



*Massachusetts Institute of Technology*

# **Rheology**

Ulrich Faul

(Ian Jackson, Chris Cline, ANU)

# **Outline**

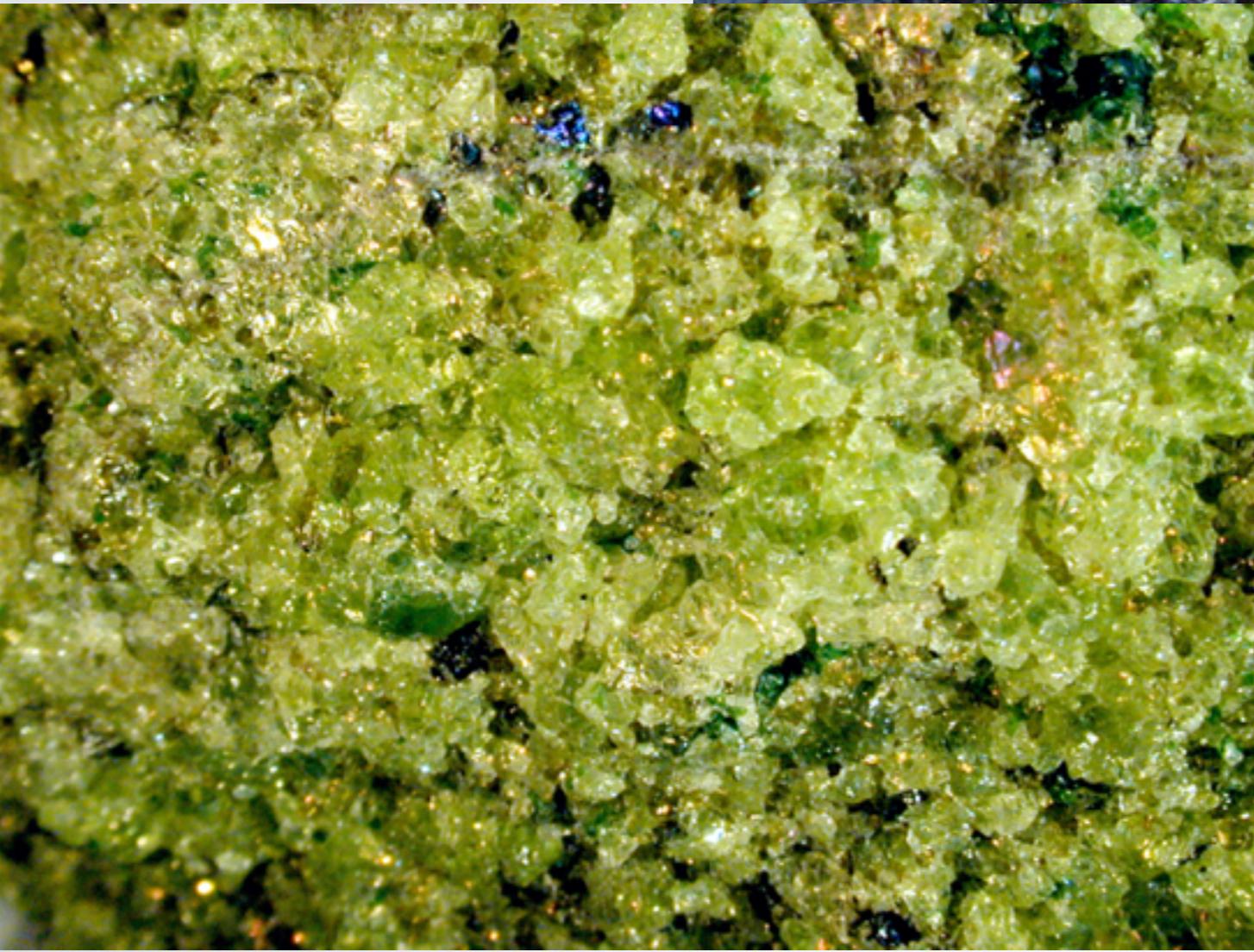
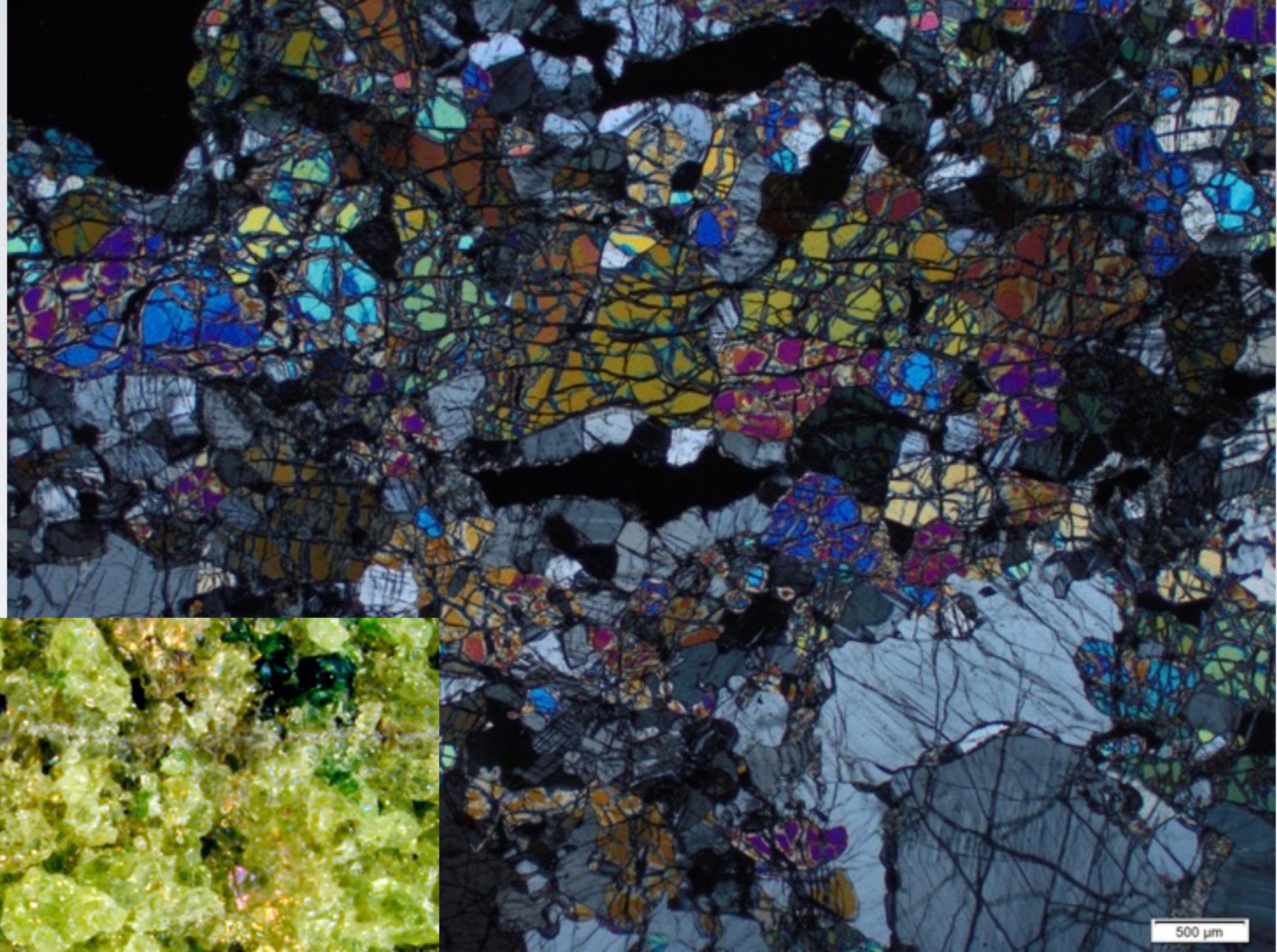
**fundamentals of defects**

**flow laws (constitutive equations)**

**extrinsic defects: water**

**seismic properties**

cross-polarized  
light image of a  
peridotite



peridotite xenolith

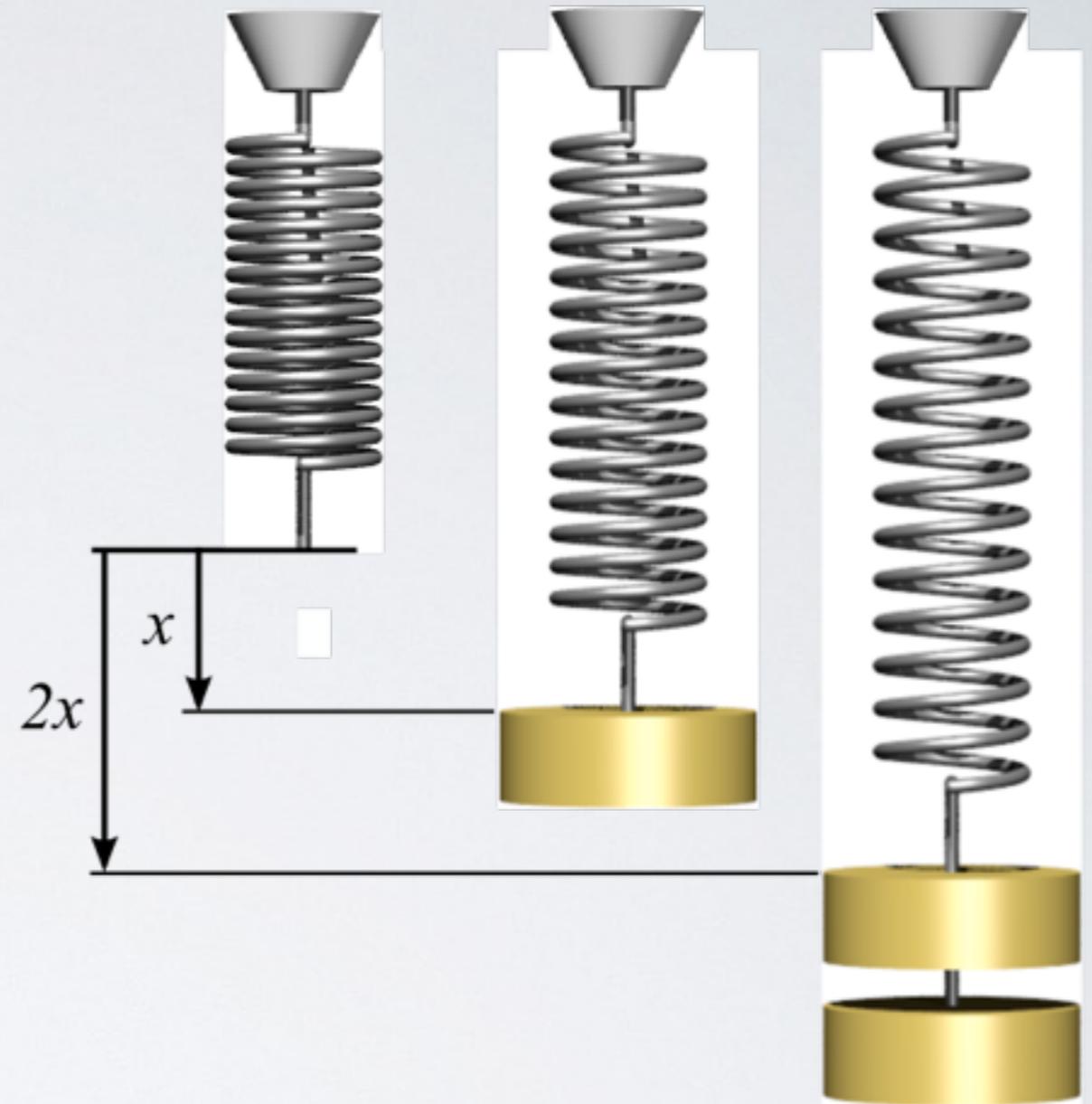
# Elastic behavior

Deformation:

Force = spring const.  $\times$  dist.

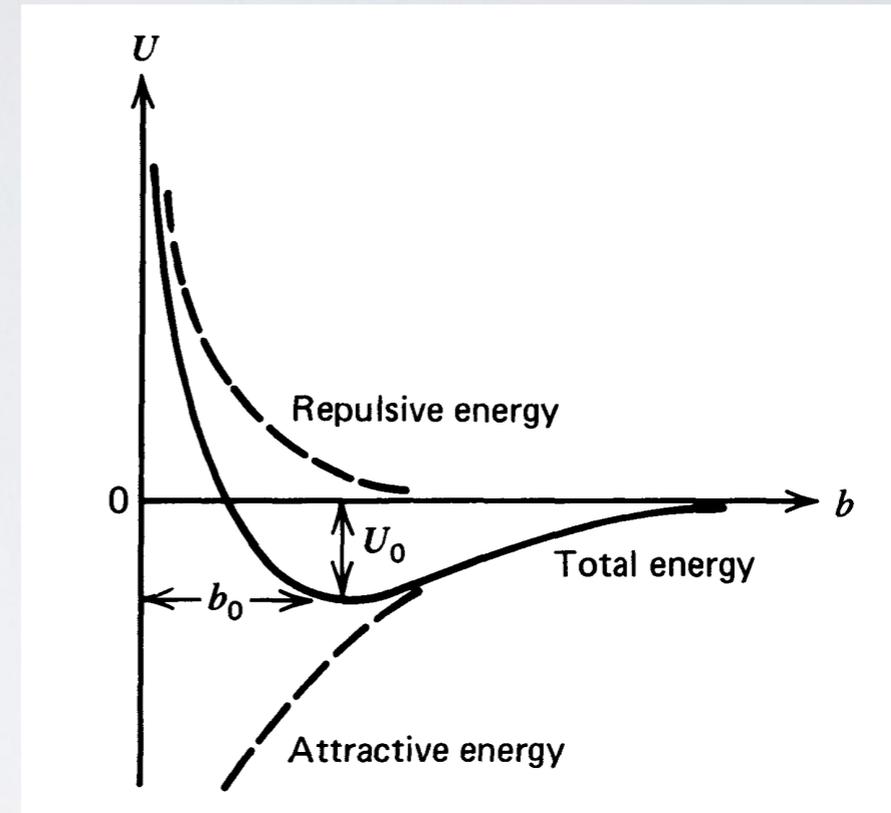
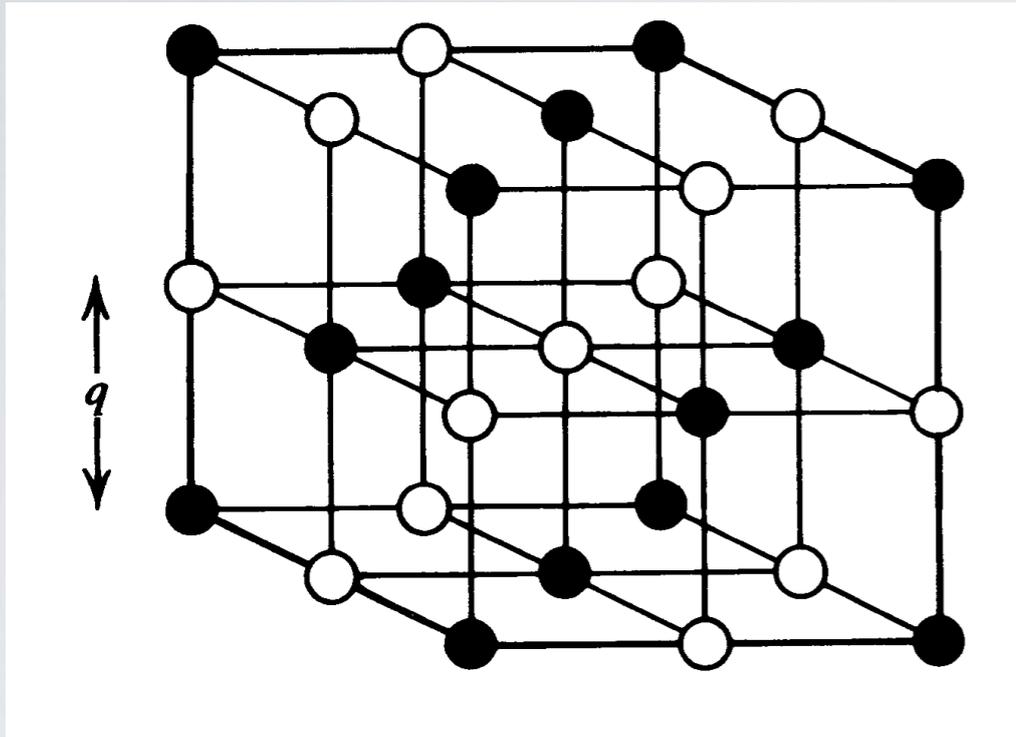
$$F = k x$$

(Hooke's law)



strain: instantaneous - recoverable

# 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



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

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



moduli of rock-forming minerals of order of 100 GPa  
convective stresses  $\sim 1 - 0.1$  MPa

**need to modify perfect elastic moduli: defects!**

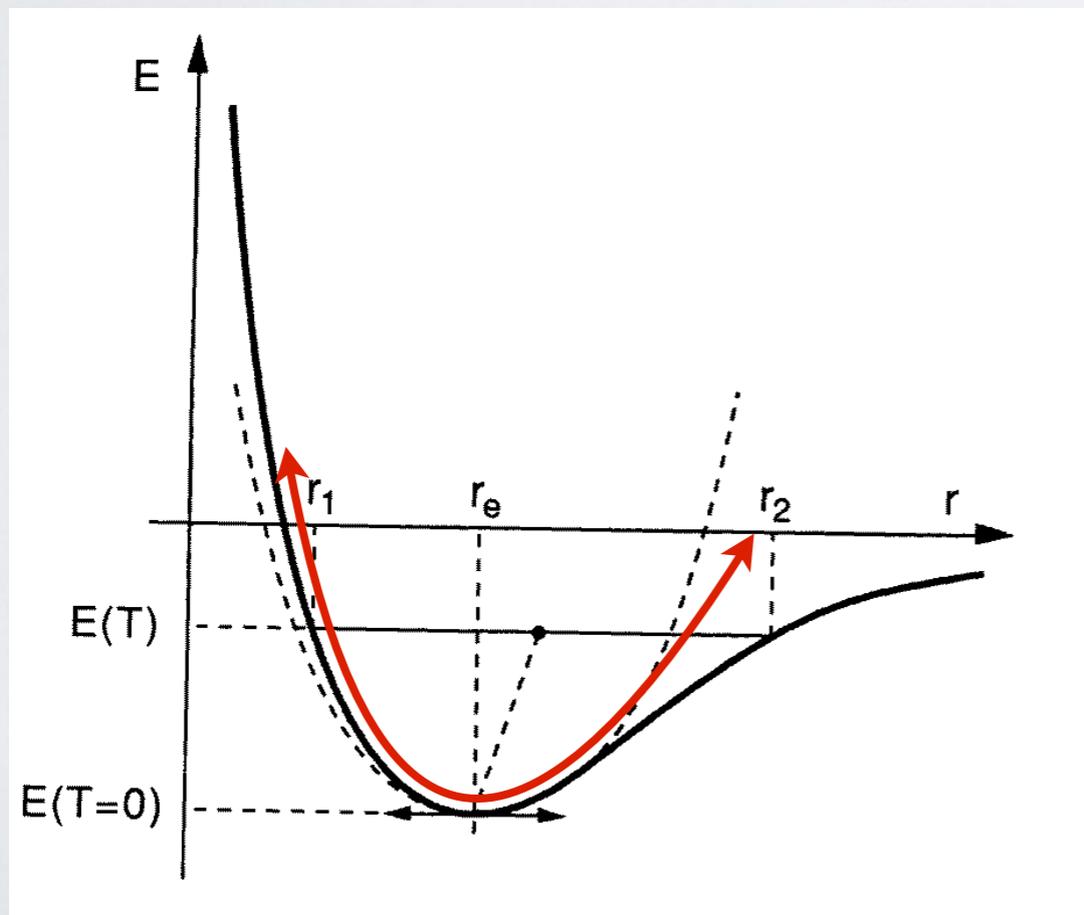
# Why do we have defects?

## **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



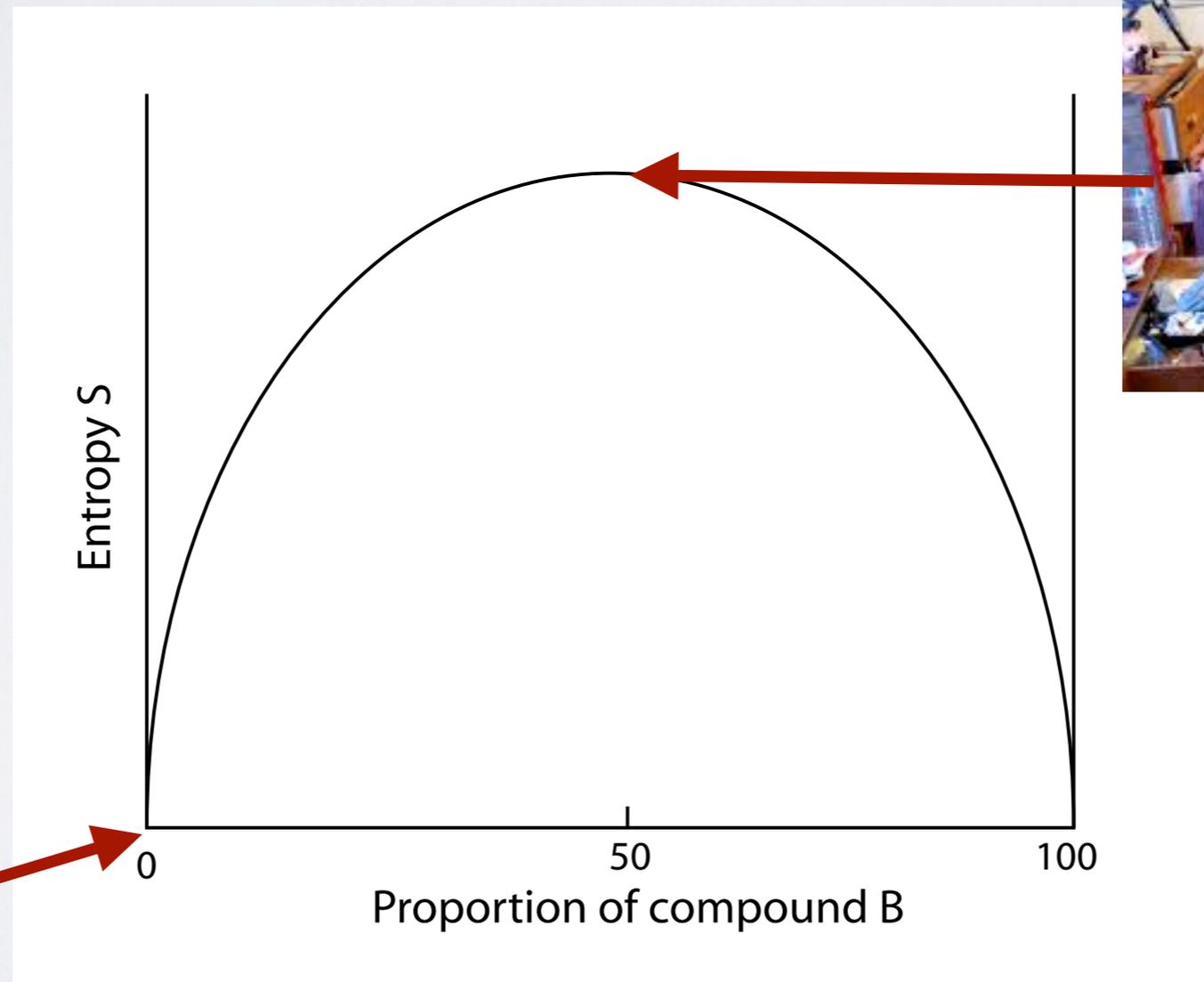
In the Earth need to account for pressure:

Enthalpy:  $H = U + PV$

# Why do we have defects?

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

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



# Thermodynamically why do we have defects?

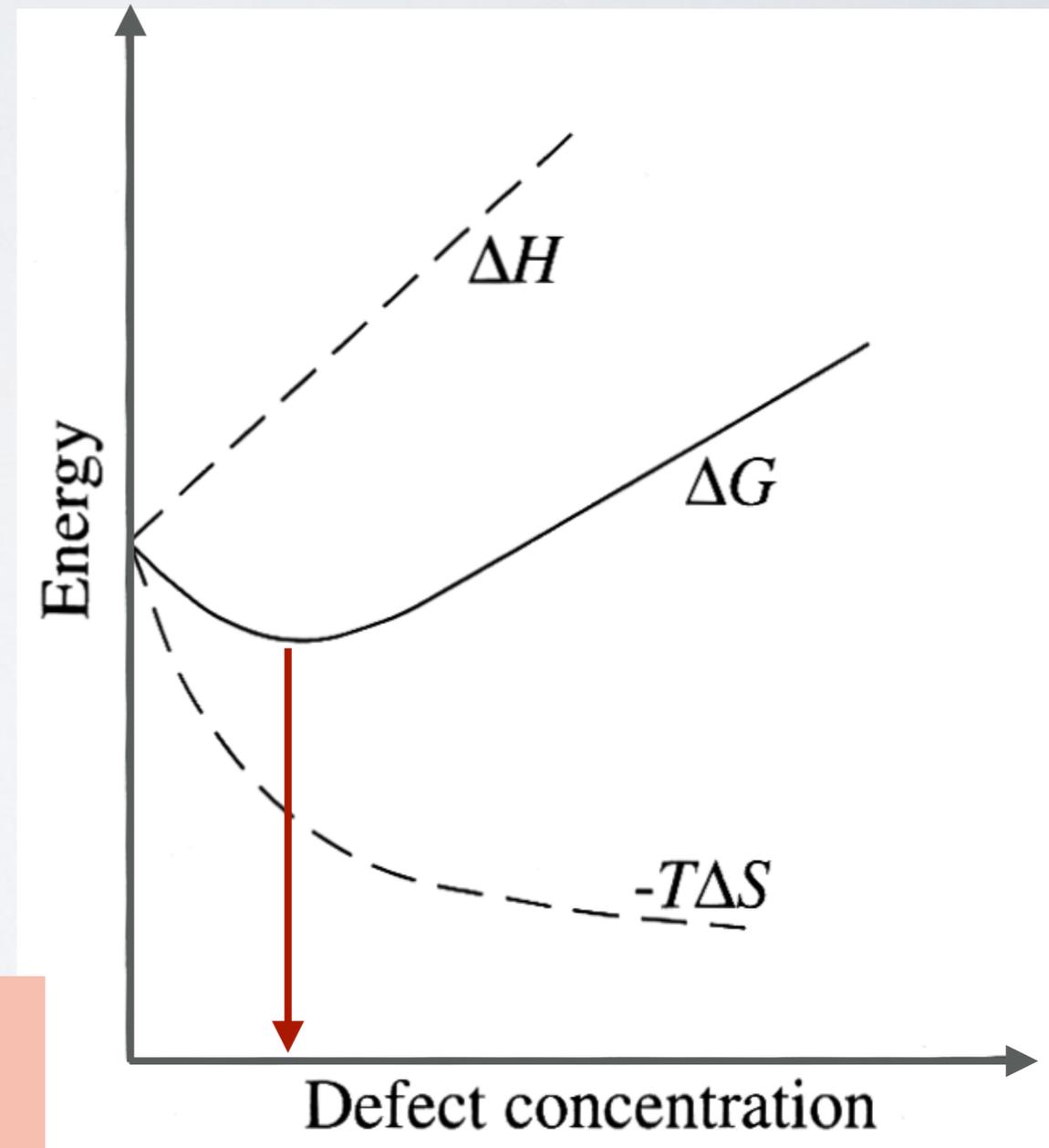
Creation of point defect requires energy:  
local distortion of lattice + imperfect satisfaction of bonding  
☞ enthalpy  $H$  increases.

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

Gibbs free energy:  $G = H - TS$

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

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



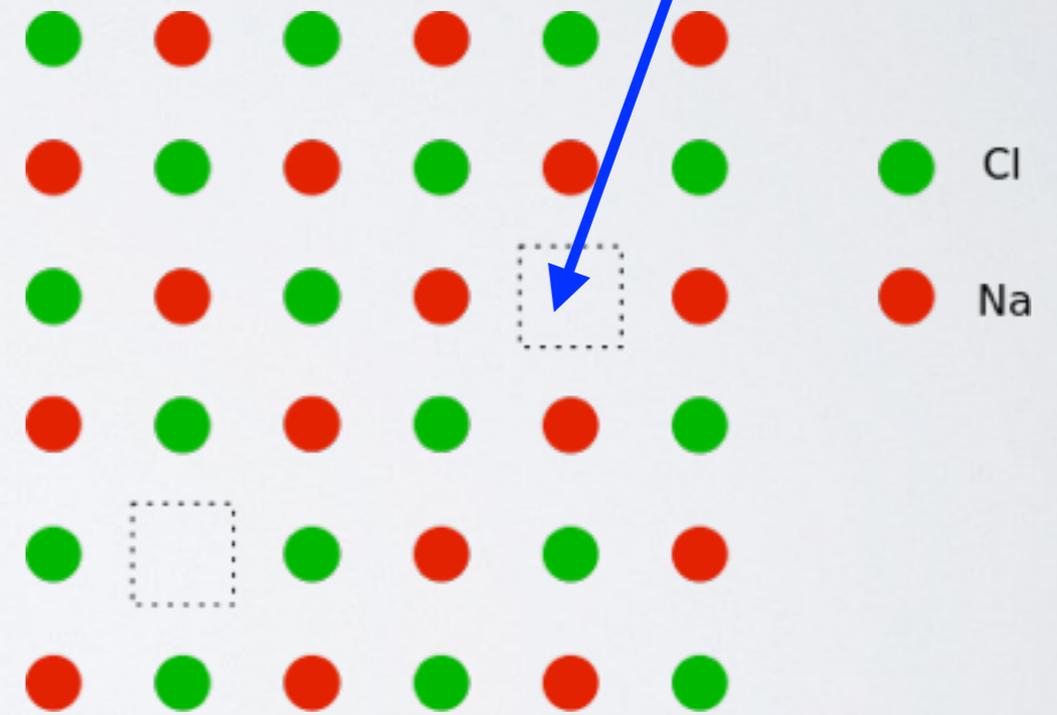
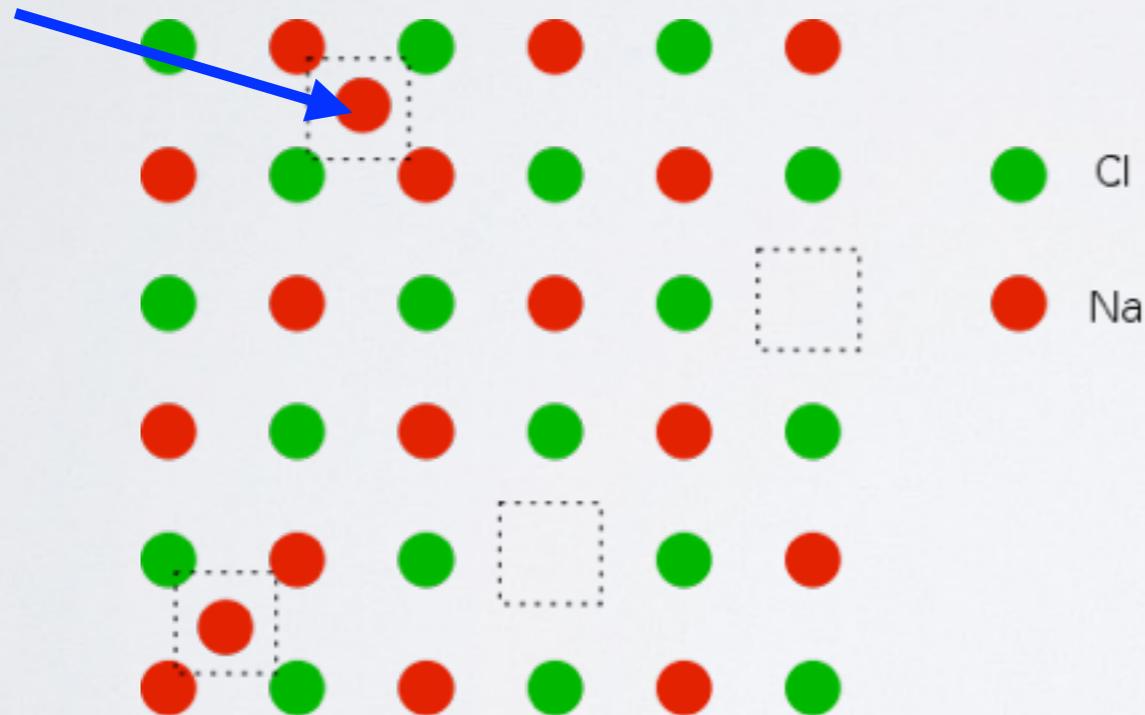
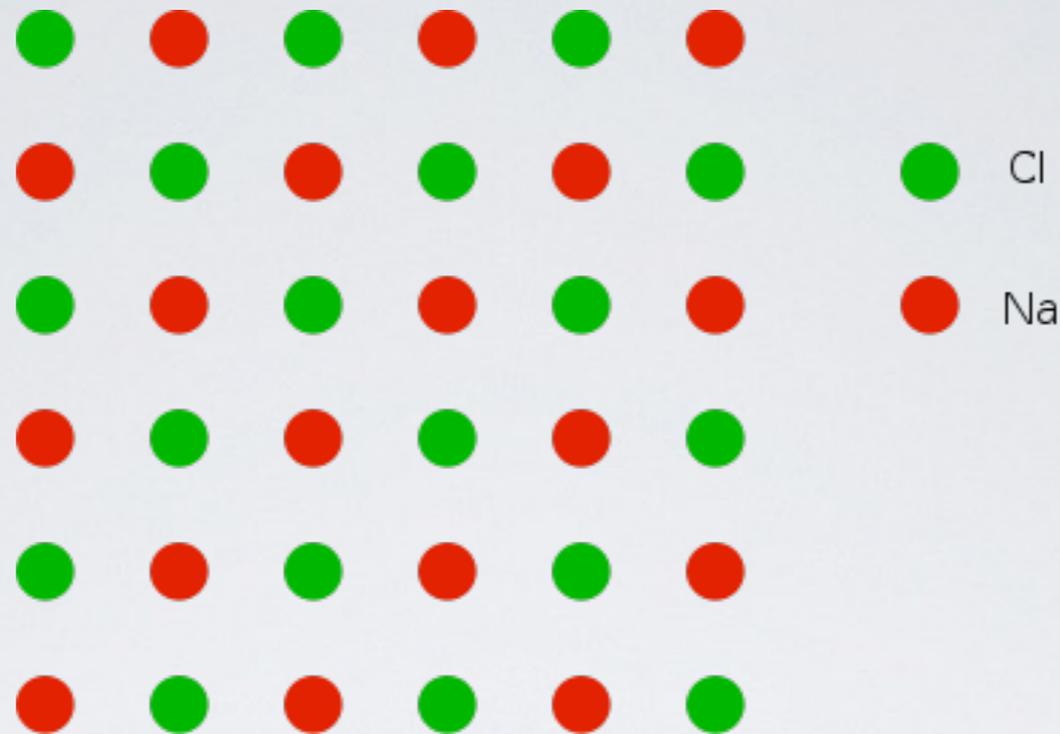
Defects!

(point defects)

intrinsic defects

interstitial

vacancy

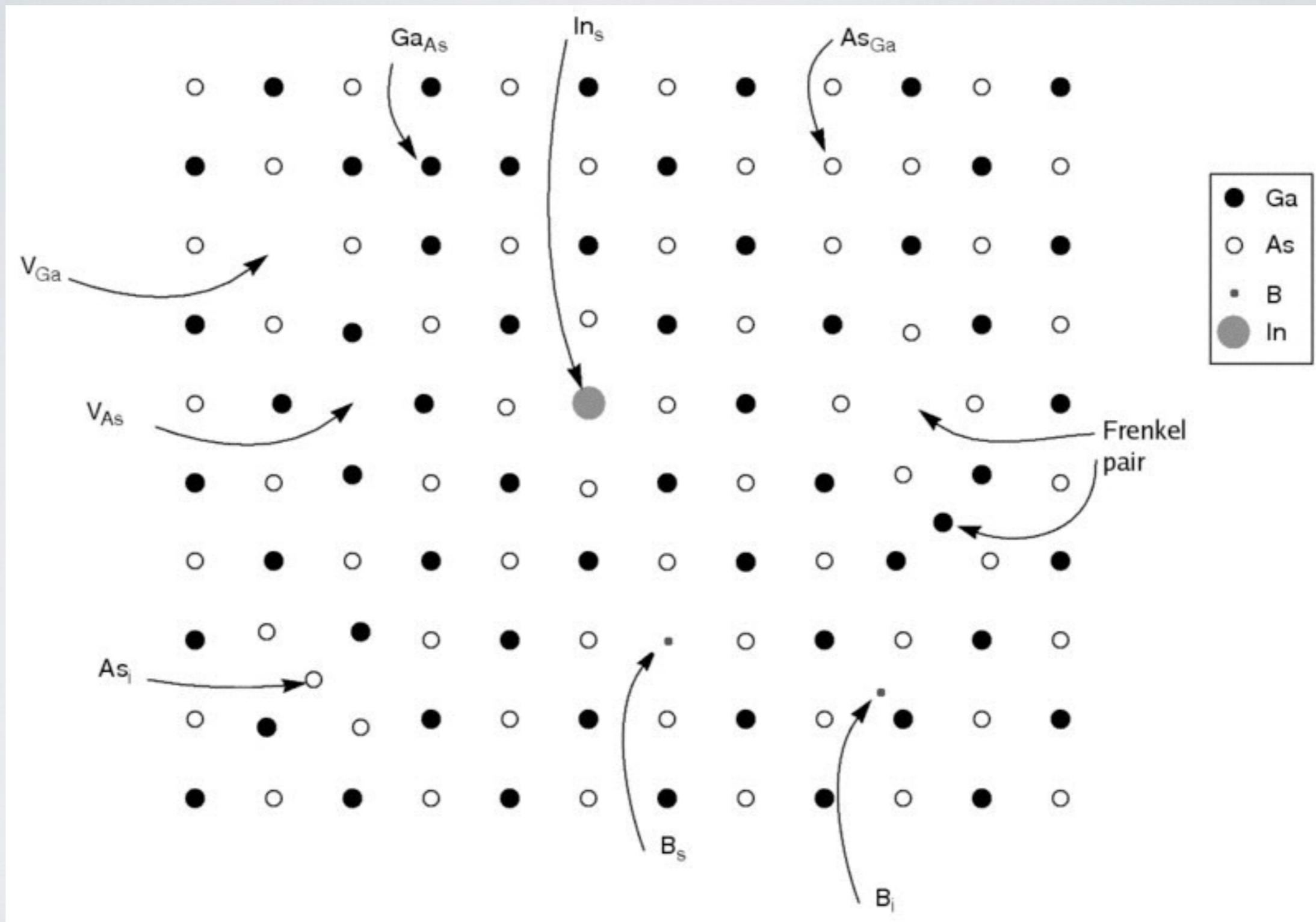


Frenkel

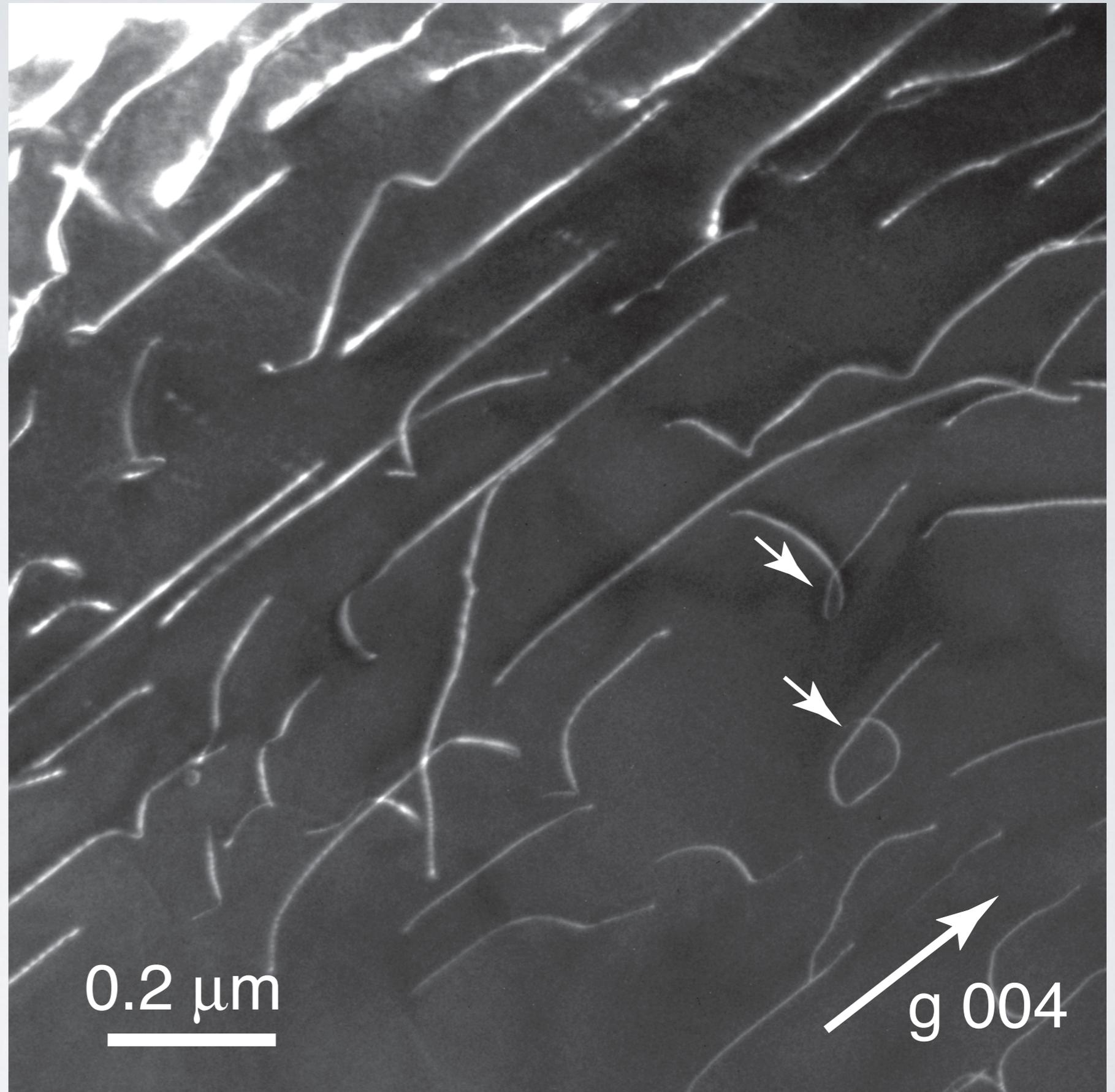
Schottky

charge balance needs to be maintained

defects can also be impurity atoms: extrinsic defects



Dislocations  
-line defects



Transmission electron microscope image of screw dislocations in olivine

# Grain boundaries

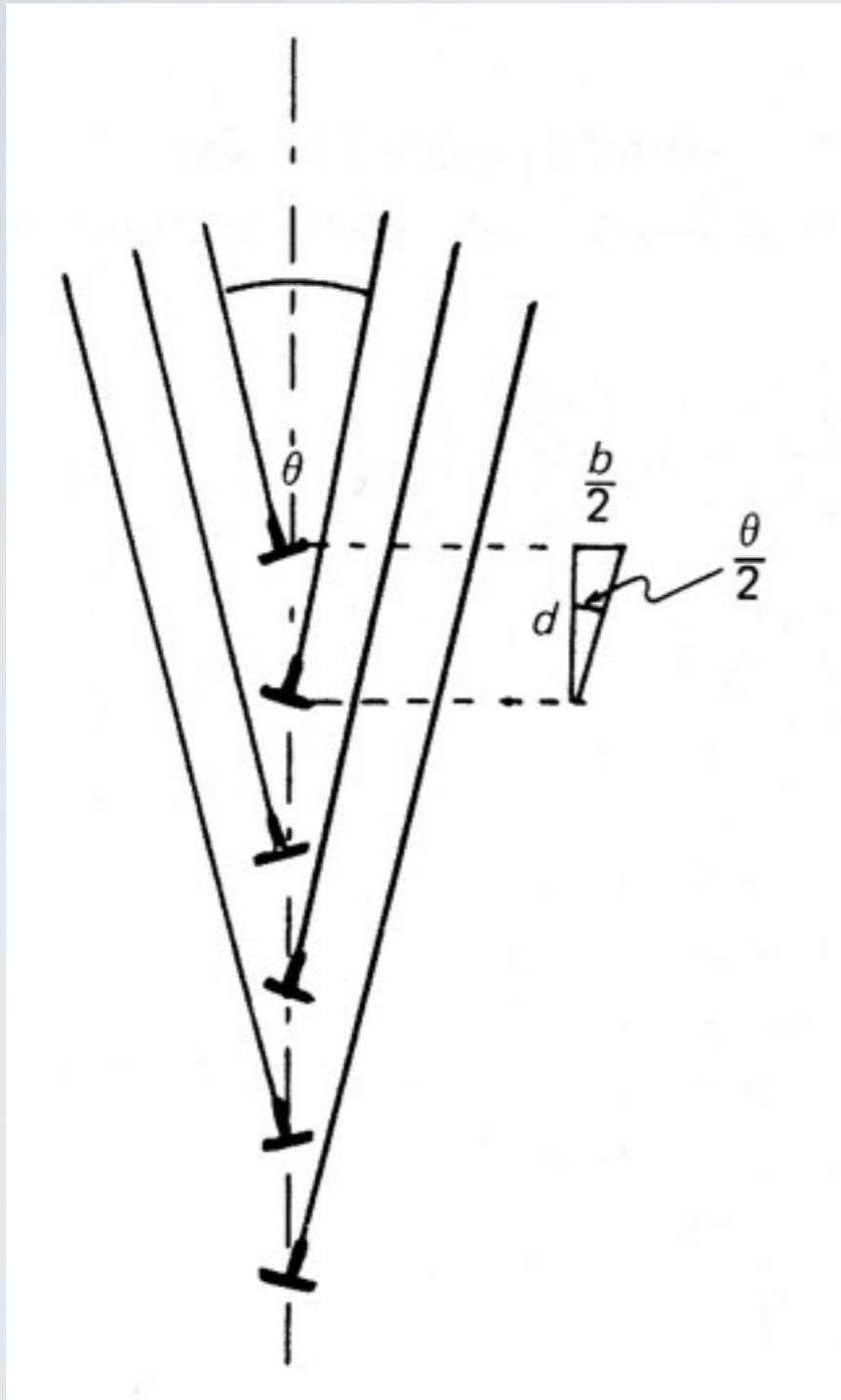
Why look at grain boundaries?

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

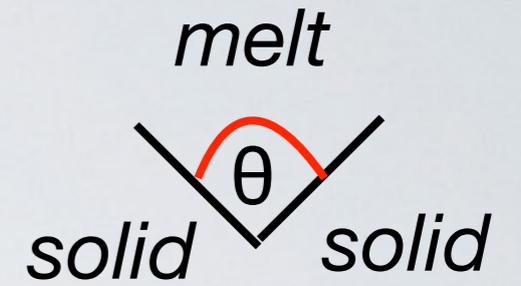
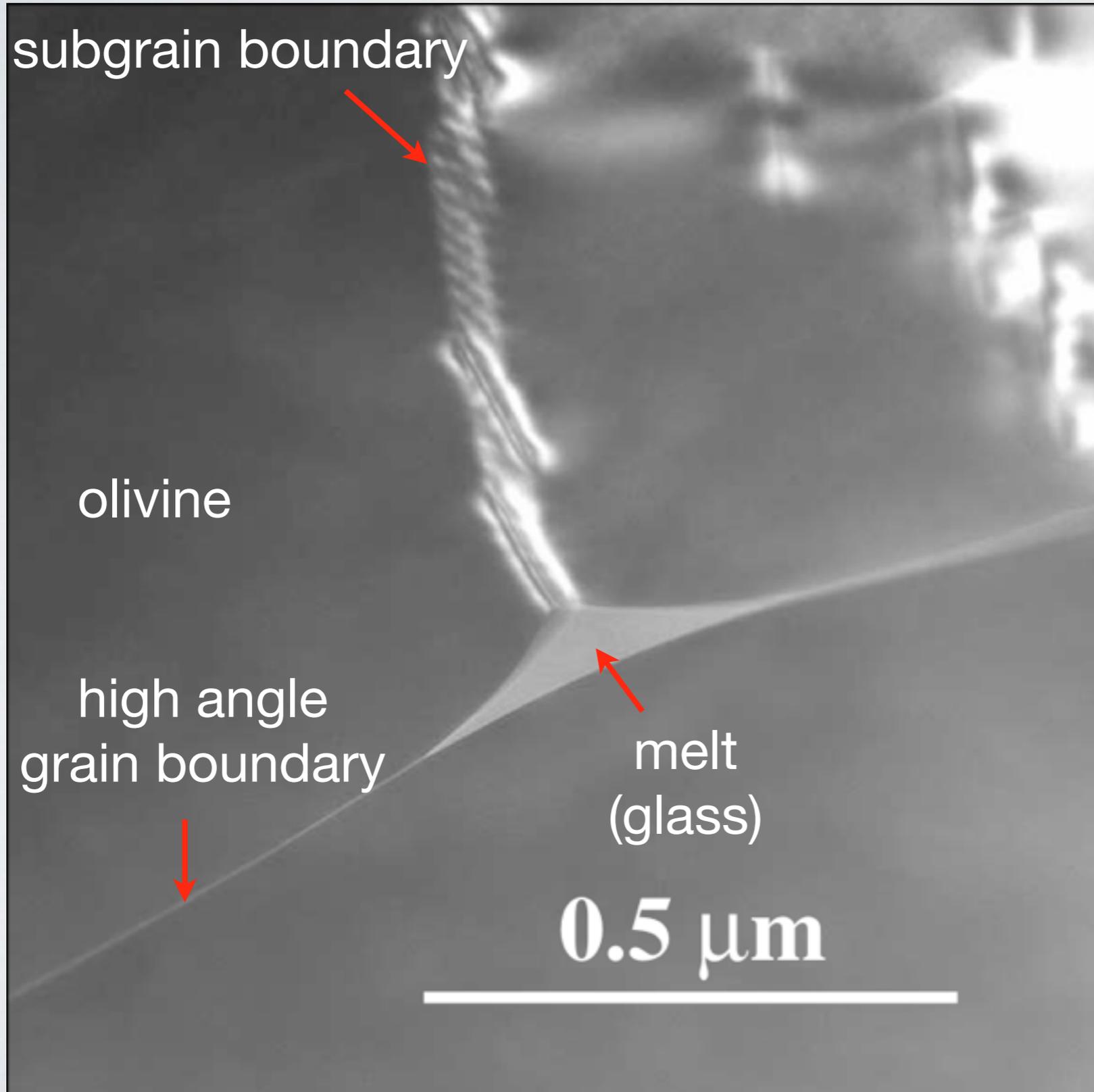
GB: 2-D lattice defect that introduces a change in lattice orientation

Lattice misorientation given by  $\theta$

grain boundaries typically defined  
by  $\theta > 10 - 15^\circ$



# Visualization of types of grain boundaries

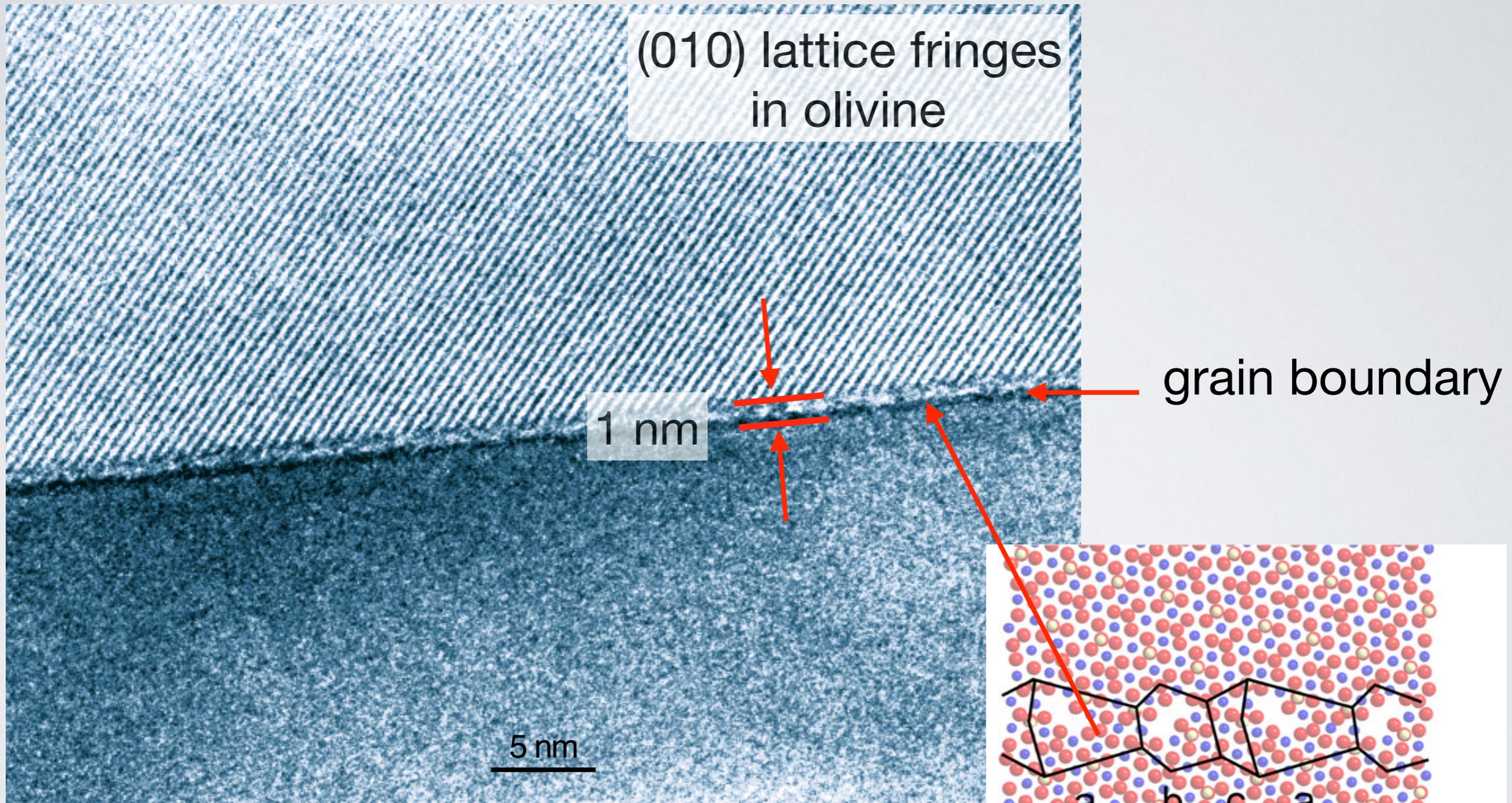


$$\cos \theta/2 = \gamma_{ss}/2\gamma_{sl}$$

$\gamma_{ss}$  = solid - solid surface energy

$\gamma_{sl}$  = solid - liquid surface energy

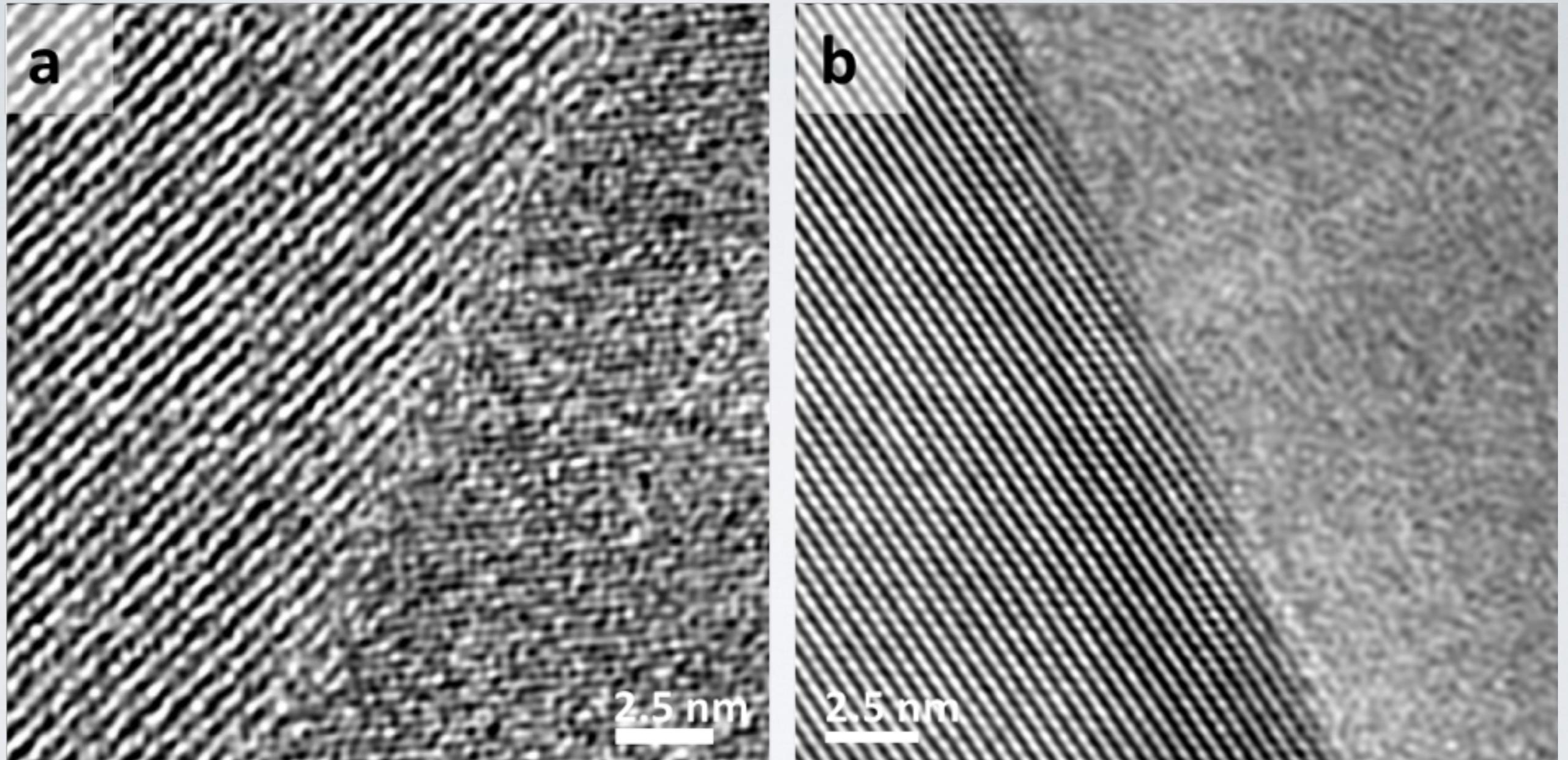
# High resolution image of olivine grain boundaries



Faul et al., 2004

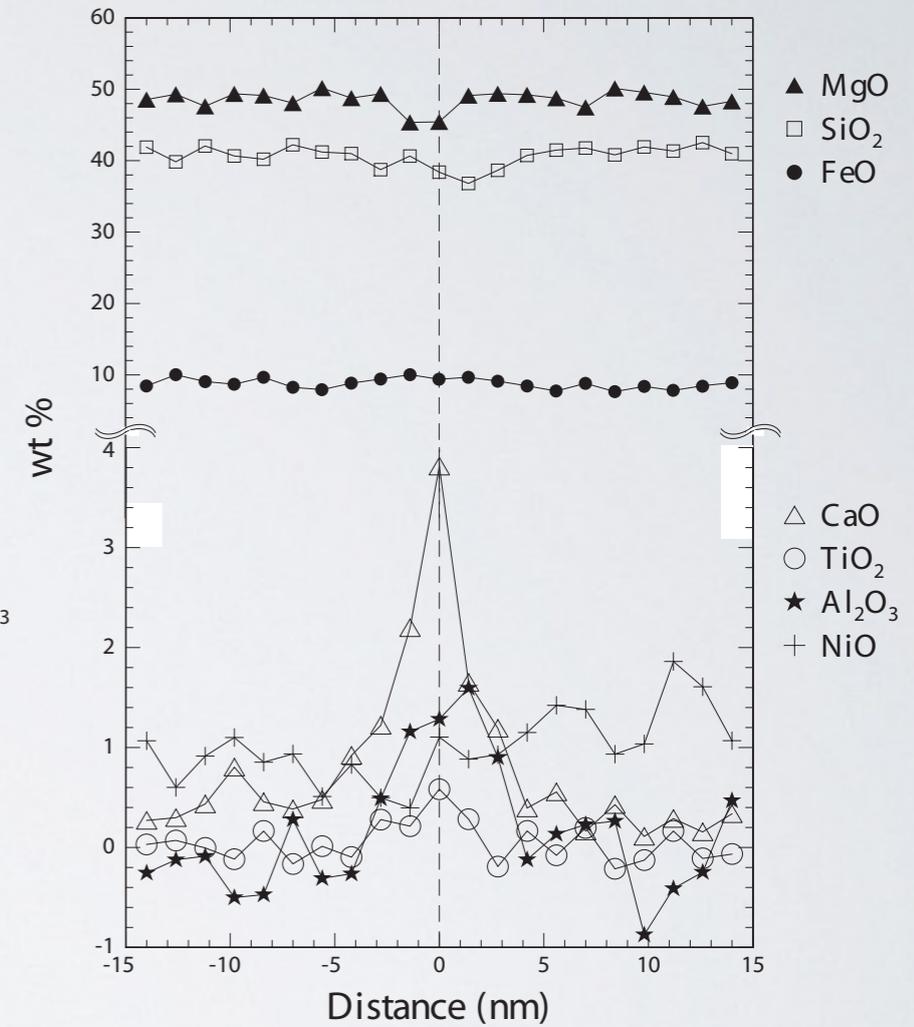
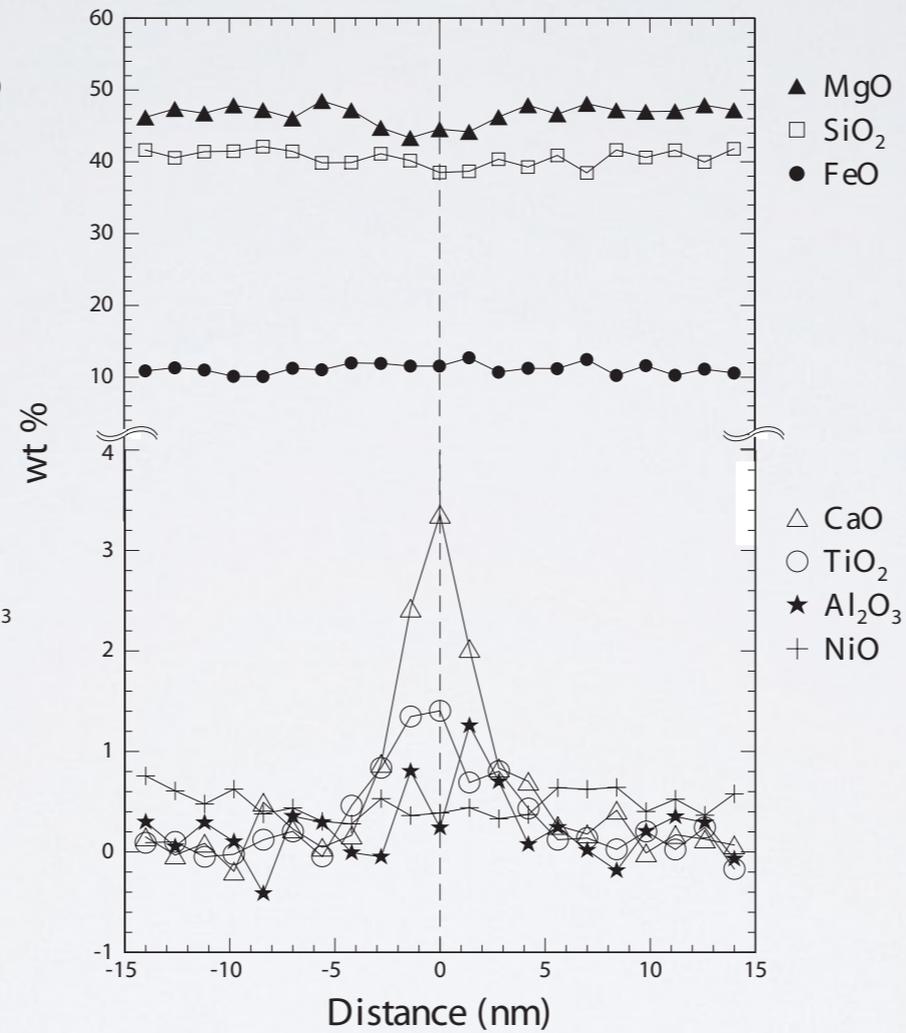
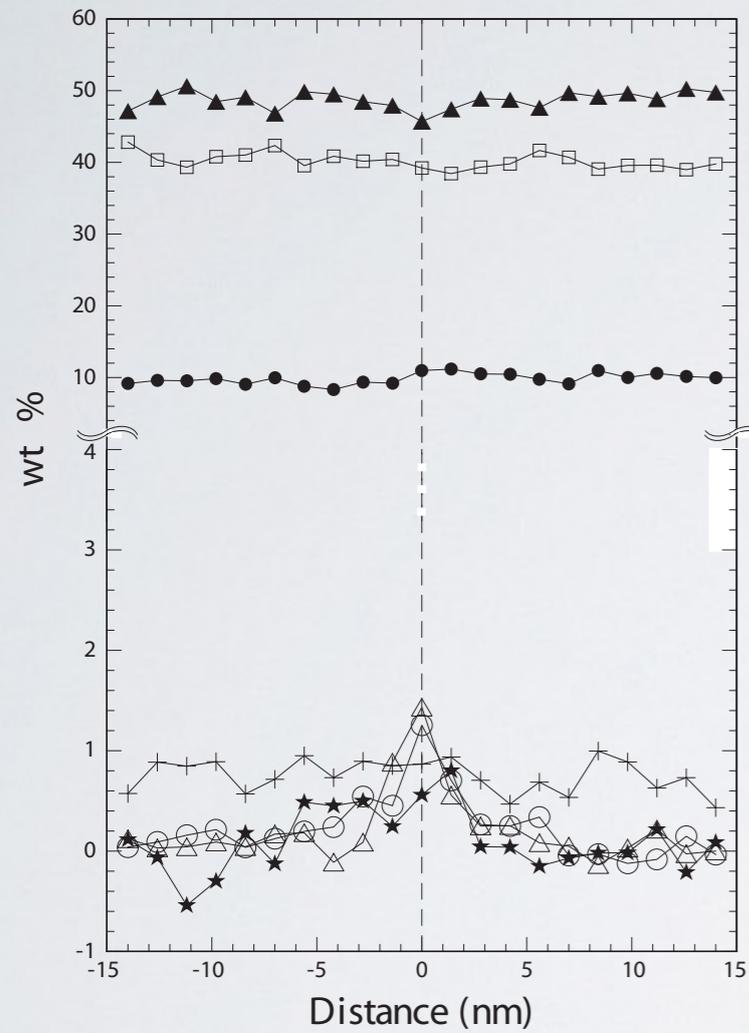
Adjaoud et al., 2012

# High resolution transmission electron microscope images showing lattice planes



K. Marquardt, Bayerisches Geoinstitute

# Grain boundaries are enriched in trace elements relative to the grain interiors



Hiraga et al., 2003

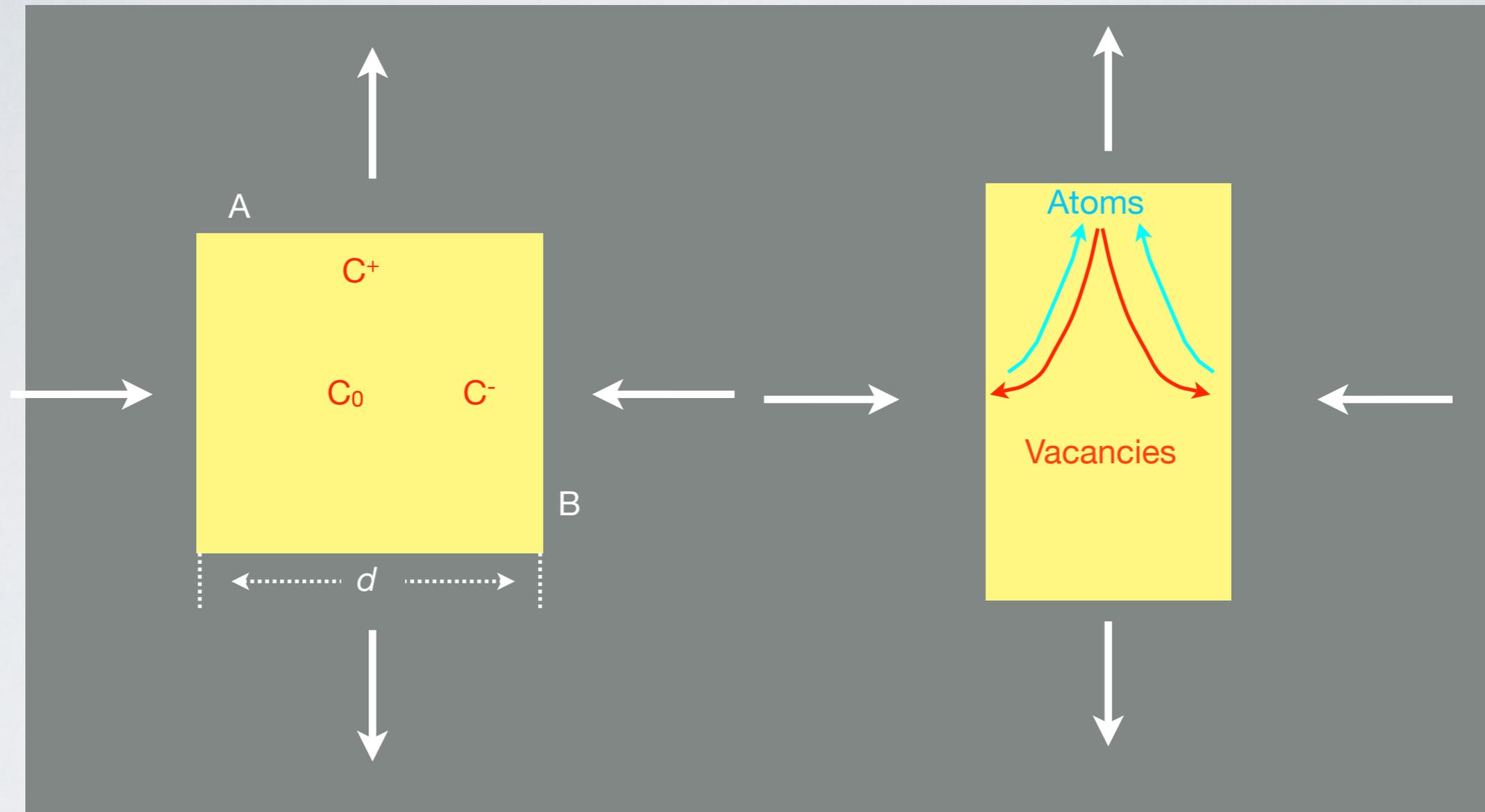
# Deformation - flow laws

,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 face A - face B: length scale (grain size  $d$ )

diffusion ~ diffusivity (atomic species, crystal structure), **temperature**

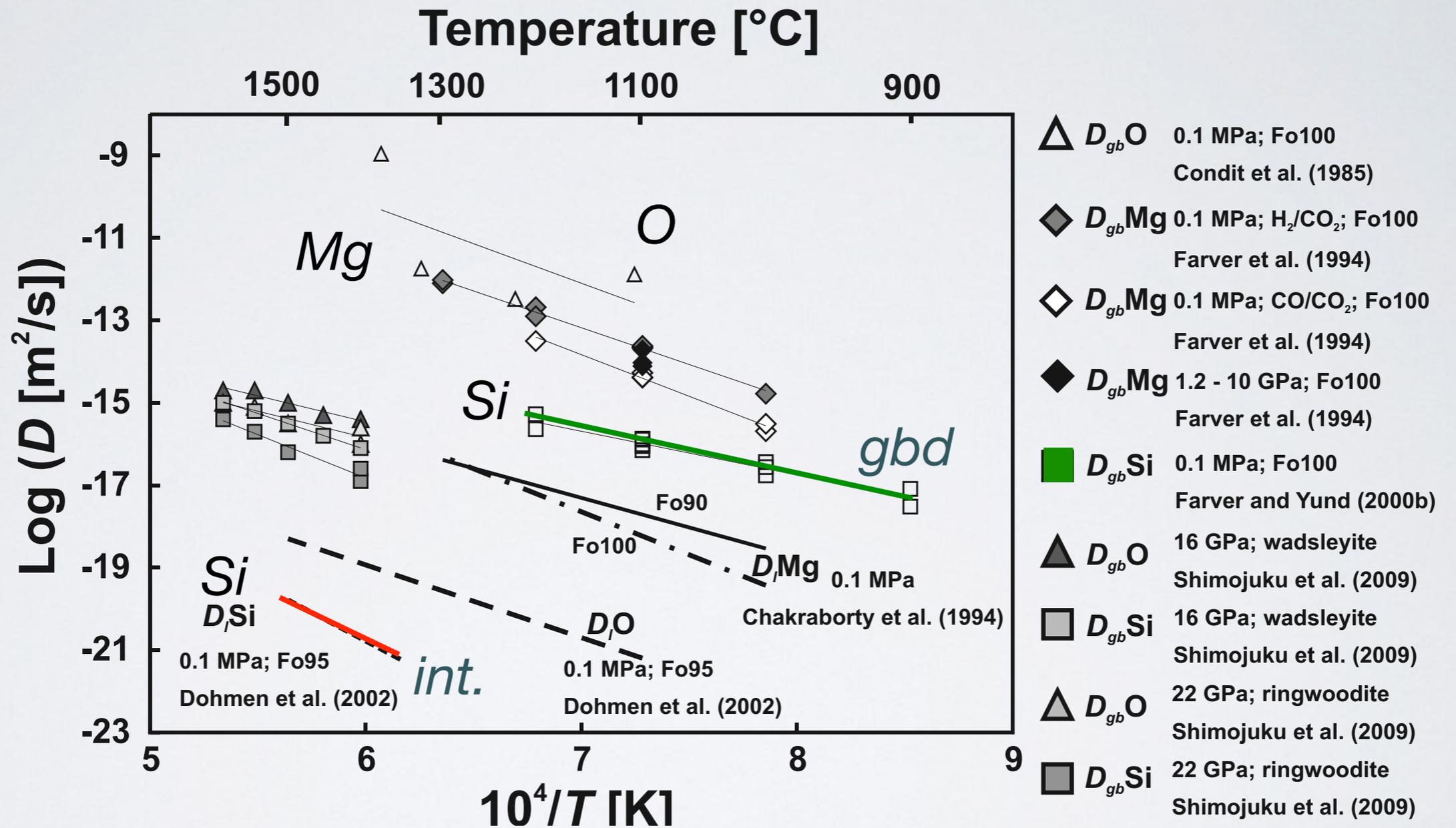
flow law (constitutive equation, strain rate  $\dot{\epsilon}$  as a function of stress  $\sigma$ ):

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

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

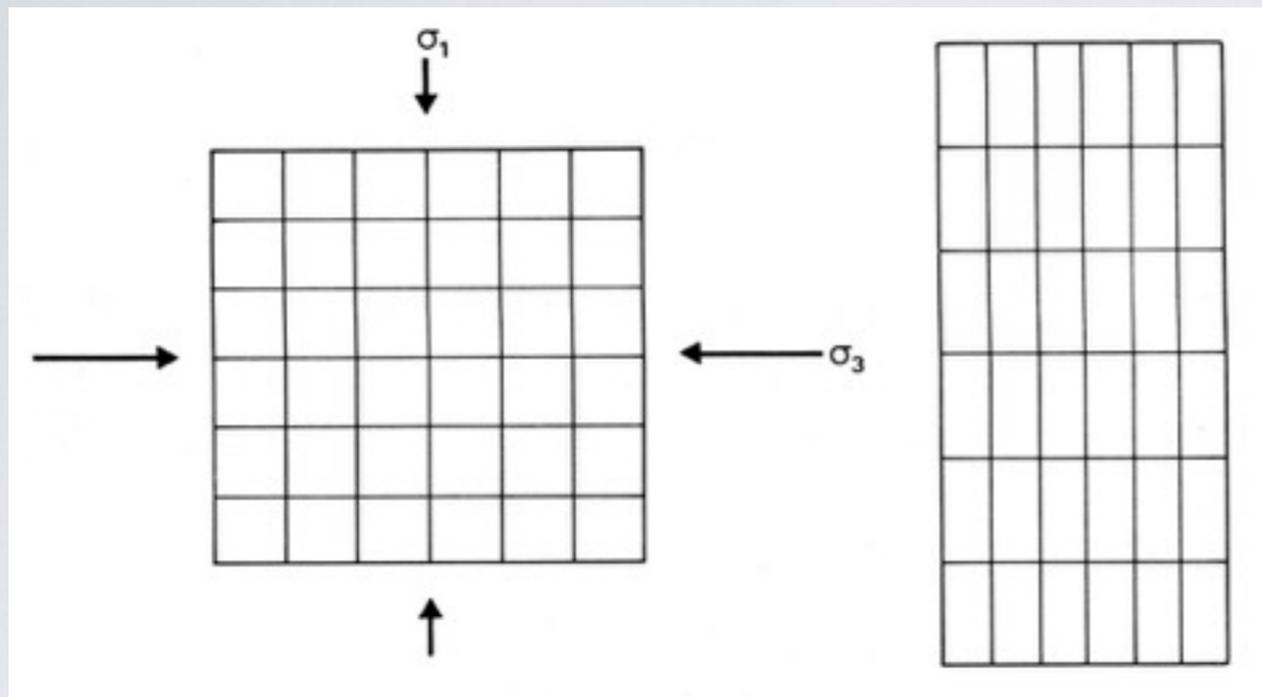
$$d\epsilon/dt = A D_{SD} \Omega \sigma / kT d^2$$

# Diffusion is rate controlling: slowest species along its fastest path

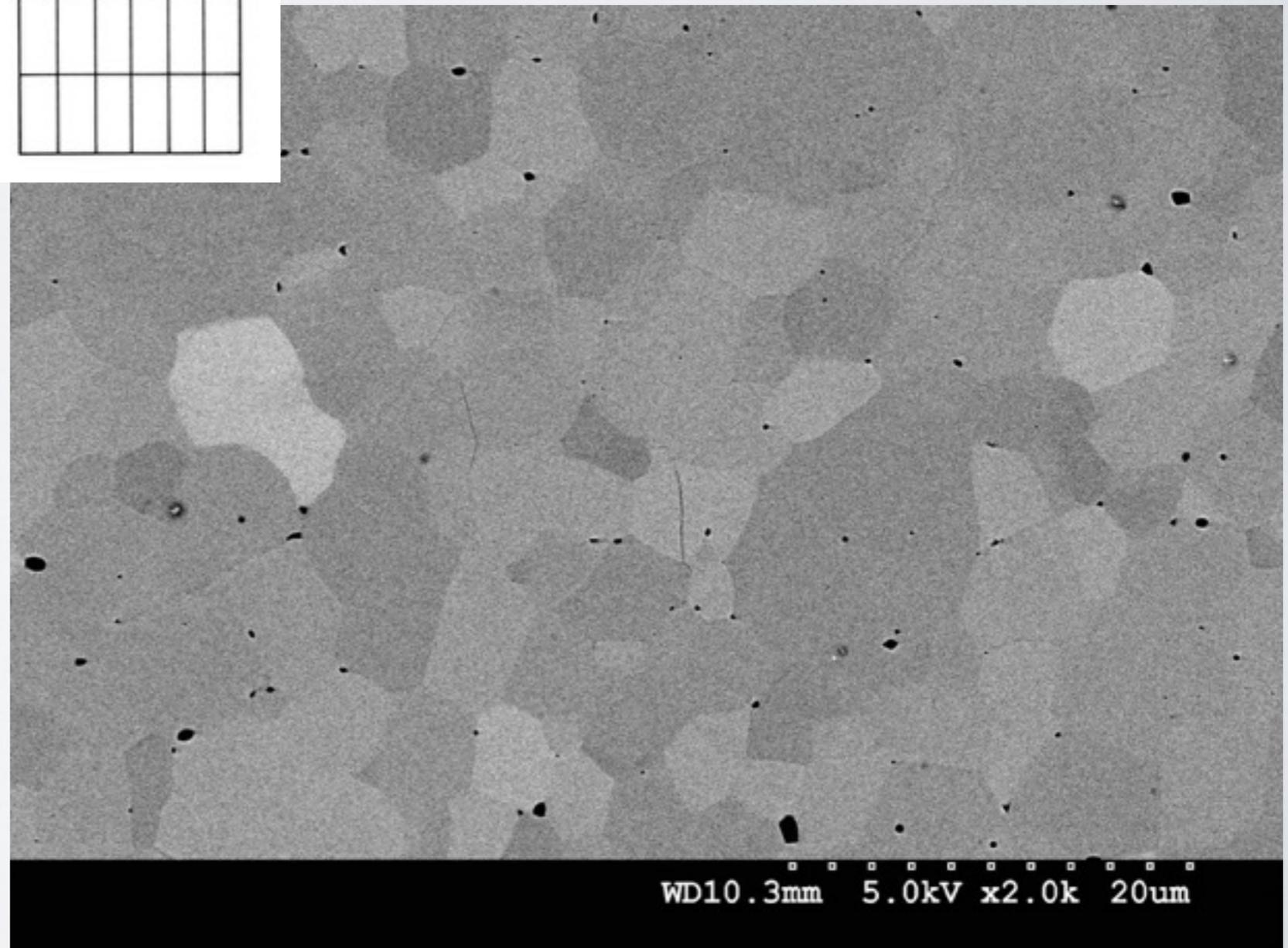


Dohmen & Milke, 2010

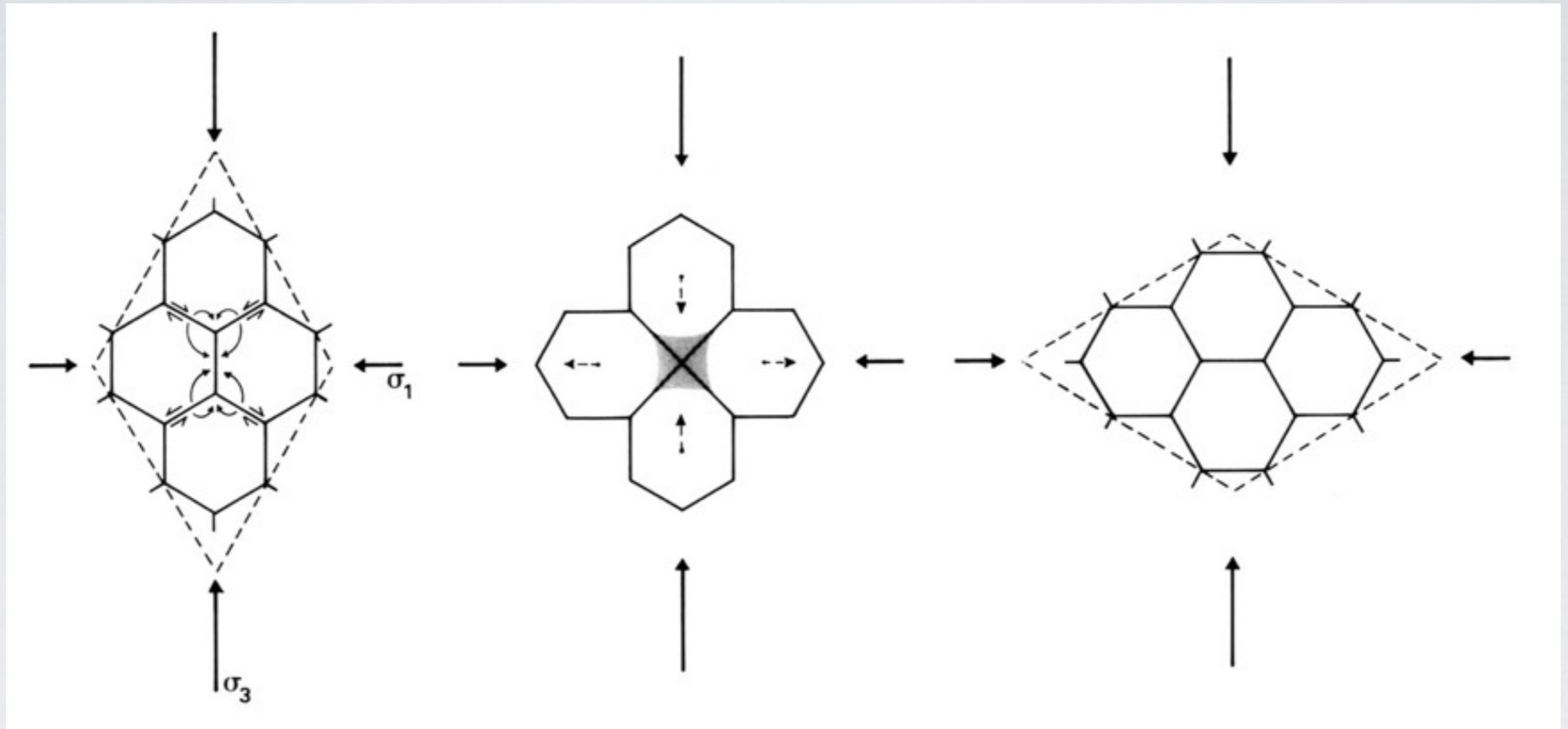
But: "Pure" diffusion creep would lead to shape change of grains:



Observation: Grains remain equiaxed after deformation



# Diffusionally accommodated grain boundary sliding (diffusion creep)



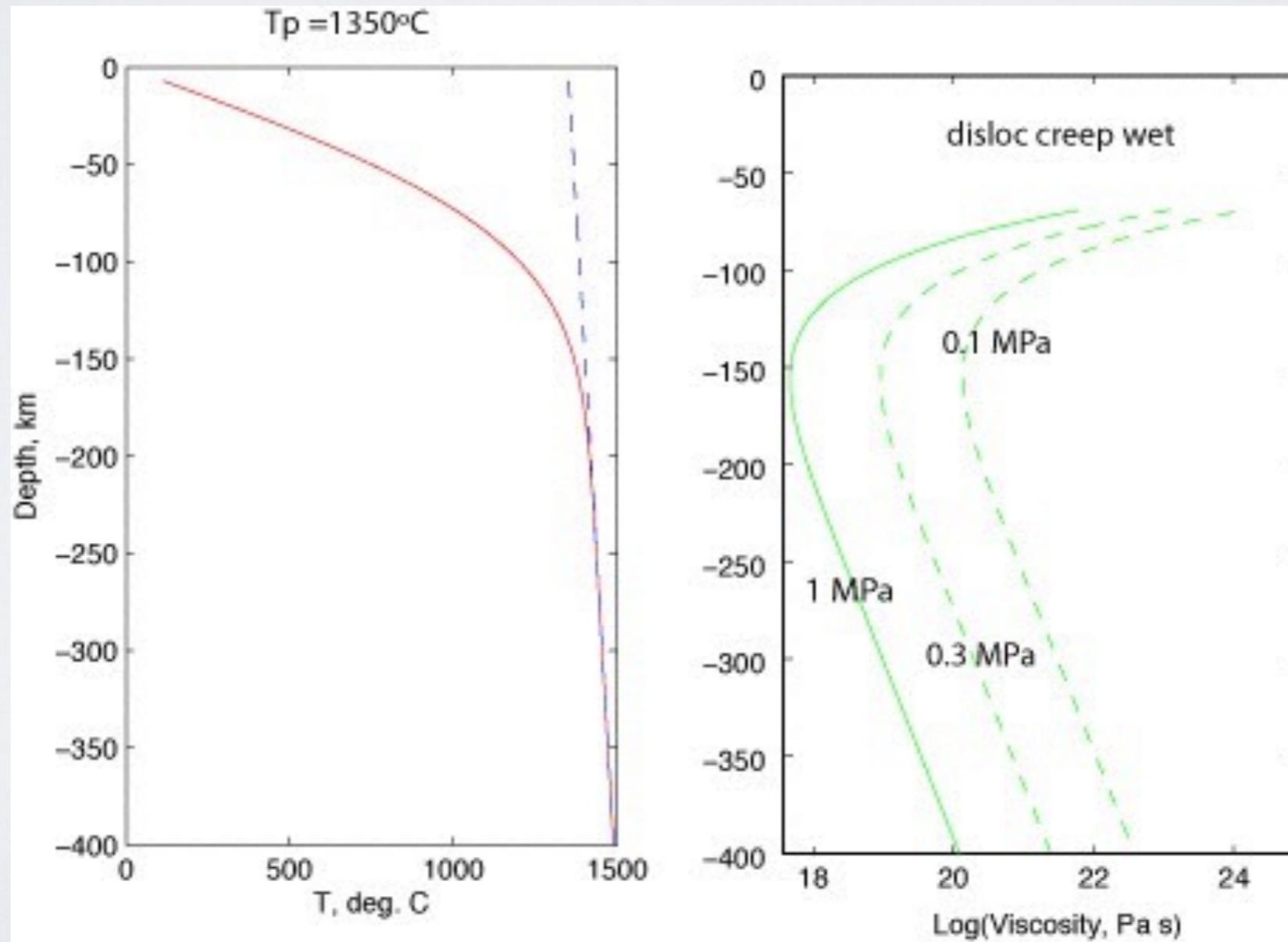
Macroscopic shape change without grain  
shape change



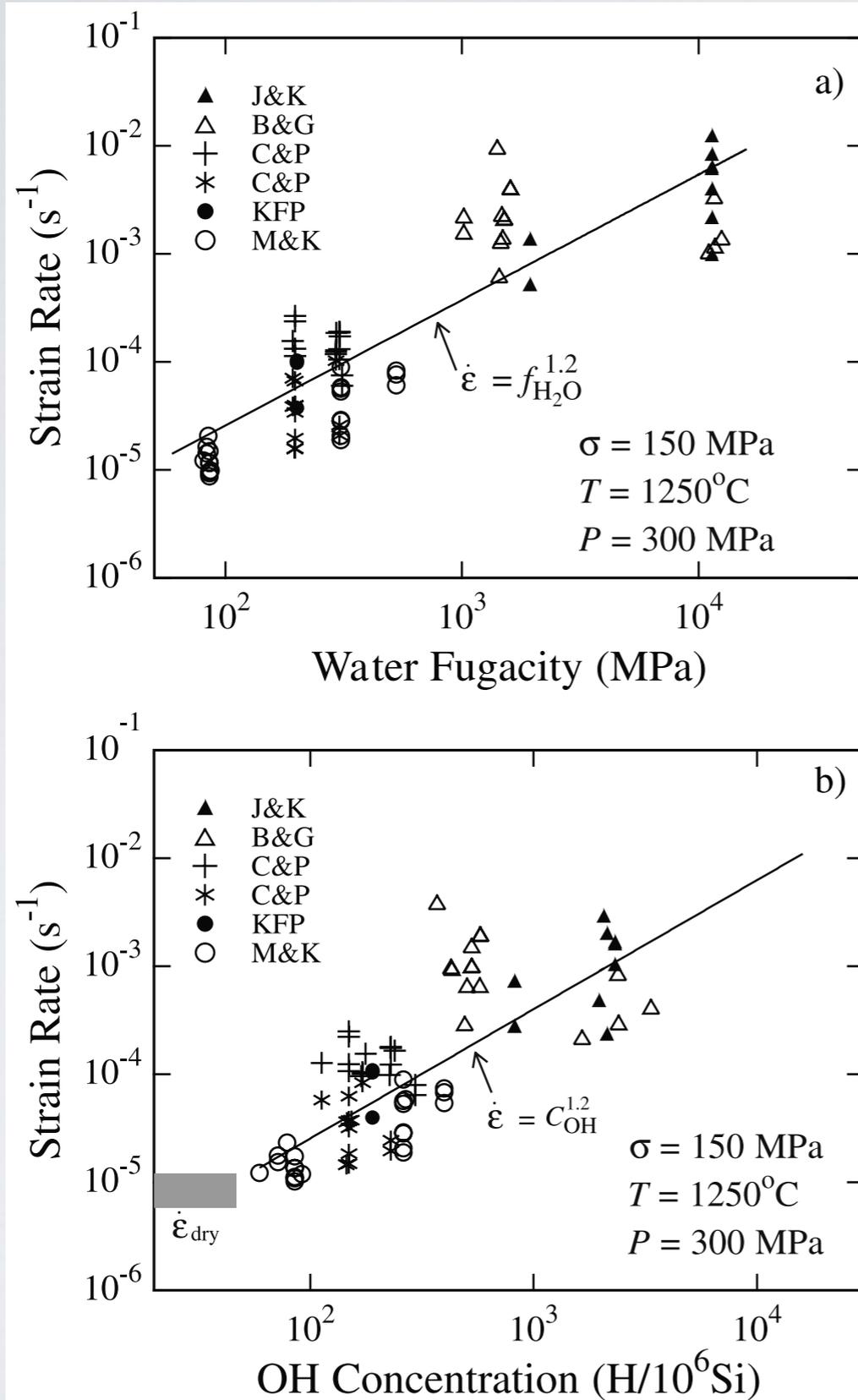
## Influence of water

$$\dot{\epsilon} = A \sigma^n d^{-p} f_{H_2O}^r \exp\left(\frac{-Q}{RT}\right)$$

viscosity  $\eta = \sigma / 2\dot{\epsilon}$  (Newtonian)



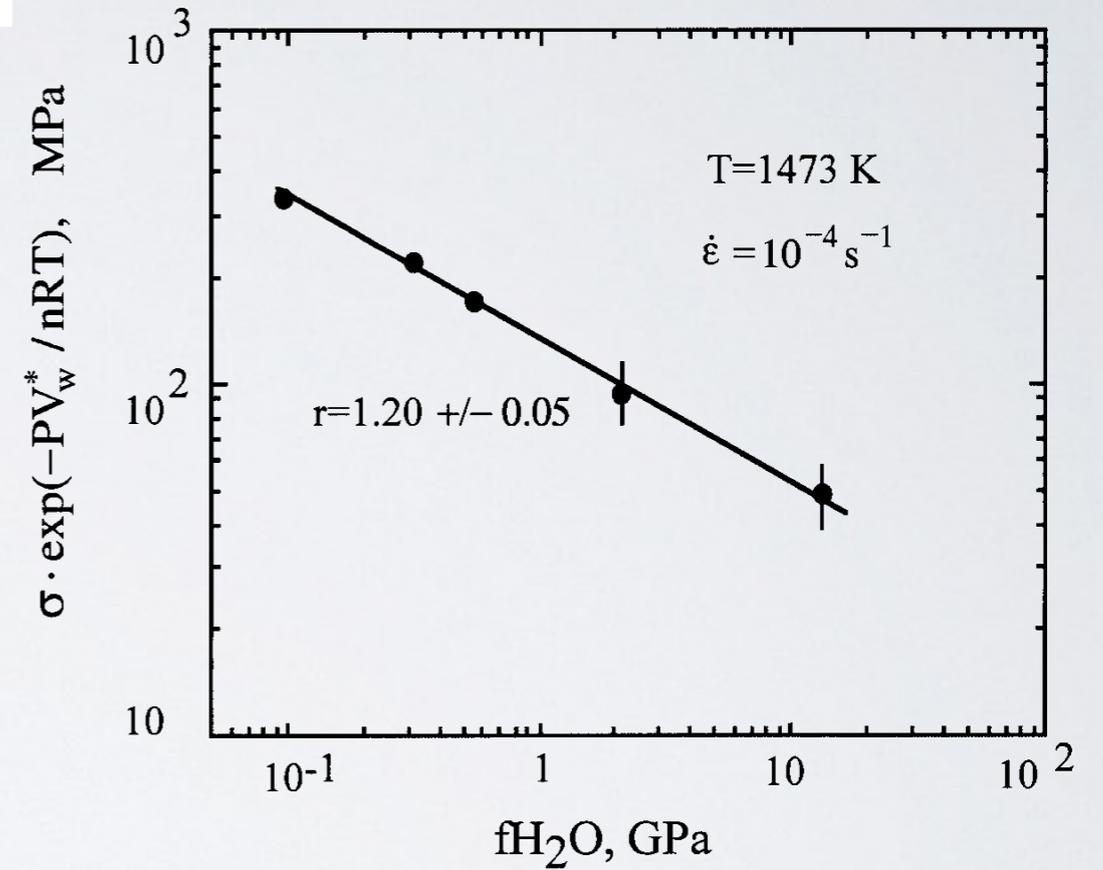
# Hirth and Kohlstedt, 2003



# Karato and Jung, 2003

S. Karato and H. Jung

olivine, "wet" condition

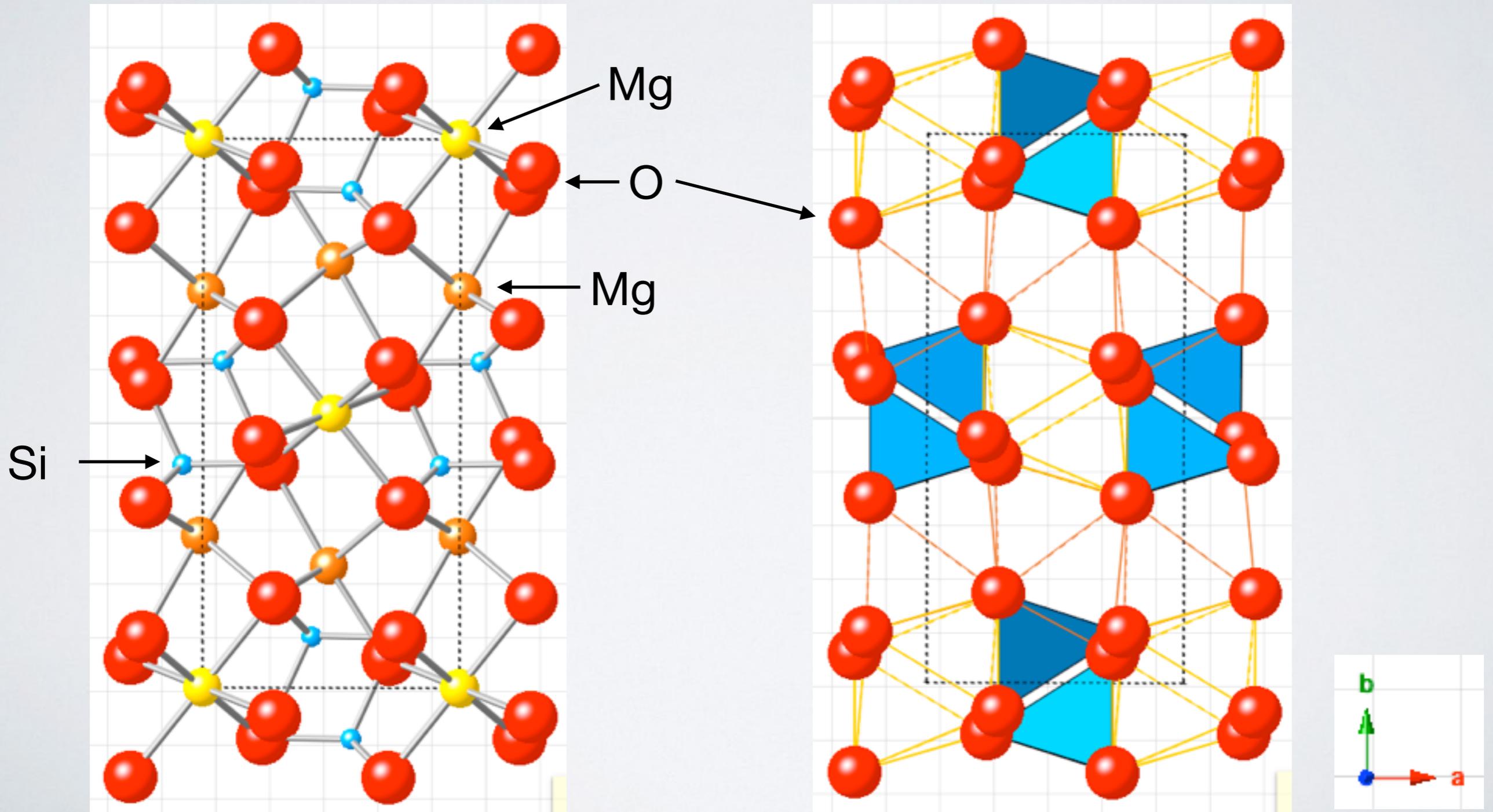


Near linear relationship between water content and strain rate

What does 'water' mean for a nominally anhydrous mineral?

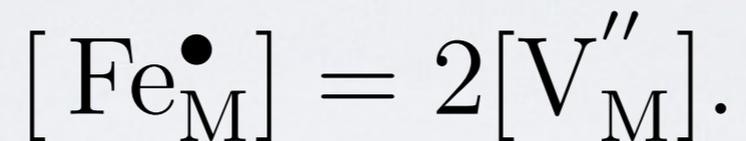
# Olivine ( $\text{Mg}_2\text{SiO}_4$ )

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



## Back to defects

Dry 'model':



dominant (most abundant) defects are M-site vacancies (charge: 2-), charge balanced by  $\text{Fe}^{3+}$  on M-sites

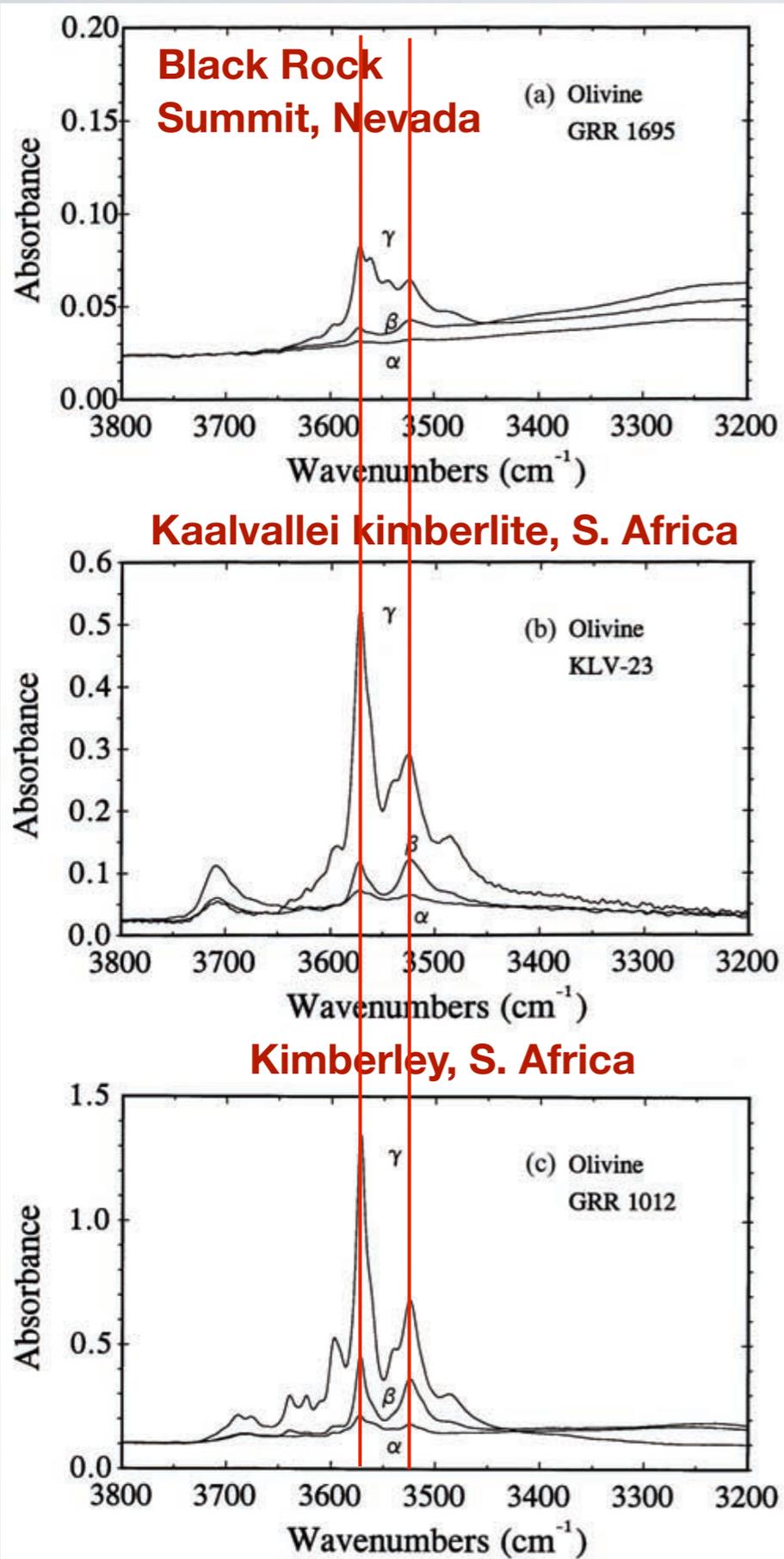
Nakamura and Schmalzried 1983,  
Kohlstedt, Karato and Co-workers

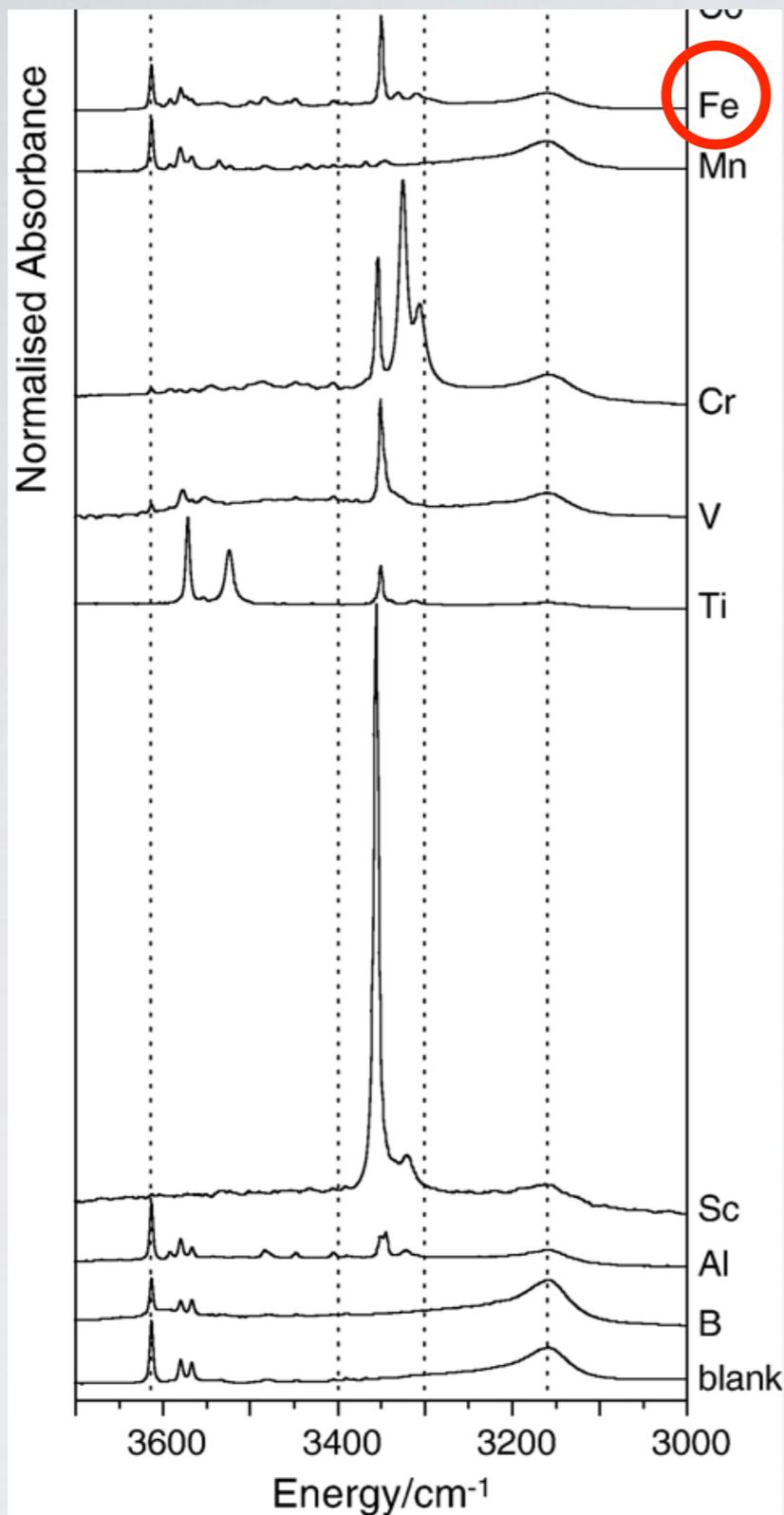
# Water in olivine: a brief background

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  $\text{cm}^{-1}$





# Site-specific absorbance

tetrahedral  
Ti  
trivalent  
octahedral

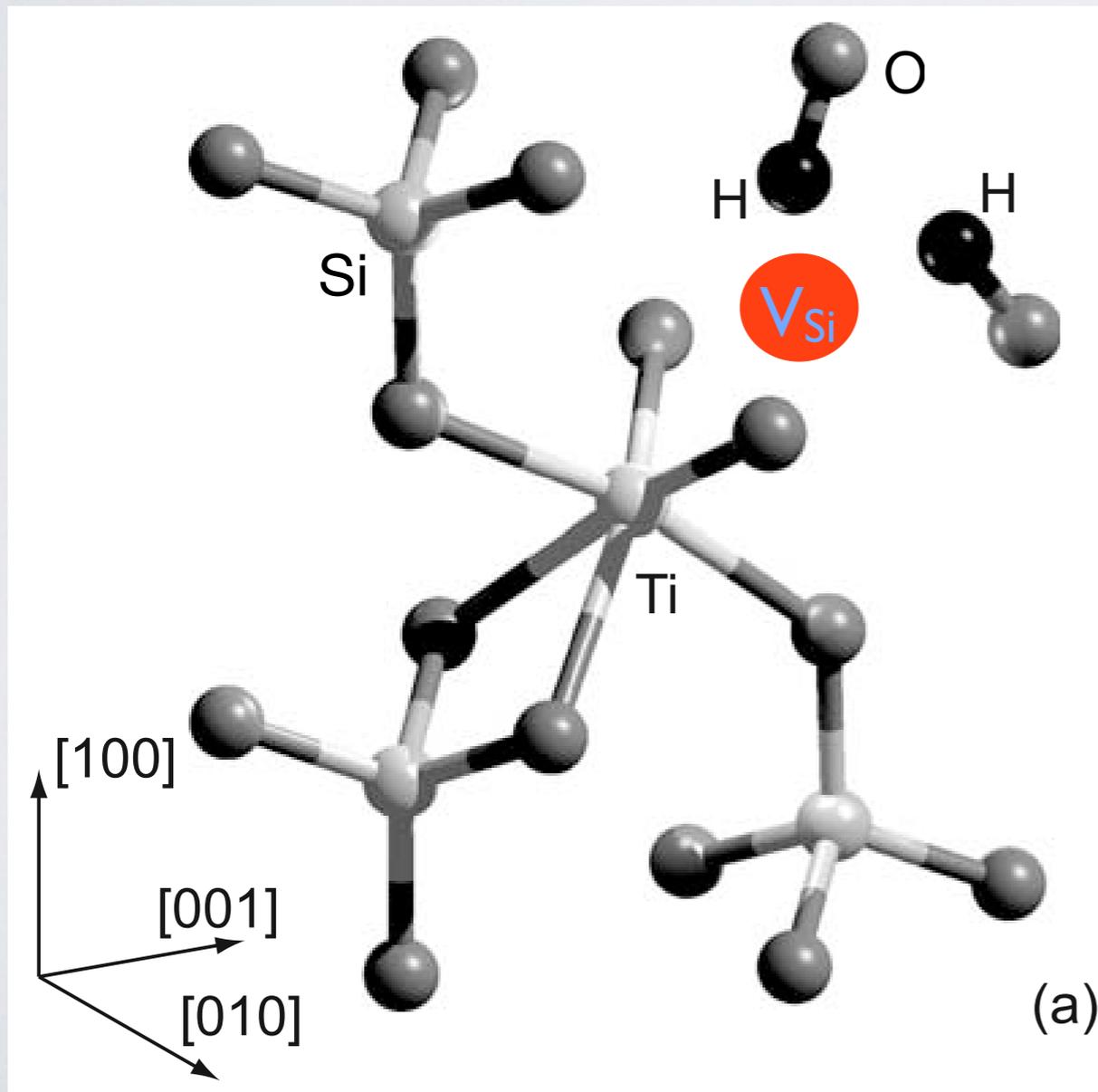
Berry et al., 2007

# 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

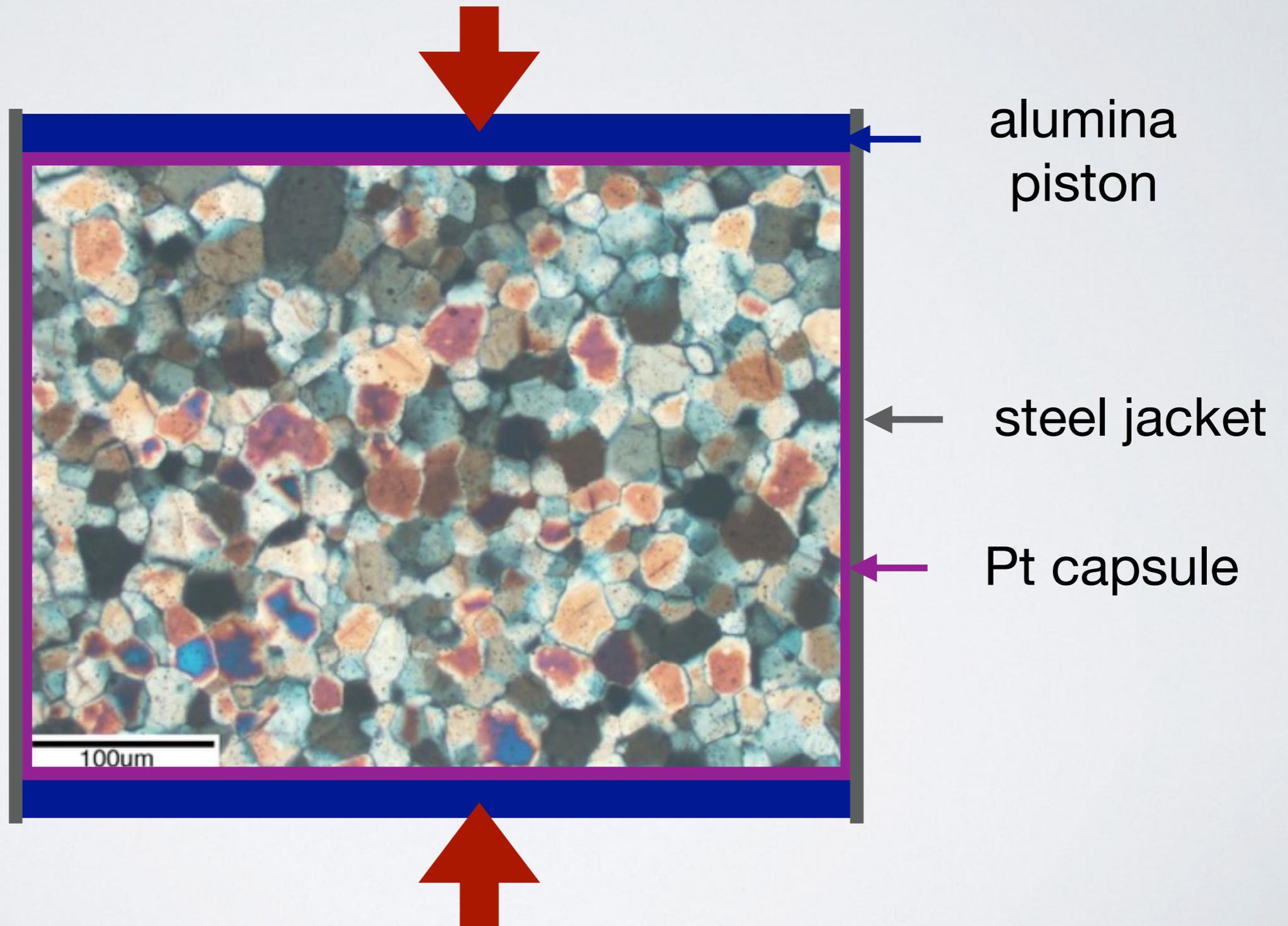


calculated OH -  
vibrational frequencies:  
3572 and 3525  $\text{cm}^{-1}$

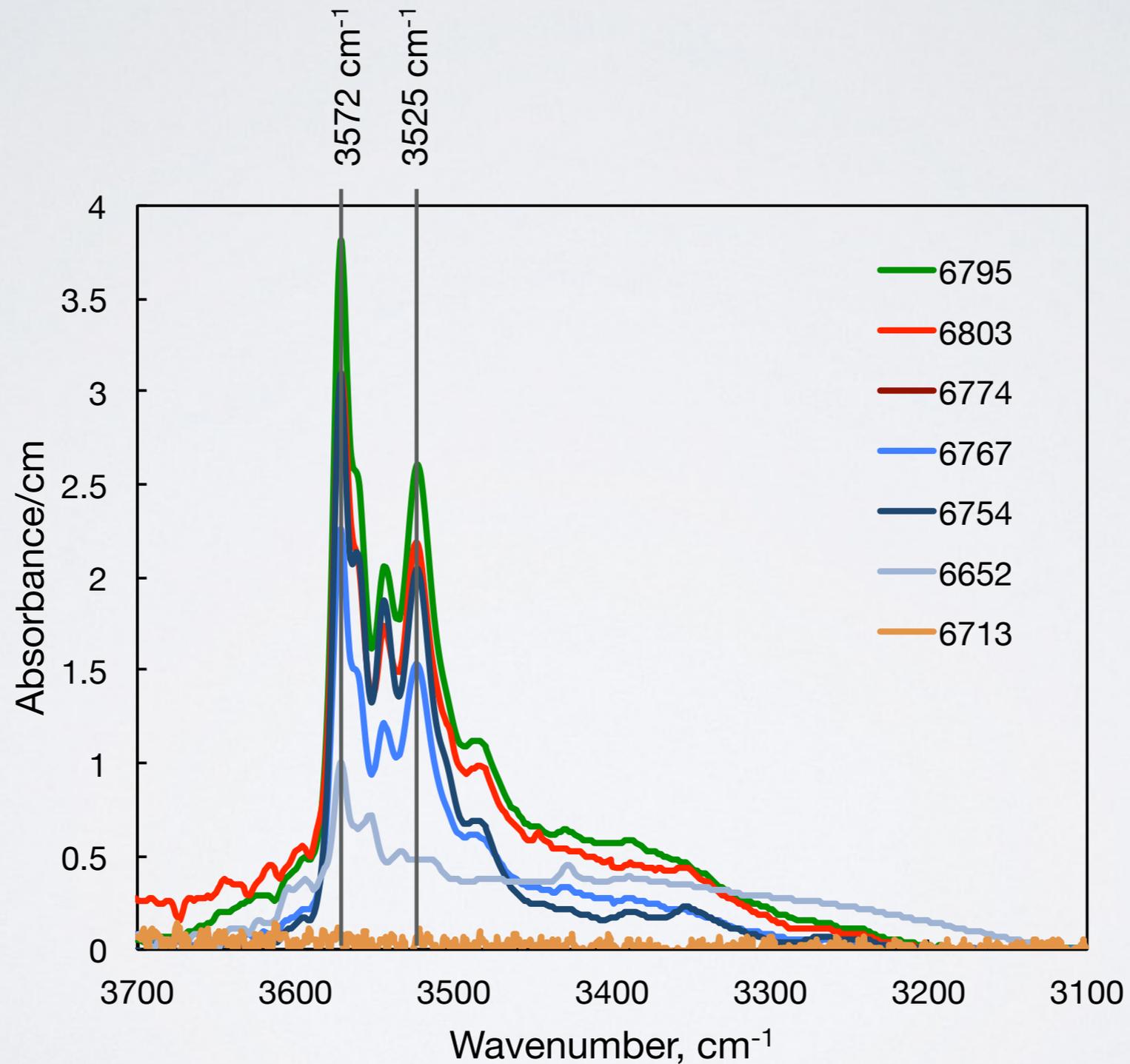
Berry et al., 2005, Walker et al., 2007

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

Fo<sub>90</sub> olivine doped with 0.04 wt% TiO<sub>2</sub>

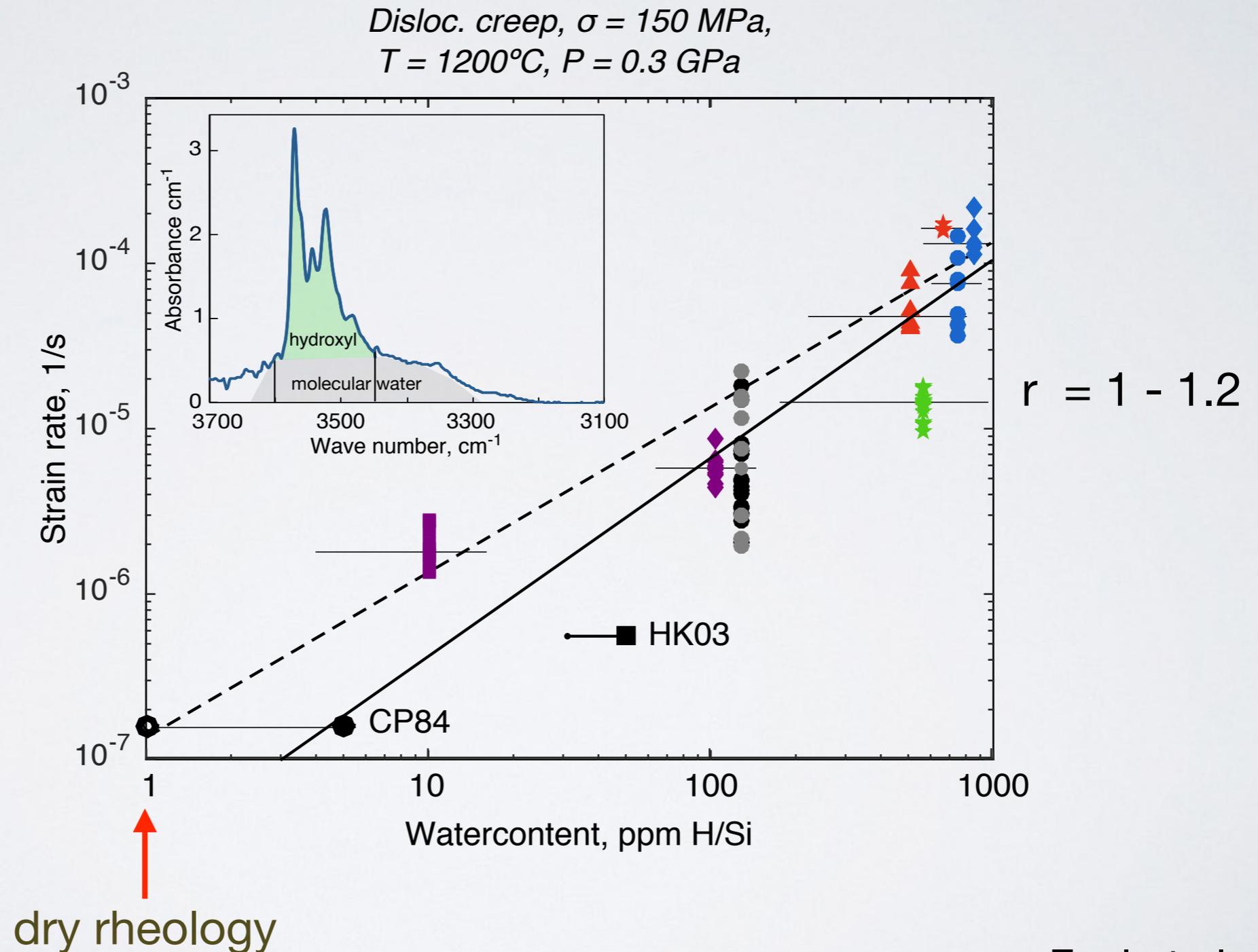


# Absorption of infrared light reveals structural location of hydrogen in olivine crystal lattice

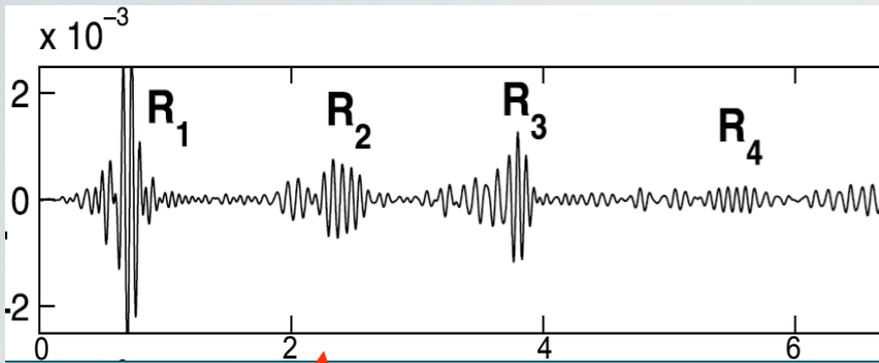


- rheology controlled by structurally bound water (hydroxyl)
- water incorporation linked to titanium:

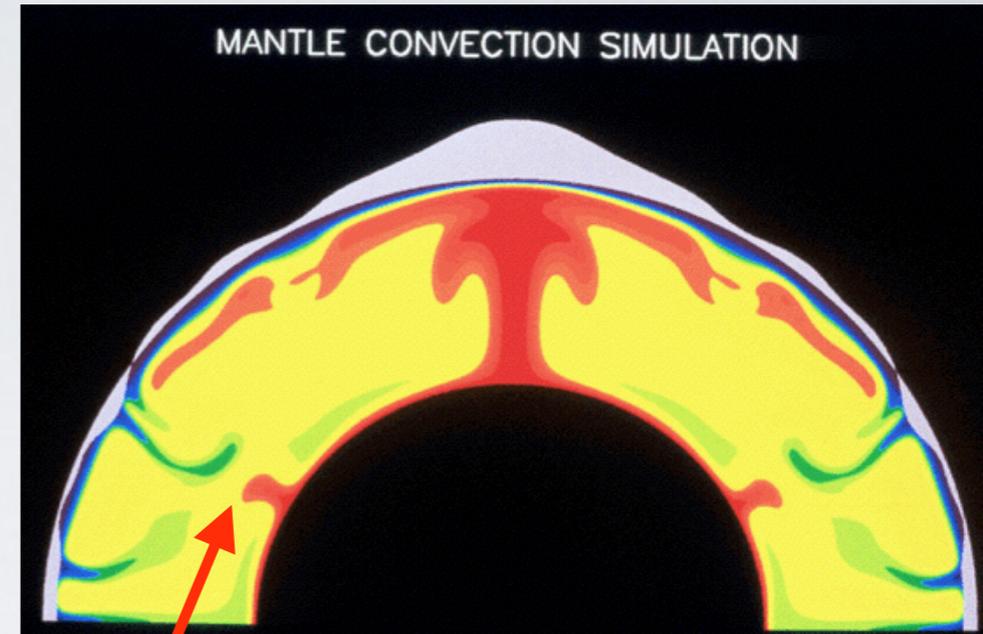
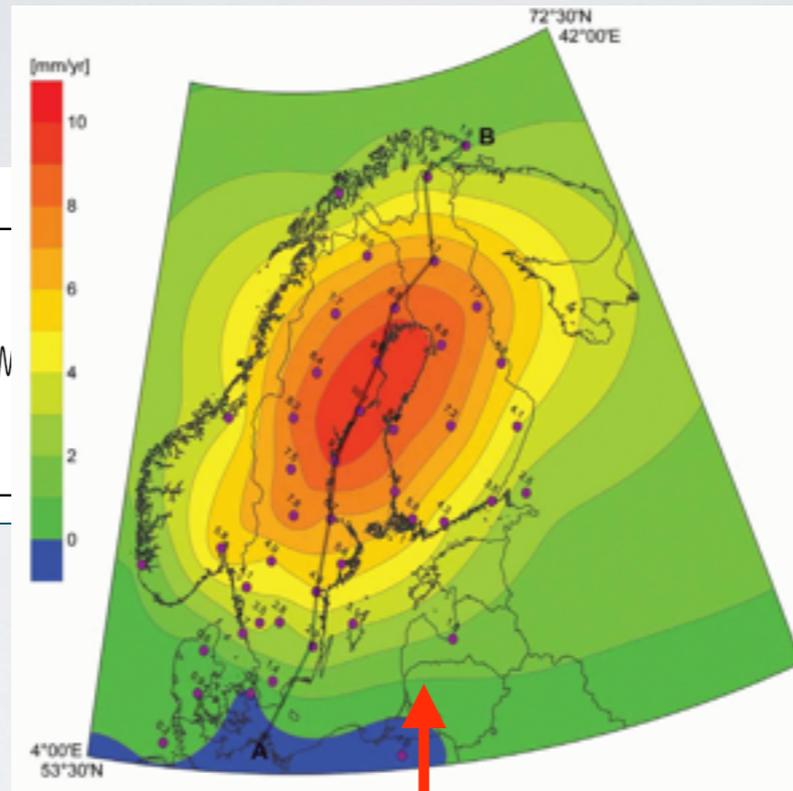
extrinsic defects control water incorporation and rheology



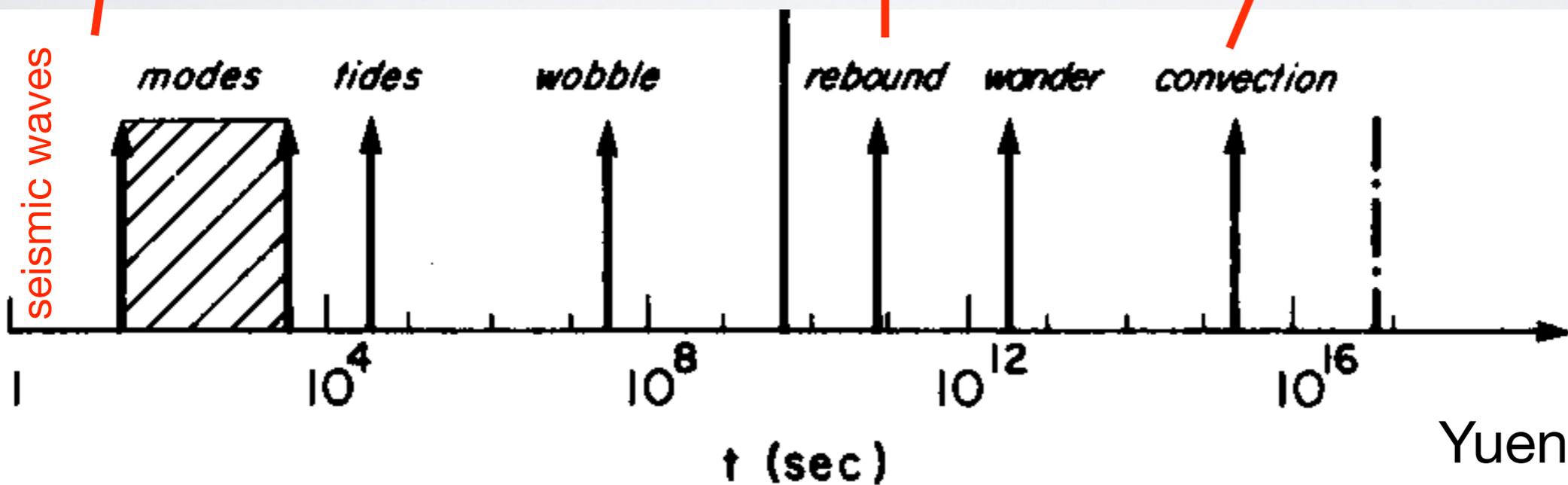
# Deformation at a range of time scales



$\epsilon < 10^{-4}$

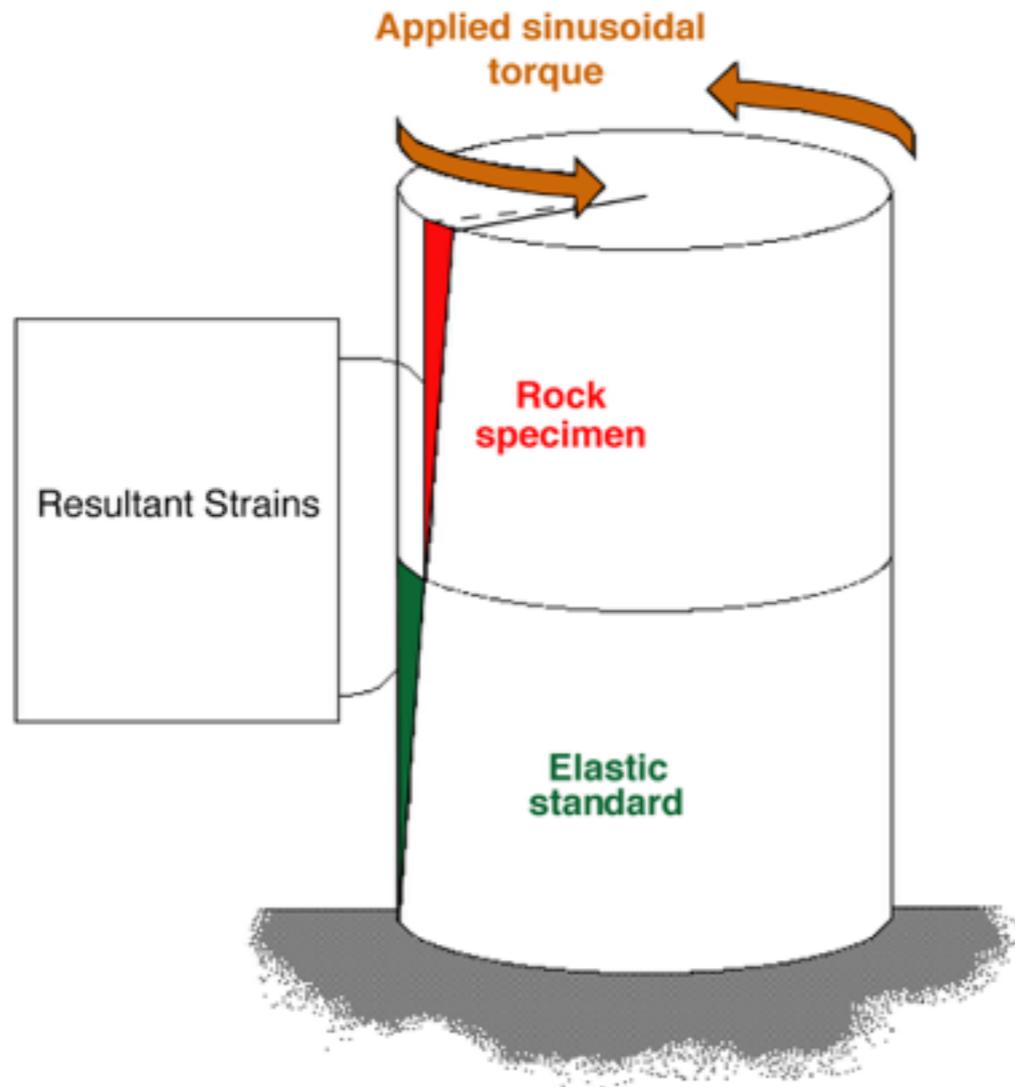


$\epsilon \gg 1$



Yuen & Peltier, 1982

# Experiments: Measurement of shear modulus (G) and attenuation (1/Q)



Research School of Earth Sciences,  
Australian National University

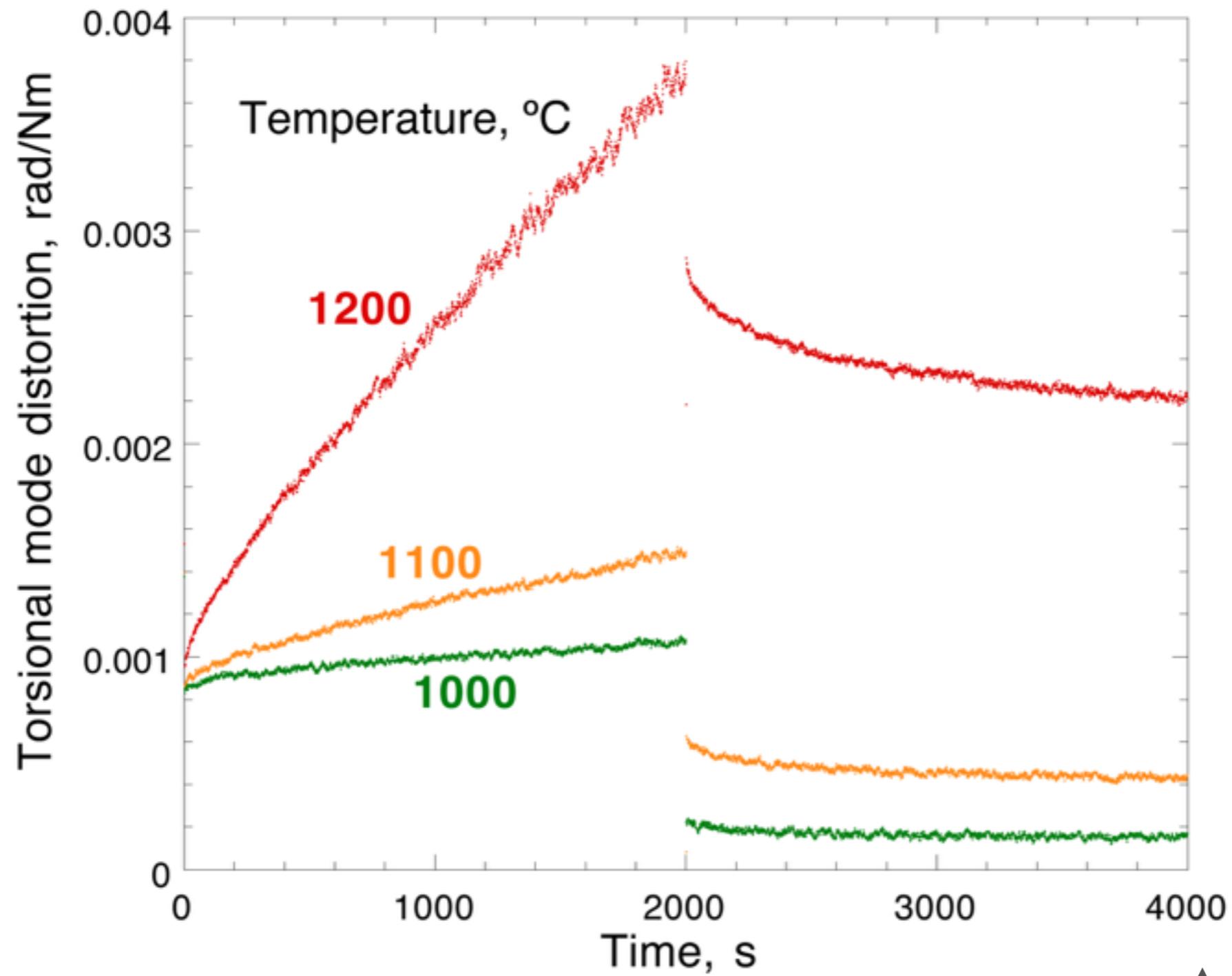
Experiments at

- temperatures to 1300°C
- periods 1 - 1000s
- 200 MPa confining pressure

Measure shear modulus G  
and dissipation/attenuation

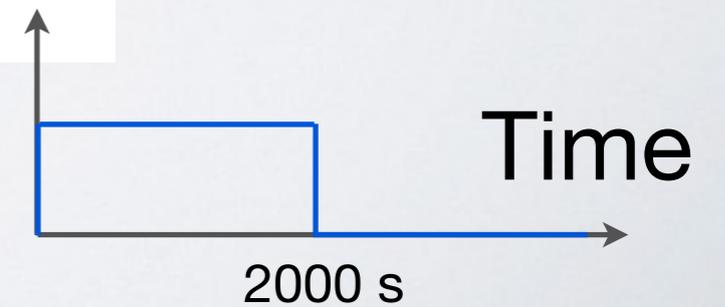
Attenuation (1/Q): energy loss  
per cycle

# Microcreep experiments (time domain)



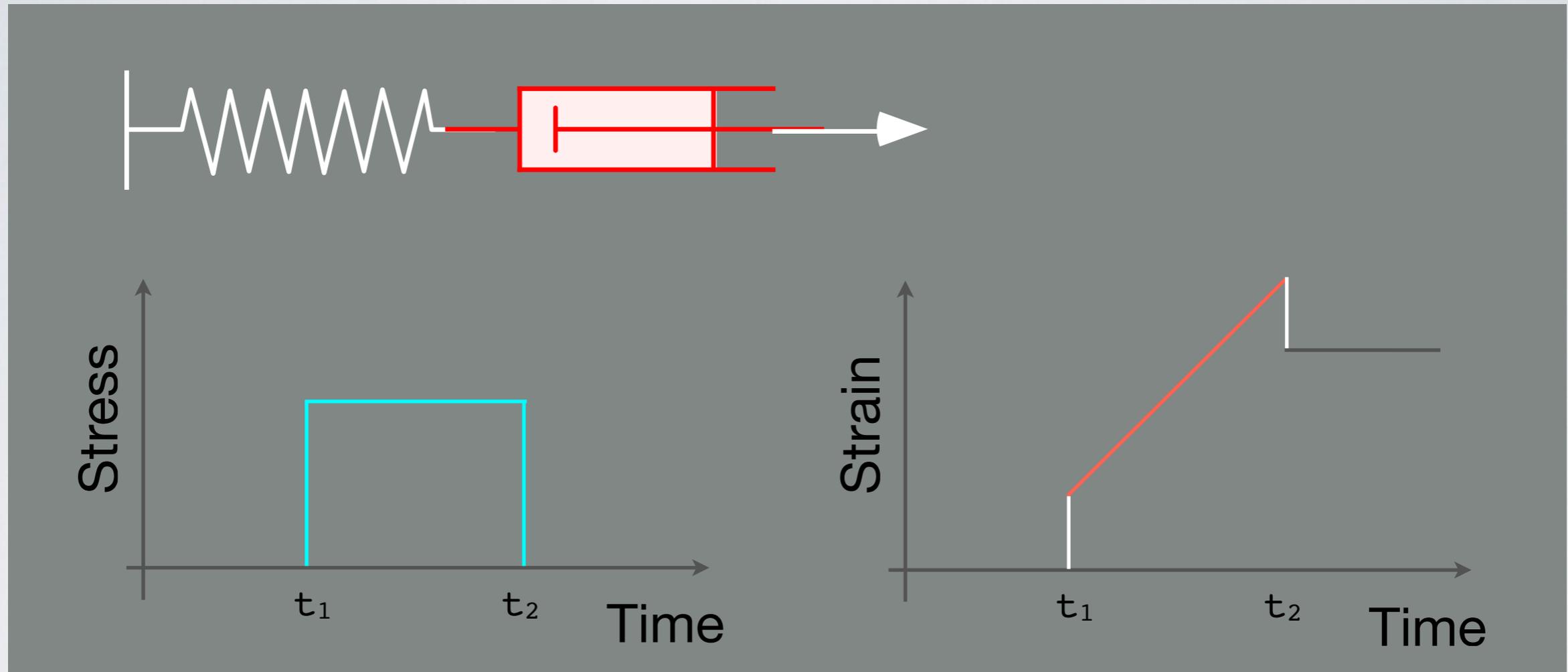
$$\varepsilon < 10^{-4}$$

Stress



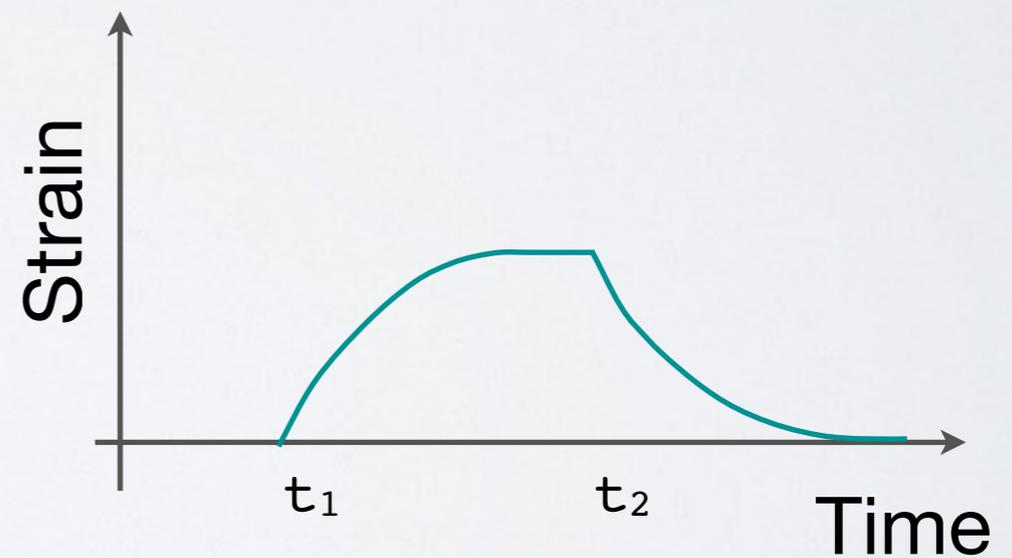
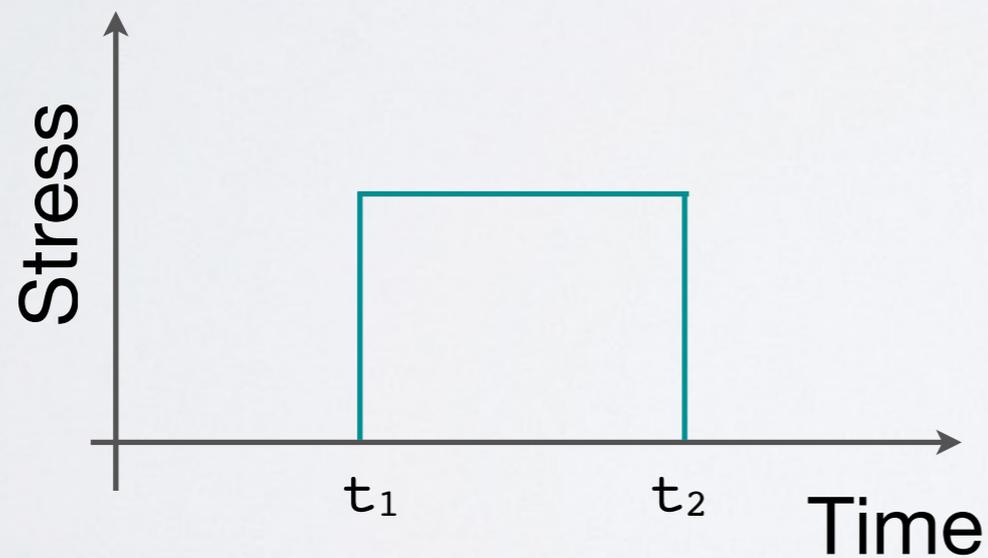
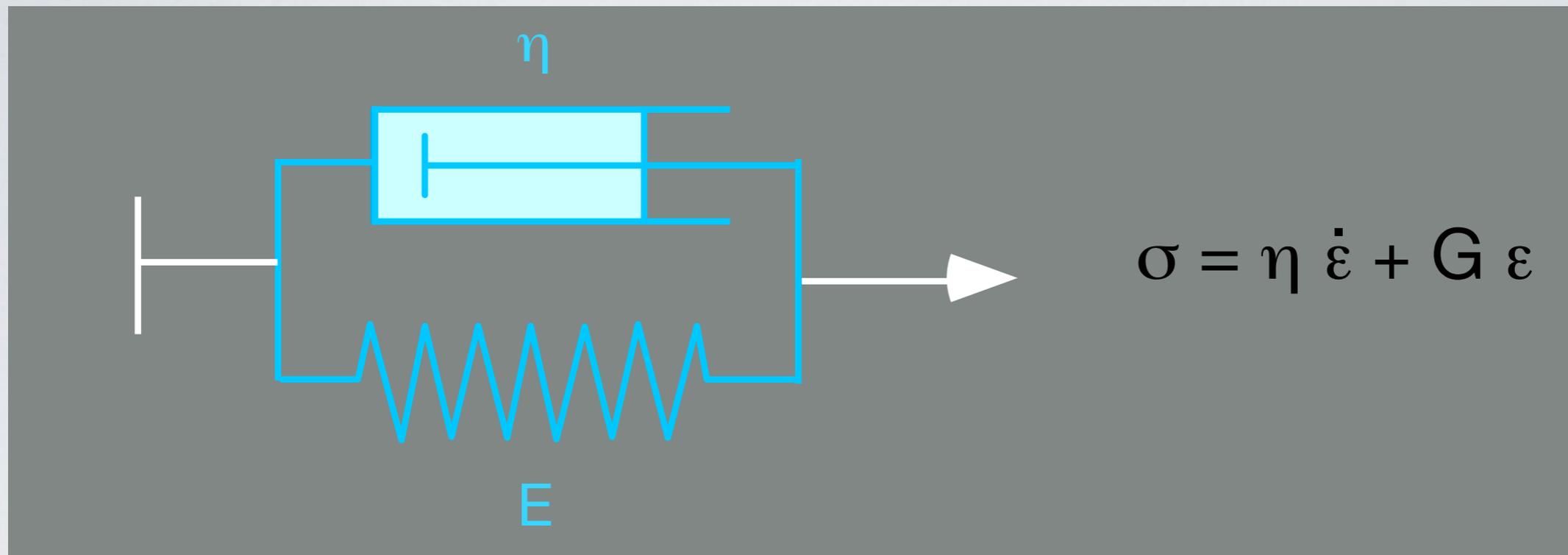
2000 s

# Maxwell body: viscoelastic



instantaneous, reversible + time-dependent permanent

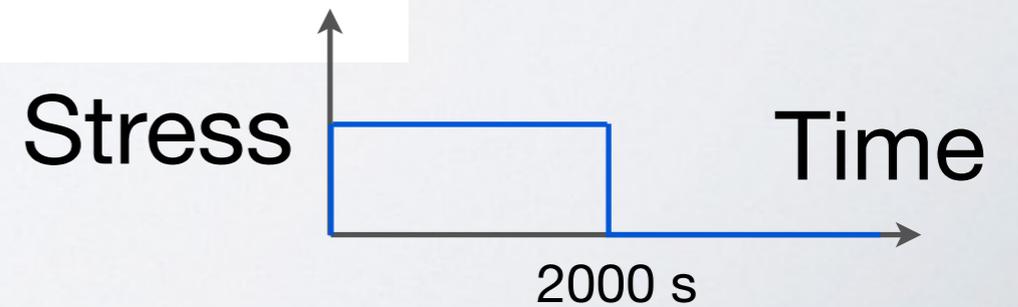
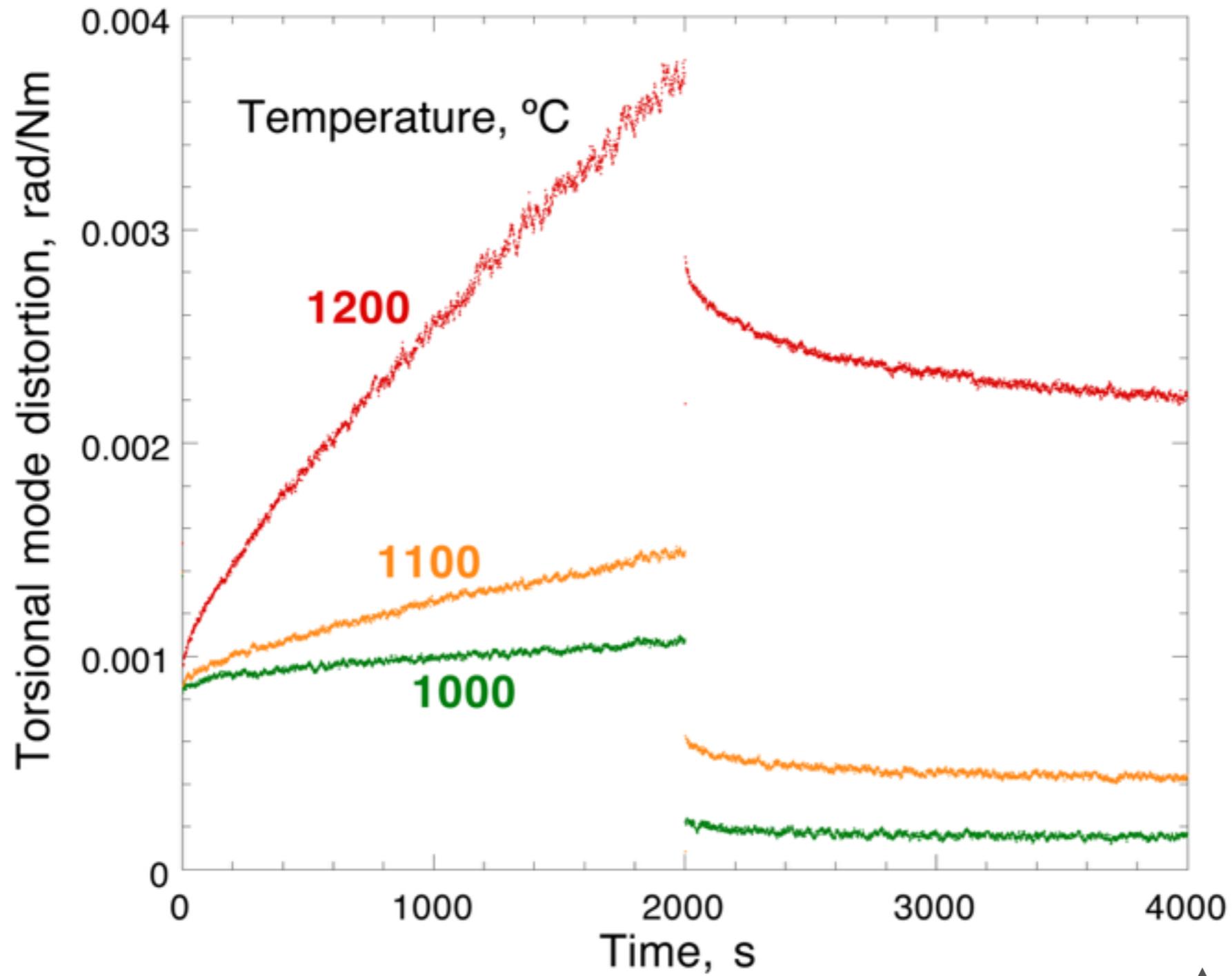
# Anelastic behavior (transient creep)



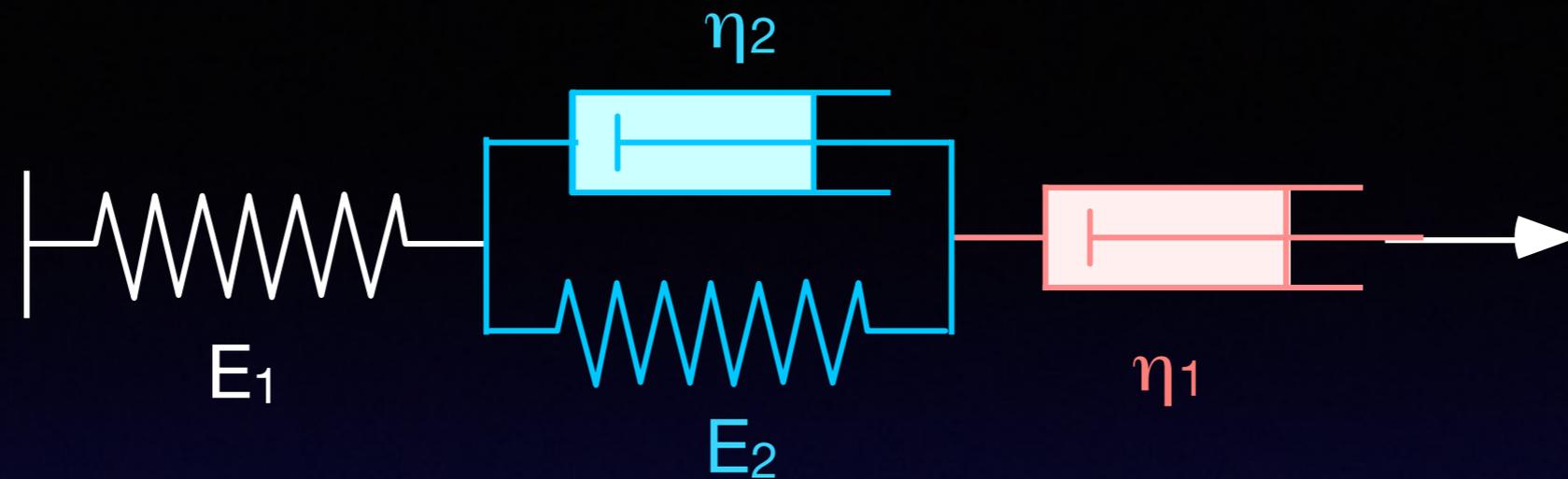
time-dependent, unique equilibrium, recoverable

# Microcreep experiments

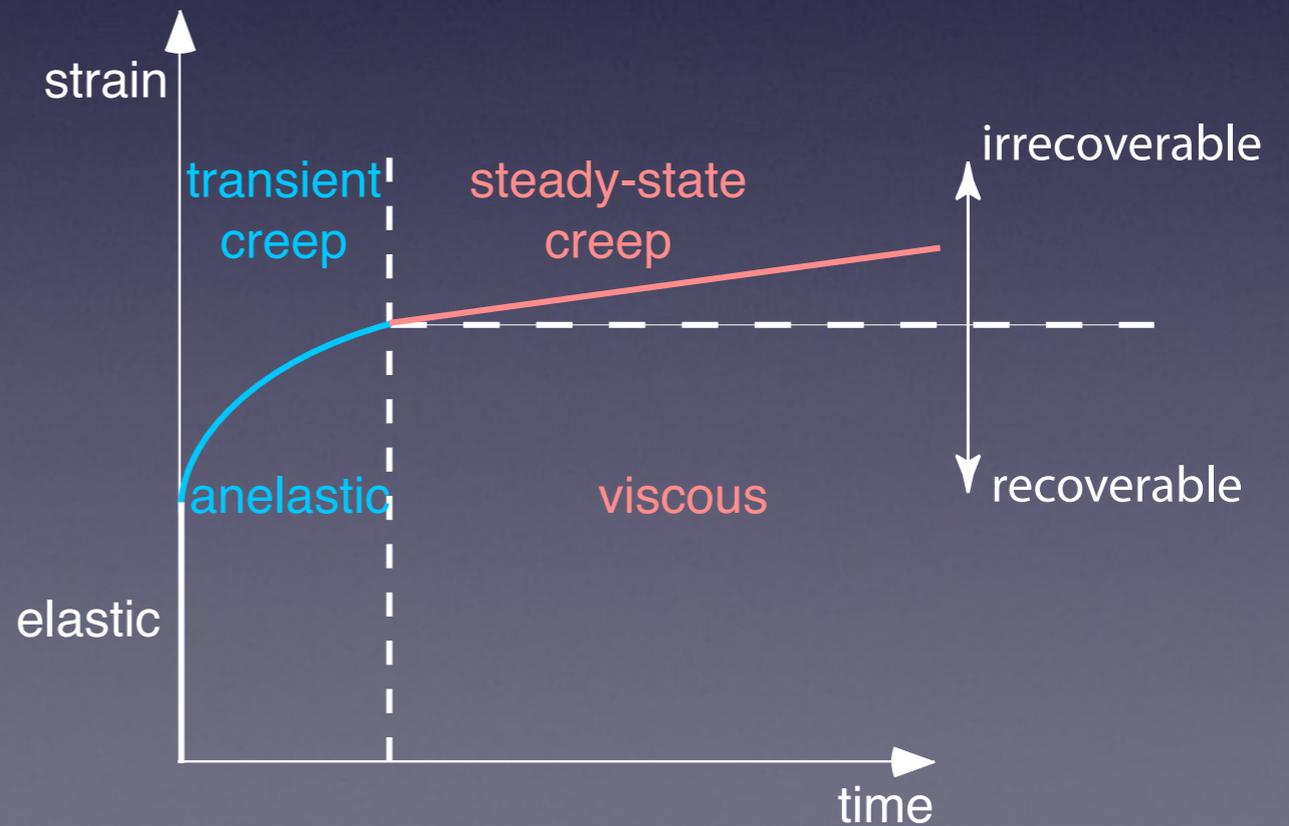
$$\epsilon < 10^{-4}$$



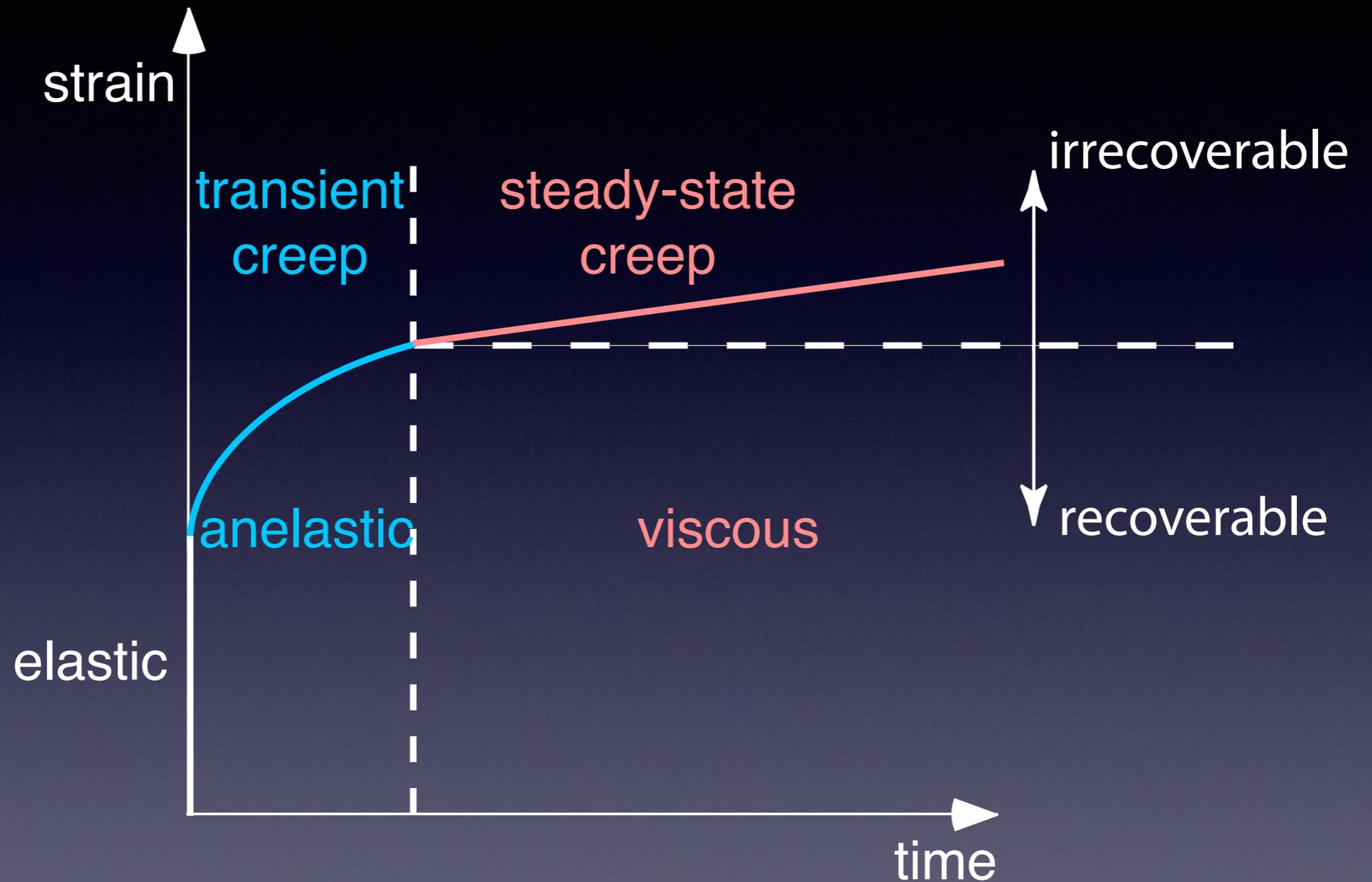
# Viscoelastic behavior: Burgers Model



$$\epsilon(t) = \epsilon_e + \epsilon_t(t) + \dot{\epsilon}t$$



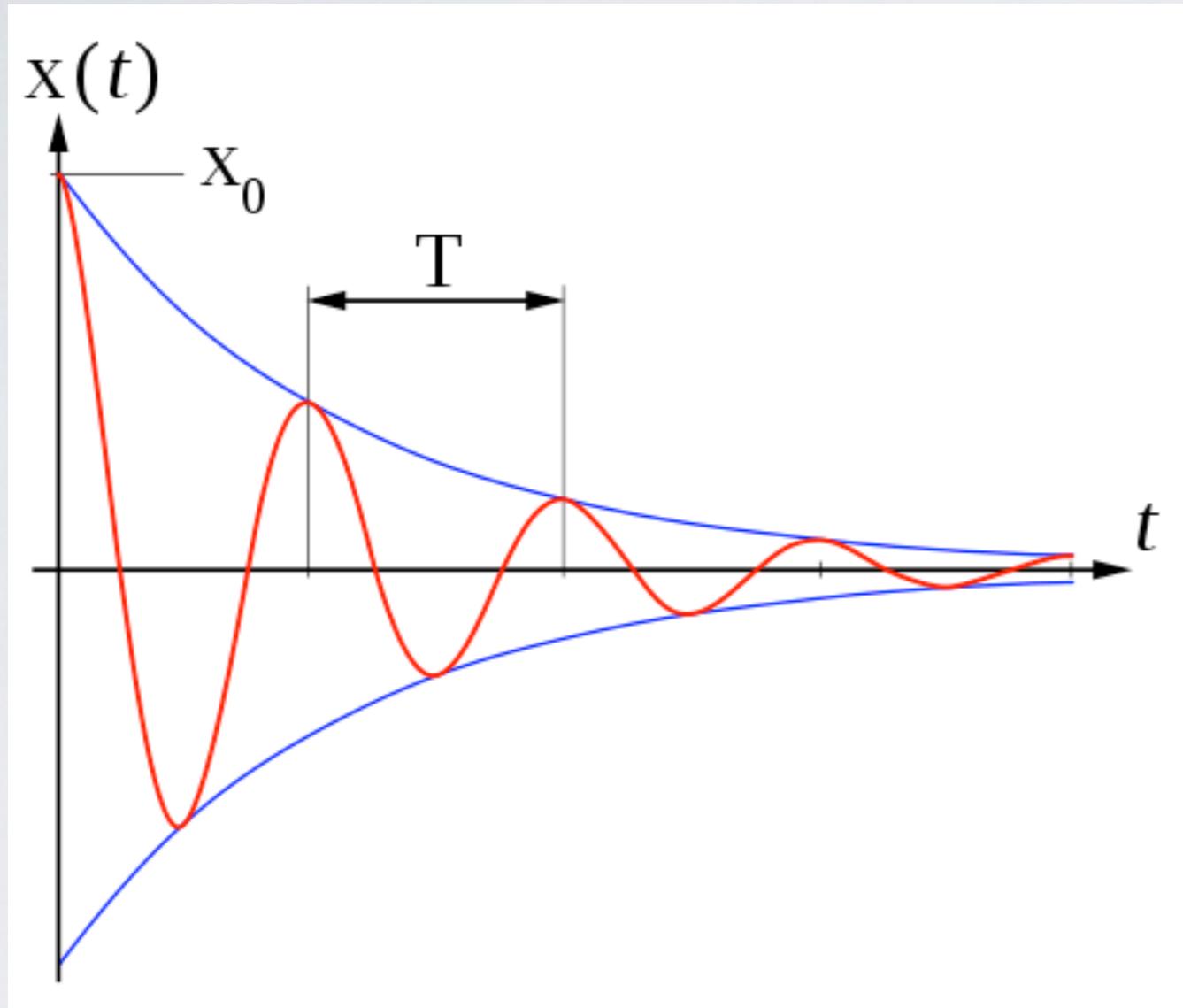
# Timescales of deformation in the Earth



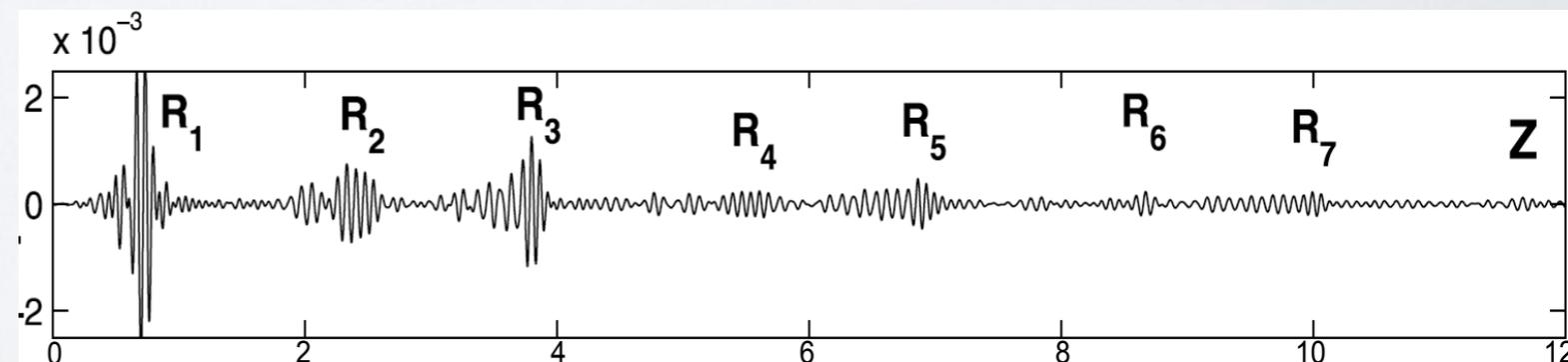
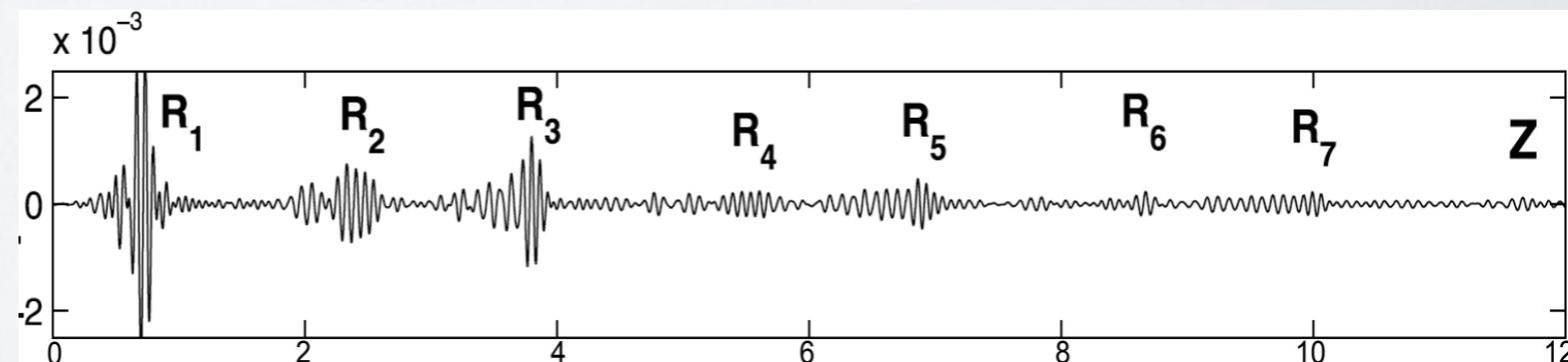
(Earth-  
quakes) Seismic waves Post-glacial rebound

Mantle convection

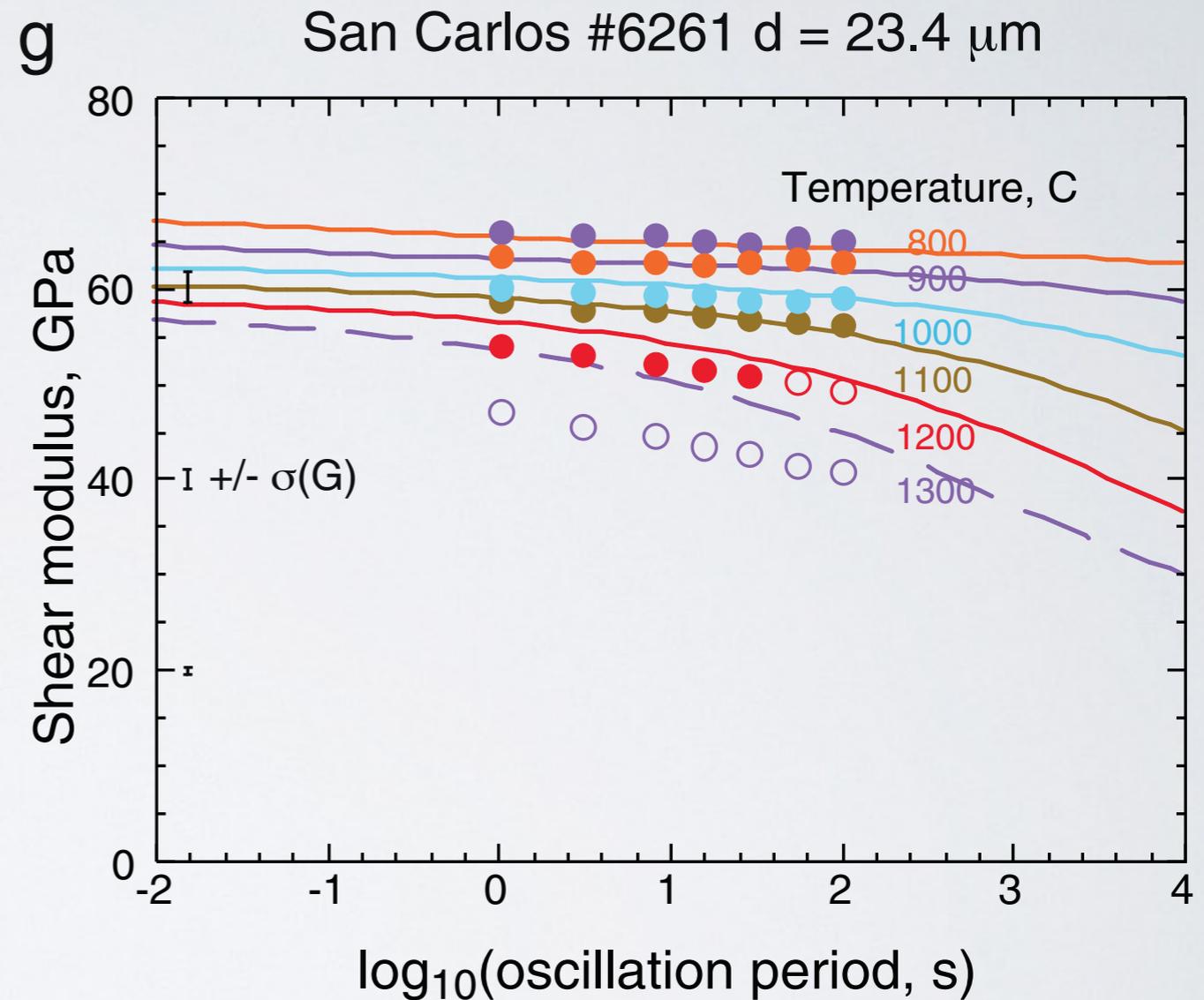
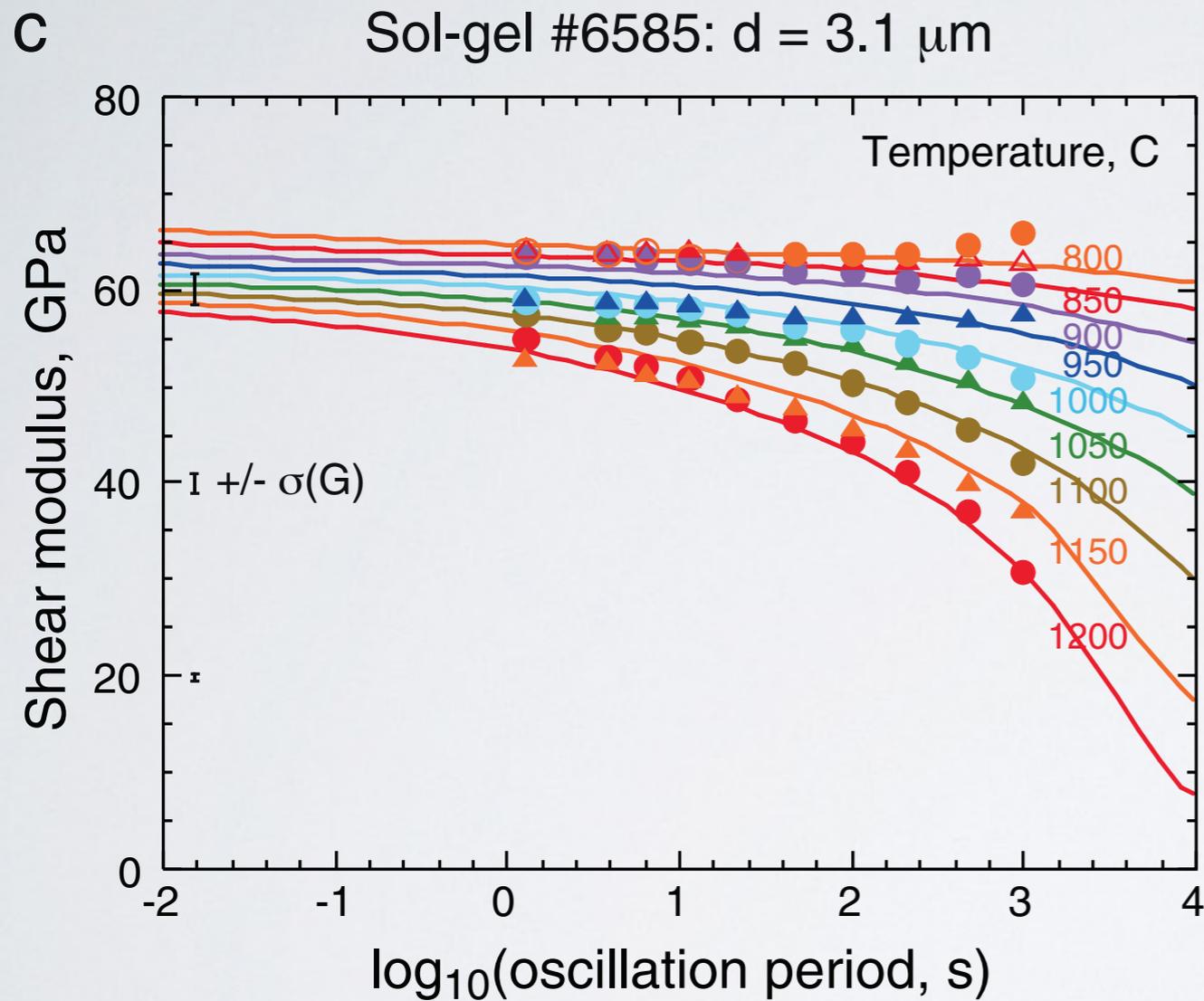
Attenuation/dissipation (frequency domain)  
amplitude decreases with each cycle



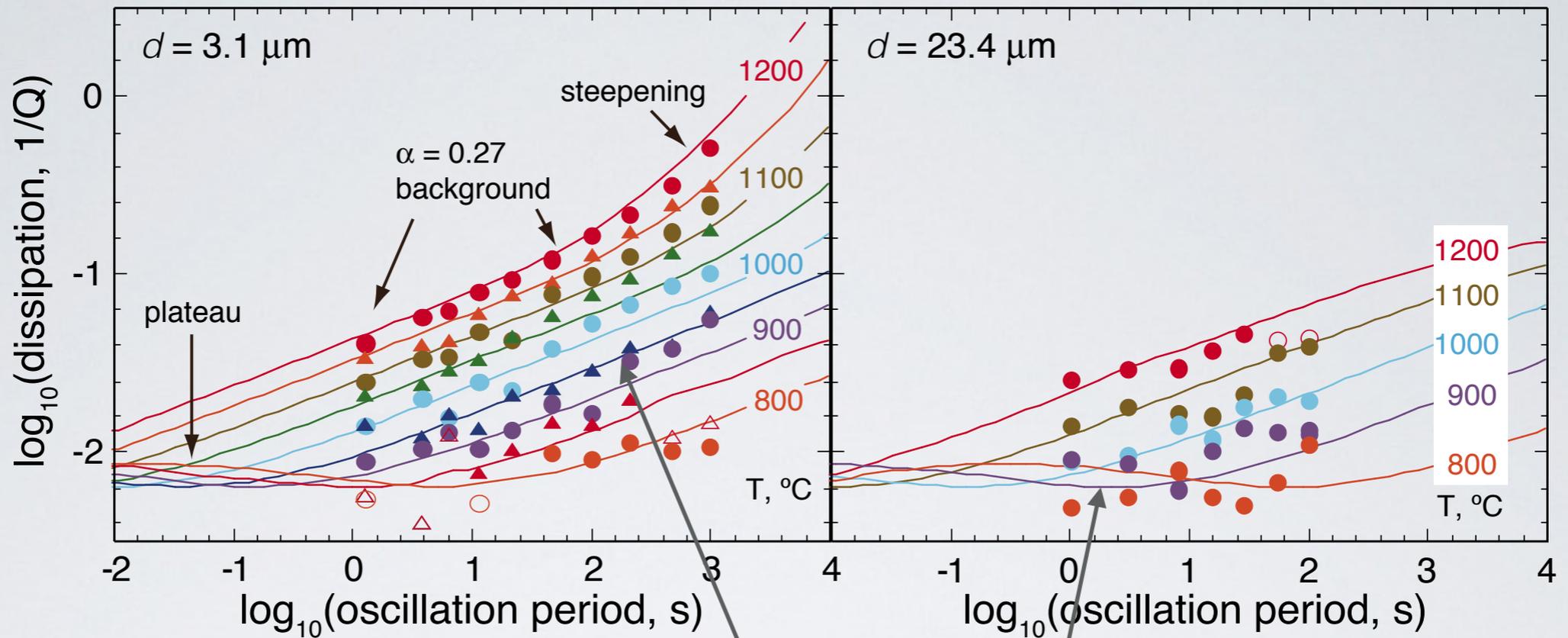
$$Q^{-1} = \delta E/E * 1/2\pi$$



# Forced torsional oscillation (frequency domain): Temperature, grain size and frequency dependence of dry, melt-free polycrystalline olivine



Jackson and Faul, 2010



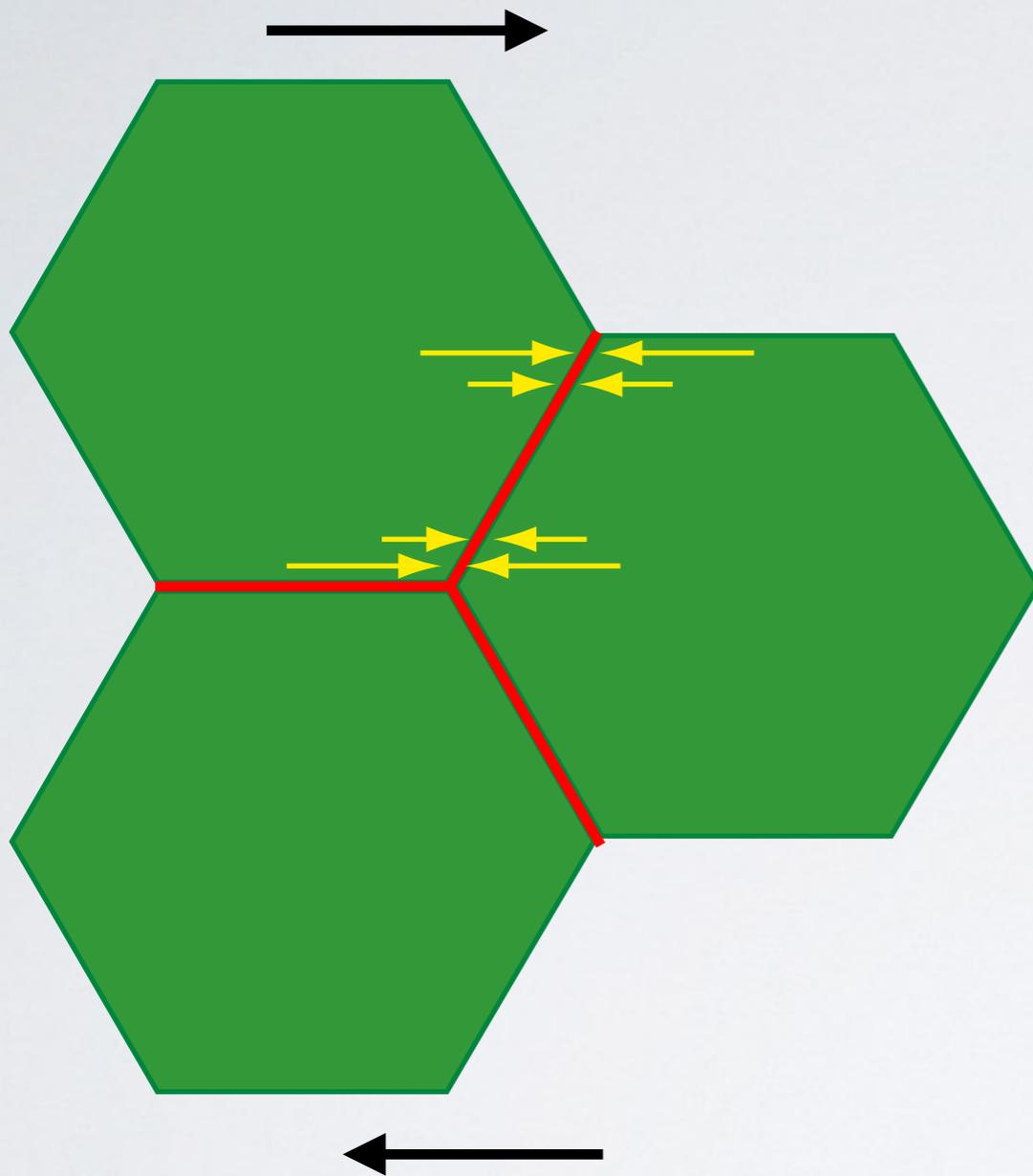
distribution of relaxation times

$$J_1(\omega) = J_U \left\{ 1 + \frac{\alpha \Delta_B}{\tau_H^\alpha - \tau_L^\alpha} \int_{\tau_L}^{\tau_H} \frac{\tau^{\alpha-1}}{1 + \omega^2 \tau^2} d\tau \right. \\ \left. + \frac{1}{\sigma \sqrt{(2\pi)}} \Delta_P \int_0^\infty \frac{1}{\tau} \frac{\exp\left(\frac{-[\ln(\tau/\tau_P)/\sigma]^2}{2}\right)}{1 + \omega^2 \tau^2} d\tau \right\}$$

plateau

$$J_2(\omega) = J_U \left\{ \frac{\omega \alpha \Delta_B}{\tau_H^\alpha - \tau_L^\alpha} \int_{\tau_L}^{\tau_H} \frac{\tau^\alpha}{1 + \omega^2 \tau^2} d\tau \right. \\ \left. + \frac{\omega}{\sigma \sqrt{(2\pi)}} \Delta_P \int_0^\infty \frac{\exp\left(\frac{-[\ln(\tau/\tau_P)/\sigma]^2}{2}\right)}{1 + \omega^2 \tau^2} d\tau + \frac{1}{\omega \tau_M} \right\}$$

# 1. Elastically accommodated sliding

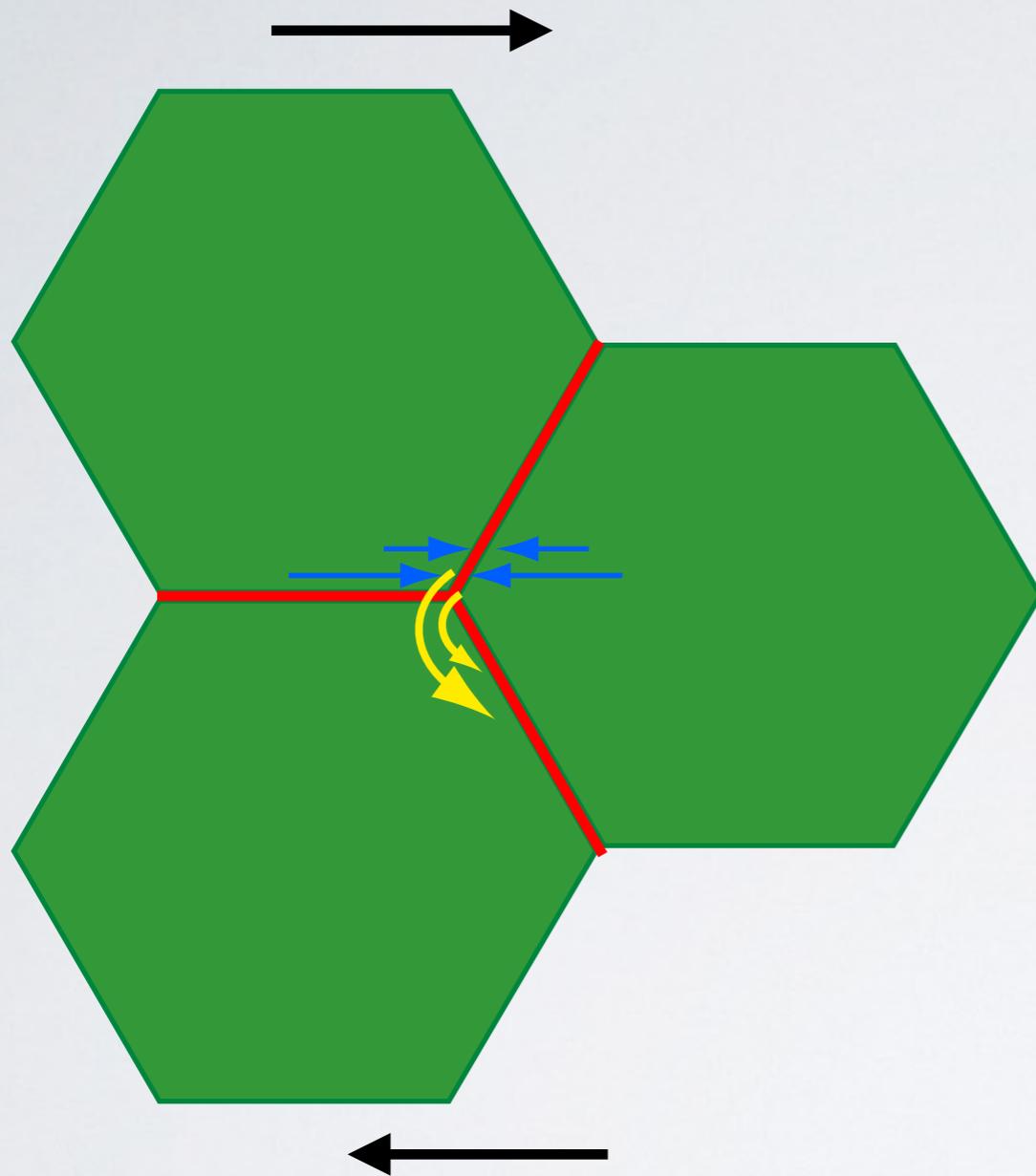


viscous sliding of grain boundaries  
leads to elastic stress  
concentrations at grain corners

$$\text{time scale: } \tau_E = \eta_{gb} d/G \delta$$

recoverable strain, anelastic process, dissipation peak

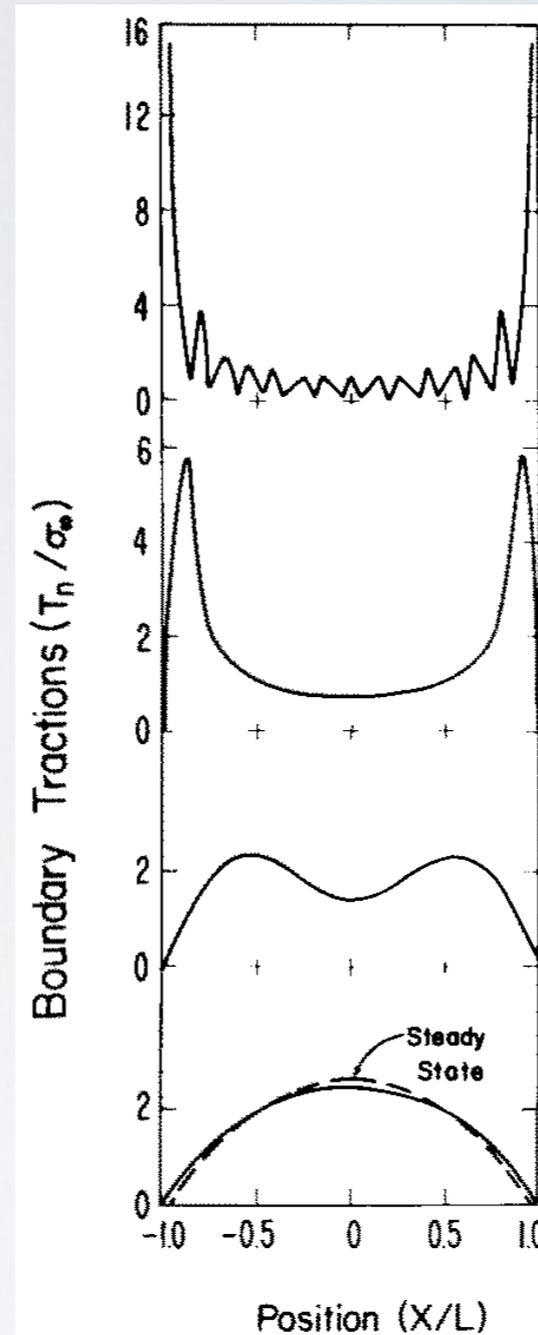
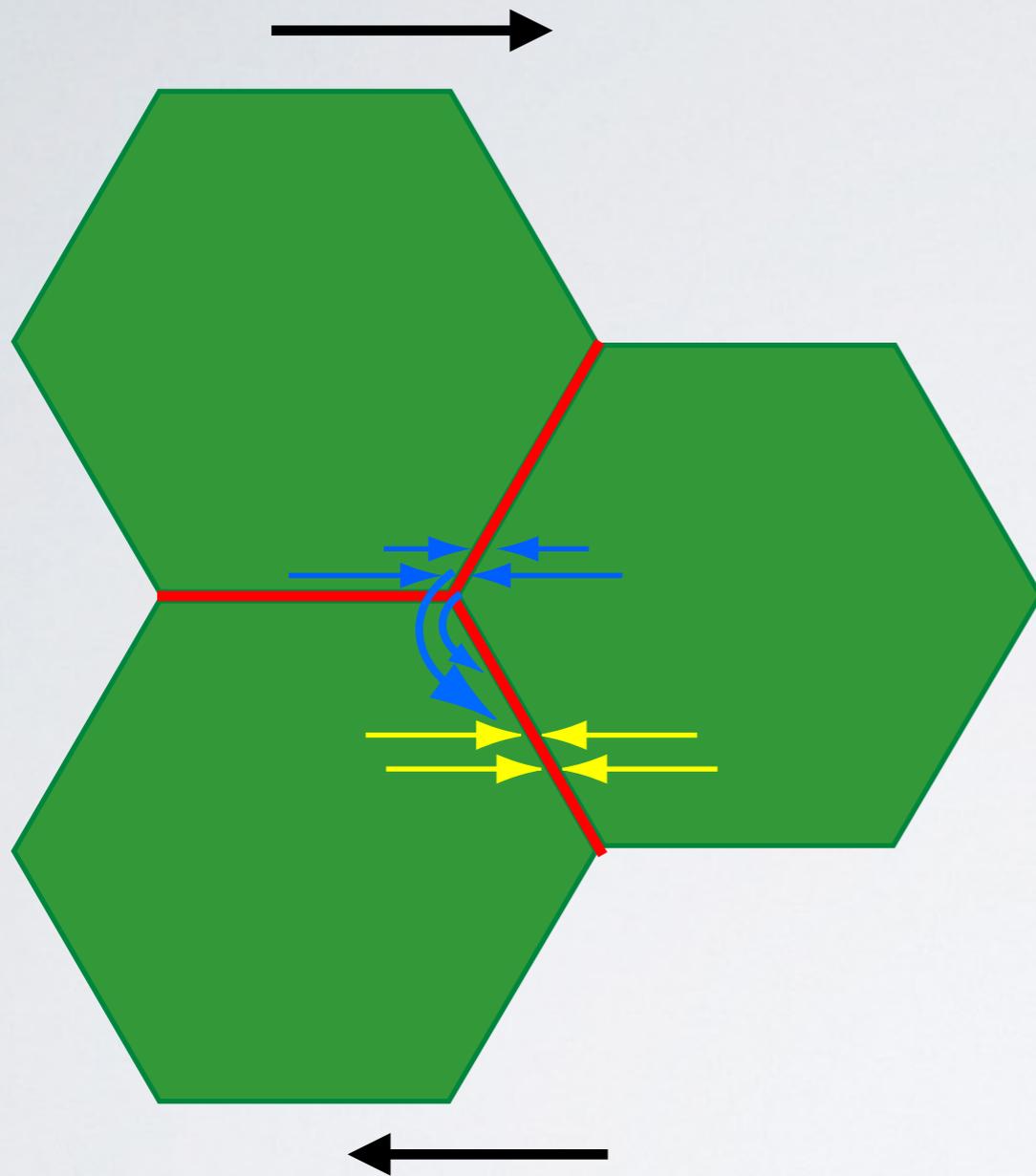
## 2. Diffusionally assisted sliding



- stress concentrations cause diffusion away from corners
- transient phase is characterised by diffusion over increasing length scales

distribution of relaxation times, transient, recoverable

### 3. Diffusionally accommodated sliding (steady state)



1. end of elastically accommodated sliding

2. diffusionally assisted sliding

3. steady state creep

Raj 1975,

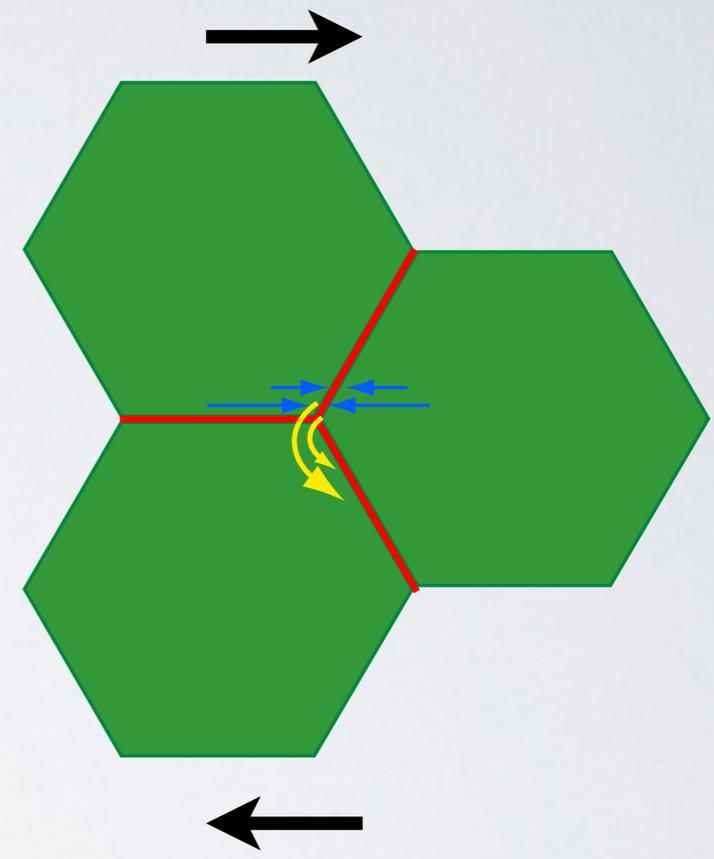
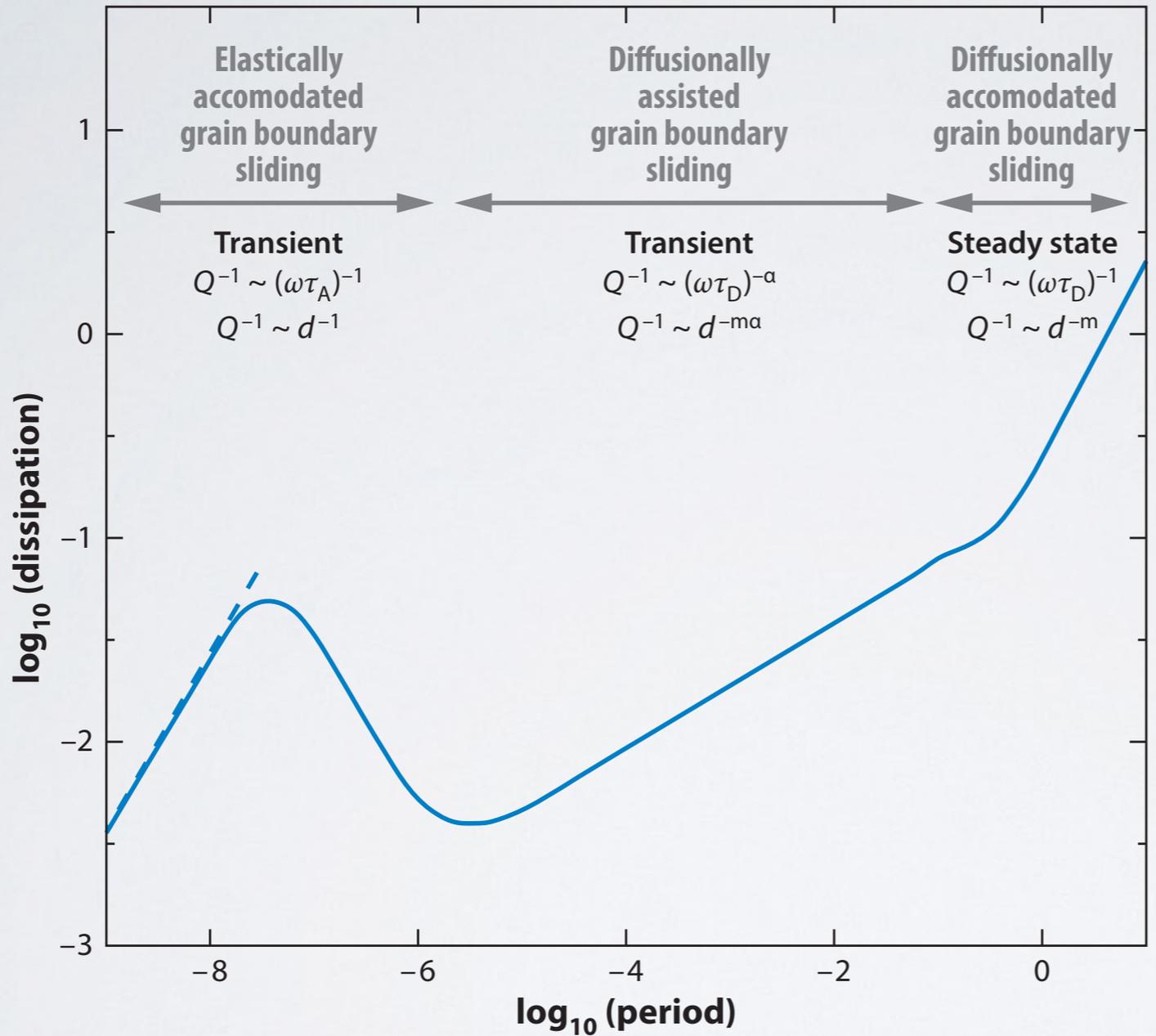
Gribb and Cooper, 1998

time scale:  $\tau_D \sim T d^3 / G \delta D_{gb}$

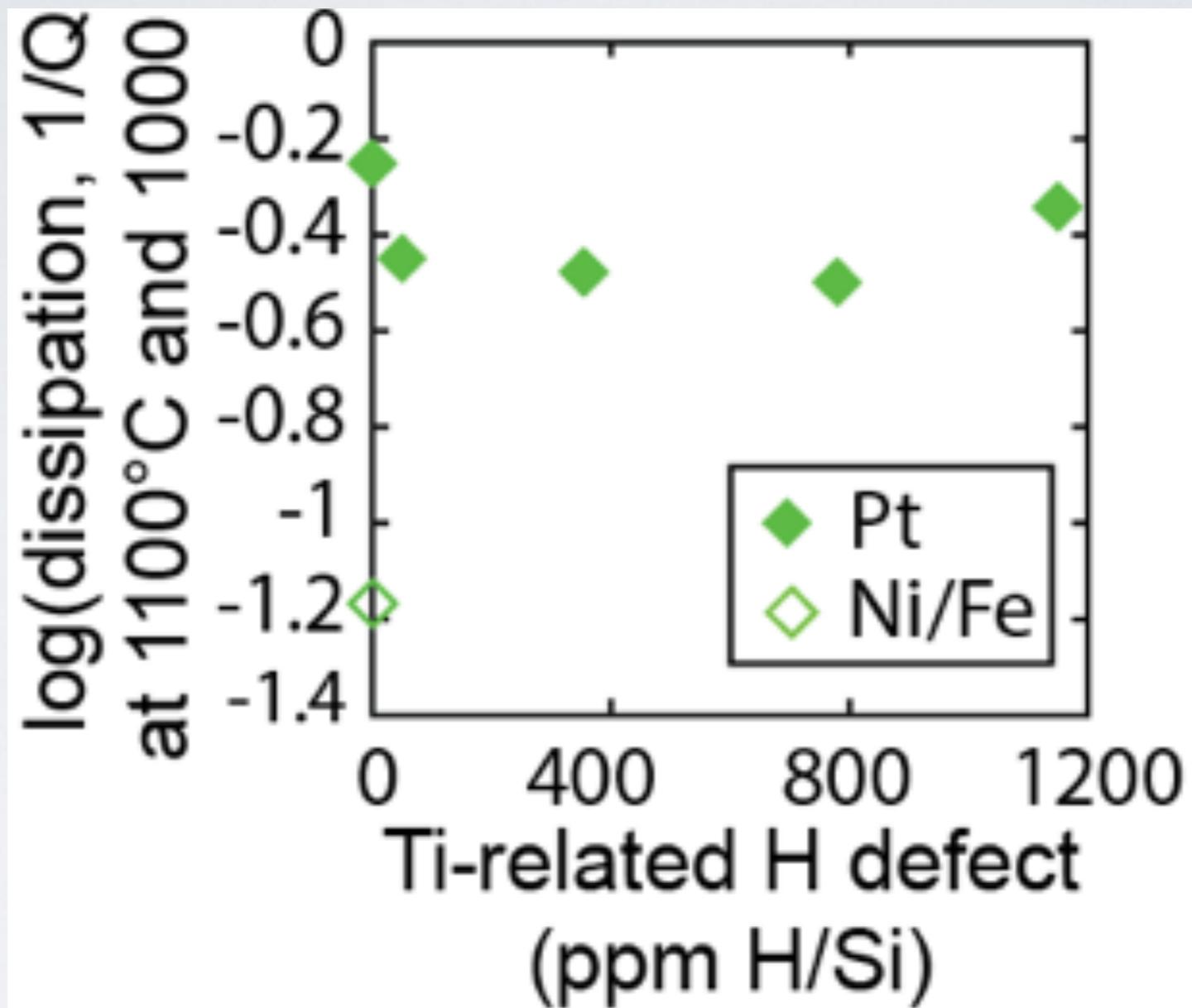
gb normal stresses are highest in center between grain corners (steady state diffusion creep)

Microphysical model: Continuum of relaxation times (absorption band) is required.

Diffusionally assisted grain boundary sliding

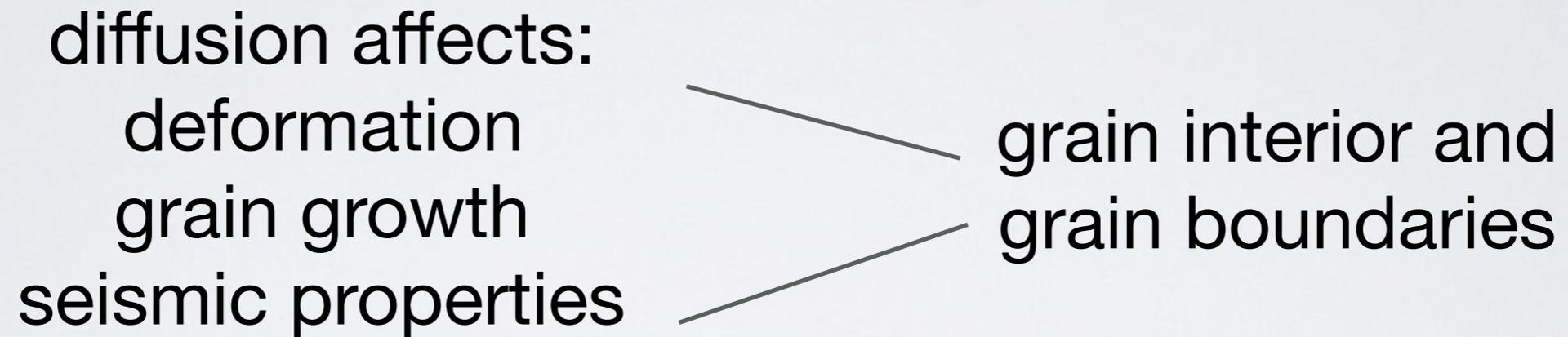


seamless transition from transient creep to steady-state deformation



# Defects

point defects, affect diffusion



Factors affecting diffusion rates: temperature, 'water'?, melt, oxygen fugacity