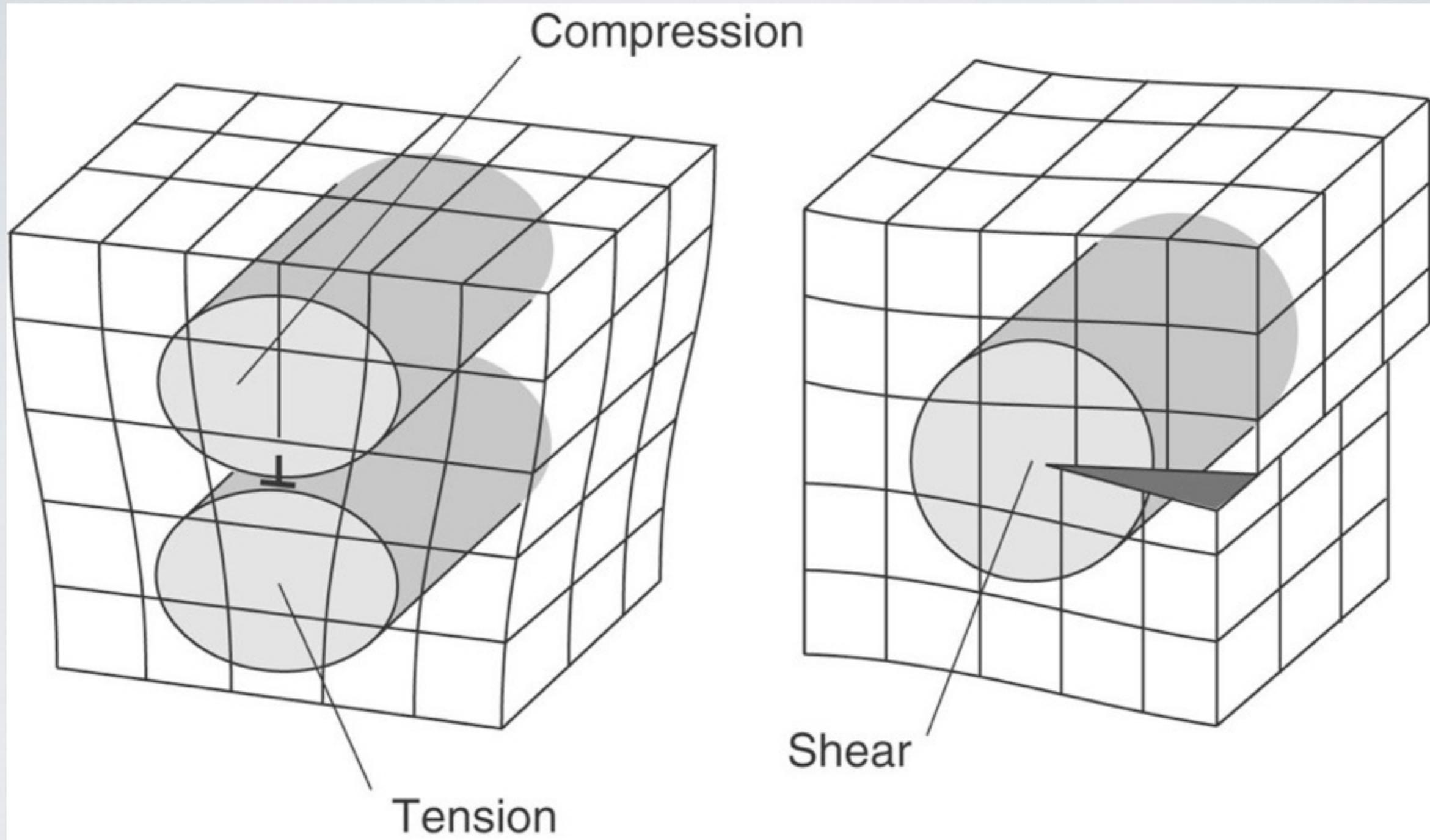
Strain due to dislocation creep



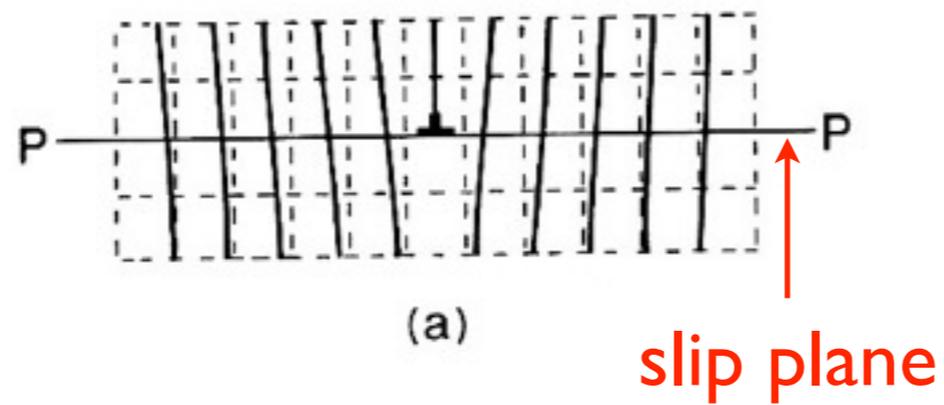
Movement in a glide plane



stress (strain) field surrounding dislocations

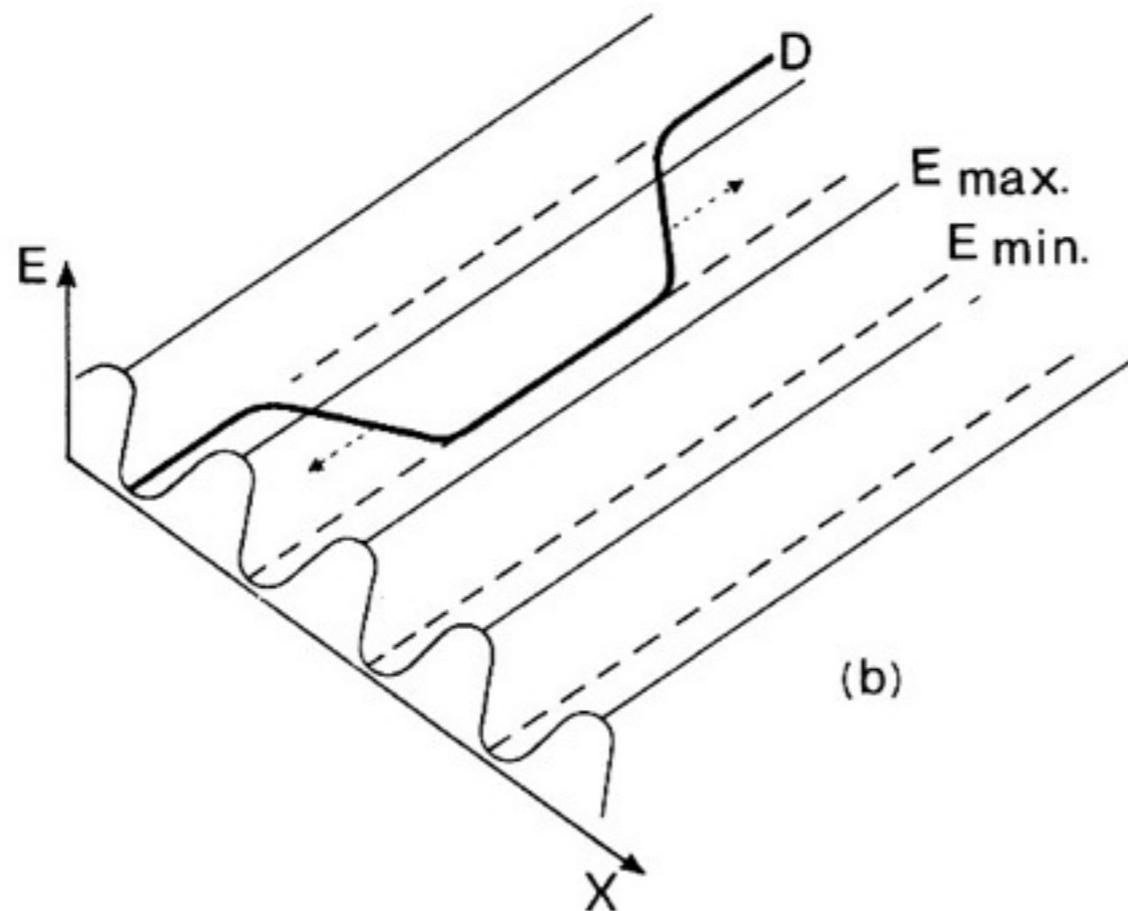


Dislocation geometry is controlled by crystal lattice

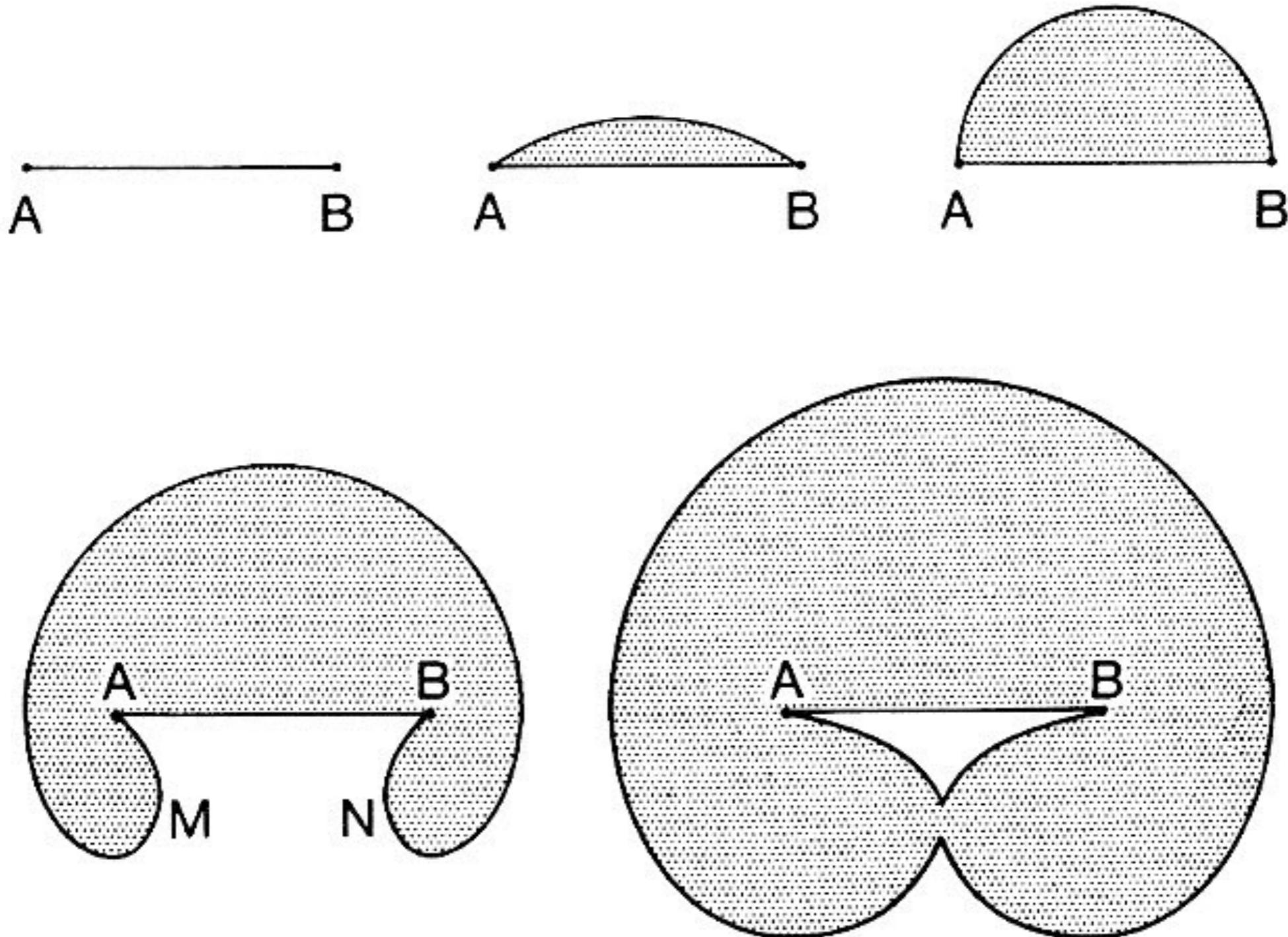


dislocations move on glide planes

Peierls potential

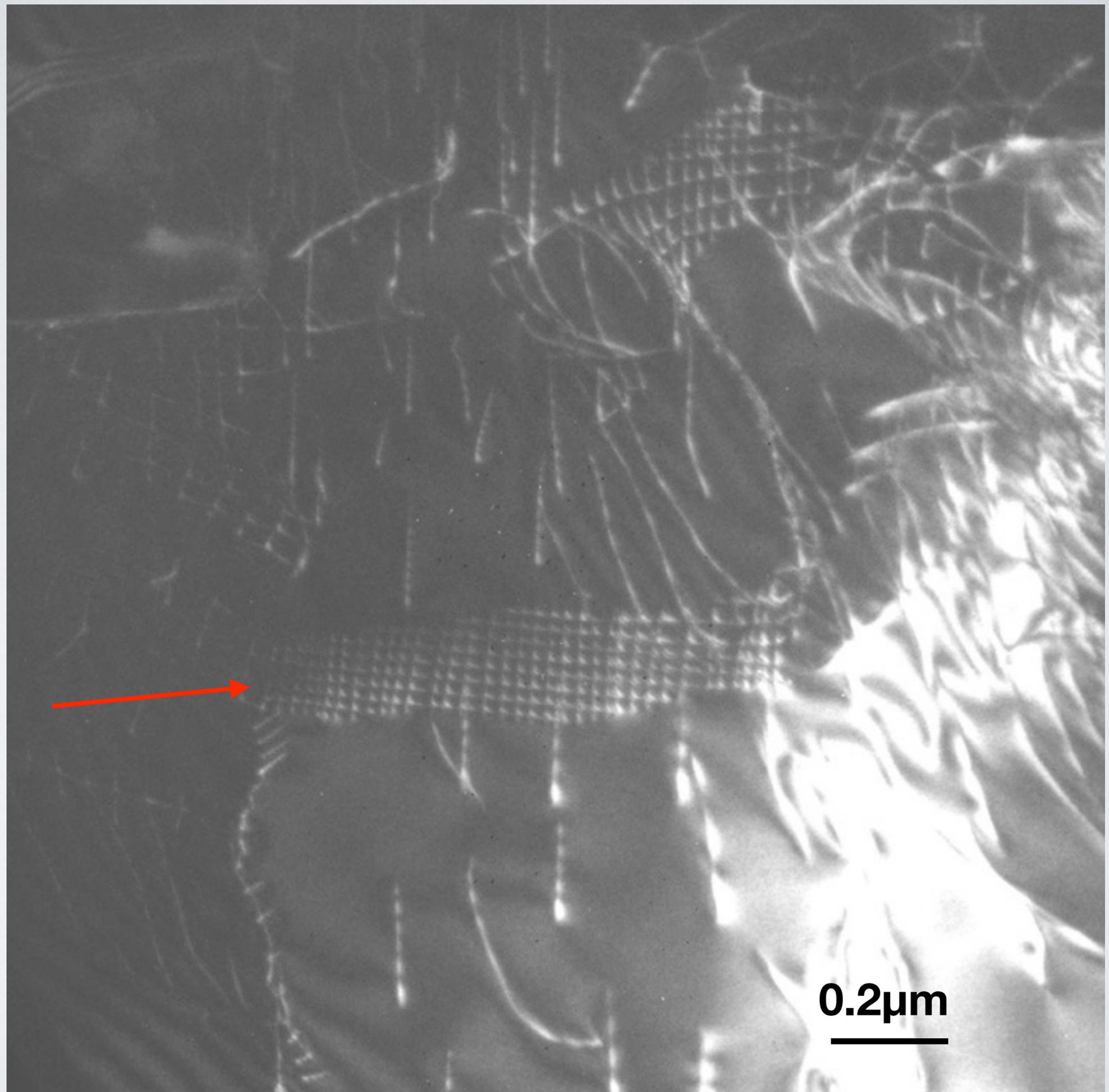


Generation of dislocations: Frank-Read sources (dislocation multiplication due to stress/strain)



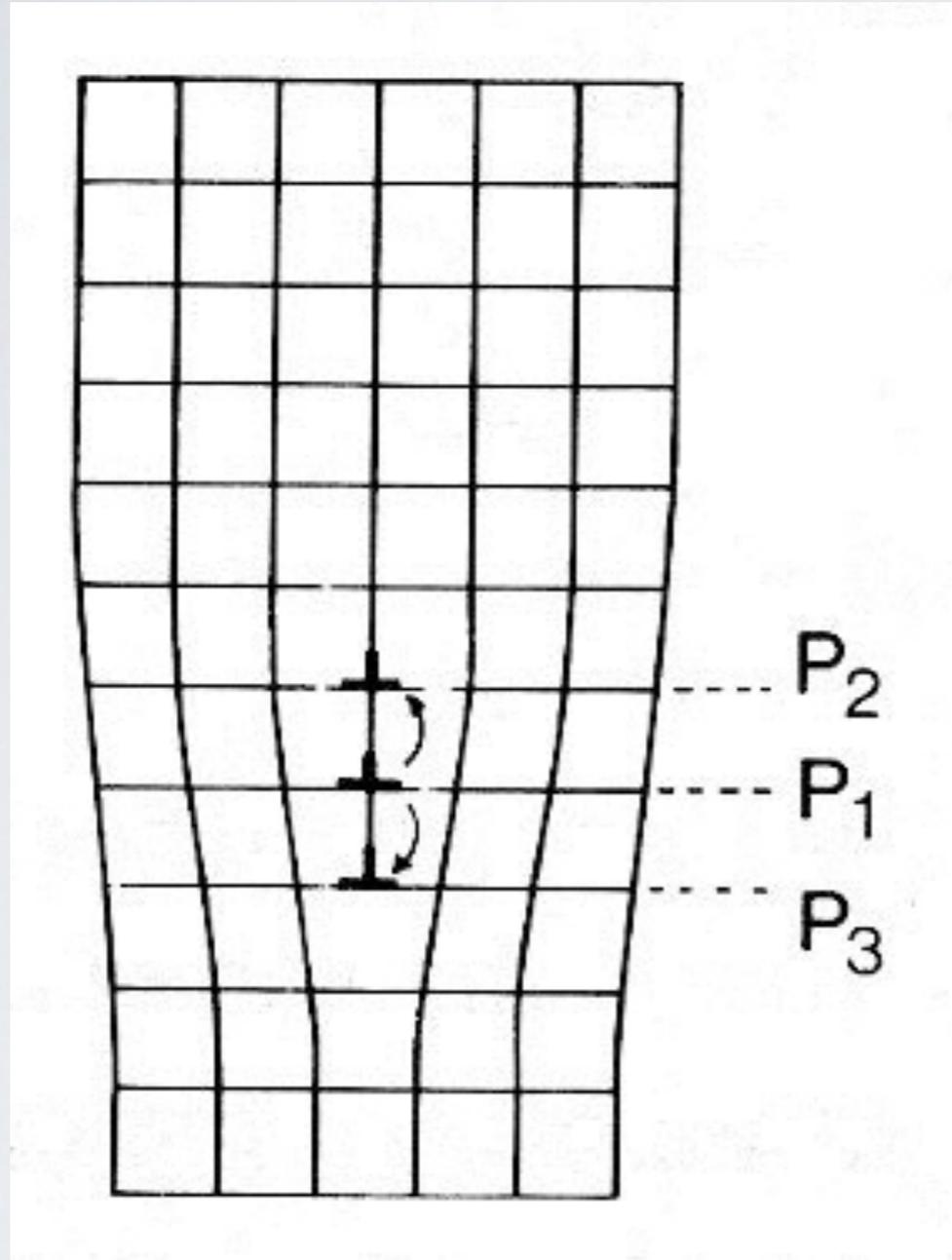
Obstacles
to
dislocation
motion

subgrain
boundary



0.2μm

Climb of an edge dislocation



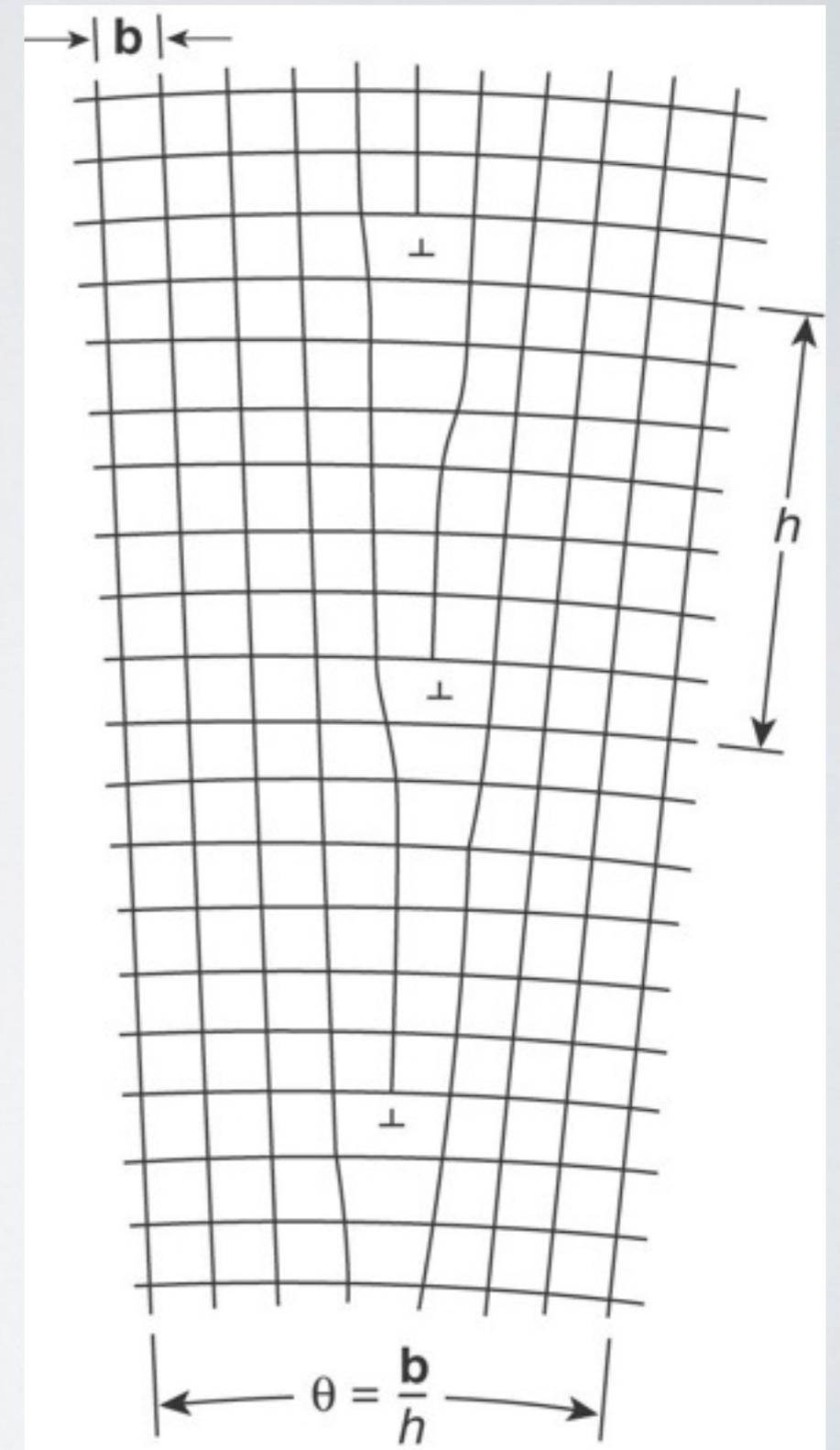
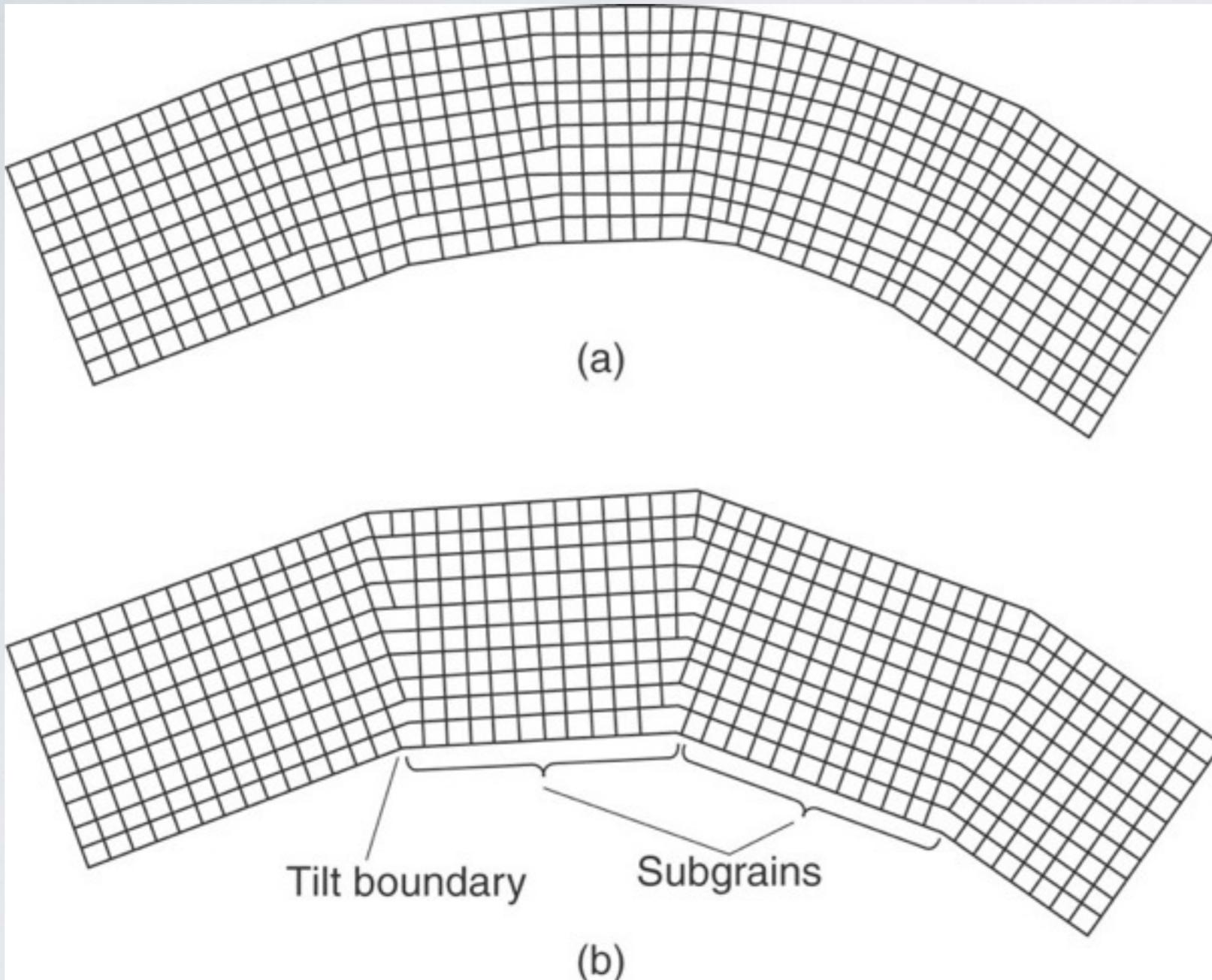
Climb by diffusion of a row of atoms from the extra half plane.

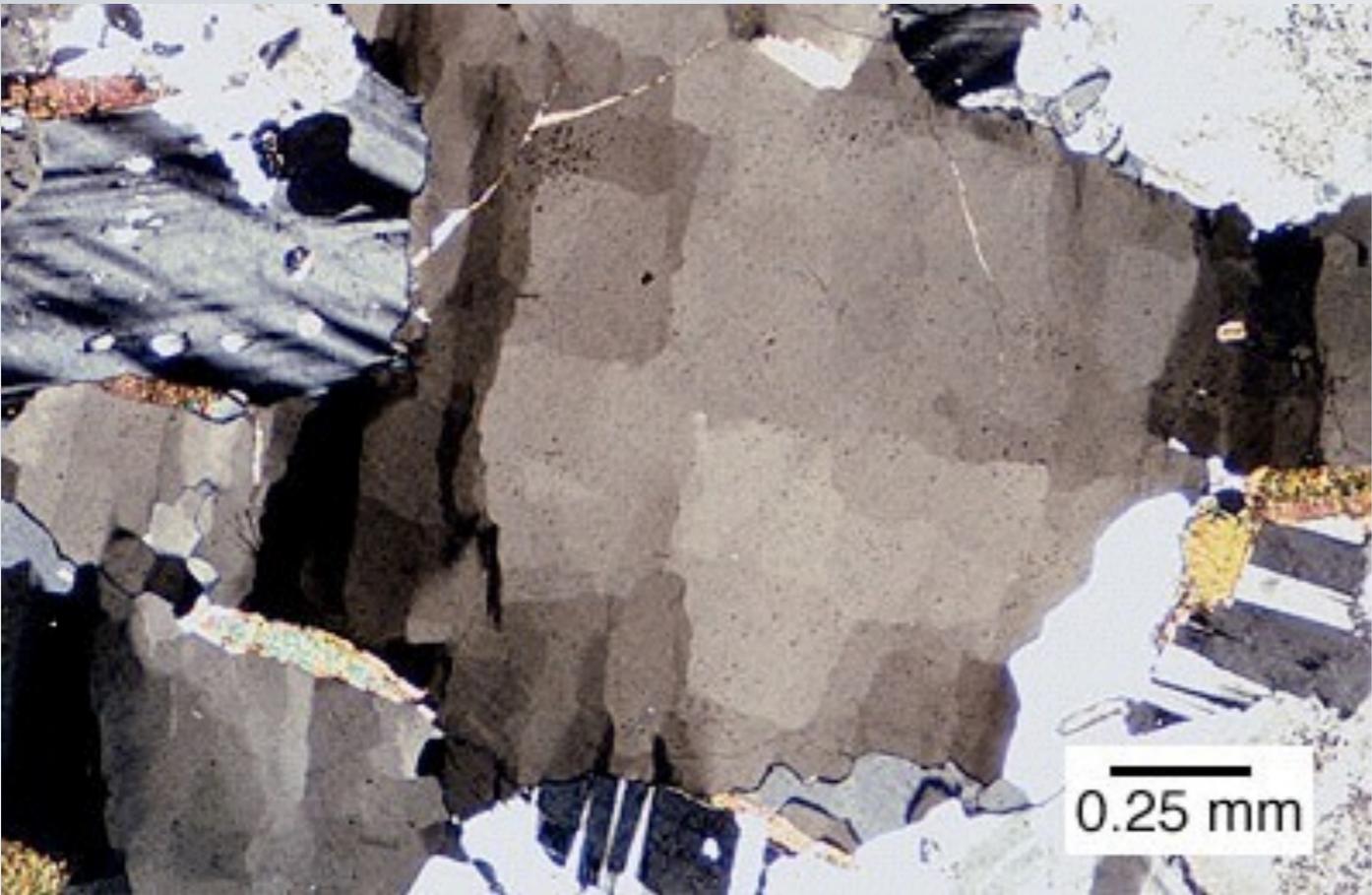
Screw dislocations have no extra half plane and cannot climb.

	temperature	shear stress
dislocations (number density)	<ul style="list-style-type: none">•not produced by,•annealed by,•mobility T dep.	sensitive to and interact with
point defects	dependent	do not interact

From dislocations to grain boundaries

Arrays of dislocations: subgrain boundaries



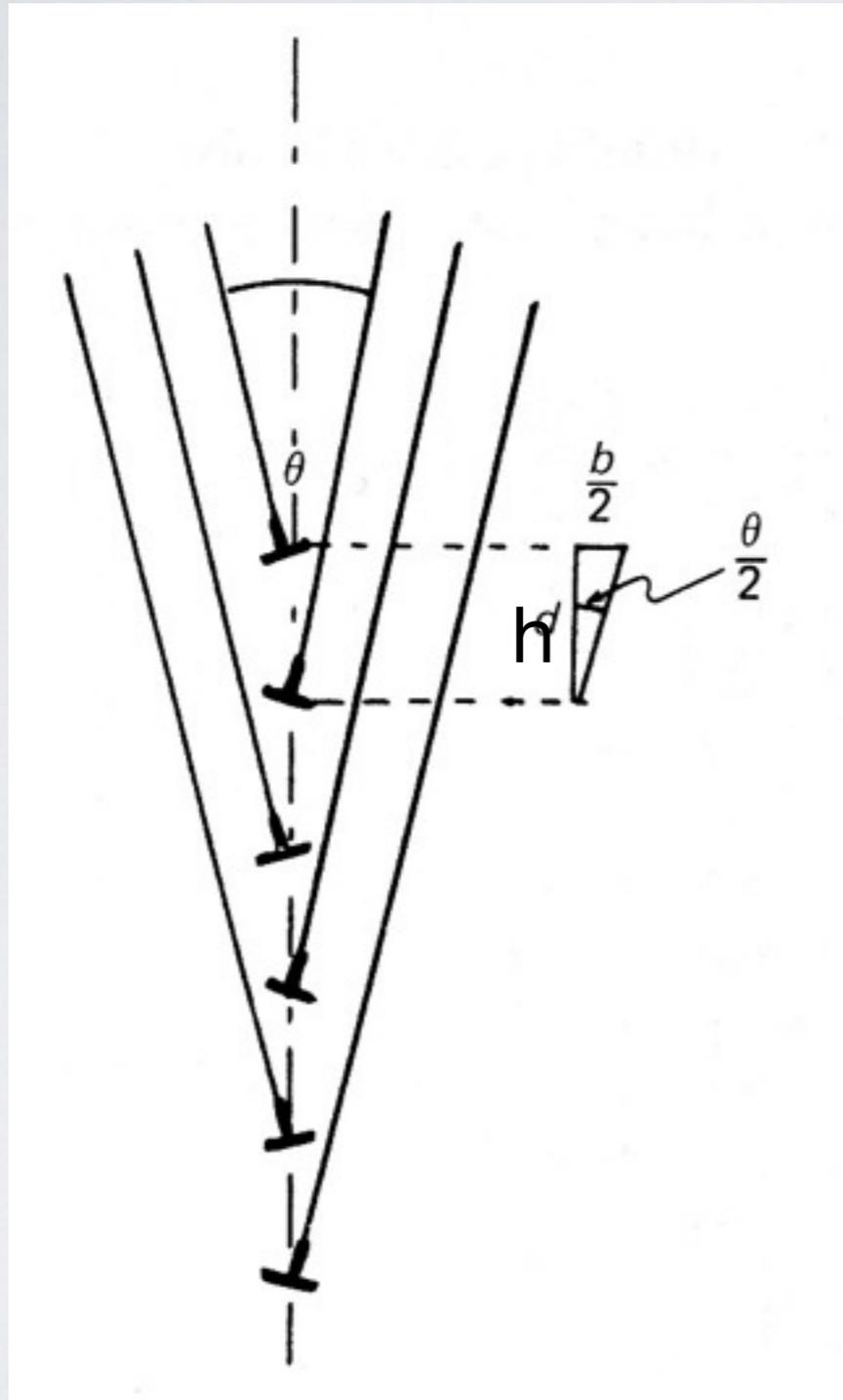


subgrain boundaries in quartz



undulose extinction in quartz

Construct grain boundaries from arrays of dislocations



Low angle tilt boundary

Misorientation angle:

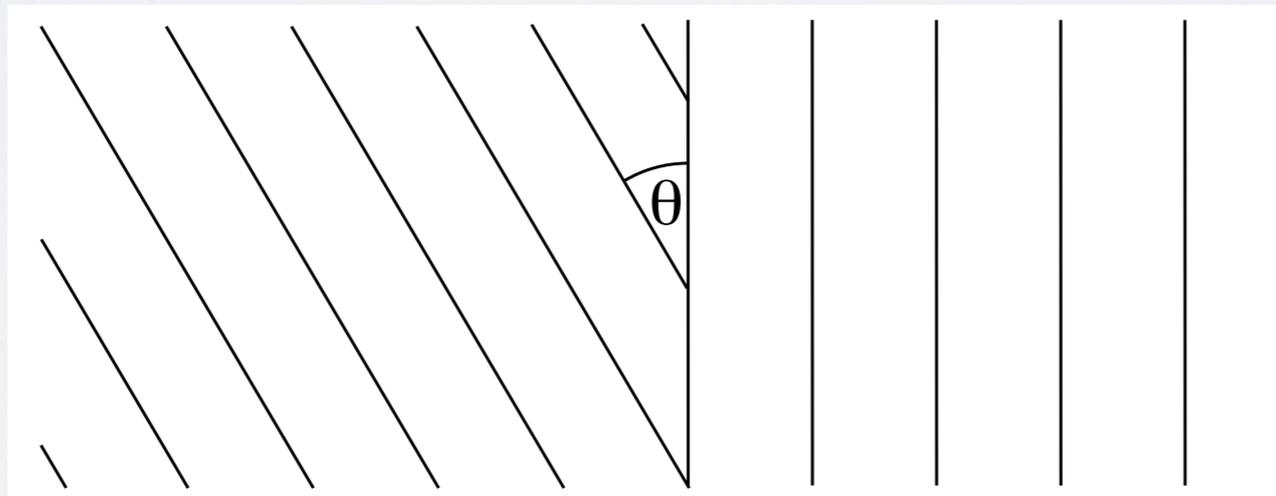
$$\theta = 2 \tan((b/2)/h) \approx b/h$$

Grain boundaries

Why look at grain boundaries?

1. GB as crystalline defect present in all rocks.
2. GB affect
 - diffusion
 - deformation
 - seismic properties
 - electrical conductivity....

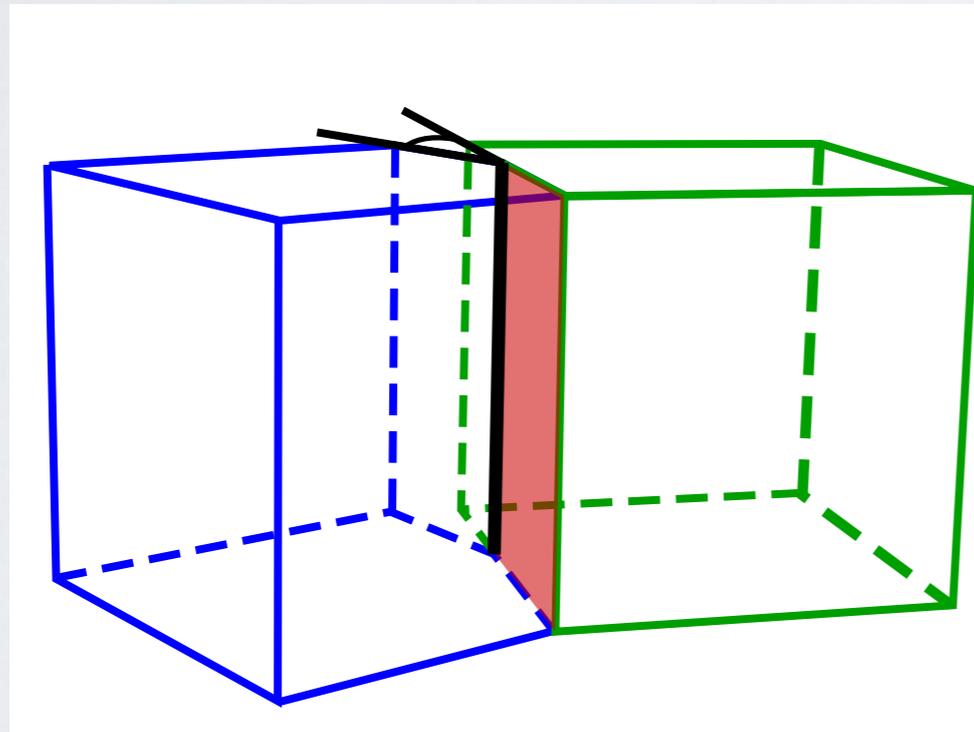
GB: 2-D lattice defect that introduces a change in lattice orientation



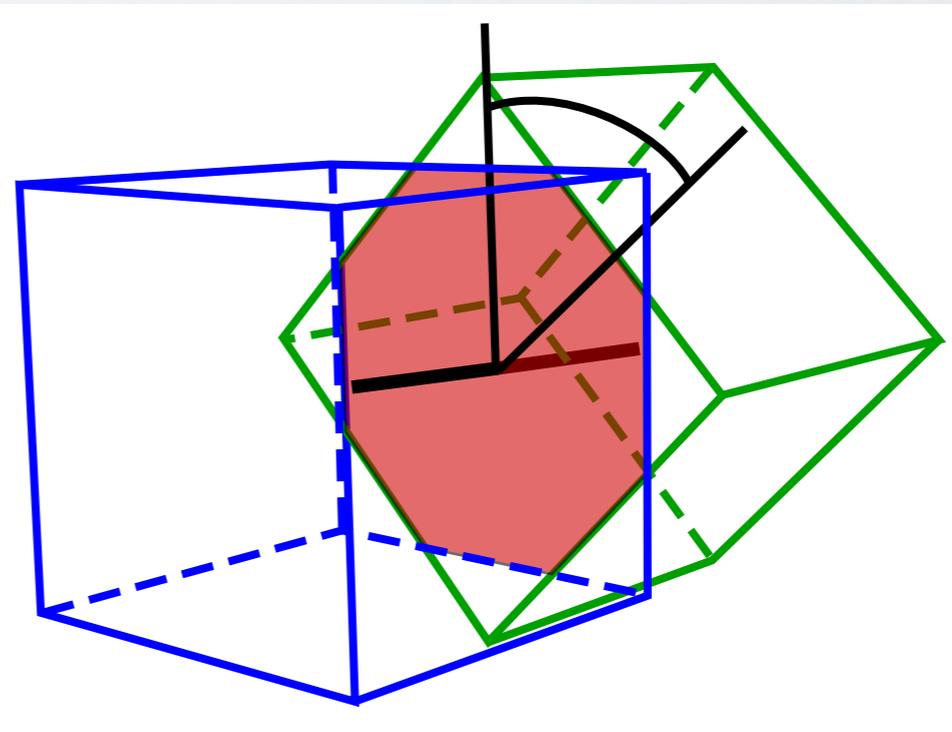
Lattice misorientation given by θ

Boundary type as a function of relative orientation of neighboring grains

Tilt boundary
rotation axis is parallel to
boundary plane
misorientation generated by
inserting edge dislocations



Twist boundary
rotation axis is
perpendicular to boundary
plane
misorientation generated
by 2 sets of screw
dislocations

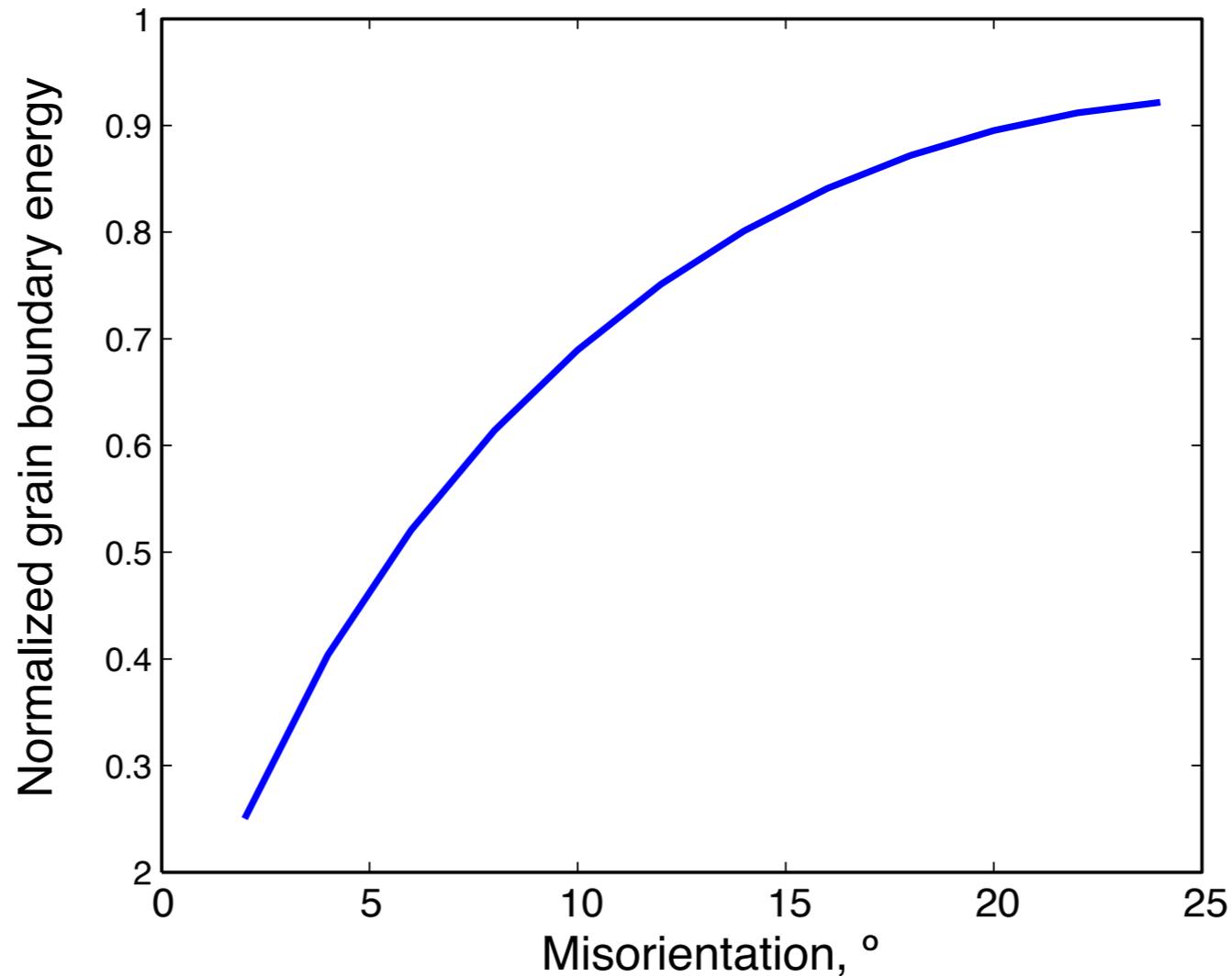


Read-Shockley dislocation model for grain boundary energy γ

$$\gamma_s = \gamma_0 \theta (C - \ln \theta)$$

where the relative rotation $\theta = b/d$, with b Burgers Vector d dislocation spacing

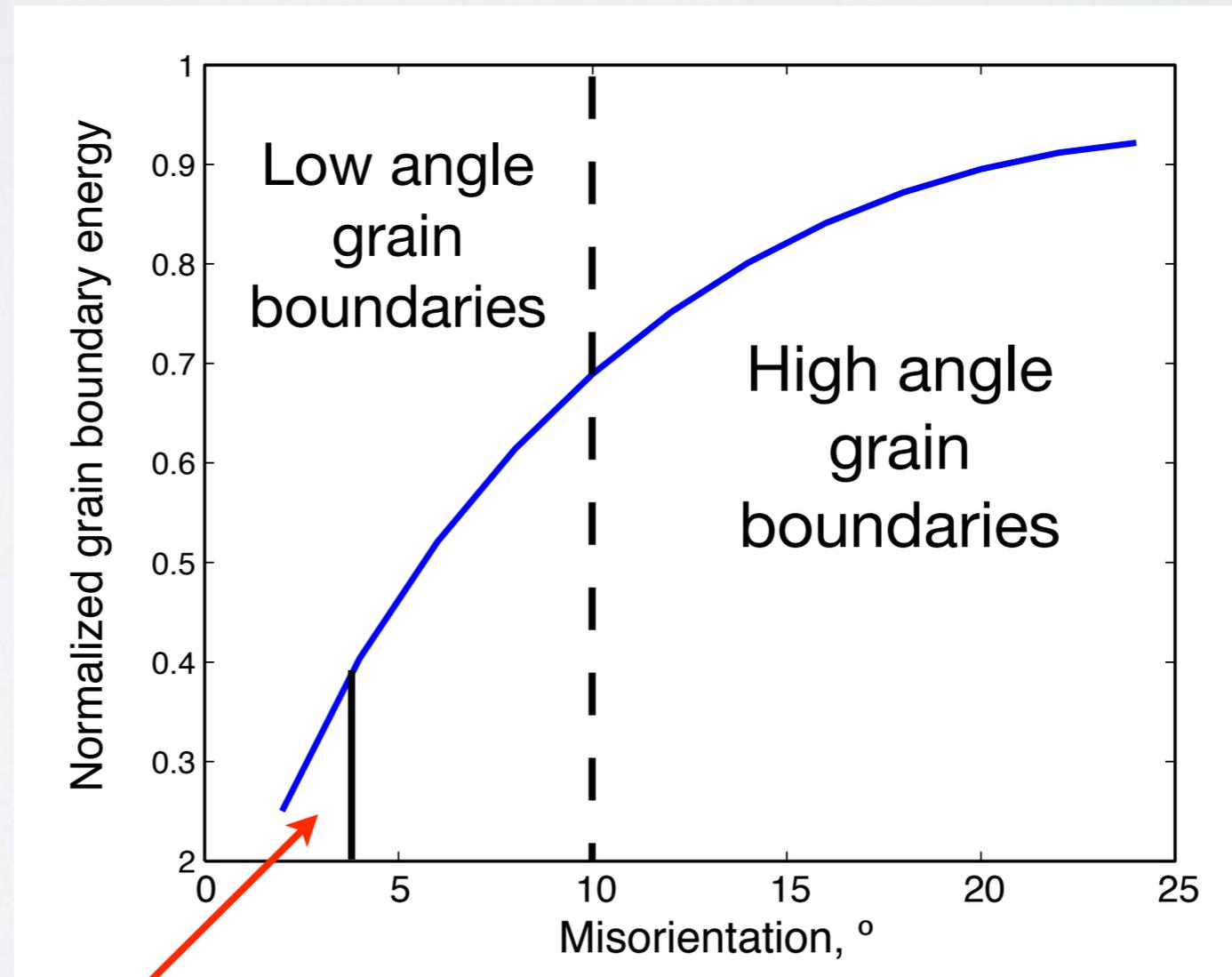
$\gamma_0 = Gb/4 \pi(1-\nu)$, with G shear modulus and ν Poisson's ratio,
 $C = 1 + \ln(b/2 \pi r_0)$ with r_0 radius of the dislocation core



Definitions

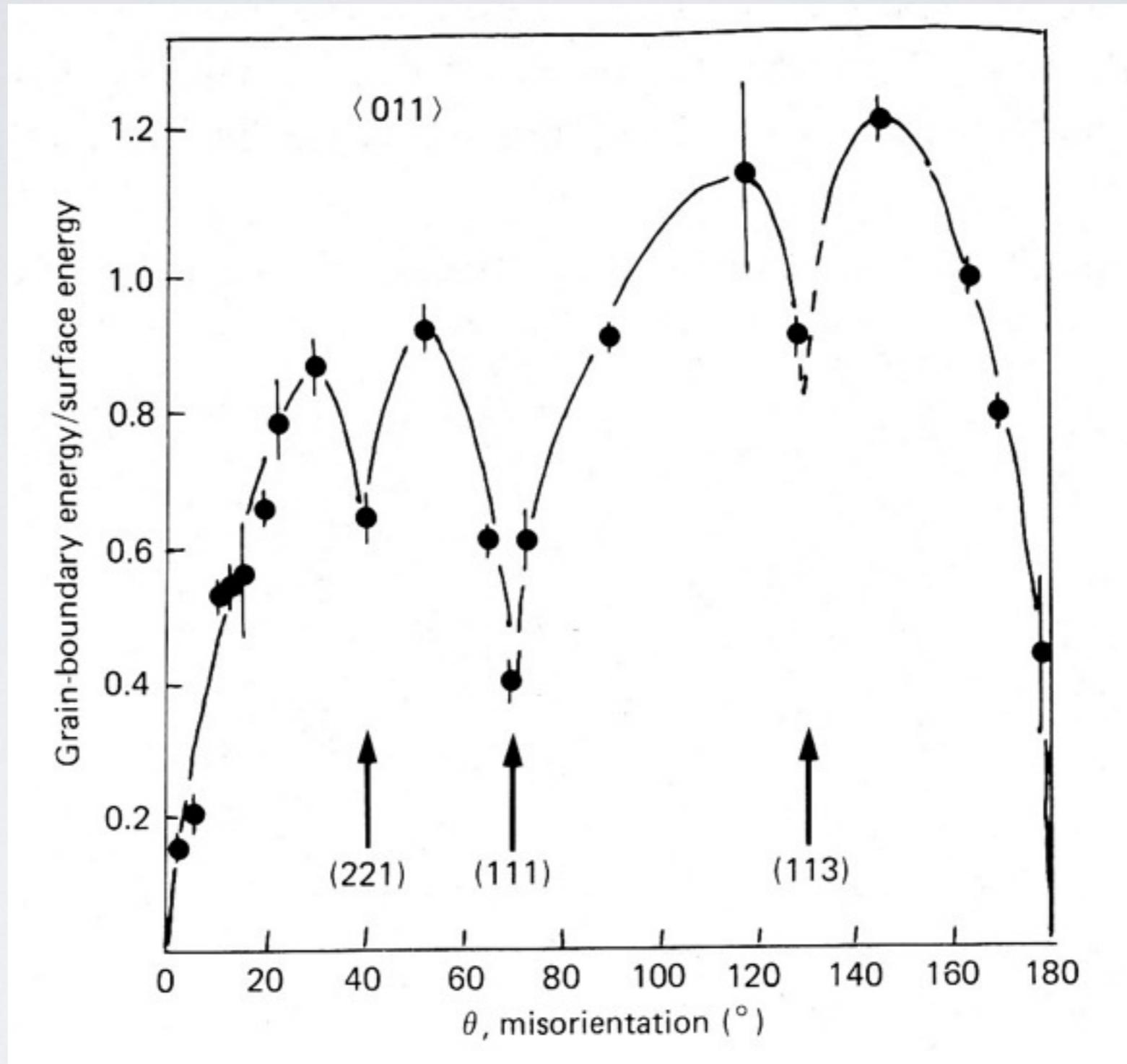
Subgrain boundaries: Dislocation cores non-overlapping, boundary consists of a (more or less ordered) array of dislocations.

High angle grain boundaries: Dislocations can no longer be identified, boundary structure and properties independent of misorientation angle.

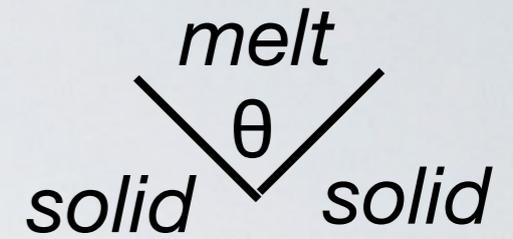
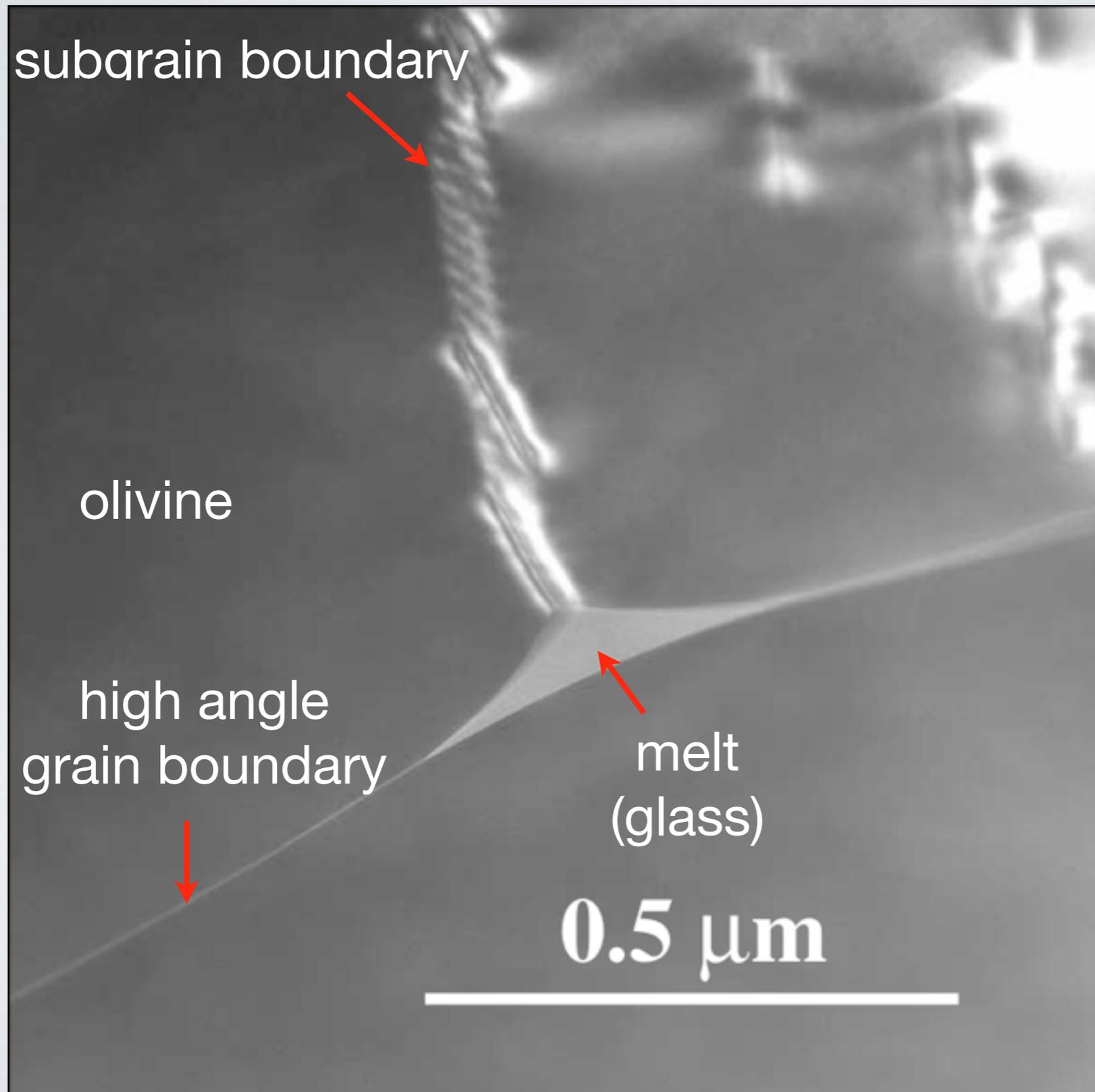


subgrain boundaries

Dependence of relative grain boundary energy on misorientation for NiO



Visualization of types of grain boundaries

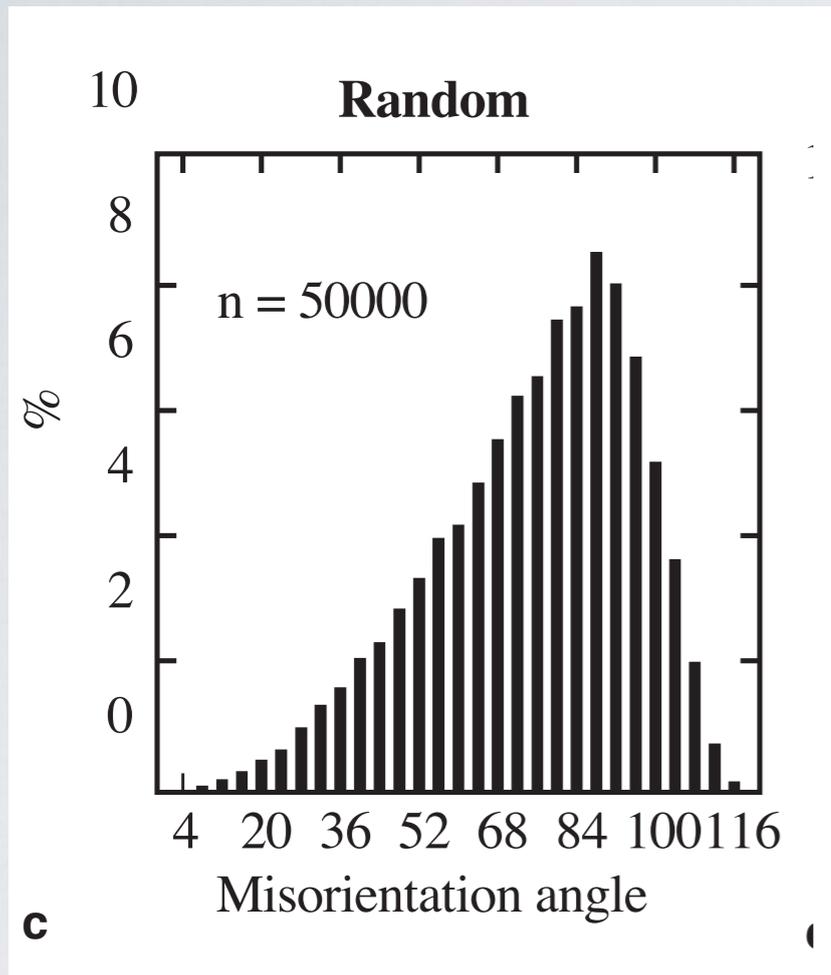


$$\cos \theta/2 = \gamma_{ss}/2\gamma_{sl}$$

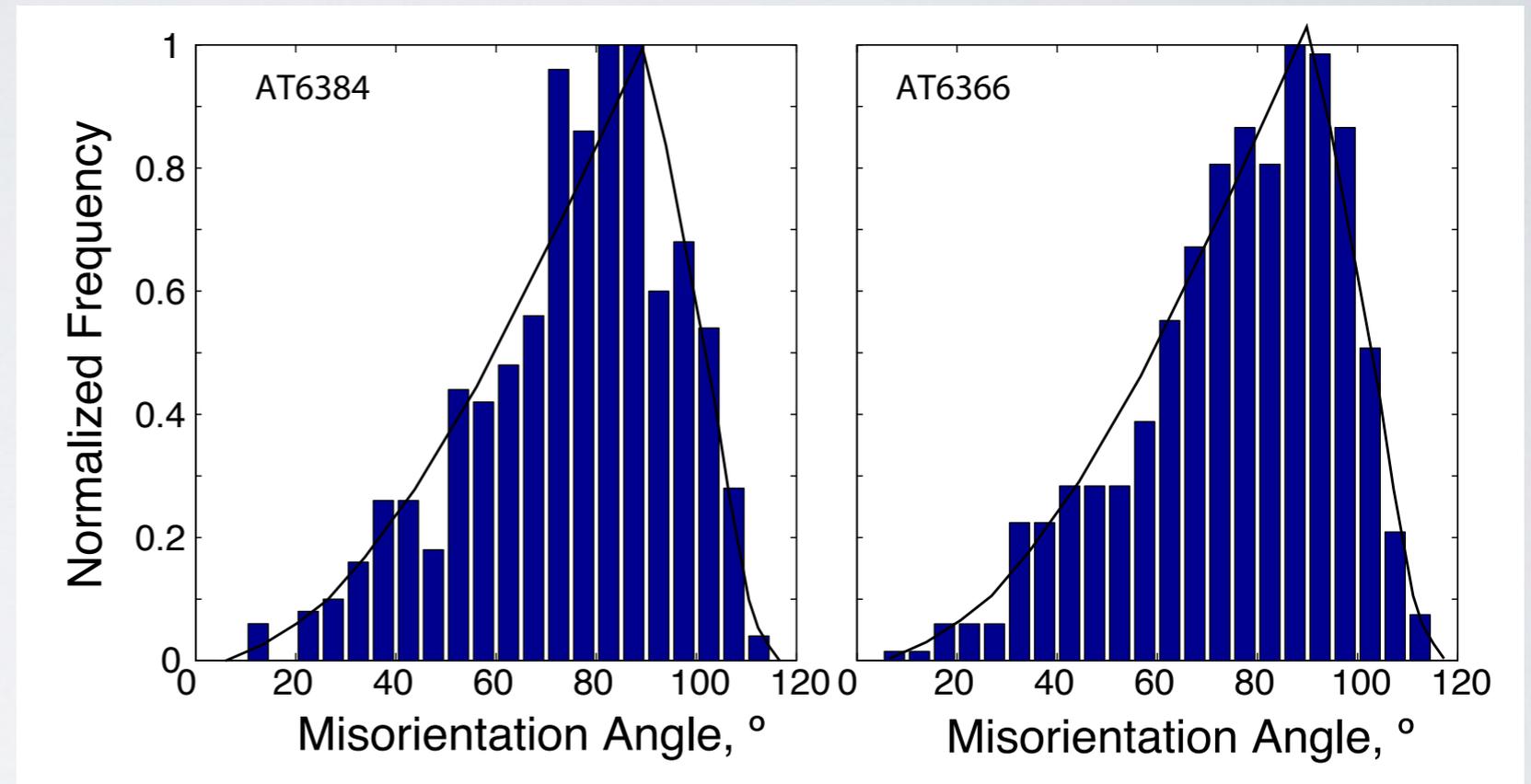
γ_{ss} = solid - solid surface energy

γ_{sl} = solid - liquid surface energy

predicted

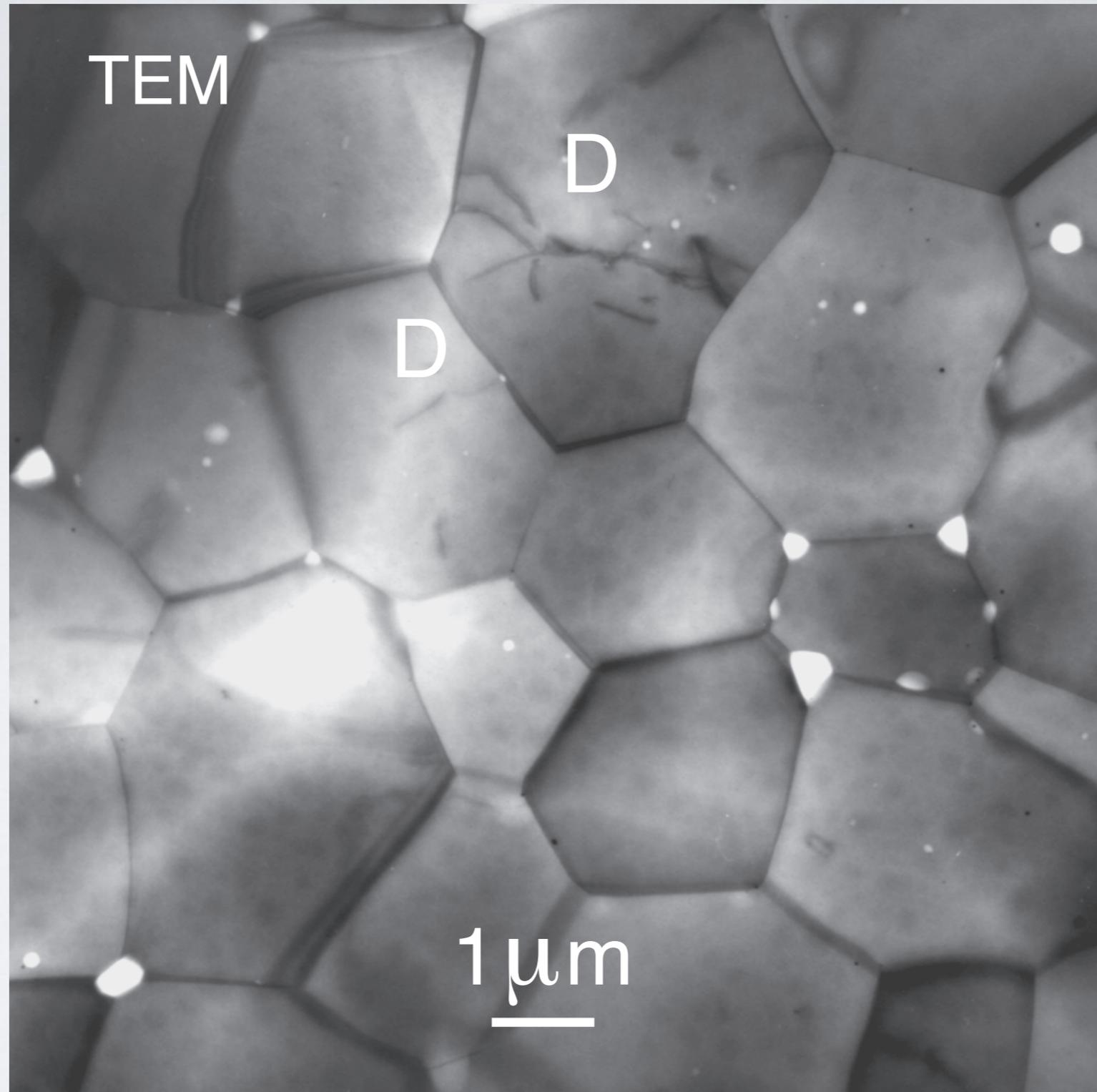


observed



-> the vast majority of grain boundaries are general, high angle grain boundaries

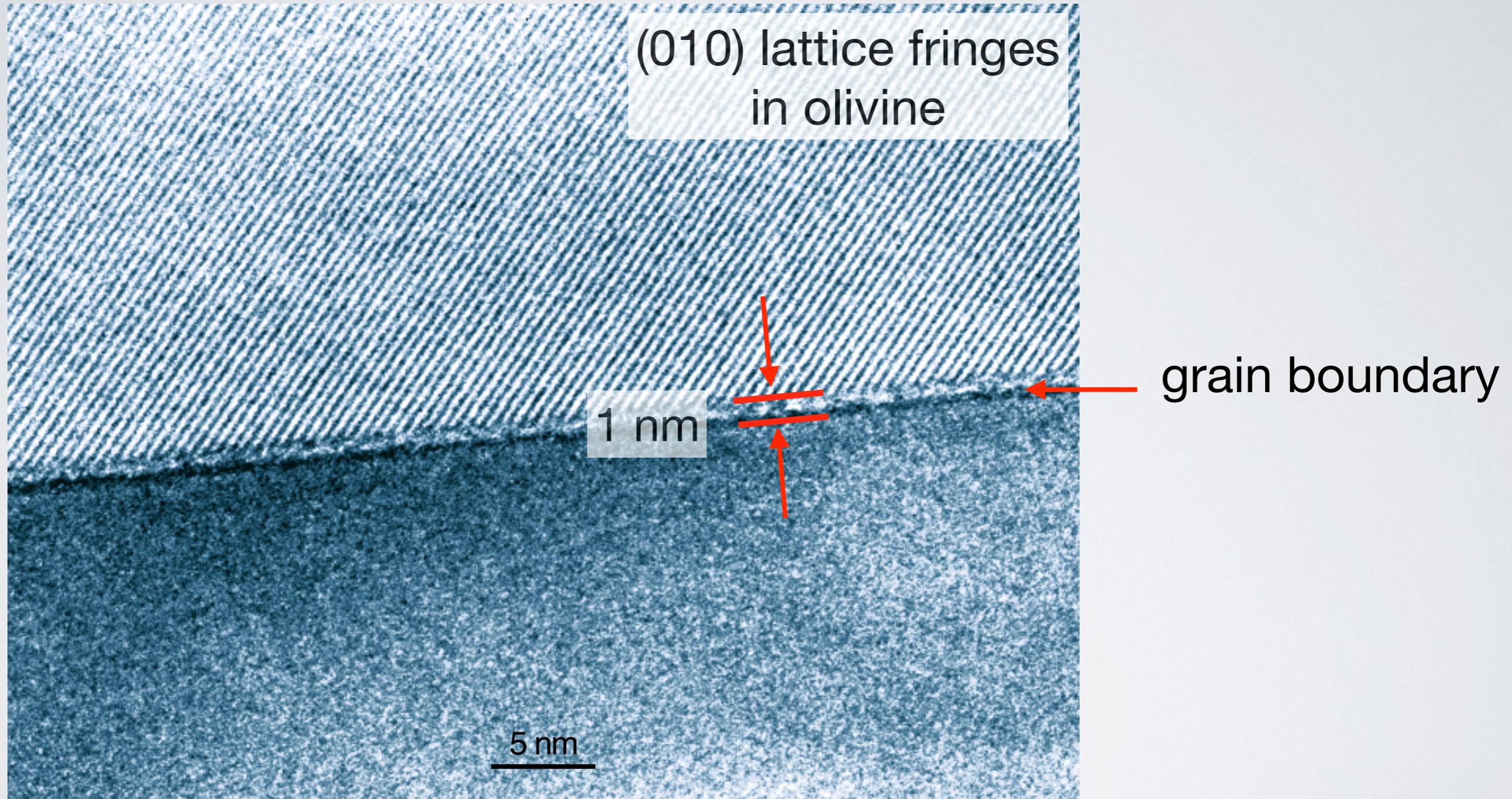
Grain boundaries: melt-free polycrystalline olivine



Jackson et al.,
2002

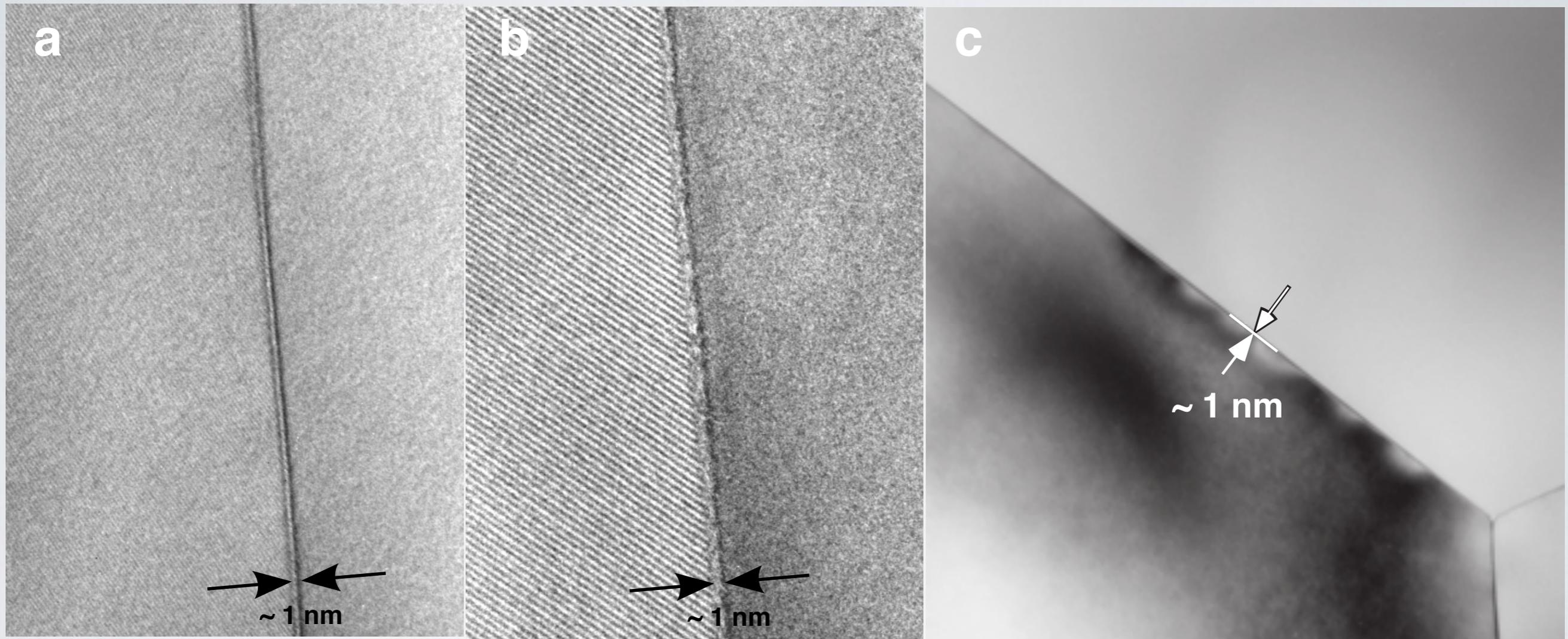
defects: grain boundaries, dislocations

High resolution image of olivine grain boundaries

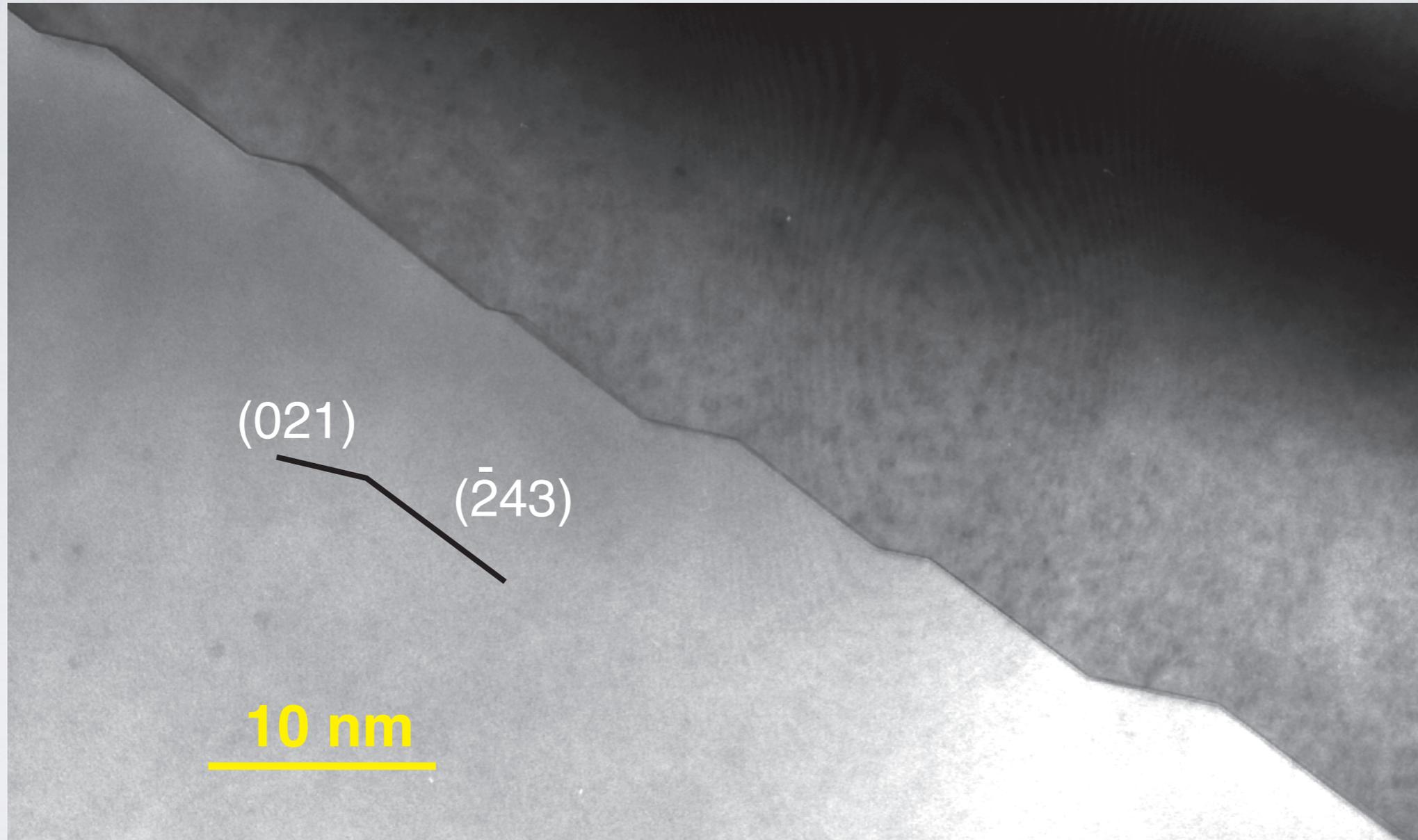


Faul et al., 2004

Grain boundaries in olivine: no evidence for dislocations, no steps, about 1 nm wide

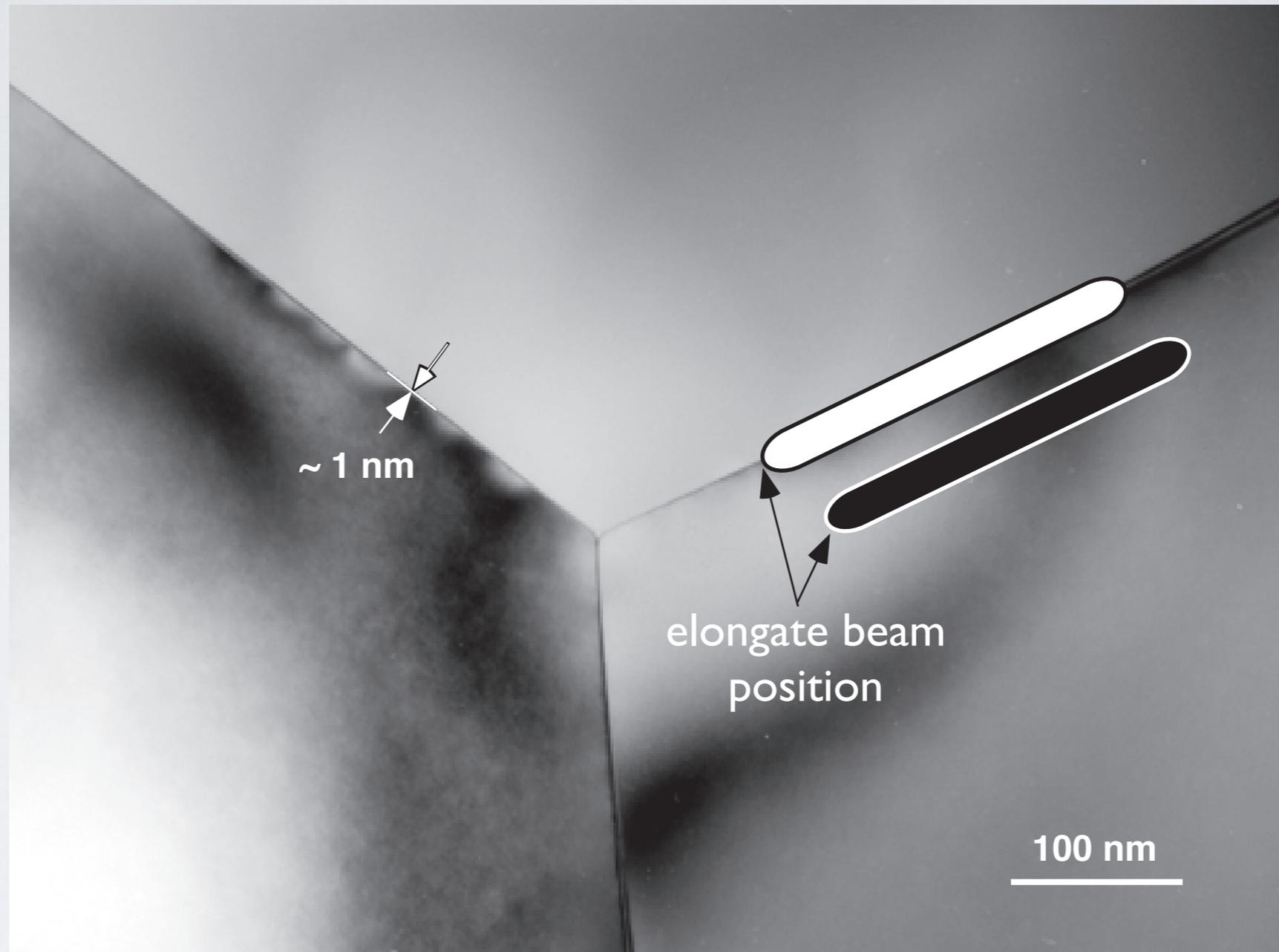


For comparison: Steps on high angle grain boundary of titanate-perovskite (SrTiO_3)

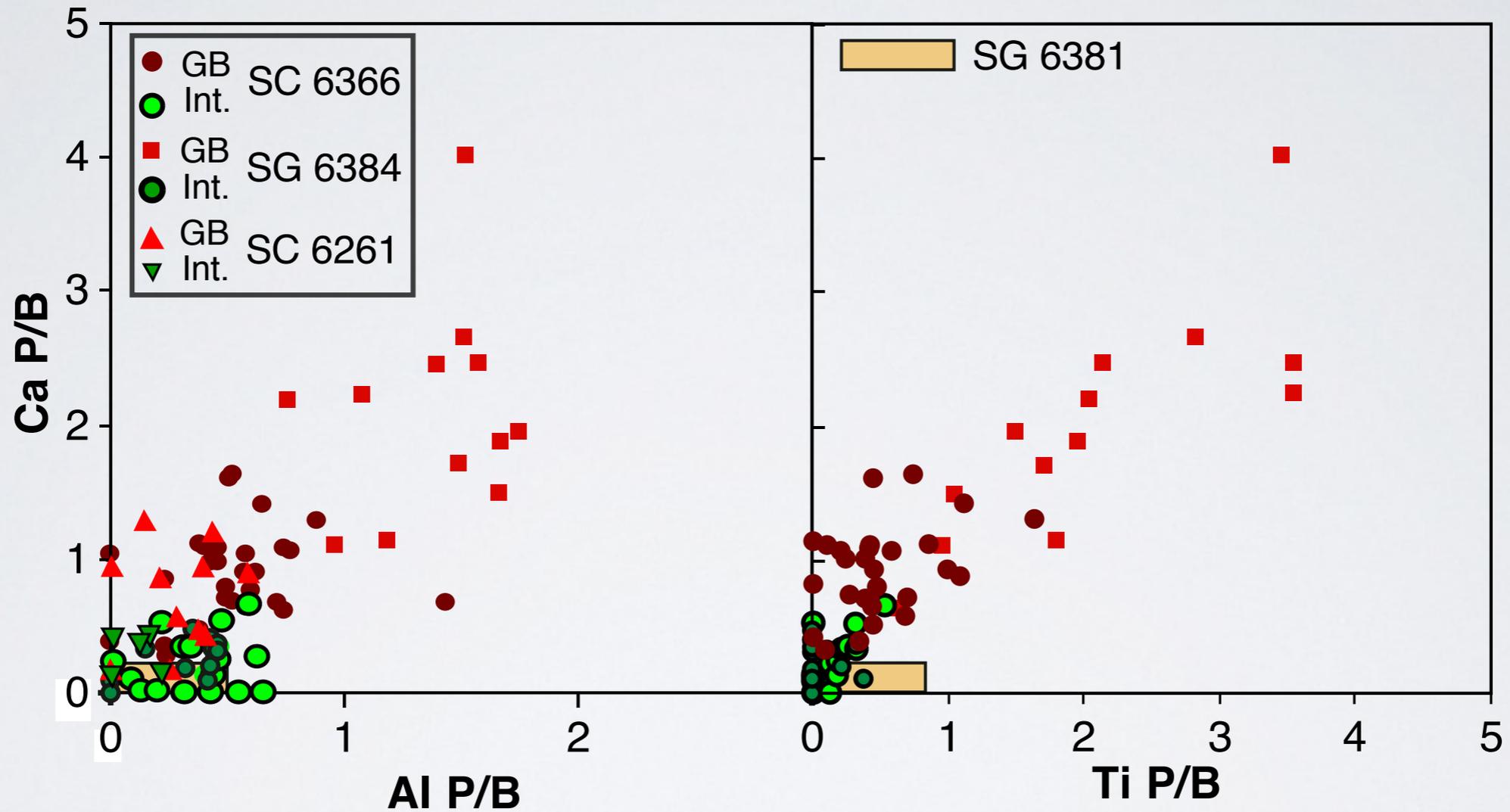


Webb et al., 1999

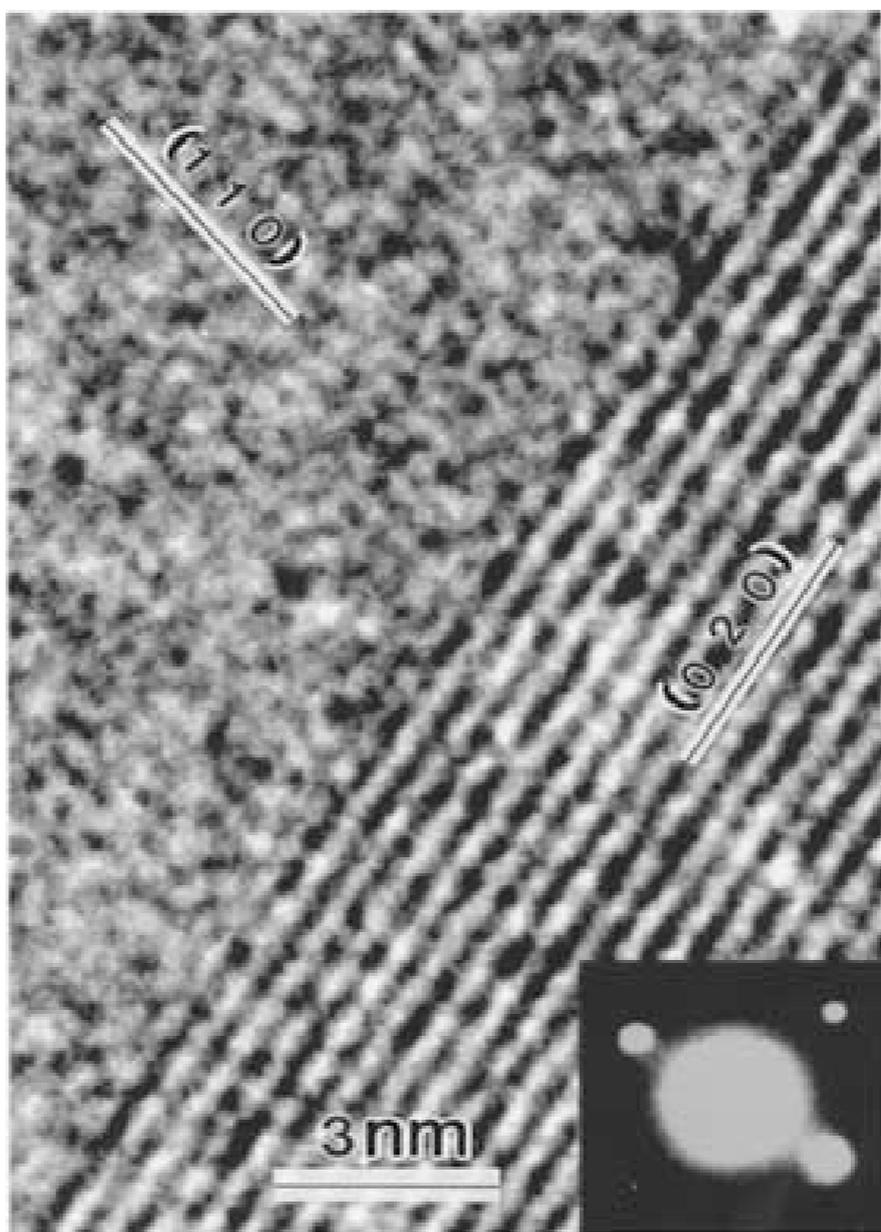
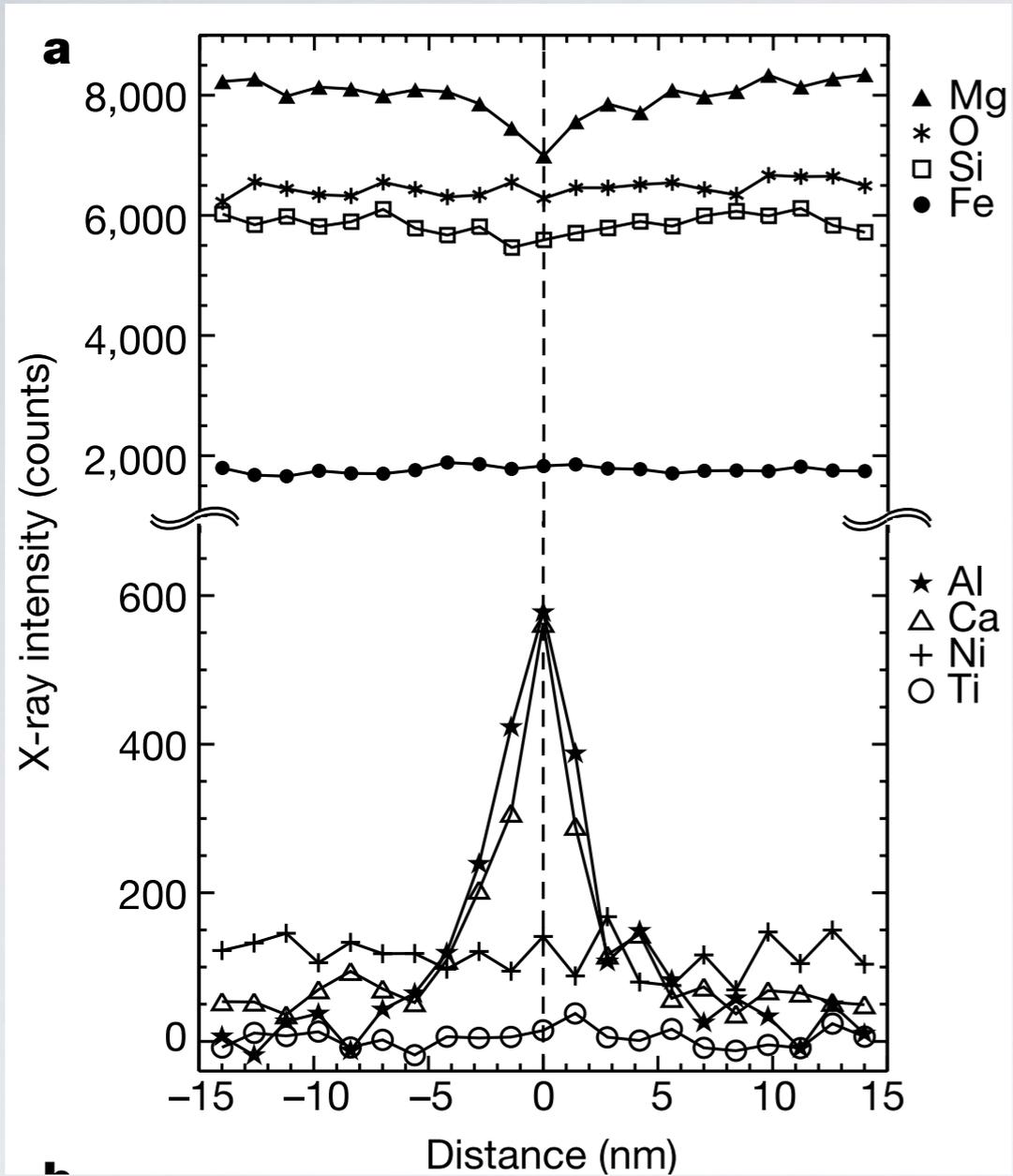
Grain boundary analysis by TEM



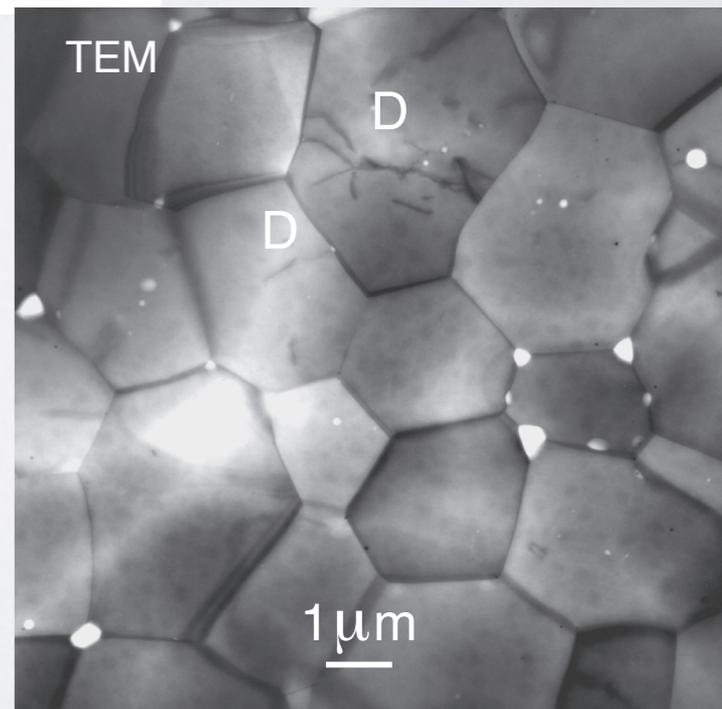
TEM EDS spectroscopy peak/background ratios of trace elements in olivine



Grain boundary composition distinct from grain interior,
correlates with grain interior composition



Hiraga et al., 2004



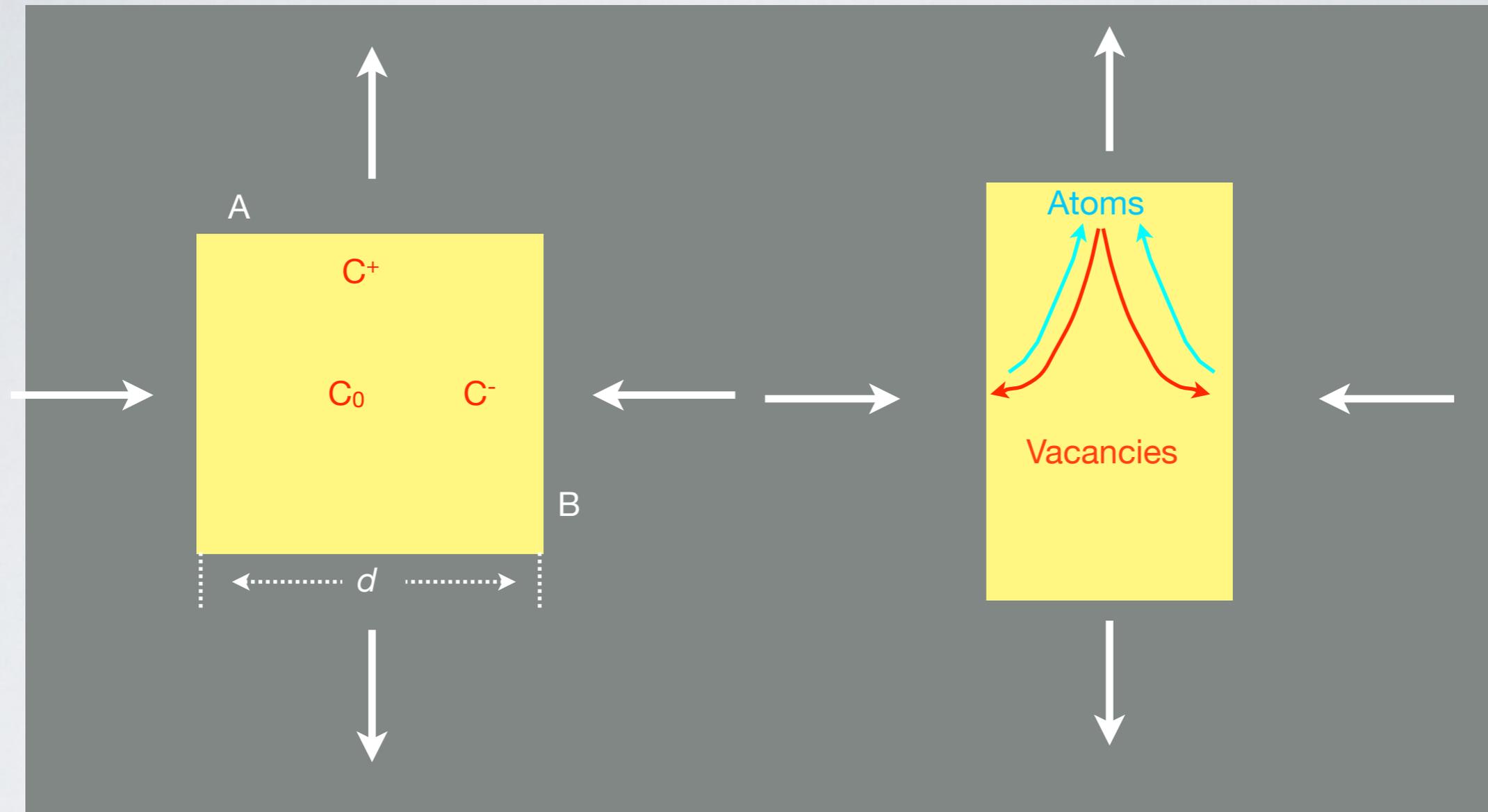
Deformation - flow laws

,first principles' derivations - physical model

constitutive equations relating strain rate to stress

Poirier, Creep of Crystals, 1985

Pure shear deformation of a single crystal: Nabarro- Herring creep



Compressive stress at face B reduces the number of vacancies.
Tensile stress at face A increases the number of vacancies.

differential stress -> concentration gradients -> diffusion

concentration gradient ~ grain size (face A - face B)

diffusion ~ diffusivity (atom species, crystal structure), temperature

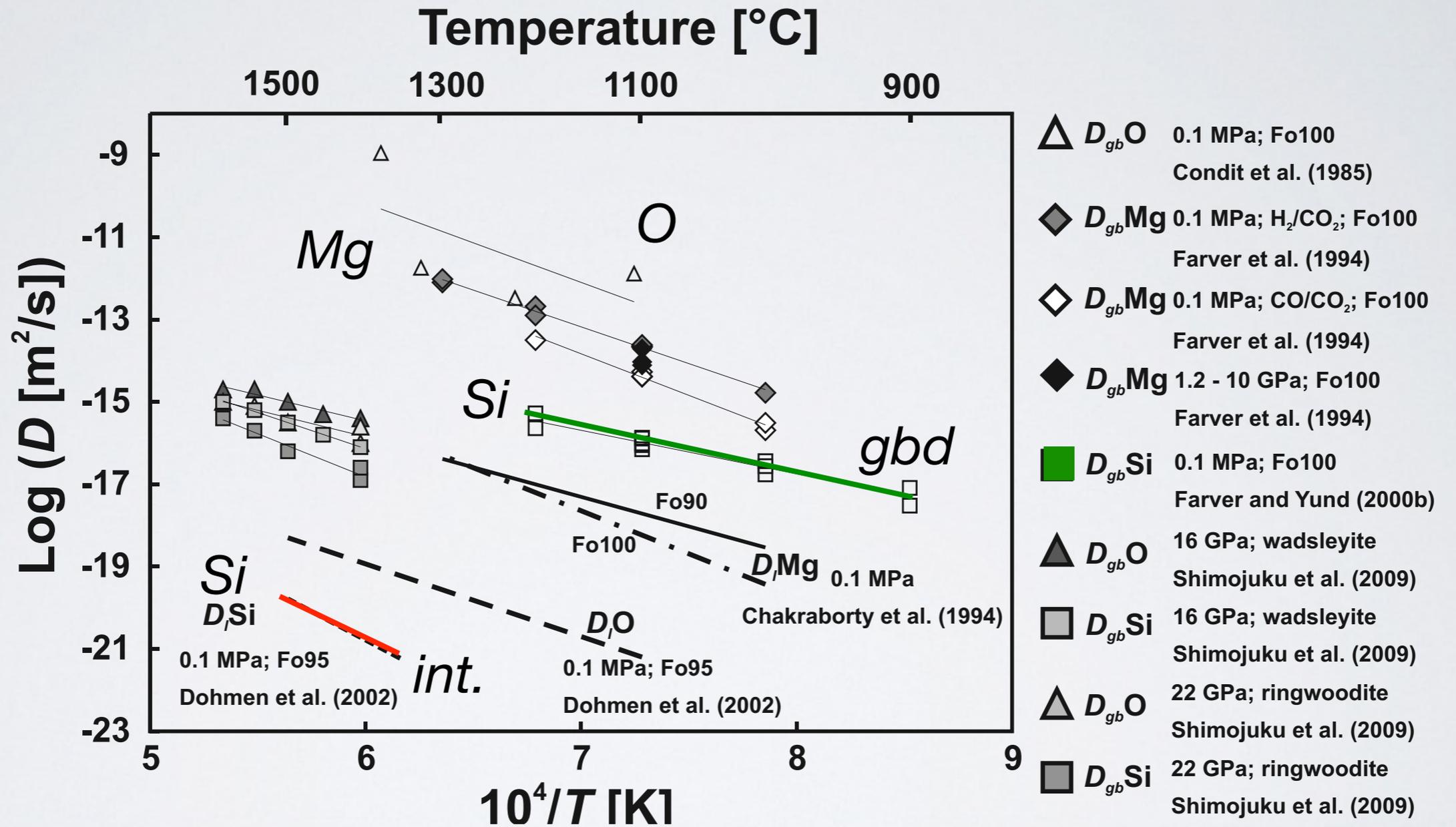
flow law (constitutive equation, strain rate $\dot{\epsilon}$ as a function of stress σ):

$$d\epsilon/dt = \dot{\epsilon} = A \sigma d^{-2} \exp[-(E+PV^*)/RT]$$

A constant (experimentally determined), d grain size,
 E activation energy, V^* activation volume

$$d\epsilon/dt = A D_{SD} \Omega \sigma / kT d^2$$

Diffusion is rate controlling: slowest species along its fastest path

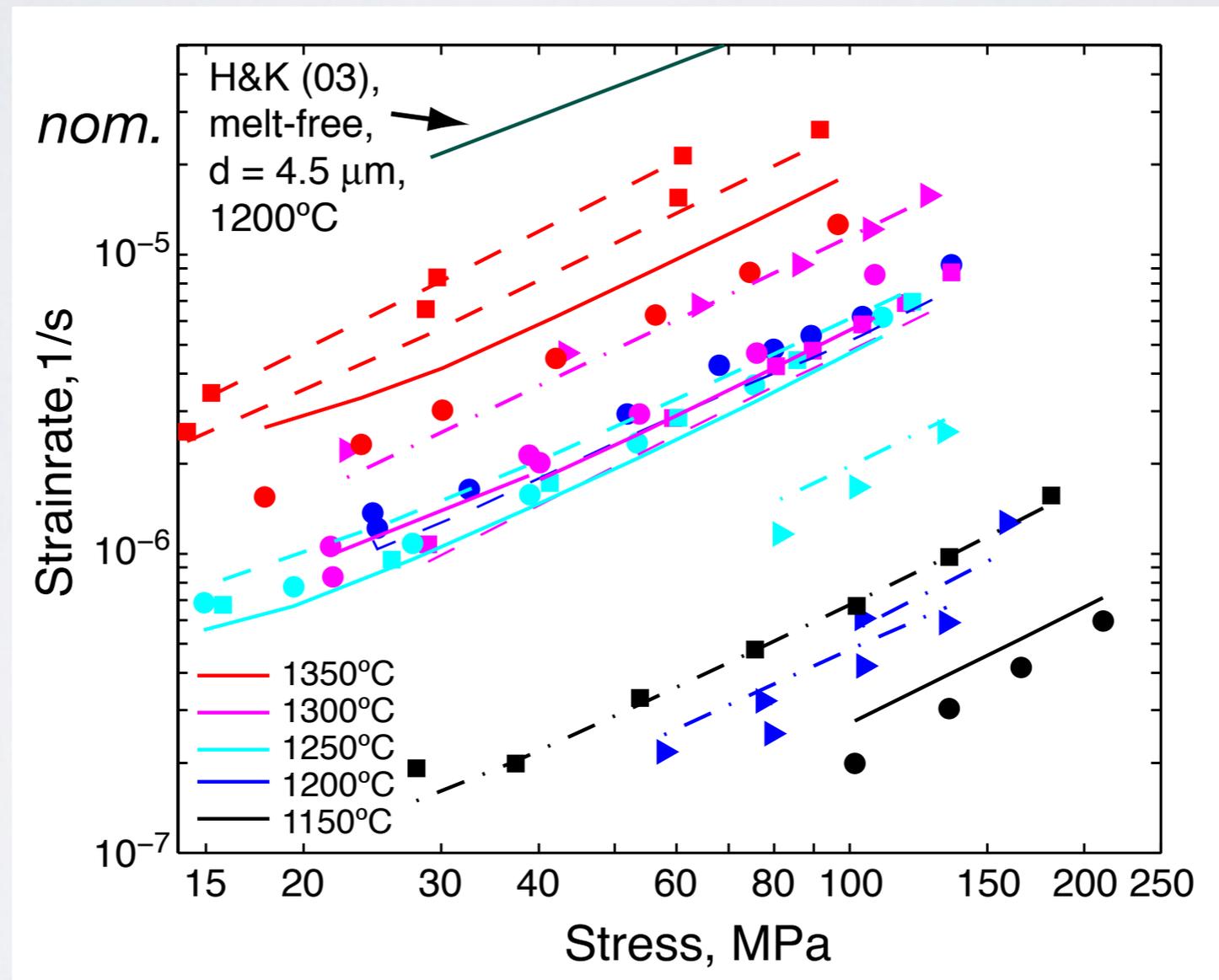


Dohmen & Milke, 2010

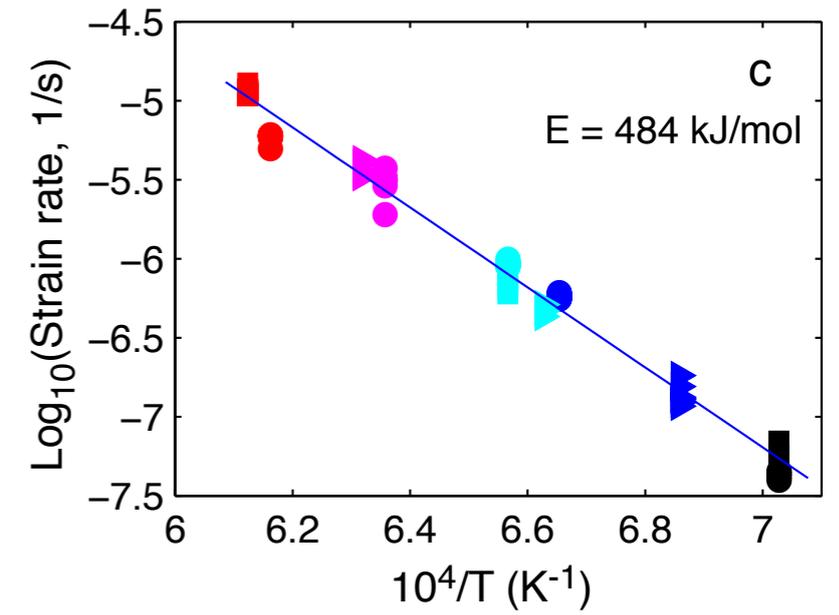
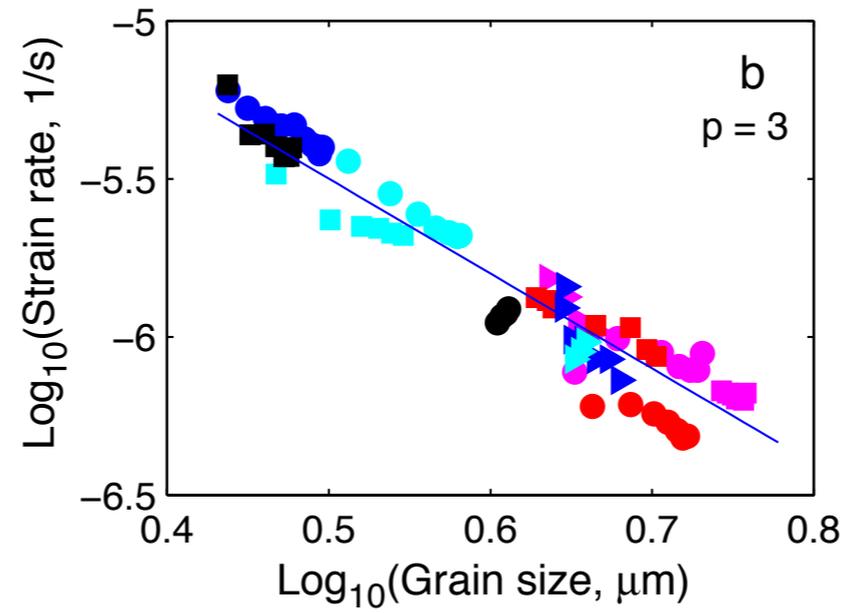
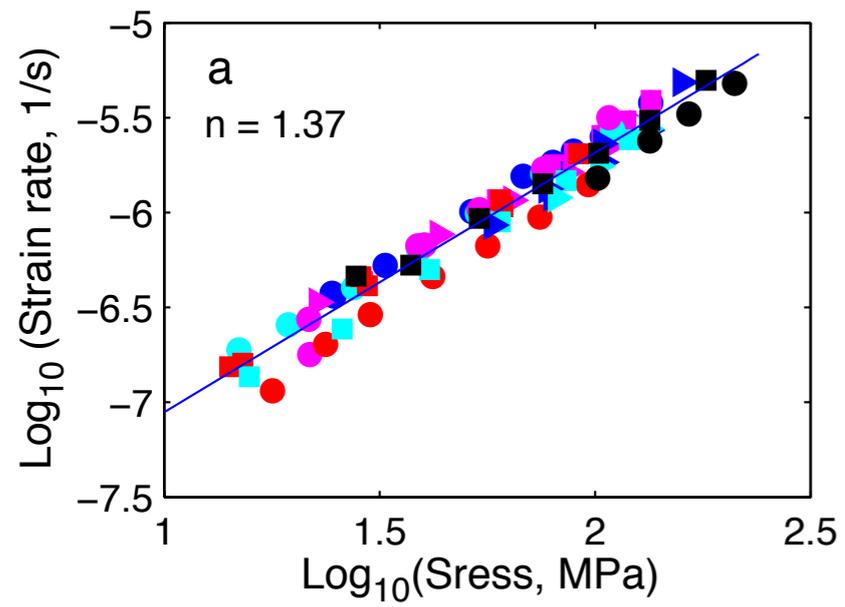
flow law for grain boundary diffusion

$$\dot{\epsilon} = A \sigma d^{-3} \exp[-(E+PV^*)/RT]$$

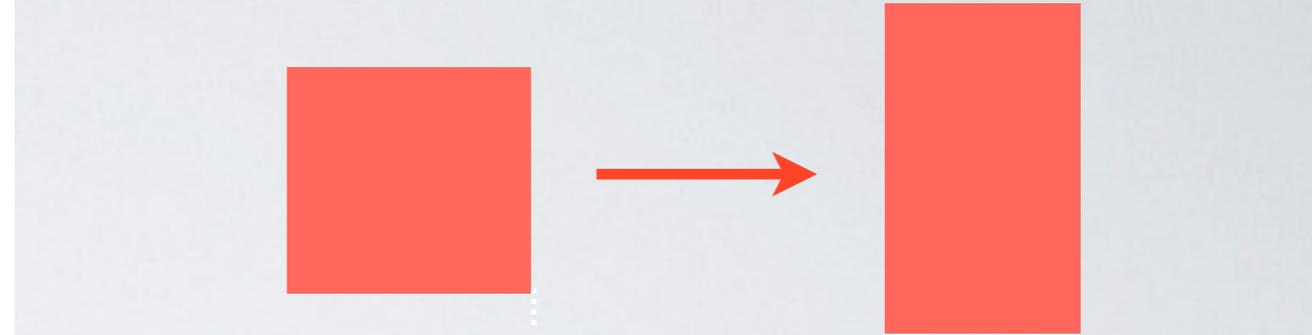
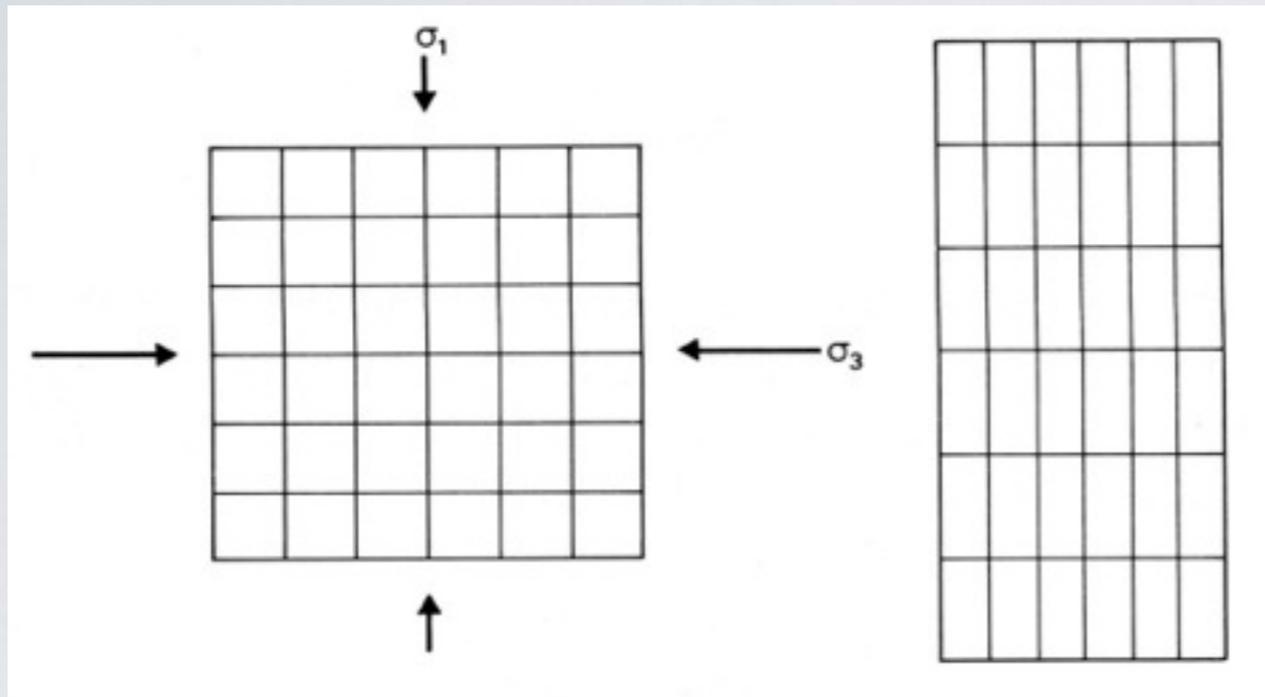
but A , E , V^* are also specific to diffusion mechanism



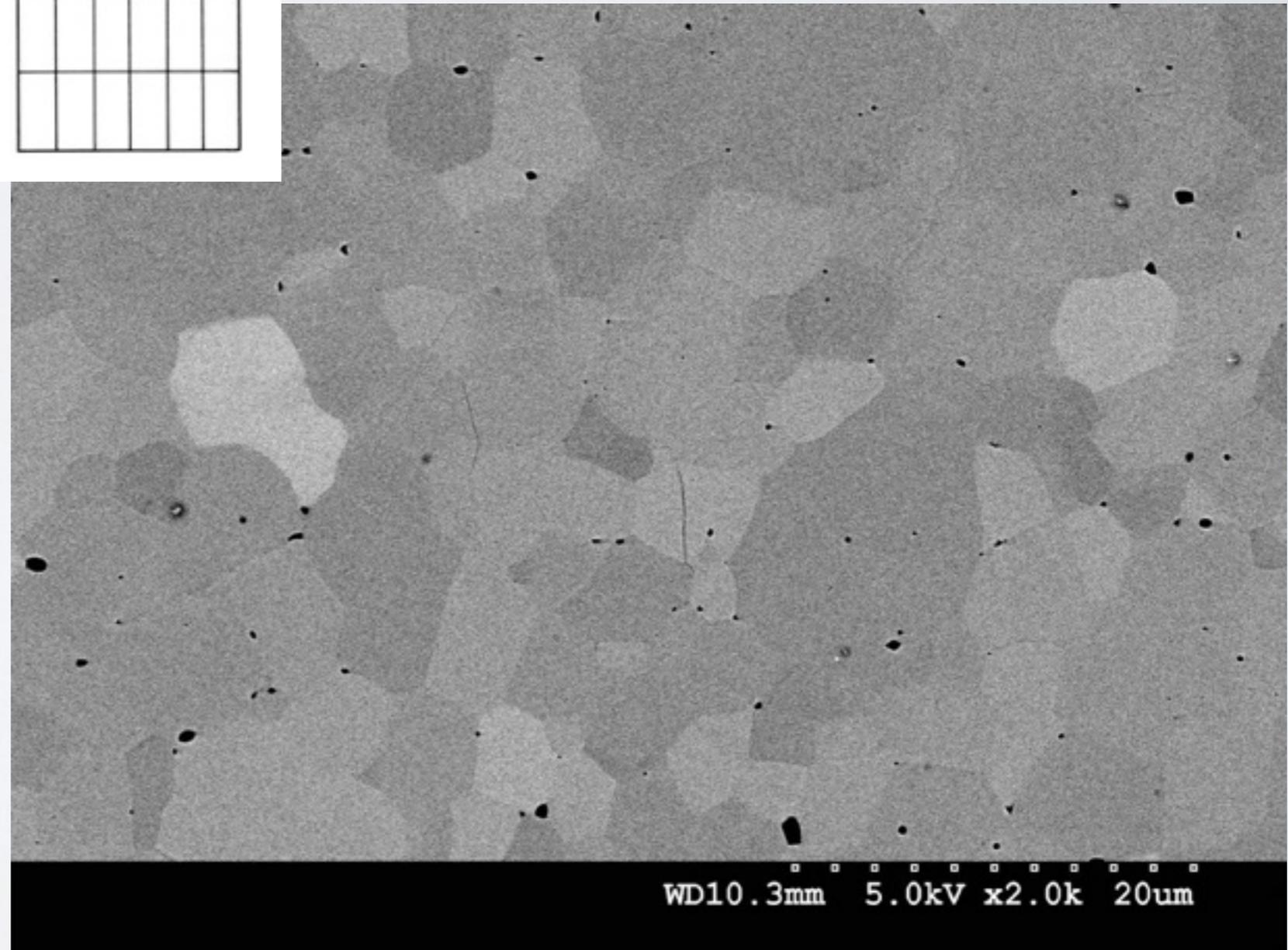
Fit parameters



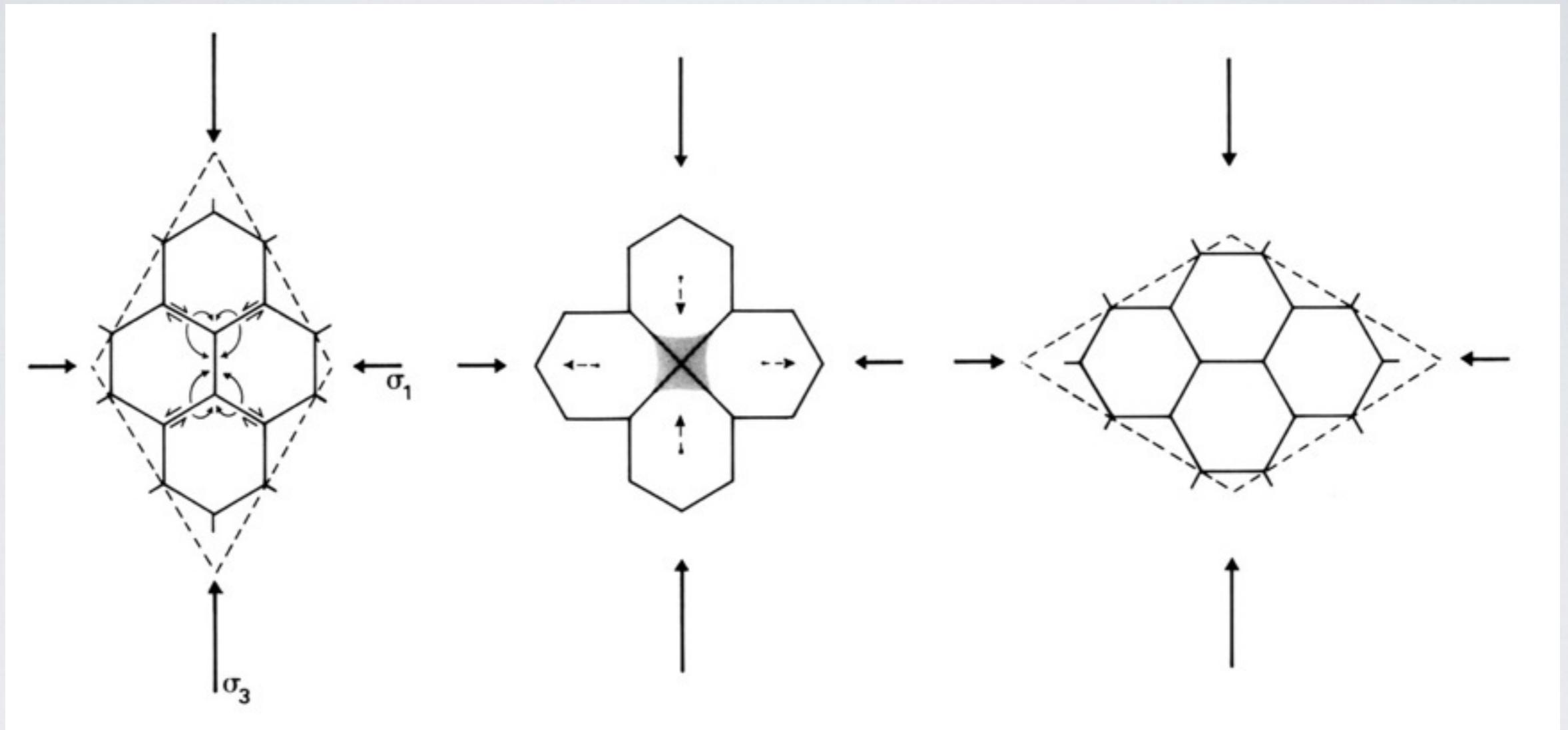
But: "Pure" diffusion creep would lead to shape change of grains:



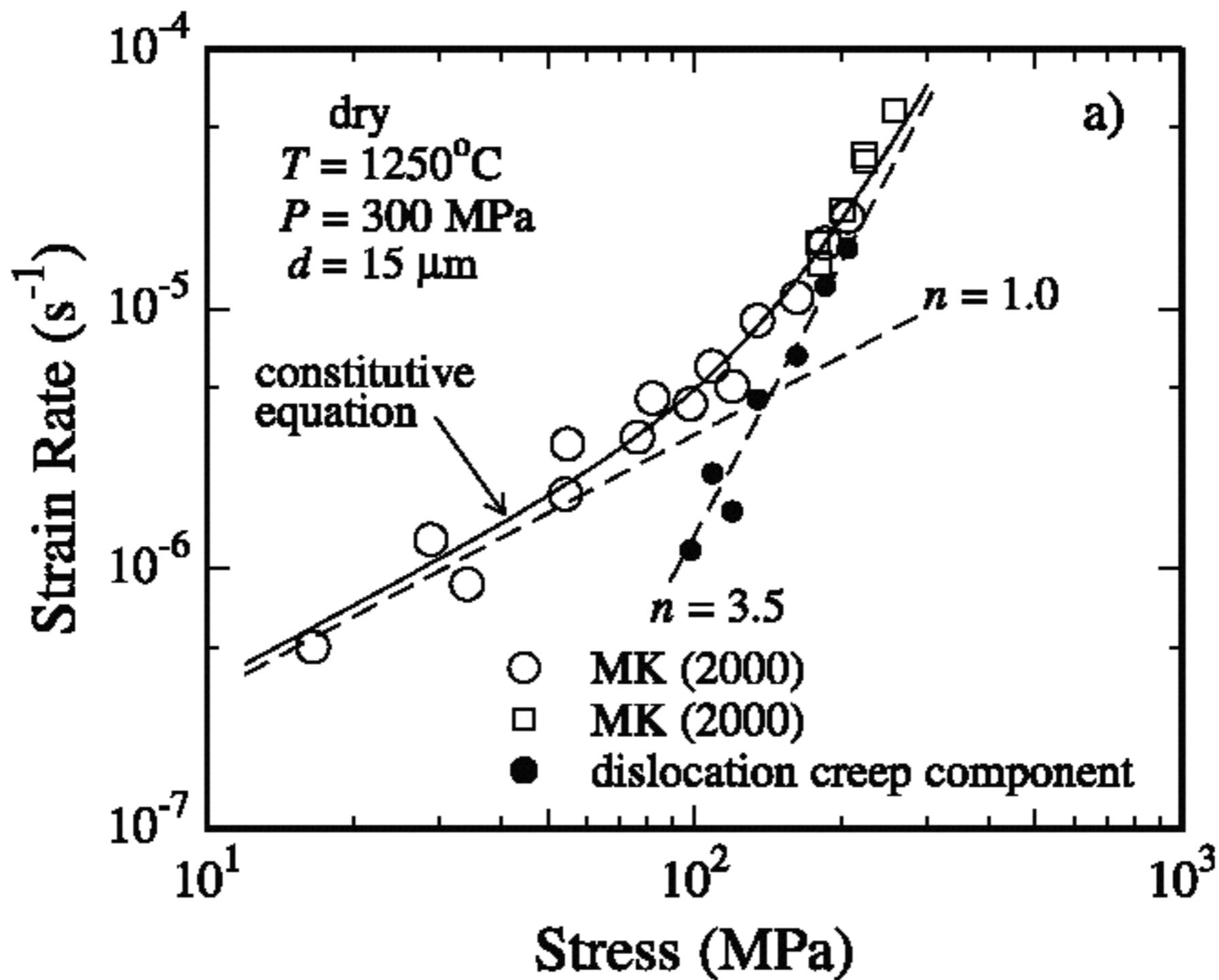
Observation: Grains remain equiaxed after deformation



Diffusionally accommodated grain boundary sliding (diffusion creep)



Macroscopic shape change without grain
shape change



Hirth, 2003

Dislocation creep (Weertman creep)

glide velocity: $v \sim b v_0 \exp(-E/kT)$
(b Burgers vector)

but dislocations get 'stuck' (entangled): edge dislocations have to 'climb' out of their glide plane, climb is rate limiting. Climb is a diffusive process.

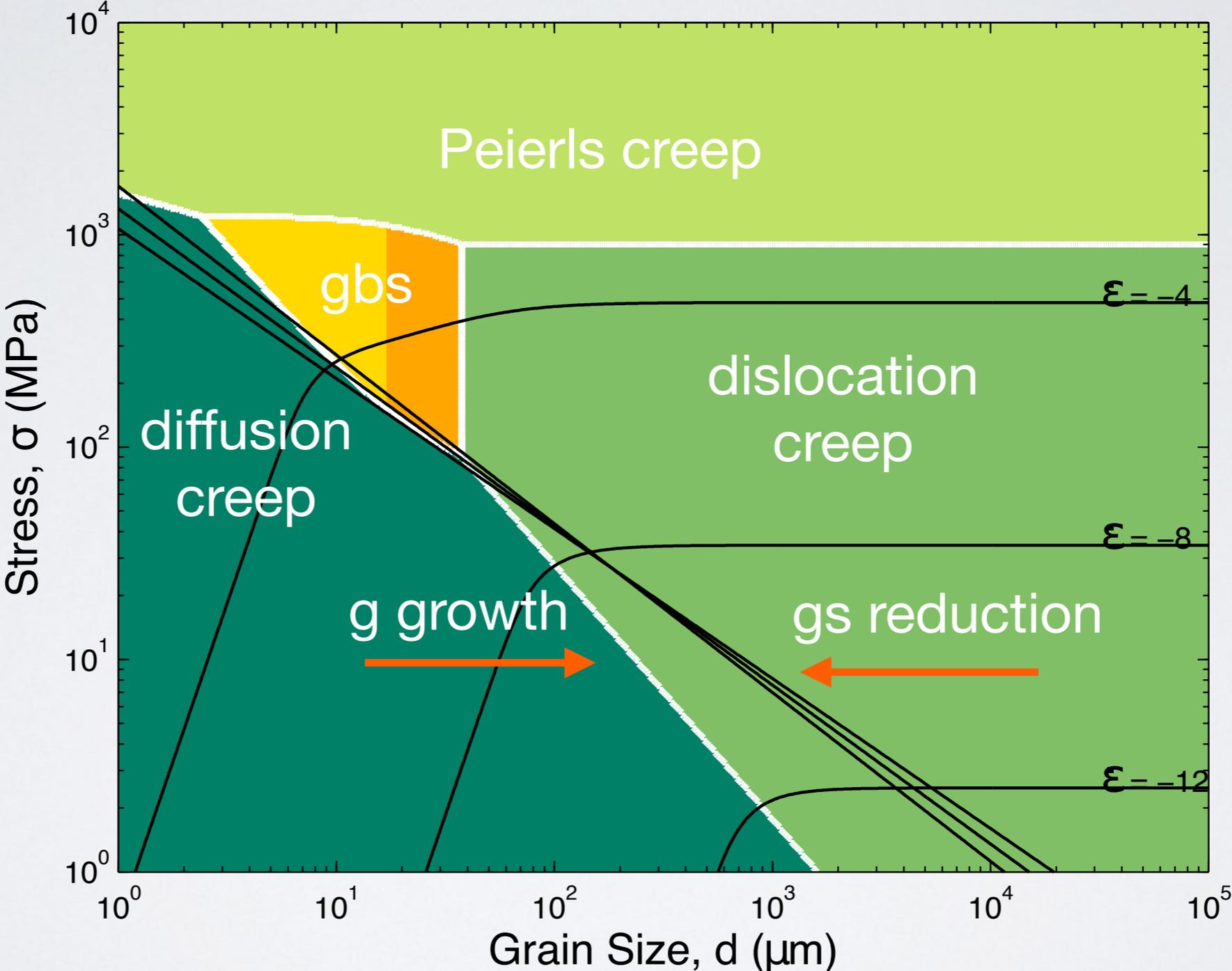
$$\dot{\epsilon} = A \sigma^n \exp[-(E+PV^*)/RT]$$

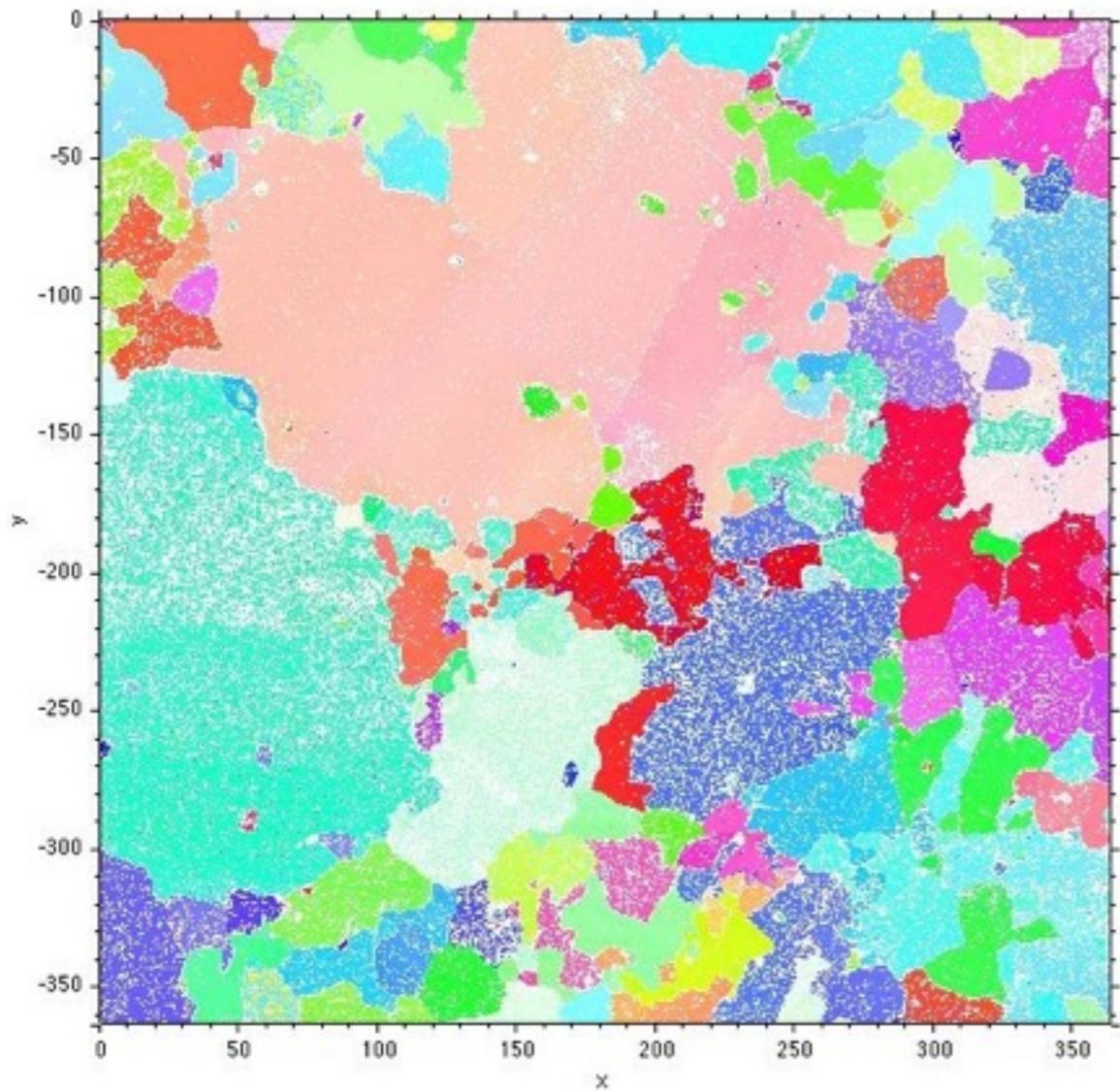
dislocation density \sim stress: strain rate depends on stressⁿ

dislocations are intracrystalline, no grain size dependence

Deformation Mechanism Map

Olivine, 1250°C, 0.4 GPa





Electron backscatter diffraction map

