

Rheology

Ulrich Faul

Massachusetts Institute of Technology

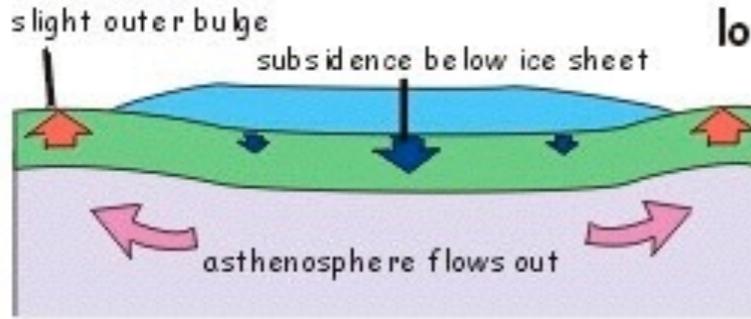
model for post-glacial rebound

ice sheet



elastic lithosphere

viscous asthenosphere



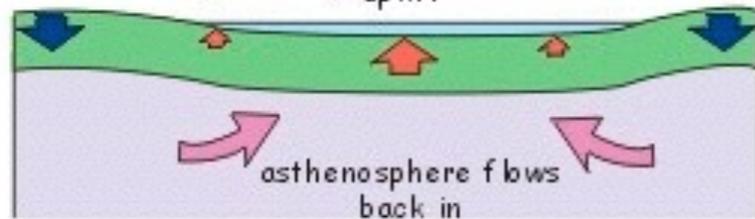
loads the plate

curvature of outer bulge is a function of elastic lithosphere thickness

ice melts quickly

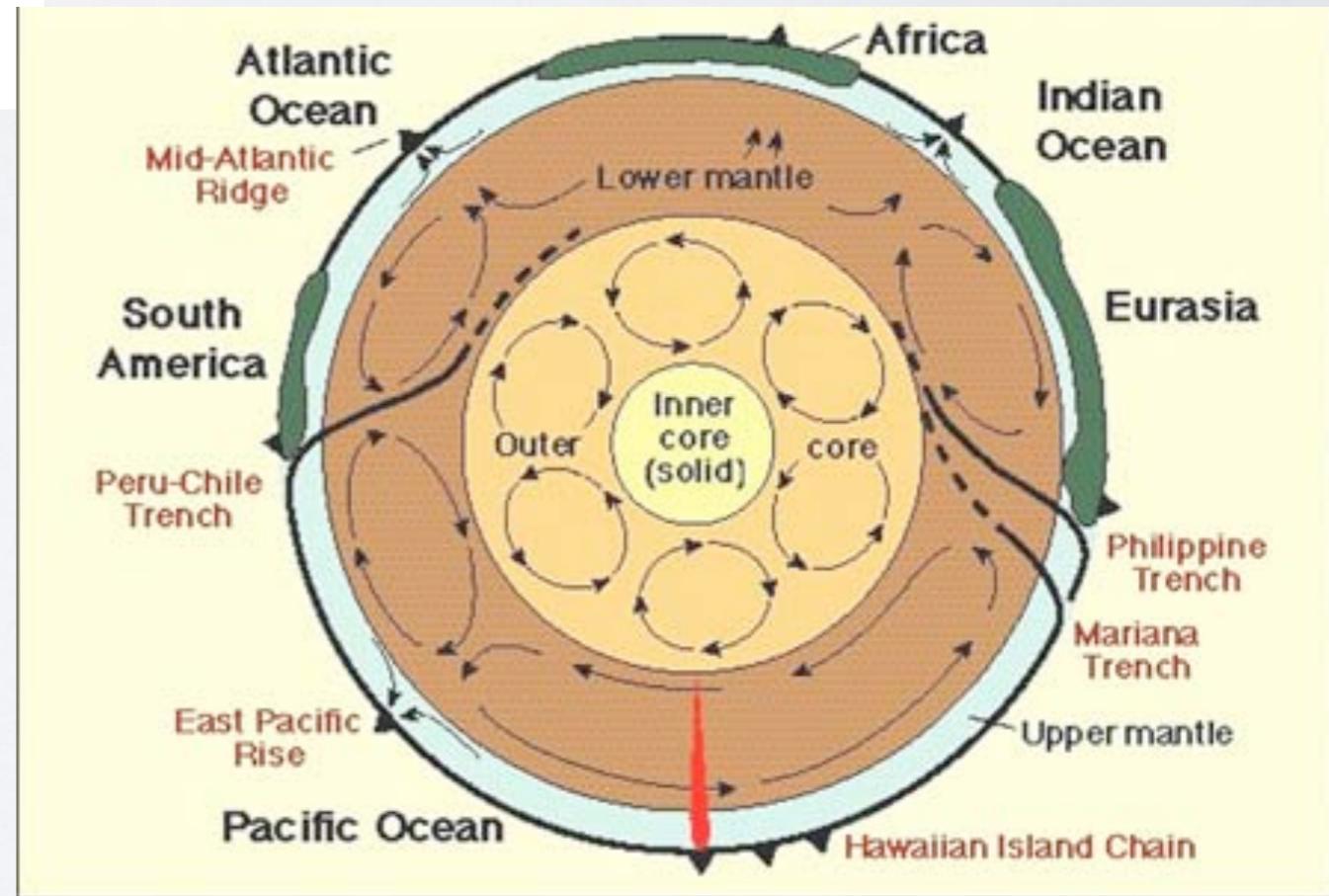
uplift

over thousands of years



rate is a function of asthenosphere viscosity

rheology - viscous deformation
- flow



Outline

fundamentals of defects

types of defects

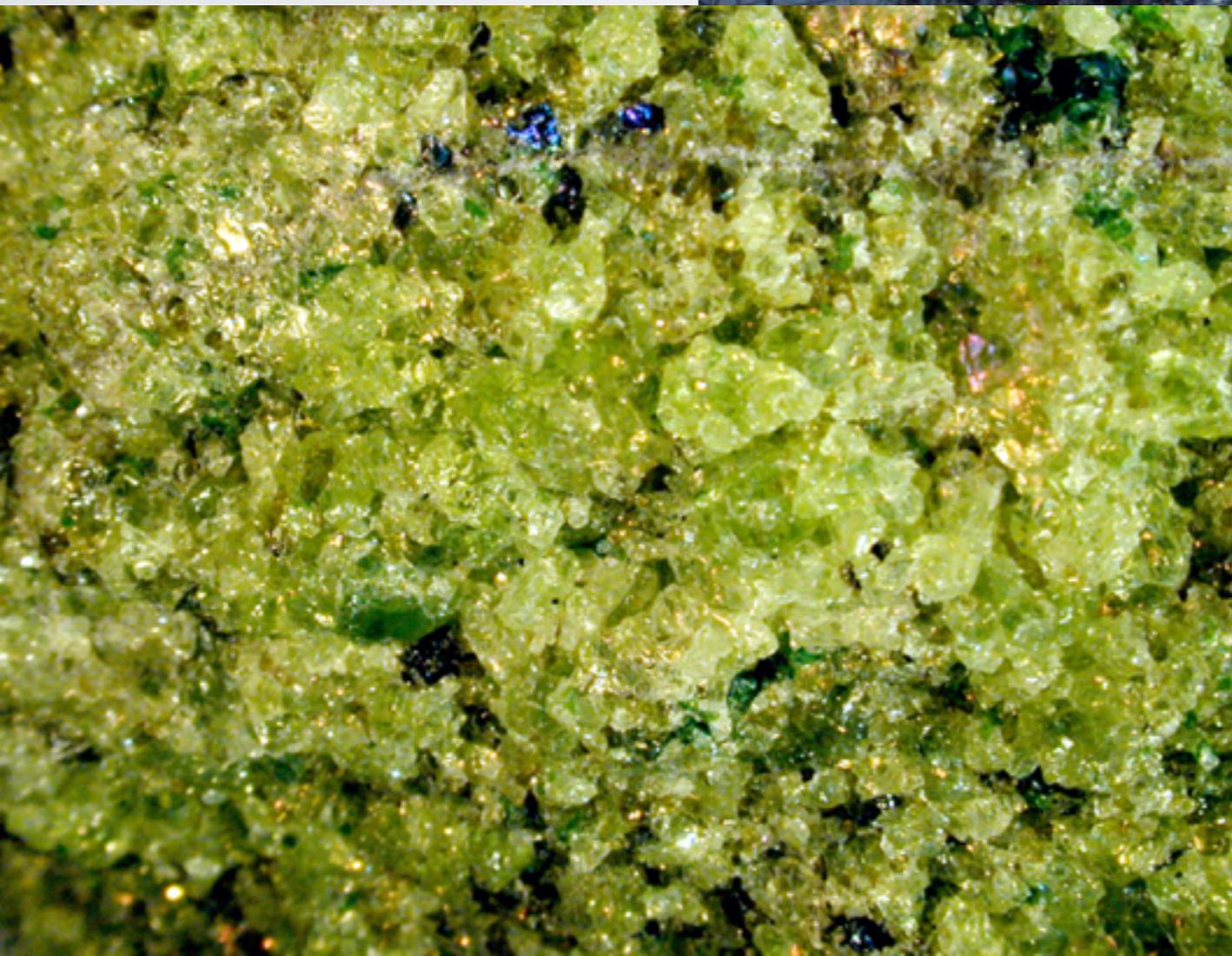
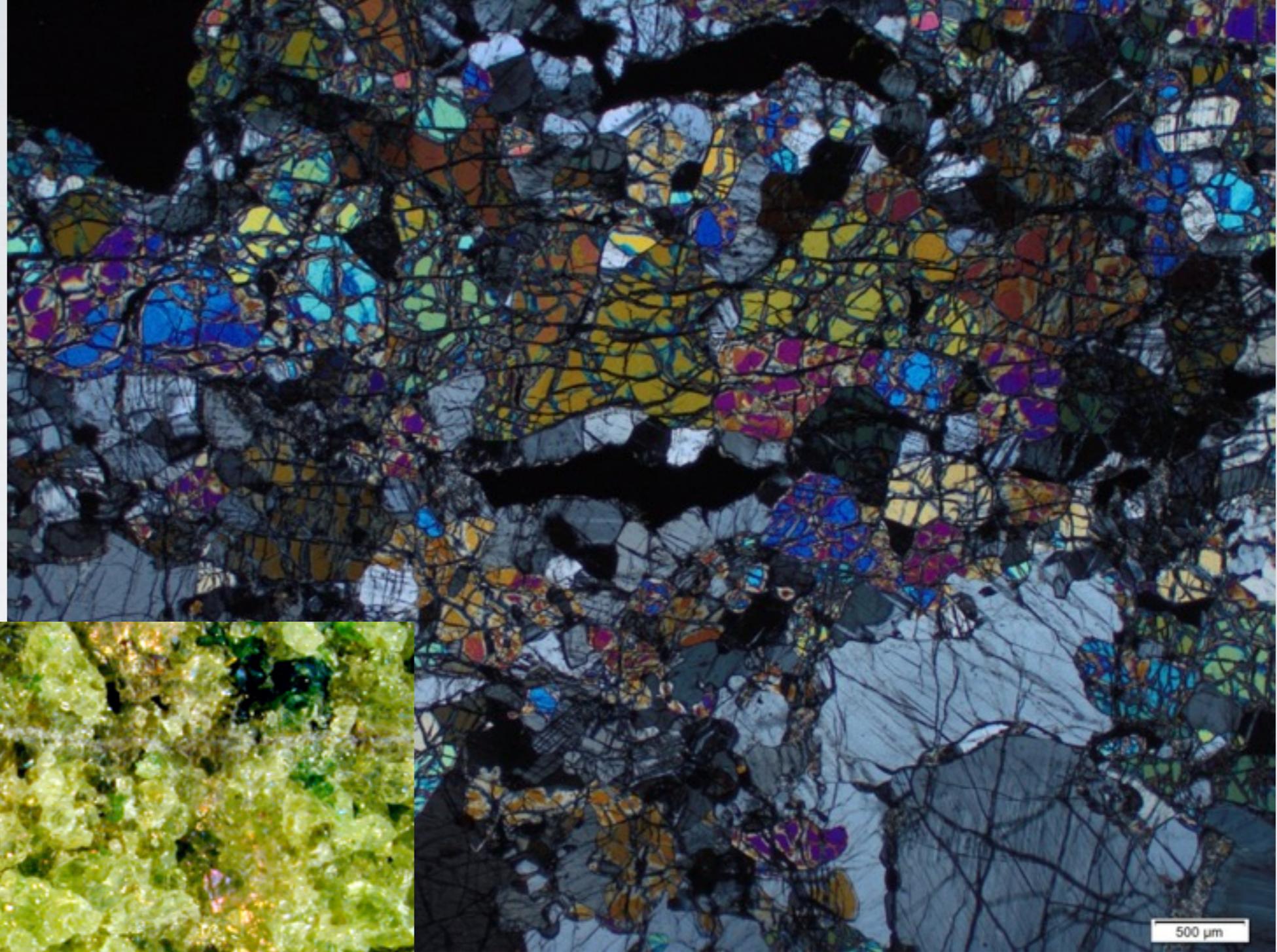
flow laws

effect of temperature

melt

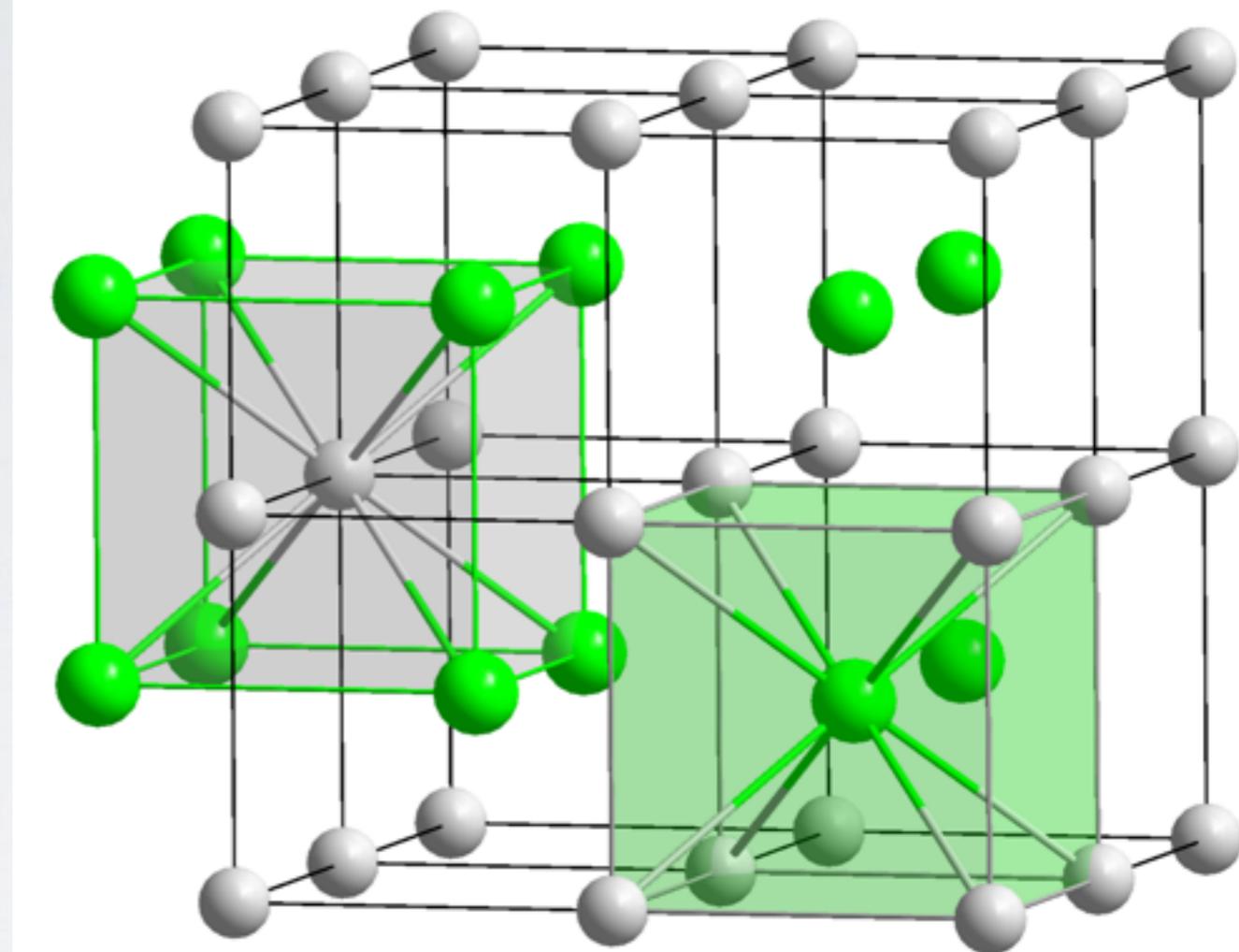
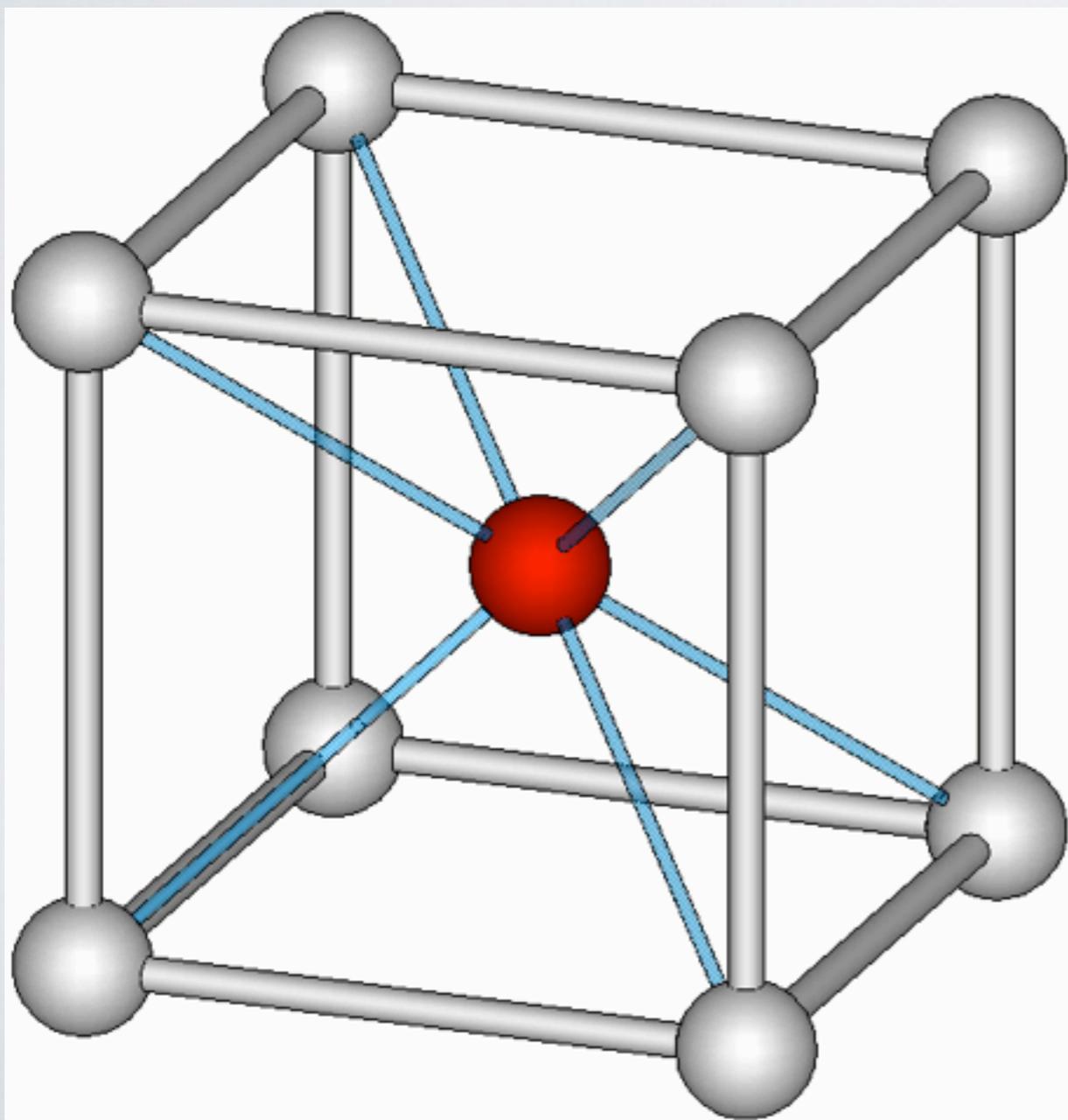
water

cross-polarized
light image of a
peridotite

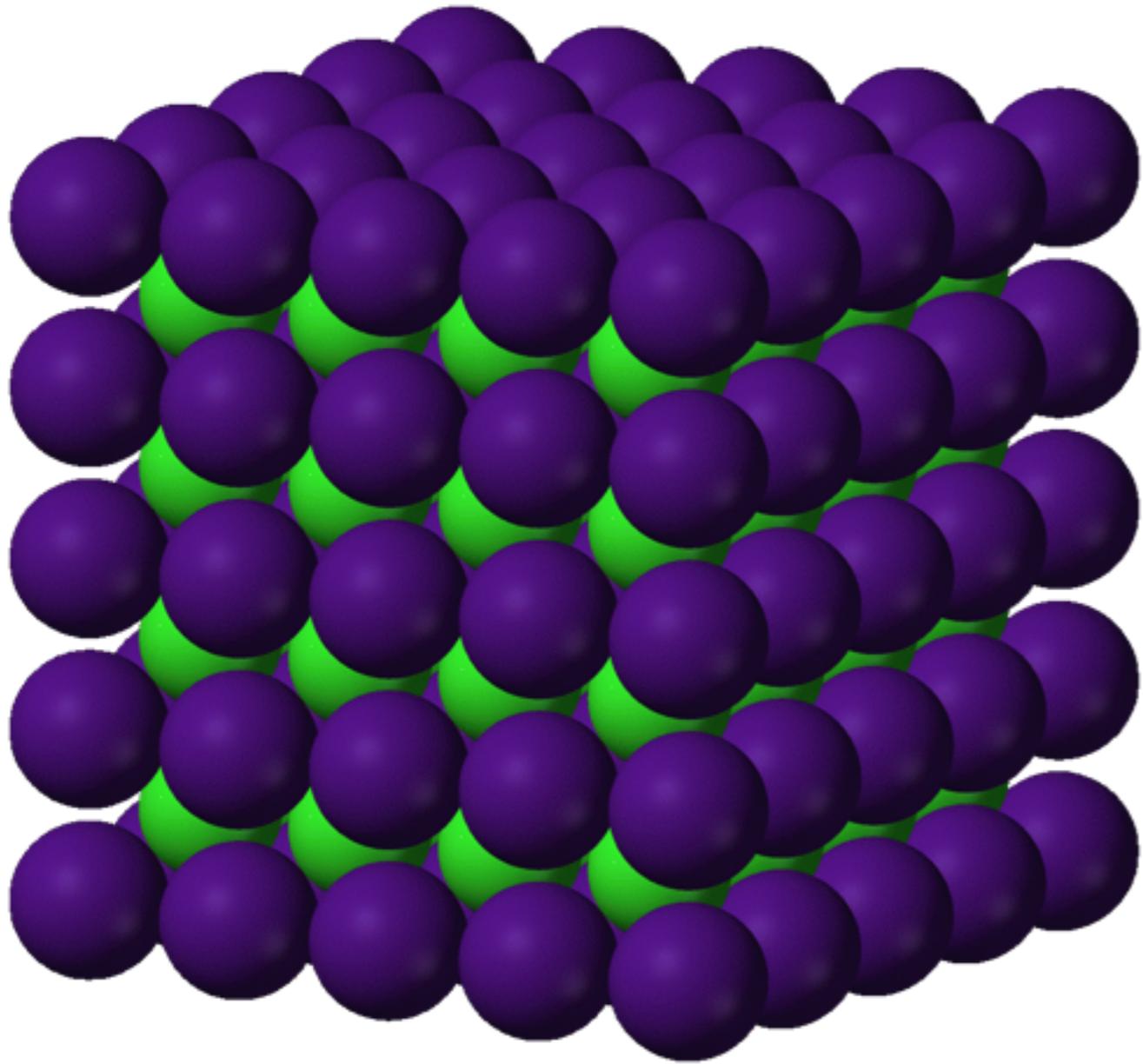


peridotite xenolith

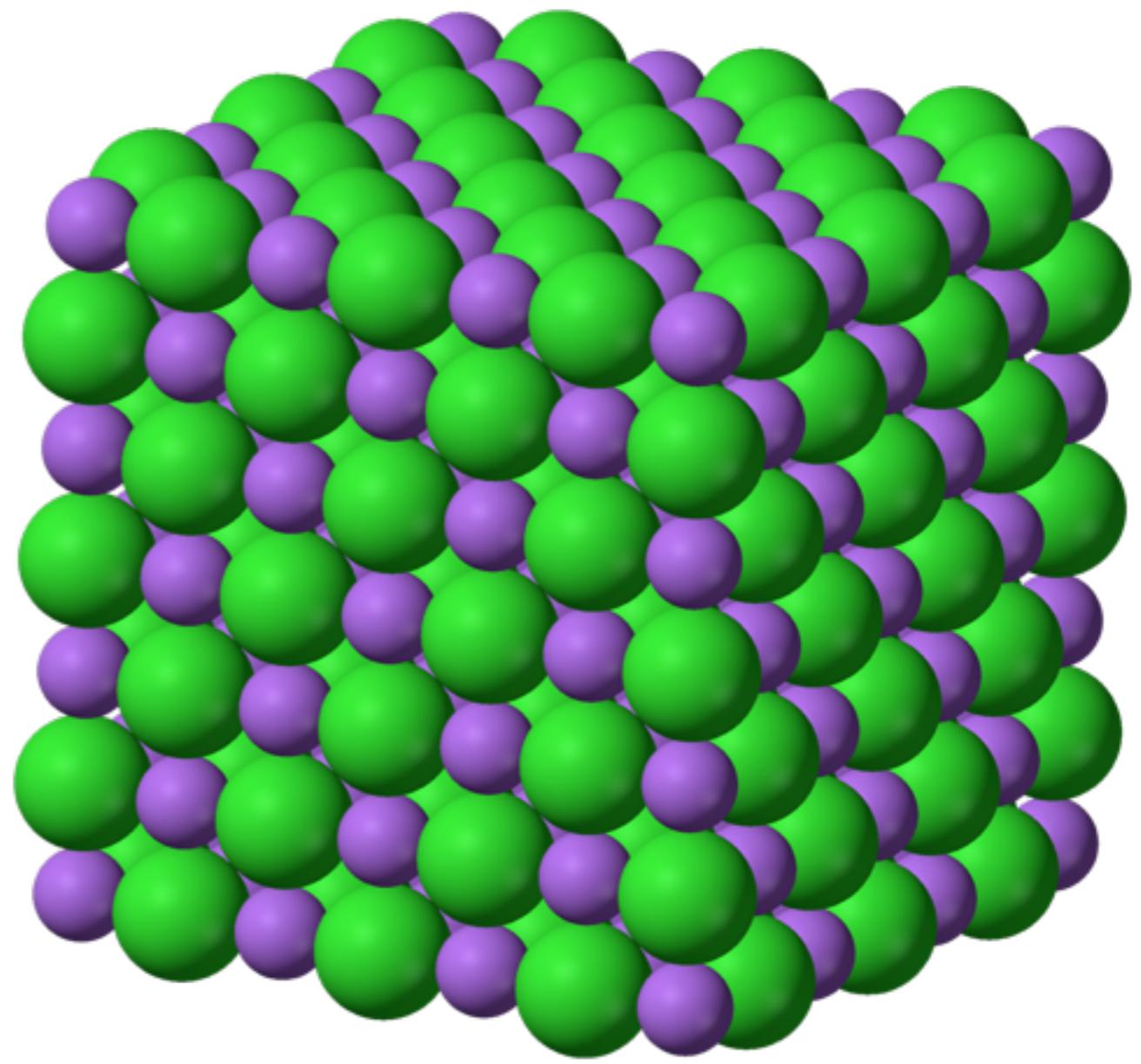
CsCl



Ionic bonding



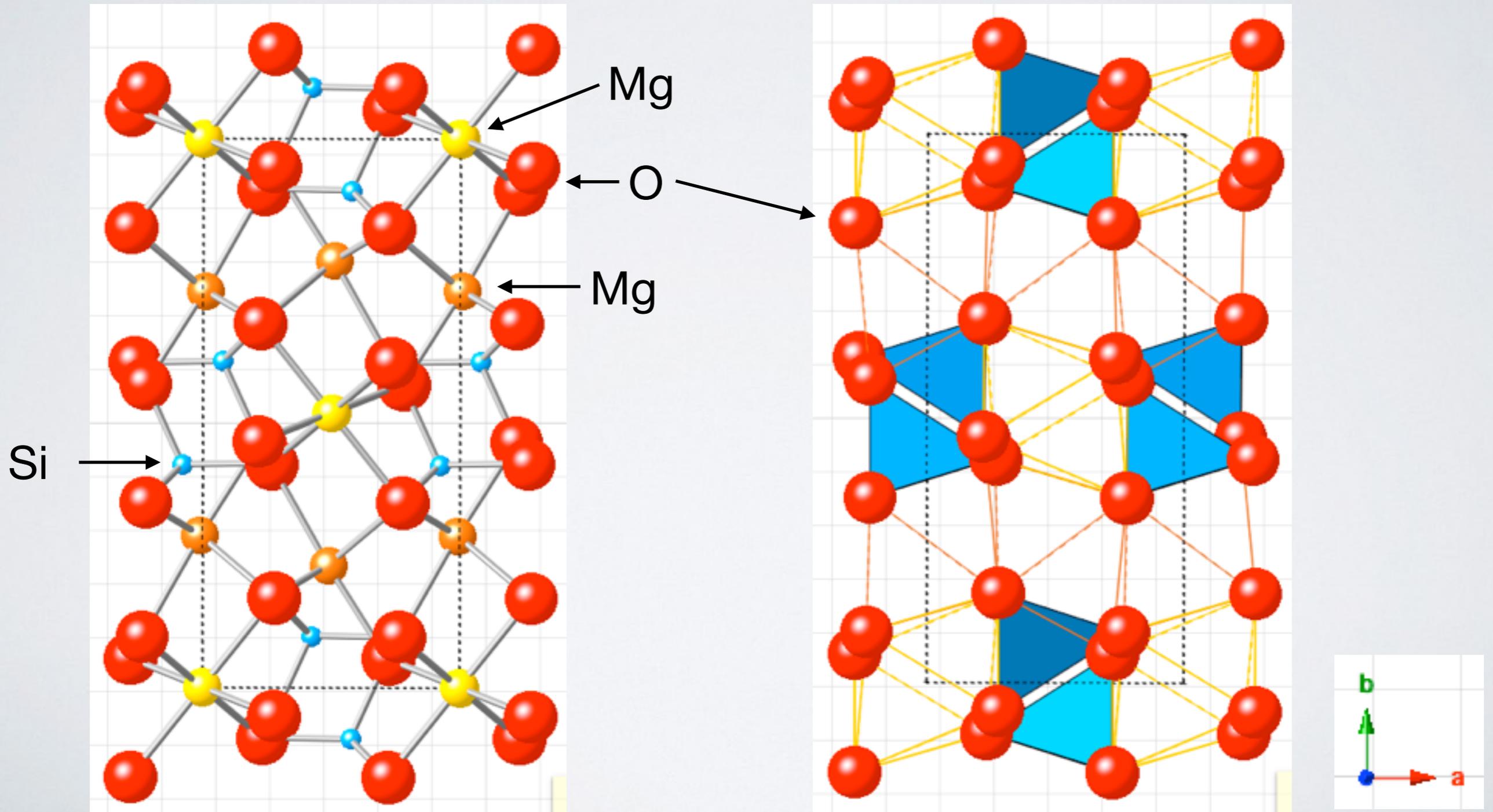
CsCl - simple cubic



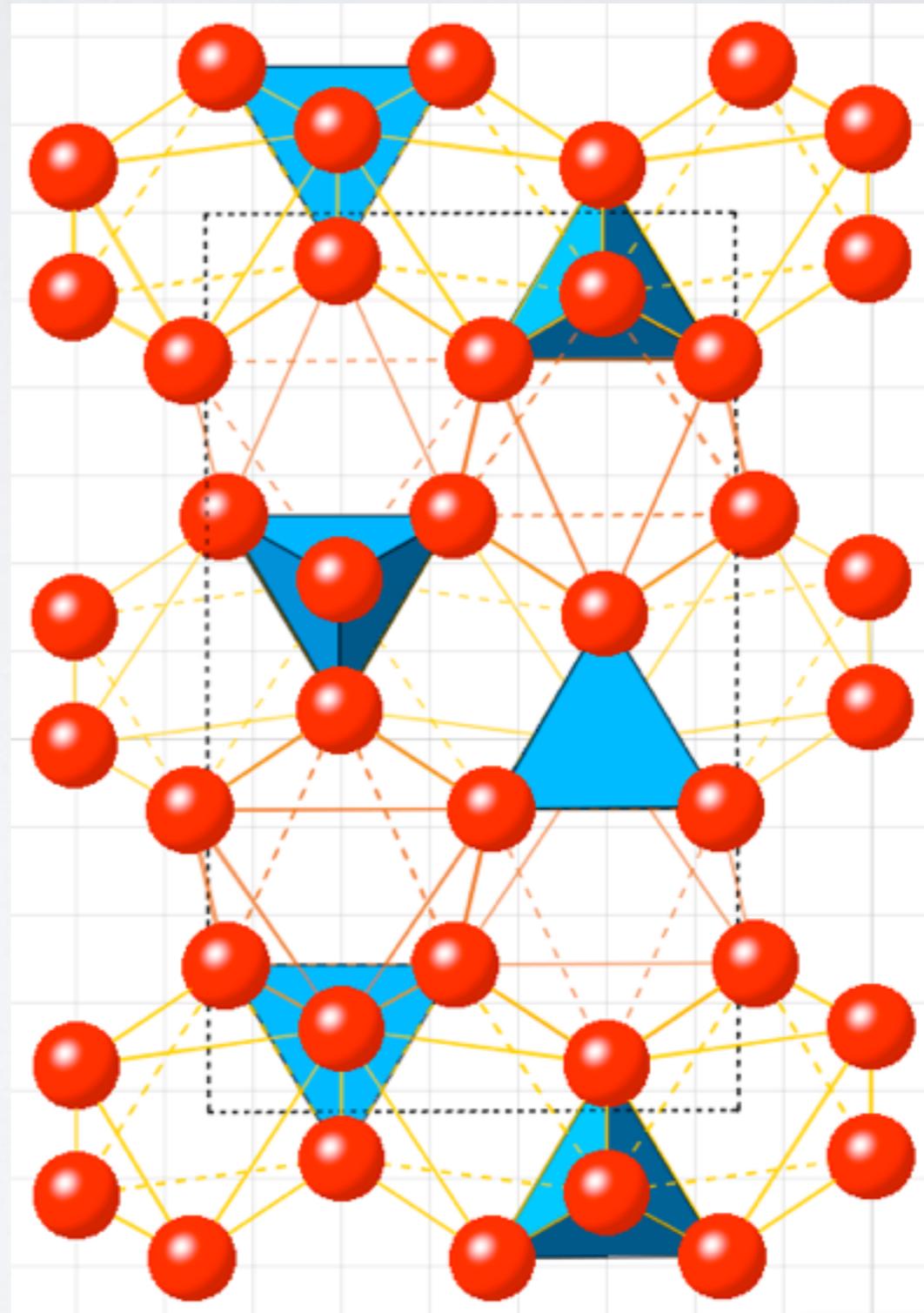
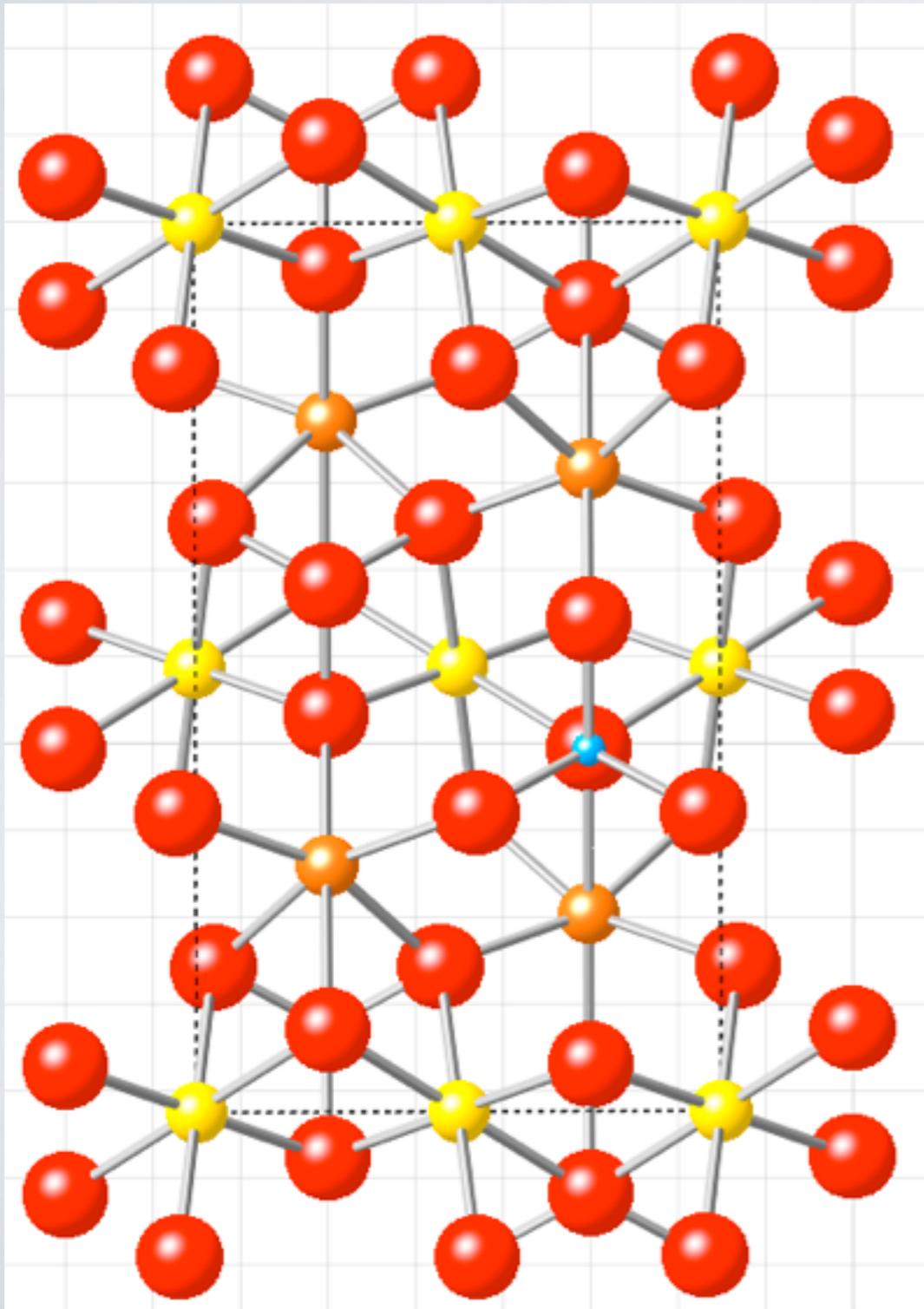
NaCl - face centered cubic

Olivine (Mg_2SiO_4)

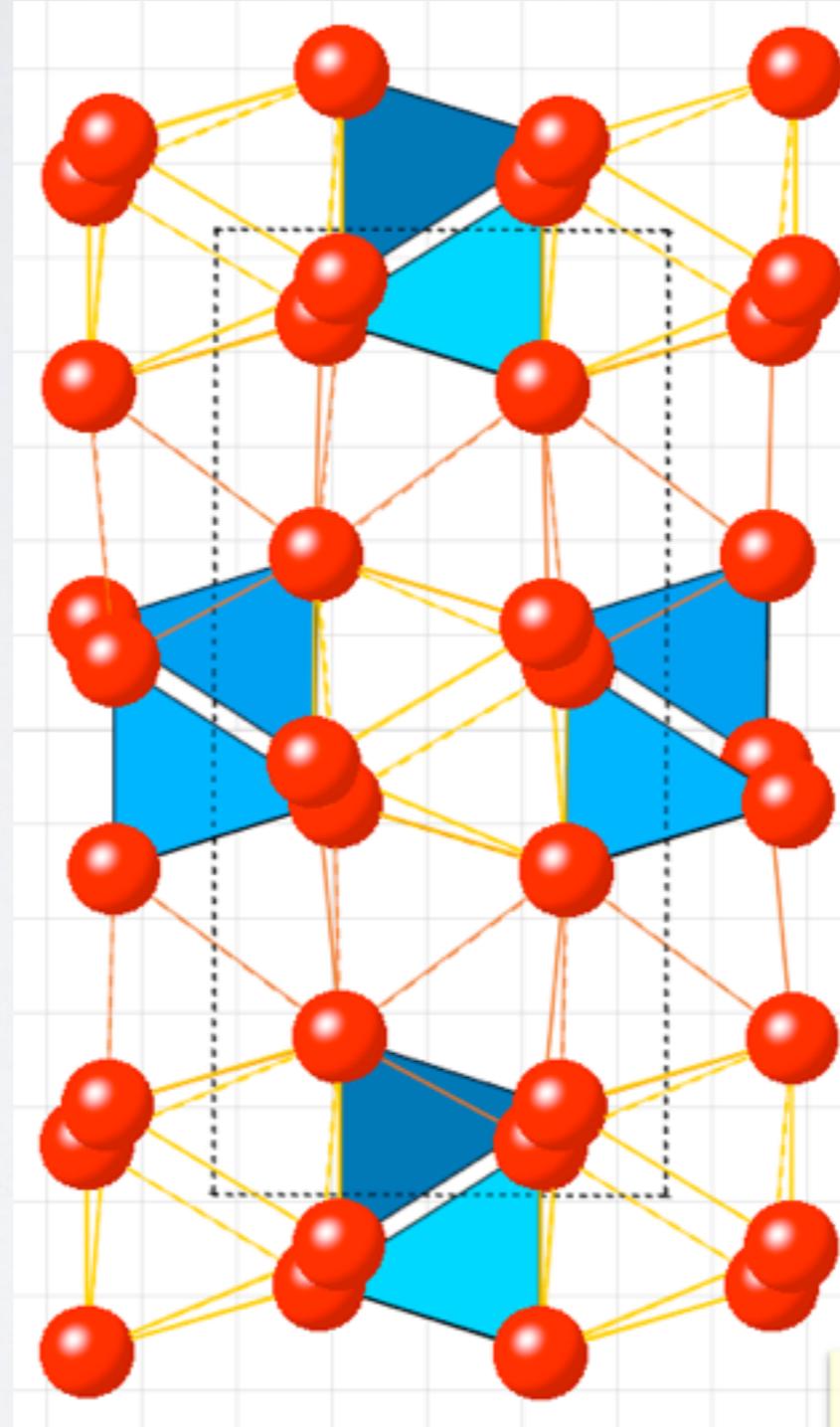
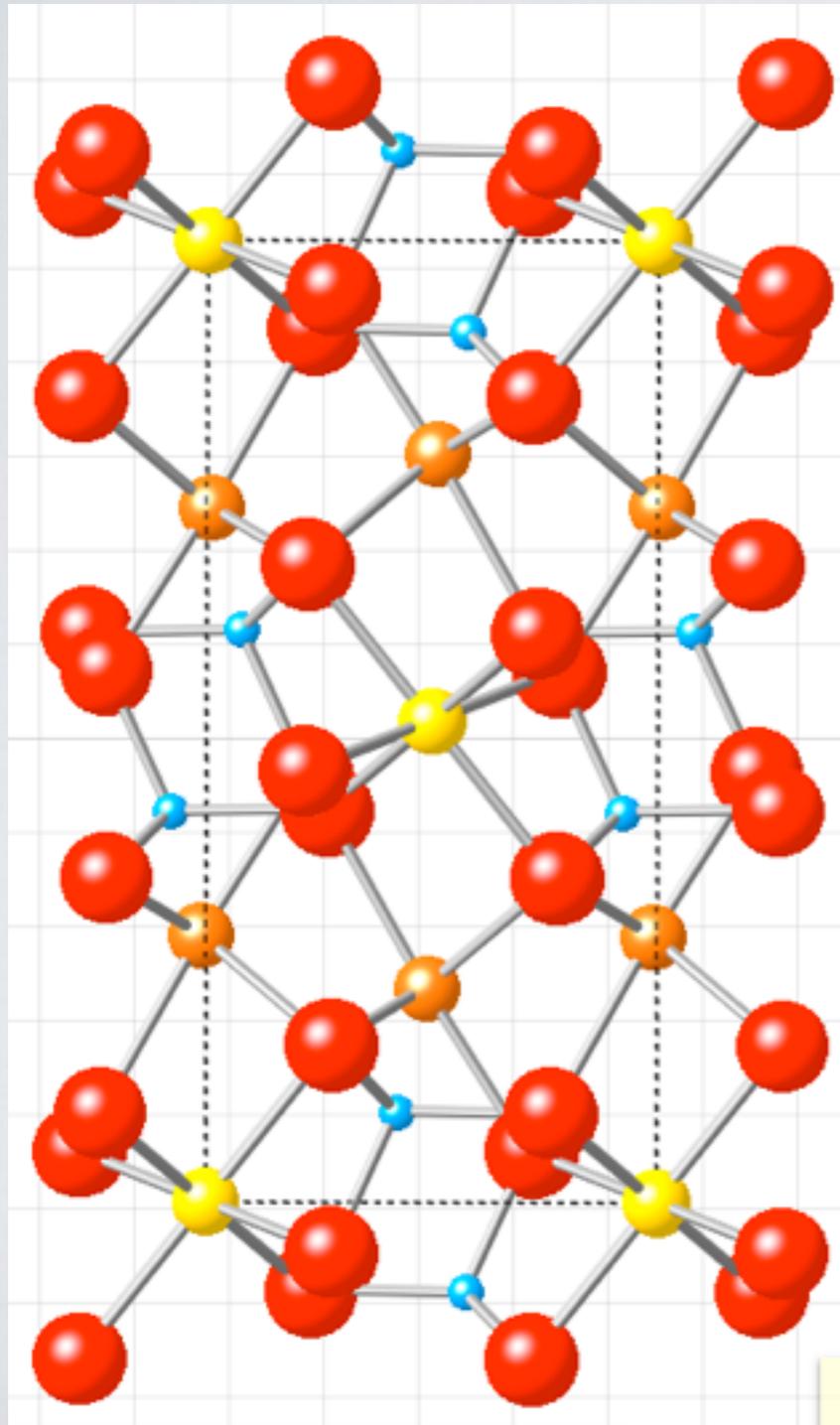
- Tetrahedrally coordinated Si, octahedrally coordinated M sites.
- Si-O bonds shortest and strongest.
- Large spacing of (010) planes and close spacing of (100) planes.



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



Anisotropy due to crystal structure

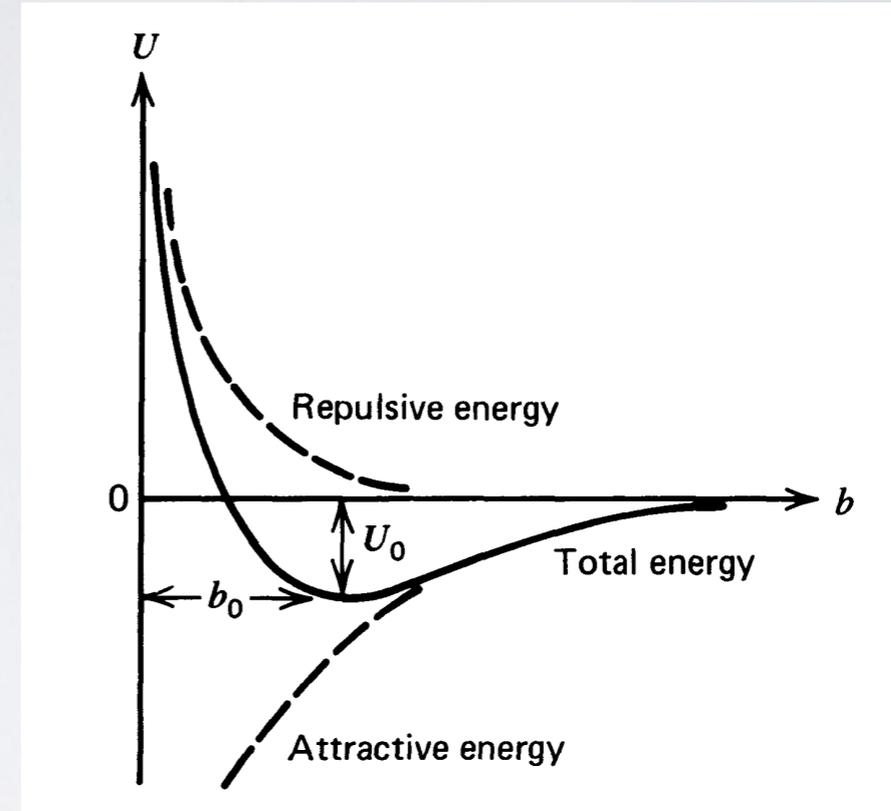
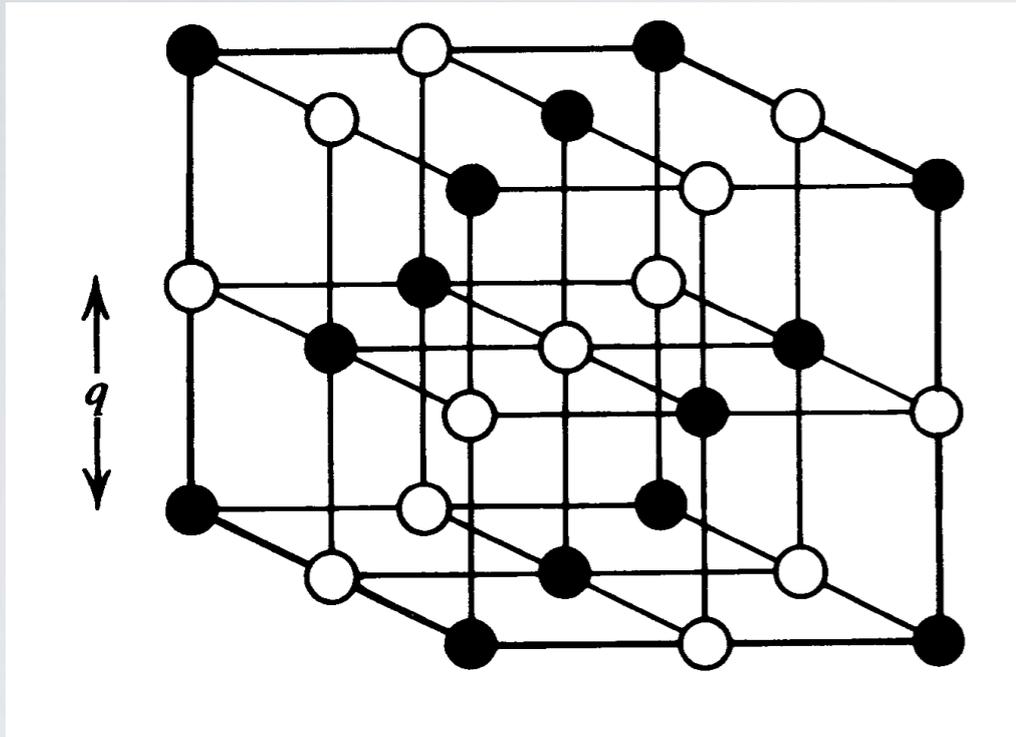


	a	b	c
unit cell dim. (Å)	4.78	10.25	6.3
V_p , km/s	9.89	7.72	8.43
V_s , km/s	4.89	4.42	4.87

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



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

Thermodynamics *(Fundamental state functions)*

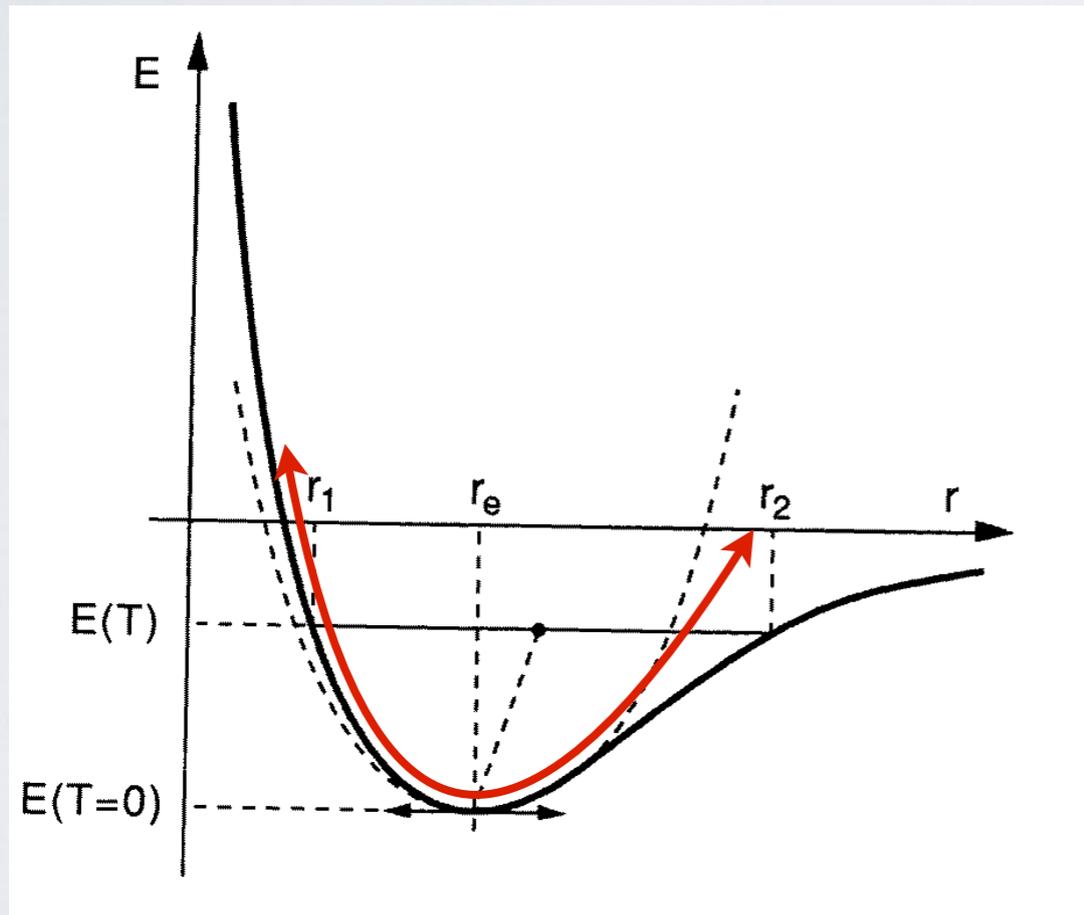
Internal energy U: Energy content of a system, the sum of the potential energy stored in interatomic bonding (electrostatic energy) plus the kinetic energy of atomic vibrations.



Temperature

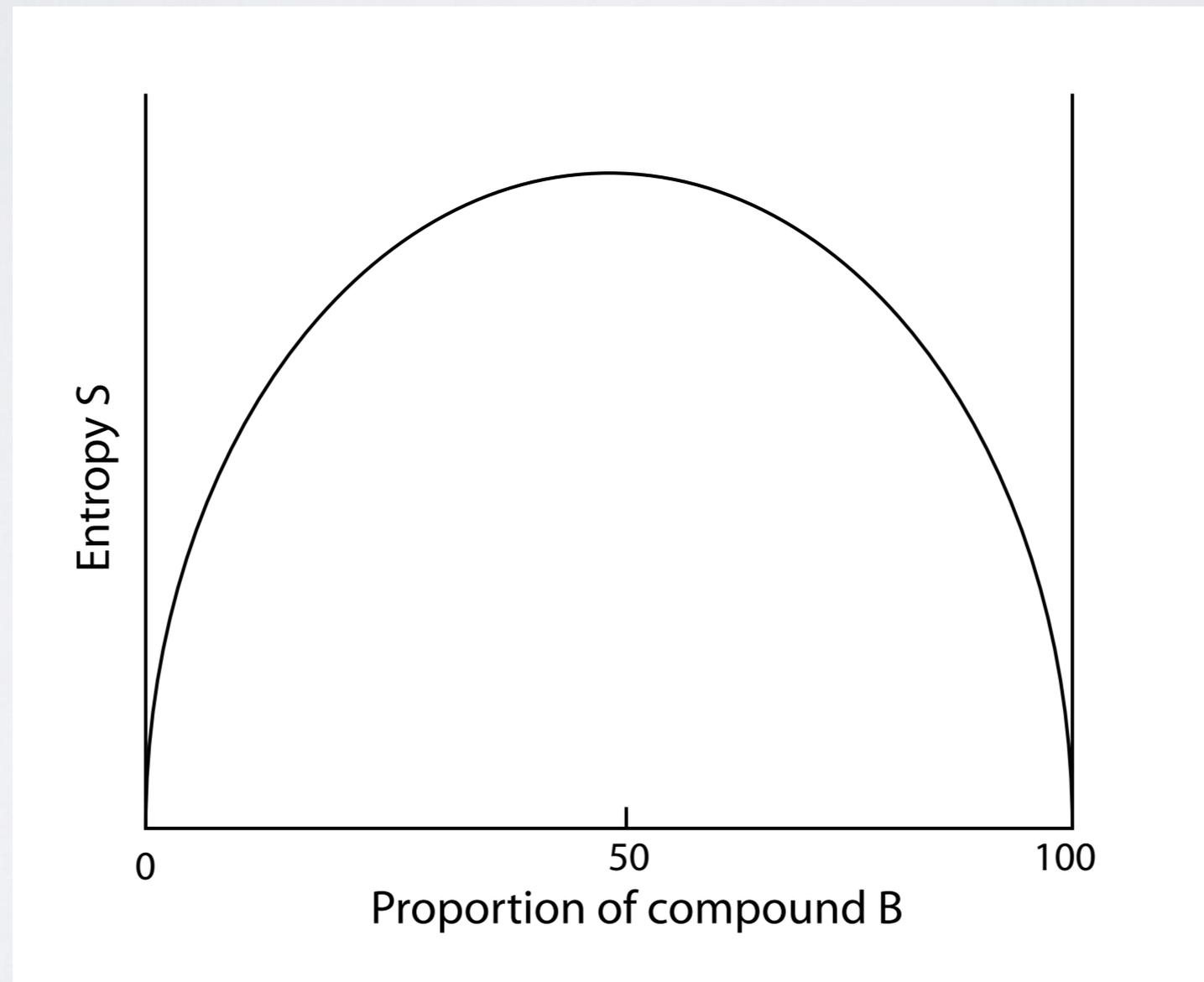
In the Earth need to account for pressure:

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:

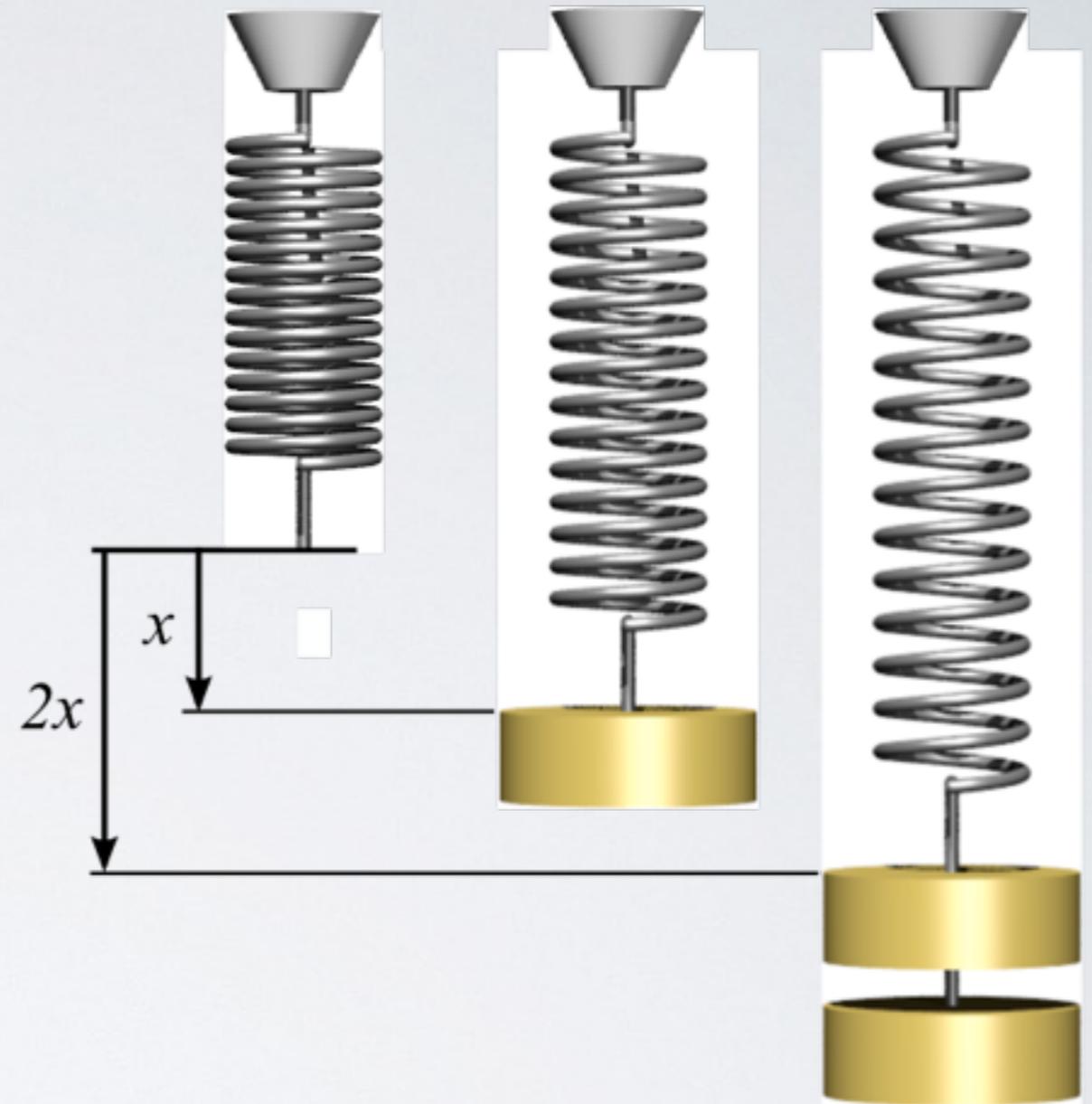
Force = spring const. \times dist.

stress = modulus \times strain

$$F = k x$$

$$\sigma = E \varepsilon$$

(Hooke's law)





Deformation:

stress = modulus x strain

$$\sigma = G \varepsilon$$

Ice:

$$G \sim 4 \text{ GPa} = 4 \times 10^9 \text{ Pa},$$

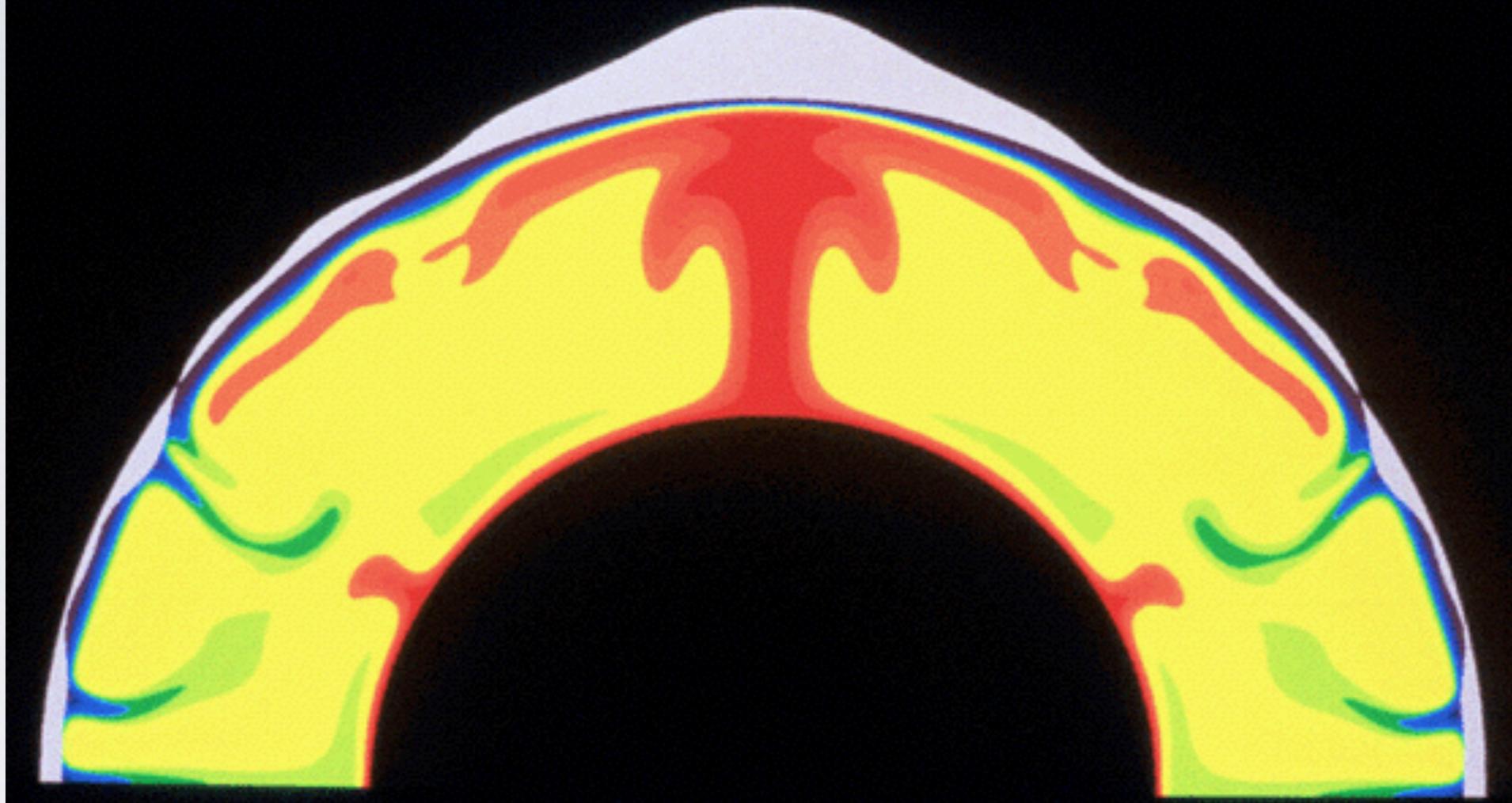
$$\varepsilon \sim 1$$

stress \sim modulus

driving flow of ice: gravity

$$\begin{aligned} \text{Pressure (stress)} &= \text{density} \times g \times \text{thickness} \\ &= 1000 \text{ kg/m}^3 \times 10 \text{ m/s}^2 \times 1000 \text{ m} = 10^7 \text{ Pa} \end{aligned}$$

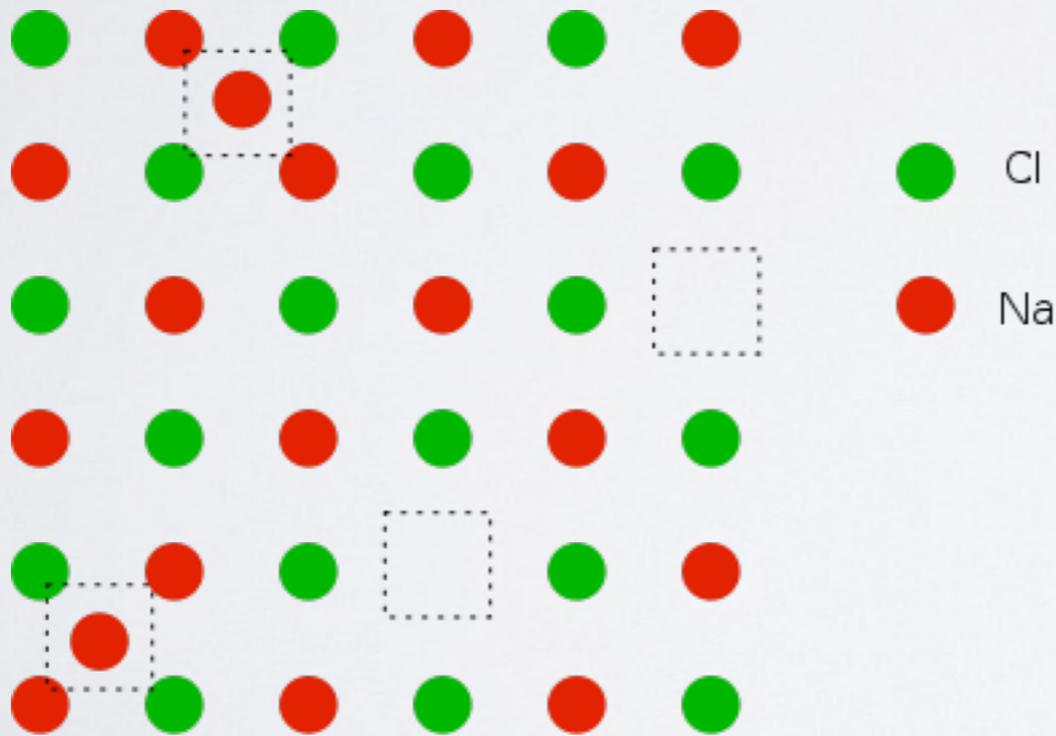
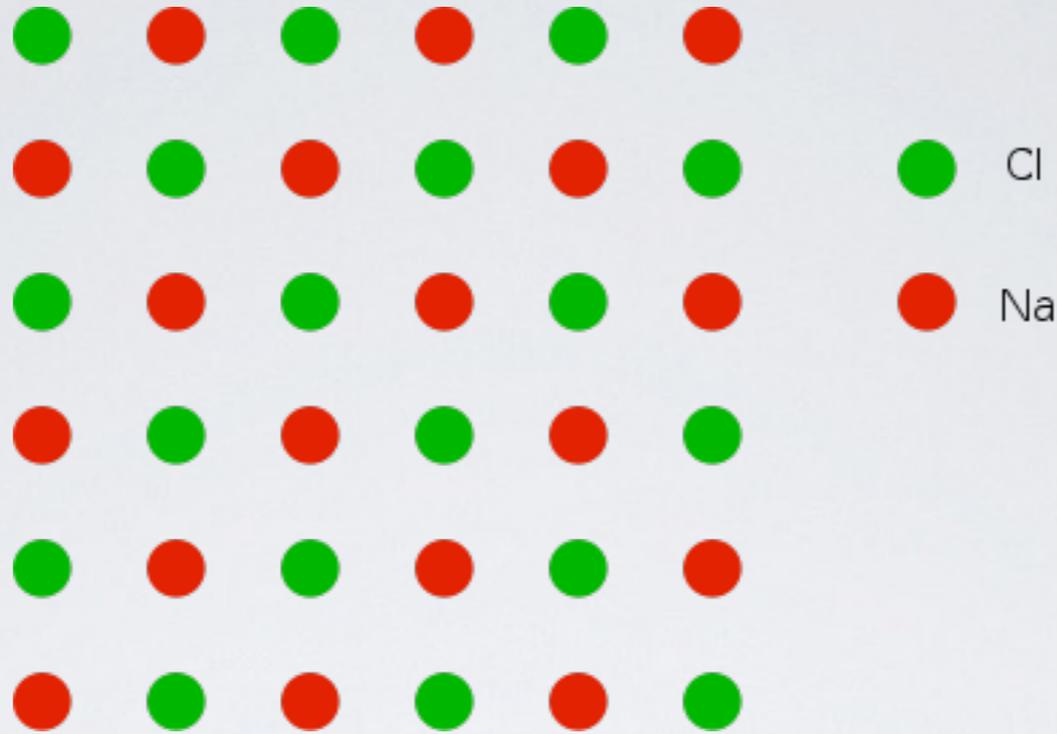
MANTLE CONVECTION SIMULATION



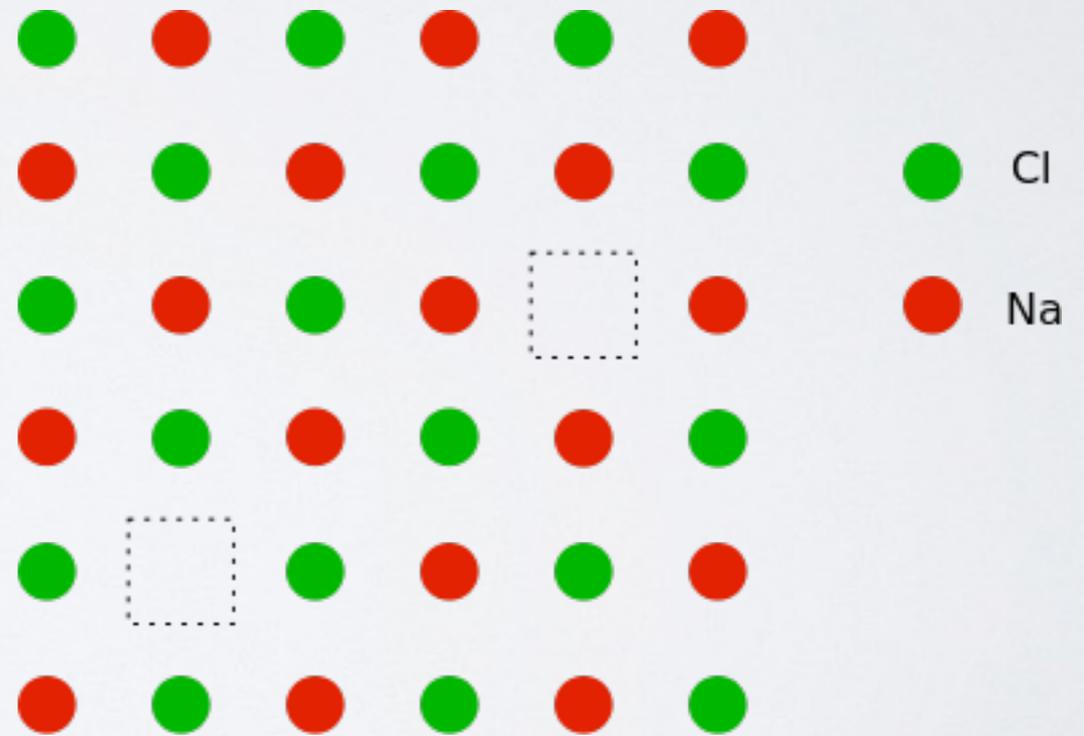
moduli of rock-forming minerals of order of 100 GPa
convective stresses ~ 0.1 MPa

Defects!

(point defects)

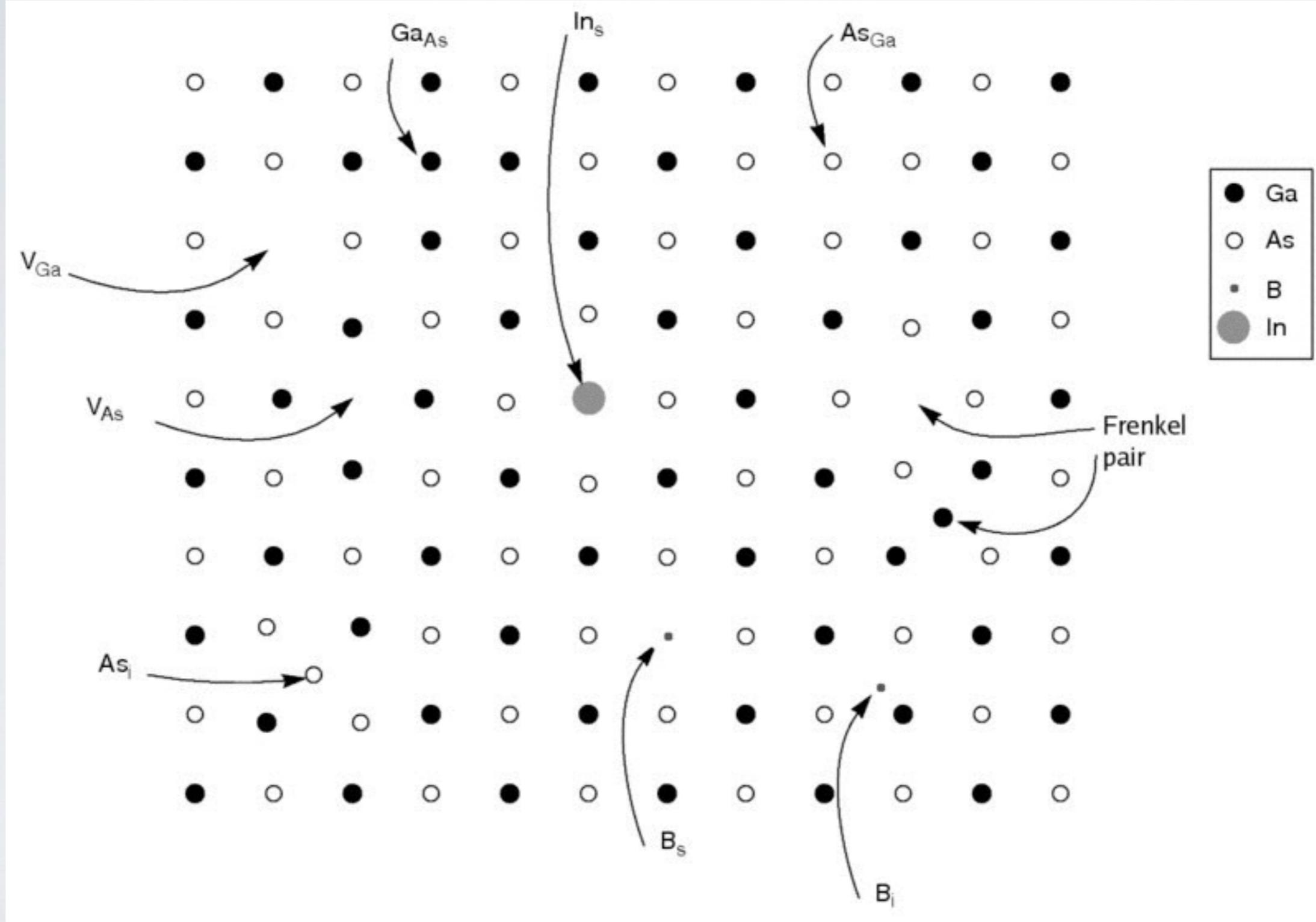


Frenkel



Schottky

defects can also be impurity atoms



Thermodynamically why do we have defects?

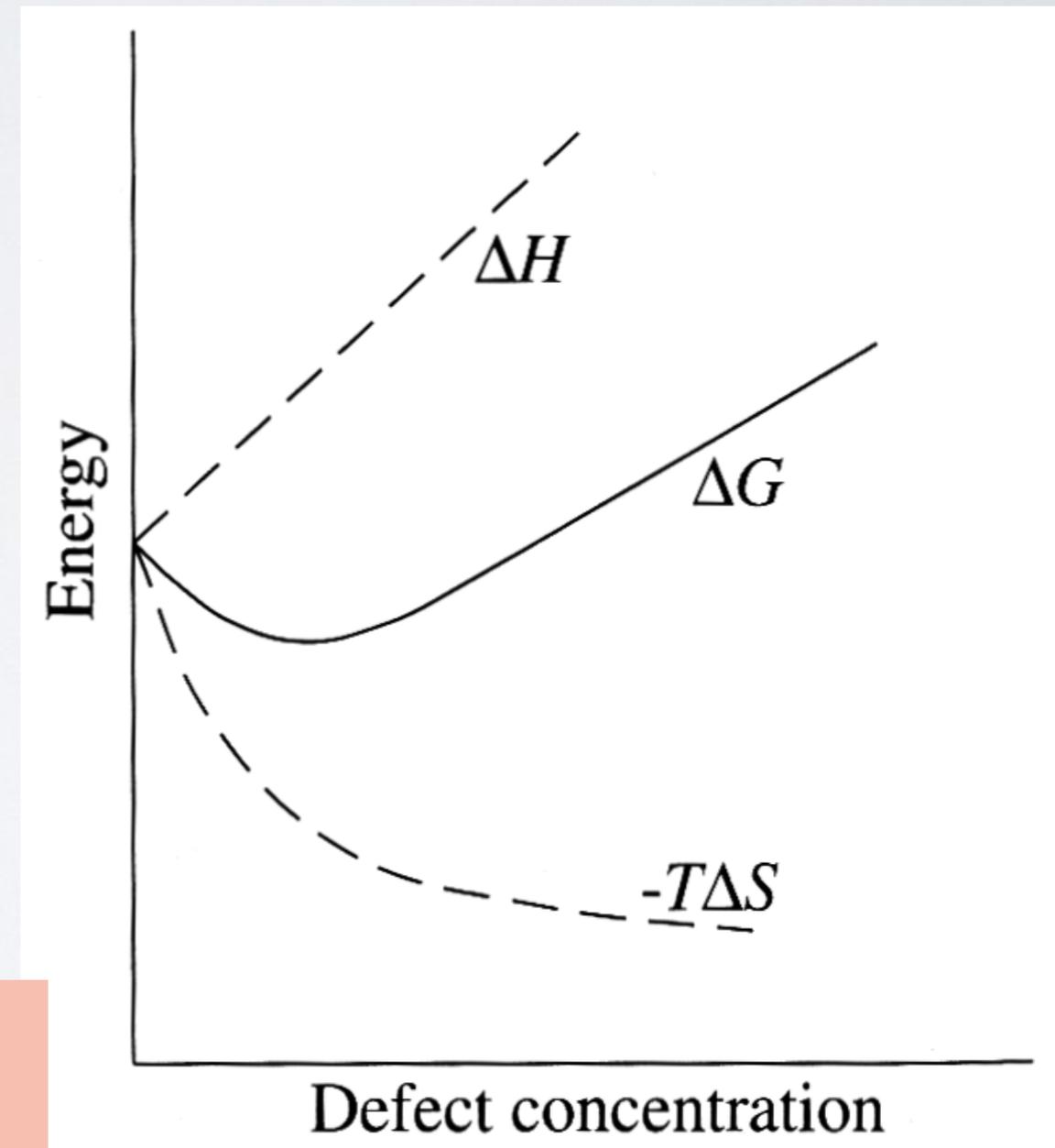
Creation of point defect requires energy:
local distortion of lattice + imperfect satisfaction of bonding
➡ enthalpy H increases.

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.)

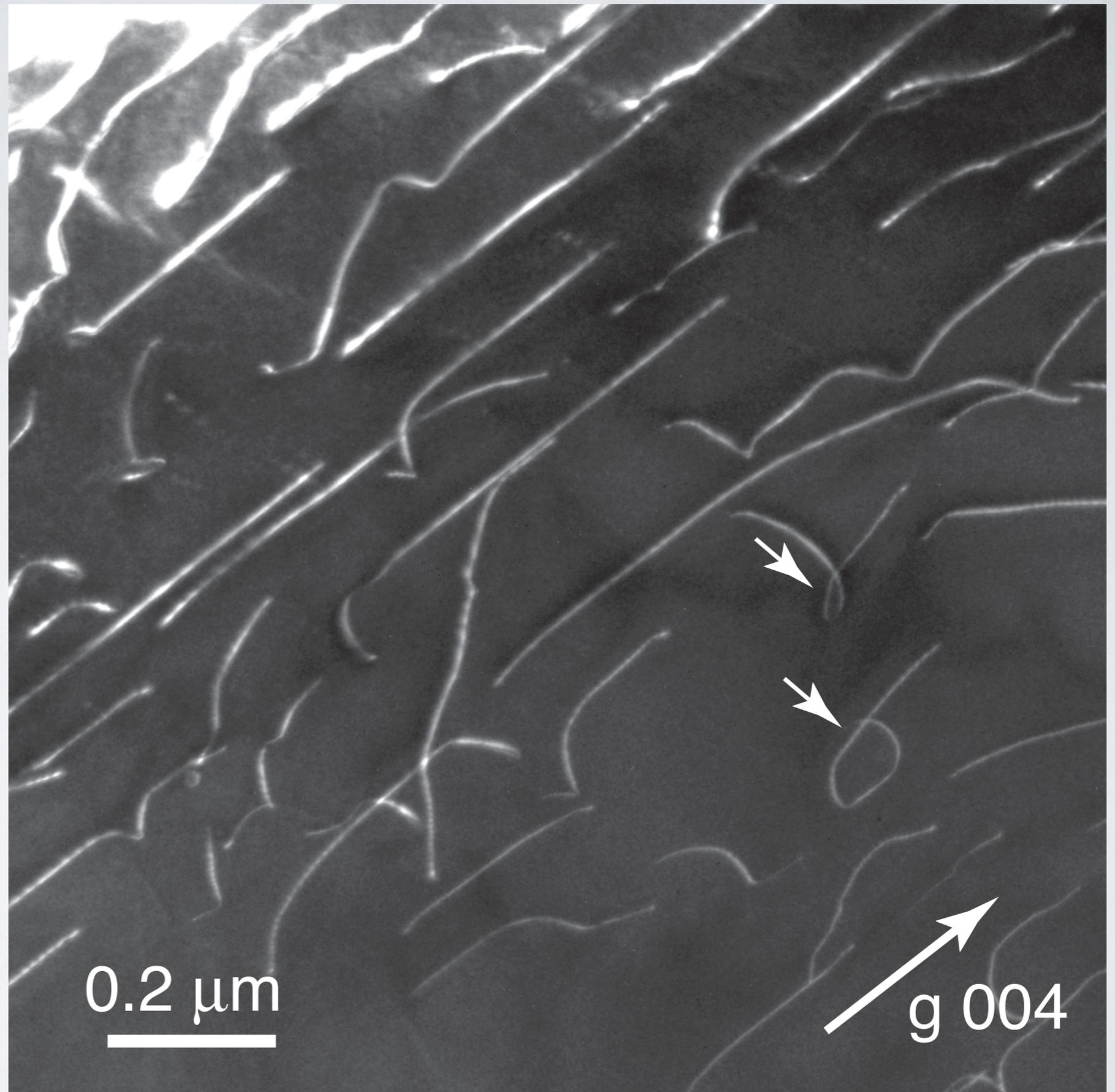
For small defect concentrations entropy
increase is *greater* than enthalpy
increase, for larger defect
concentrations enthalpy increase
dominates:

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



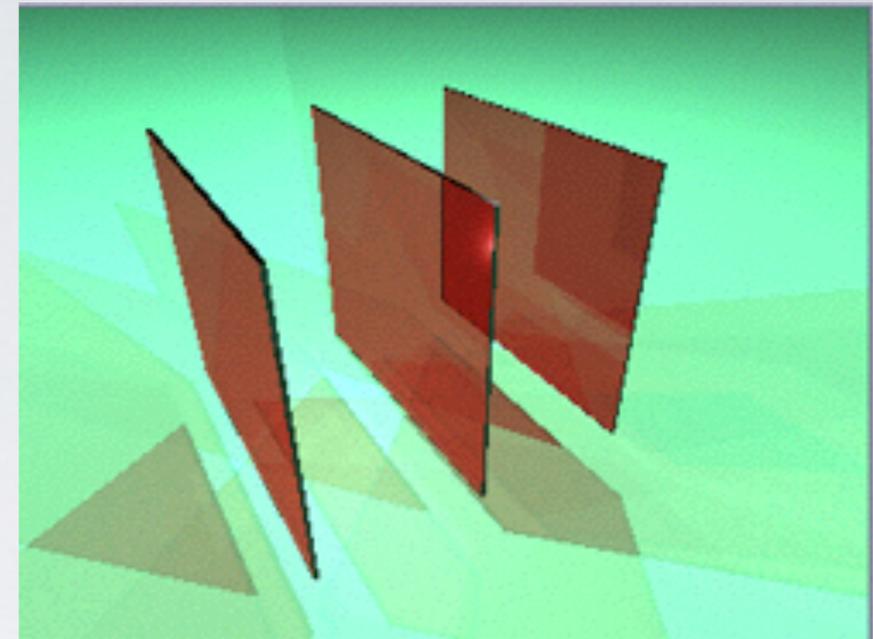
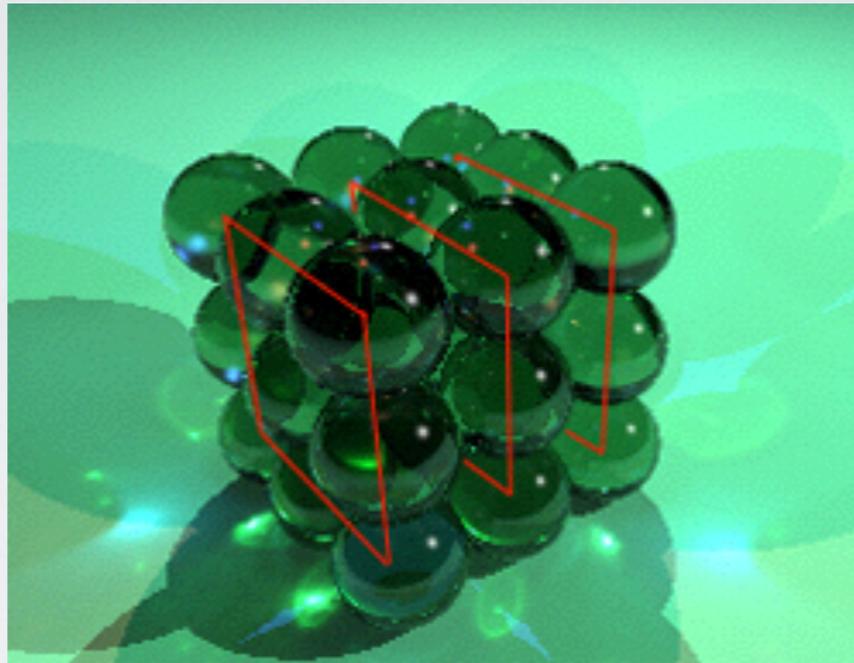
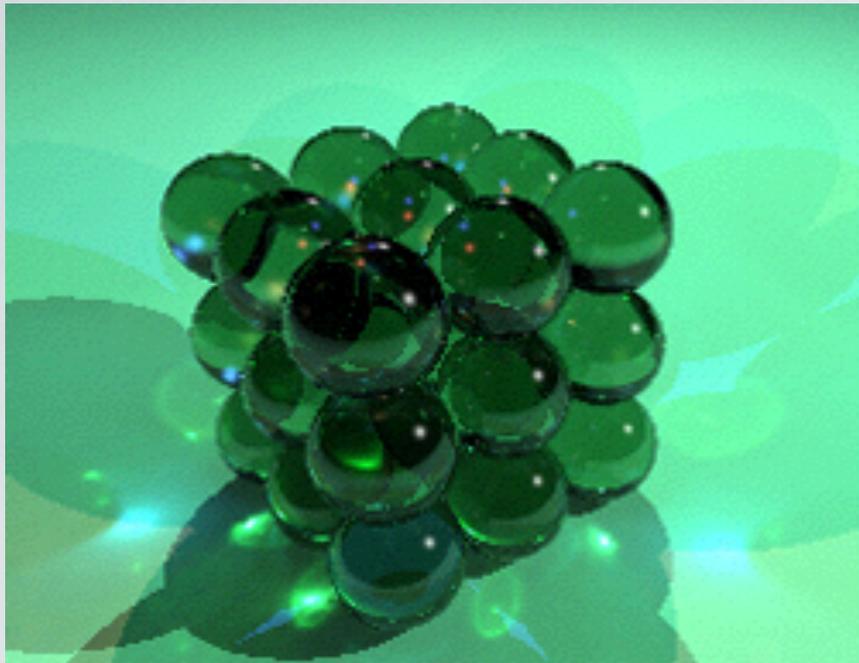


Dislocations
-line defects



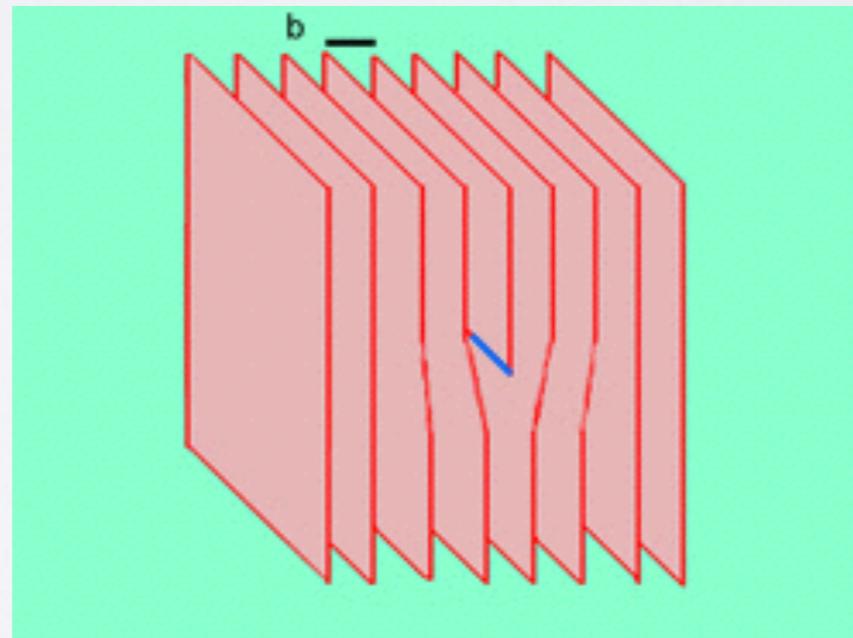
Transmission electron microscope image of screw dislocations in olivine

What is a dislocation?

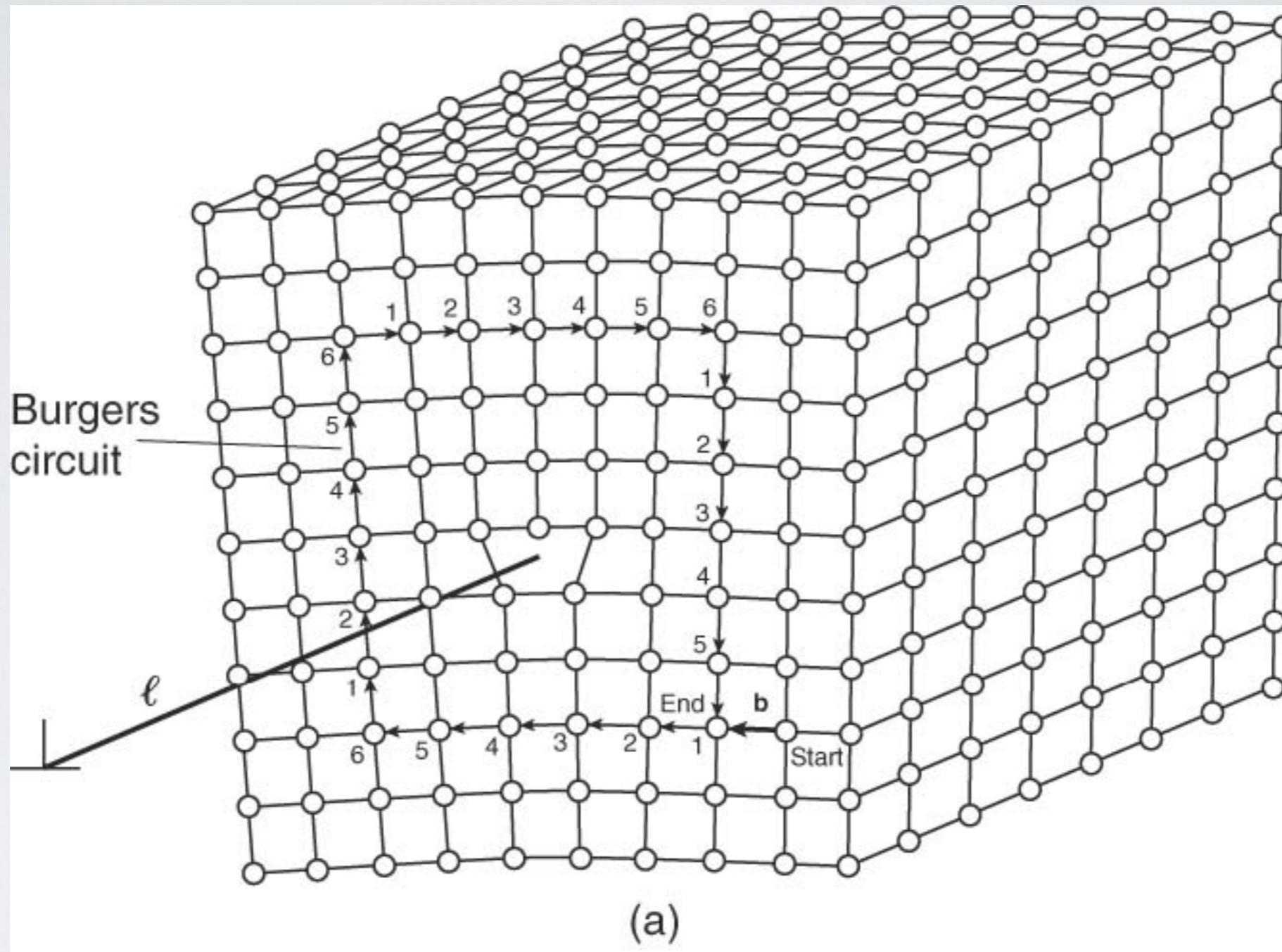


Lattice planes in a cubic crystal

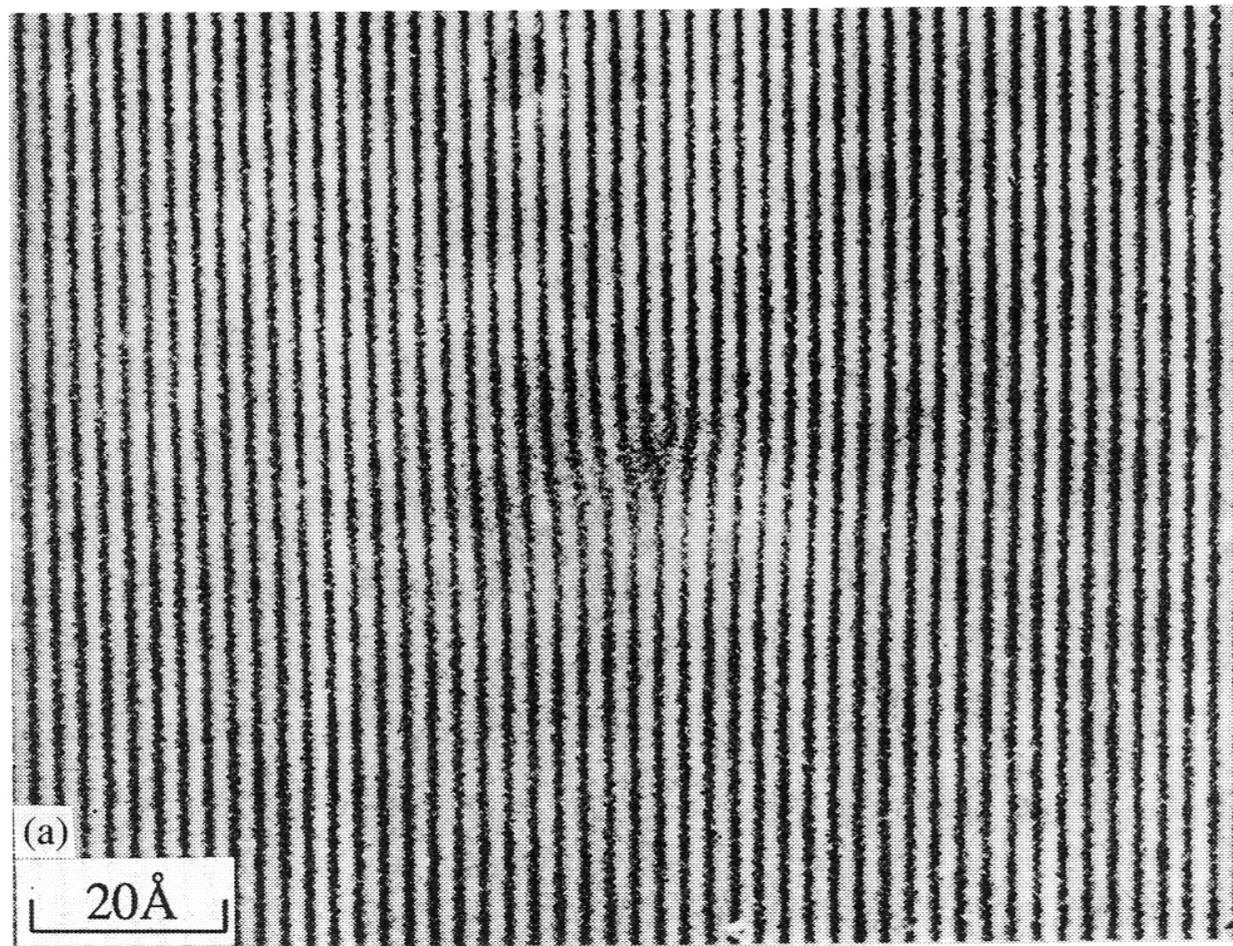
Insert an extra half plane



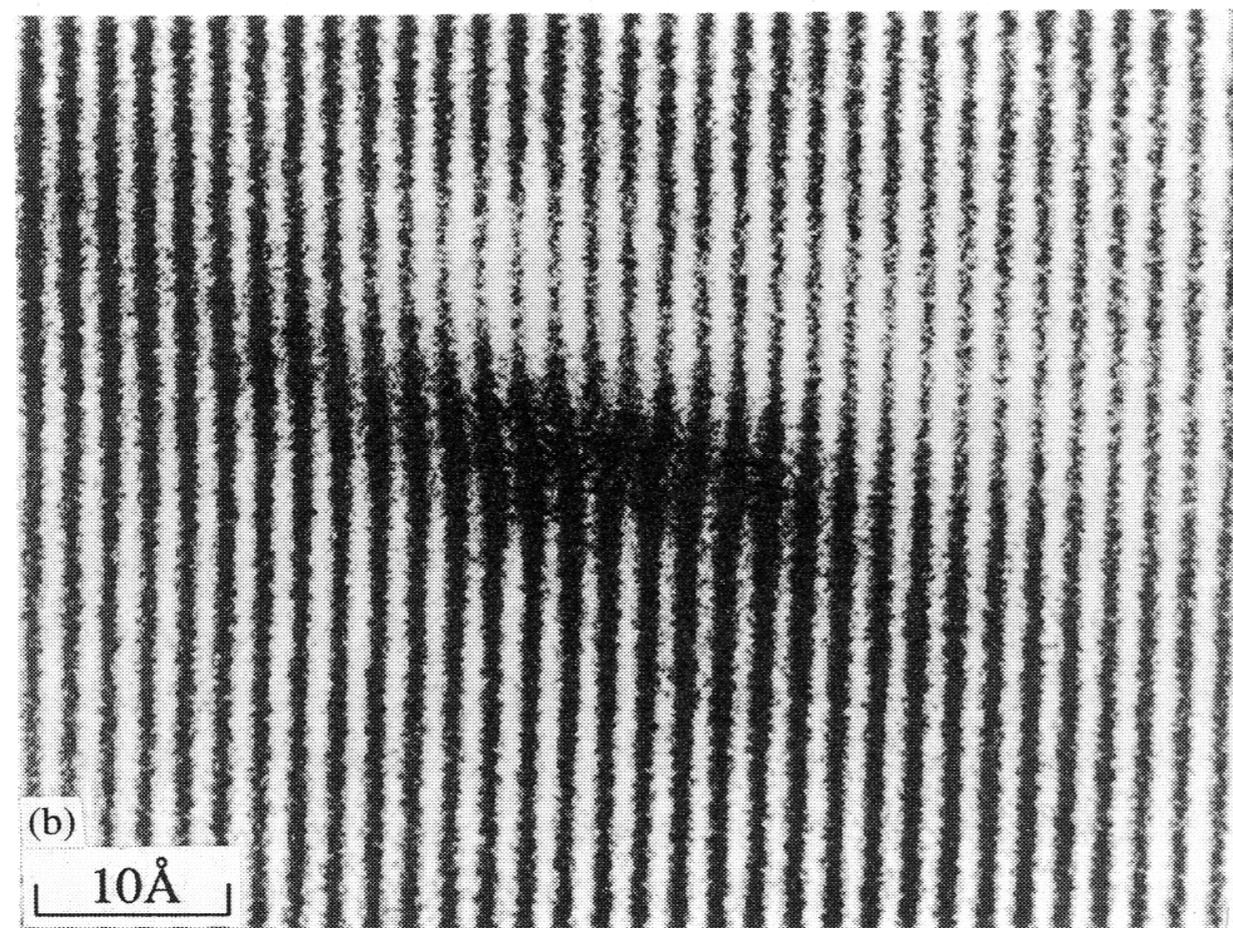
Edge dislocation

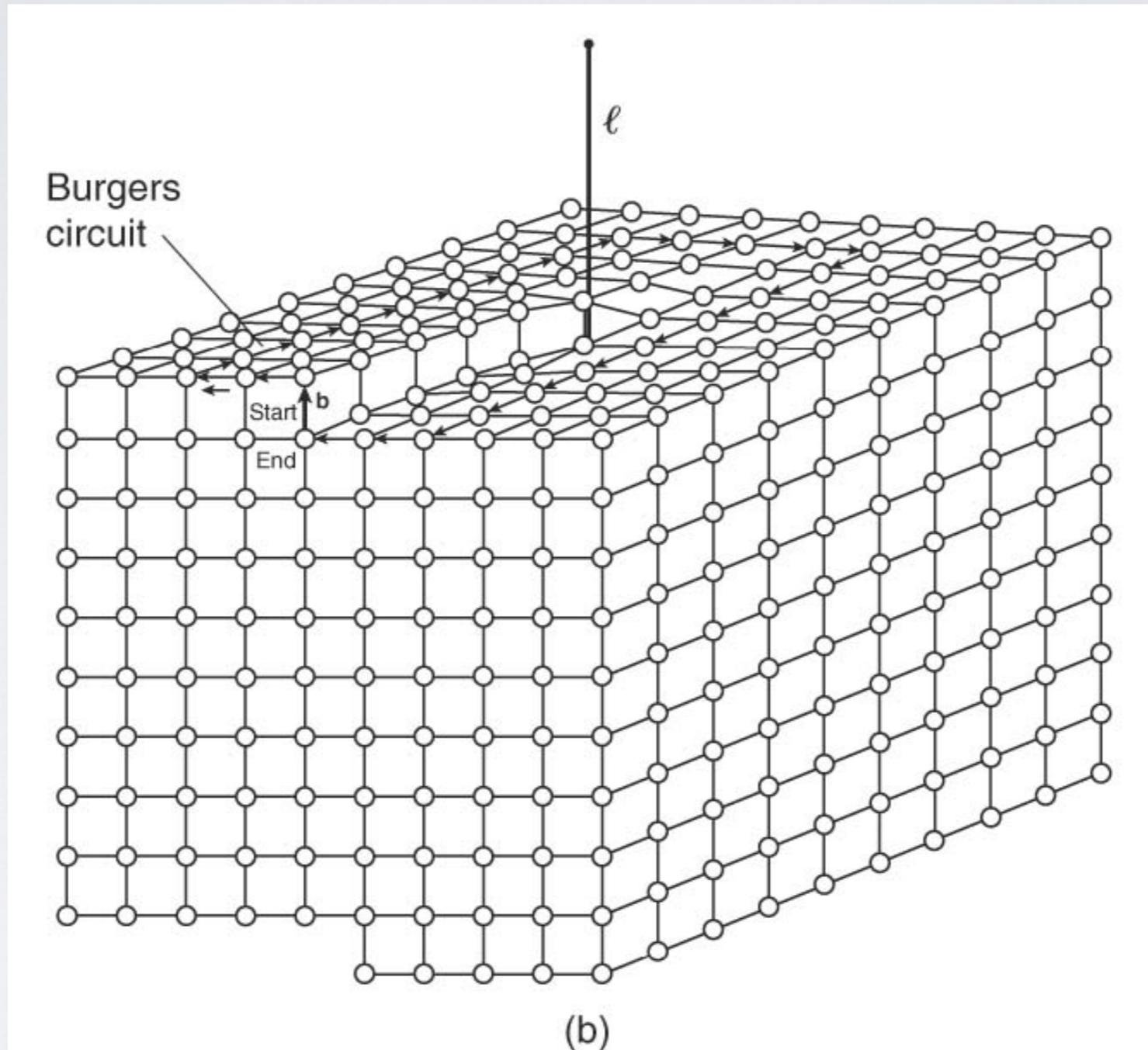


edge dislocation: Burgers vector perpendicular to dislocation line l

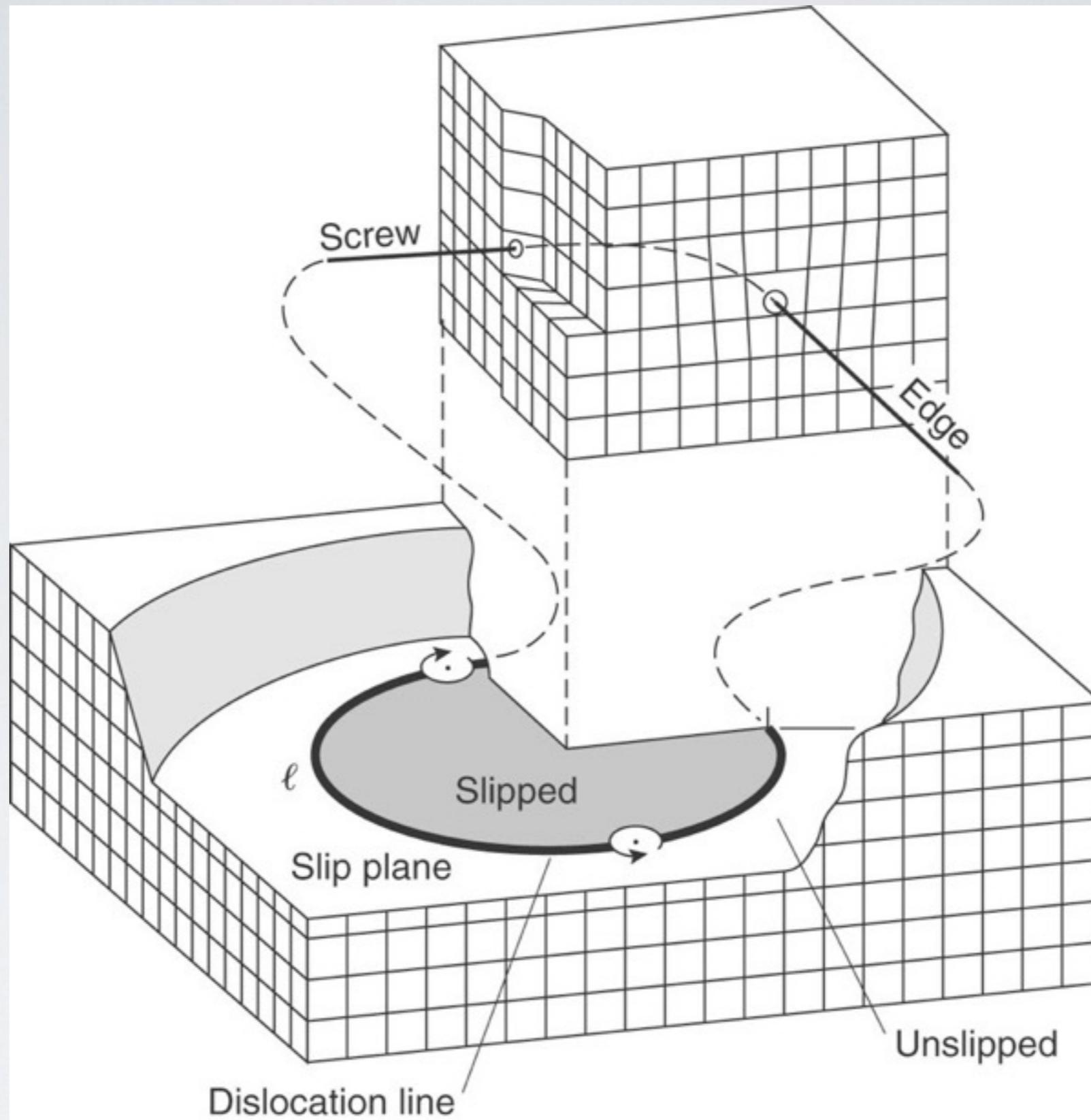


TEM lattice-fringe
images with electron
beam parallel to
dislocation line



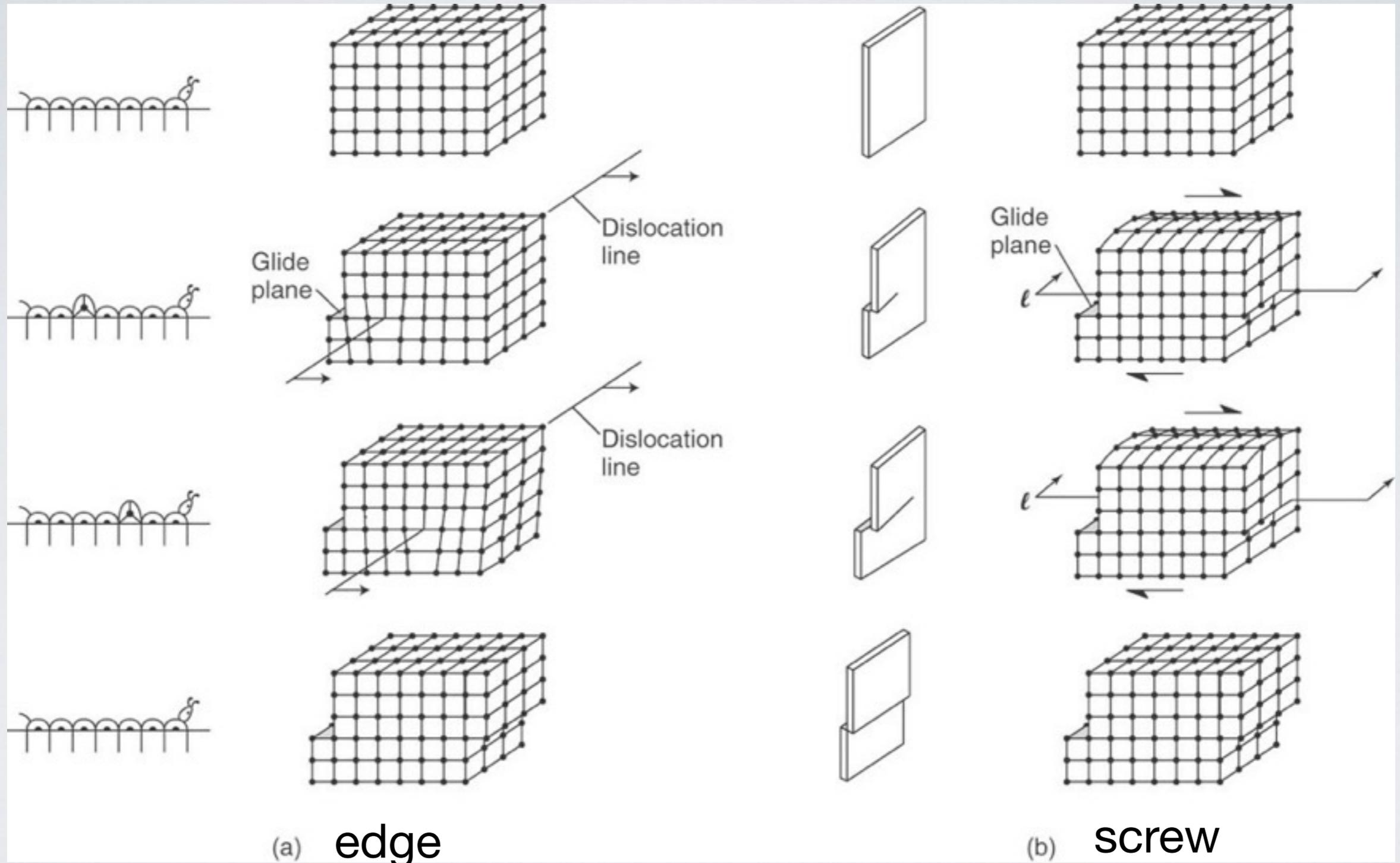


screw dislocation: Burgers vector parallel to dislocation line ℓ

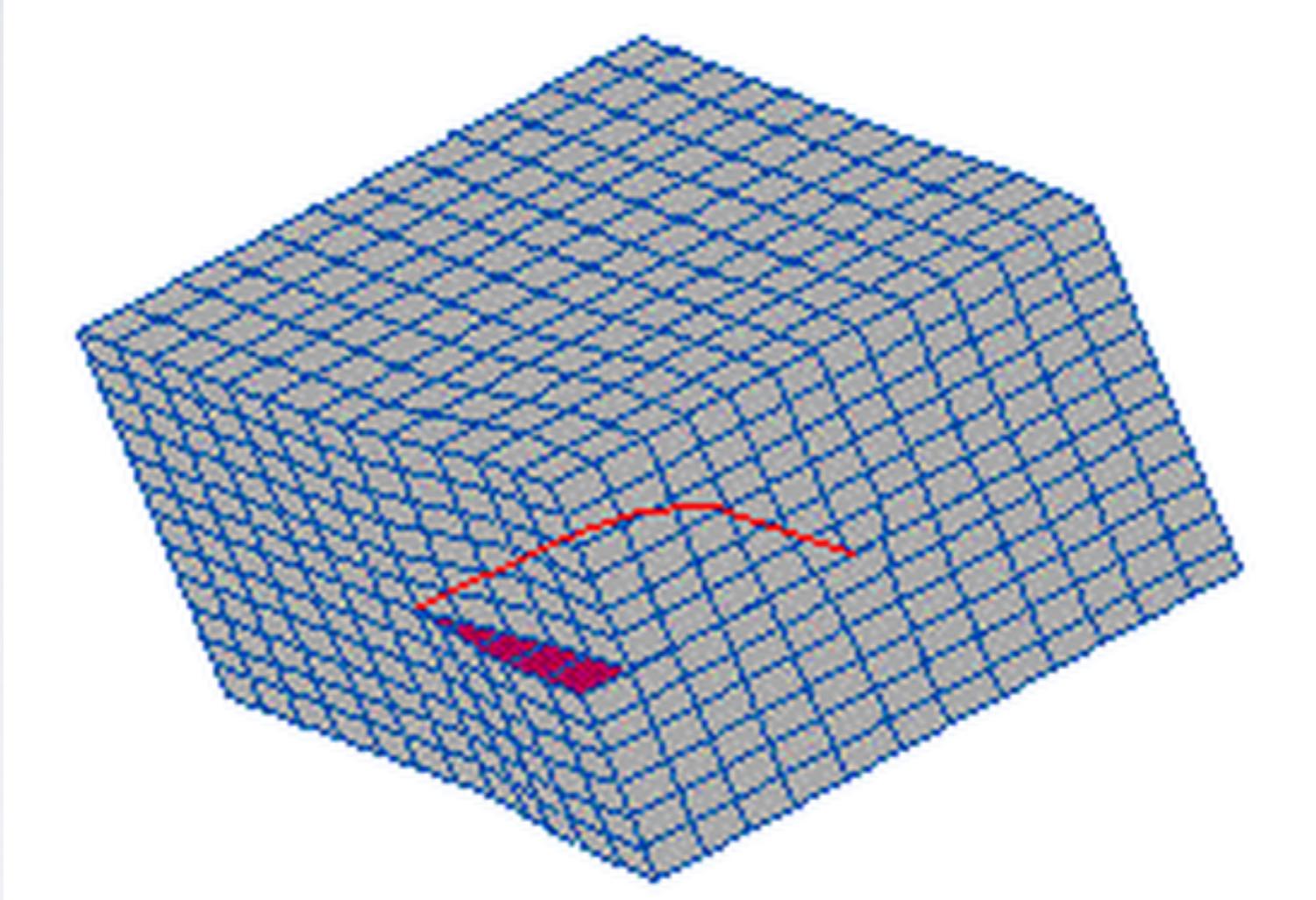


dislocations: mixed character

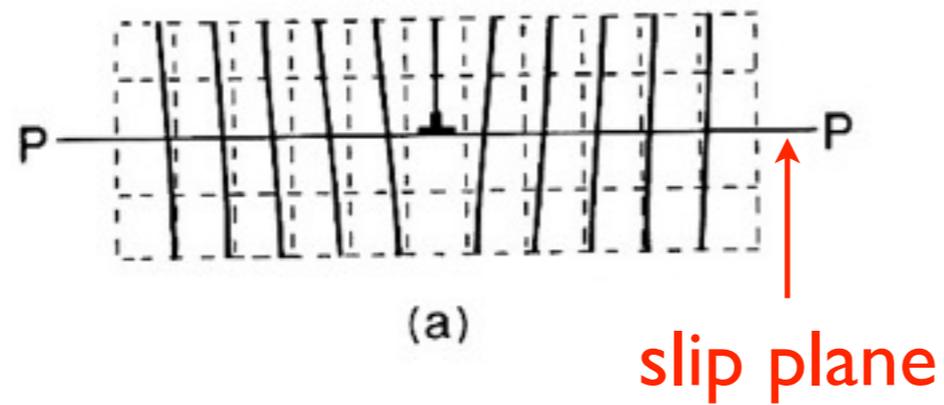
Strain due to dislocation creep



Movement in a glide plane

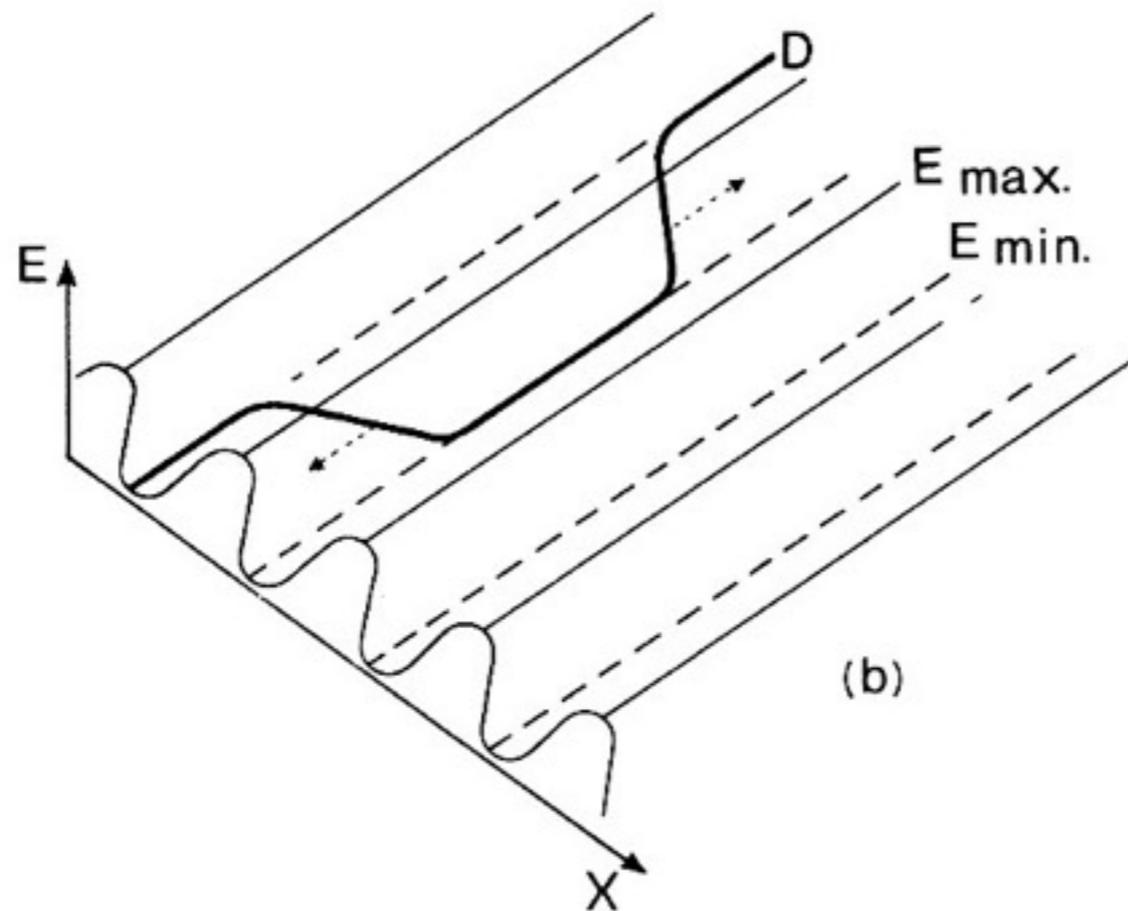


Dislocation geometry is controlled by crystal lattice

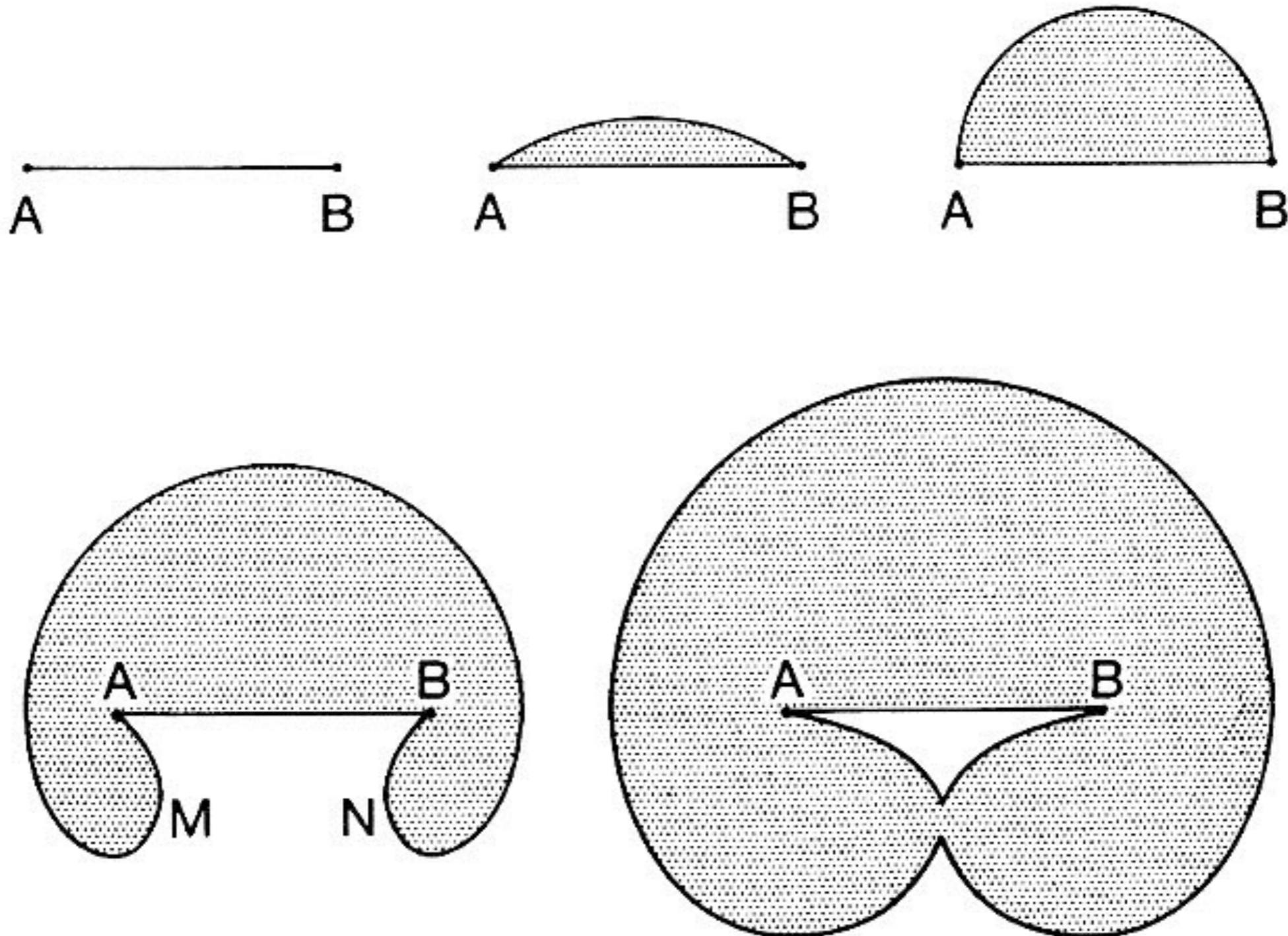


dislocations move on glide planes

Peierls potential

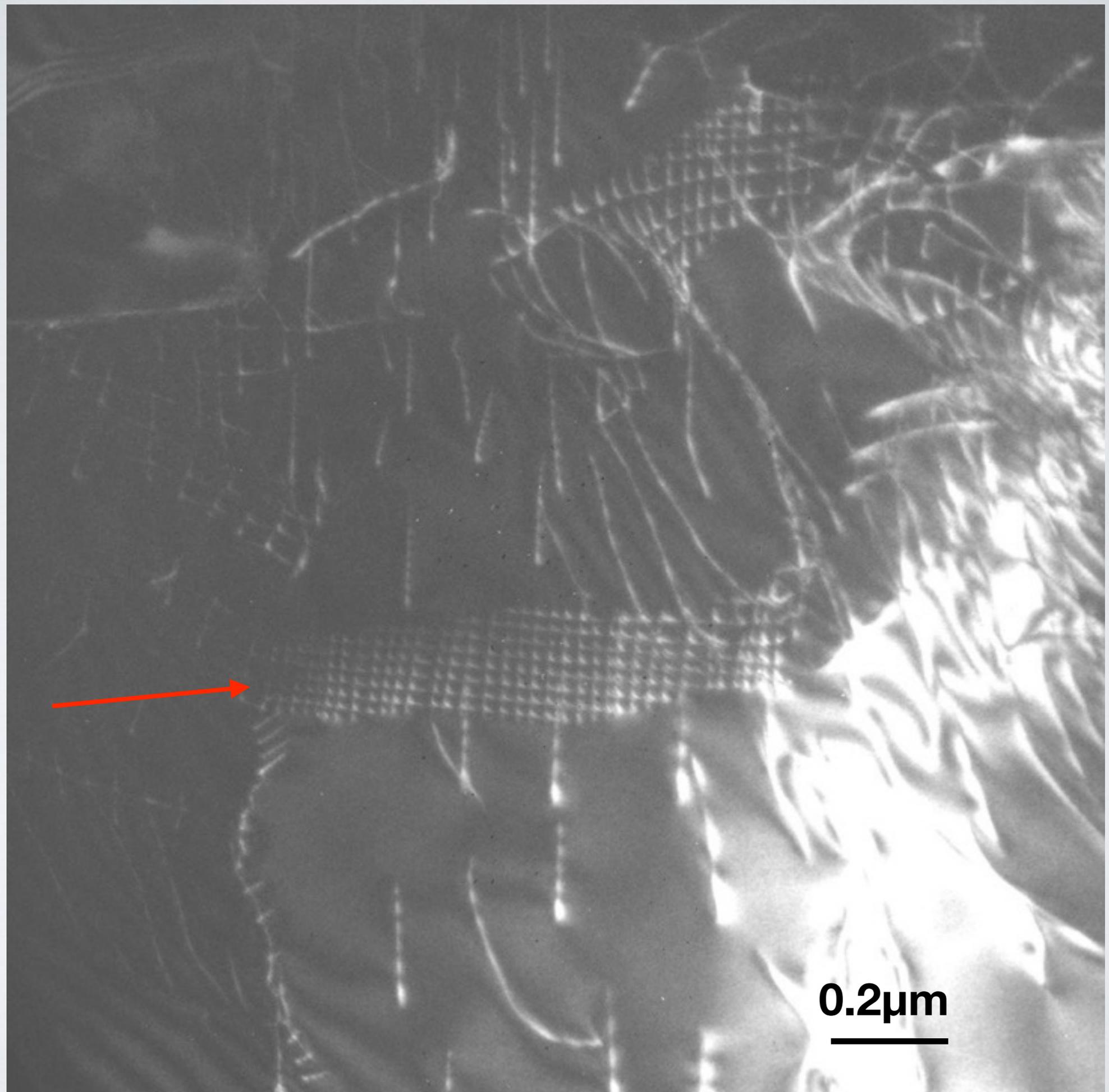


Generation of dislocations: Frank-Read sources (dislocation multiplication due to stress/strain)



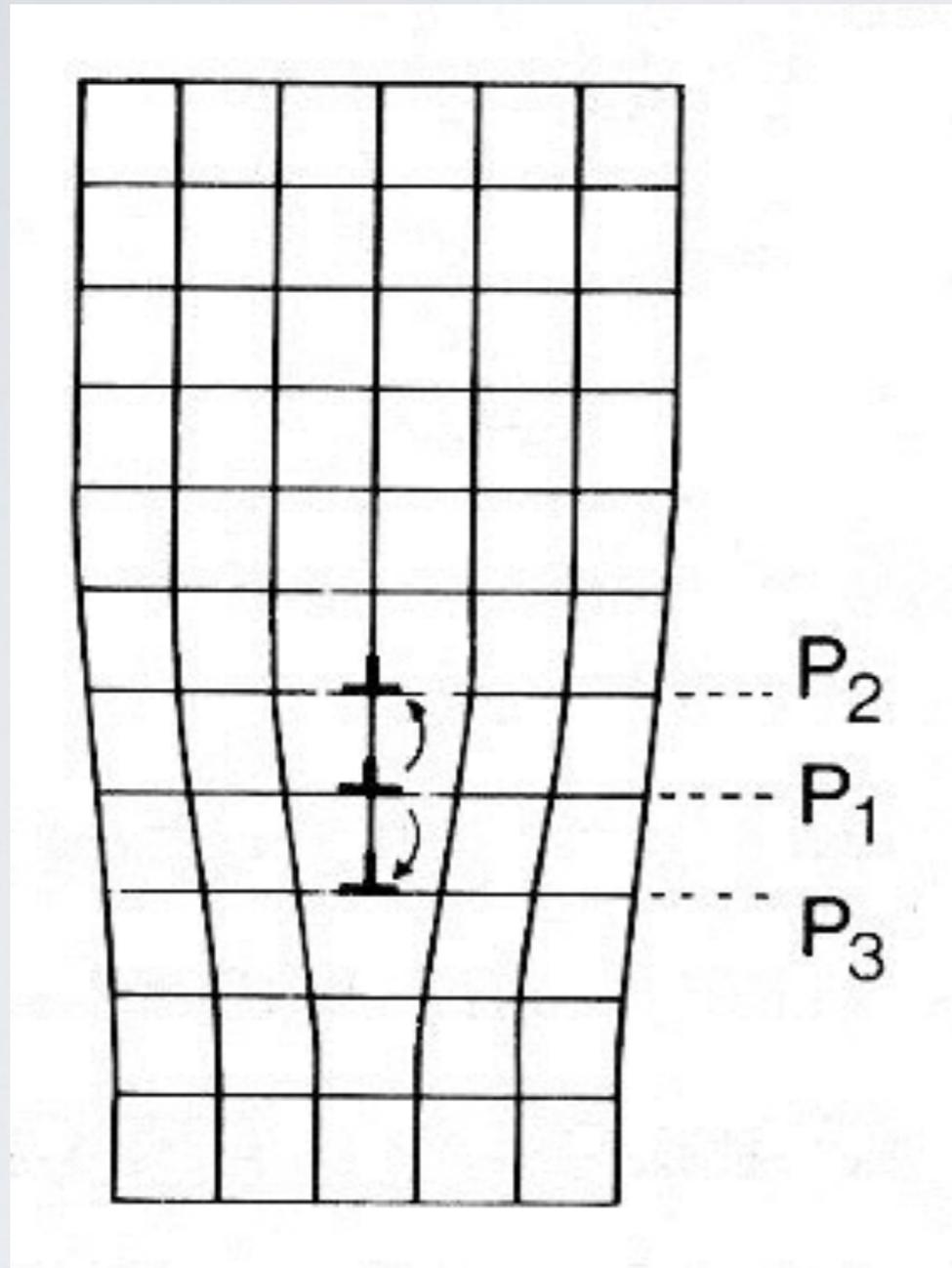
Obstacles
to
dislocation
motion

subgrain
boundary



0.2μm

Climb of an edge dislocation



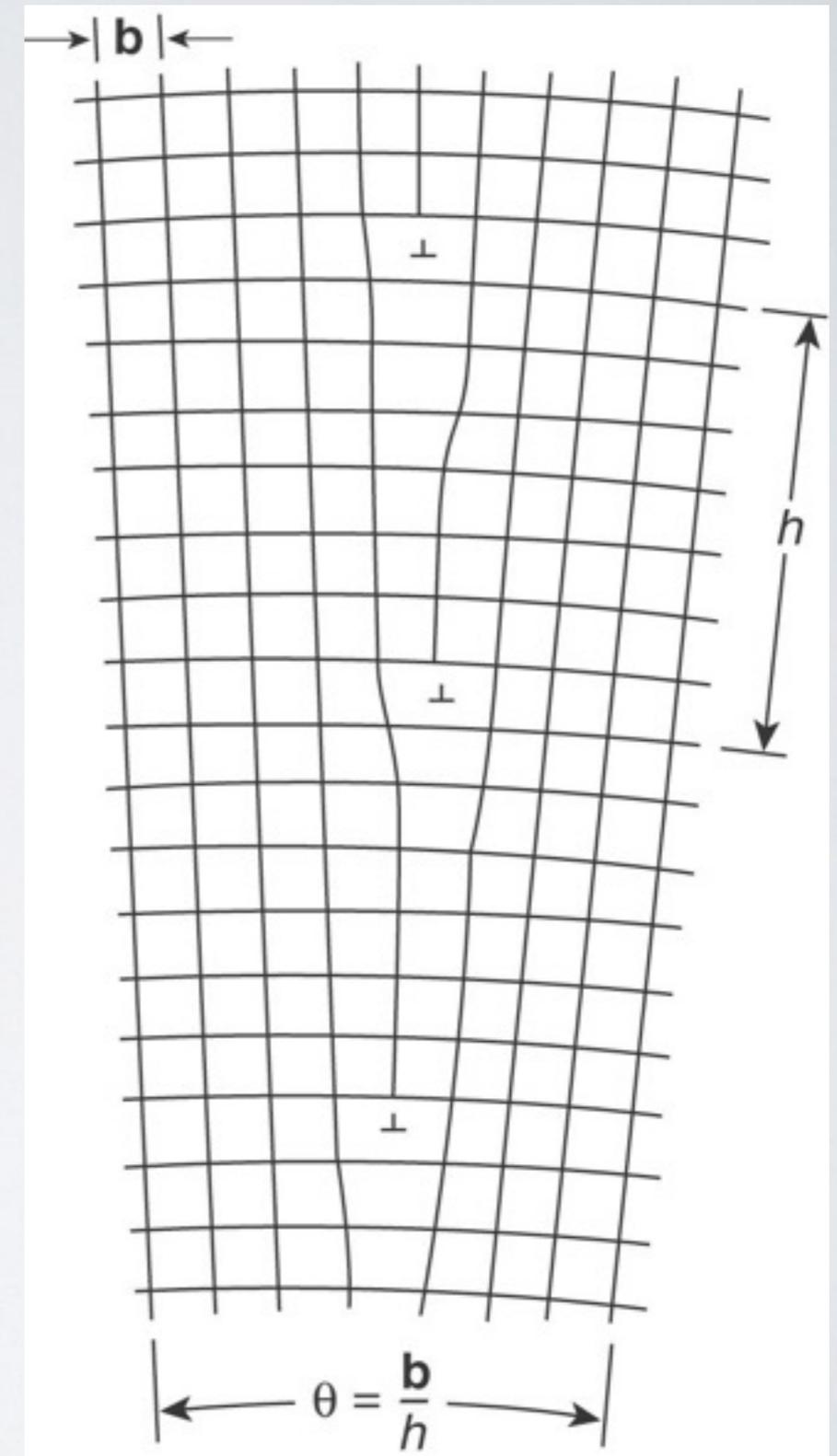
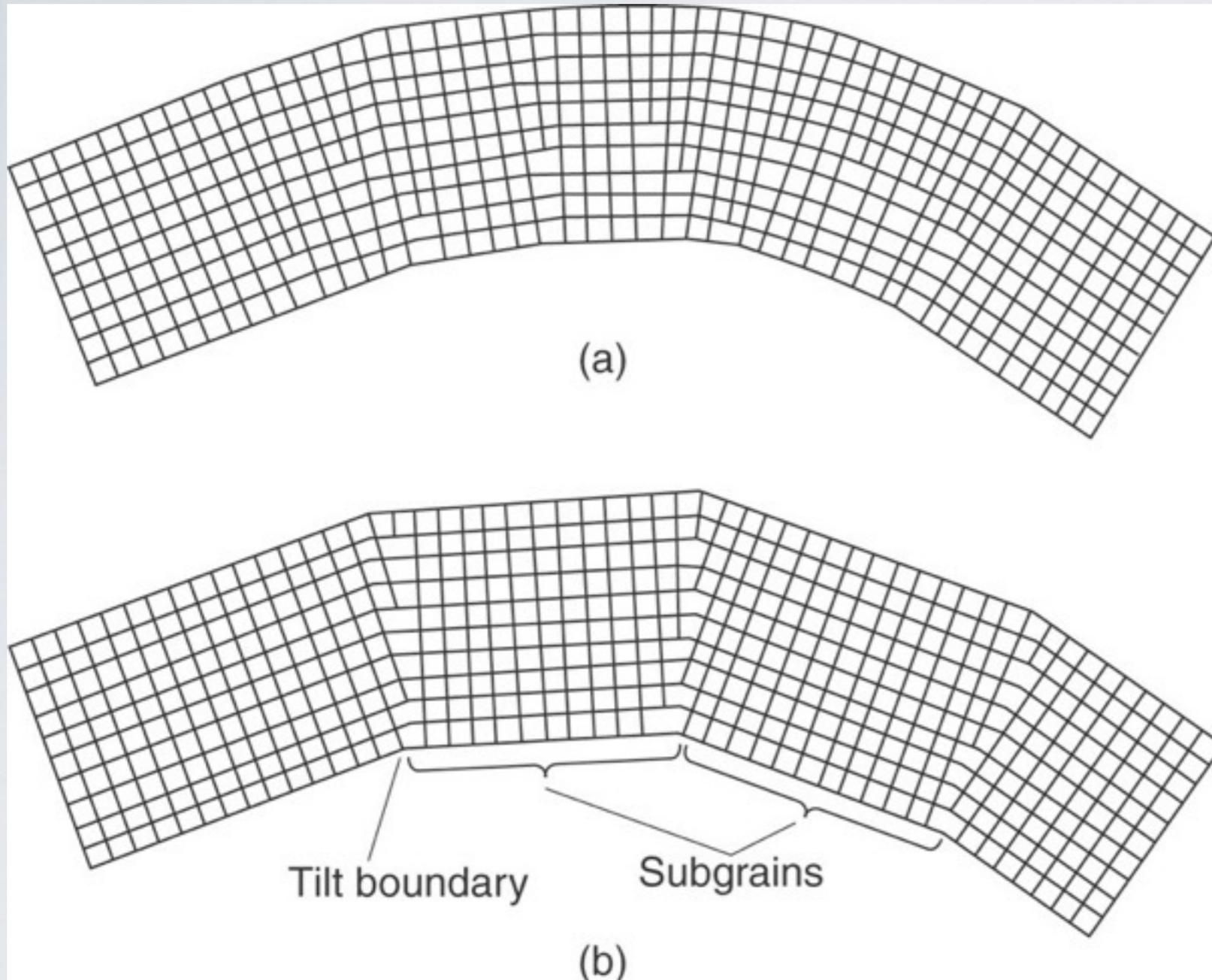
Climb by diffusion of a row of atoms from the extra half plane.
Screw dislocations have no extra half plane and cannot climb.

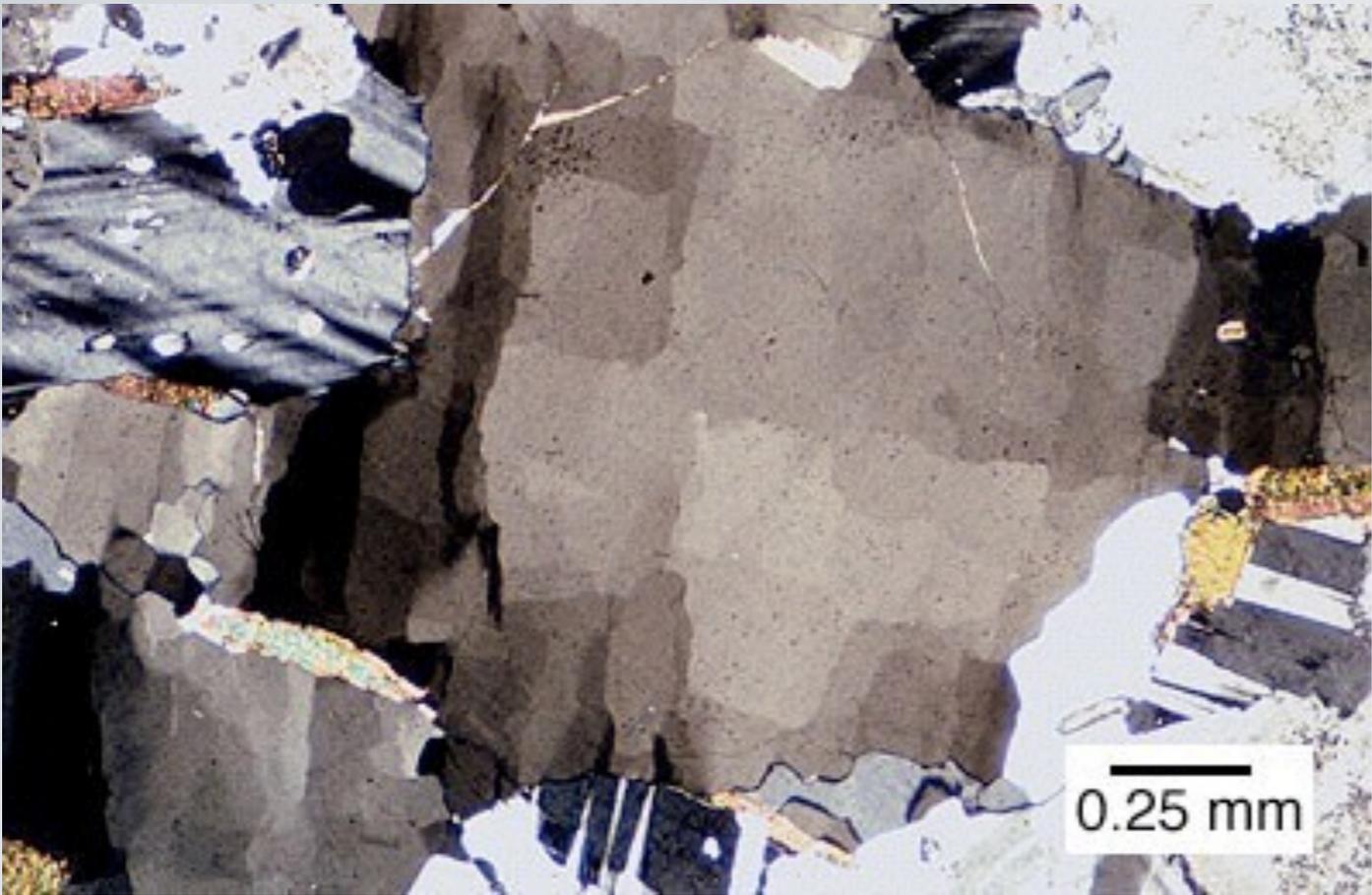
Dislocation creep: strain produced by glide of dislocations, rate limited by diffusion

	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

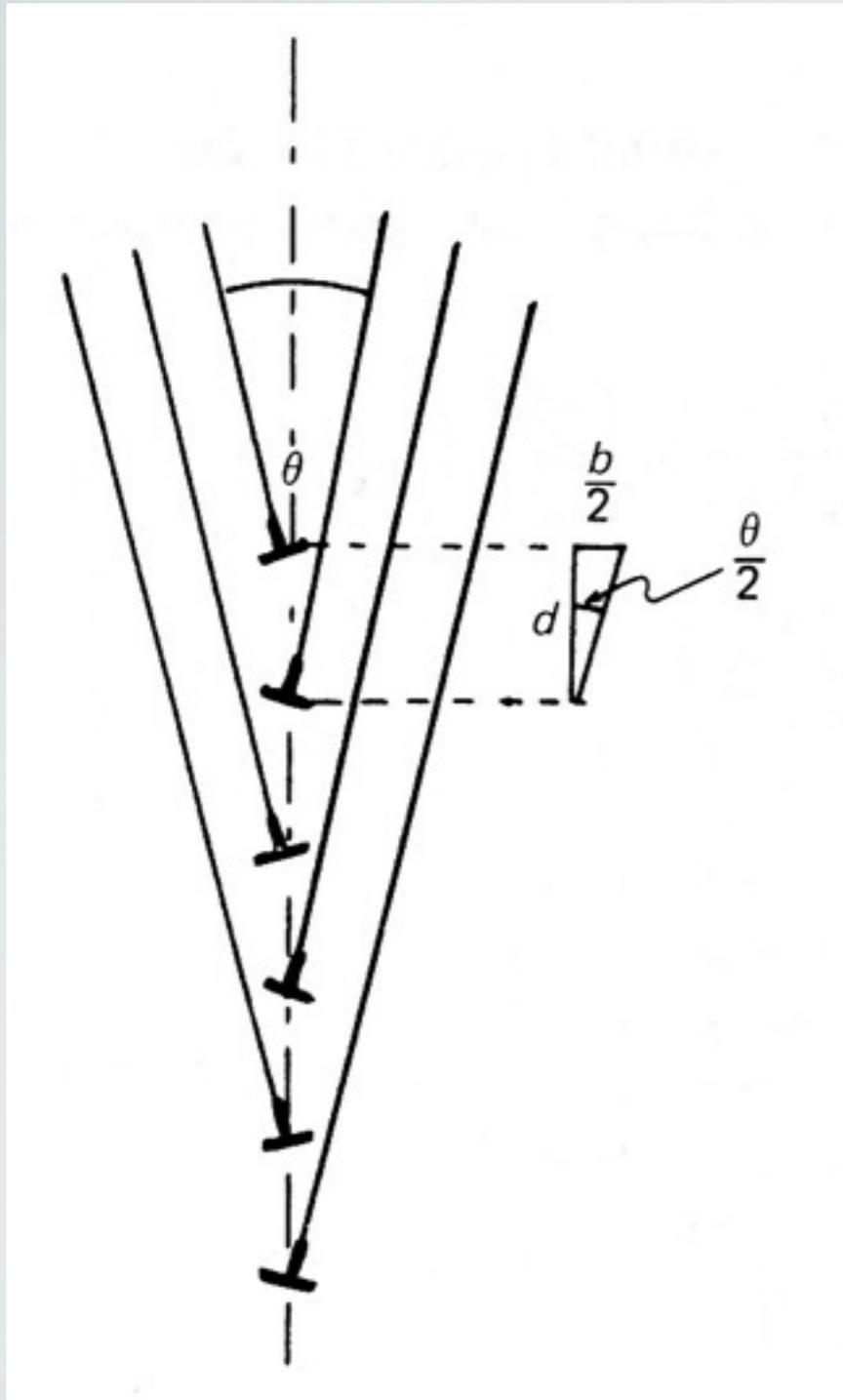
Grain boundaries

Why look at grain boundaries?

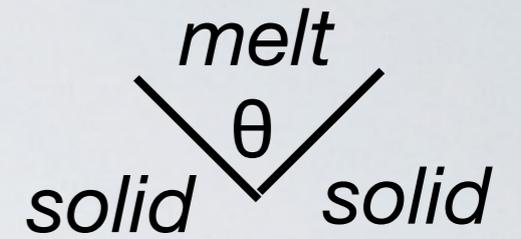
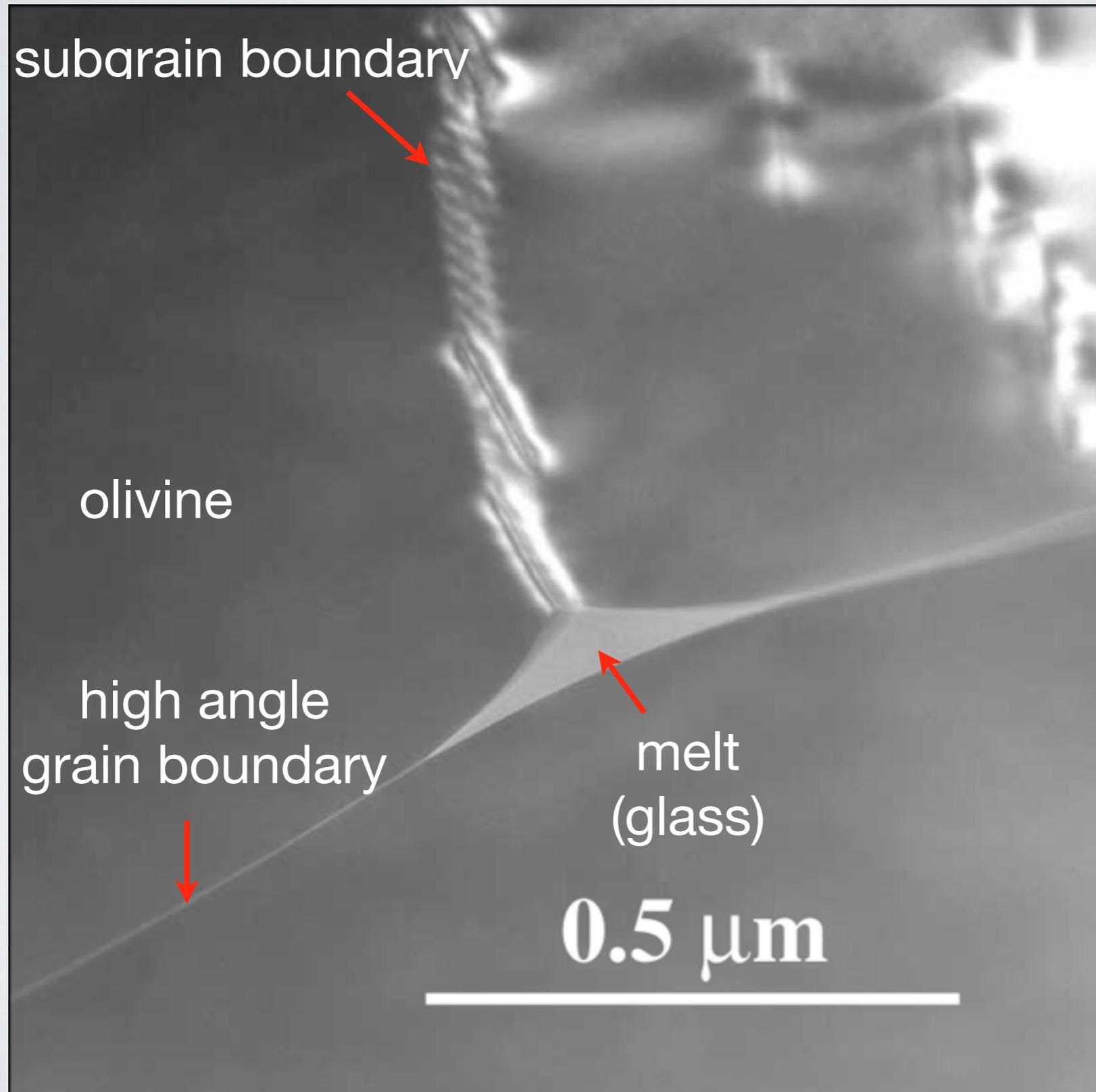
1. GB as crystalline defect present in all rocks.
2. GB affect
 - diffusion
 - deformation
 - seismic properties
 - electrical conductivity....

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

Lattice misorientation given by θ



Visualization of types of grain boundaries

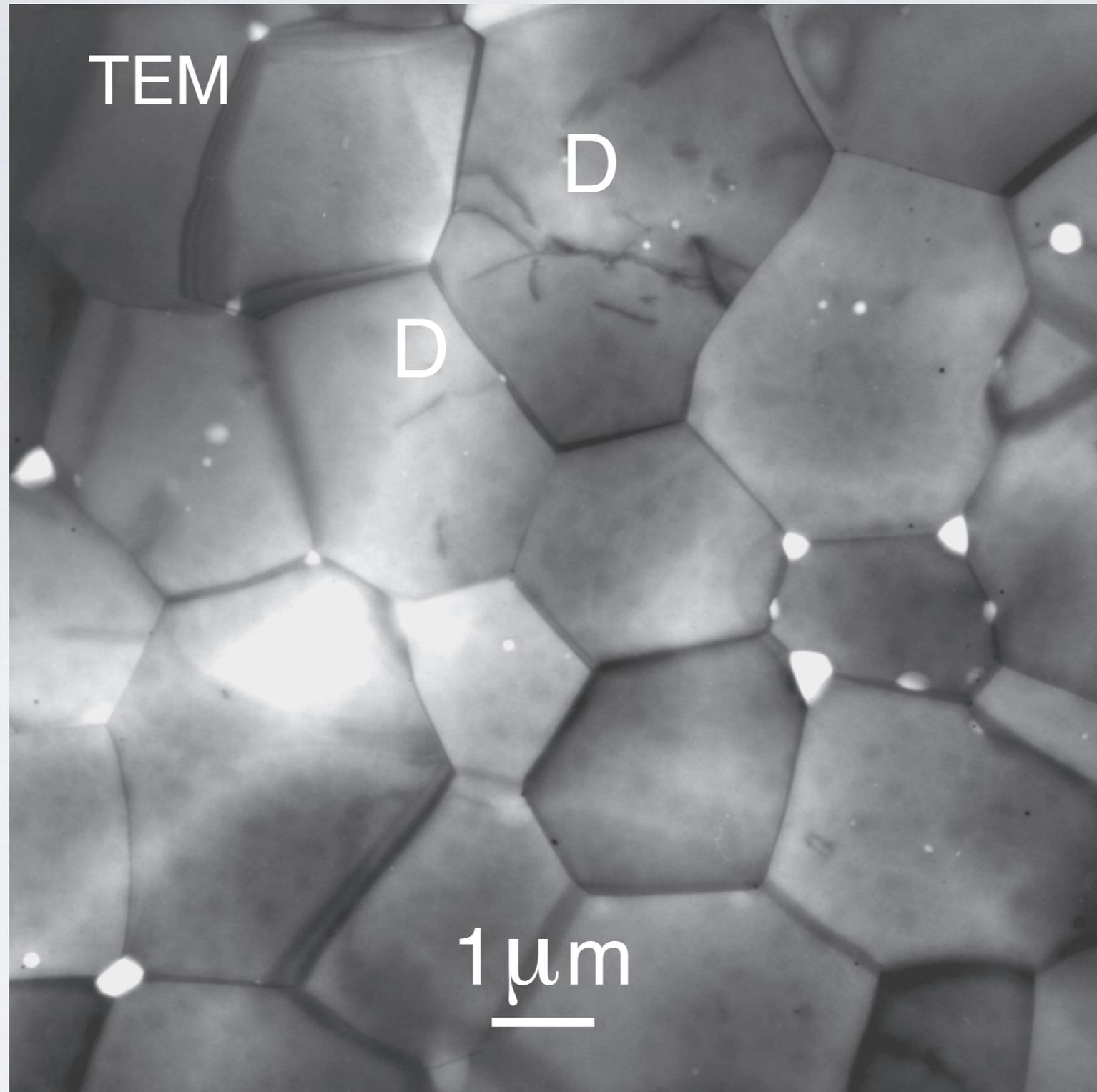


$$\cos \theta/2 = \gamma_{ss}/2\gamma_{sl}$$

γ_{ss} = solid - solid
surface energy

γ_{sl} = solid - liquid
surface energy

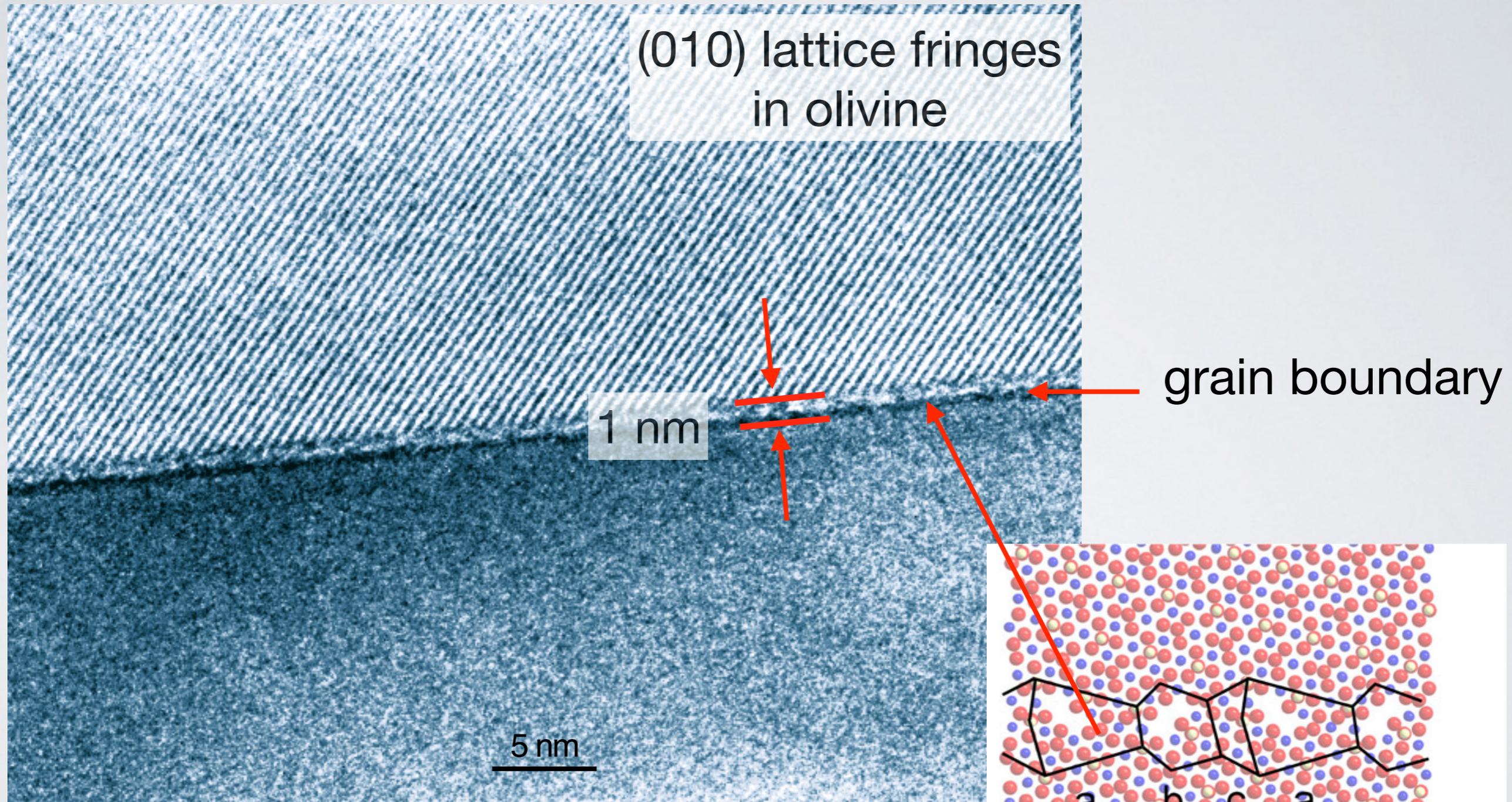
Grain boundaries: melt-free polycrystalline olivine



Jackson et al.,
2002

defects: grain boundaries, dislocations

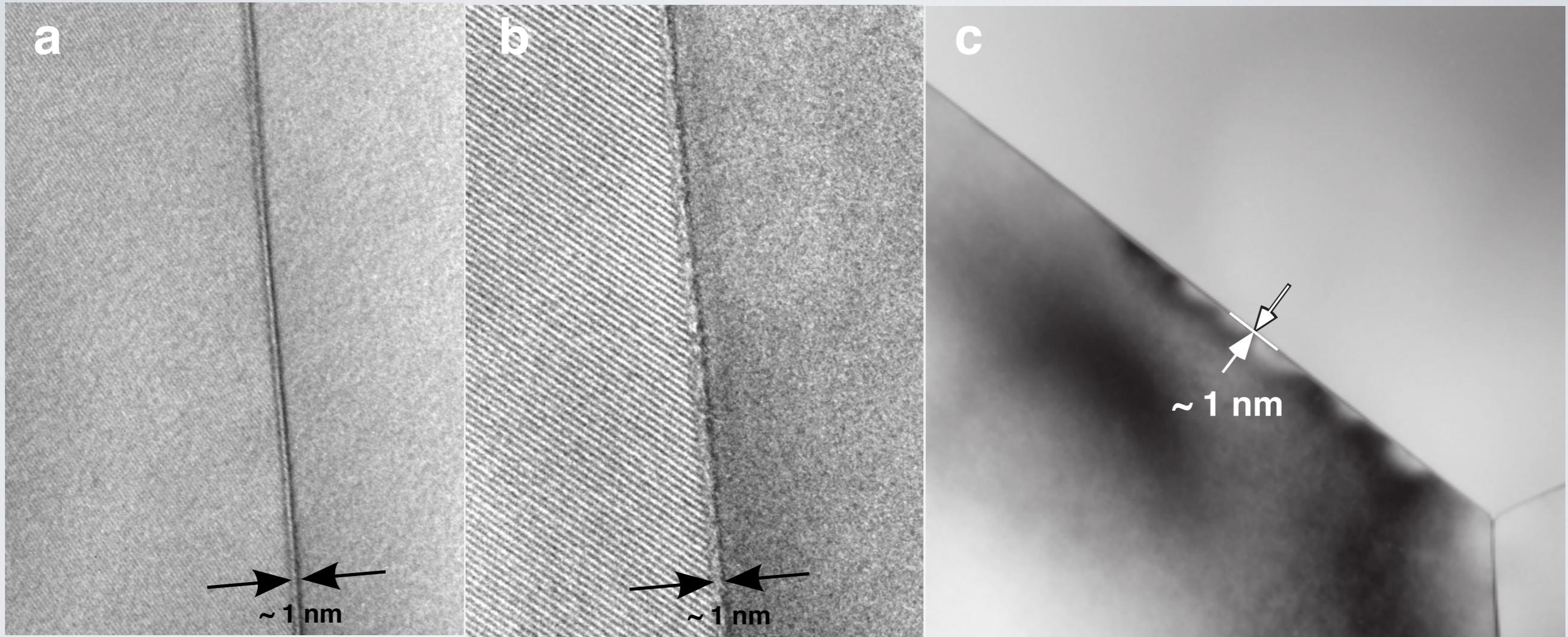
High resolution image of olivine grain boundaries



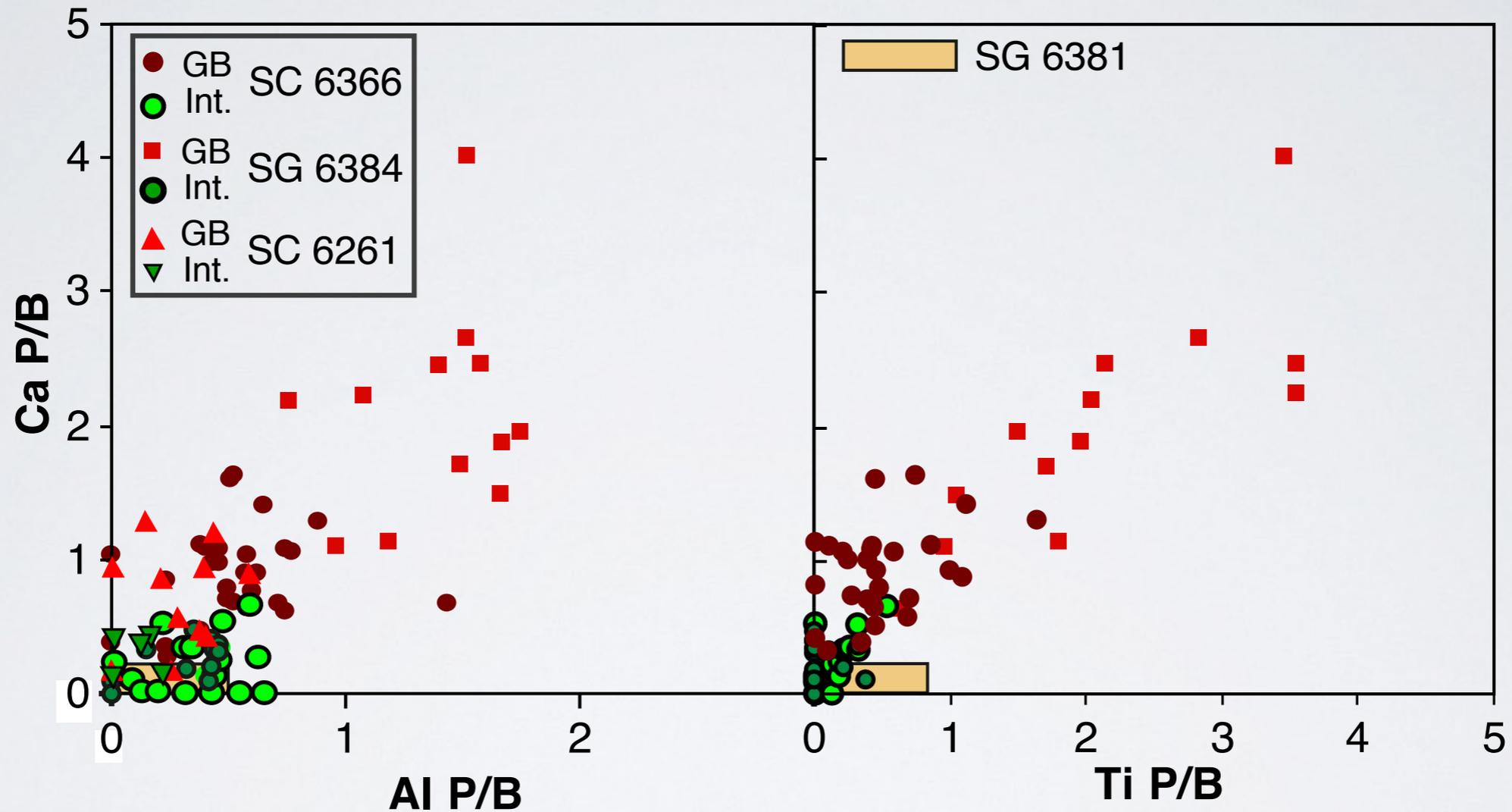
Faul et al., 2004

Adjaoud et al., 2012

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



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



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

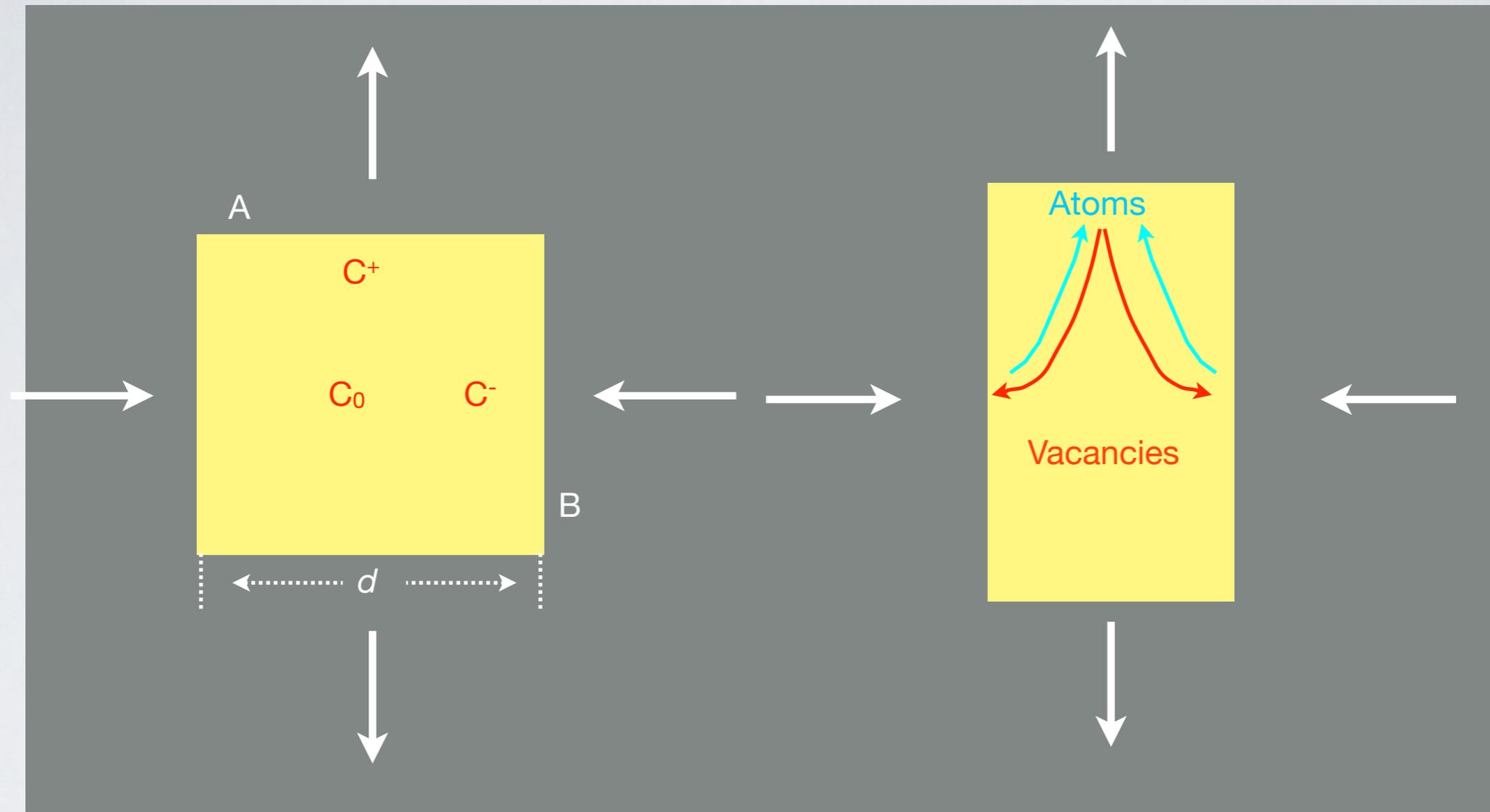
Deformation - flow laws

,first principles' derivations - physical model

constitutive equations relating strain rate to stress

Poirier, Creep of Crystals, 1985

Application of a differential stress:
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 \sim grain size (face A - face B)

diffusion \sim diffusivity (atom species, crystal structure), temperature

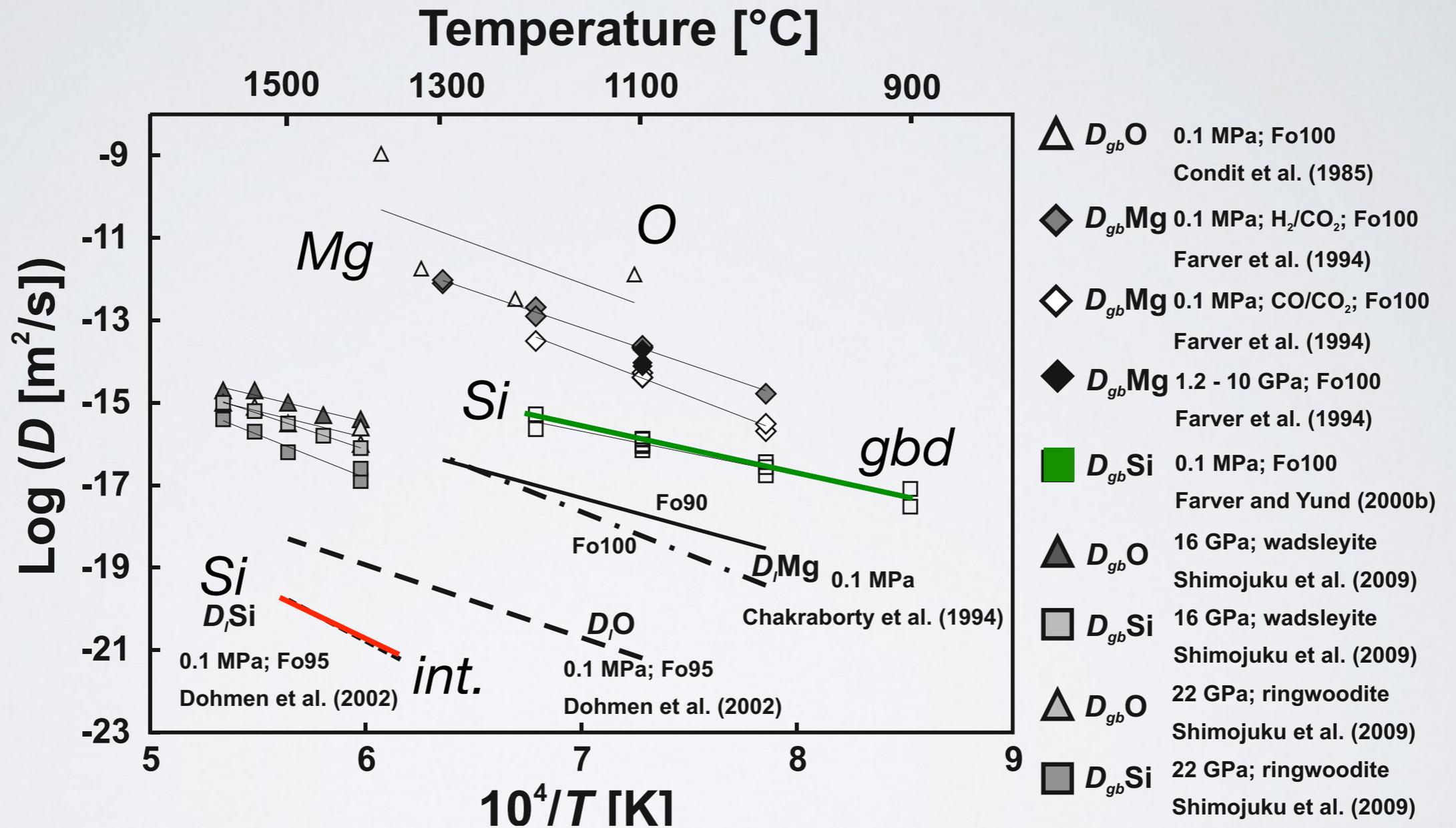
flow law (constitutive equation, strain rate $\dot{\epsilon}$ as a function of stress σ):

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

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

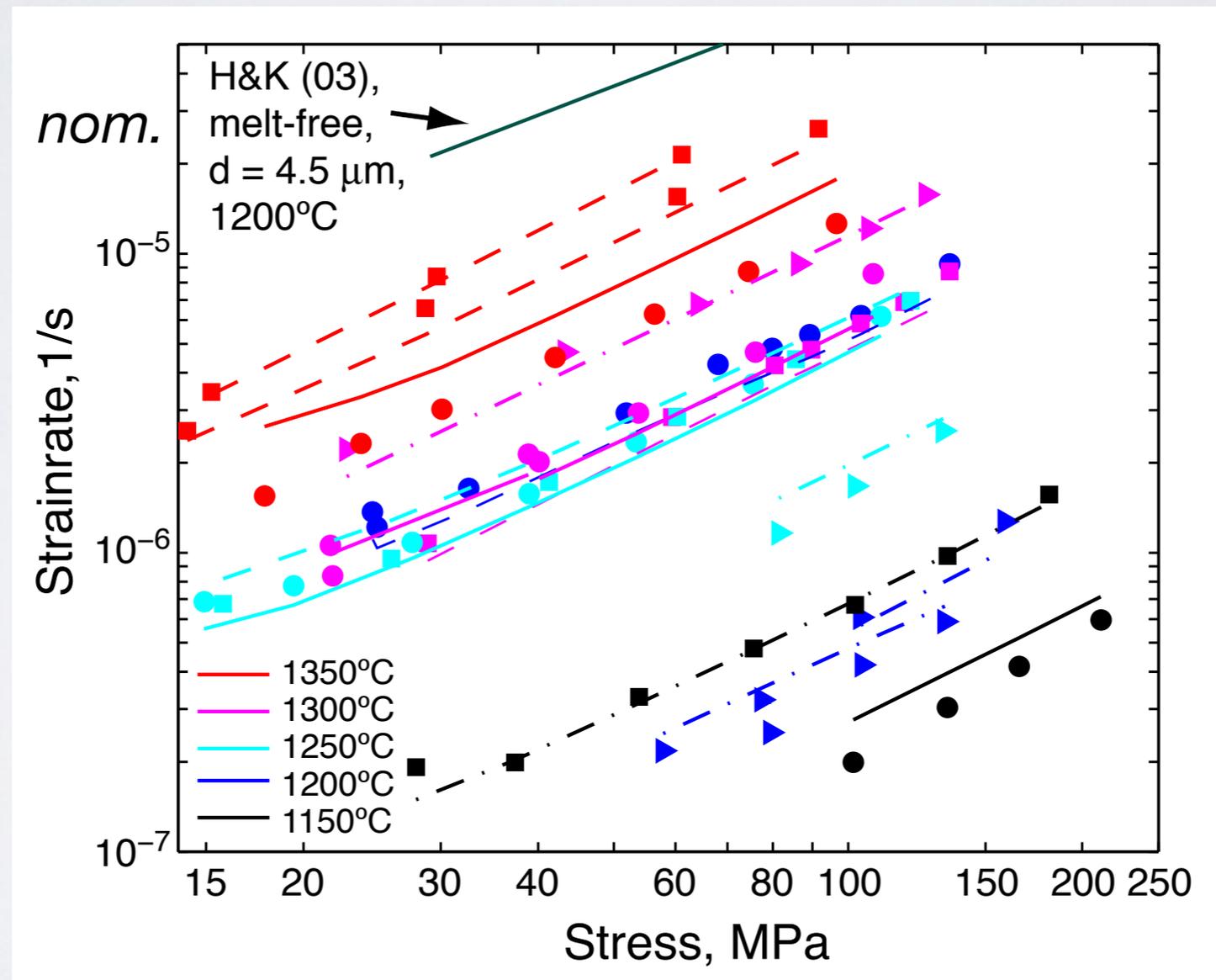


Dohmen & Milke, 2010

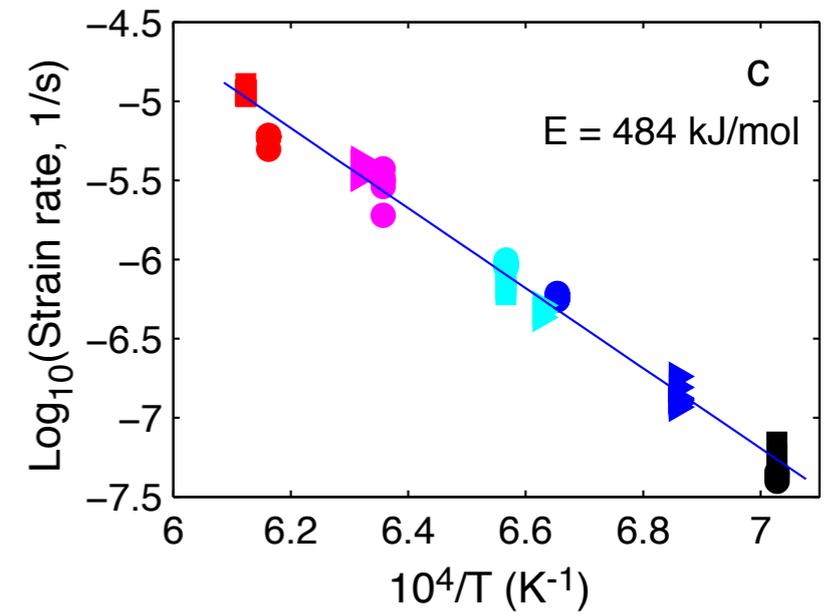
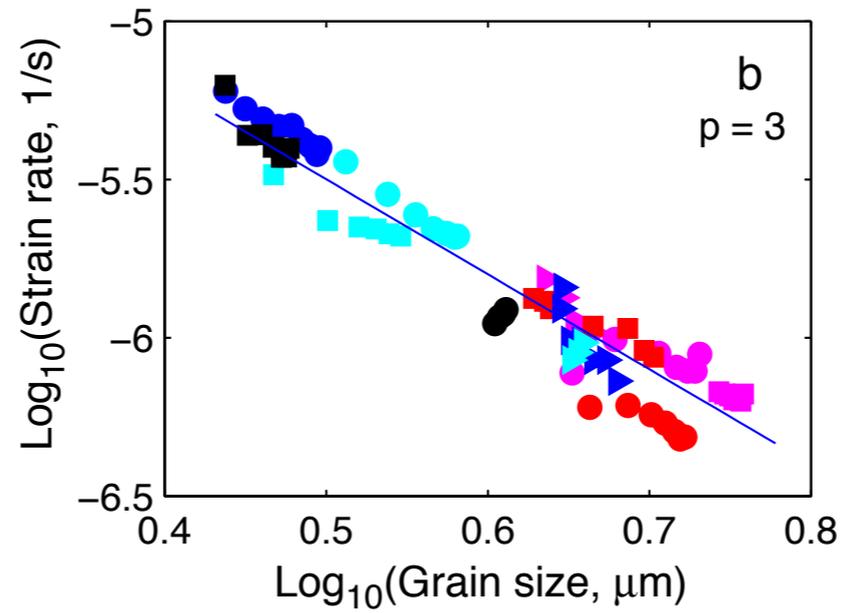
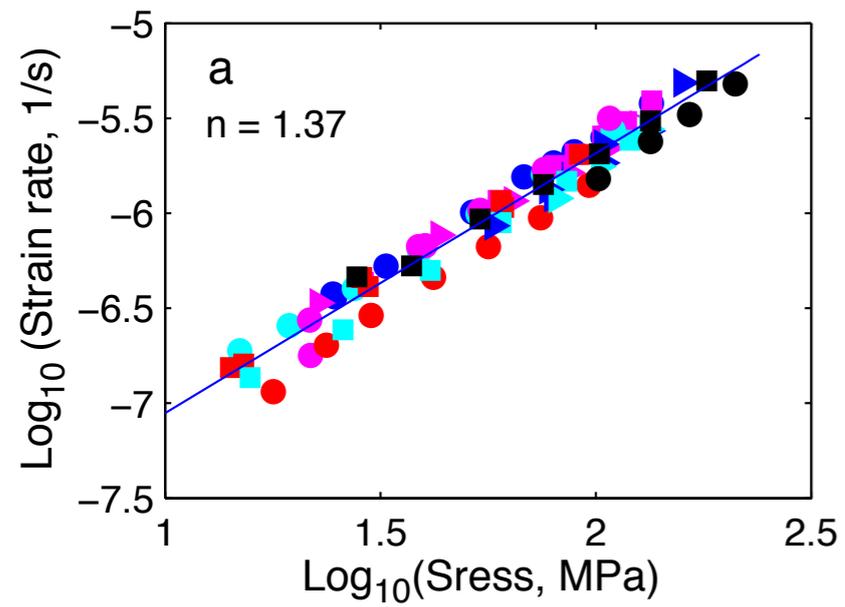
flow law for grain boundary diffusion

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

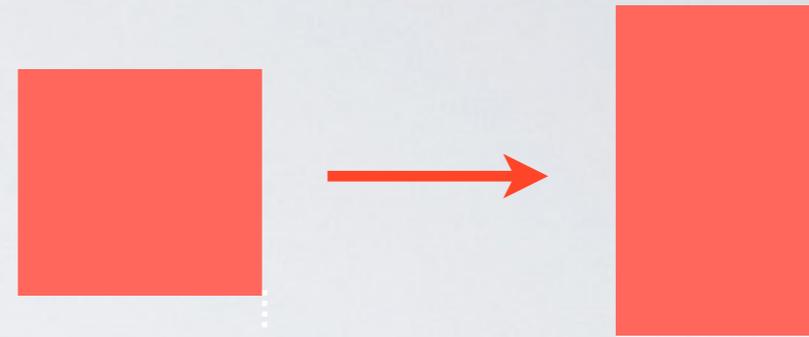
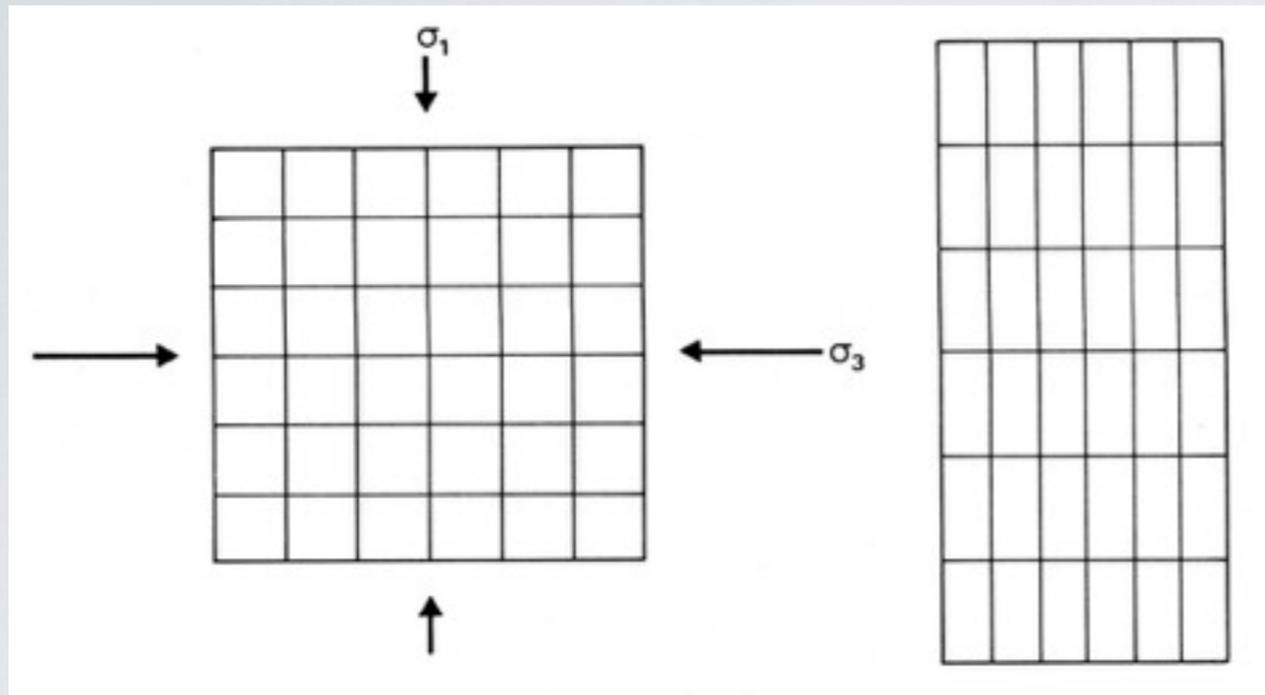
but A , E , V^* are also specific to diffusion mechanism



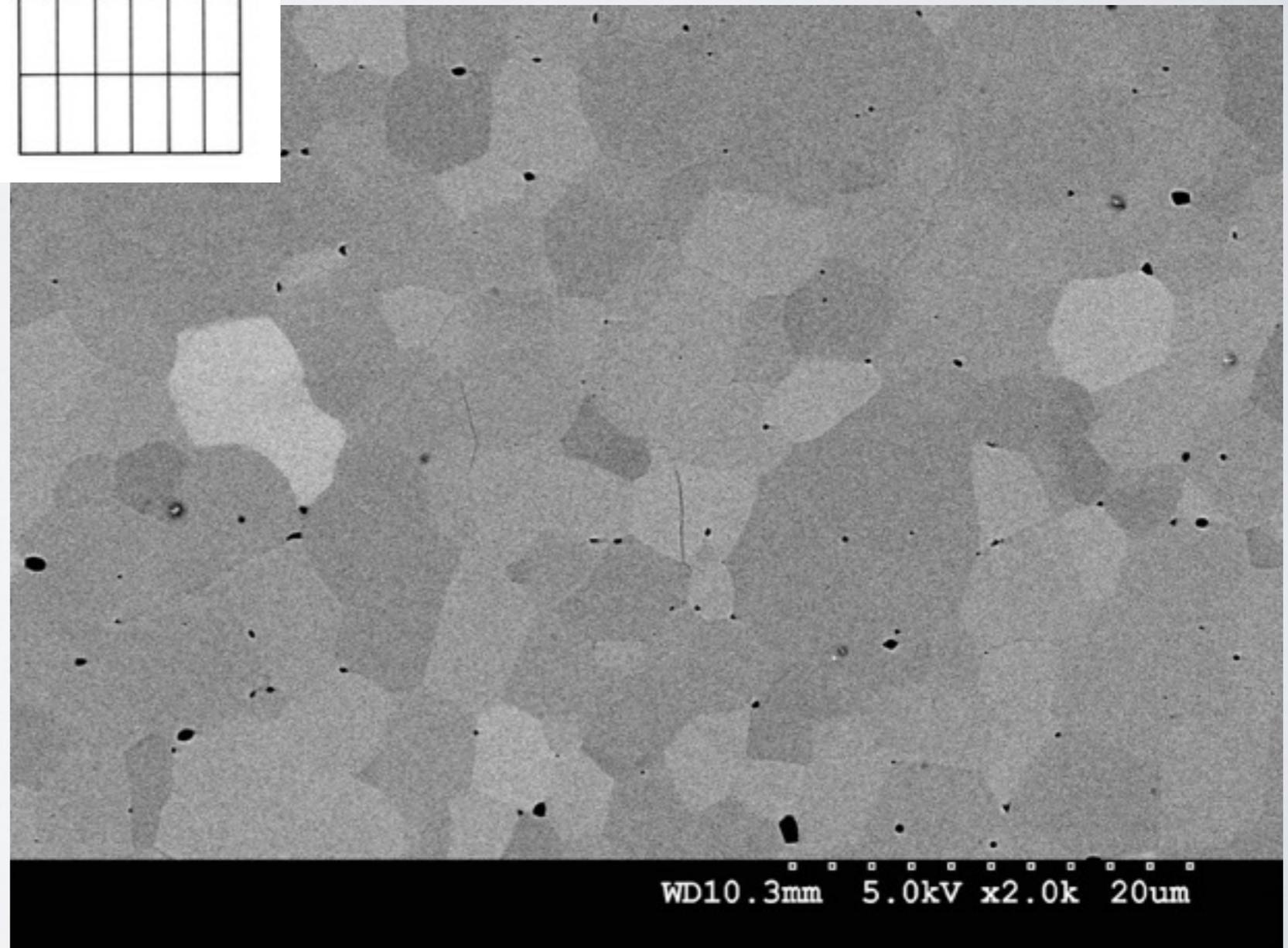
Fit parameters



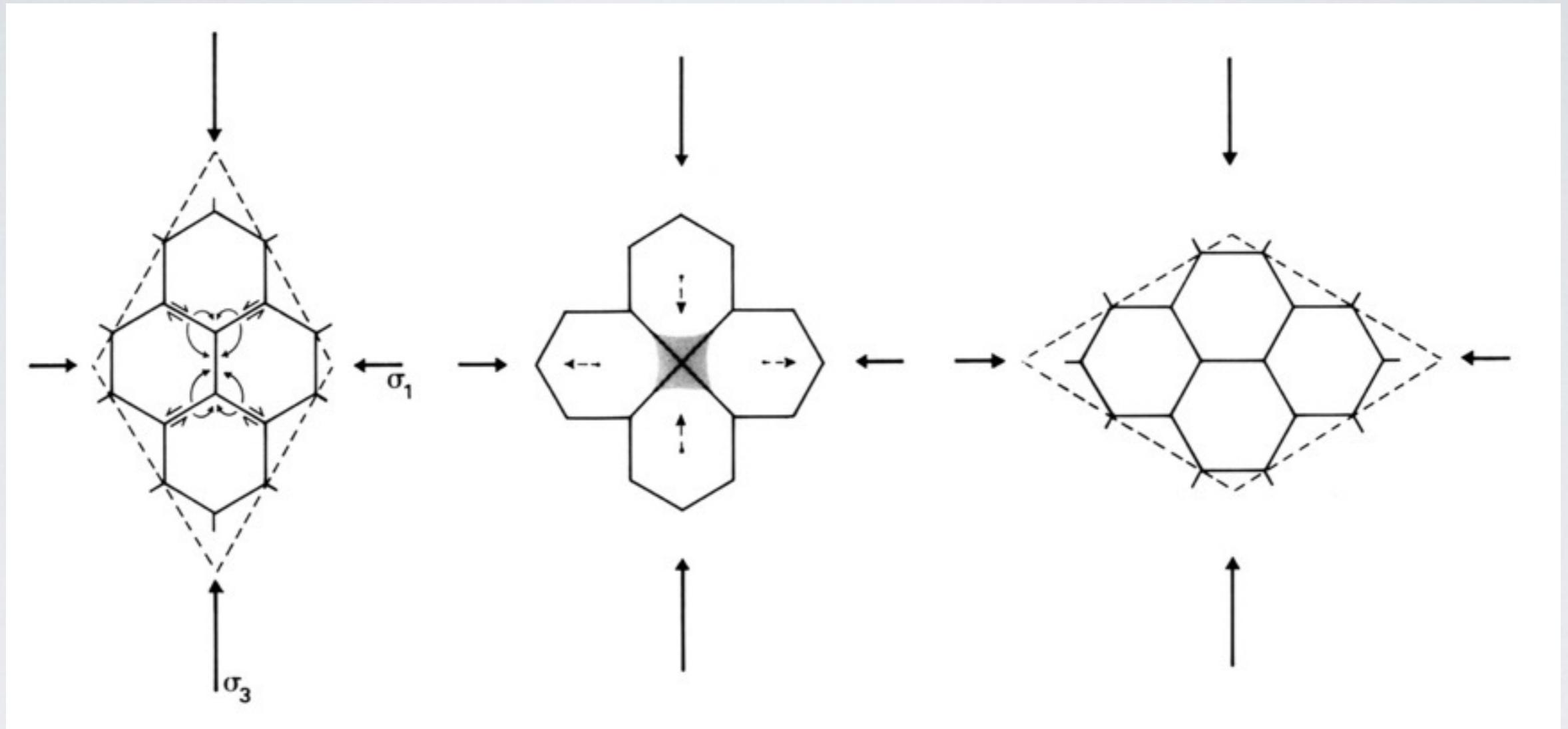
But: "Pure" diffusion creep would lead to shape change of grains:



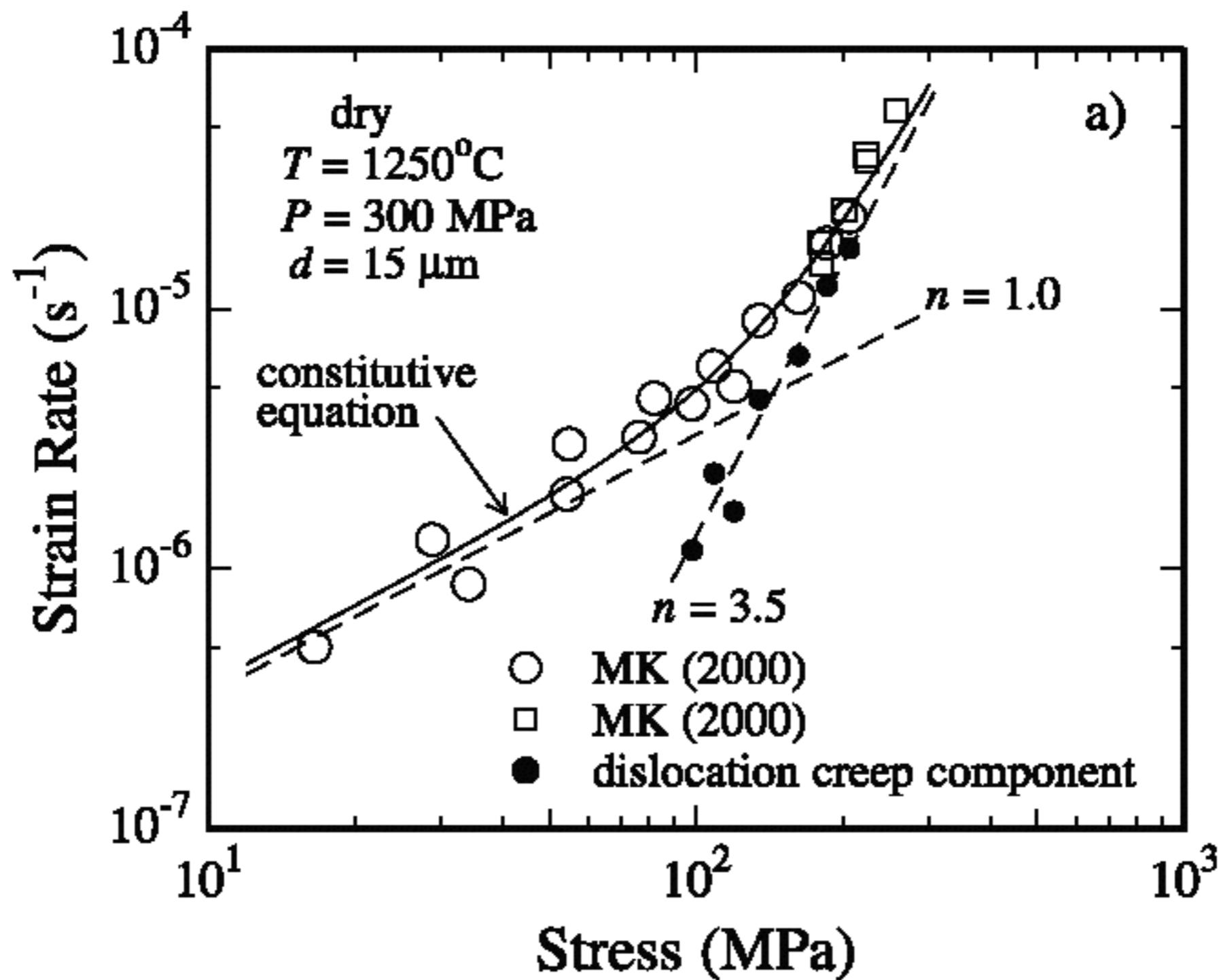
Observation: Grains remain equiaxed after deformation



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.

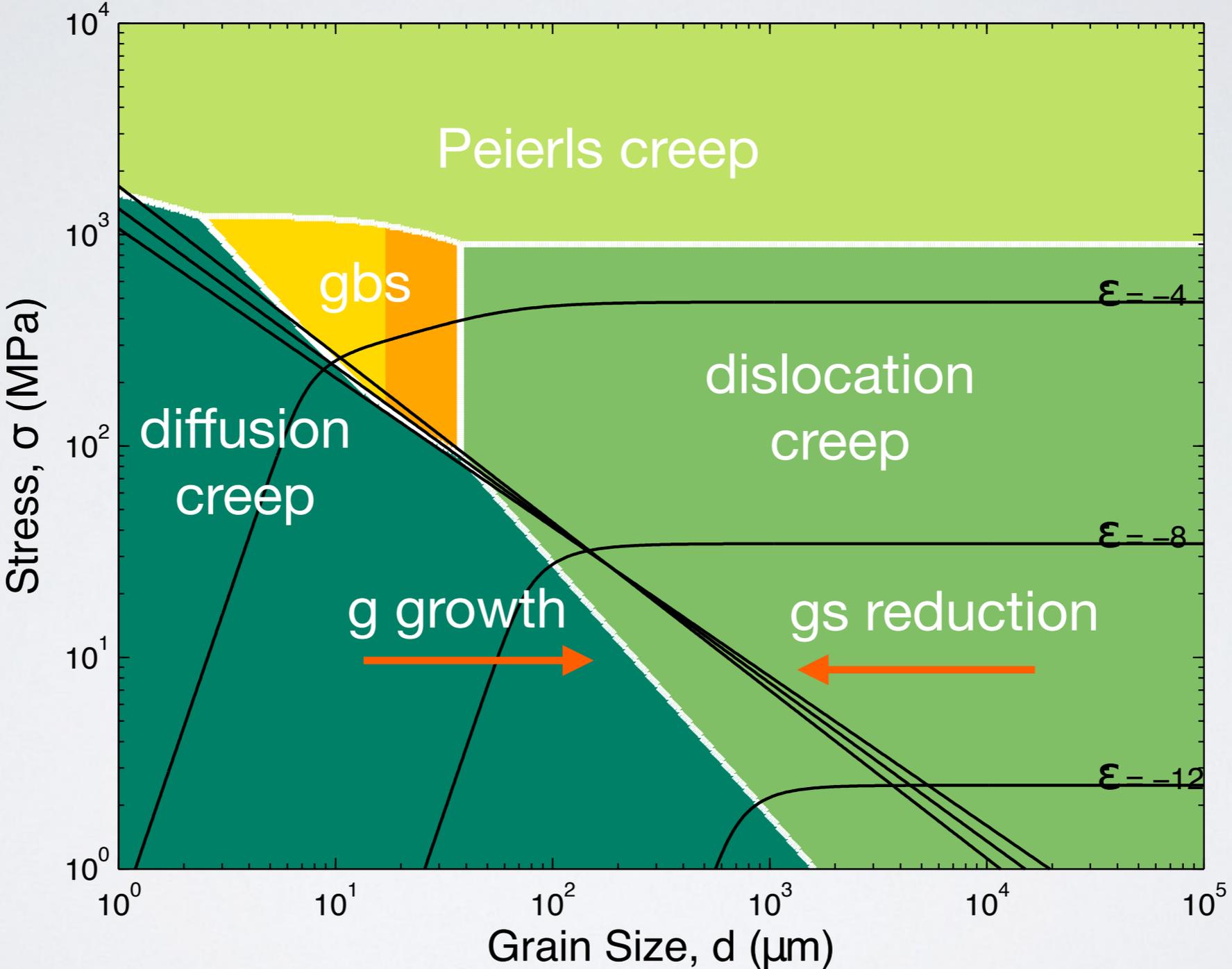
$$\dot{\epsilon} = A \sigma^n \exp[-(E+PV^*)/RT]$$

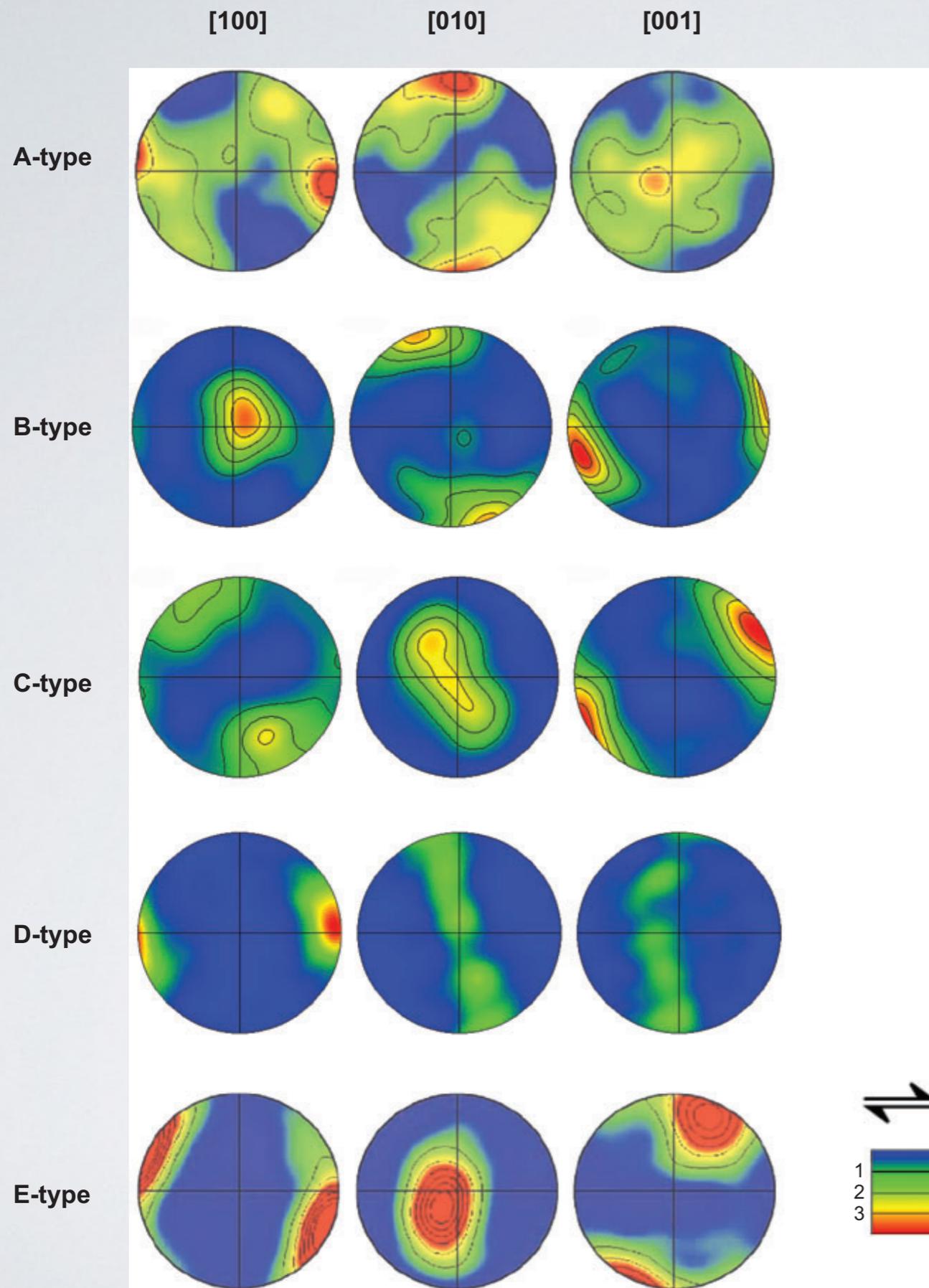
dislocation density \sim stress: strain rate depends on stressⁿ

dislocations are intracrystalline, no grain size dependence

Deformation Mechanism Map

Olivine, 1250°C, 0.4 GPa

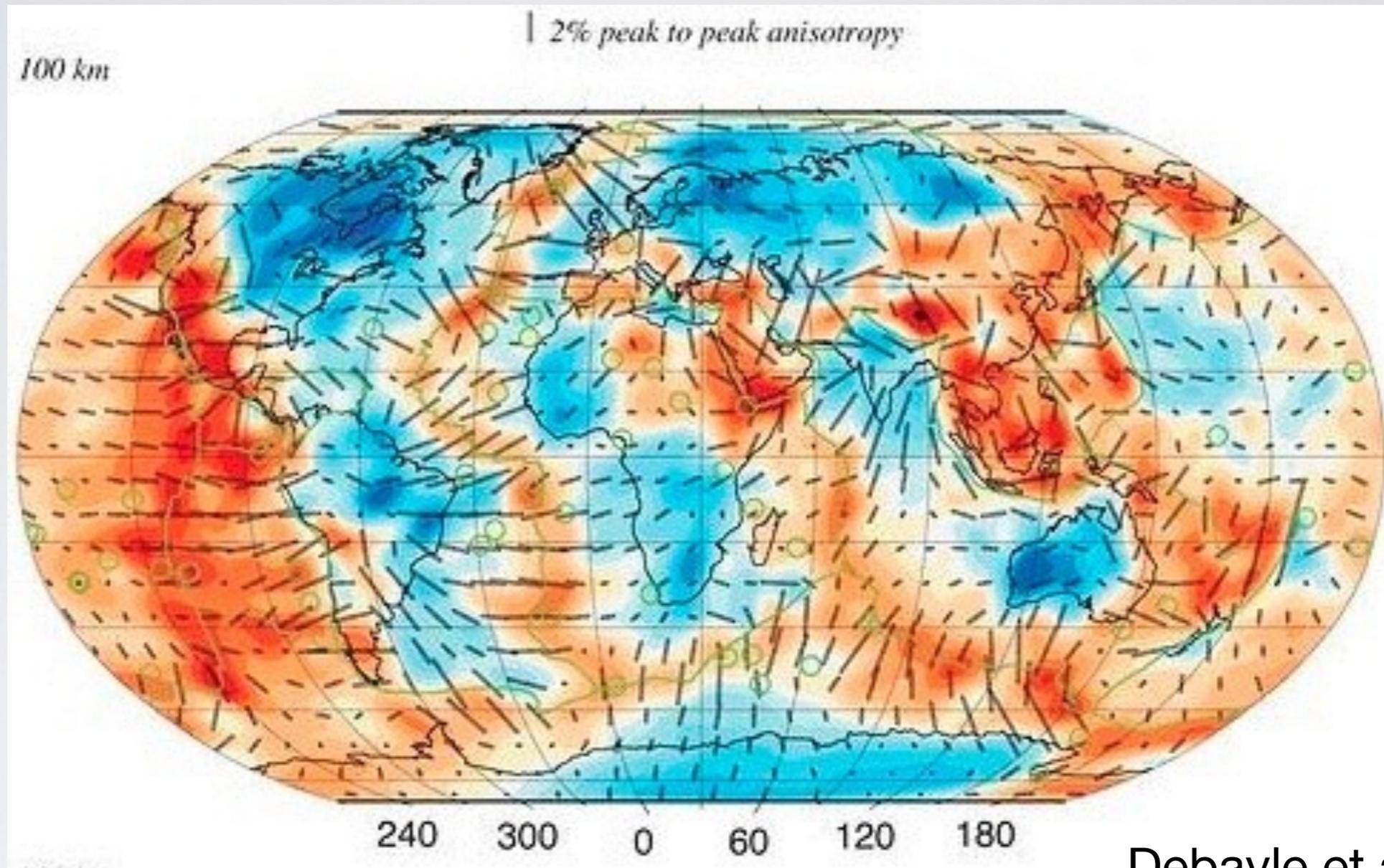




Pole figures showing the alignment of olivine crystallographic axes - consequence of dislocation creep, i.e. the glide of dislocations on certain planes in certain directions

Karato et al., 2008

Dislocation creep leads to seismic anisotropy



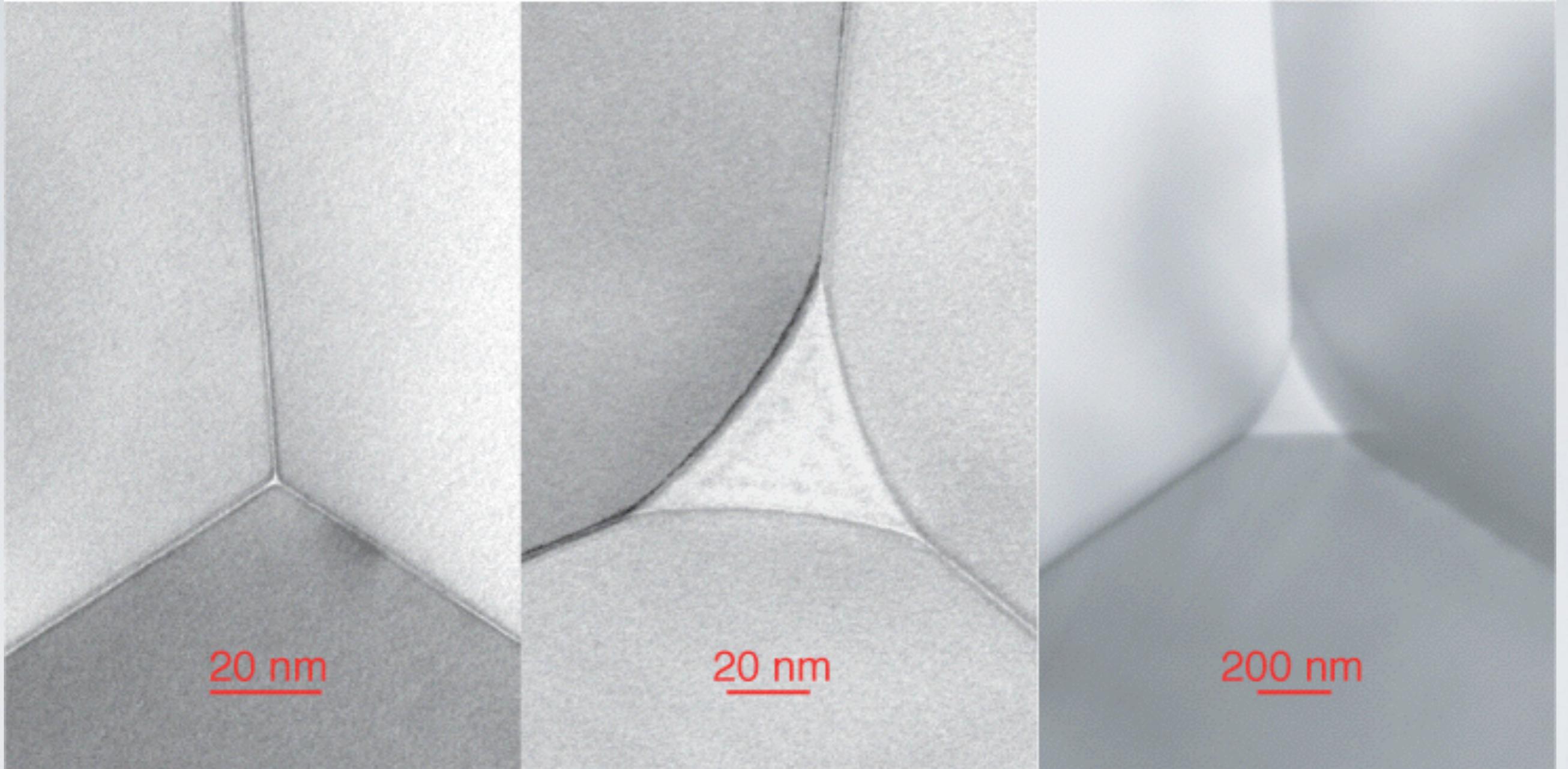
Debayle et al., 2005

color scale represents velocity variation (slow - red e.g. at MOR,
fast - blue cartons)

lines represent direction and magnitude of anisotropy,
alignment of olivine indicates flow

Influence of melt

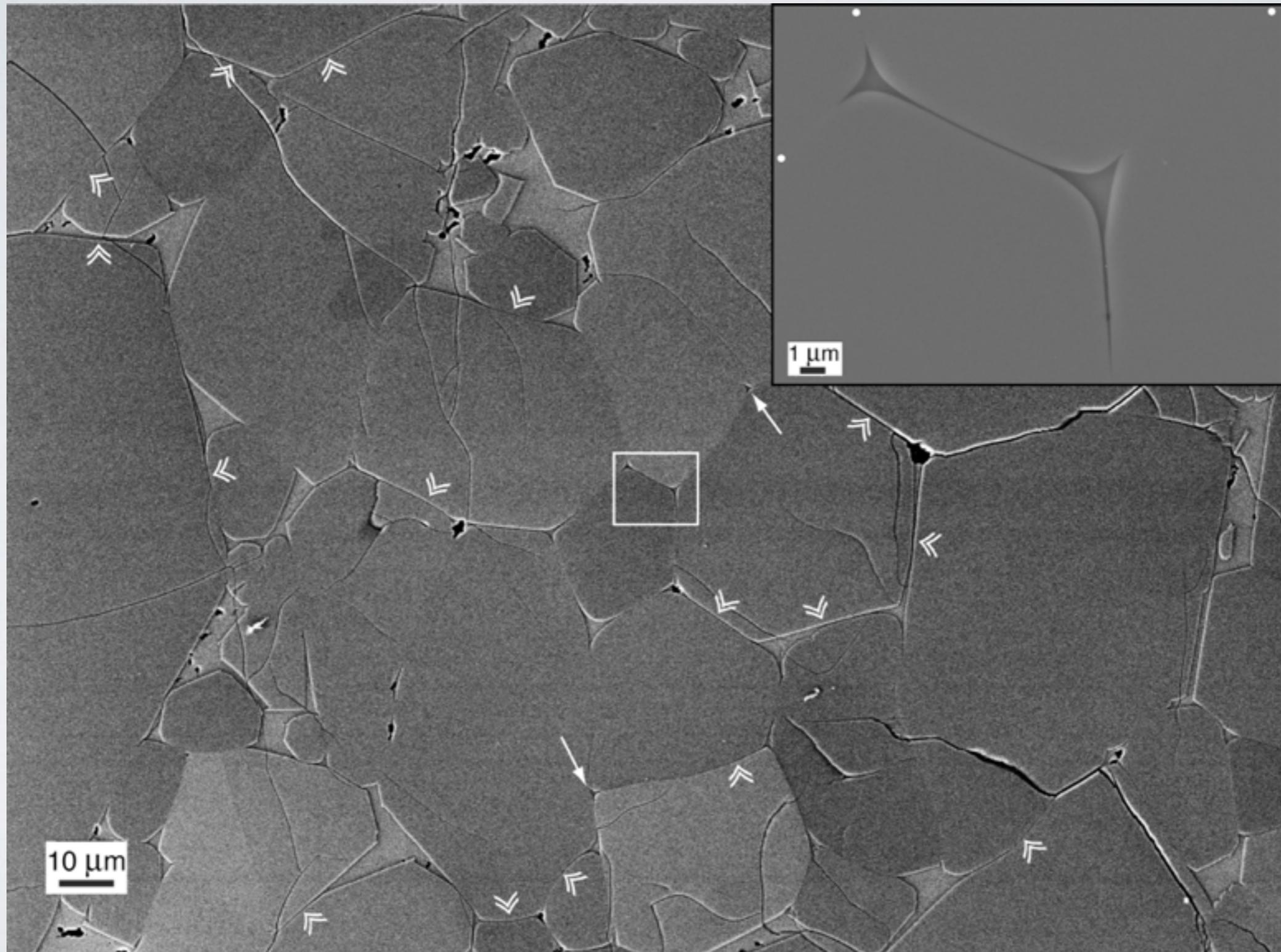
TEM images of three-grain edges



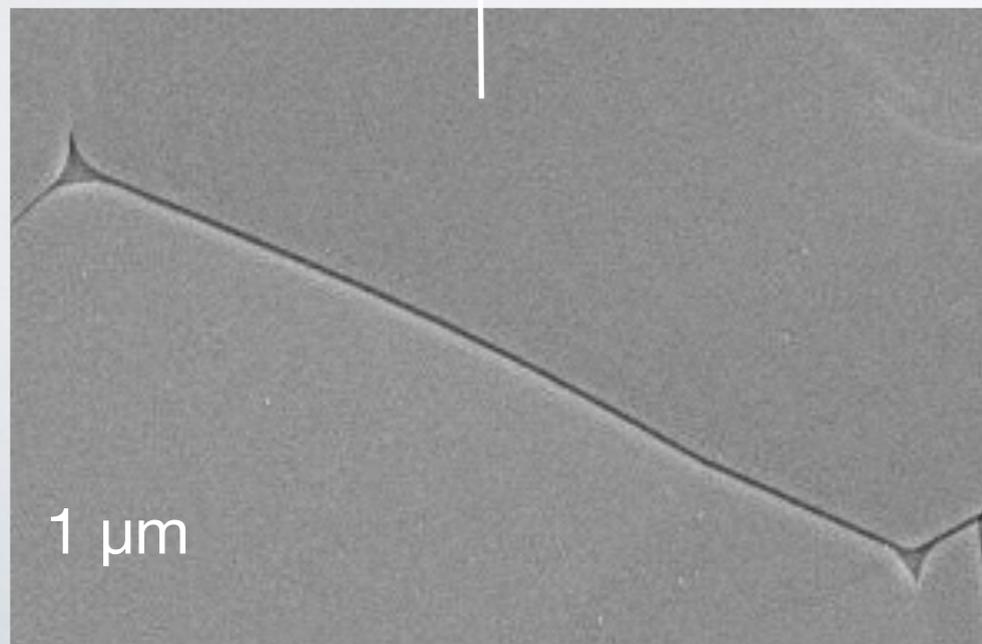
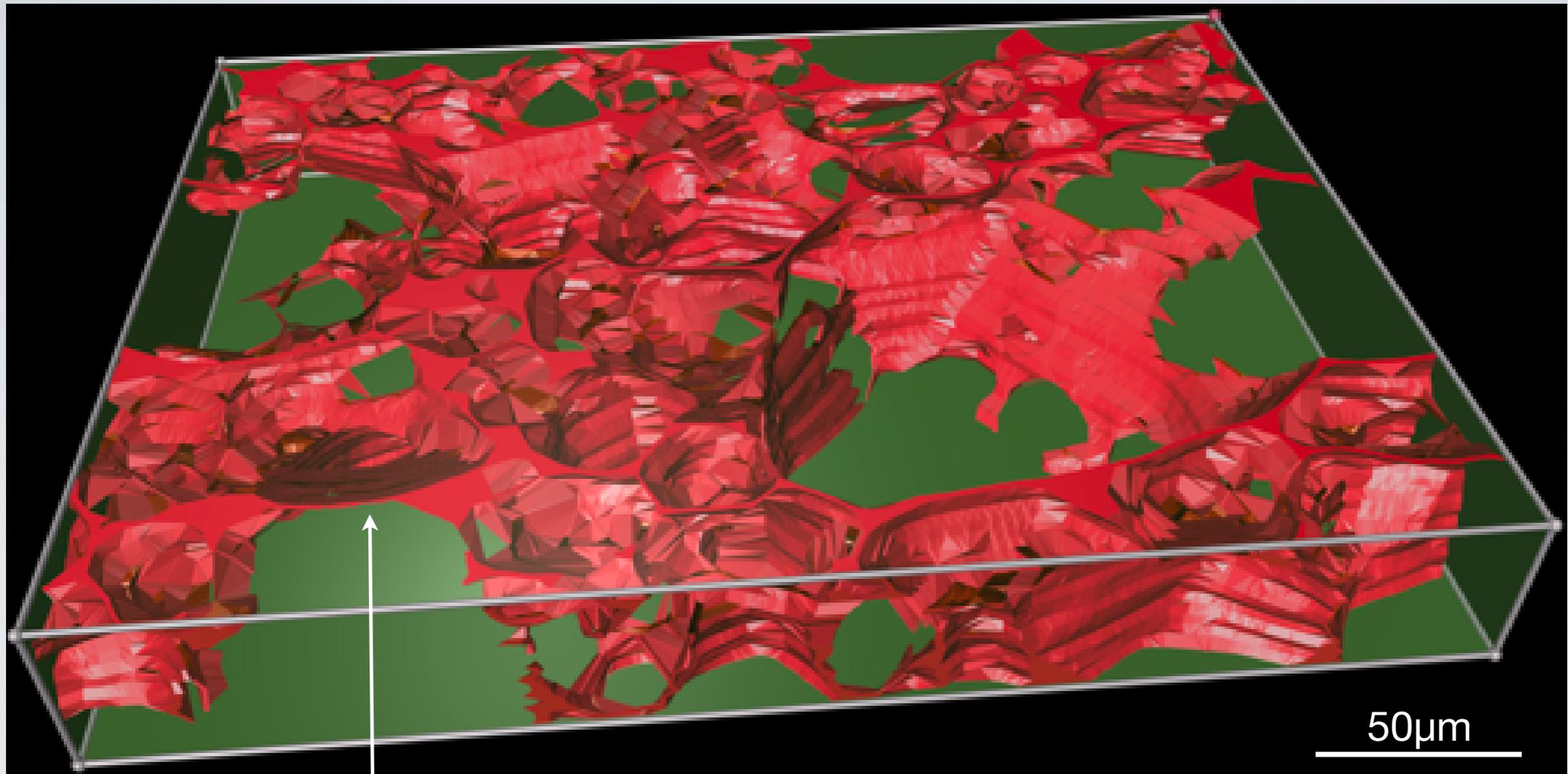
Solgel olivine

San Carlos olivine

Melt distribution in polycrystalline olivine



$P = 1 \text{ GPa}, 1350^\circ\text{C}, 432 \text{ hours}$

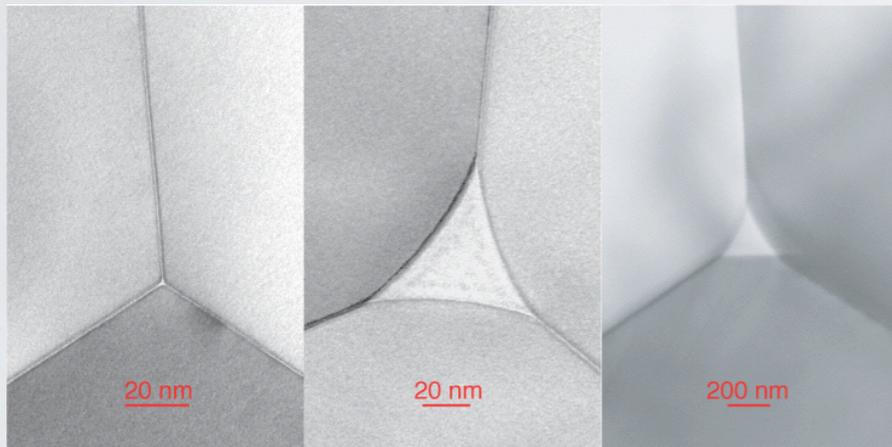


3-D view of the melt distribution
3.6% melt, 30 μm grain size

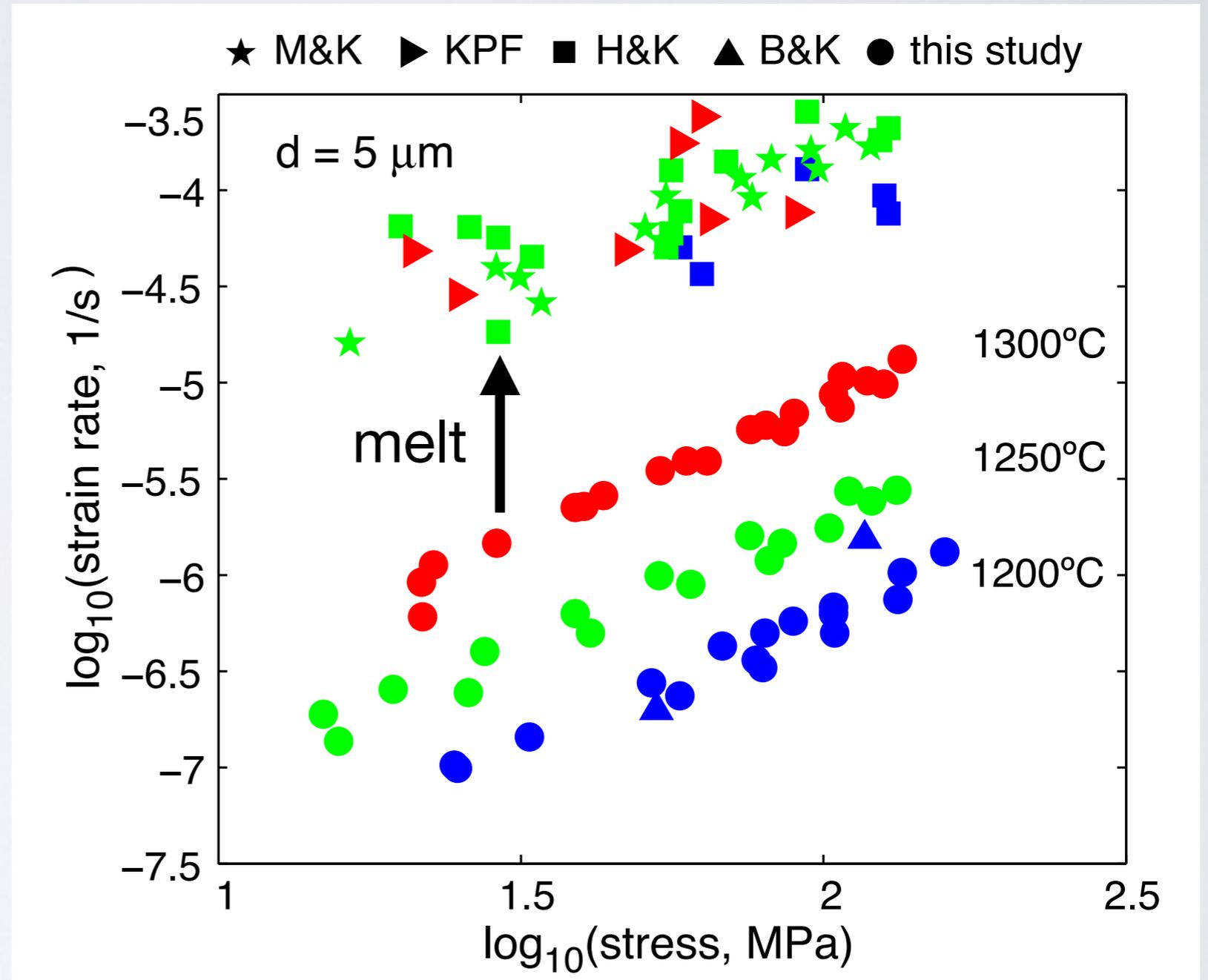
Garapić, Faul and Brisson, G^3 , 2013

Influence of melt on rheology

Small amount (1%) of melt enhances strain rate by about an order of magnitude (in diffusion creep)



connected melt produces short circuit diffusion paths



Influence of Water

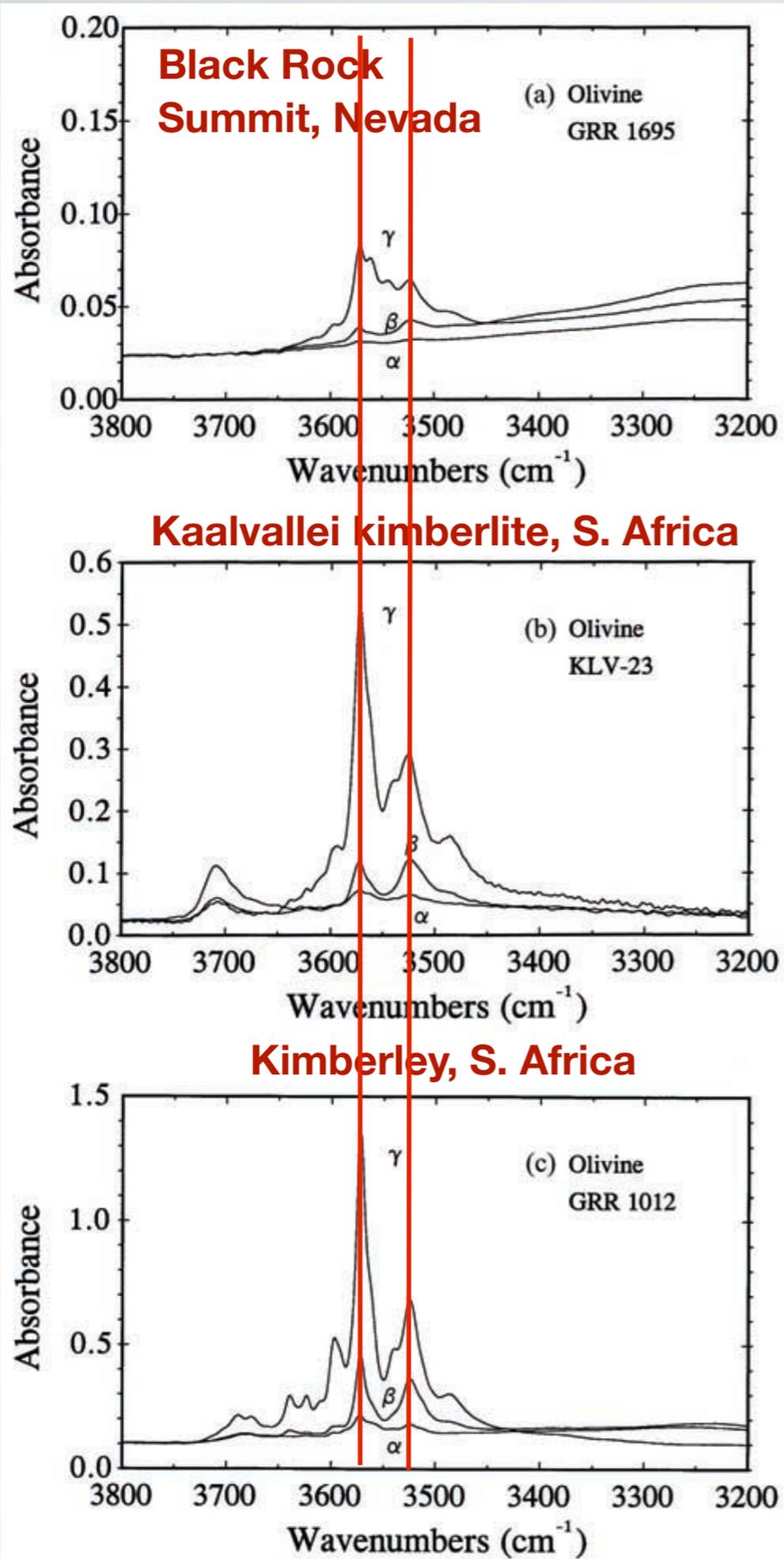
Water is a trace element in olivine at the 10s of ppm level
key aspect: hydrogen is very mobile (high diffusivity)

Water in olivine: a brief background

water (hydrogen) is a trace element

observable by Fourier Transform
Infrared Spectroscopy (FTIR)
(absorption of IR light)
advantage: absorption depends
on bonding environment

Most natural olivine has two
dominant absorption bands in IR
spectra, at 3525 and 3572 cm^{-1}

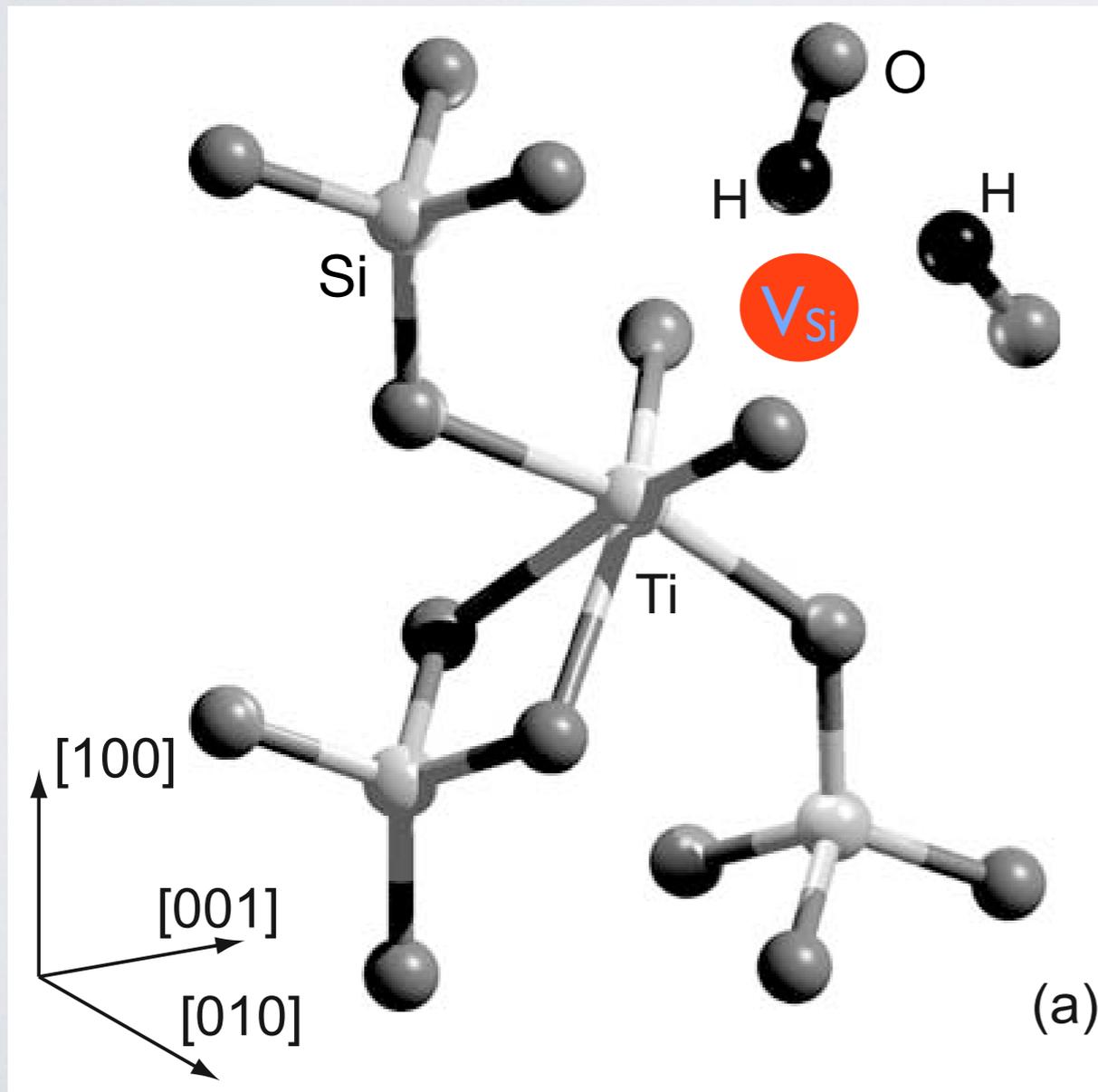


Where is the water?

Titanium clinohumite “Point Defect”: Coupled substitution of 6-fold coordinated Ti on M1 site with 2 H on Si vacancy.

Energetically the most stable.

Supported by synchrotron observations

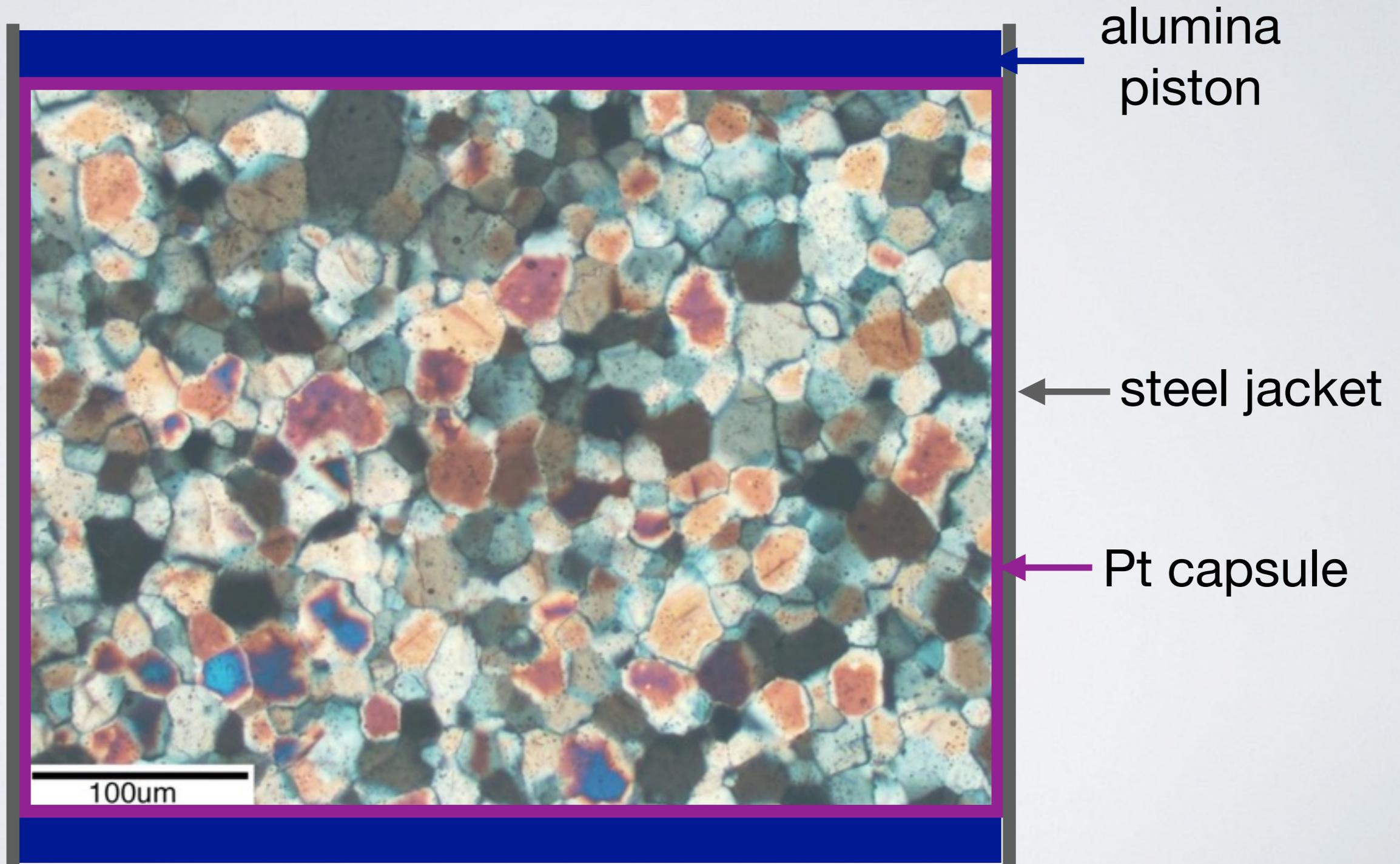


calculated OH -
vibrational frequencies:
3572 and 3525 cm^{-1}

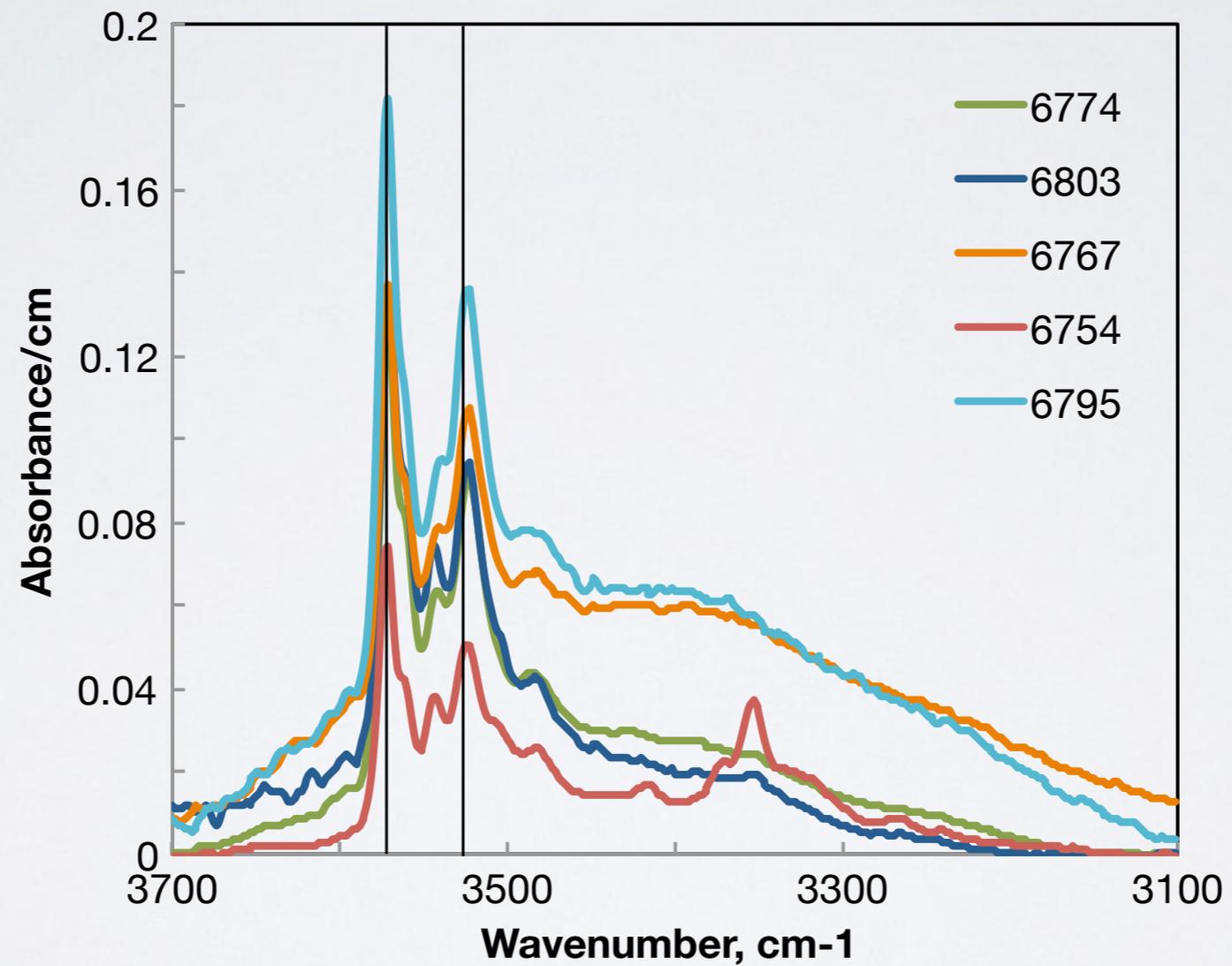
Walker et al., 2007

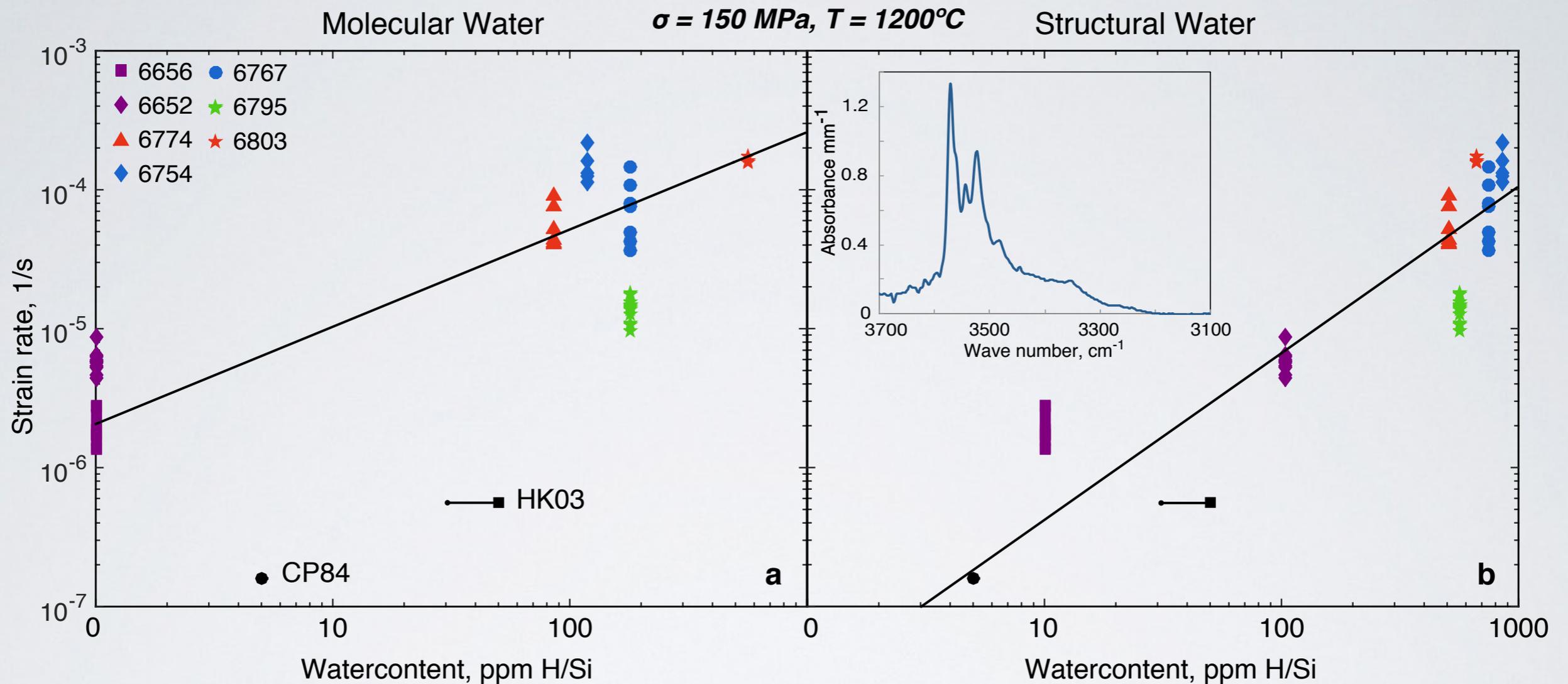
Experiments in Paterson (gas medium) apparatus,
300 MPa (200 MPa) confining pressure, 1200 - 1350°C.
Water not buffered, samples encapsulated in Pt.

Fo₉₀ olivine doped with 0.02 wt% TiO₂



IR spectra of experimental olivine: absorption bands at 3525 and 3572 cm⁻¹

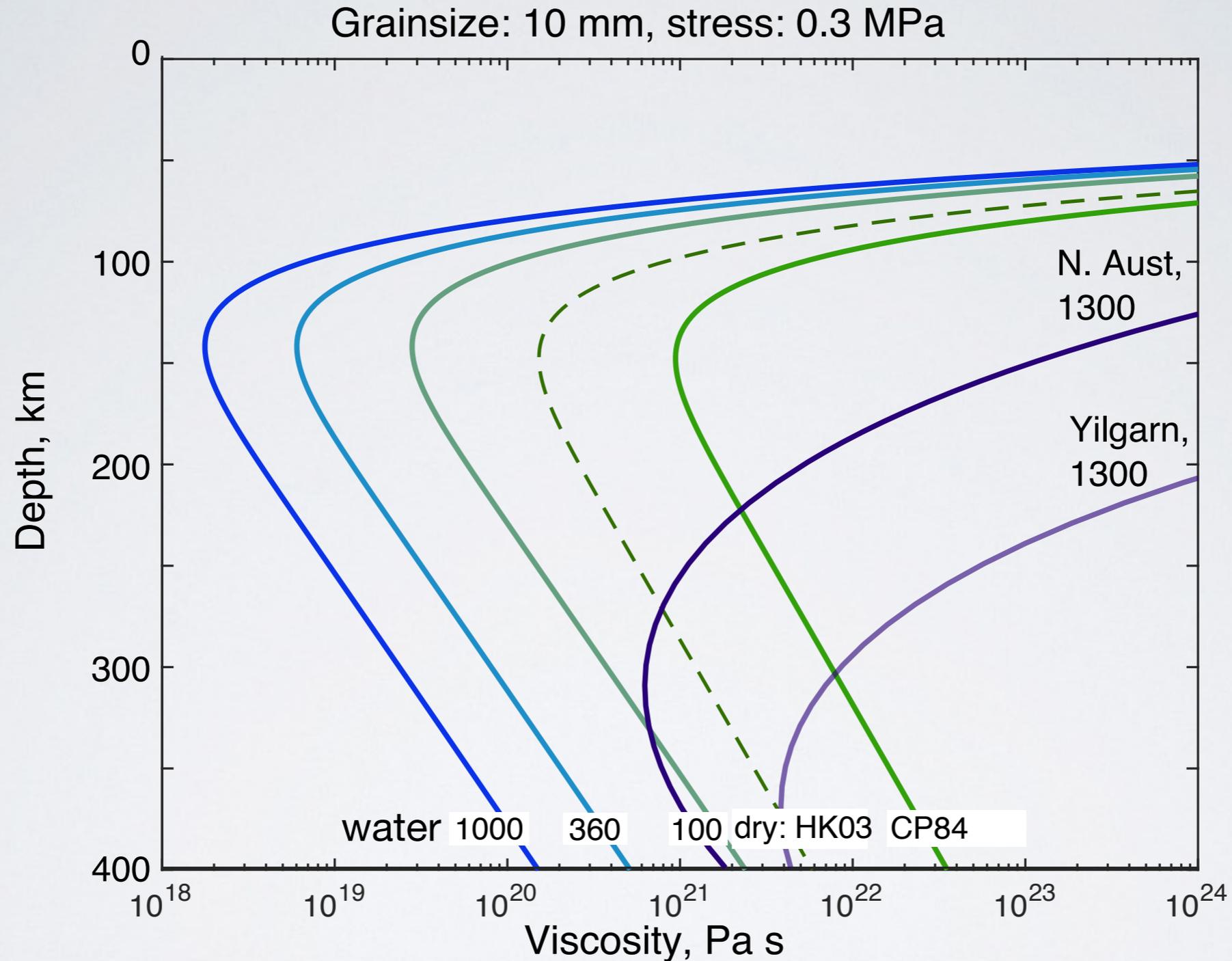




linear relationship between water content and strain rate

$$\dot{\epsilon} = A \sigma^n d^{-p} f H_2 O^r \exp\left(\frac{-Q}{RT}\right)$$

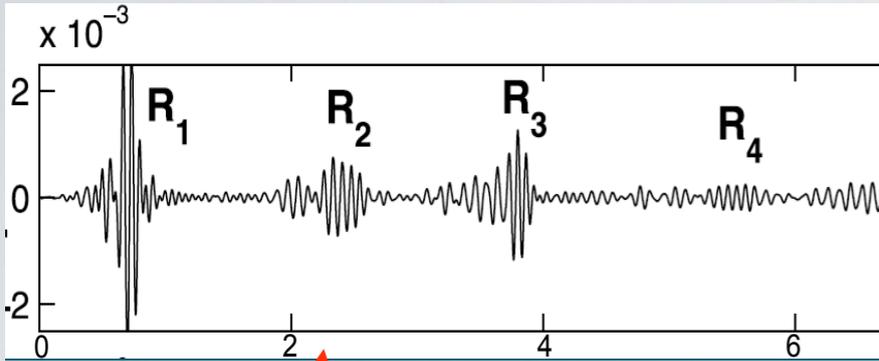
Upper mantle viscosity as a function of water



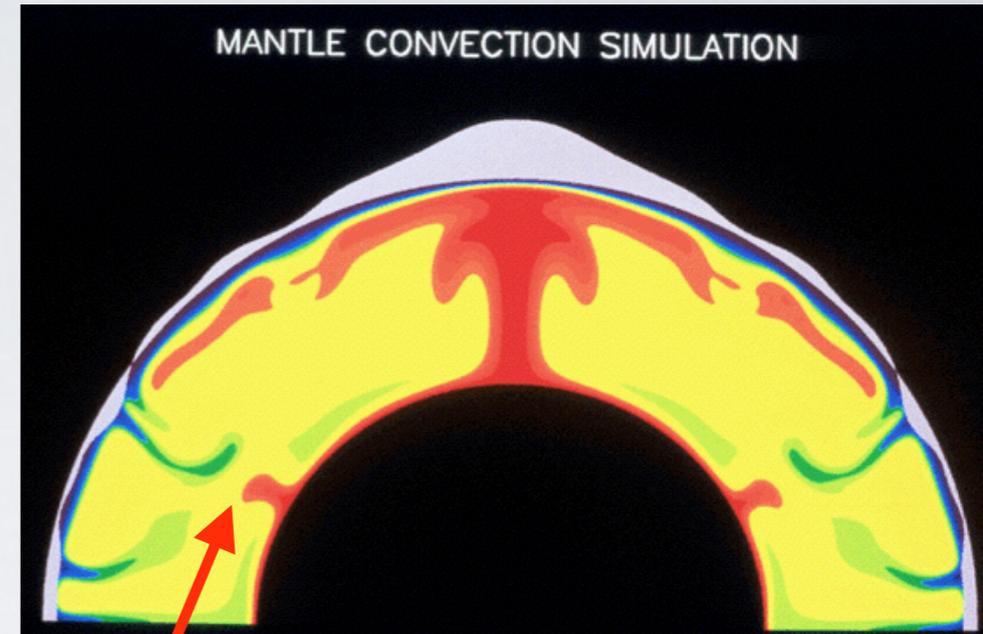
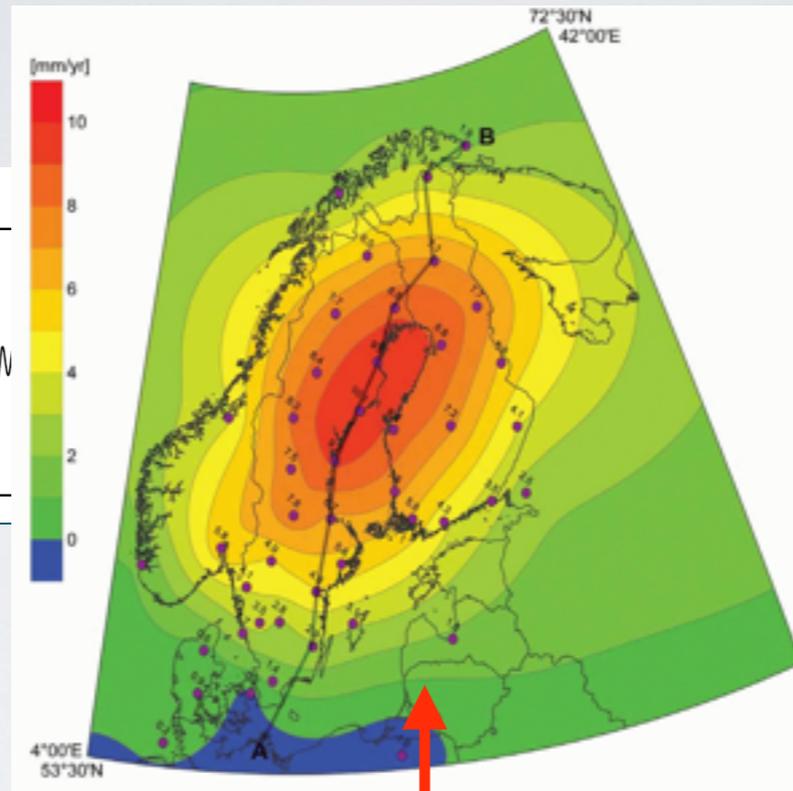
$$\text{viscosity } \eta = \sigma / 2\dot{\epsilon}$$

water content in olivine in ppm H/Si; 1000 ppm H/Si \approx 60 ppm H₂O

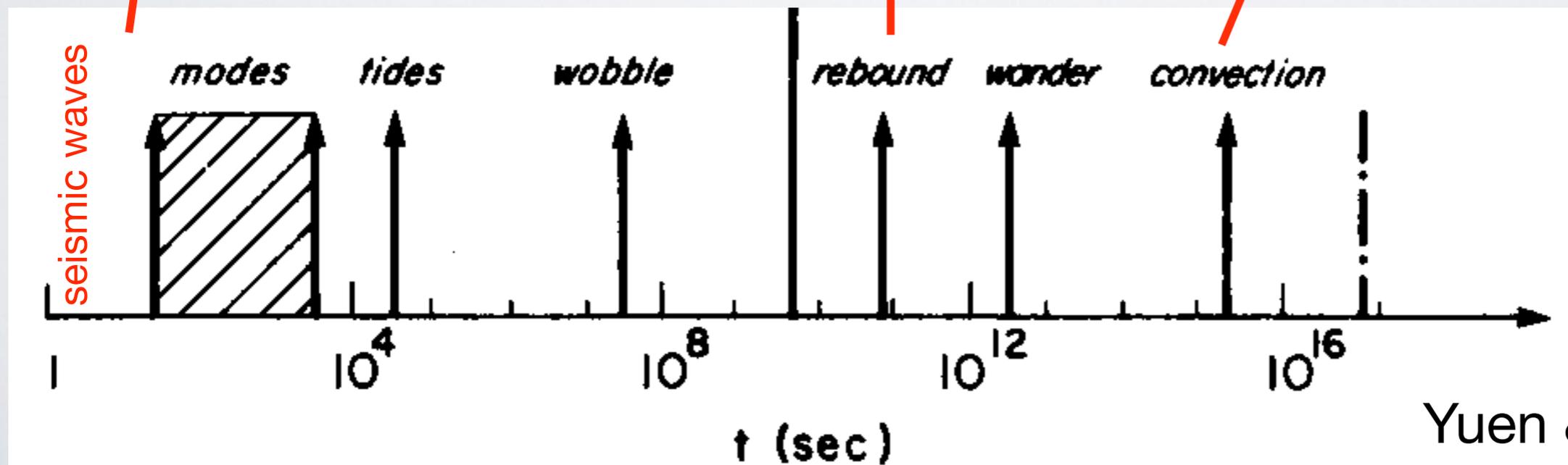
Deformation at a range of time scales



$\epsilon < 10^{-4}$



$\epsilon \gg 1$



Yuen & Peltier, 1982