CRYSTAL2PLATE

**How does plate tectonics work:
From crystal-scale processes to mantle
convection with self-consistent plates**

Introduction to crystal plasticity: deformation mechanisms, microstructures, and crystal preferred orientations

Andréa Tommasi

Short course on "Microstructures, textures & anisotropy"
Geosciences Montpellier (F) - 28 June - 2 July, 2010

ductile deformation

crystal plasticity

dislocation creep

diffusion creep

dislocation glide

recrystallization

visco-plastic behavior

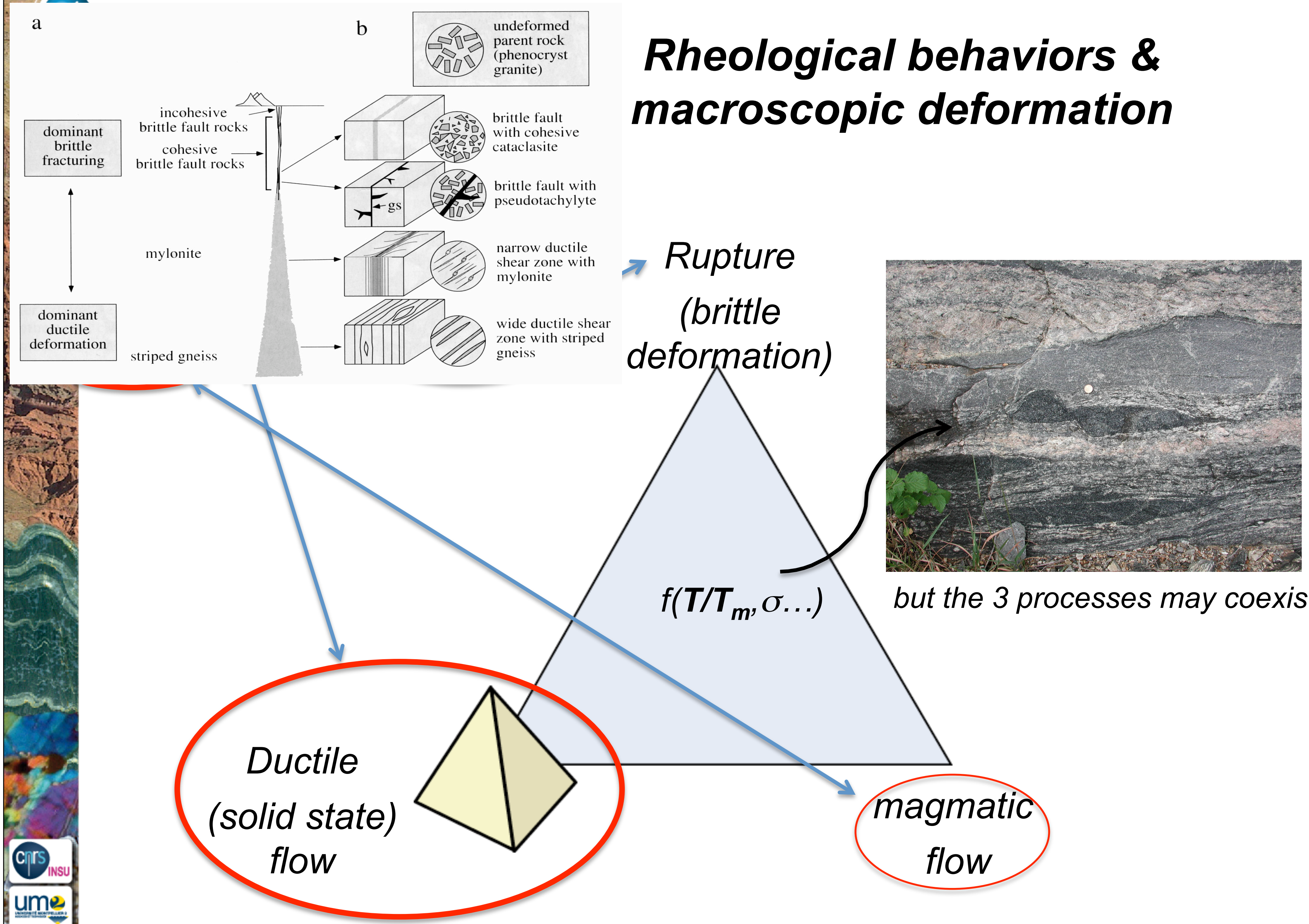
$$\sigma = \sigma_y + f(\dot{\varepsilon})$$

viscous behavior

$$\sigma \propto \dot{\varepsilon}$$

linear – non-linear?

Rheological behaviors & macroscopic deformation



Rupture

(brittle deformation)

$f(\mathbf{T/T_m}, \sigma\ldots)$

Ductile

(solid state)

flow

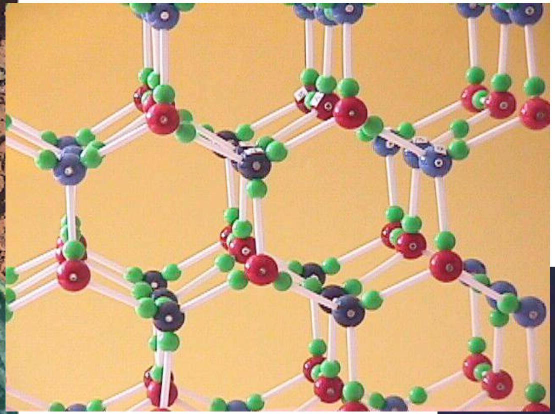
magmatic

flow

but the 3 processes may coexist

Crystal plasticity = main process in ductile deformation

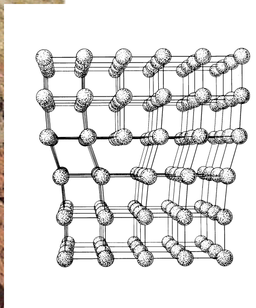
- ✓ *deformation (change in shape ± crystals orientation) without loss of physical continuity (≠ brittle behavior)*
- ✓ *viscoplastic behavior :* $if\, \sigma \geq \sigma_y \Rightarrow \sigma \propto \dot{\varepsilon}$

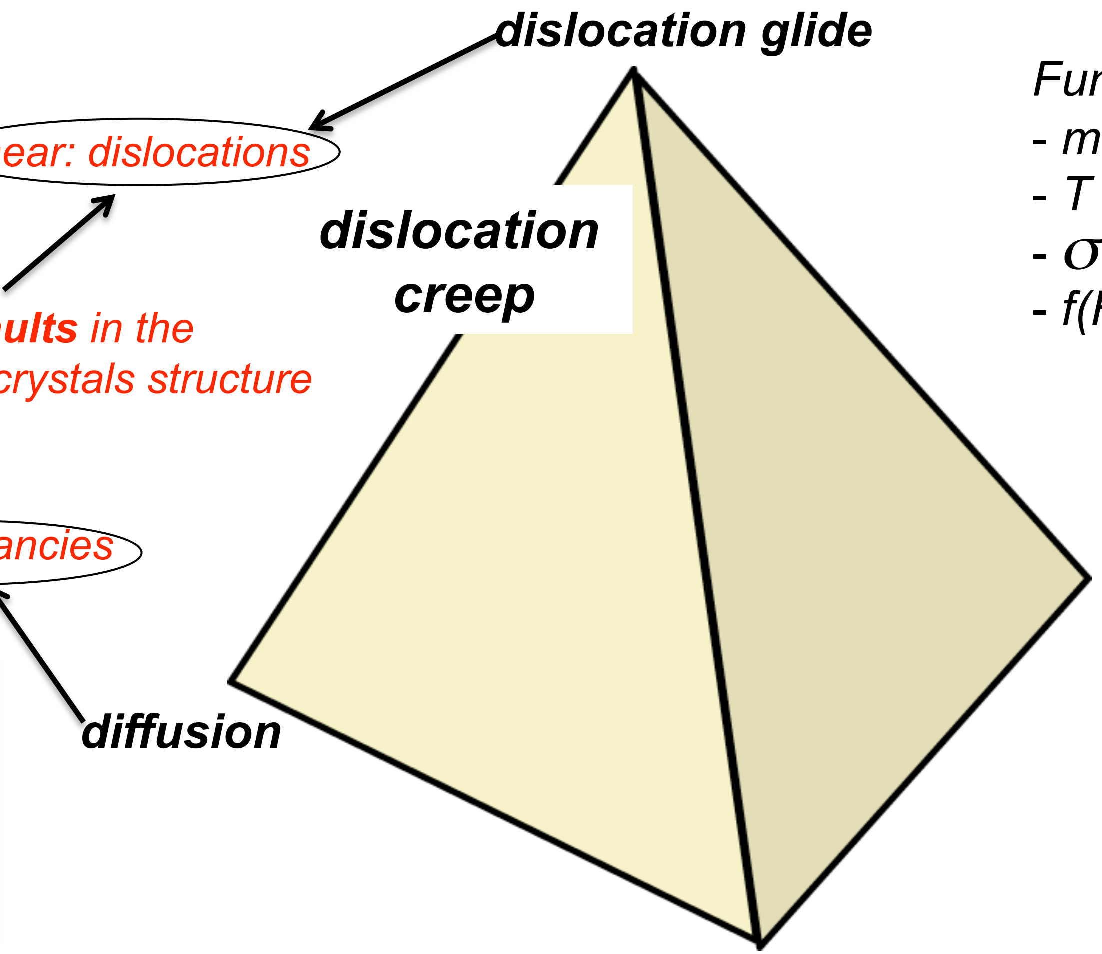


Ice Ih
hexagonal

Which processes ?

Ductile deformation = solid-state flow





dislocation glide

linear: dislocations

dislocation creep

*Motion of **defaults** in the crystals structure*

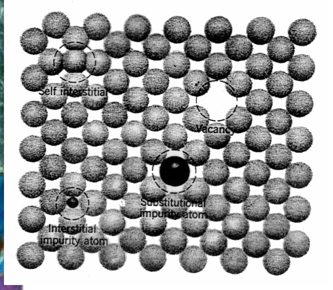
point: vacancies

diffusion

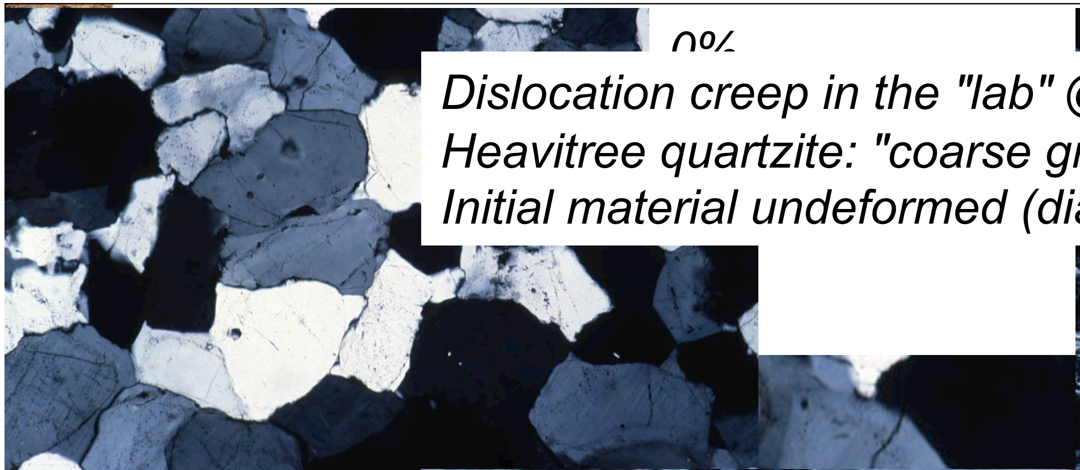
twinning

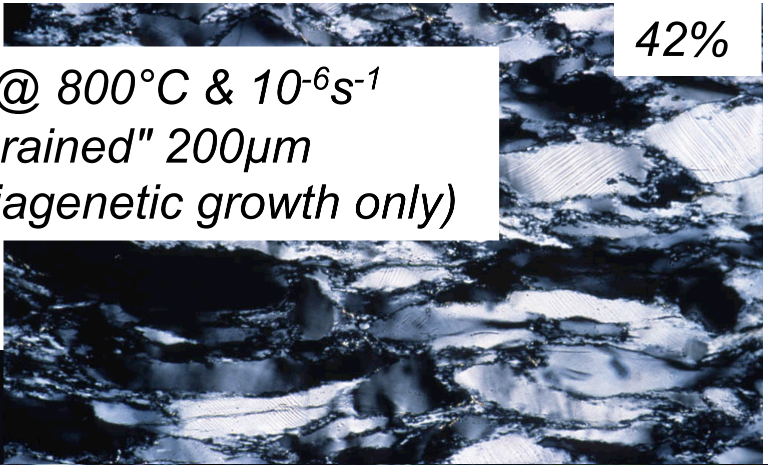
grain boundary sliding ?
needs an additional mechanism!

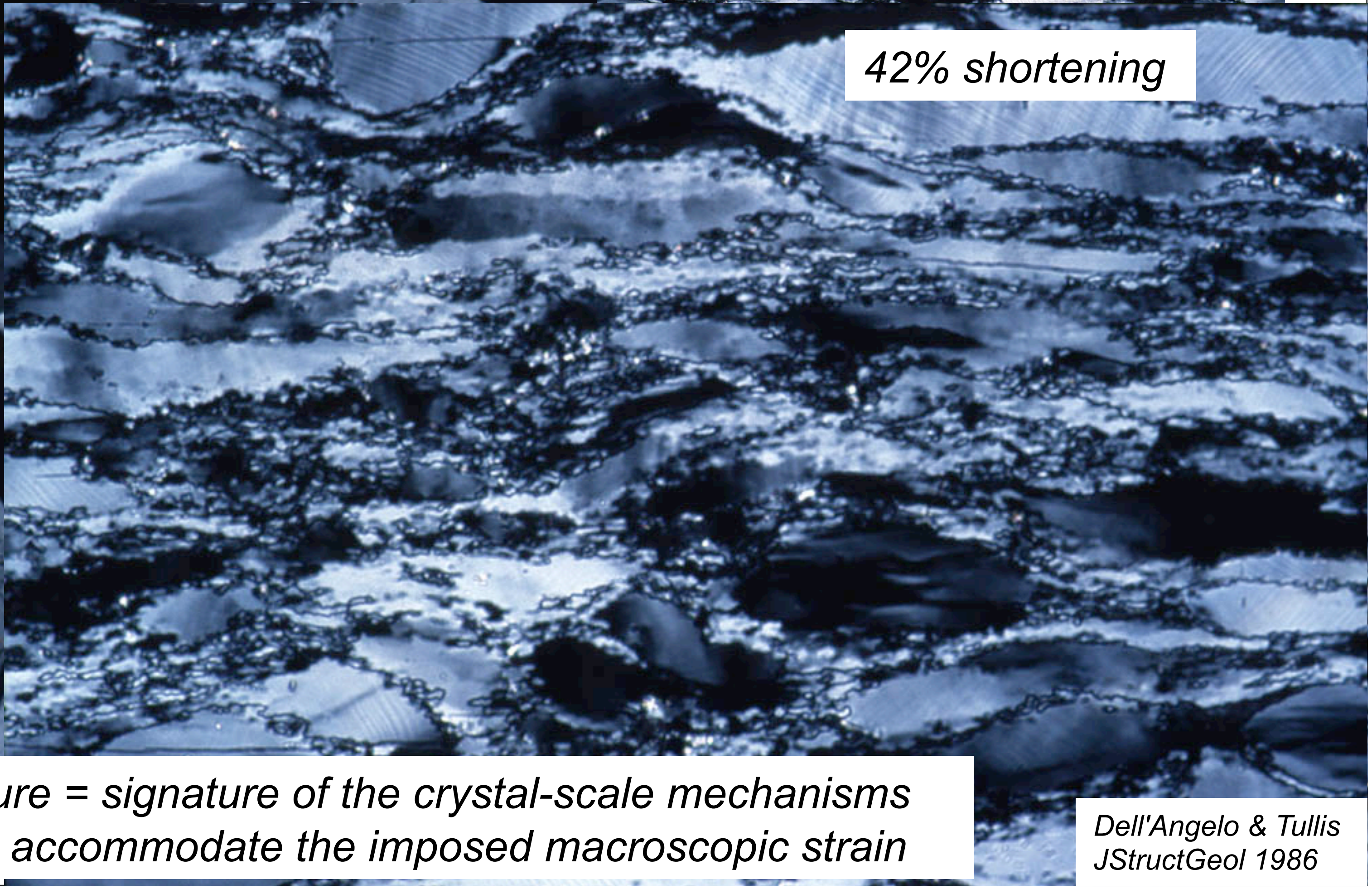
Function of:
- *mineral structure*
- *T*
- $\sigma, \dot{\varepsilon}$
- *f(H_2O, O_2)…*



Dislocation creep in the "lab" @ 800°C & $10^{-6}s^{-1}$
Heavitree quartzite: "coarse grained" 200µm
Initial material undeformed (diagenetic growth only)



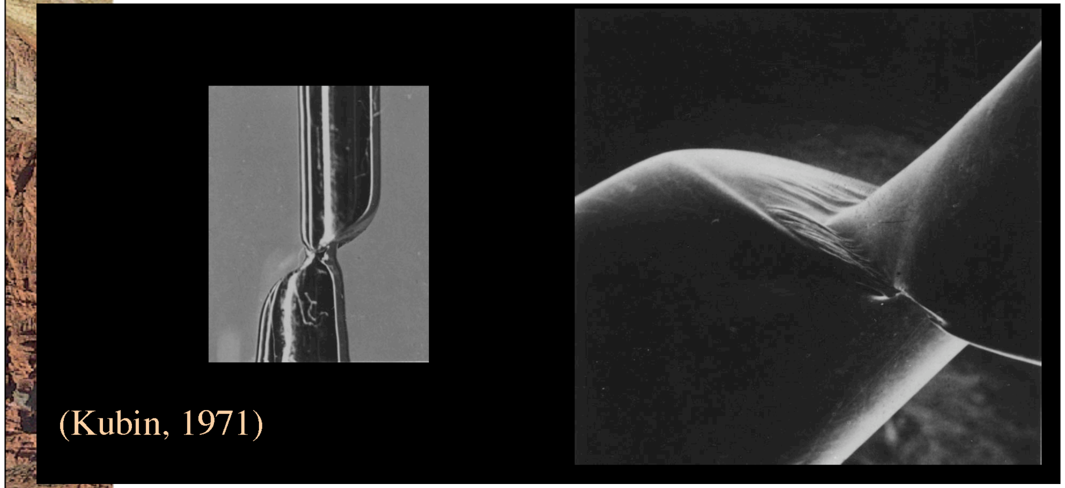




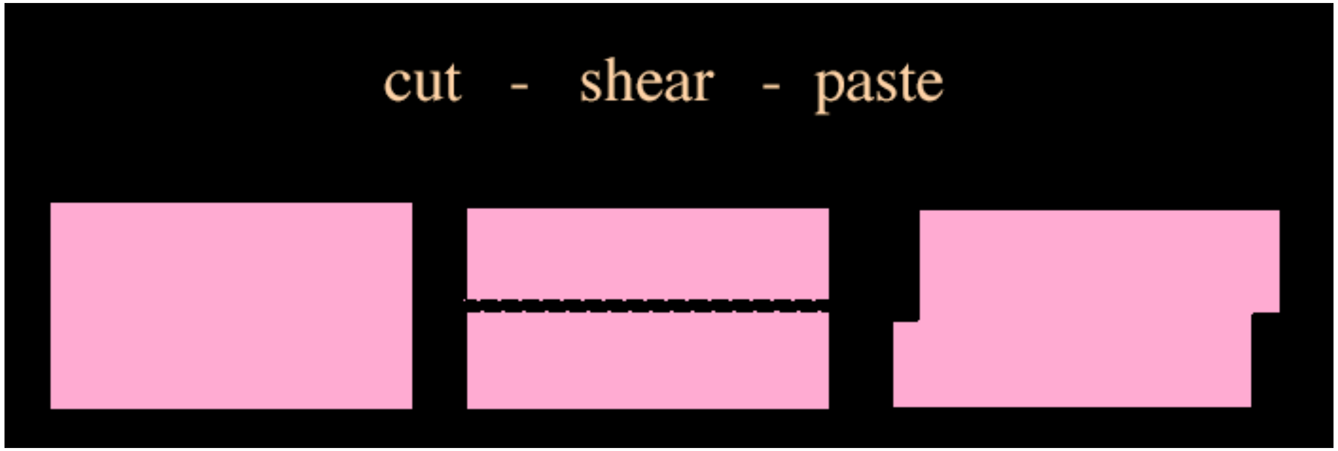
Microstructure = signature of the crystal-scale mechanisms activated to accommodate the imposed macroscopic strain

Dell'Angelo & Tullis
JStructGeol 1986

Deformation of metals : shear along well-defined crystallographic planes


(Kubin, 1971)


Frenkel's early model

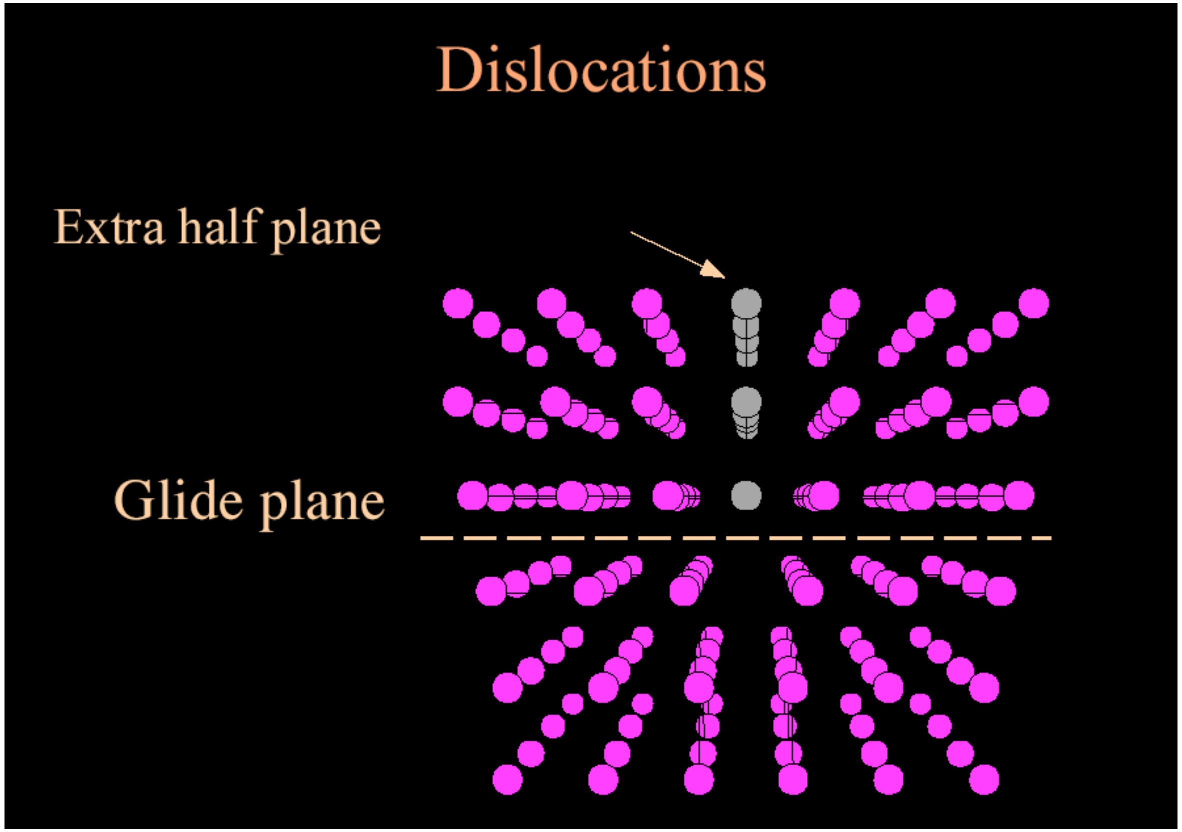


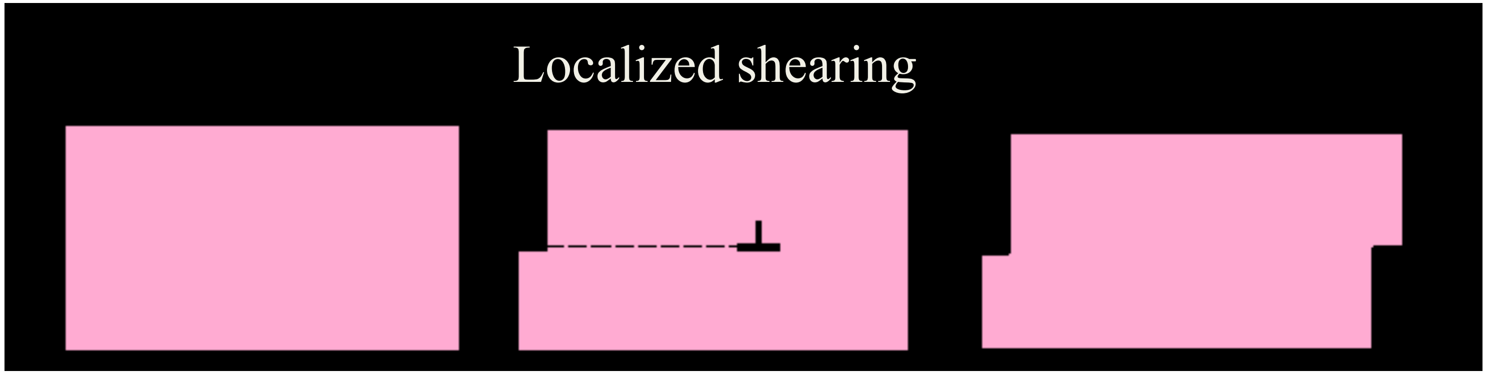
high energy cost : rupture and reconstruction of a large number of atomic bonds

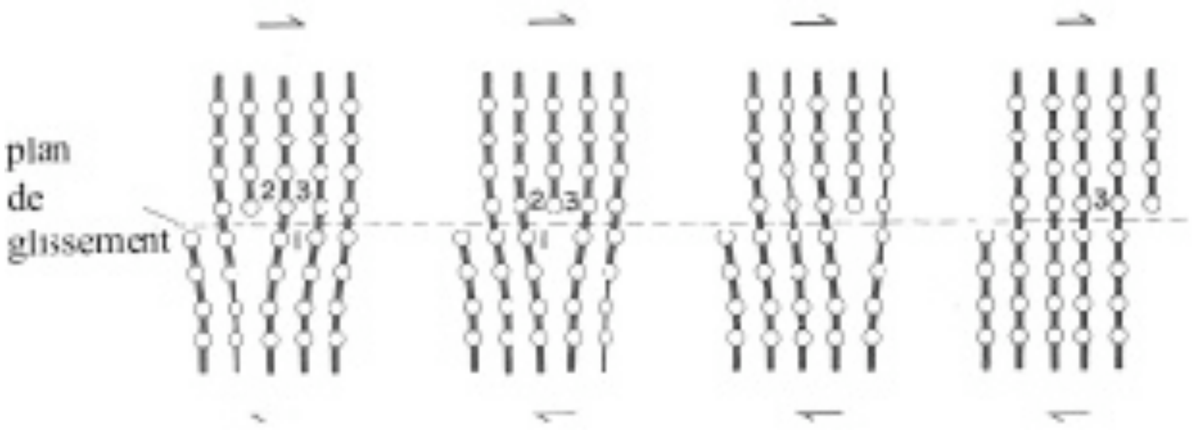
➢*crystal strength much higher than observed experimentally*

Solution?

Solution? Defaults in the crystalline structure

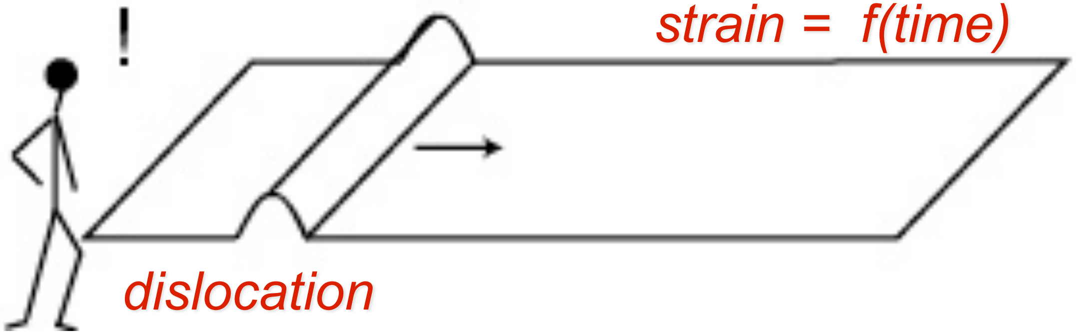






Instantaneous strain

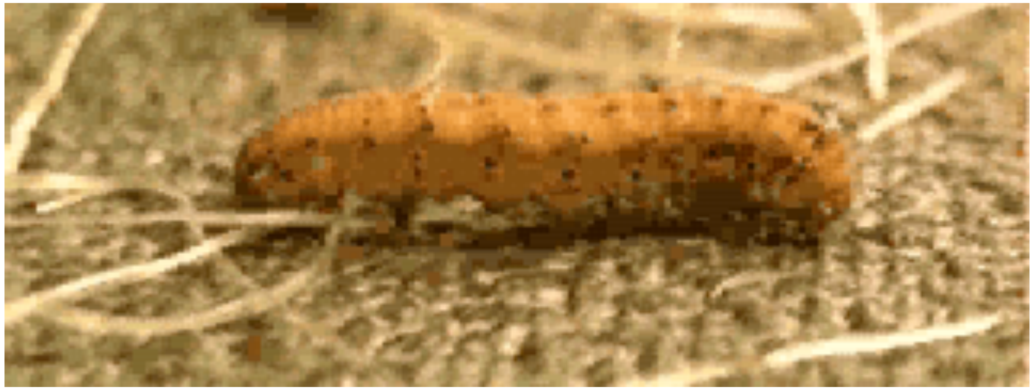
strain = f(time)



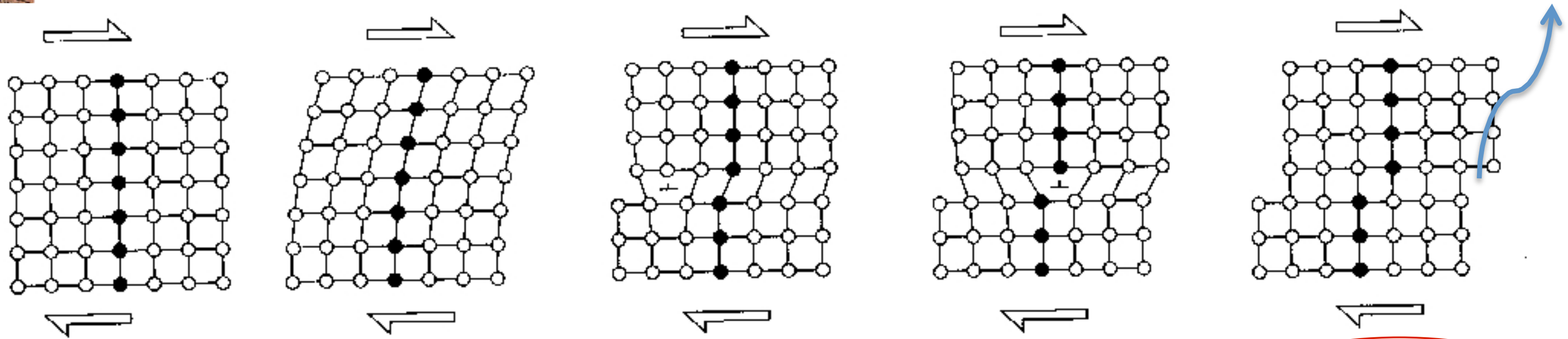
dislocation

Same final result, but lower energy consumption!

the principle…



Displacement by a crystal lattice unit = Burgers vector $\vec{b}$



elastic deformation

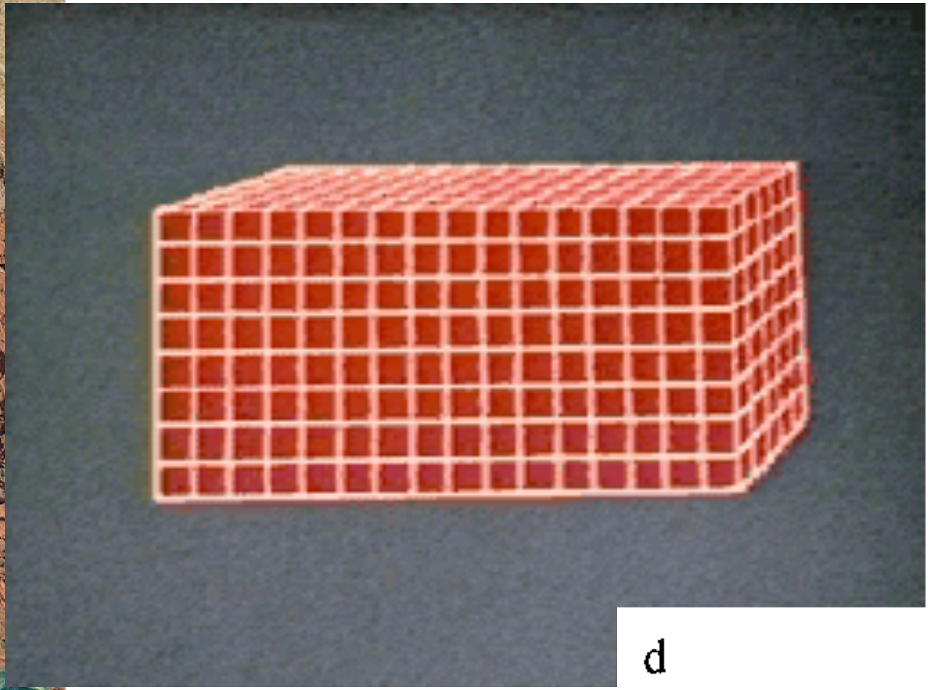
introduction of dislocation

migration of dislocation

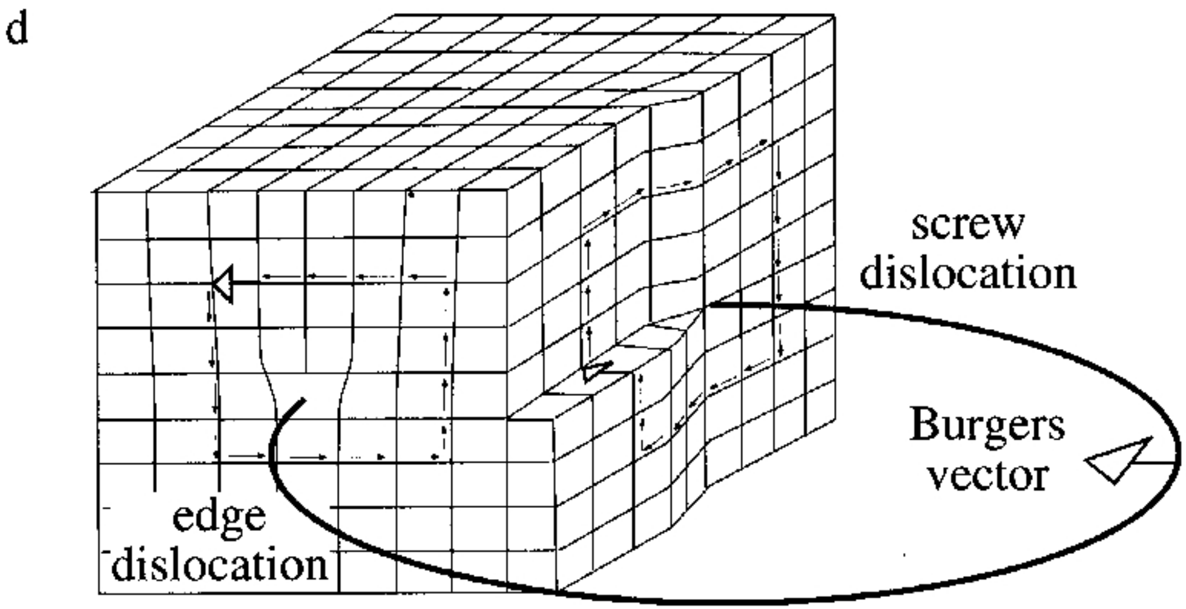
crystal shape has changed without mechanical fracturing or loss of crystal structure

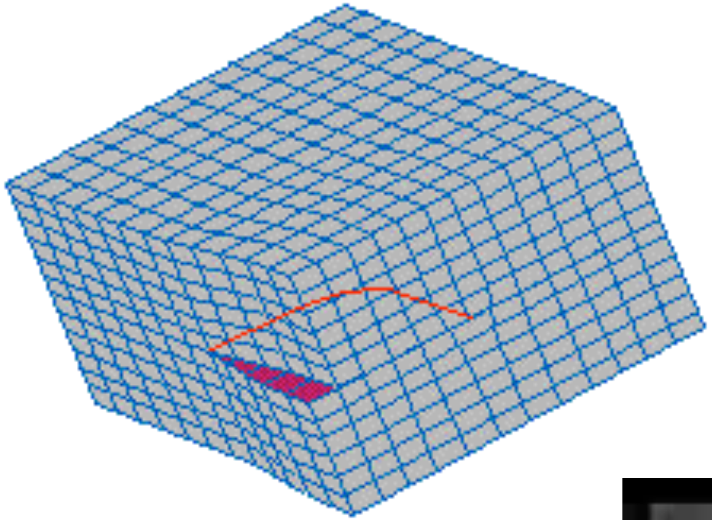
Deformation = motion of dislocations = dislocation glide

Dislocations in 3D = dislocation loops



- *The dislocation line separates the sheared volume of the crystal from the non-sheared one*
- *The Burgers vector is the dislocation motion (shear) direction*

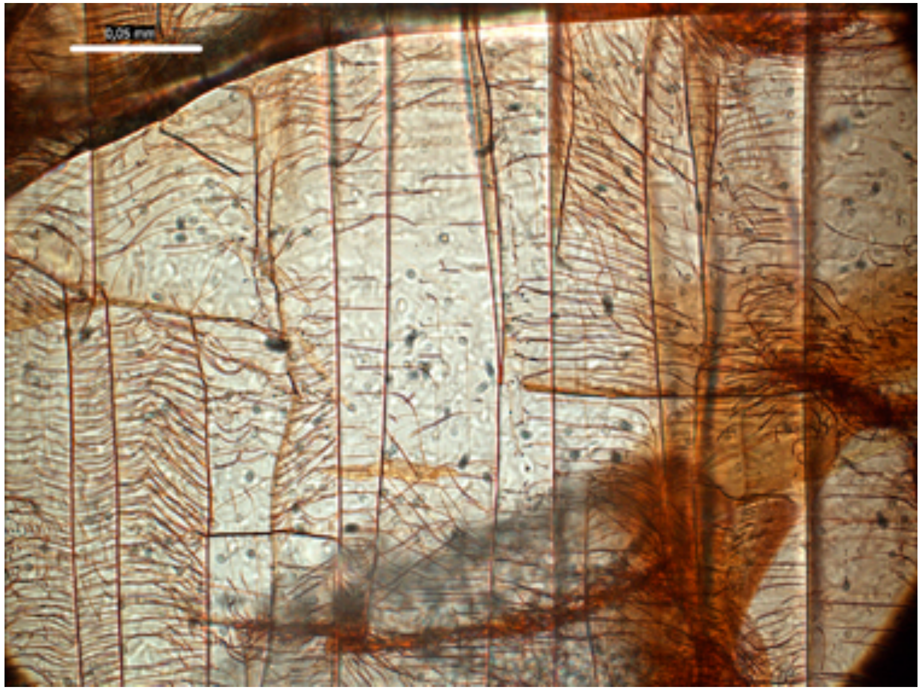




YouTube - Dislocations in motion

How do we observe dislocations?

- ***decoration (olivine: oxyde depots)***

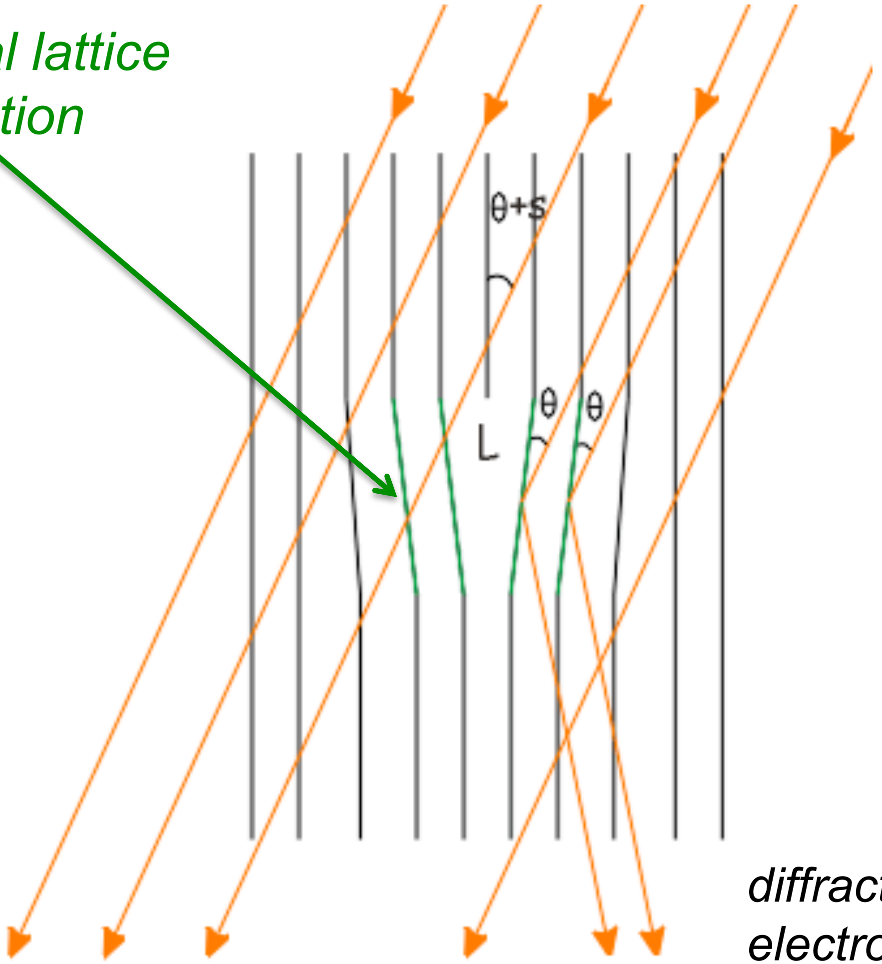


Kamchatka xenolith, Soustelle et al. J. Petrol. 2010

- ***transmission electron microscopy (TEM)***

Dislocations imaging by TEM

Deformation of the crystal lattice in the vicinity of a dislocation



transmitted electrons

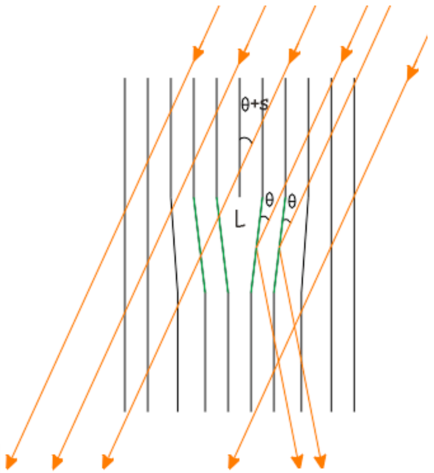
diffracted electrons

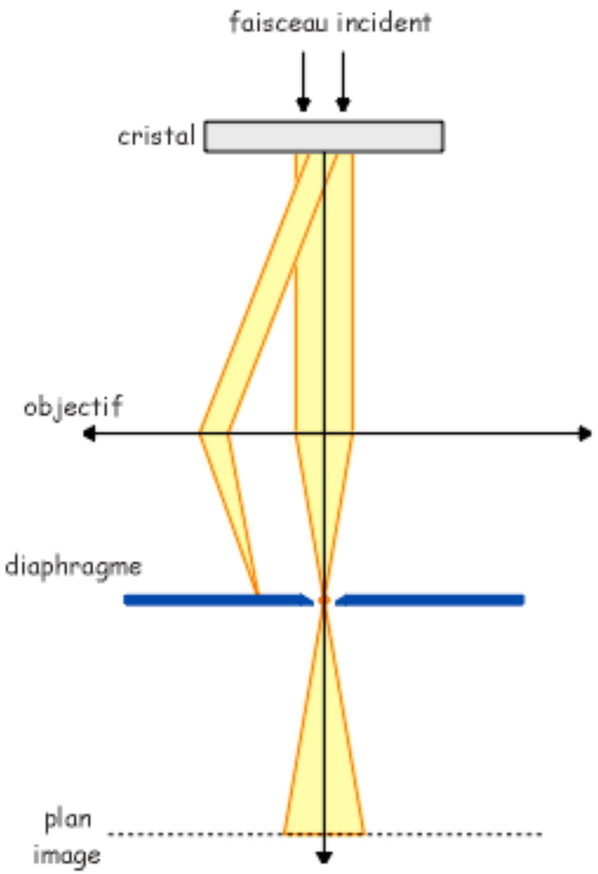
(L: dislocation line
s: deviation relatively to Bragg angle)

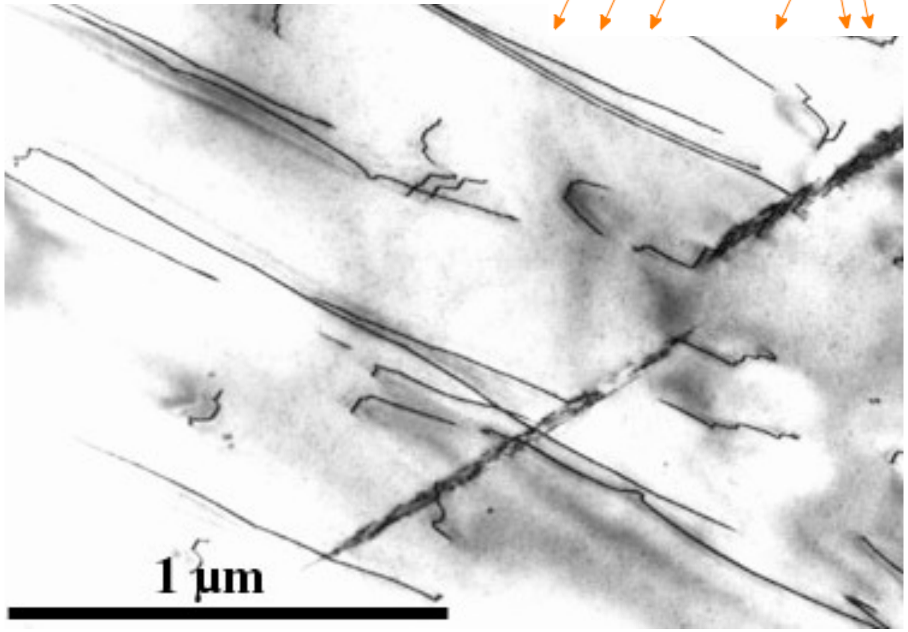
Dislocations : TEM

Using an aperture, one may select

- *the transmitted electrons*

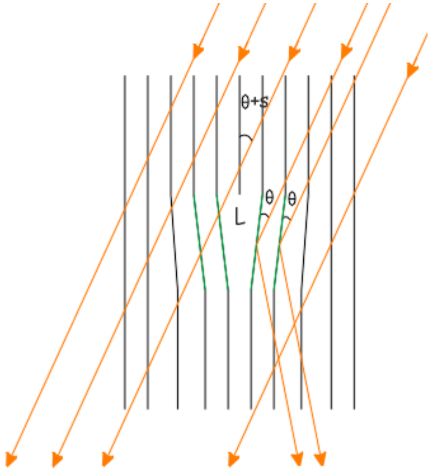






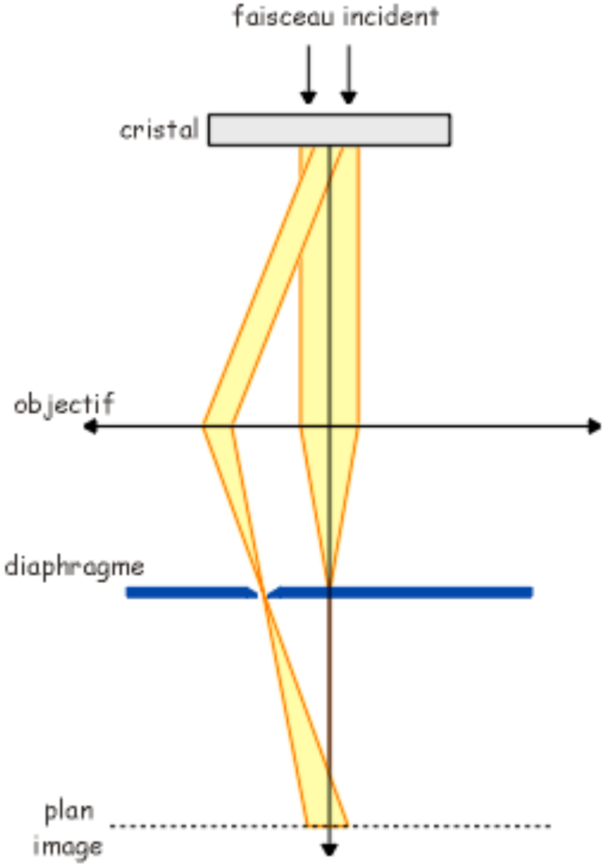
Dislocations in glide configuration in a Zr alloy
Foto H. Leroux, LSPES- USTLille

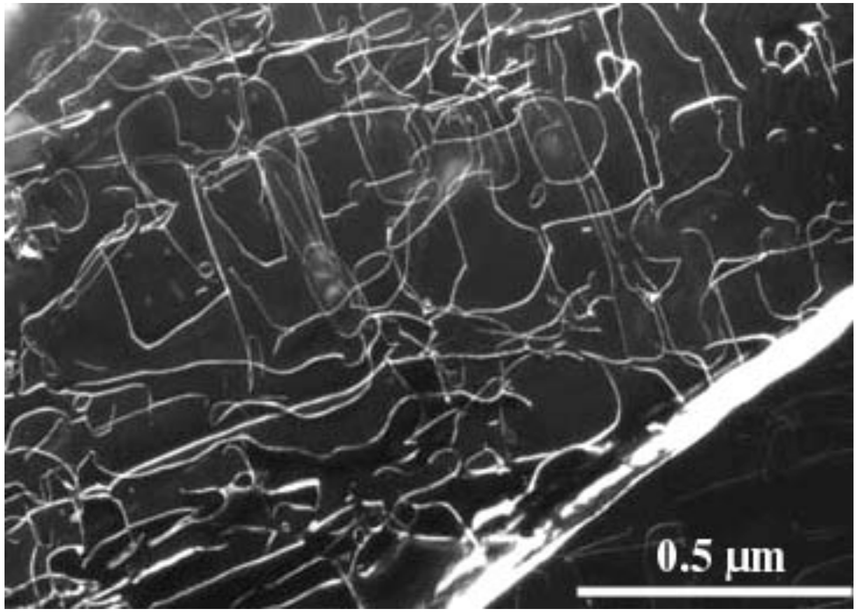
Dislocations : TEM



Using an aperture, one may select

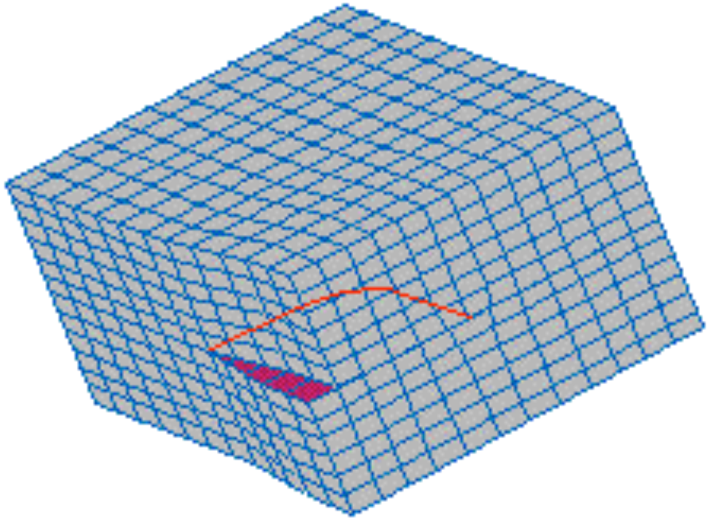
- *the diffracted electrons*





Dislocations in olivine © H. Couvy, USTLille

Deformation = Dislocation glide



Burgers vector

strain rate

$$\dot{\varepsilon} \propto \rho_m b v$$

glide velocity
(also depends on σ)

density of free dislocations

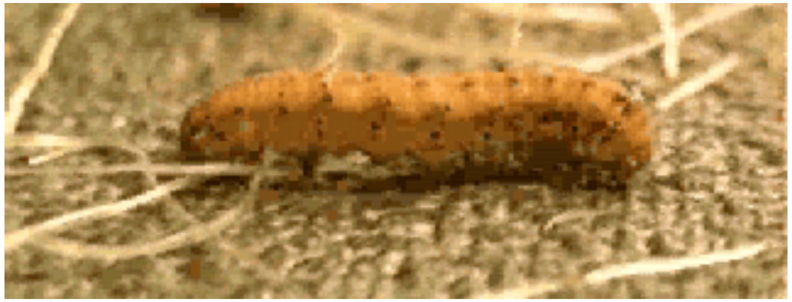
$$\rho_m \propto \left(\frac{\sigma}{\mu b}\right)^2$$

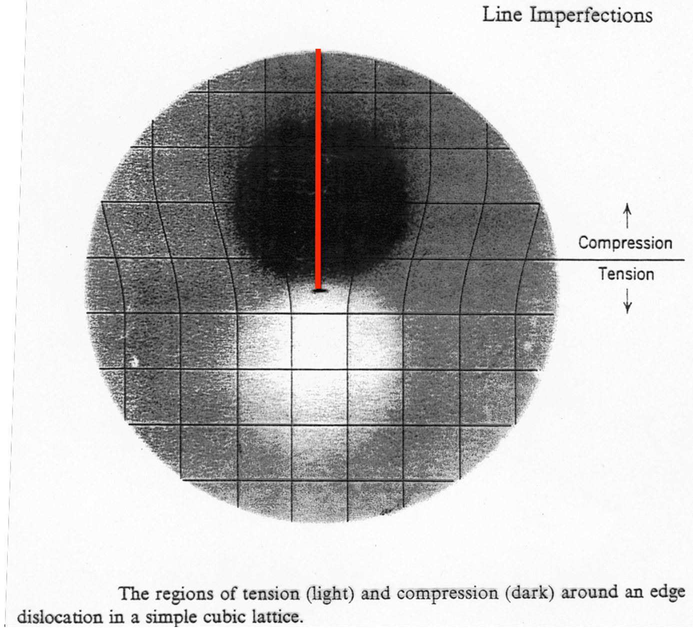
shear modulus

$$\boxed{\dot{\varepsilon} \propto \sigma^2}$$

Dislocations & energy

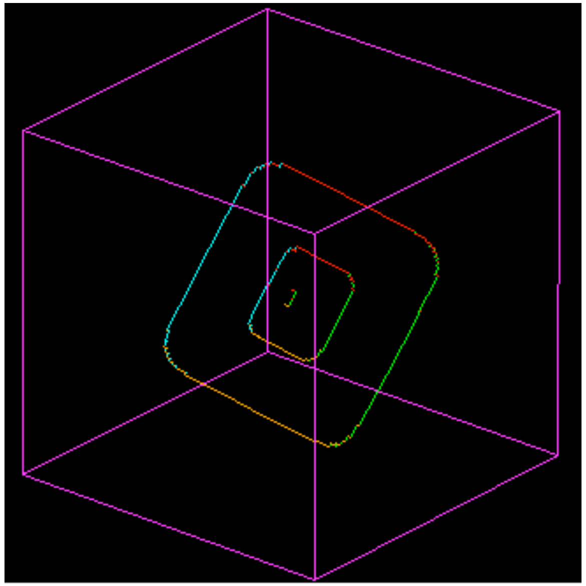
- *Potential energy = elastic deformation of the lattice around a dislocation*



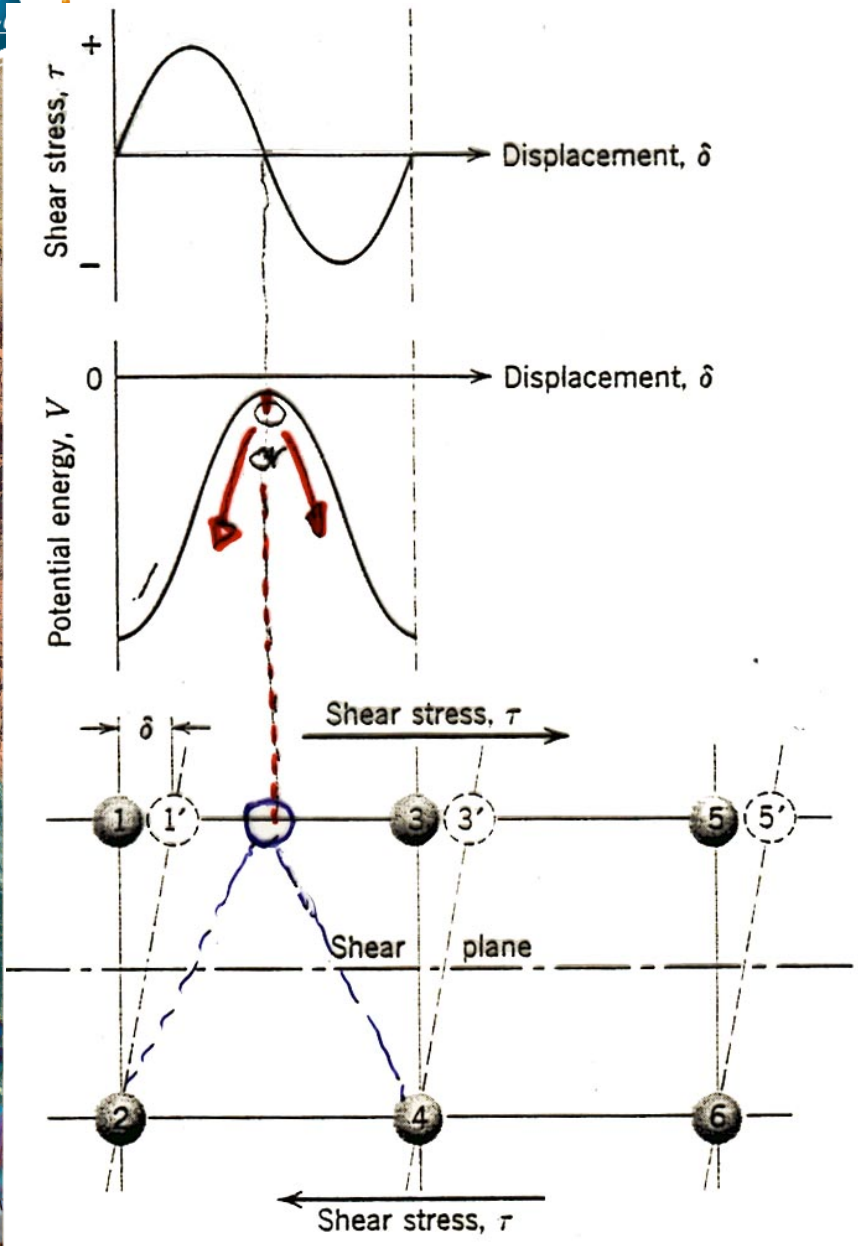


The regions of tension (light) and compression (dark) around an edge dislocation in a simple cubic lattice.

- *Activation energy (formation & **glide**)*



http://zig.onera.fr/~devincre/DisGallery/index.html



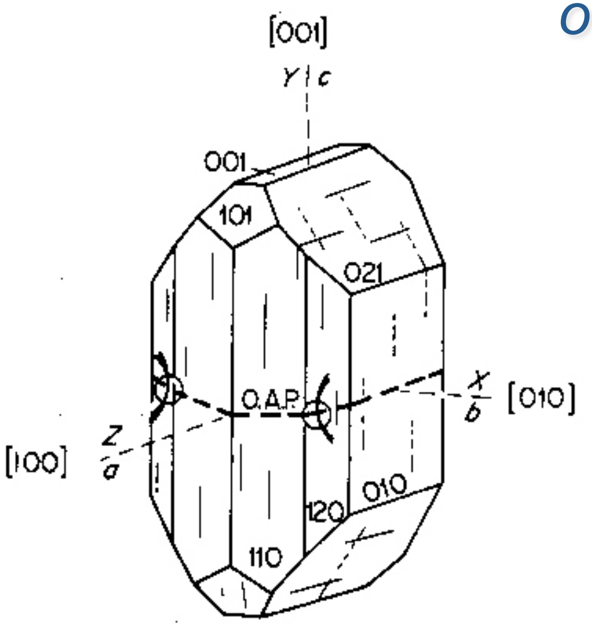
Variation of shear stress, τ, and potential energy, V, with displacement, δ.

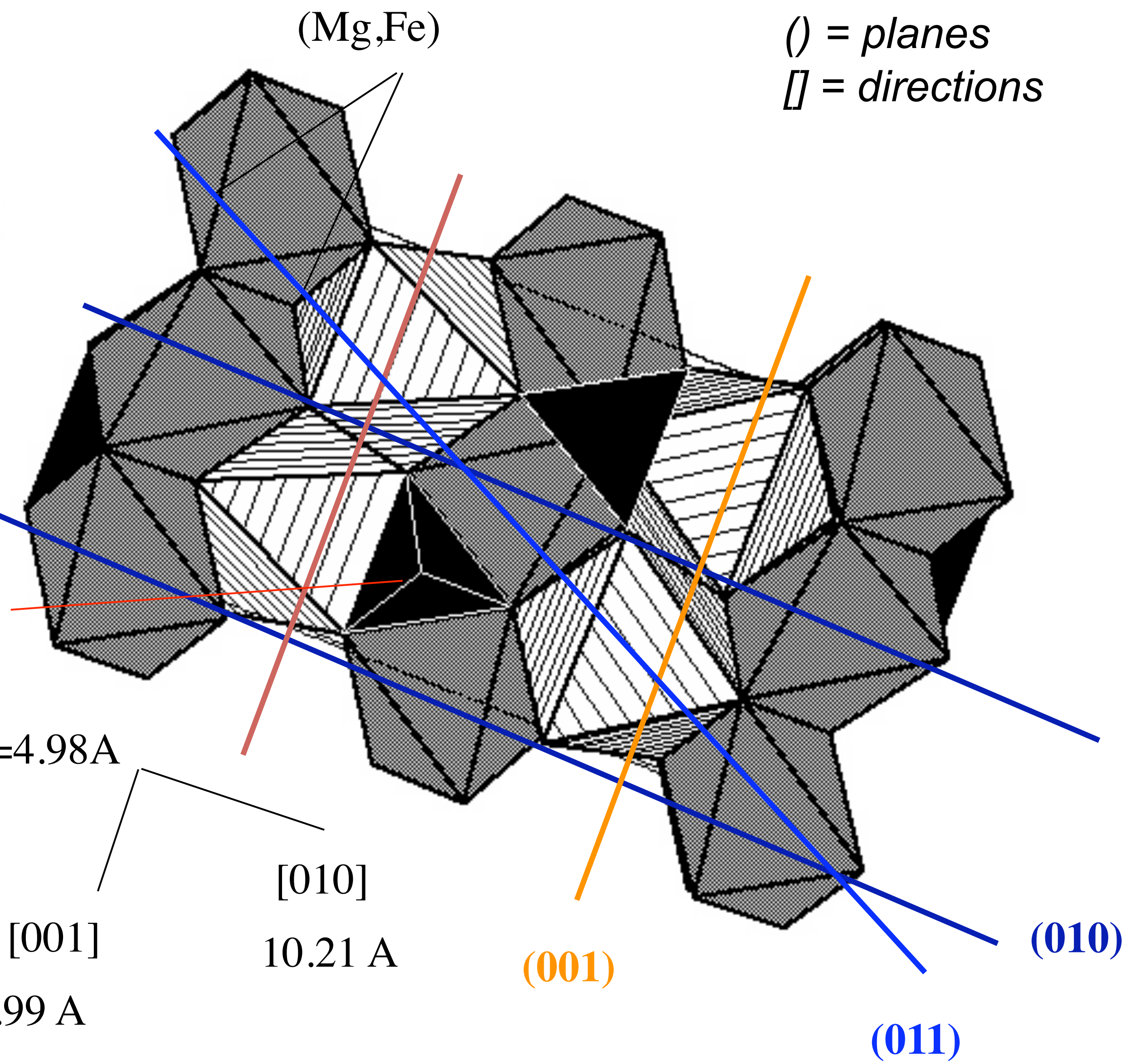
• *Activation energy : **glide***

Dislocation glide: reorganisation of atomic bonds

- ➢ *f(σ, T)*
- ➢ *f (crystal structure): some planes & directions are favored because bonds are weaker*

olivine crystal seen along the [100] direction





() = planes
[] = directions

$Si0_2$ tetraedra

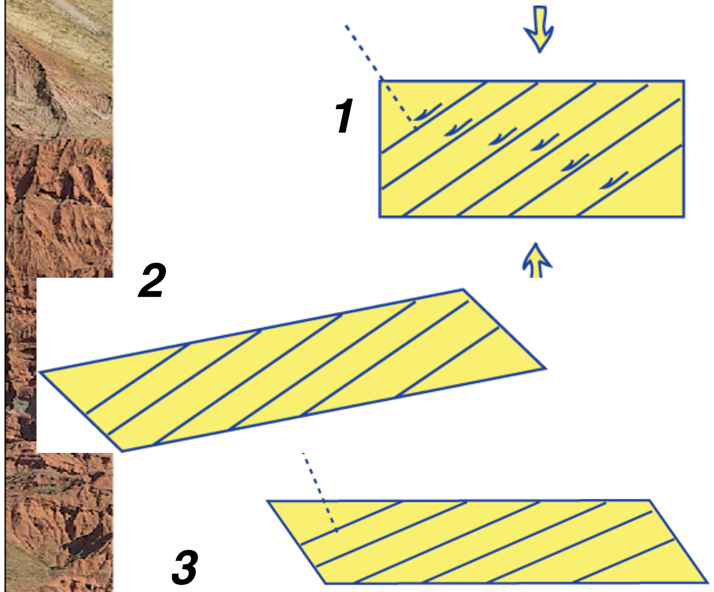
Covalent bonds
= strong!

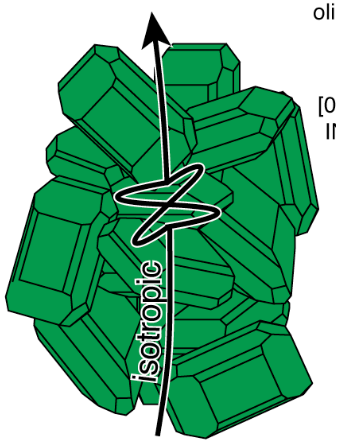
Cations: Mg, Fe

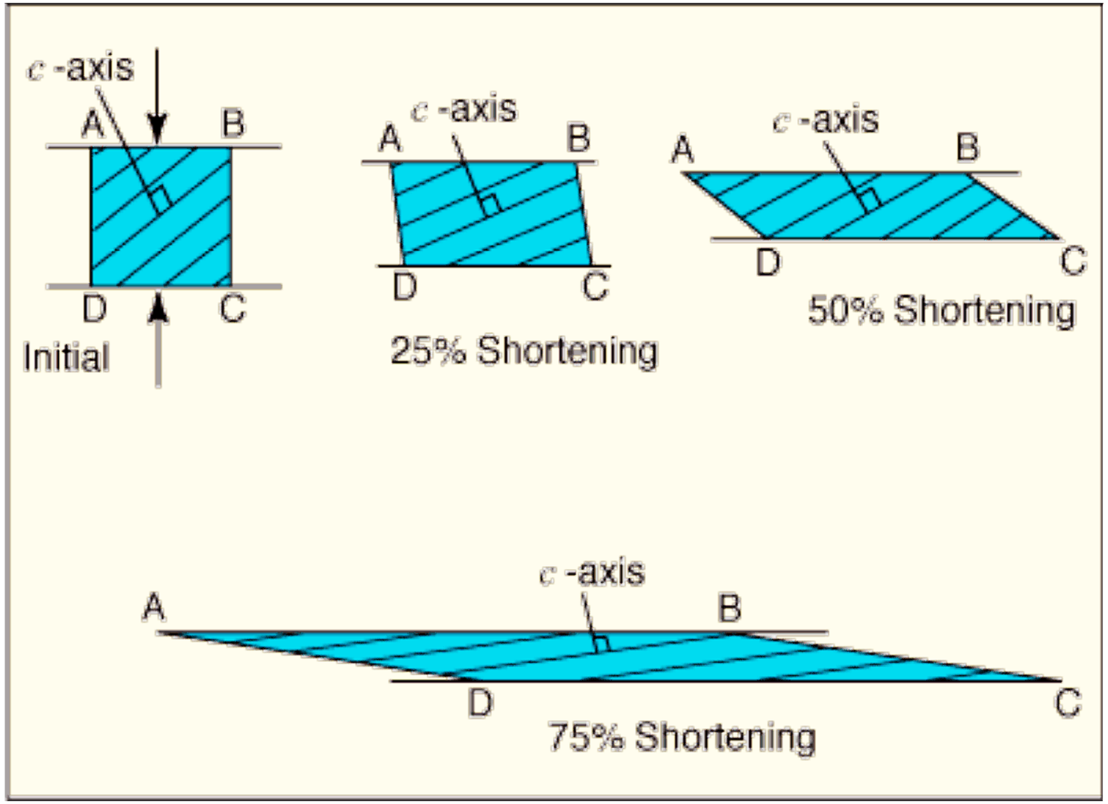
Ionic bonds
= weak

motion of dislocationson well-defined crystal planes & directions = crystal deformation has a limited degree of freedom

- strain compatibility = rotation of the crystal
- development of a crystal preferred orientation



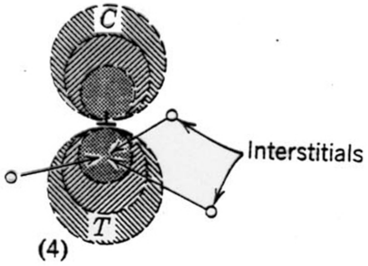




Dislocations interactions

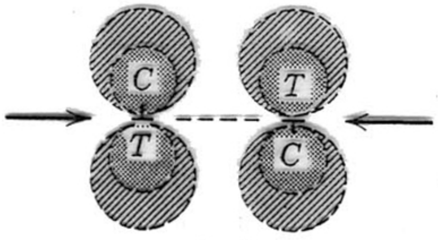

http://zig.onera.fr/~devincre/DisGallery/index.html

repulsion: tangling E ↗

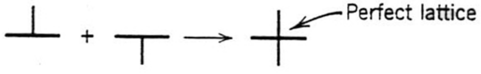


(4)

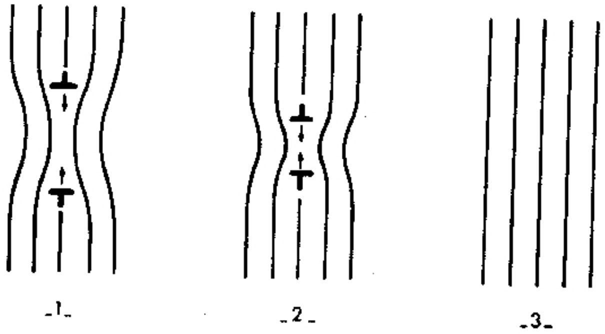
atraction: anhilation E ↘



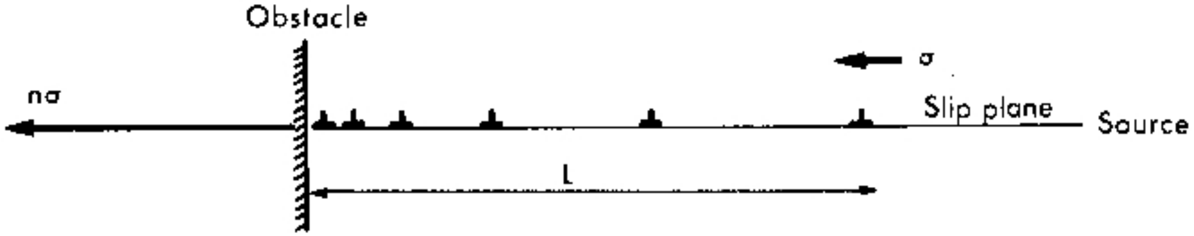
3(a)



3(b)



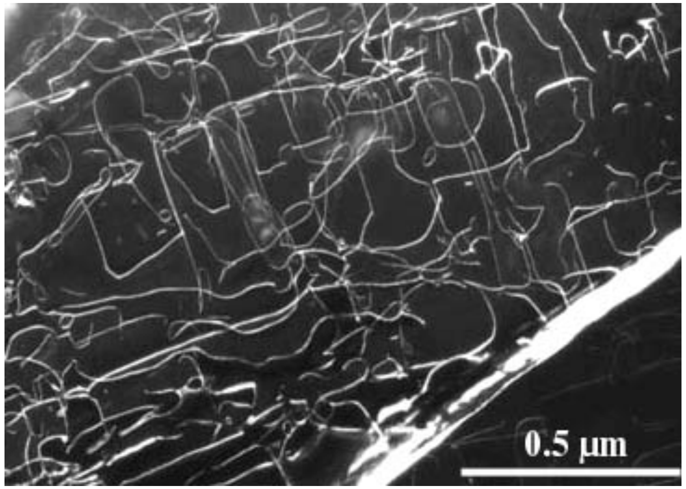
obstacle = grain boundary, another dislocation, impurity…

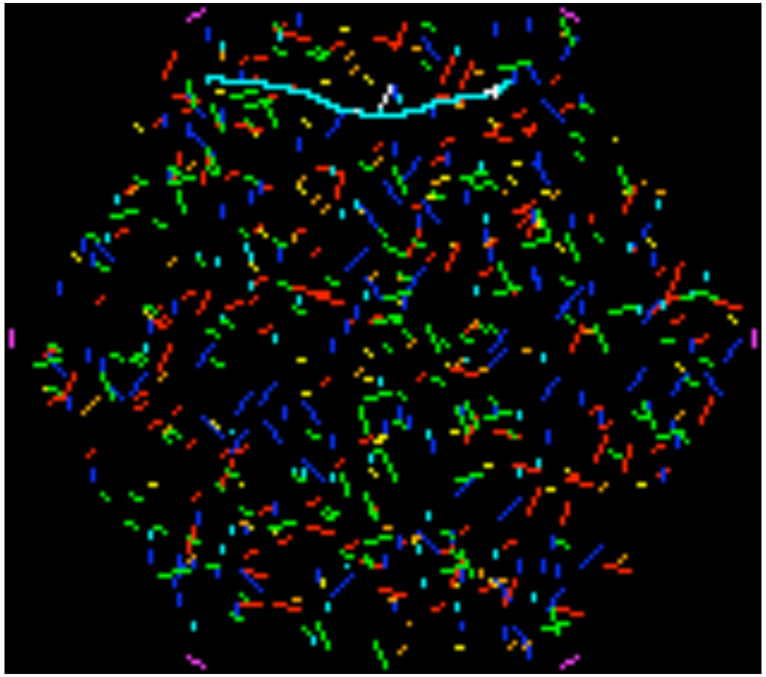


accumulation of dislocations = tangling = forests

increase of the crystal internal energy

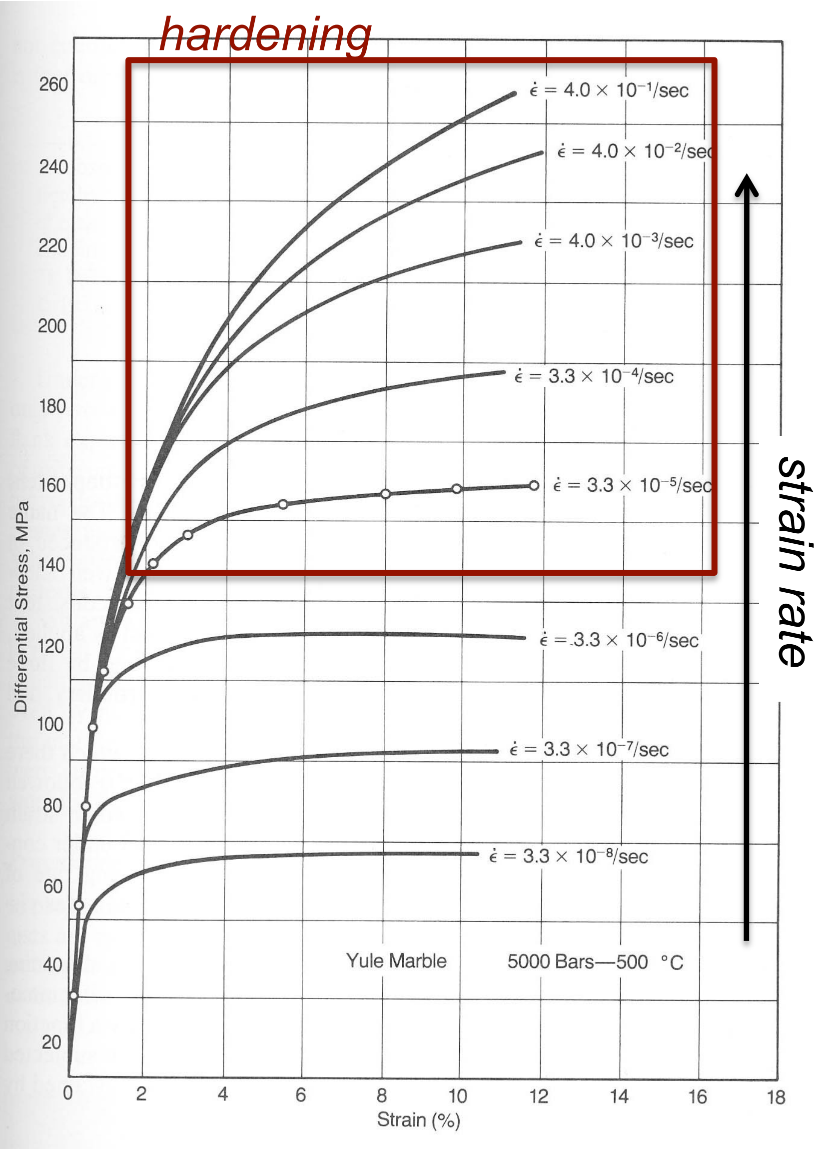
➢ hardening





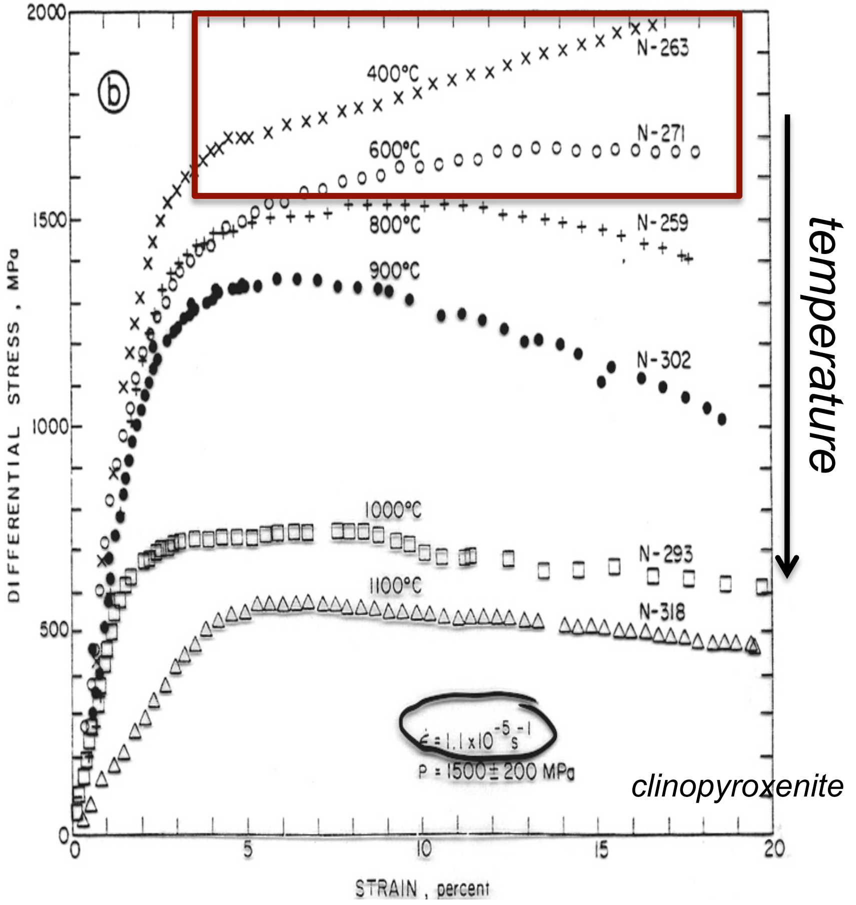
http://zig.onera.fr/~devincre/DisGallery/index.html

Experimental data: change in mechanical behavior as a function of strain rate & temperature



hardening

strain rate

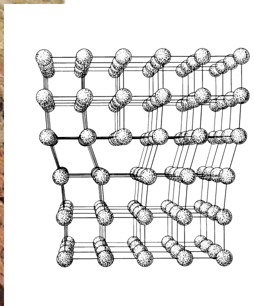


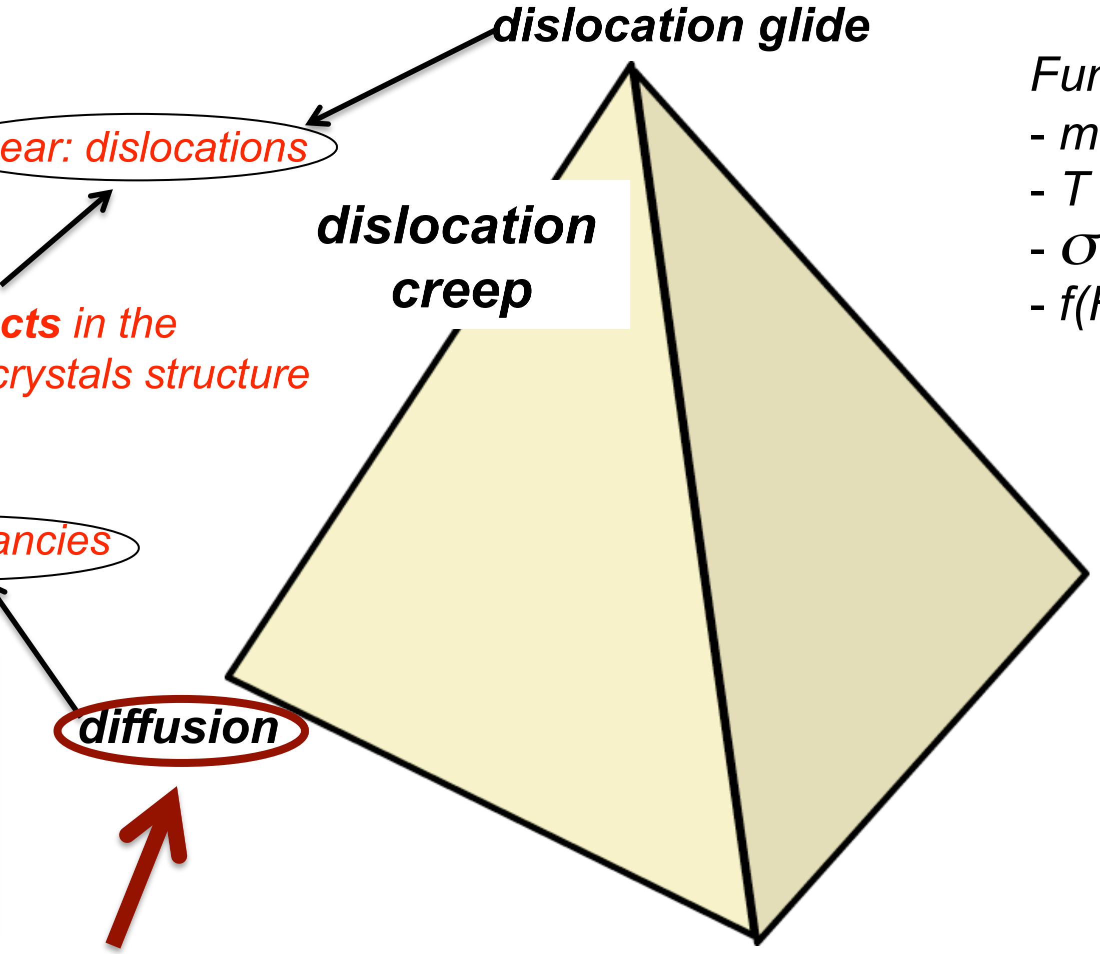
temperature

clinopyroxenite

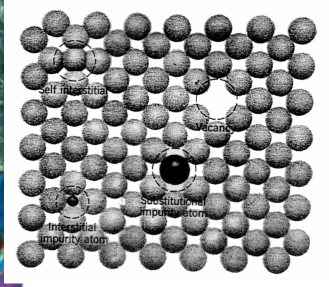
Hardening avoided by a process that is "slow" and T dependent!

Ductile deformation = solid-state flow





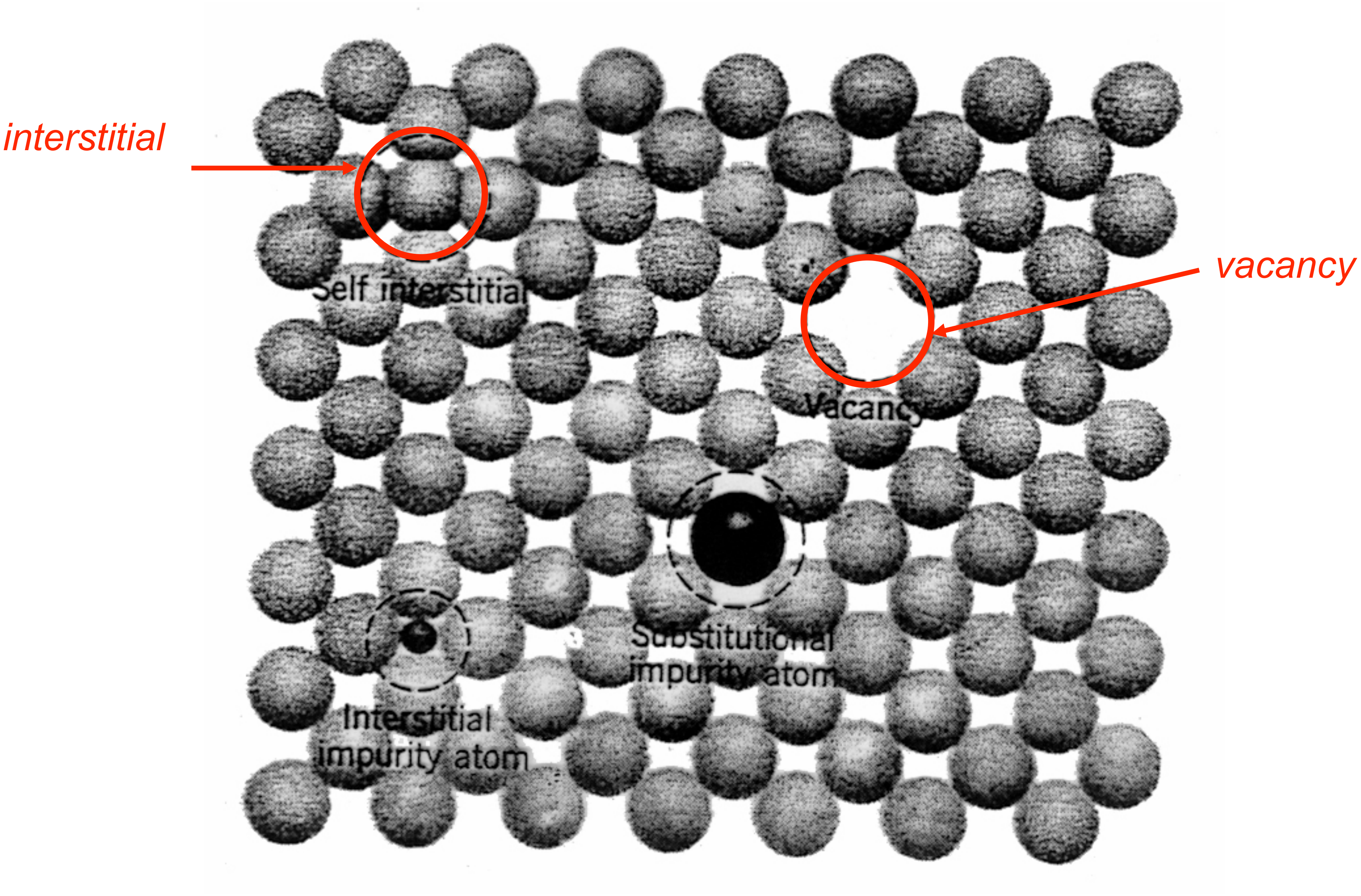
Motion of **defects** in the crystals structure



Function of:
- *mineral structure*
- *T*
- $\sigma, \dot{\varepsilon}$
- $f(H_2O, O_2)$…

grain boundary sliding ?
needs an additional mechanism!

Point defects in a crystal



difusion = mass transport
motion of atoms & vacancies

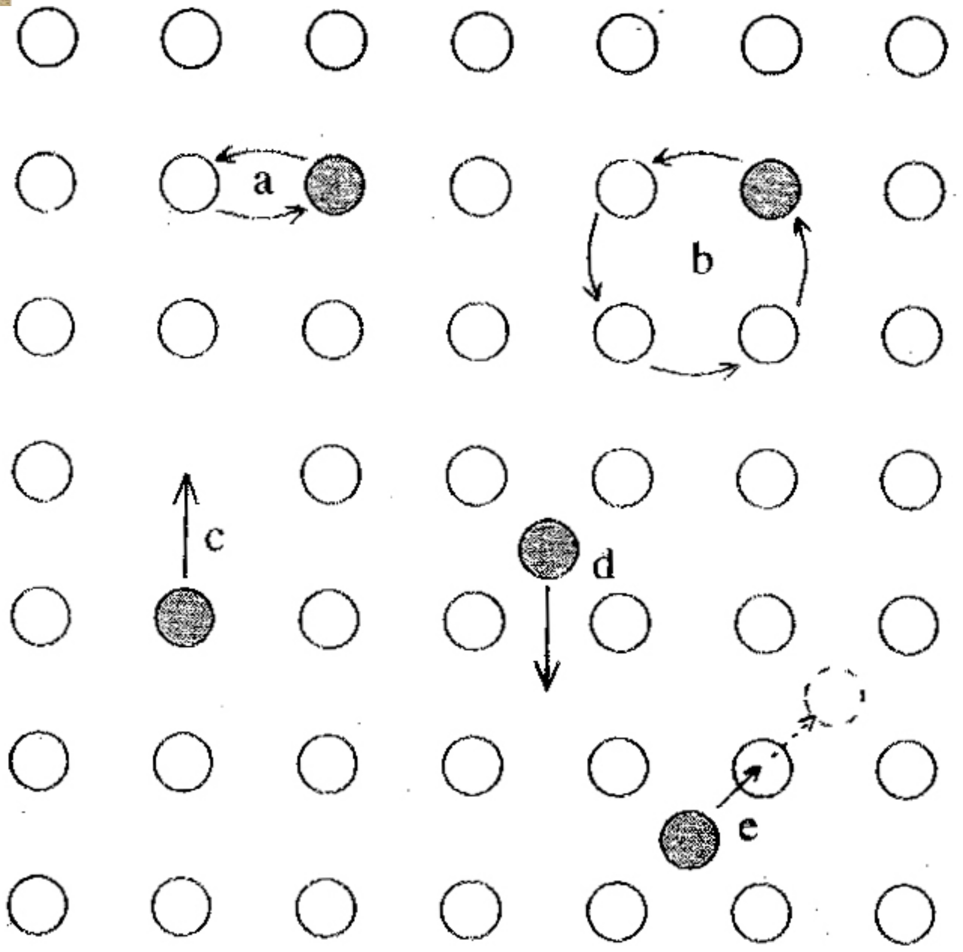
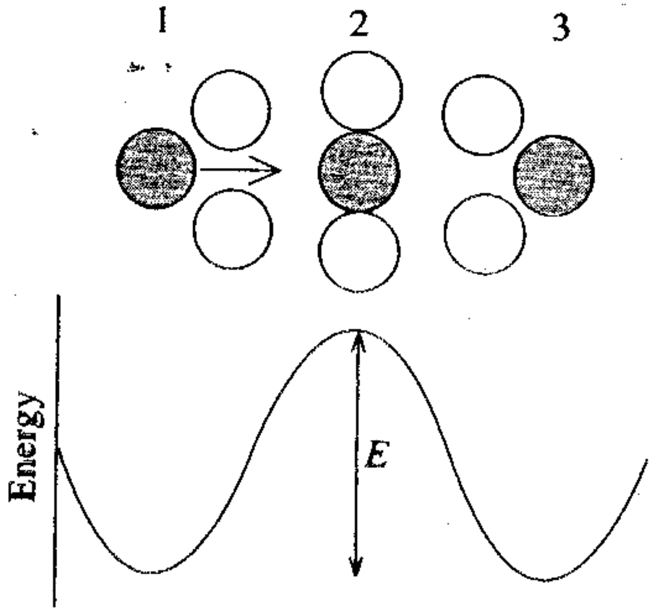


Figure 7.5. Various atomic mechanisms of diffusion. (a) and (b) are exchange mechanisms without involving vacancies, (c) is a vacancy migration mechanism, (d) and (e) are interstitial migration mechanisms.



energy = T, σ

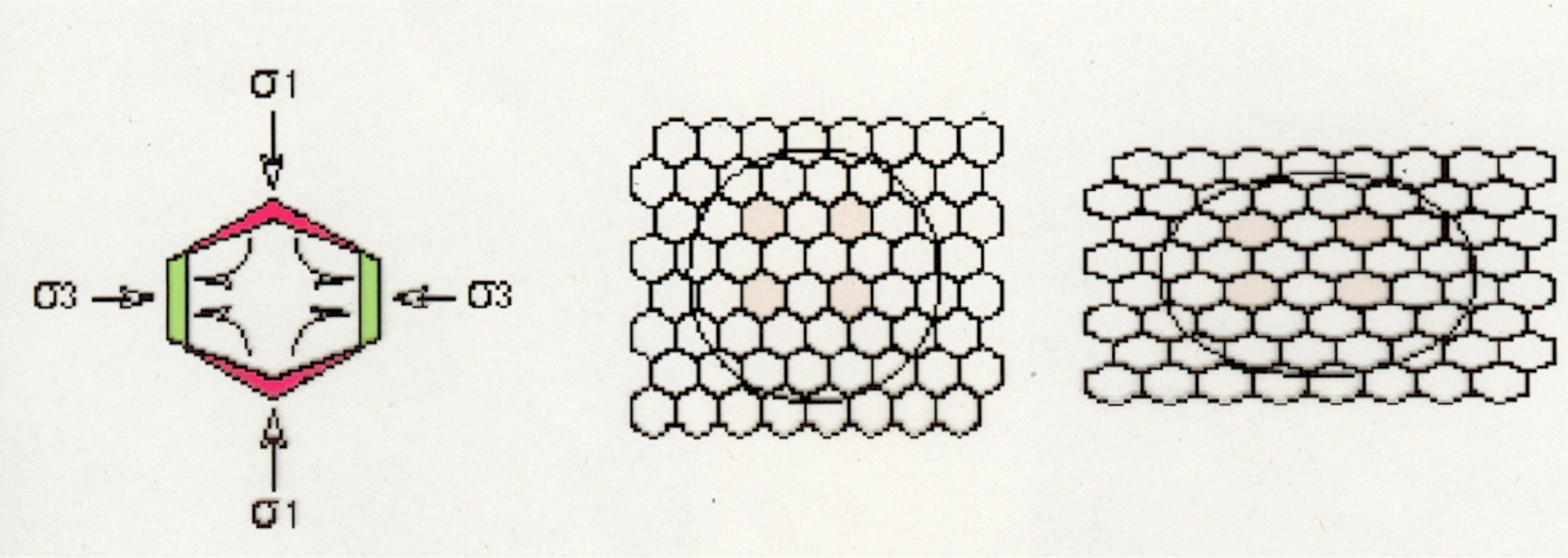
difusion = mass transport
motion of atoms & vacancies

Fick law (1-D) – flux is a function
of the diffusivity D &
of the concentration gradient

$$J = -D.\frac{\partial c}{\partial x}$$

F(mineral, T, …)

from high stress (compressive) to low stress (extensive) regions

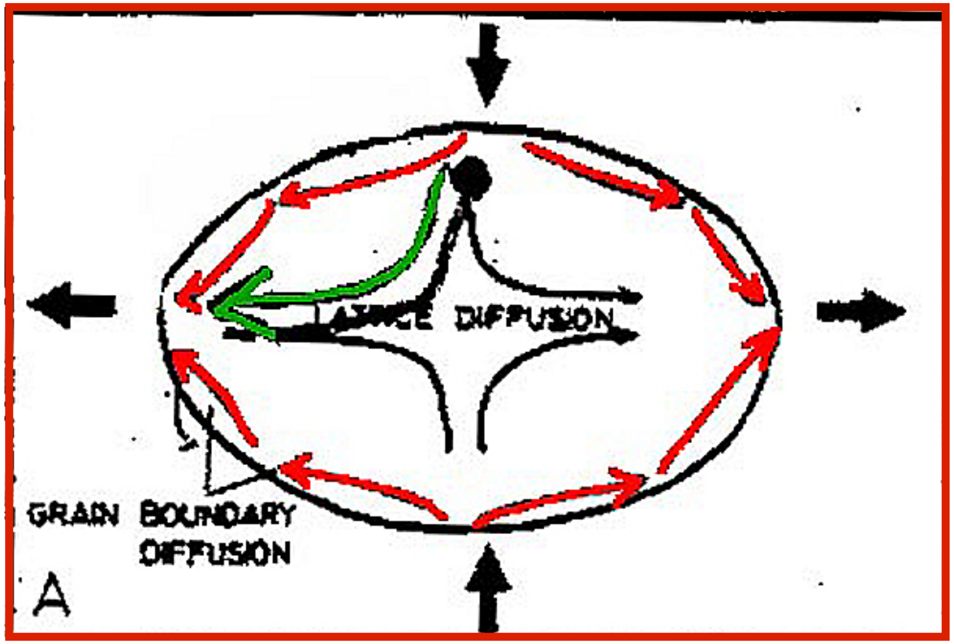


Changes the shape, but not the orientation of the crystals

Diffusion mechanisms

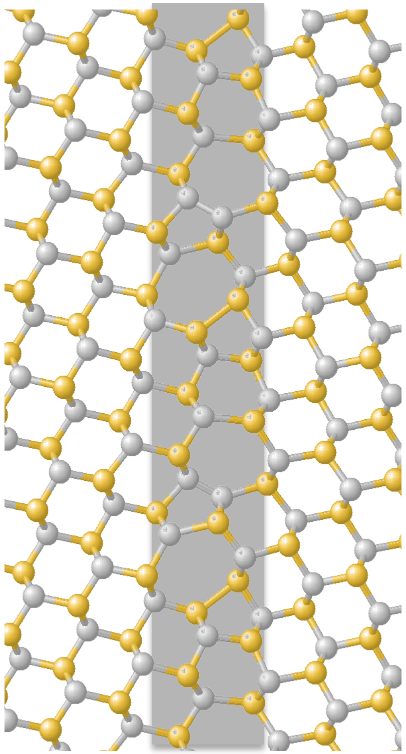
-Nabarro-Herring creep : intracrystalline diffusion

-Coble creep: diffusion along grain boundaries



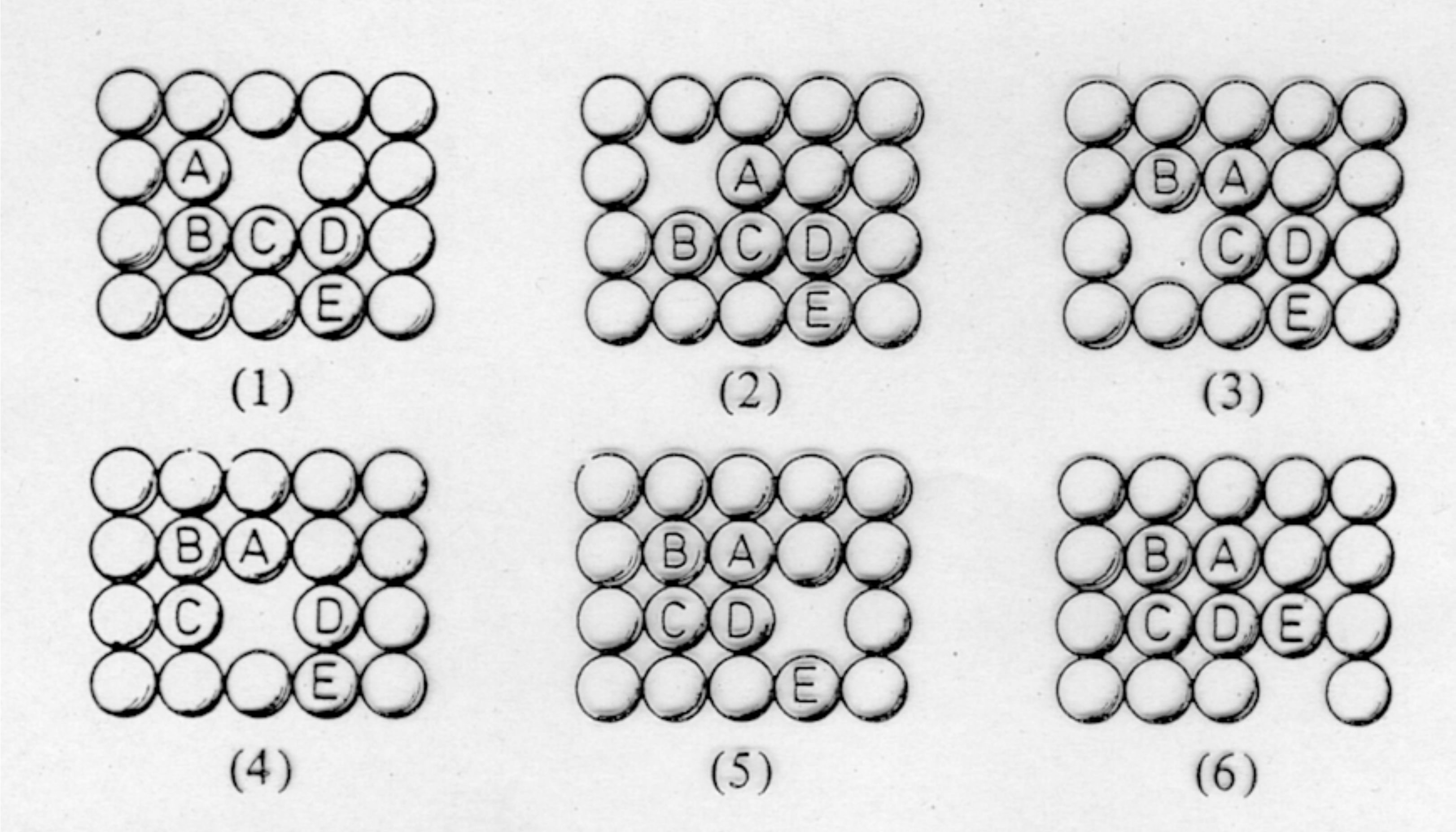
Vacancies & atoms move in opposite directions (arrows indicate atoms flow, but it is the vacancies that really move along large distances!)

grain boundary



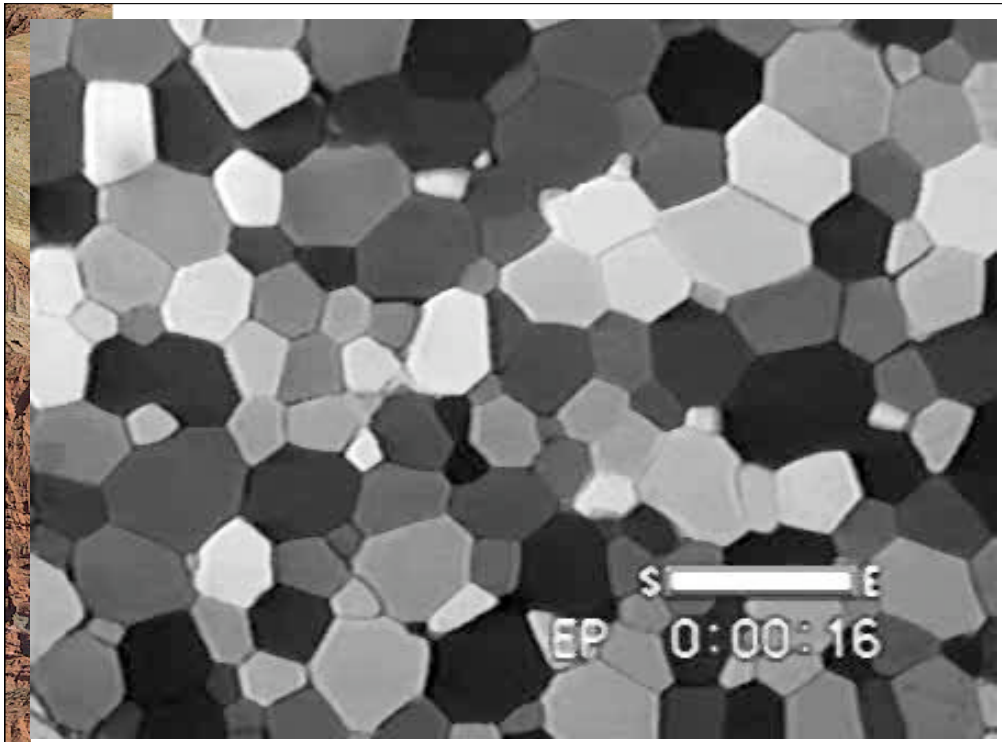
- *not an empty space!*
  - *rocks are cohesive*
- *region of discontinuity in the crystalline arrangement = more defects*

difusion = mass transport
motion of atoms & **vacancies**



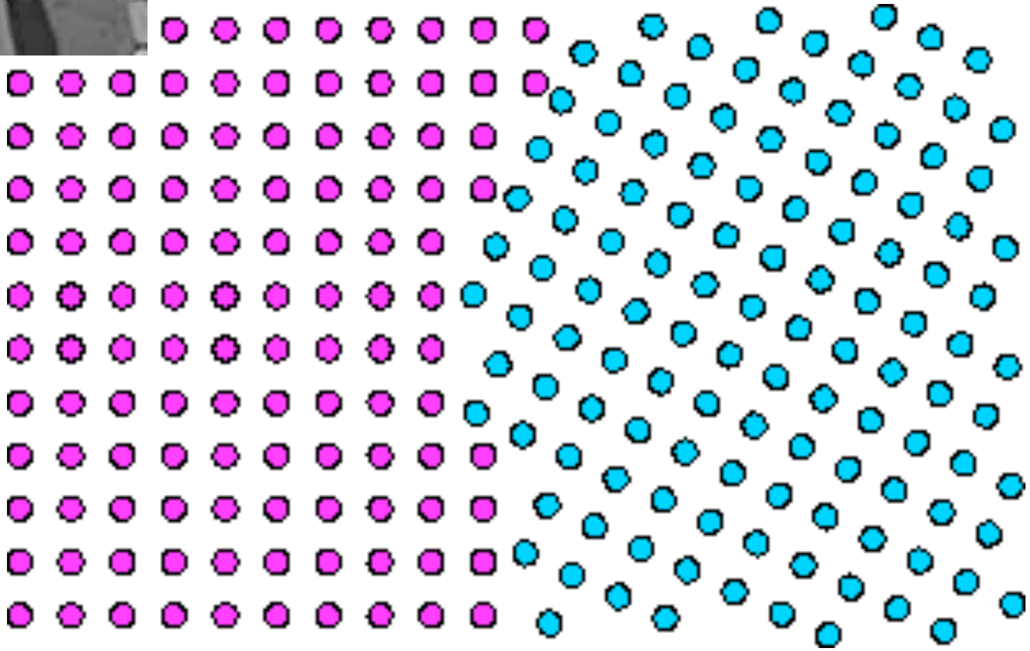
Vacancies & atoms move in opposite directions, but it is the vacancies that move along large distances

An easily observable diffusional process: Grain boundary migration



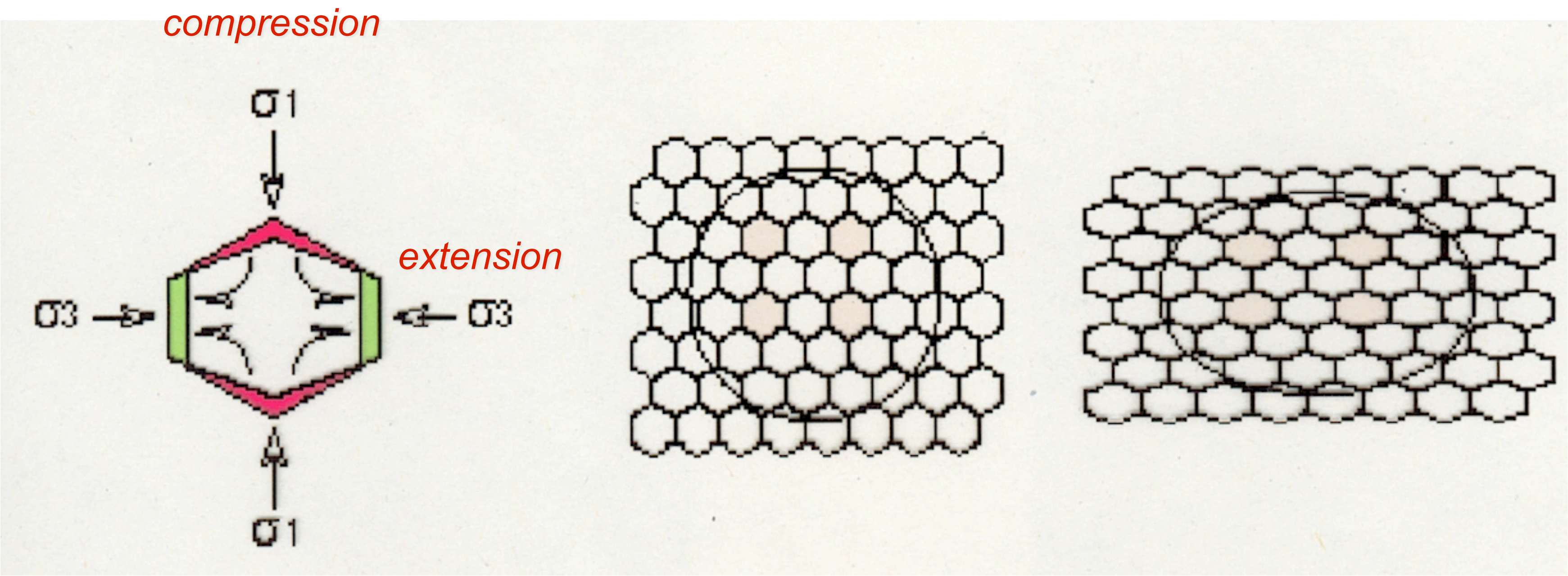
Static grain growth: octachloropropane

Park, Ree & Means, J. Virtual Explorer 2000



Jessel & Bons – Simulation using ELLE – J. Virtual Explorer 2000
virtualexplorer.com.au/.../lectures/lec2.html

Diffusion creep



Does it really exist?

- experimental evidence = linear relation between stress & strain rate
(dislocation glide = $\dot{\varepsilon} \propto \sigma^2$)

- absence of crystal preferred orientations…

+ ??

Under which conditions?

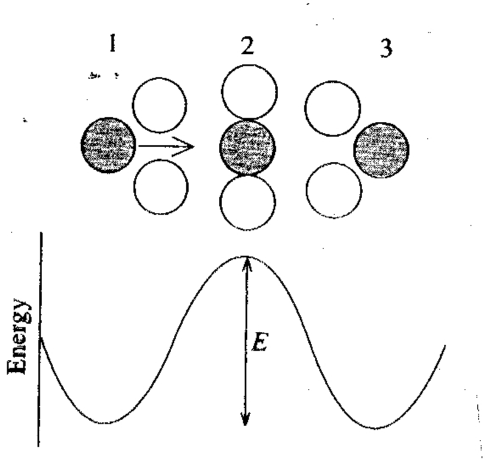
Einstein law (the drunk guy walking…)

$$d = \sqrt{\Gamma a^2 t}$$

Γ: frequency of steps
a : amplitude of the step
t : observation time
d : walked distance

In a crystal:

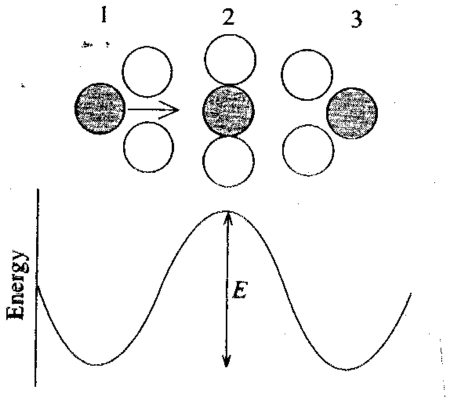
$$\Gamma = \nu.\exp\left(-\frac{\Delta G_m}{RT}\right)$$



Γ= probability of successful atomic jumps
ν= vibration frequency of the atoms (≈10^{13}Hz)

ΔG_m = *enthalpy reduction ("migration energy)*

Probability of an oscillation with a large enough amplitude : T ↗ = Γ ↗



$$\Gamma = \nu.\exp\left(-\frac{\Delta G_m}{RT}\right)$$

Γ= probability of successful atomic jumps
ν= vibration frequency of the atoms (≈10^{13}Hz)
***ΔG$_m$** = enthalpy reduction ("migration energy)*

Γ= probability of an oscillation with a large enough amplitude : T ↗ = Γ ↗

Atomic diffusion coefficient

$$D = \frac{1}{2}\Gamma.N_v.a^2 \qquad \mathbf{cm^2s^{-1}}$$

N_v = vacancy concentration (# empty sites/ total # sites)
a = interatomic distances

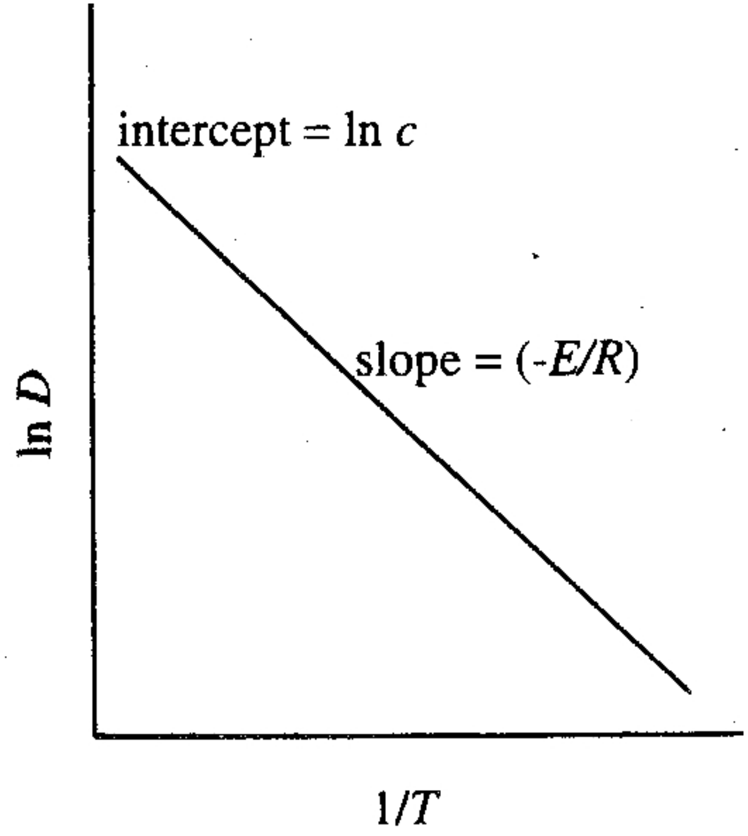
T ↗ = Γ ↗ = D ↗

Difusion = thermally–actived process

$$D \propto \frac{-E}{kT}$$

$$D \propto D_0 e^{-E/RT}$$

$$LogD \approx -\frac{E}{R} \cdot \frac{1}{T}$$



T ↗ = D ↗

Strain rate = transport velocity

$$< v >= D\frac{F_{ext}}{kT}$$

$$v \propto F$$

$$D \propto \exp\left(-{}^{1}\!/_{T}\right)$$

$$v \propto \frac{\exp\left(-{}^{1}\!/_{T}\right)}{T}$$

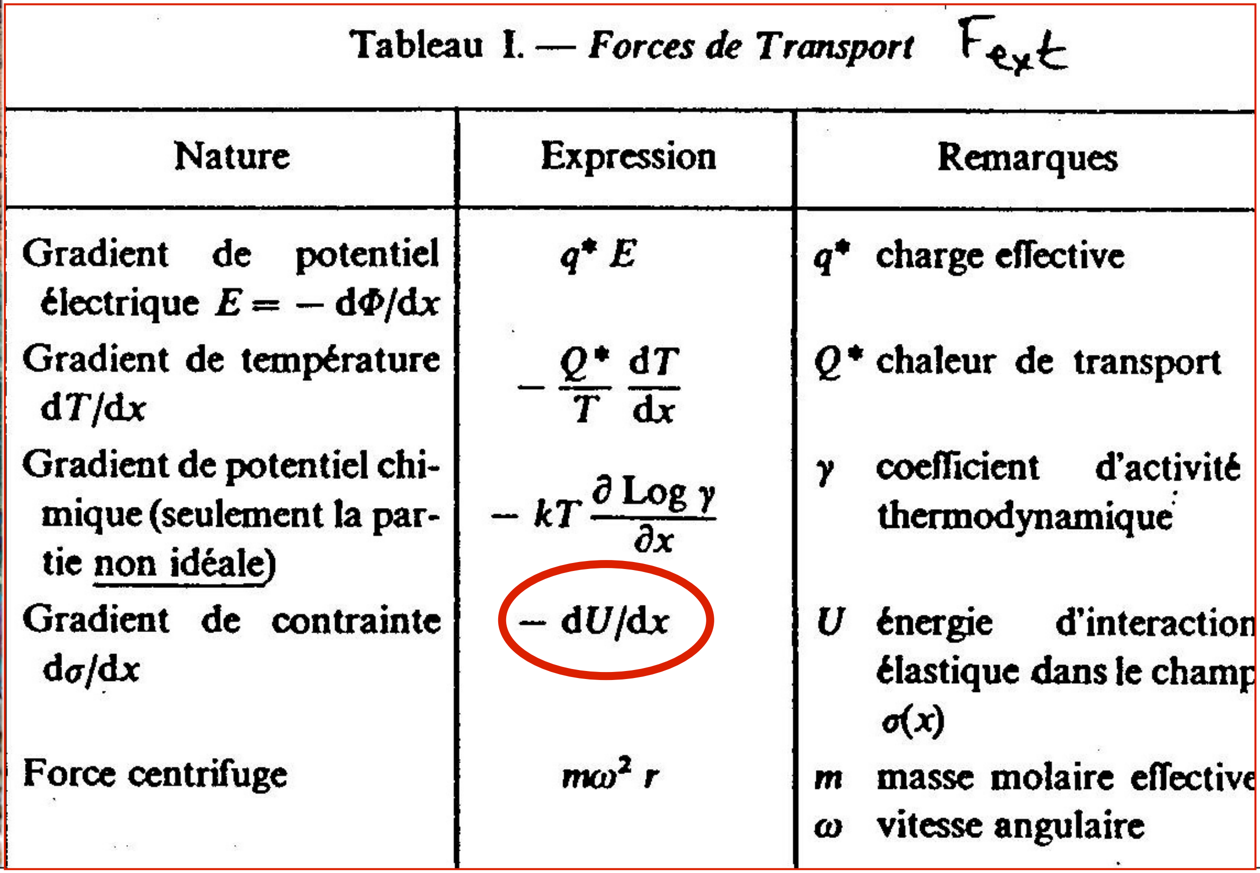
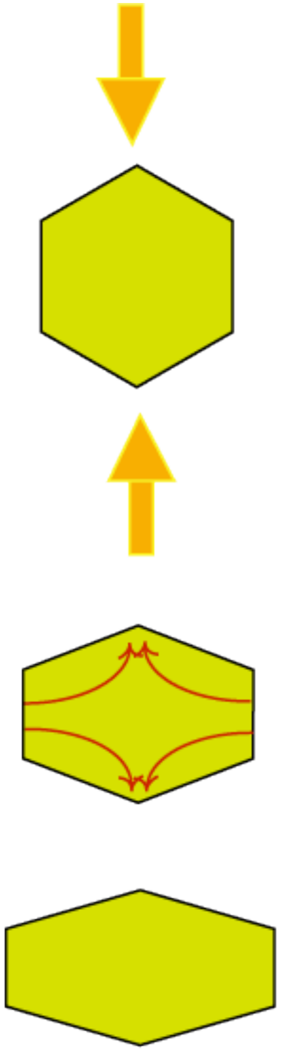


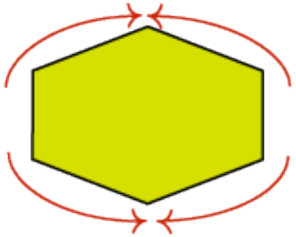
Tableau I. — *Forces de Transport* F_{ext}

Nature	Expression	Remarques
Gradient de potentiel électrique $E = -\mathrm{d}\Phi/\mathrm{d}x$	$q^* E$	q^* charge effective
Gradient de température $\mathrm{d}T/\mathrm{d}x$	$-\frac{Q^*}{T}\frac{\mathrm{d}T}{\mathrm{d}x}$	Q^* chaleur de transport
Gradient de potentiel chimique (seulement la partie <u>non idéale</u>)	$-kT\frac{\partial \operatorname{Log}\gamma}{\partial x}$	γ coefficient d'activité thermodynamique
Gradient de contrainte $\mathrm{d}\sigma/\mathrm{d}x$	$\boxed{-\mathrm{d}U/\mathrm{d}x}$	U énergie d'interaction élastique dans le champ $\sigma(x)$
Force centrifuge	$m\omega^2 r$	m masse molaire effective ω vitesse angulaire

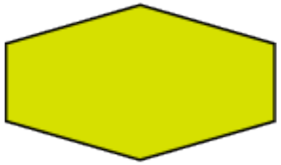
Coble vs. Nabarro-Herring creep

$$\boxed{\begin{array}{l}\dot{\varepsilon} = v/l \rightarrow l \propto d \\ \dot{\varepsilon} \propto F \rightarrow F \propto \sigma \\ \dot{\varepsilon} \propto \exp\left(-\frac{1}{T}\right)\end{array}}$$

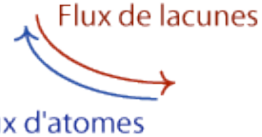




FLUAGE COBLE



$$\dot{\varepsilon} = A_B \frac{\sigma V}{RT} \cdot \frac{\delta D_B}{d^3}$$



$$\dot{\varepsilon} = A_V \frac{\sigma V}{RT} \cdot \frac{D_V}{d^2}$$

FLUAGE NABARRO-HERRING

D_v = intracrystalline diffusion coeff.
$D_b =$ grain boundary diffusion coeff
Db >> Dv
A= adimensional constant
V = molar volume
R = ideal gaz constant
d = grain size
δ = grain boundary thickness

Usually the 2 processes are associated …
General diffusion creep flow:

$$\dot{\varepsilon} = A \frac{\sigma V}{kTd^2} D_{eff}$$

$$D_{eff} = D_v \left(1 + \frac{\pi \delta D_b}{d D_v}\right)$$

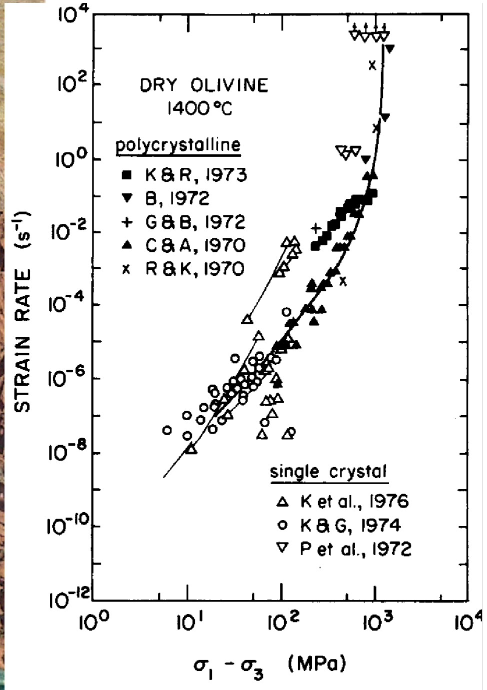
$$R = k_b N_A$$

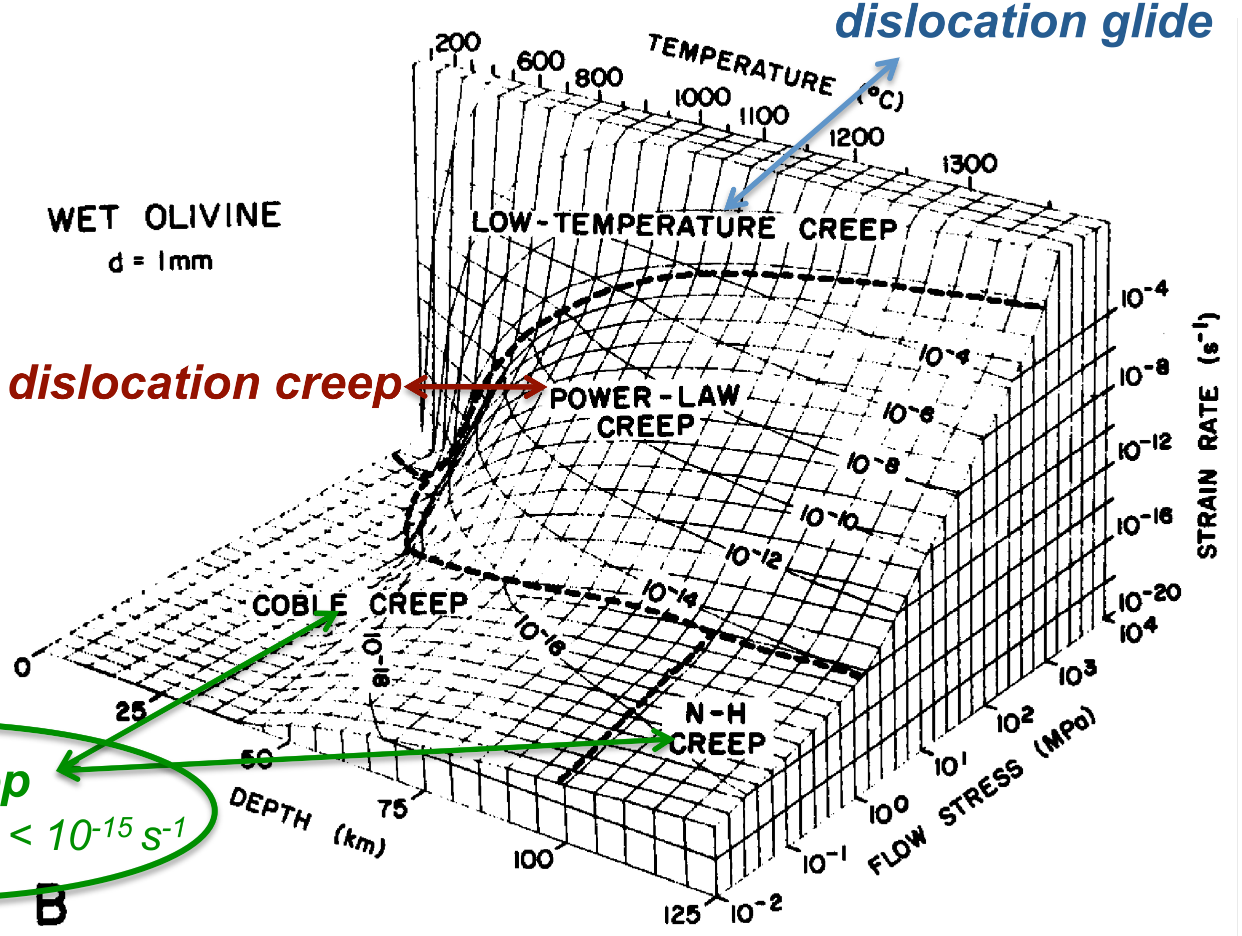
D_v = intracrystalline diffusion coeff.
D_{b} = grain boundary diffusion coeff
Db >> Dv
A= adimensional constant
V = molar volume
R = ideal gas constant
N_A = Avogadro constant
k = Boltzmann constant
d = grain size
δ = grain boundary thickness

Effective diffusion creep needs small grain sizes & high temperature

Deformation mechanisms maps

dry olivine polycrystals (dunite)





dislocation glide

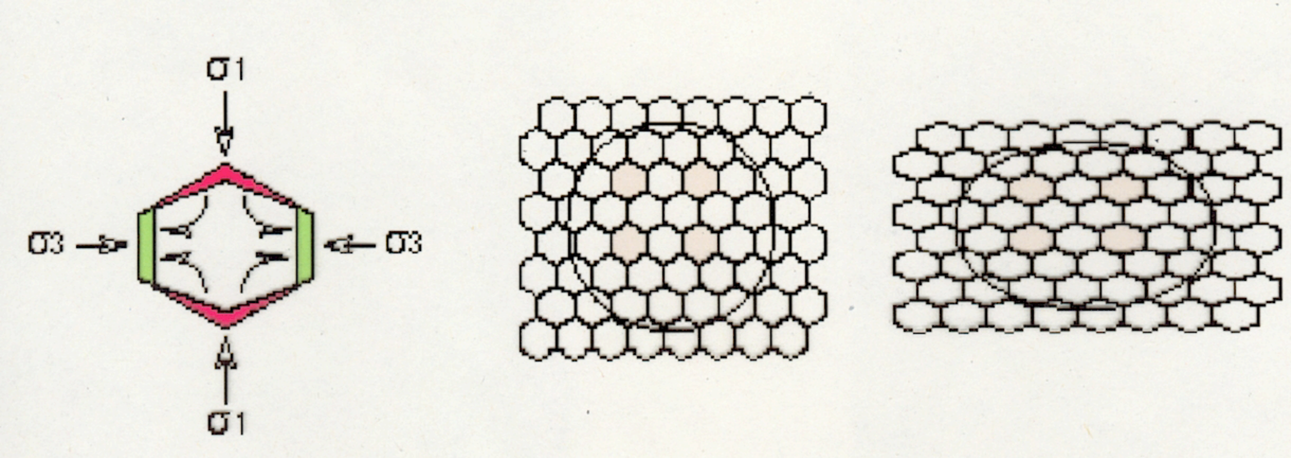
dislocation creep

diffusion creep

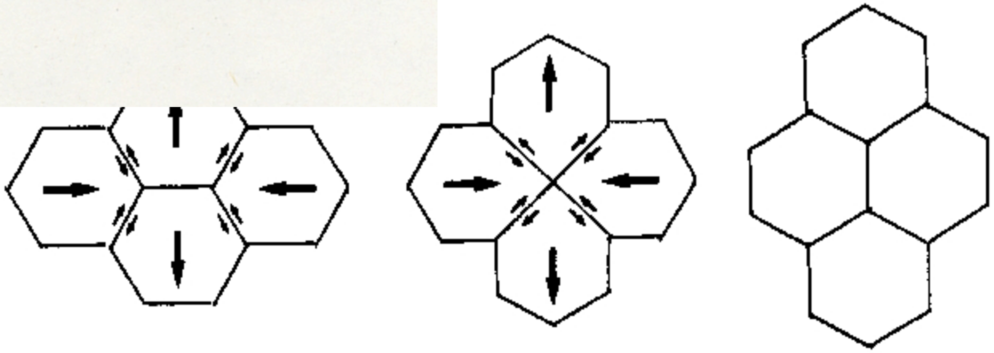
slow strain rates < 10^{-15} s^{-1}

May another process help enhance strain rates?

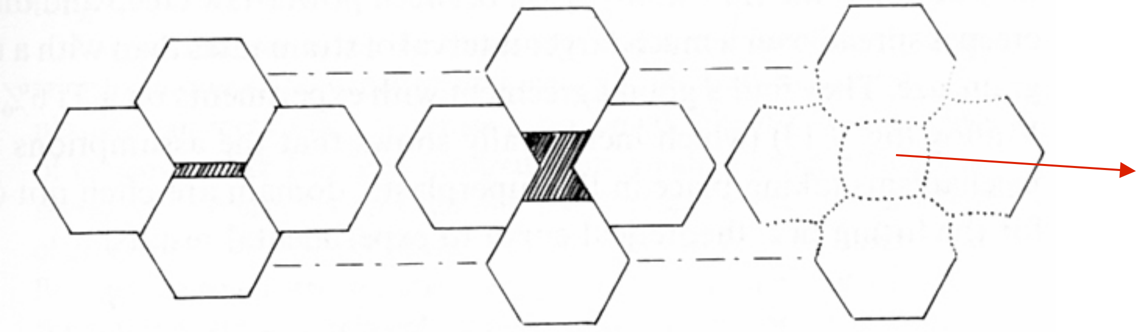
Superplasticity or grain boundary sliding assisted by diffusion:



sion accommodates
n incompatibility
lems (voids & overlaps)!

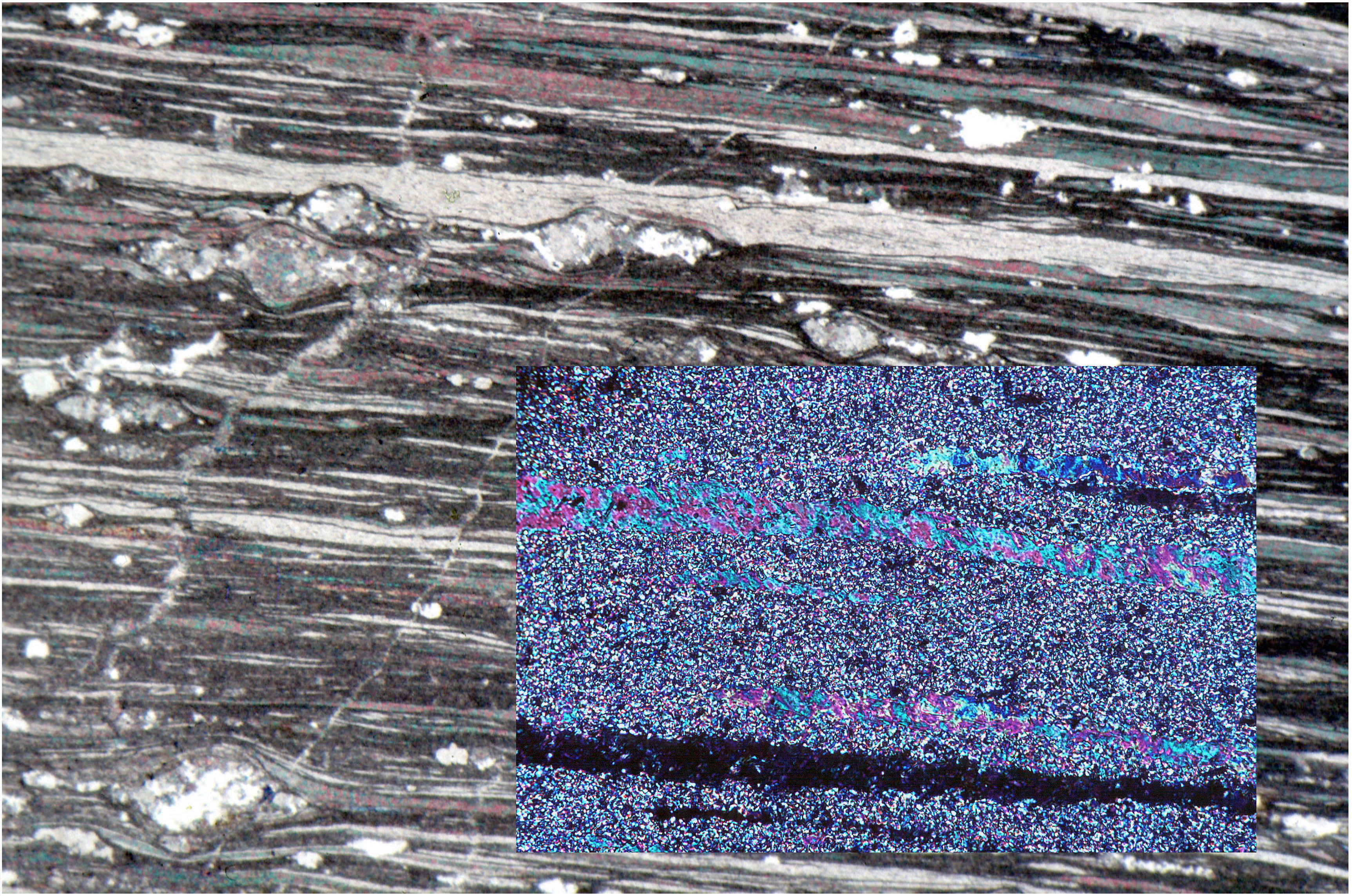


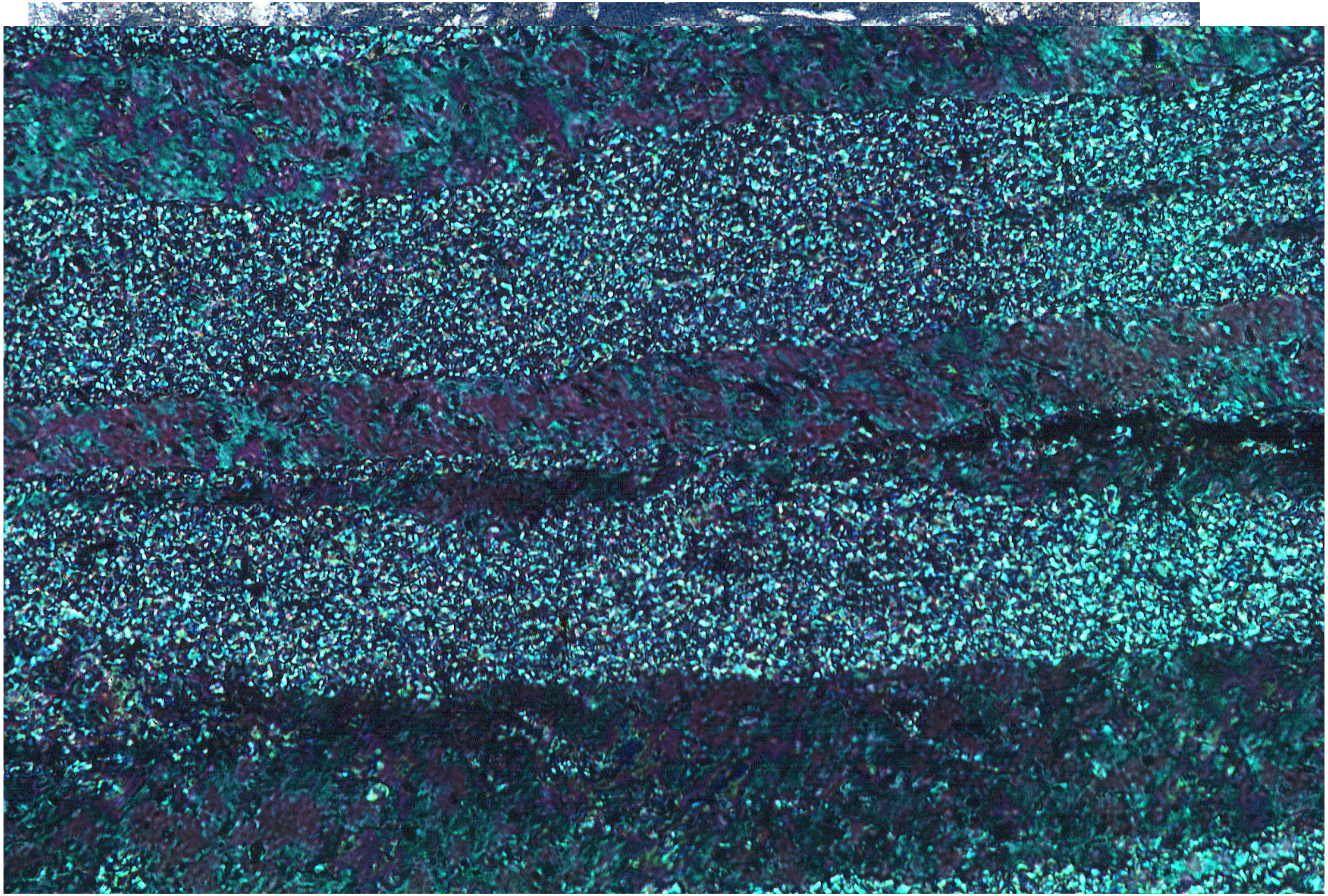
≠ from pure diffusion creep?
equiaxed grains???

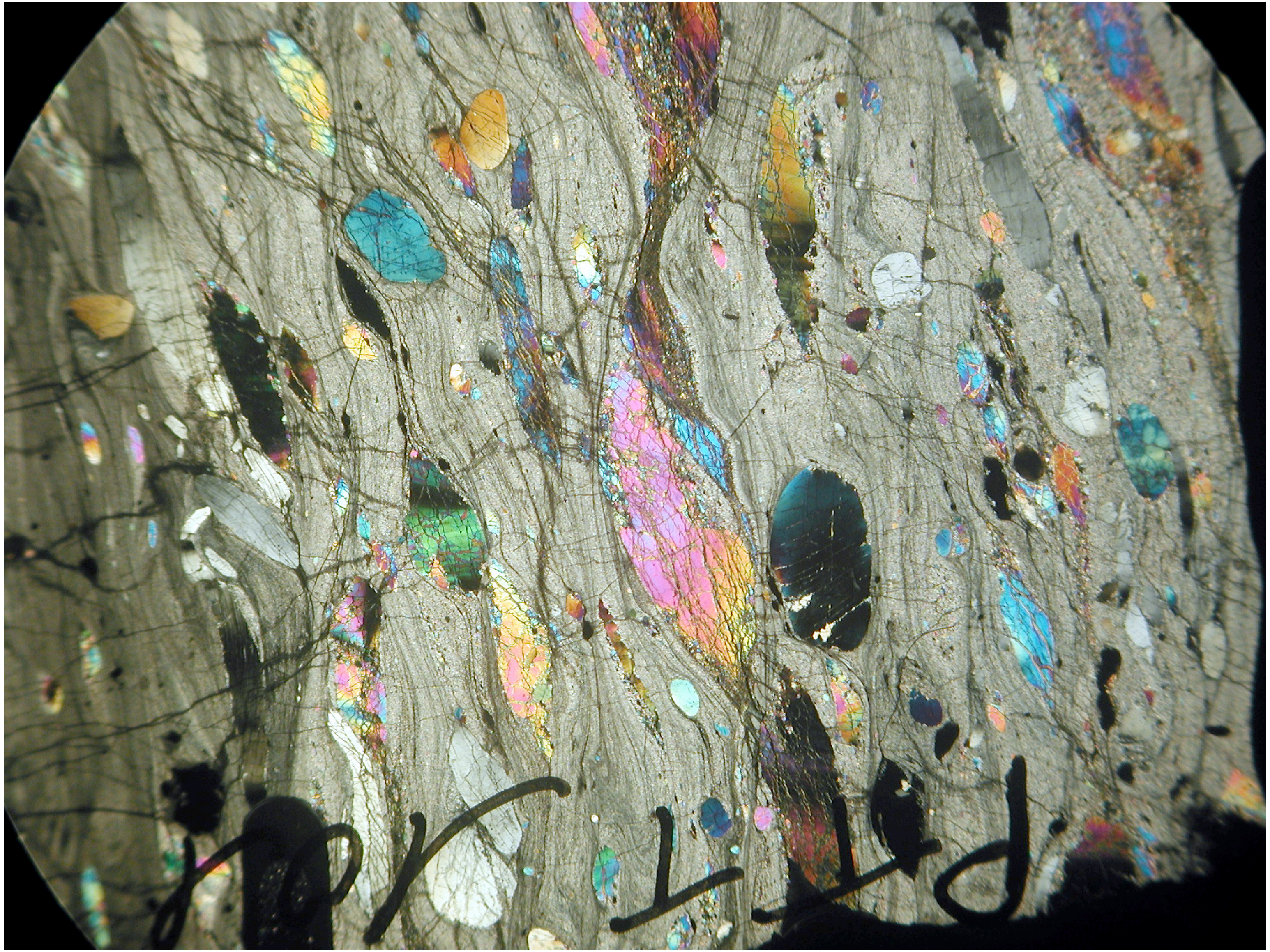


Grain growing from a lower plane
(rocks is a 3D object!)

Mylonitic limestone – Agly massif, Pyrenees

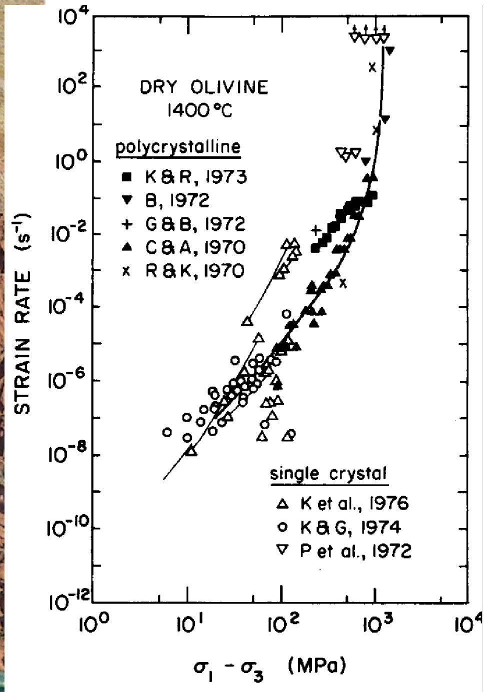


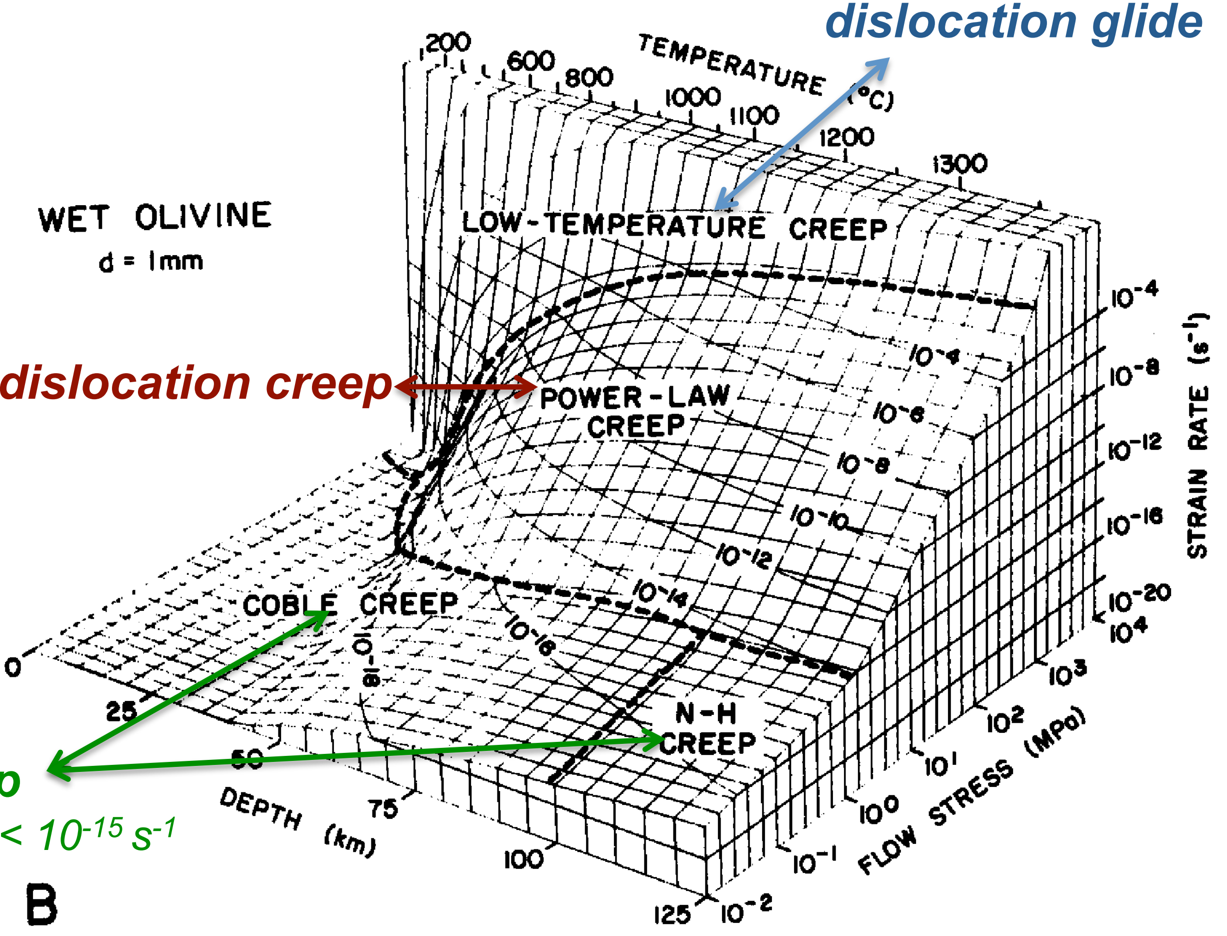




Deformation mechanisms maps

dry olivine polycrystals (dunite)





dislocation glide

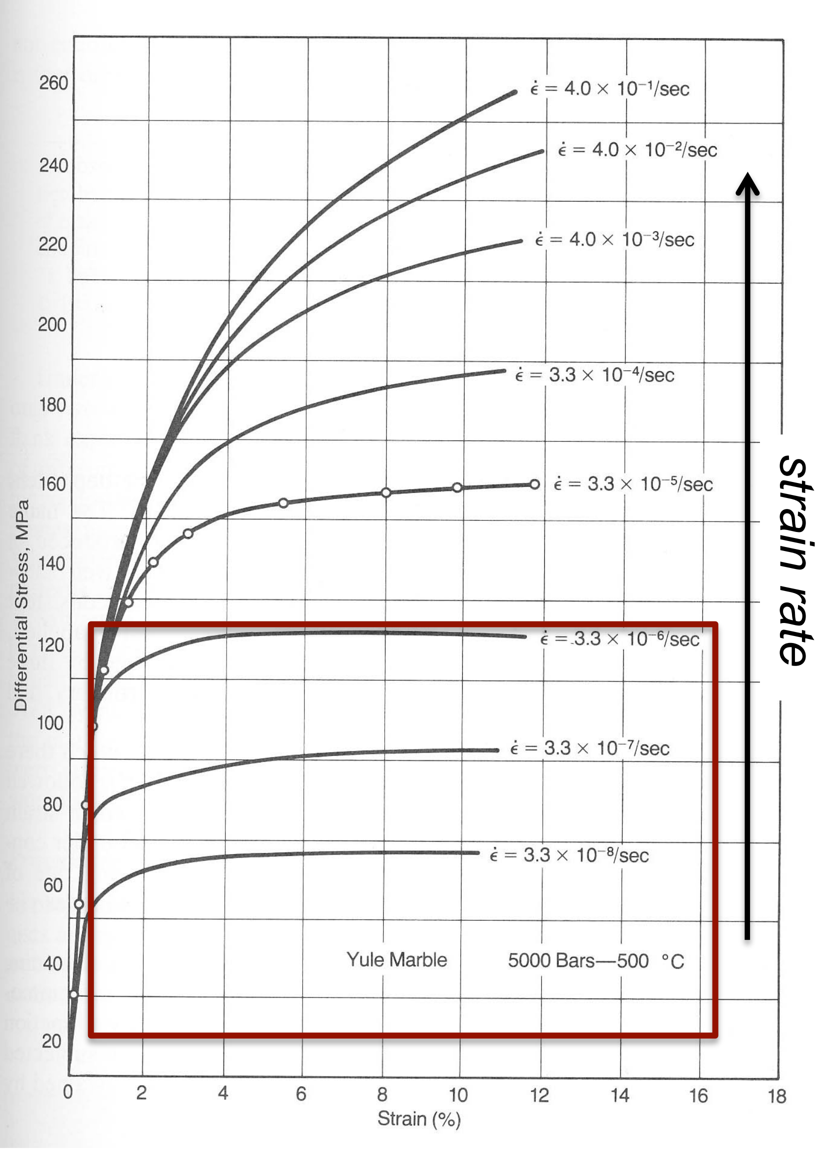
dislocation creep

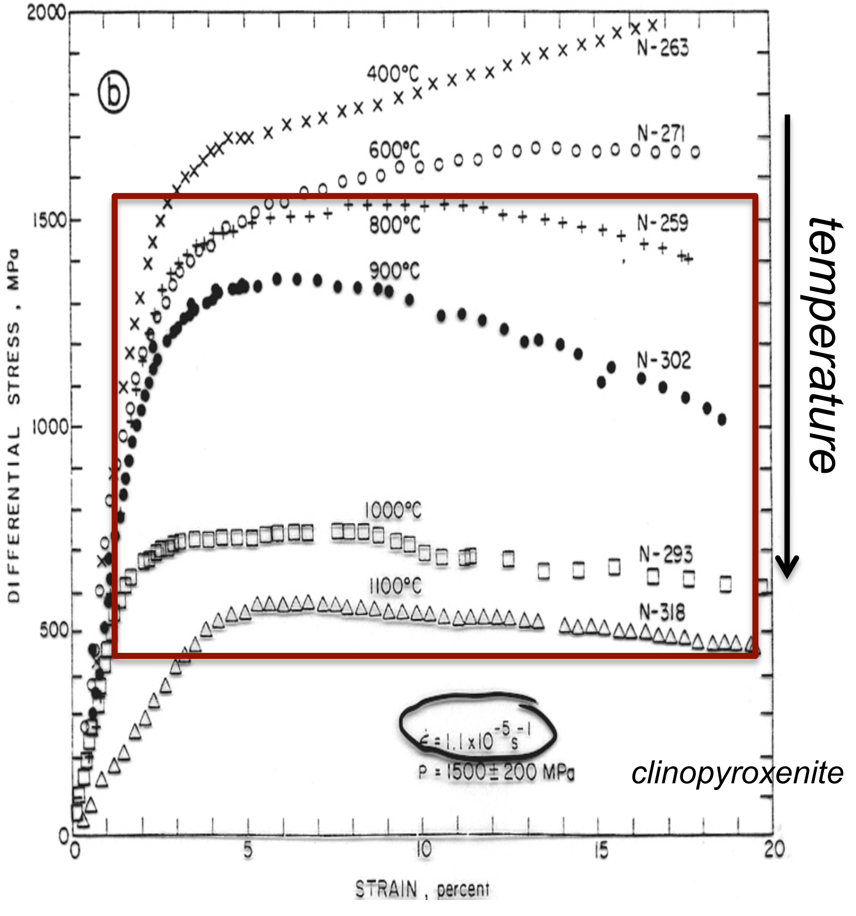
diffusion creep

slow strain rates < 10^{-15} s^{-1}

*But diffusion plays an essential in dislocation creep:
avoids hardening due to dislocation pinning*

Experimental data: change in mechanical behavior as a function of strain rate & temperature

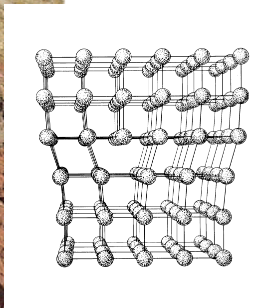


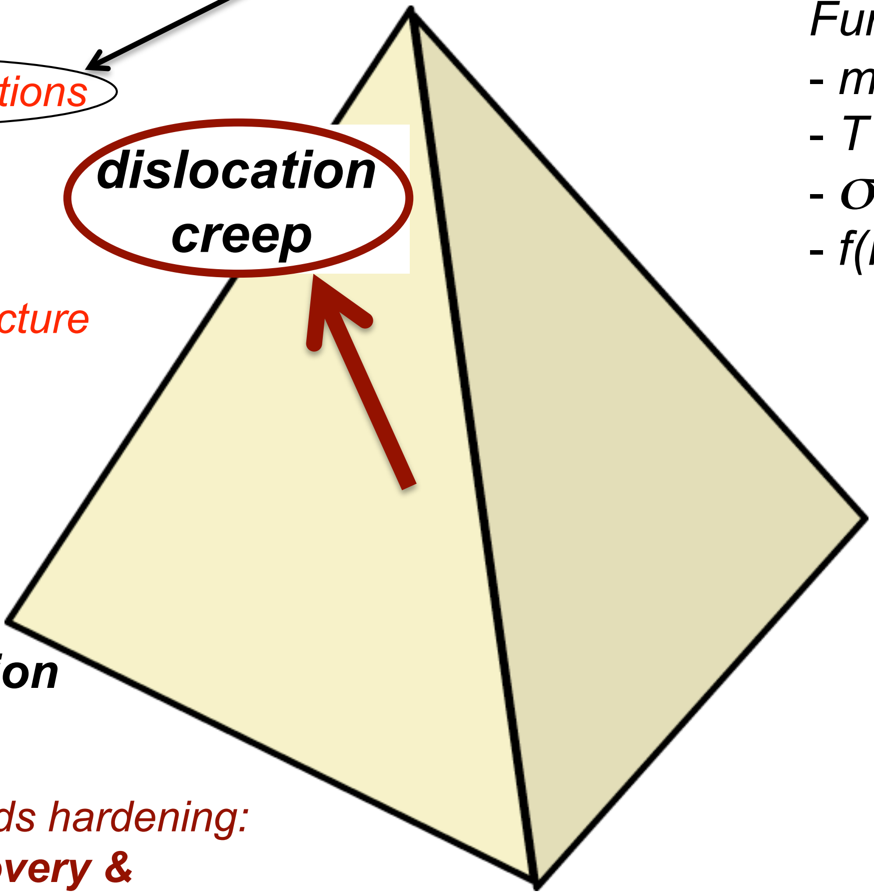


Dislocation creep

Deformation by dislocation glide, but hardening avoided by diffusional processes

Ductile deformation = solid-state flow





main deformation process

dislocation glide

Function of:
- *mineral structure*
- *T*
- $\sigma, \dot{\varepsilon}$
- *f*(H_2O, O_2)…

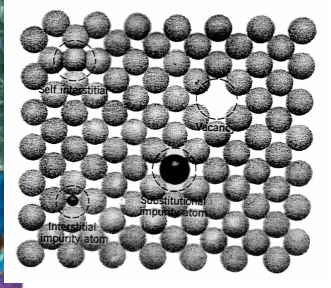
linear: dislocations

dislocation creep

Motion of ***defaults*** *in the crystals structure*

point: vacancies

twinning



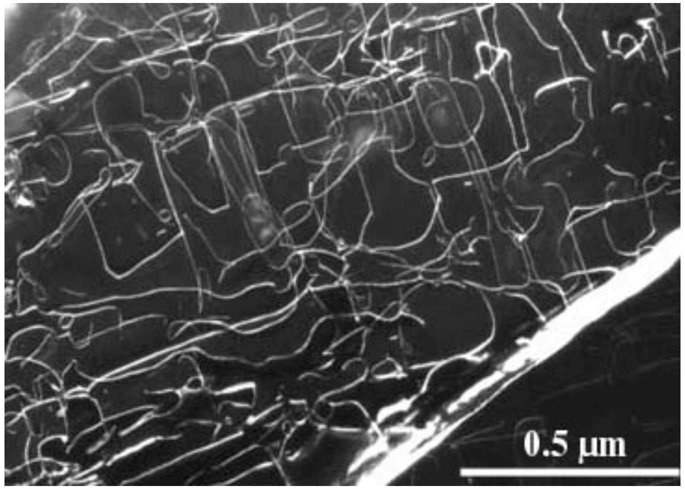
diffusion

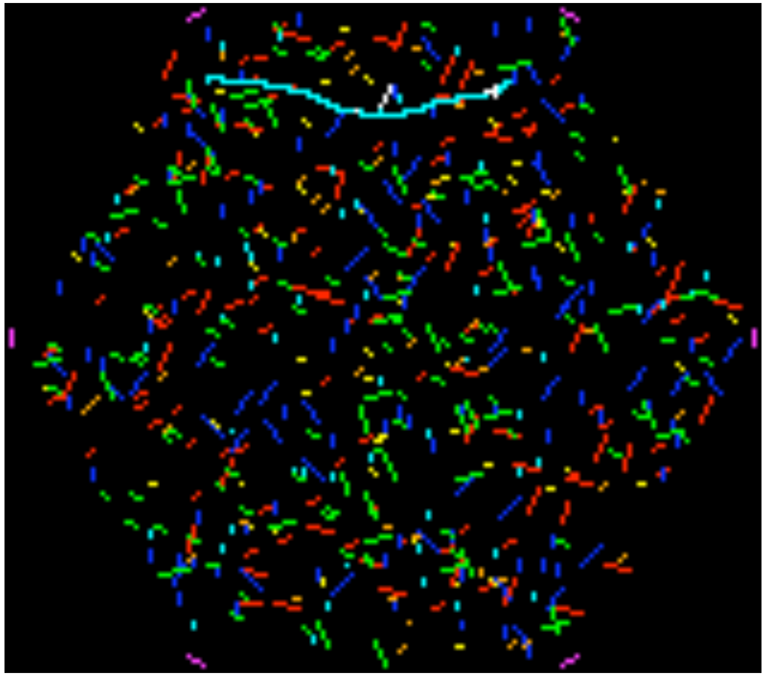
avoids hardening:
recovery &
recrystallization

grain boundary sliding
needs an additional mechanism:
diffusion*, dislocations, or cataclasis!*

obstacle = grain boundary, another dislocation, impurity…

accumulation of dislocations = tangling = forests
increase of the crystal internal energy
➢ hardening



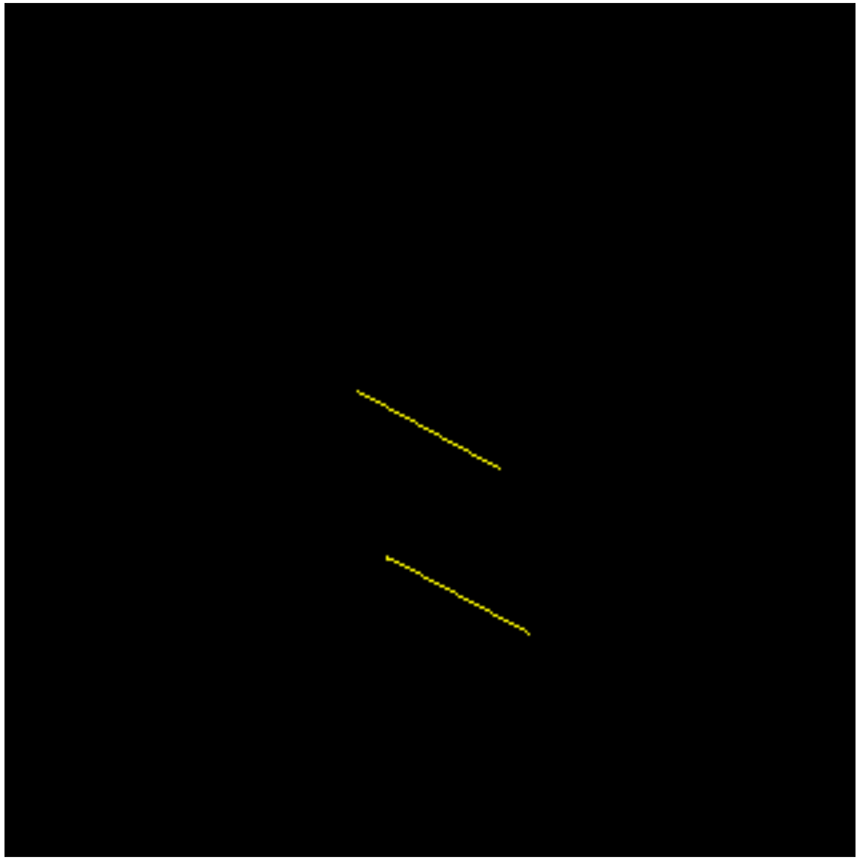


http://zig.onera.fr/~devincre/DisGallery/index.html

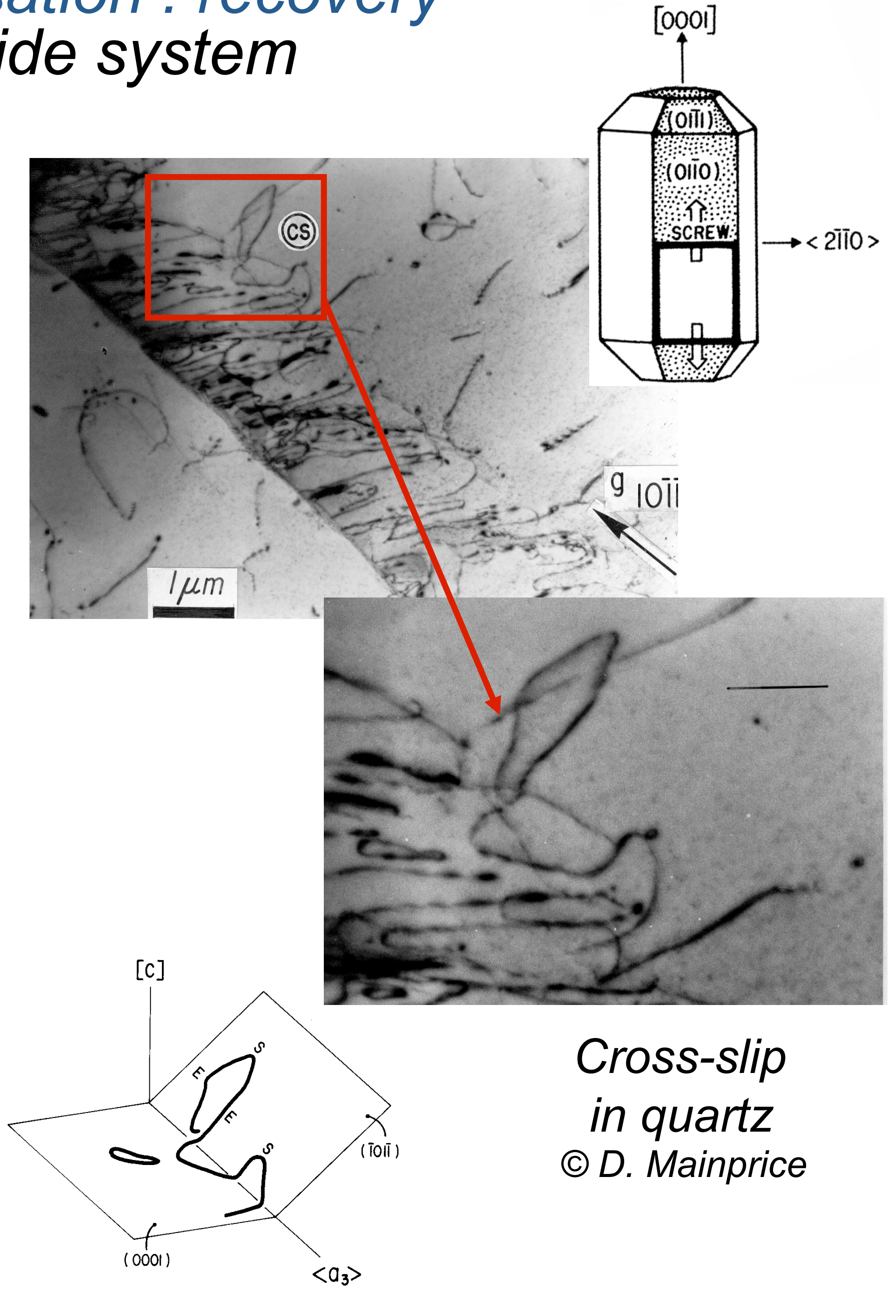
How to avoid dislocations pinning?
Dislocation reorganisation : recovery

How to avoid the blocking of dislocations?
Dislocation reorganisation : recovery
➢ change of glide system

screw dislocations: cross-slip



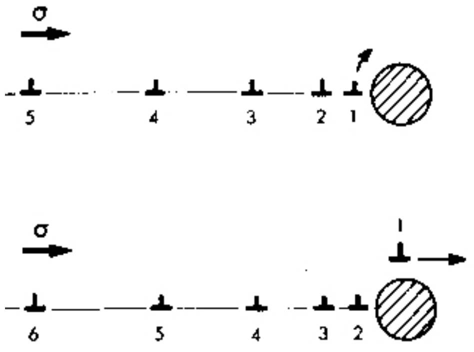
http://zig.onera.fr/~devincre/DisGallery/index.html

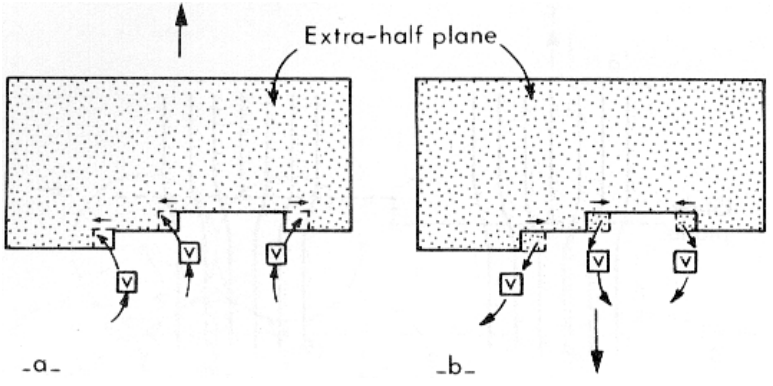


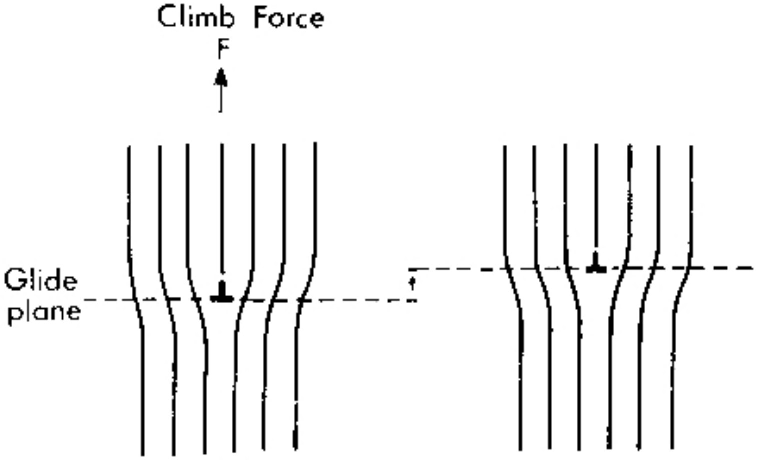
Cross-slip
in quartz
© D. Mainprice

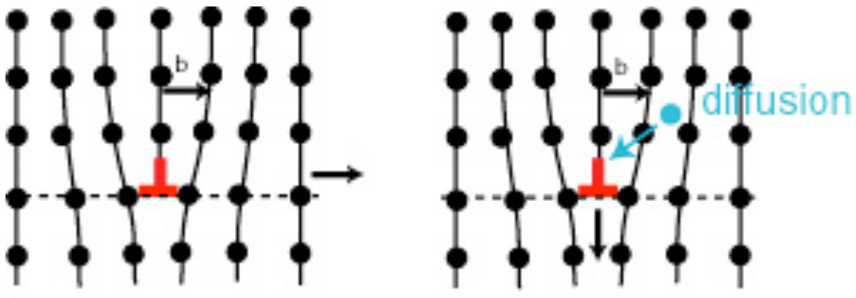
How to avoid the blocking of dislocations? Dislocation reorganisation : recovery
➢ change of glide plane

Edge dislocations : climb





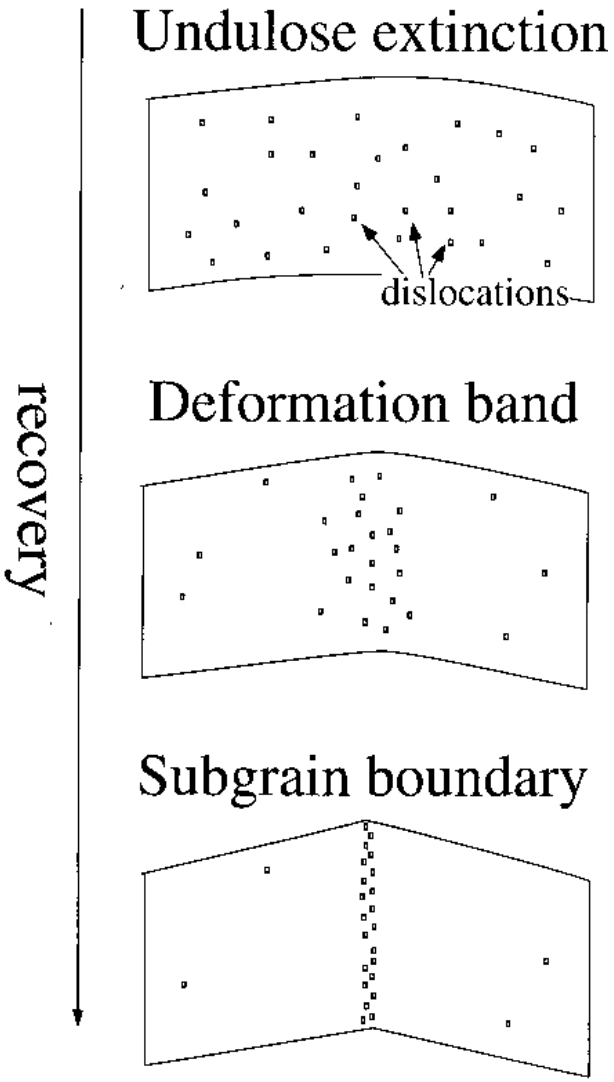


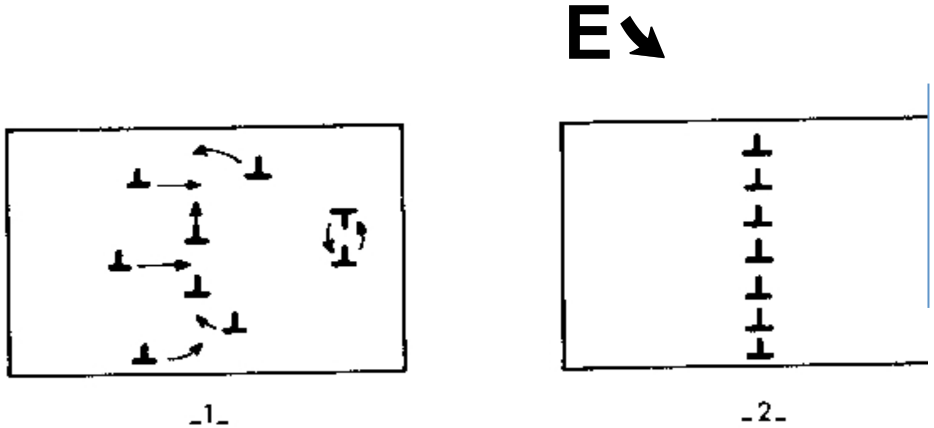


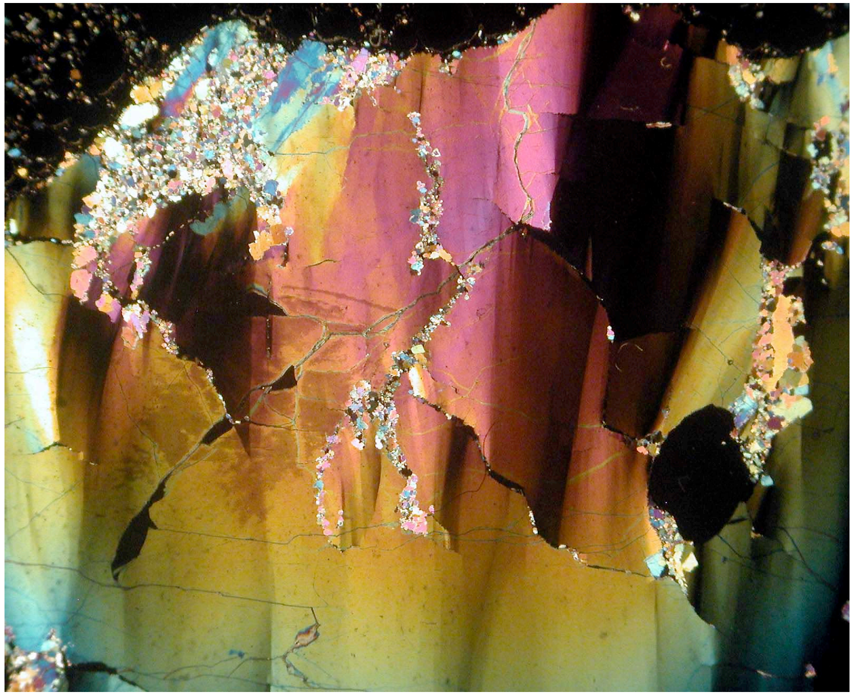
glide *climb*

Needs vacancies motion:
diffusion ➢ f(T)

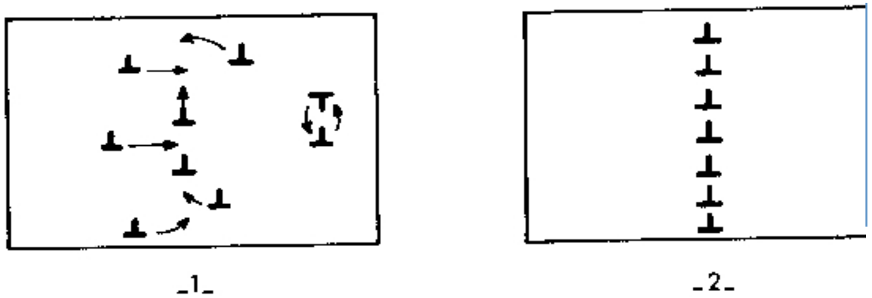
How to avoid the blocking of dislocations?
Dislocation reorganisation : recovery
➢ formation of dislocations walls & subgrains

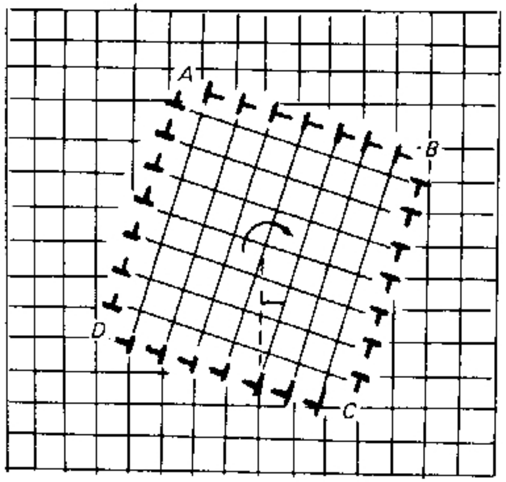


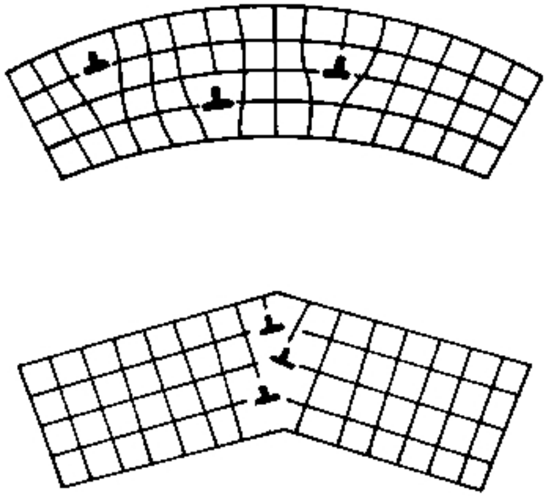


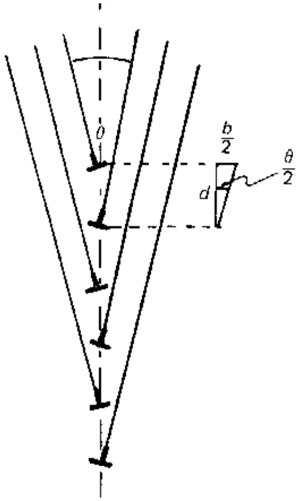


How to avoid the blocking of dislocations?
Dislocation reorganisation : recovery
➢ *formation of dislocations walls & subgrains*



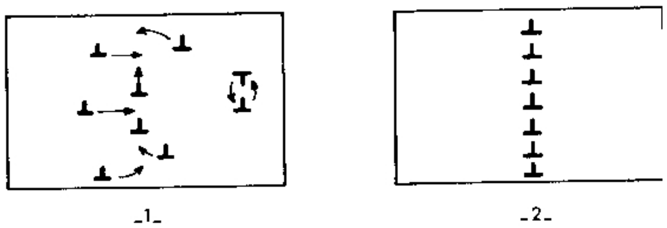






Subgrain boundary= misorientation <15°

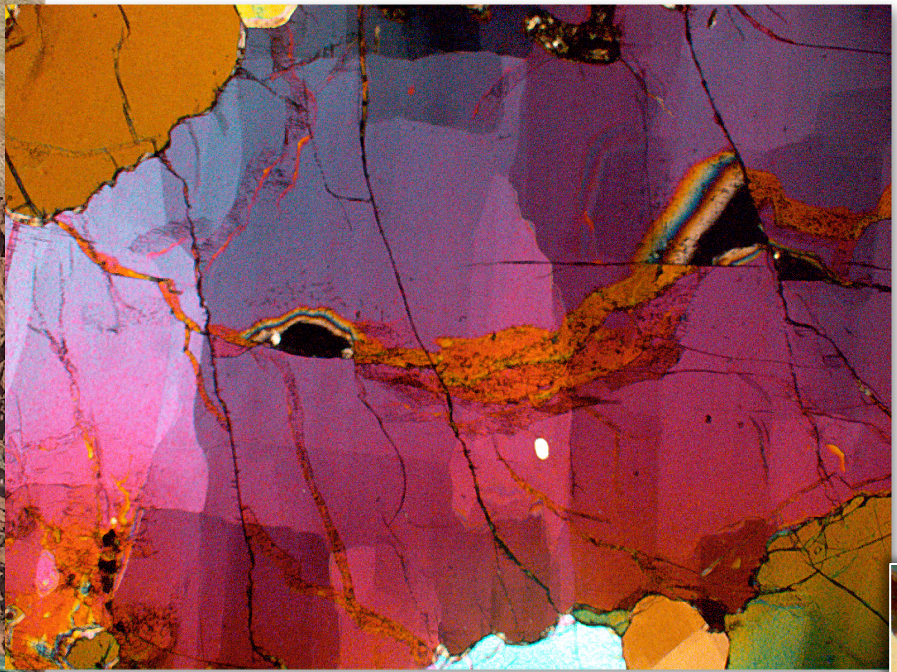
➢ *Dynamic recrystallisação by subgrain rotation*



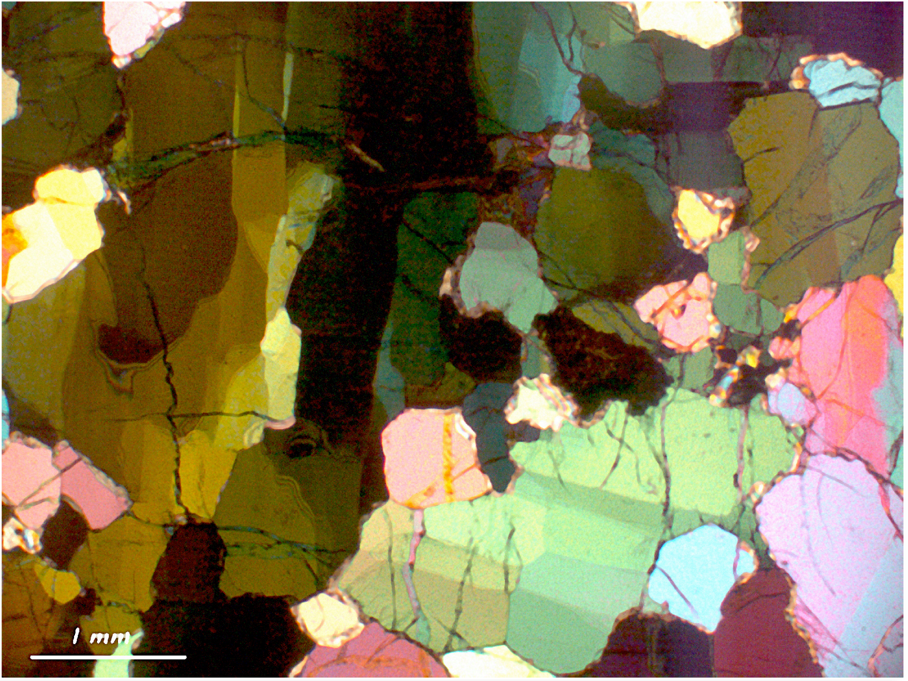
Tilt walls = formed mainly by edge dislocations

Subgrain boundary = normal to Burgers vector

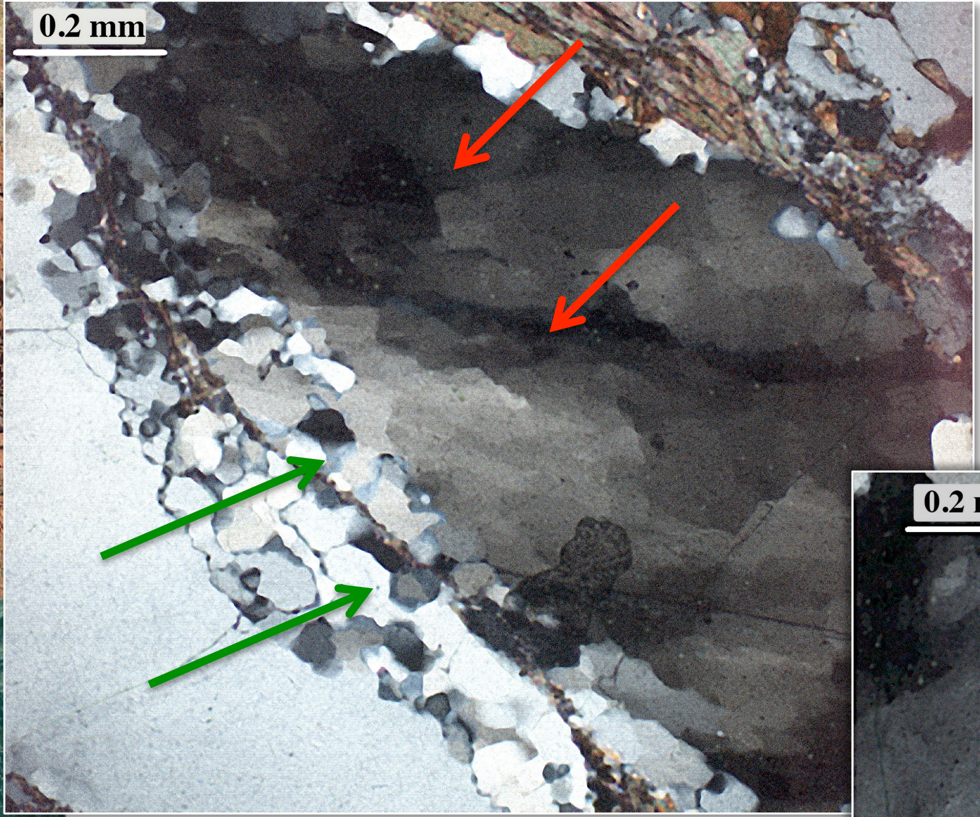
Rotation axis = normal to Burgers vector & to the normal to the glide plane



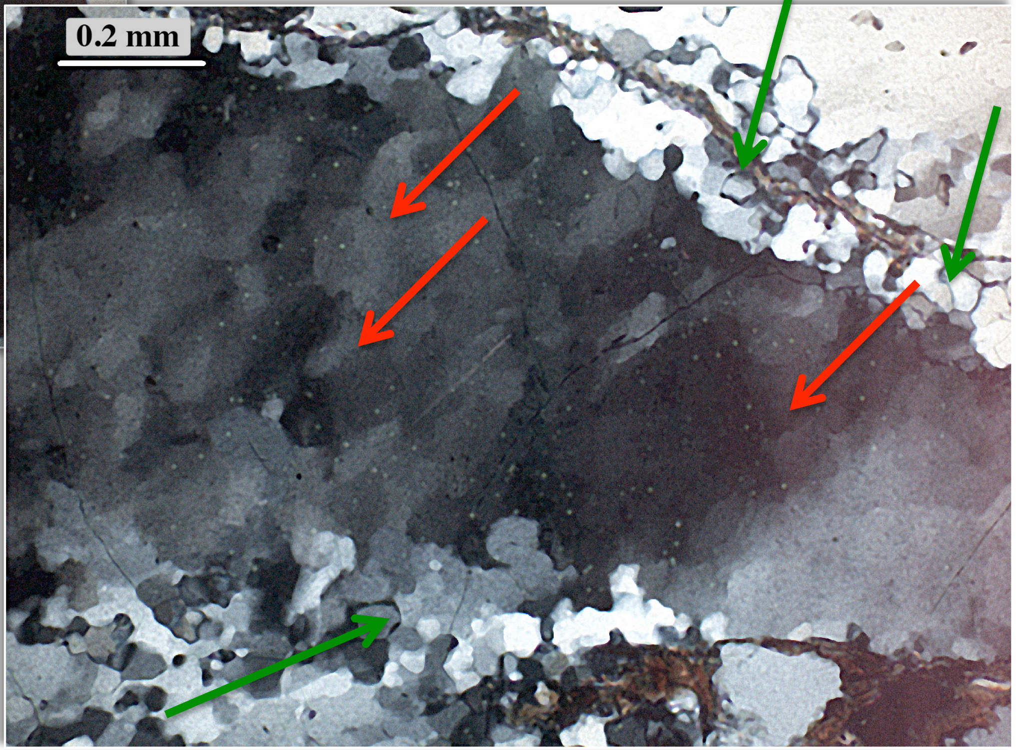
2 families of subgrain boundaries
= 2 families of slip systems



Dislocation walls and subgrains + dynamic recrystallization by subgrain rotation

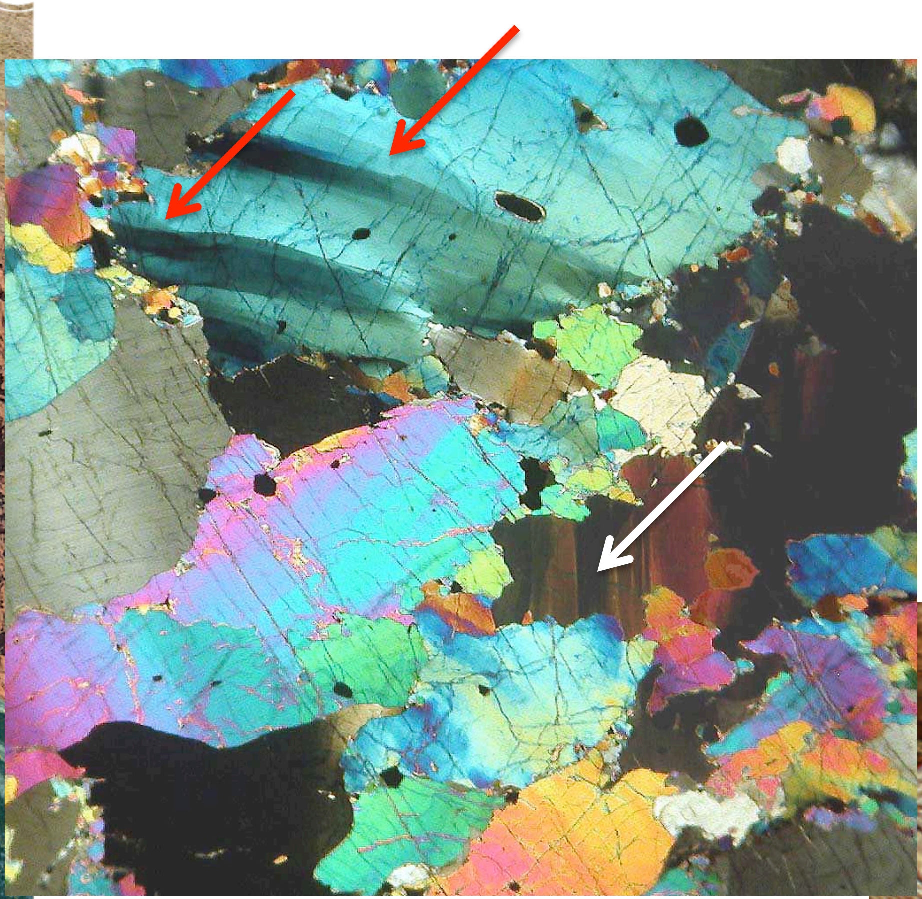


Quartz-mylonite
Crossed-polarized light

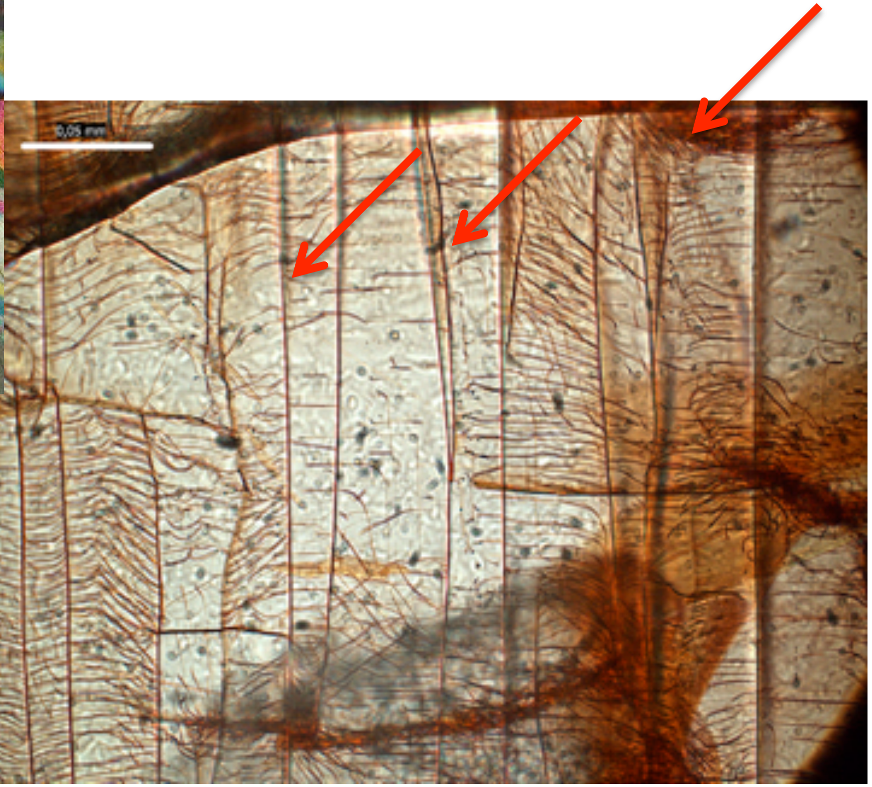


"hexagonal" subgrains:
crystal symmetry
control on slip systems

Dislocation walls and subgrains in olivine

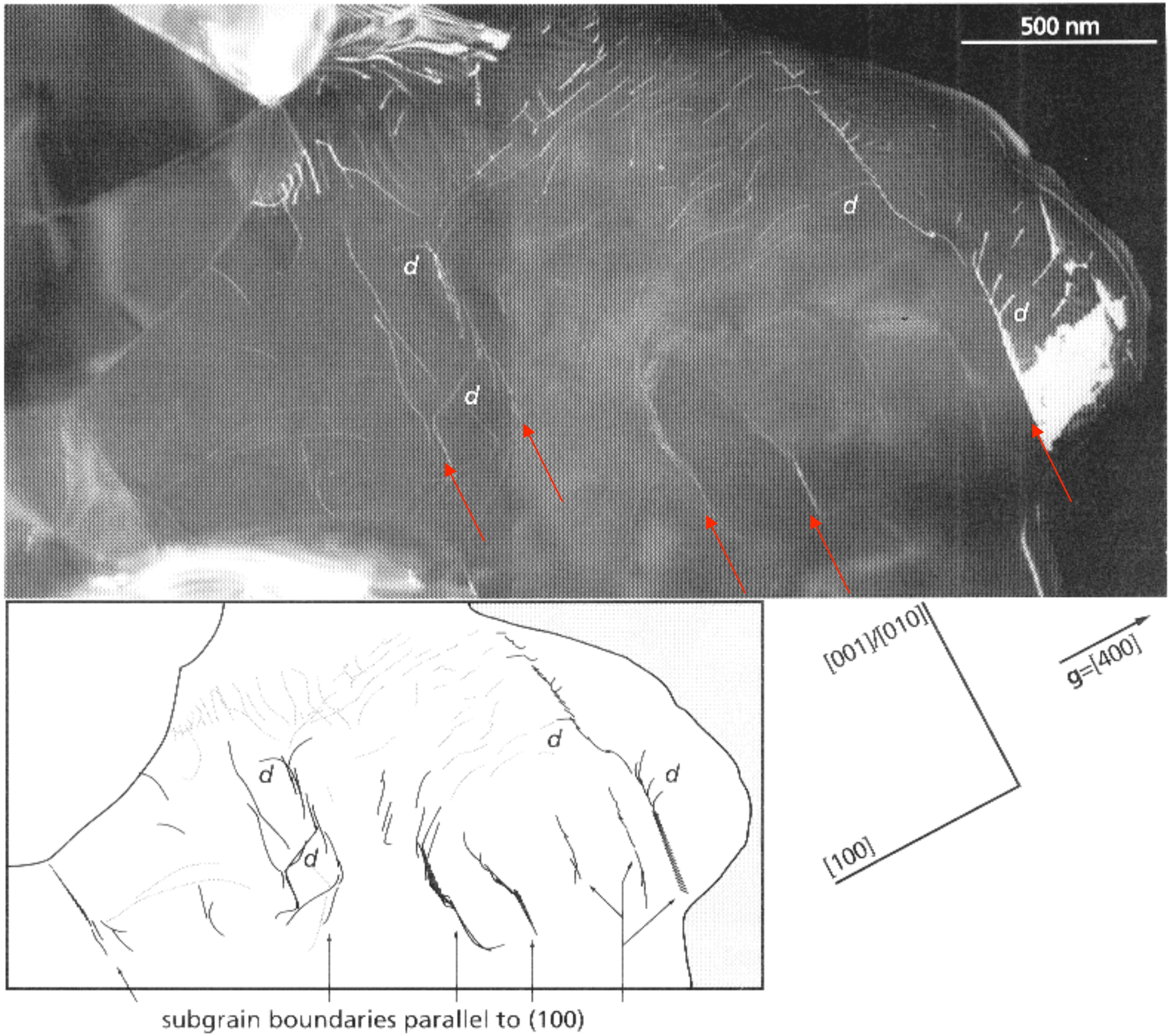


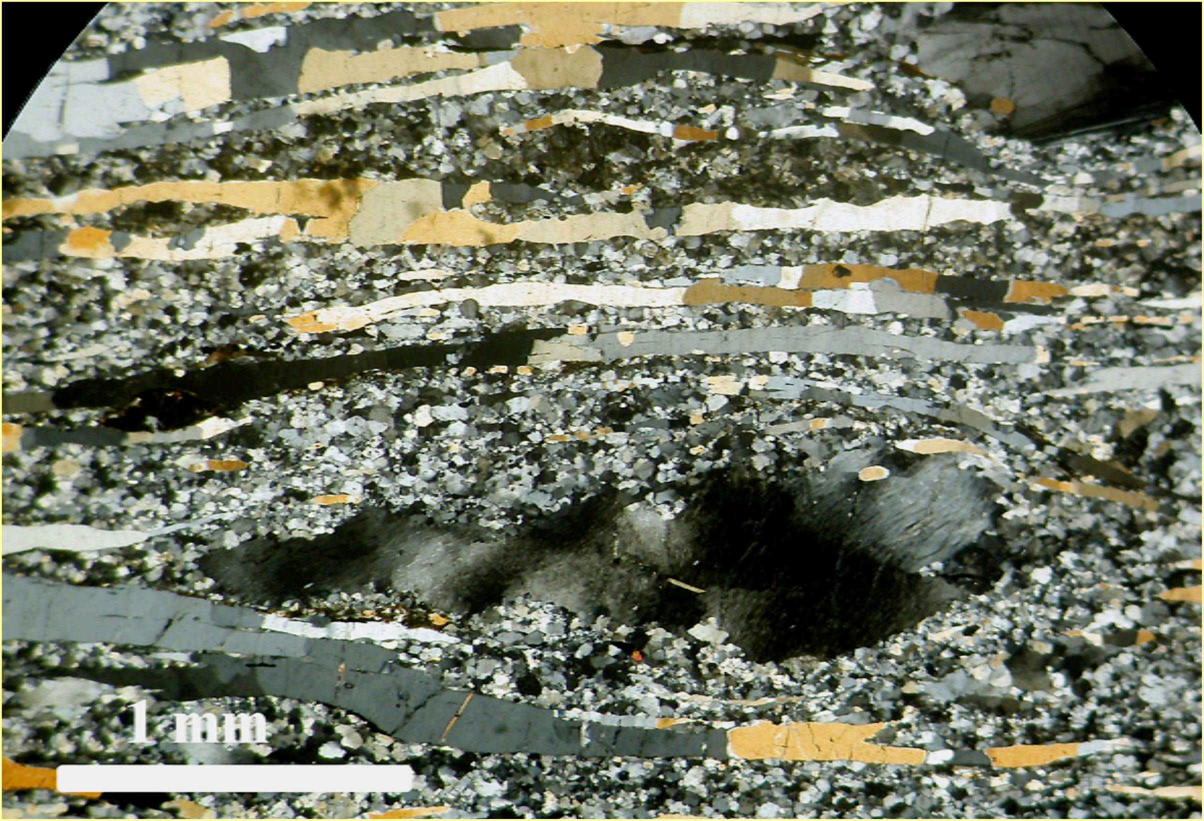
Hawaii xenolith
Crossed-polarized light

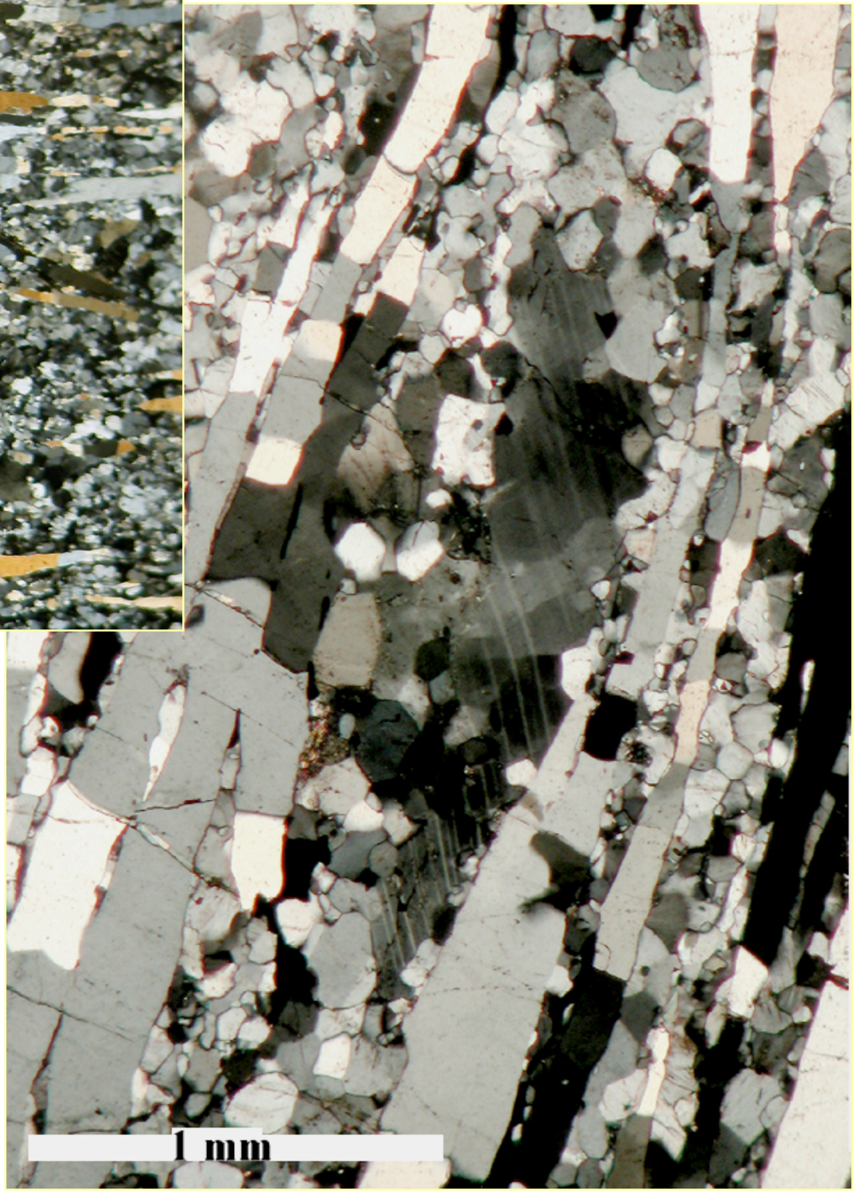


Kamchatka xenolith
Decorated (oxydized) sample
Plane-polarized light
Soustelle et al. J. Petrol. 2010

TEM observations : subgrains in olivine

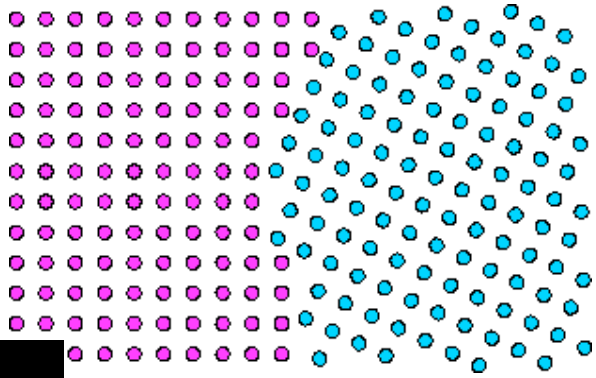






Granulite deformation:
Dynamic recrystallization
by subgrain rotation of
plagioclase

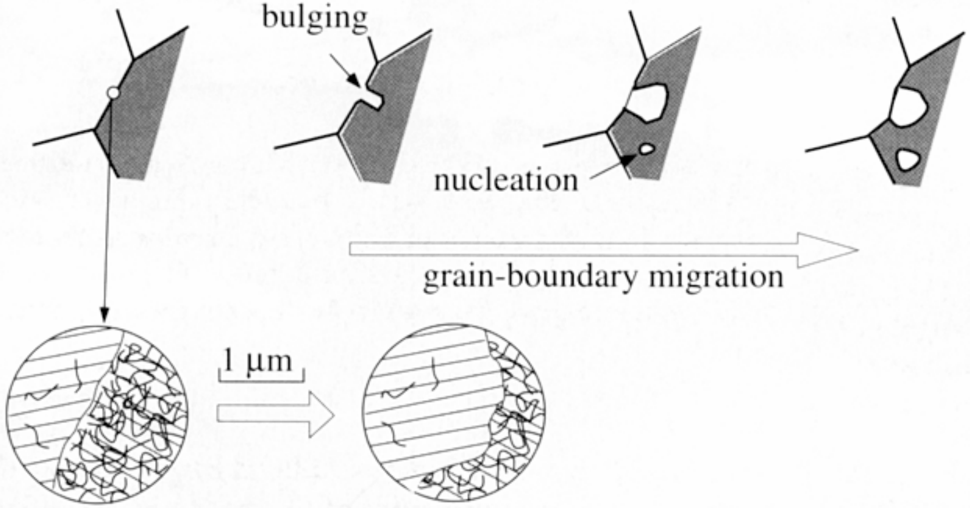
A 2nd diffusion-assisted recovery and recrystallization process: Grain boundary migration

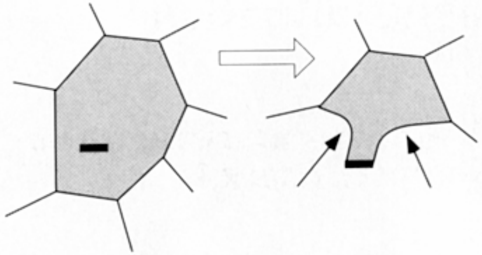


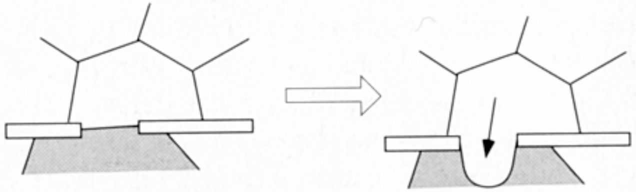
Jessel & Bons – Simulation using ELLE
virtualexplorer.com.au/.../lectures/lec2.html

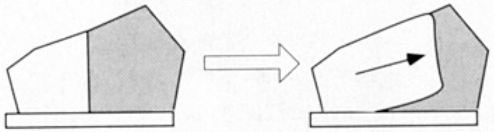
Deformation followed by static recrystallization in octachloropropane

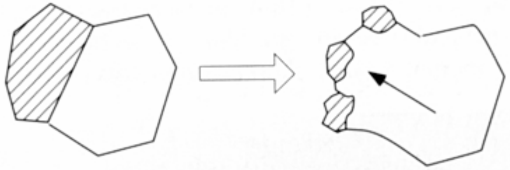
A 2nd diffusion-assisted recovery and recrystallization process: Grain boundary migration


GBM-recrystallisation


'pinning' microstructure


'window'-microstructure

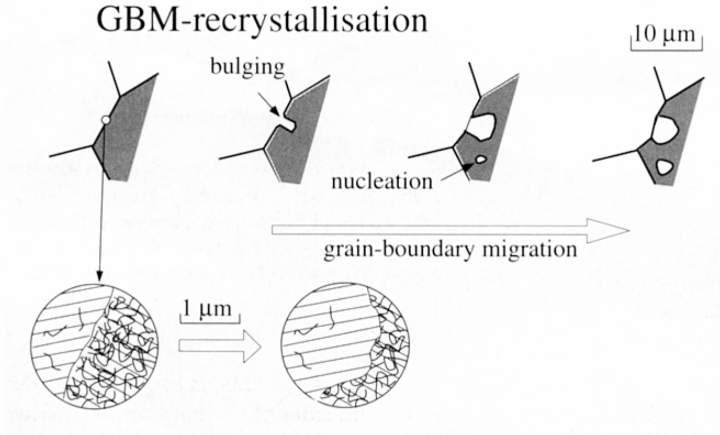

'dragging' microstructure

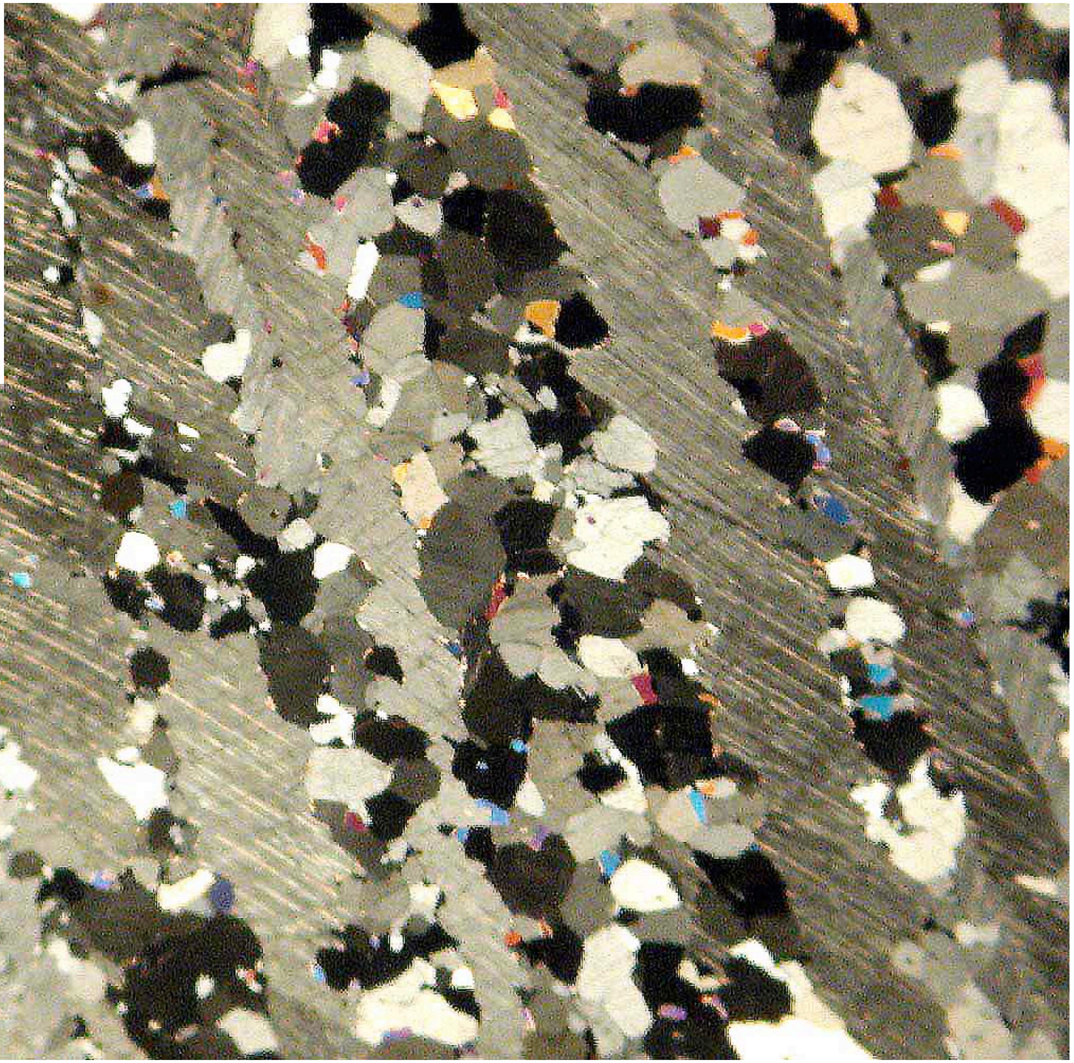

'left-over grains'

motor 1: Δ stored elastic energy (ρ of dislocations)
  - ➢ *dynamic recrystallization (synkinematic)*

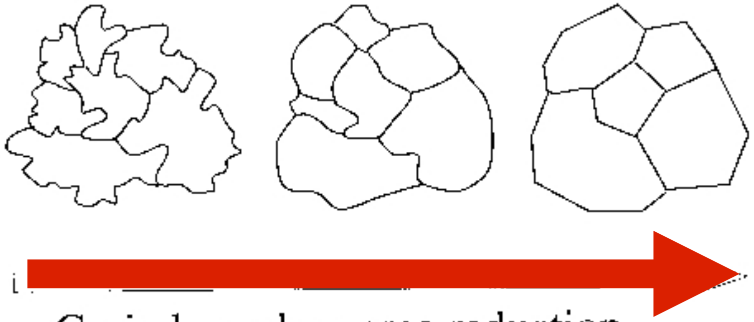
motor 2: decrease in surface energy ➔ grain growth)
  - ➢ *static recrystallization (post-kinematic)*

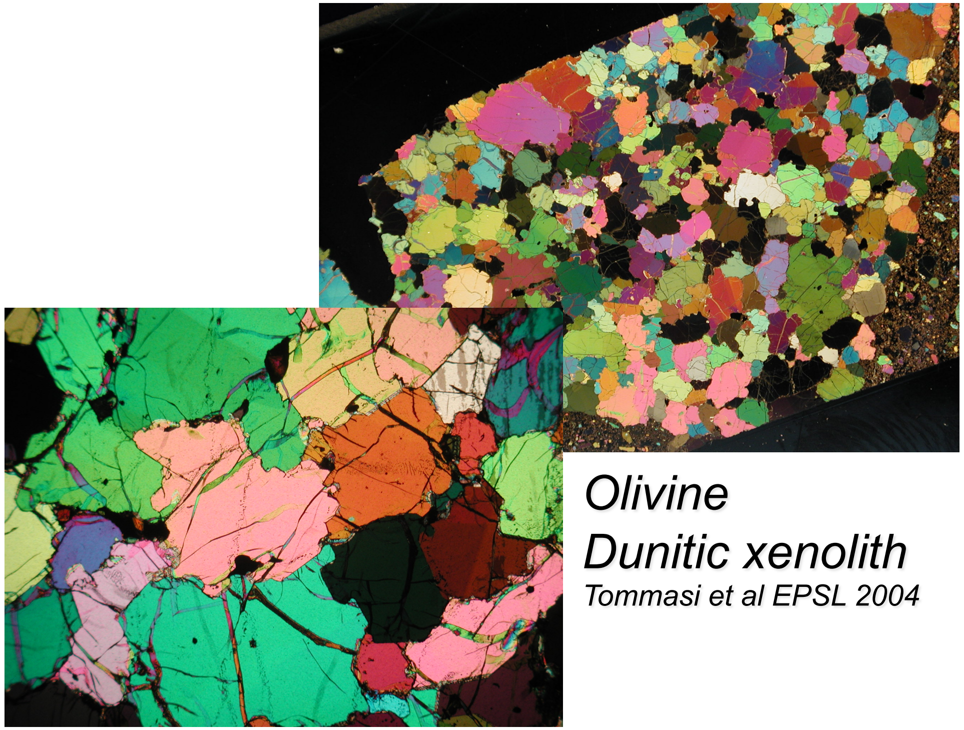
Recrystallization (nucleation) starts in high stress domains of the crystal
Enstatite (opx): Recrystallization along kink bands





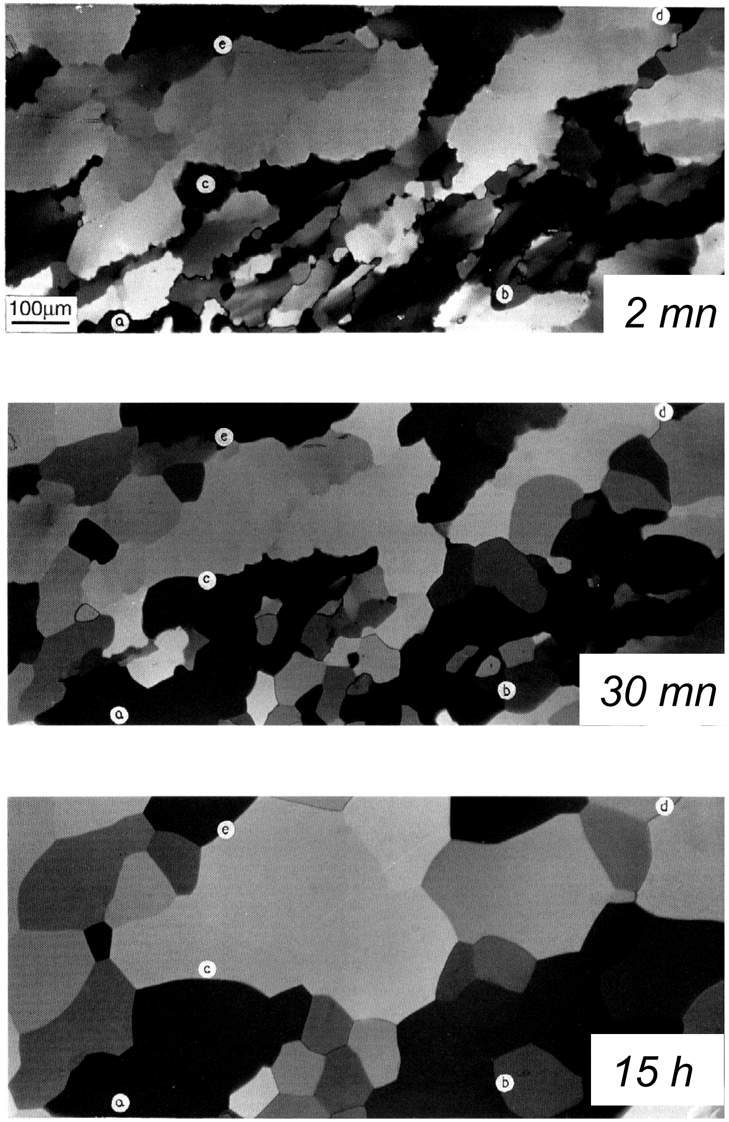
A 2nd diffusion-assisted recovery and recrystallization process: Grain boundary migration


Grain boundary area reduction


Olivine

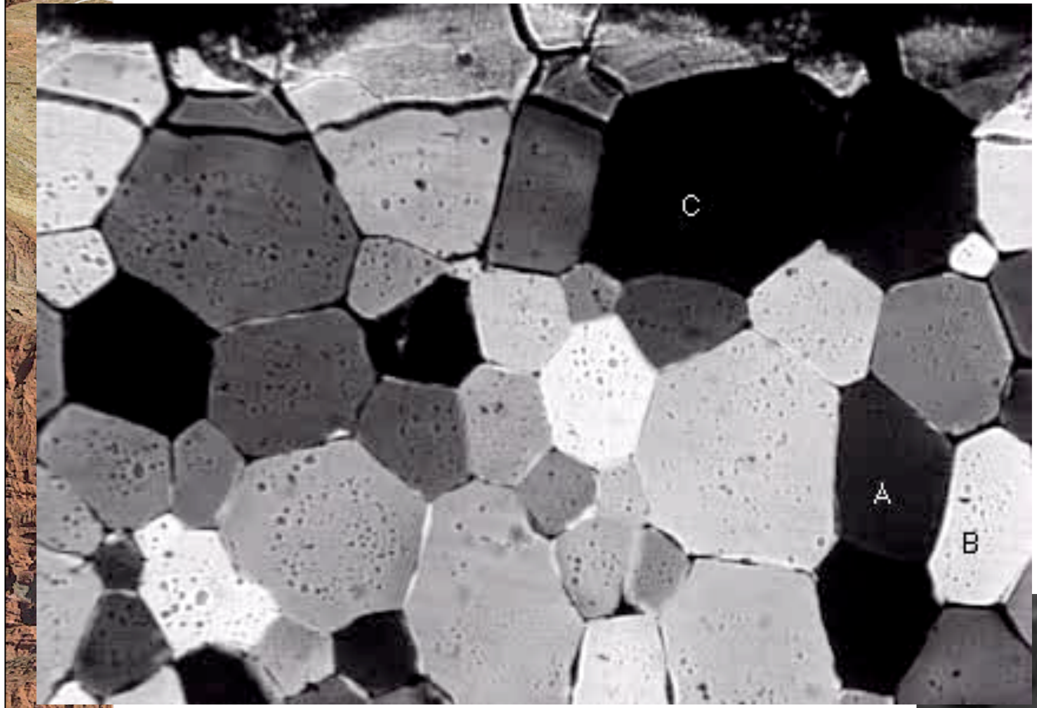
Dunitic xenolith

Tommasi et al EPSL 2004



Static grain growth: octachloropropane

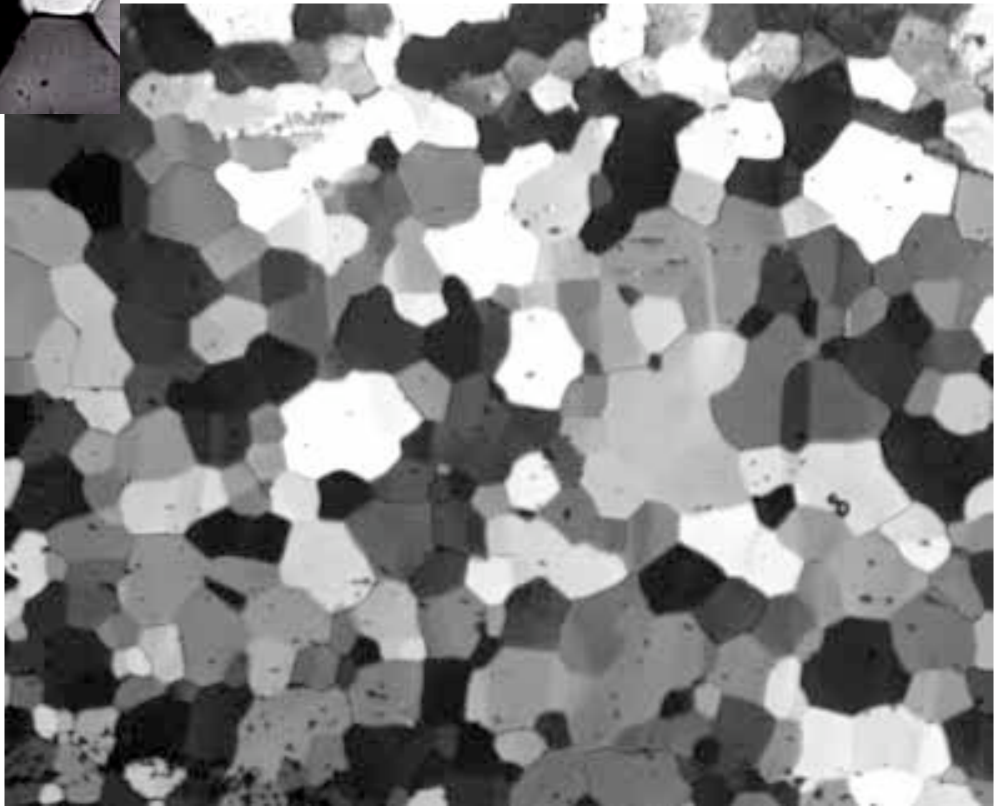
Park, Ree & Means, J. Virtual Explorer 2000



octacloropropane C_3Cl_8

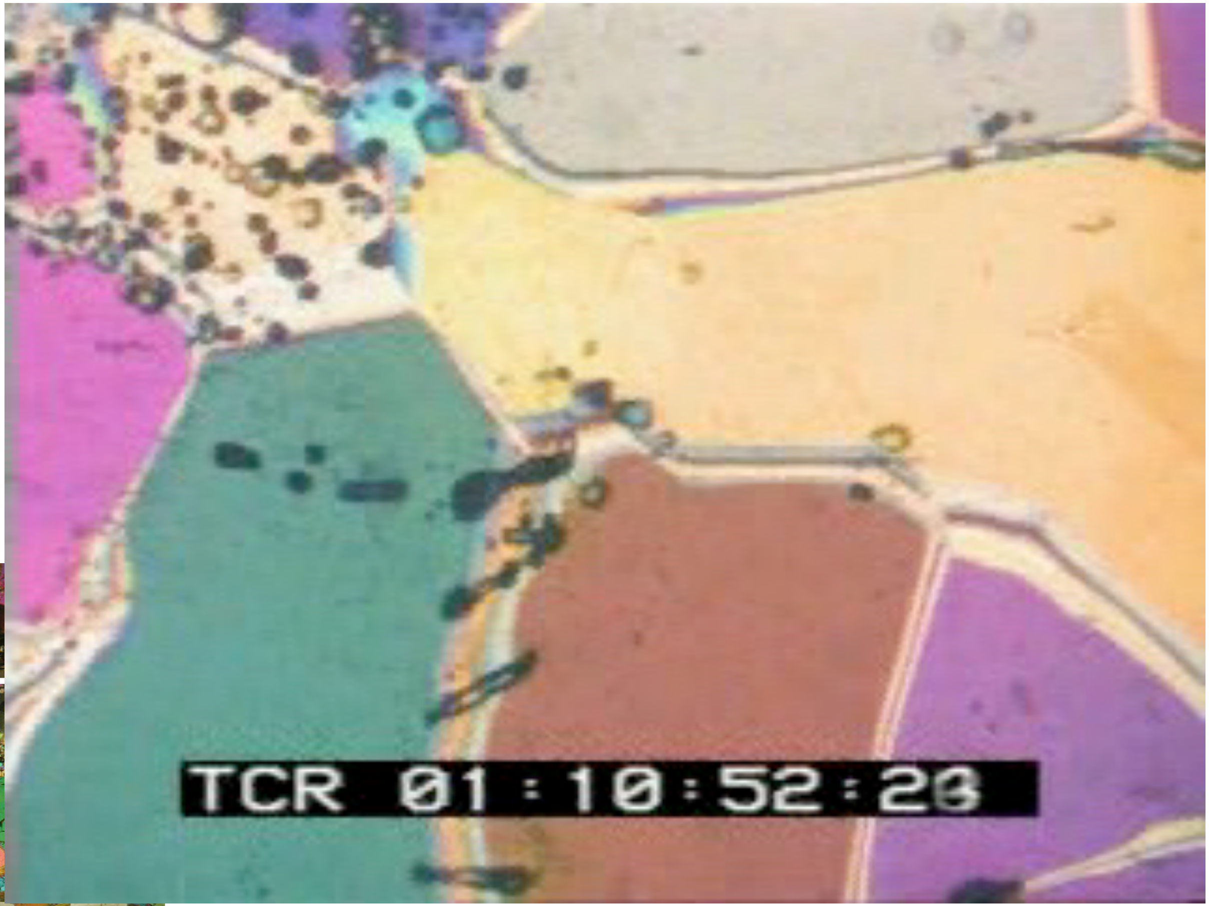
Deformation under ≠ strain rate conditions

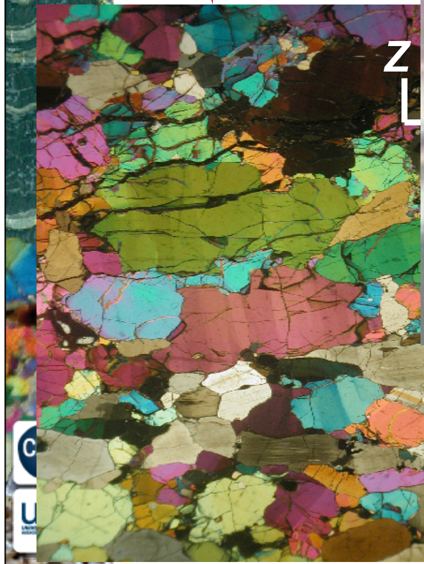
Park, Ree & Means, J. Virtual Explorer 2000



Viscoplastic deformation of ice

dislocation creep = dislocation glide + dynamic recrystallization

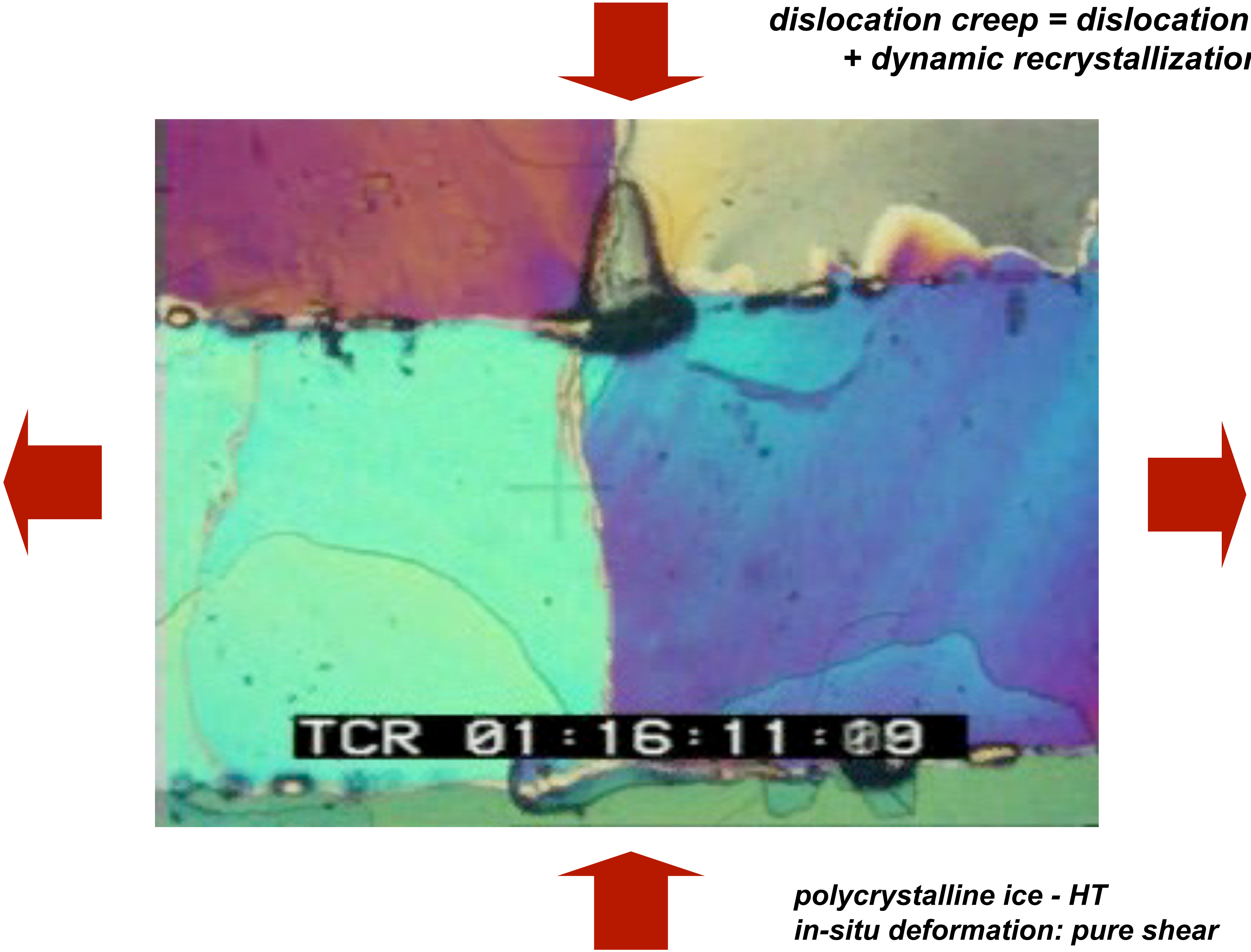




polycrystalline ice
in-situ deformation: pure shear
C. Wilson - Univ. Melbourne, Australia

Viscoplastic deformation of ice

dislocation creep = dislocation glide
+ dynamic recrystallization



polycrystalline ice - HT
in-situ deformation: pure shear
C. Wilson - Univ. Melbourne, Australia

In the experiments, it is easy, but…
may we identify the mechanisms active during and after deformation in natural systems (Earth)?

Macroscopic and microscopic observations & deformation regimes

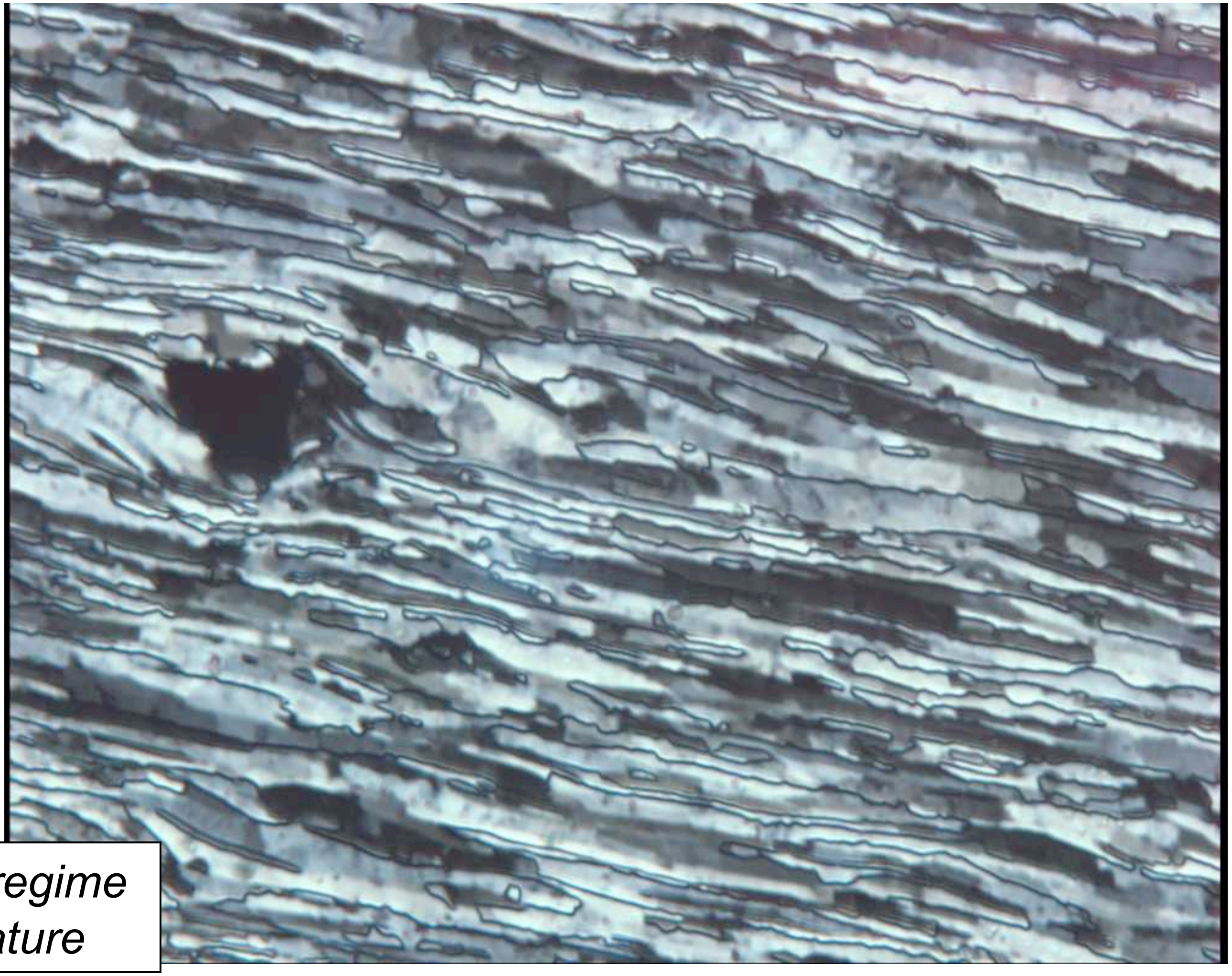
Dislocation creep:

- *Grain elongation*
  - *May be erased by recrystallization*
- *Undulose extinction, deformation bands & subgrains*
  (microstructures directely related to dislocations)
- *Crystallographic preferred orientation (CPO)*
- *Dynamic recryistallization may produce a bimodal grain size distribution at high stress (porphyroclasts vs. Neoblasts)*
- *HT: sinuous or polygonal grain boundaries : migration*
  synkinematic grain growth hinder grain size reduction

Diffusion creep or diffusion-assisted GBS:

- *Fine-grained material (µm)*
- *Weak elongation may exist, but generaly absent*
- *Absence of intracrystalline deformation features (Undulose extinction, deformation bands & subgrains)*
- *Absence of CPO*

Experimental deformation : calcite + 1% qz - 900 K – $10^{-5}s^{-1}$



High stress regime
~ low T in nature

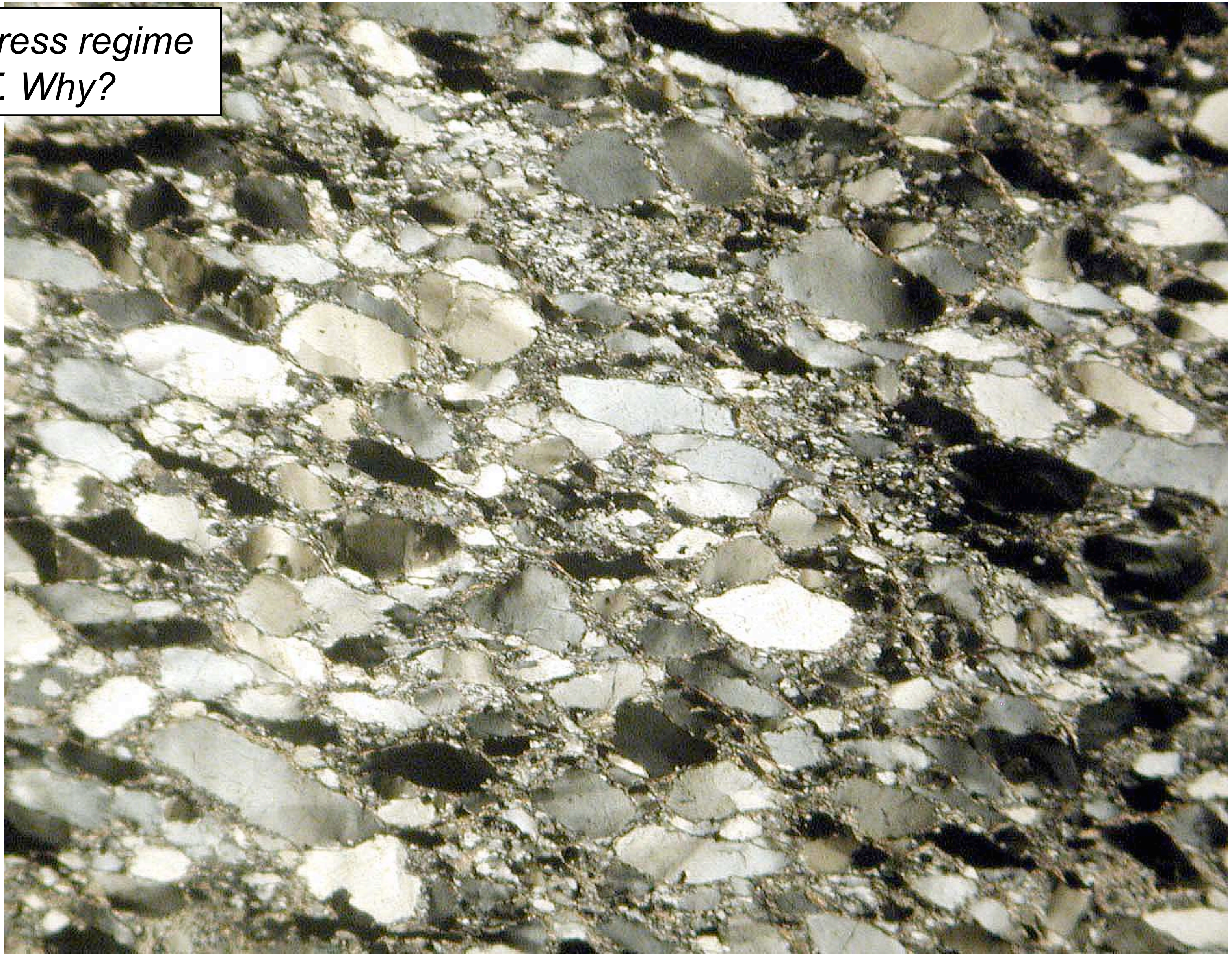
© GFZ Postdam

Crystals elongation & undulose extinction

➢ dislocation glide dominant

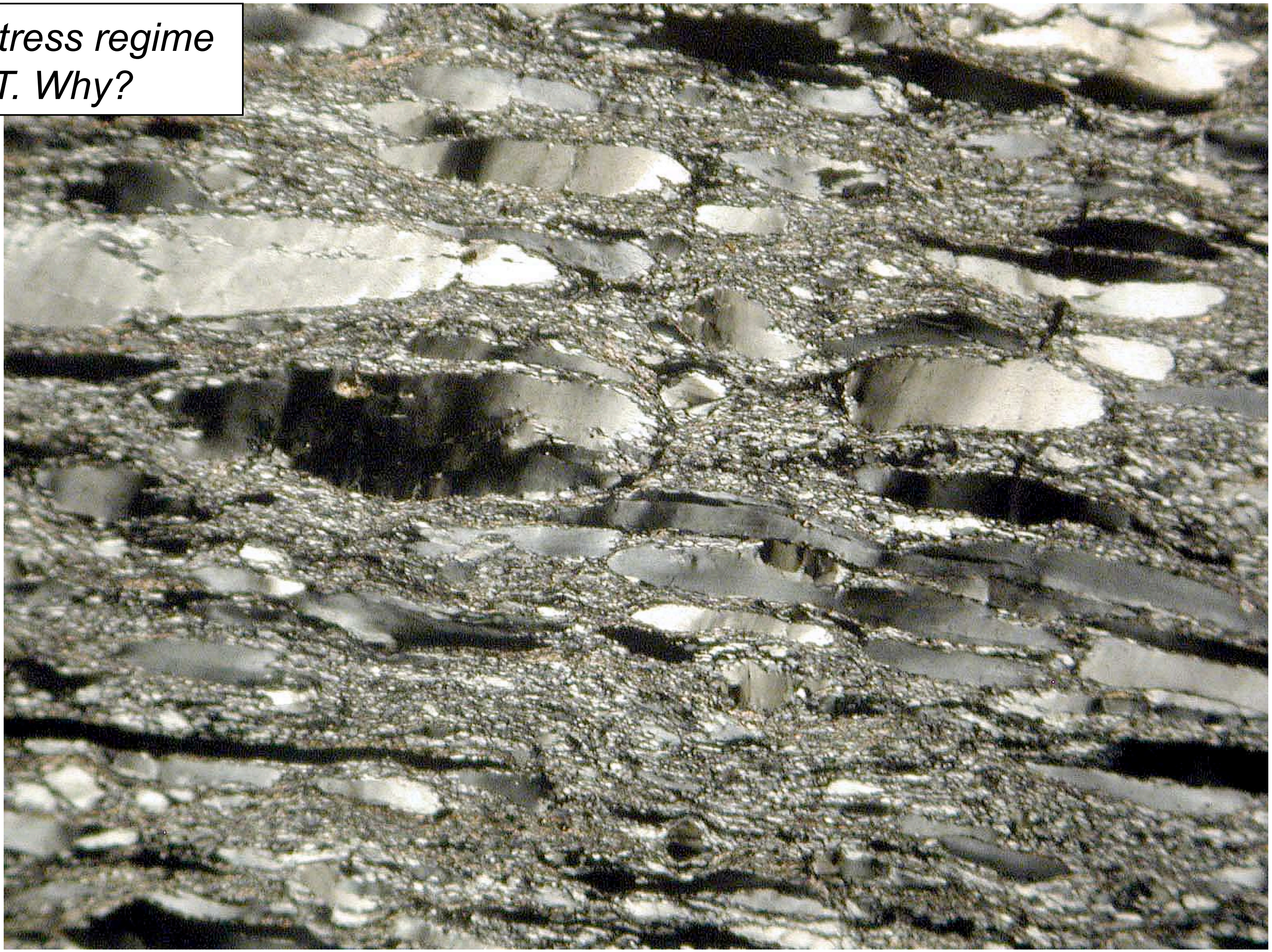
Quartz: crystals elongation & undulose extinction
+ recrystallization producing a very fine grained matrix

High stress regime
~ low T. Why?

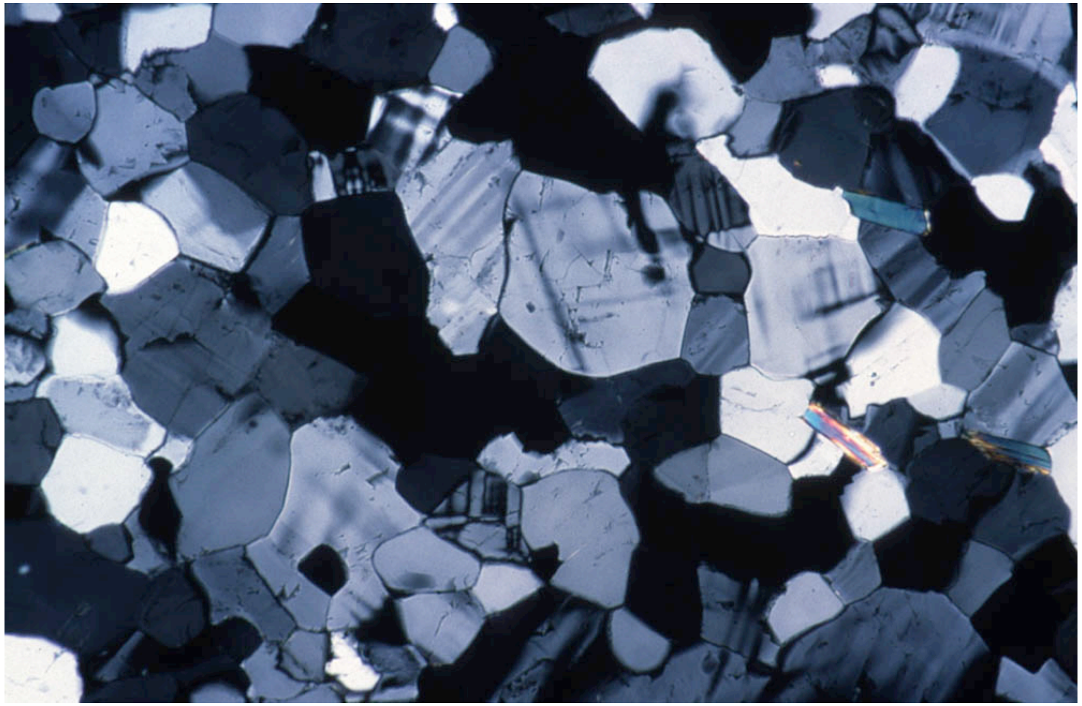


Quartz: crystals elongation & undulose extinction
+ recrystallization producing a very fine grained matrix

High stress regime
~ low T. Why?



Deformation of a polymineralic rock
Strenght contrasts between ≠ minerals = mechanical segregation

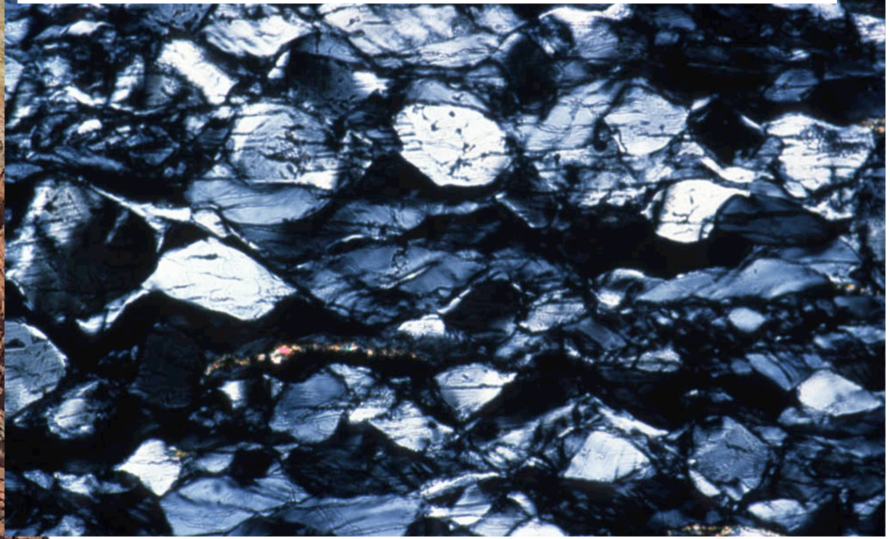


experimental deformation - Enfield aplite

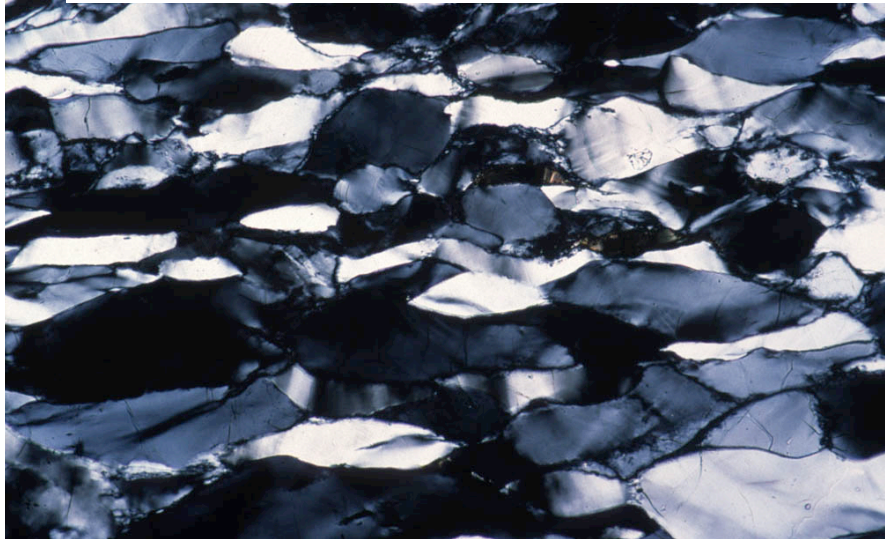
Quartz ~30%, microcline ~35%, oligoclase ~35%; 200µm in average

Quartz & feldspar = high strength contrast

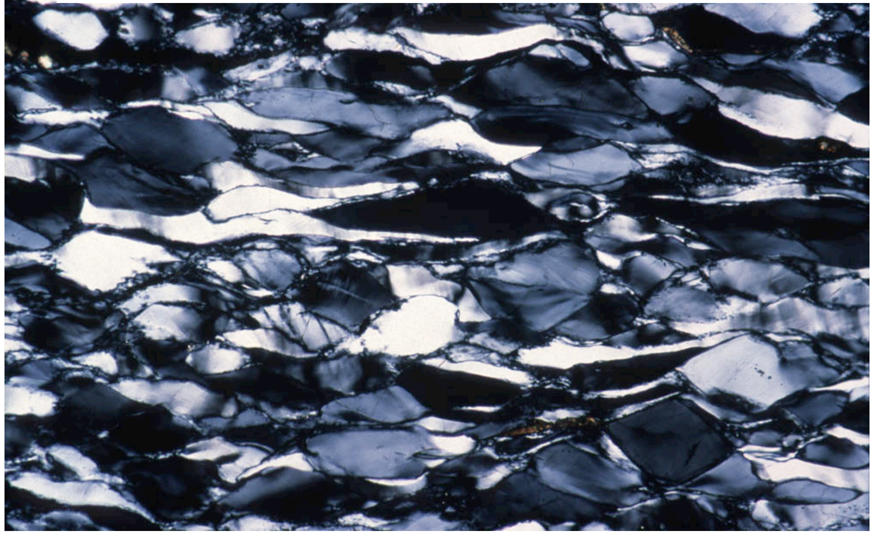
Dell'Angelo & Tullis
JStructGeol 1986



35% at 725°C, 10-6/sec, 1200 MPa



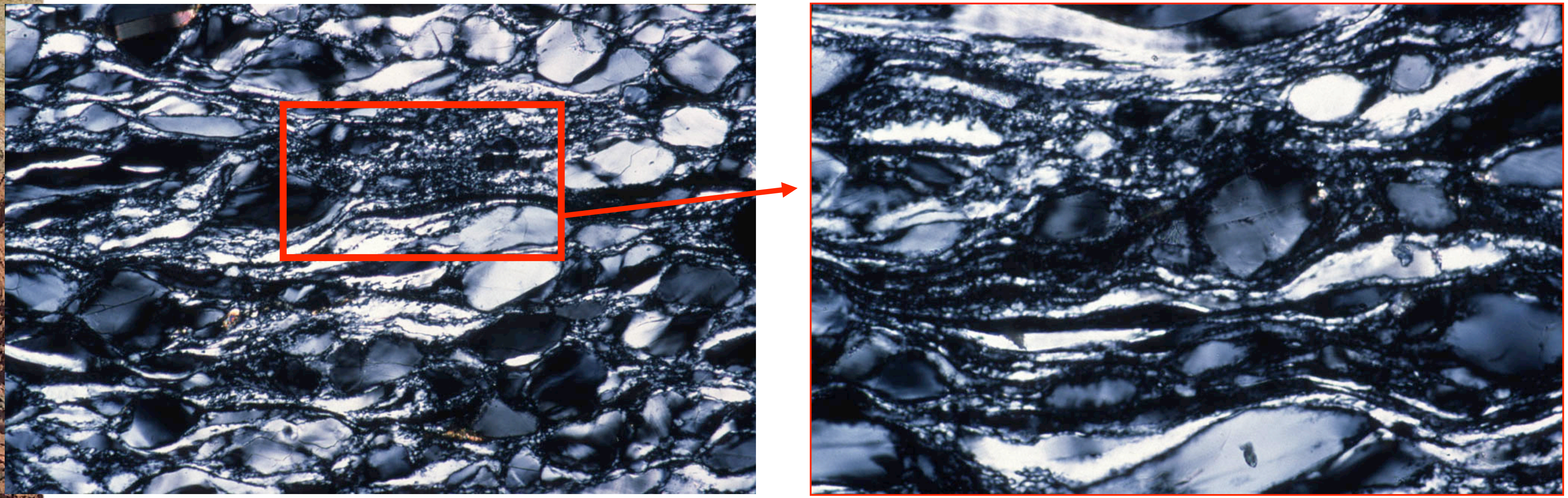
50% at 900°C, 10-6/sec, 1200 MPa.

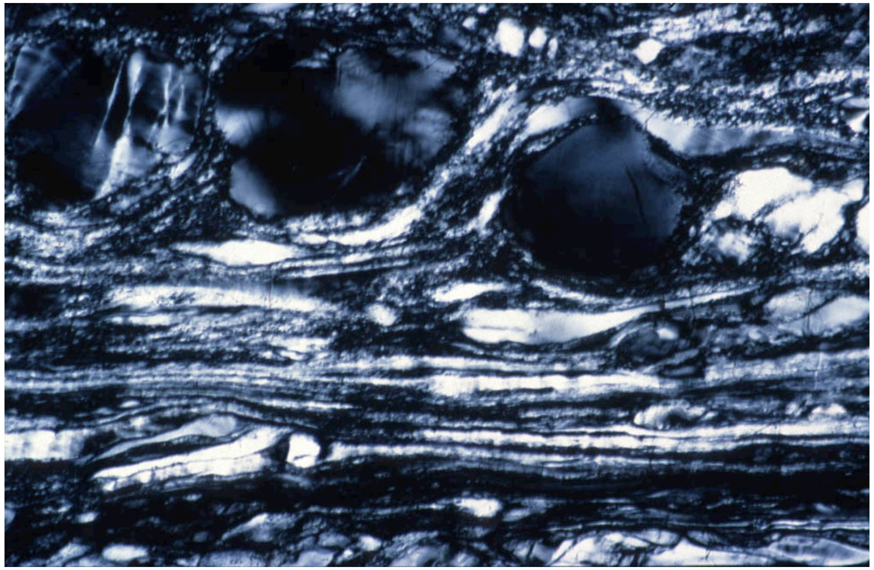


60% at 900°C, 10-6/sec, 1200 MPa

dextral shear
plus compression
= transpression

85% at 900°C, 10-6/sec, 1200 MPa

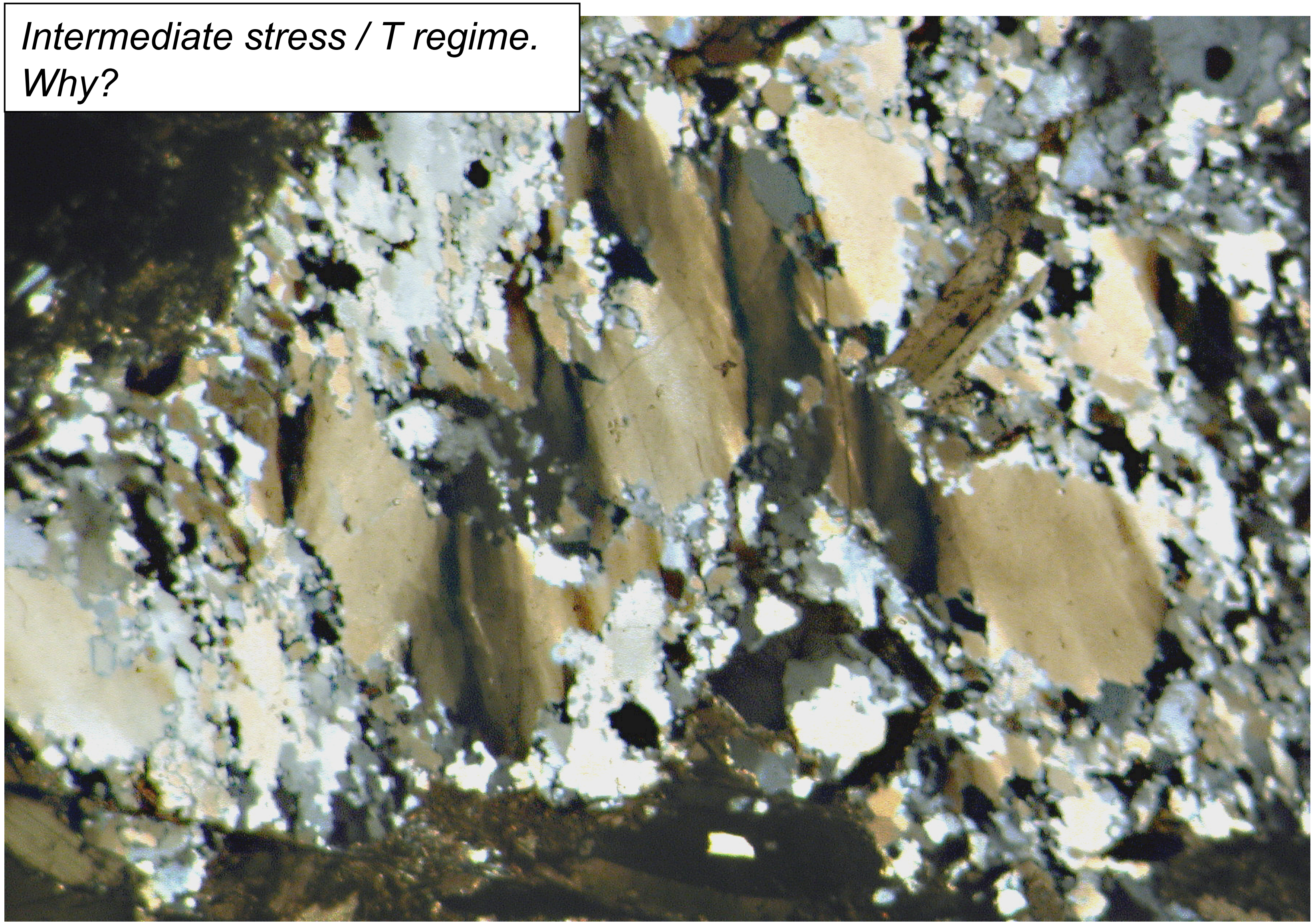




dextral shear (γ = 2.4)
plus compression
(~40% shortening)

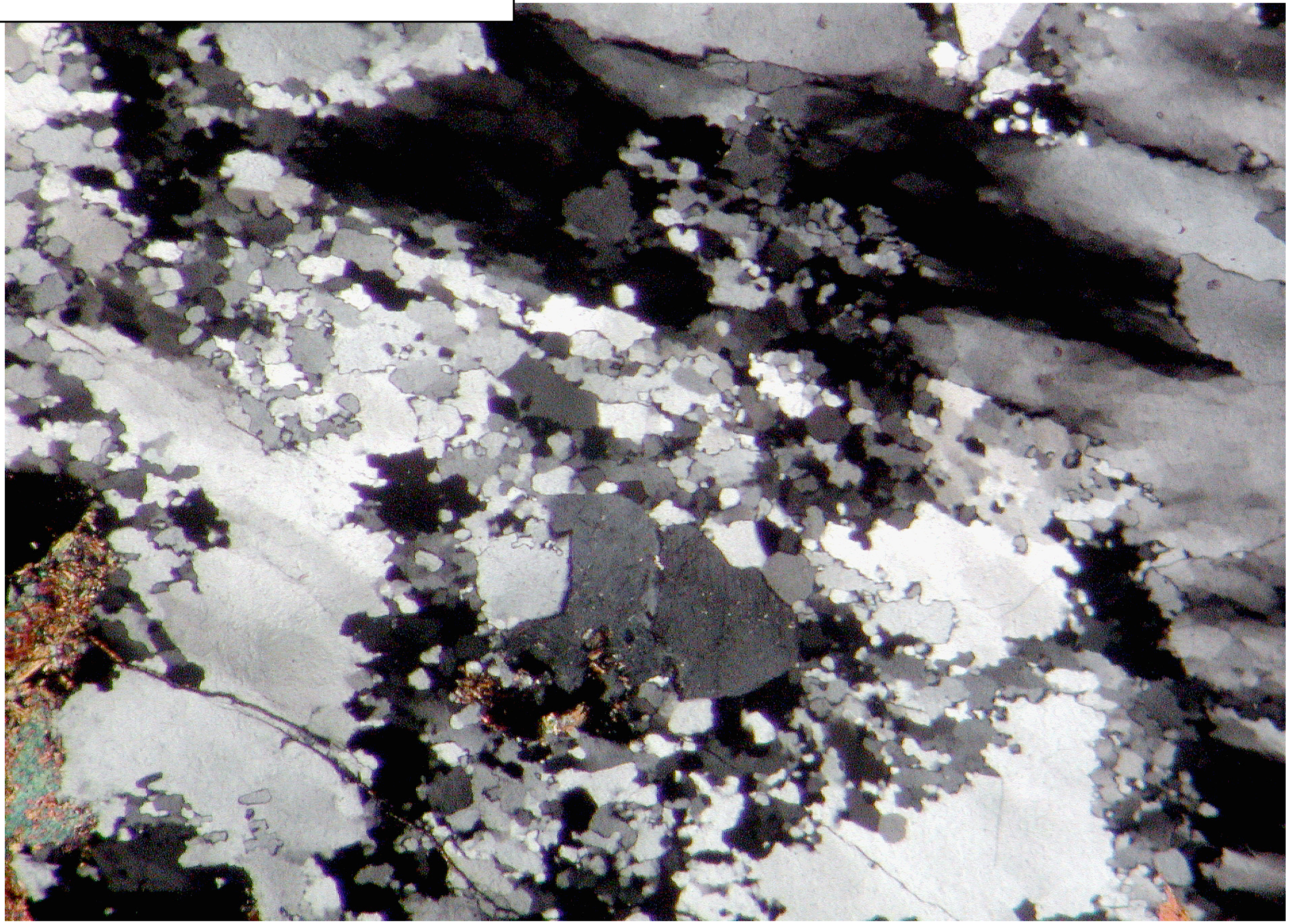
Quartz: subgrains + some (low range) grain boundary migration

Intermediate stress / T regime.
Why?



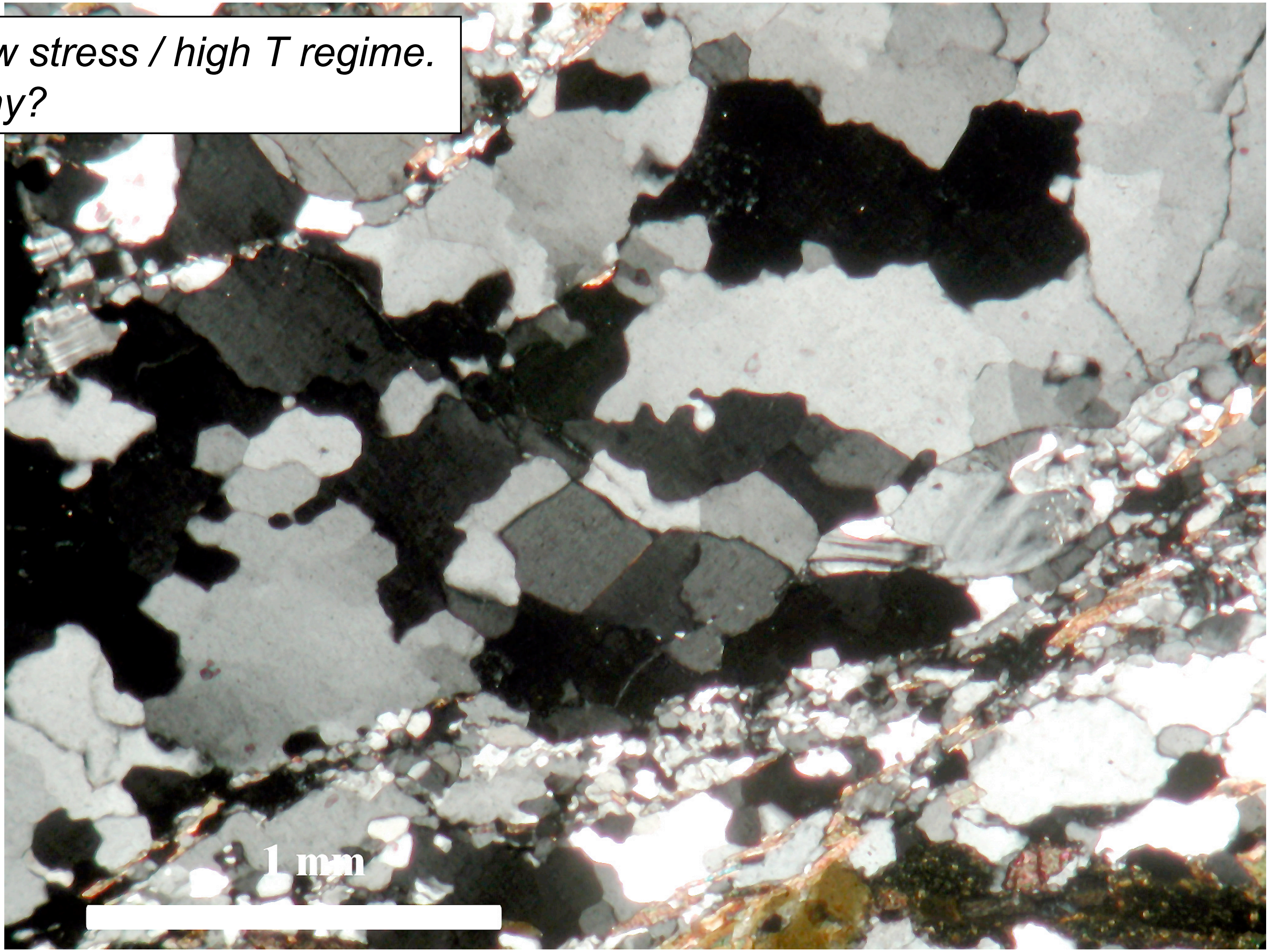
Quartz: subgrains + some (low range) grain boundary migration

Intermediate stress / T regime.
Why?



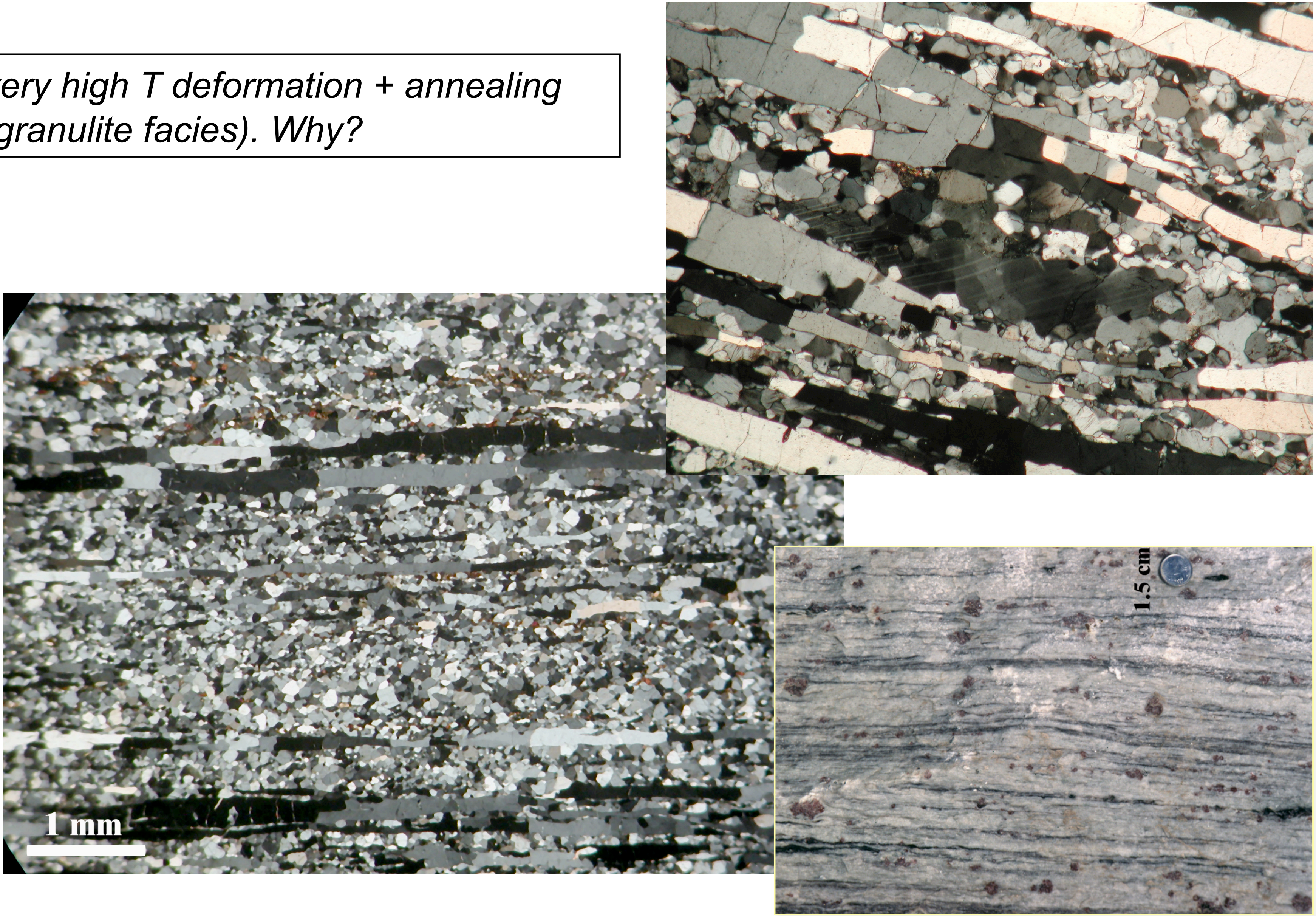
Quartz: grain boundary migration (+ subgrains)

Low stress / high T regime.
Why?

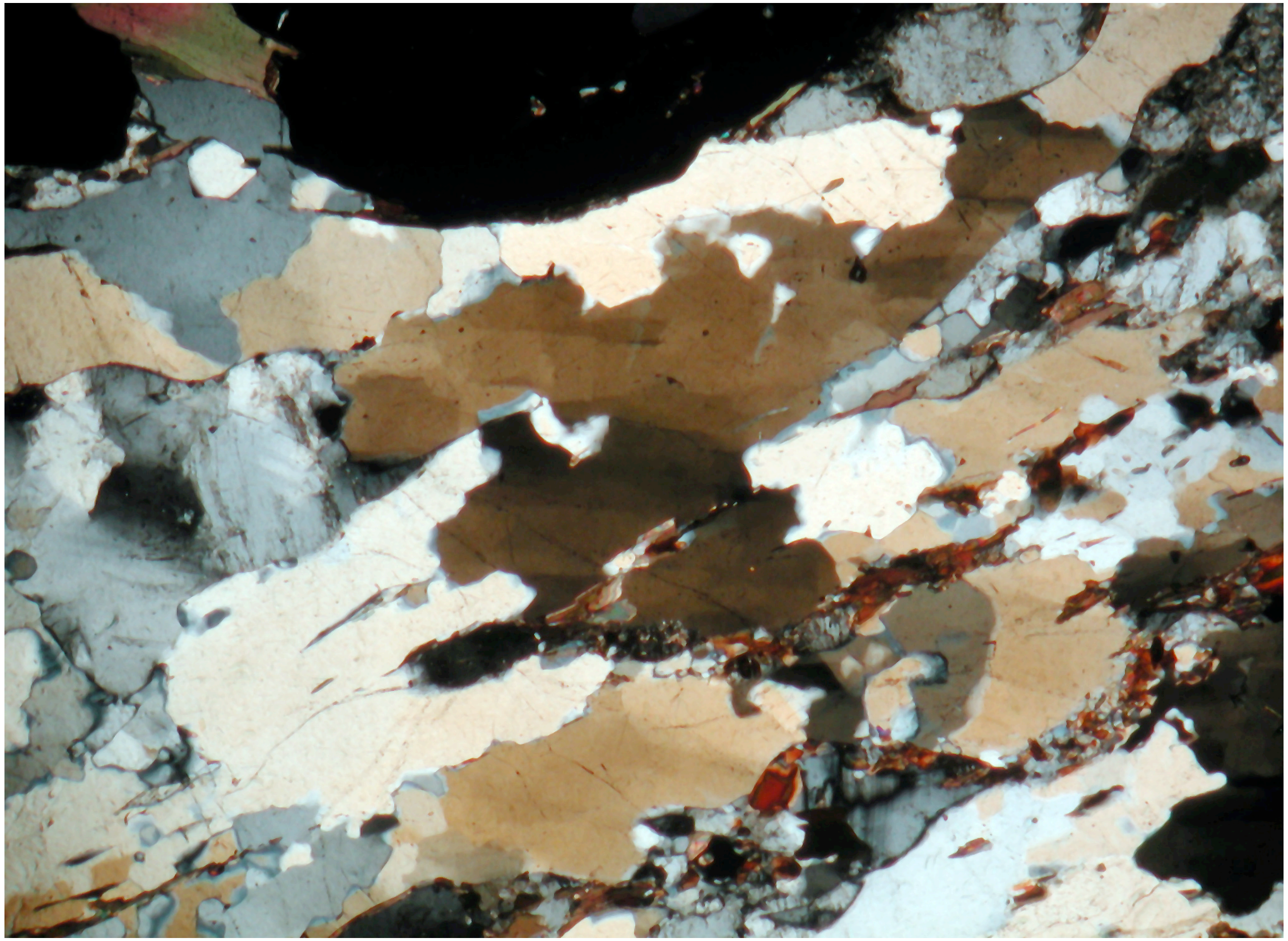


Quartz: grain boundary migration

very high T deformation + annealing (granulite facies). Why?

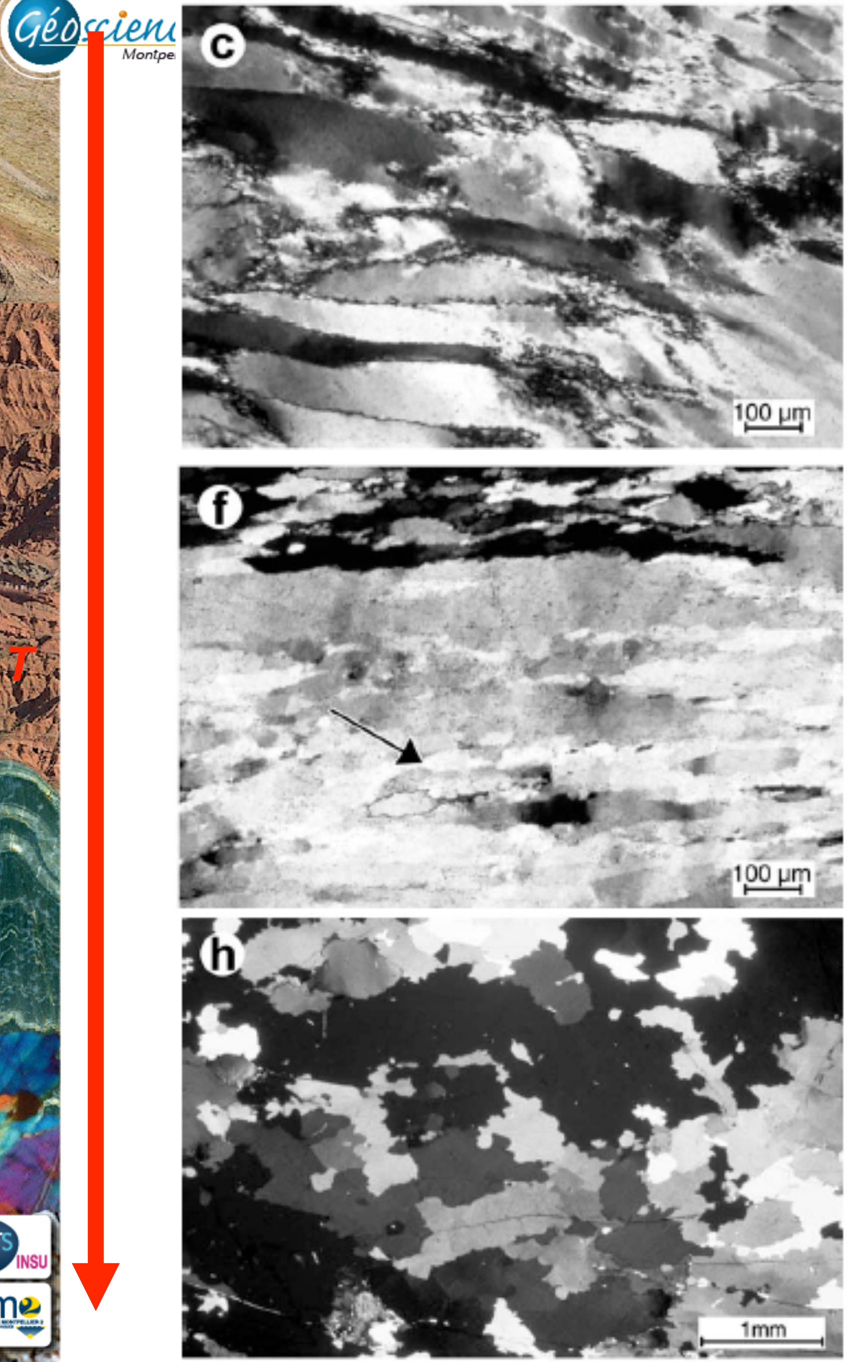


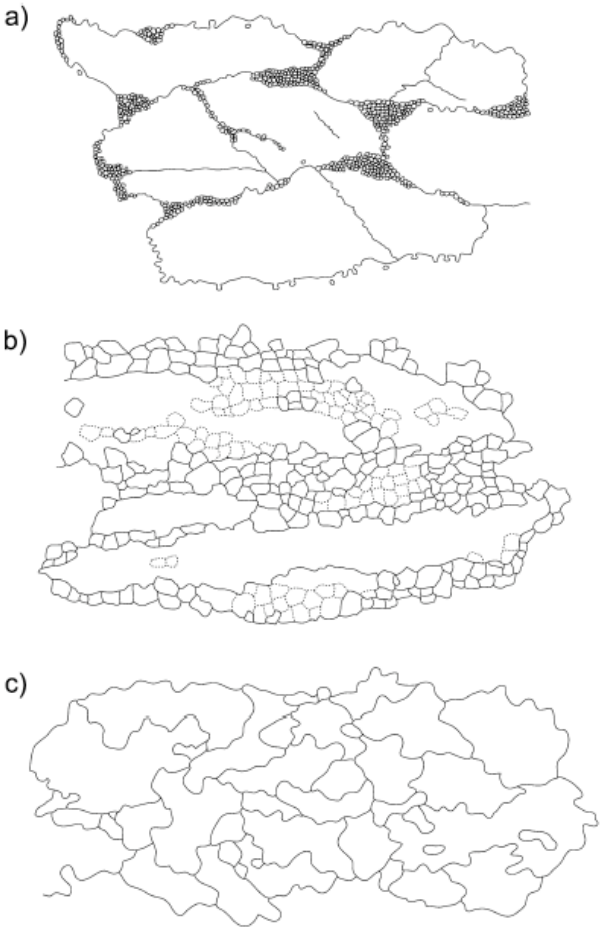
Quartz: grain boundary migration + subgrains



Superimposed deformations - decreasing T

Quartz : dynamic recrystallization





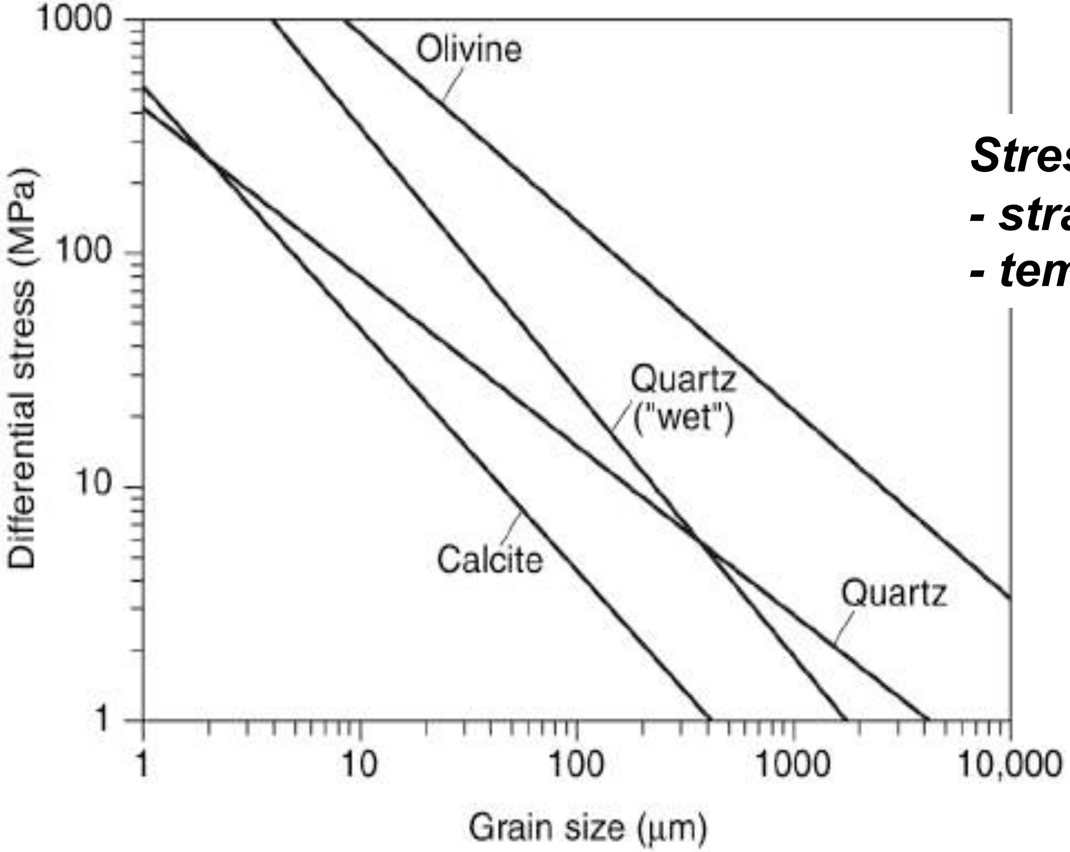
bulging

subgrain rotation

grain bondary migration

M. Stipp et al. / Journal of Structural Geology 24 (2002)

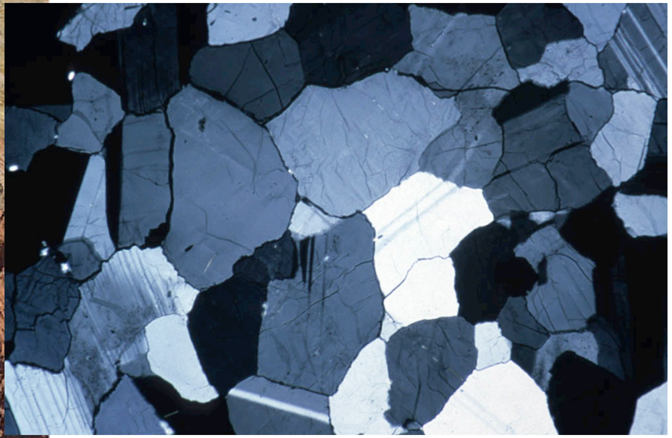
Dynamic recristallization
Relation recrystallized grain size - stress



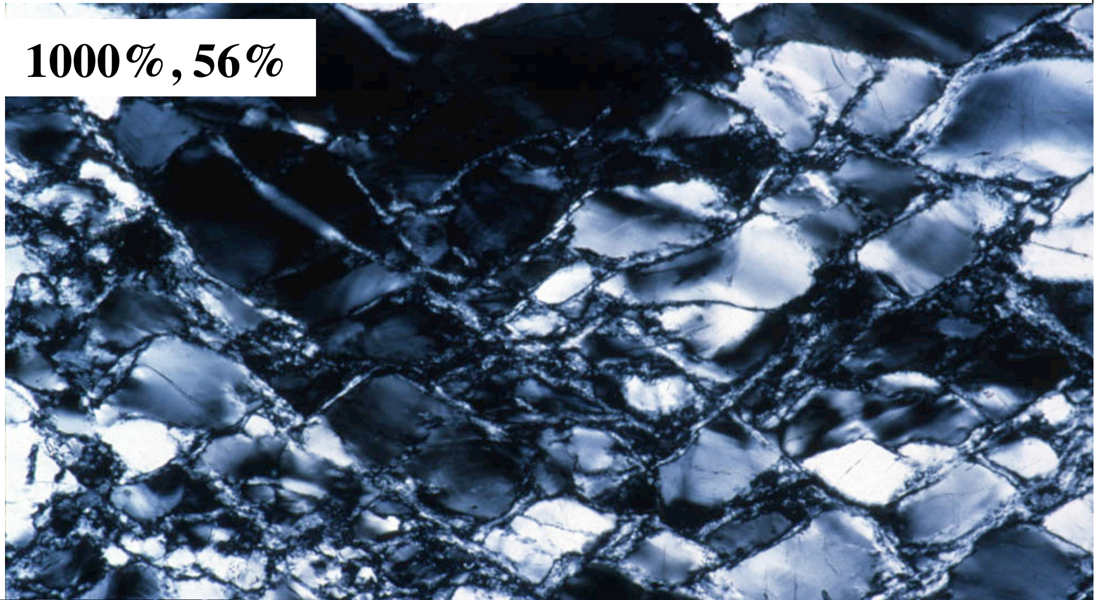
Stress depends on
- strain rate
- temperature

Deformation mechanisms depend on grain size…
May dynamic recrystallization result in a change from dislocation to diffusion creep? Under which conditions?

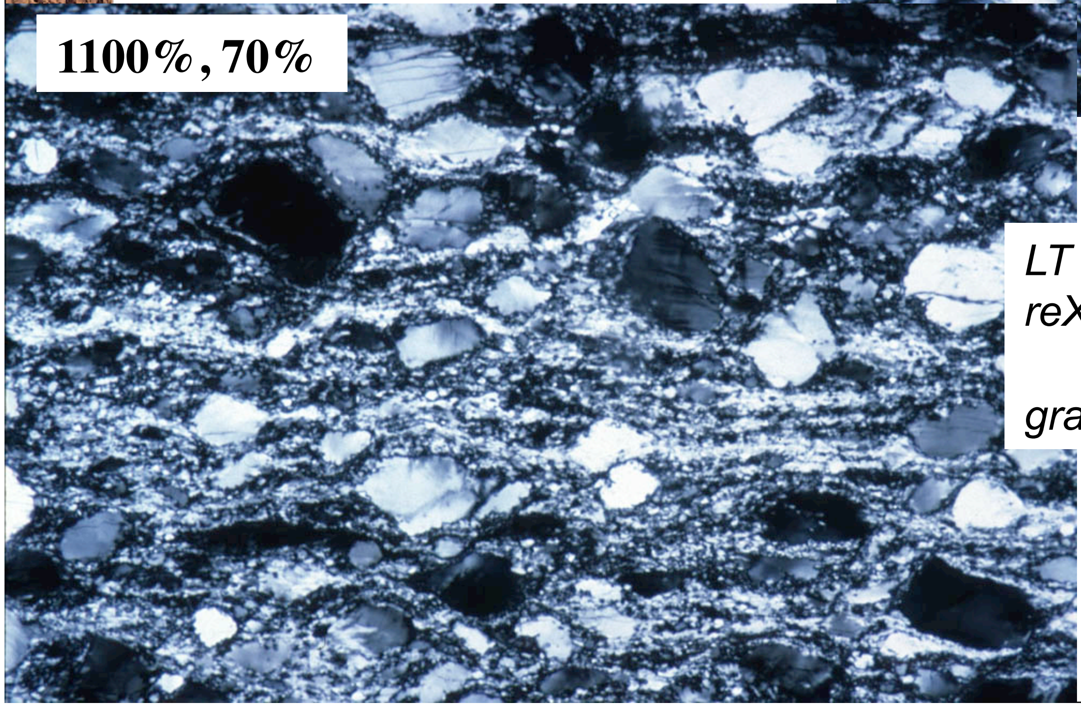
Experimentally deformed feldspar aggregate (J. Tullis)



starting material: Yale albite
10-6/sec, 1200 MPa

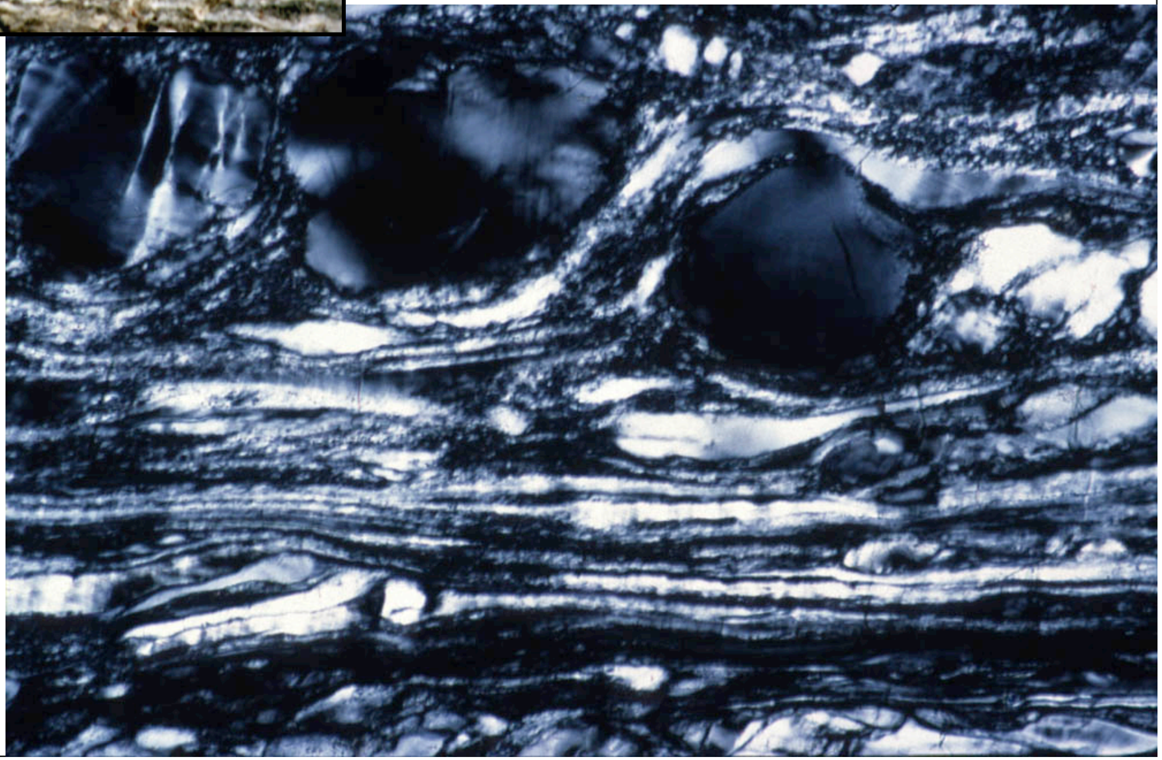


1000%, 56%

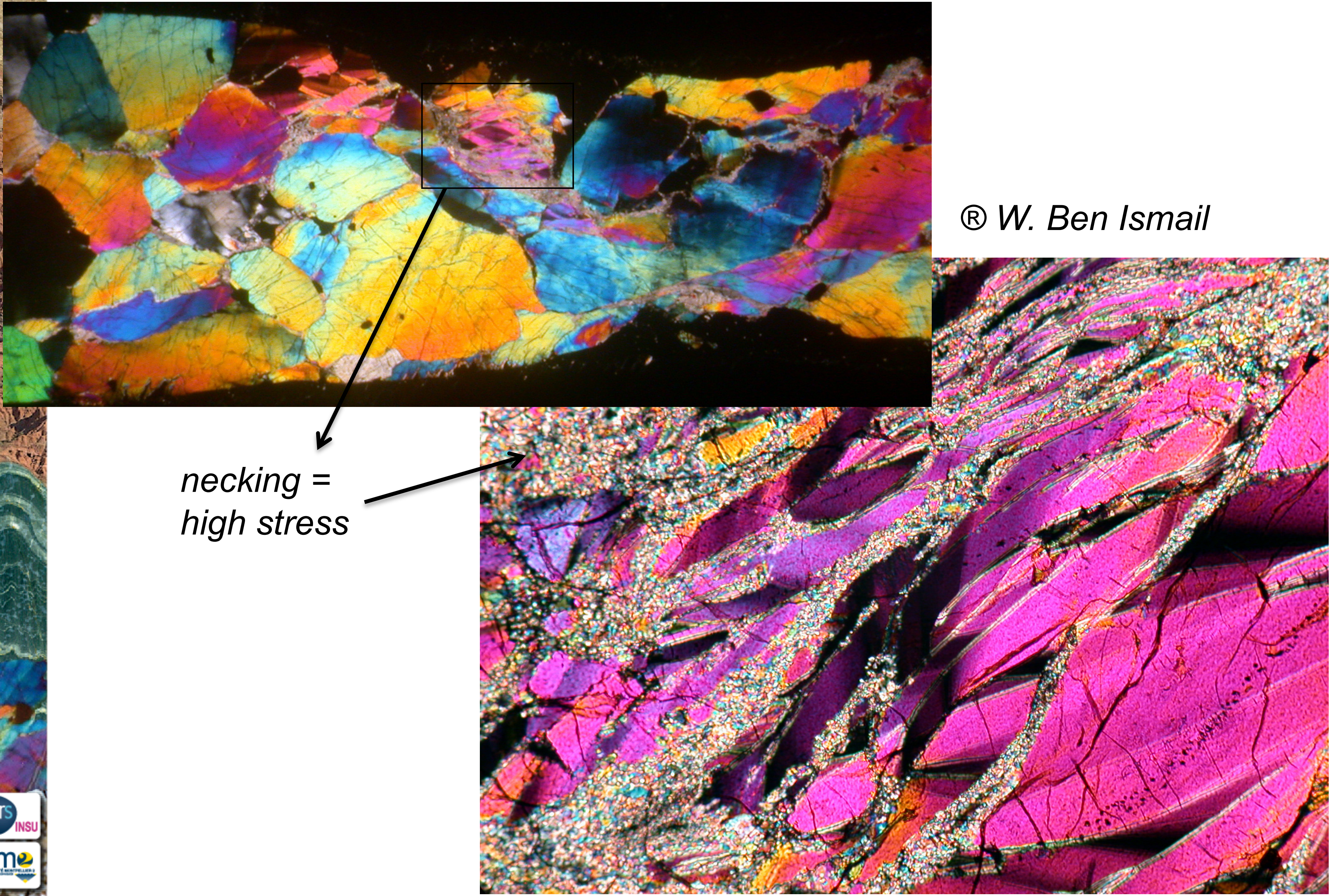


1100%, 70%

LT dislocation creep, hardening
reX bulging: low GB mobility, driving force
(stress) = high
grain size reduction by continuous reX



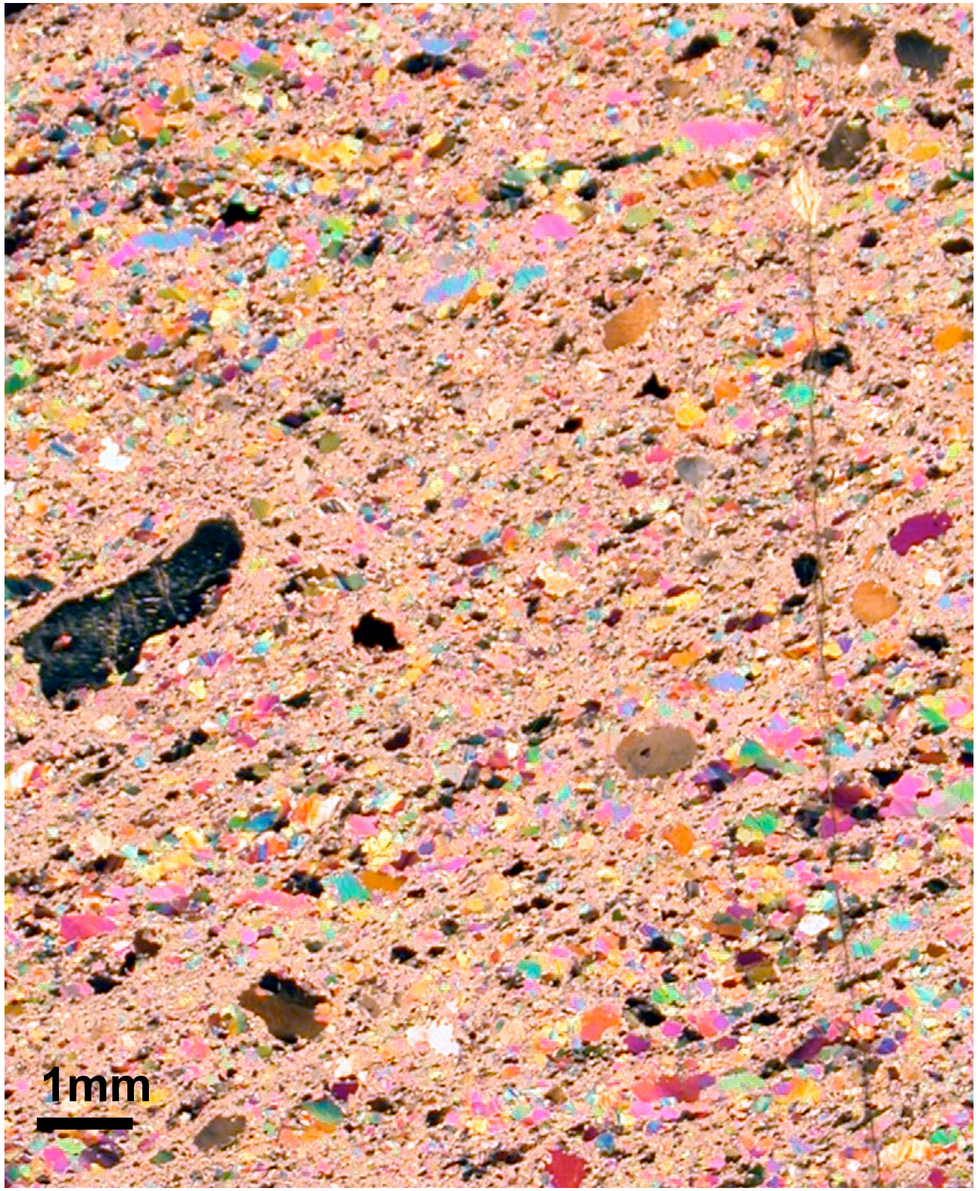
experimental deformation = extension - olivine – 1200°C & $10^{-5}s^{-1}$



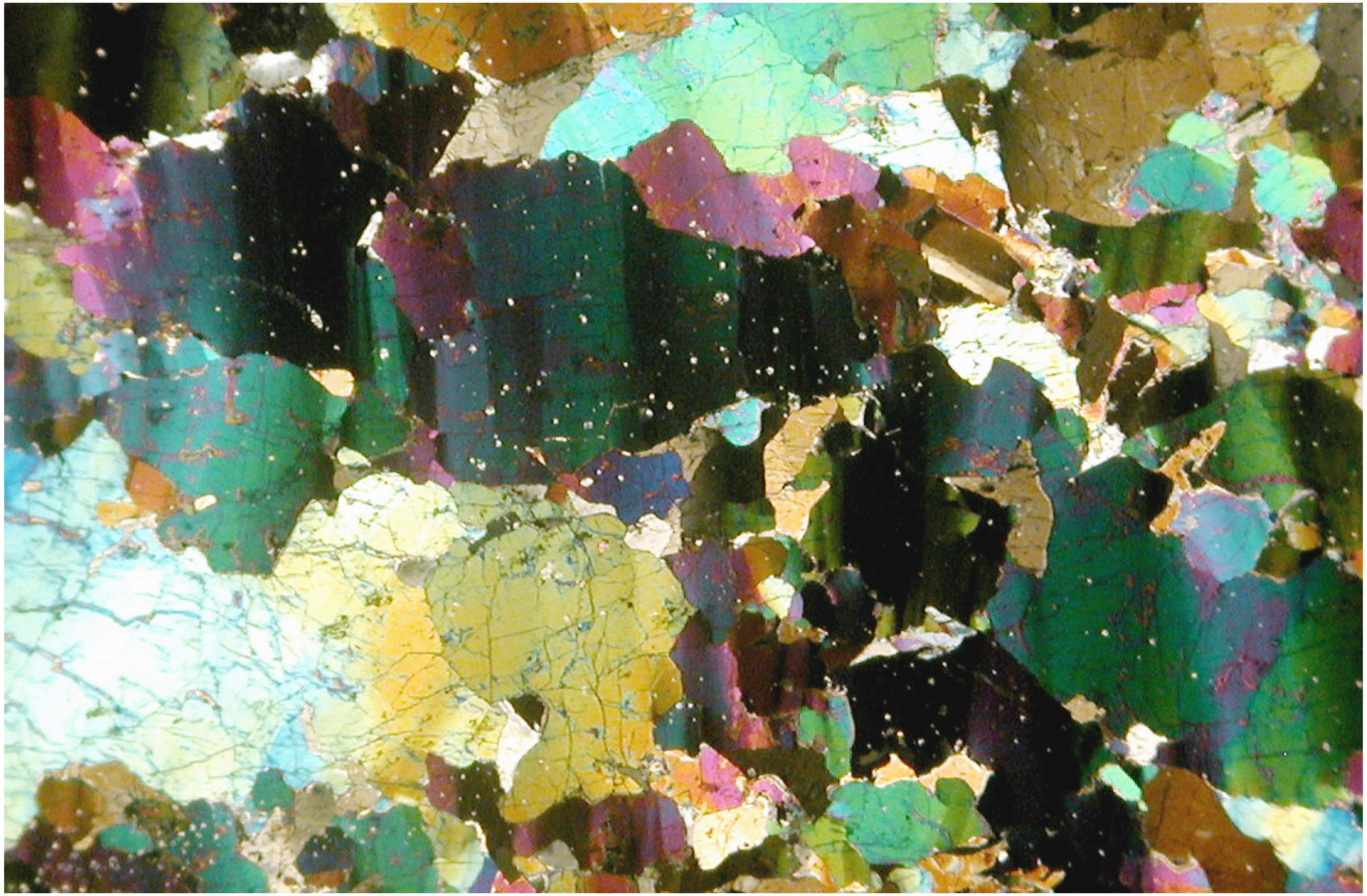
® W. Ben Ismail

necking =
high stress

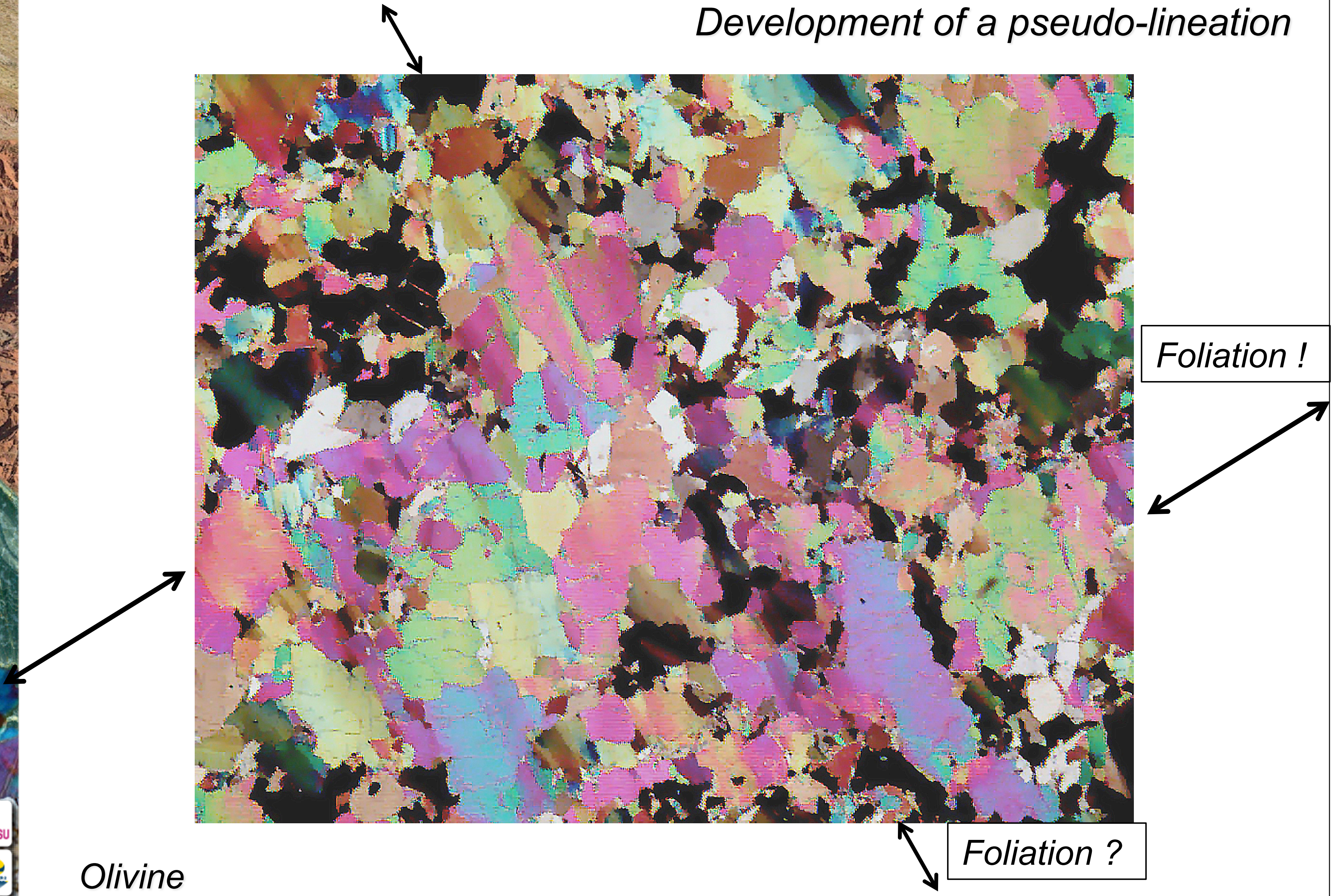
olivine – low T (~900°C) deformation
Mylonite = basal thrust of the Oman ophiolite



HT deformation of mantle rock (olivine-rich):
grain elongation & undulose extinction
well-developed subgrains & grain boundary migration
= dislocations motion and diffusion active = DISLOCATION CREEP



A possible effect of subgrain rotation recrystallization:
Change in grain shapes
Development of a pseudo-lineation

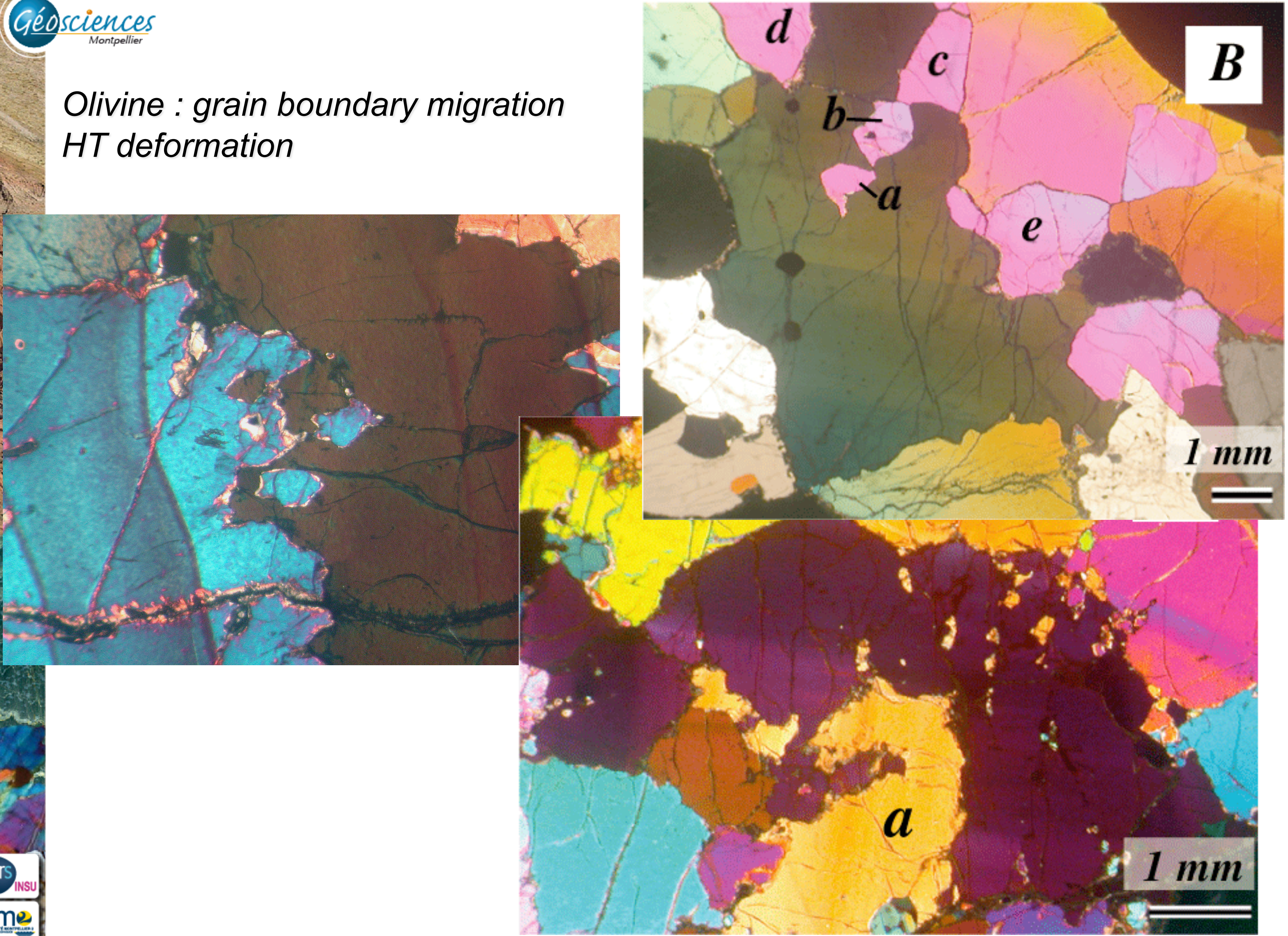


Foliation !

Foliation ?

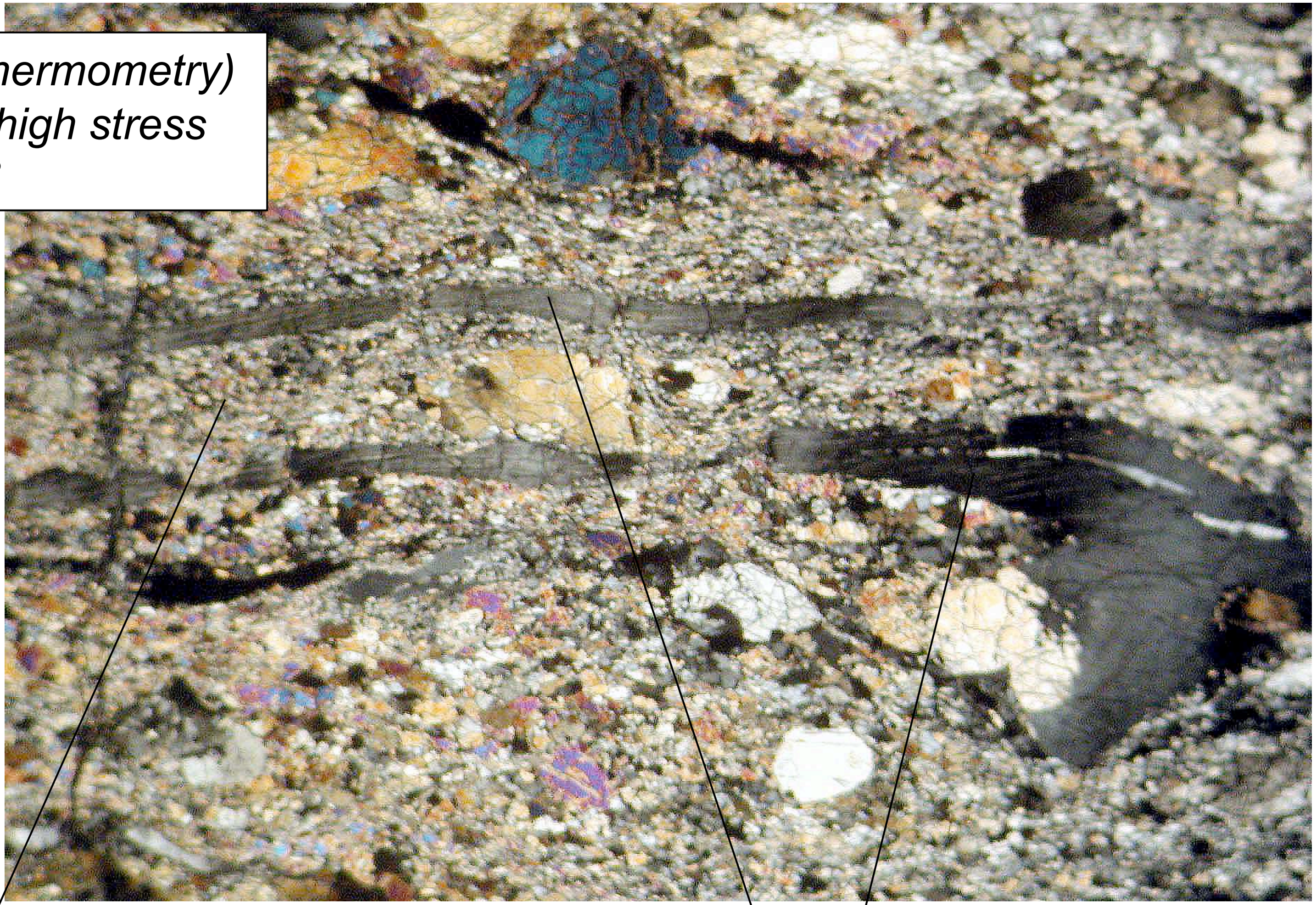
Olivine

Olivine : grain boundary migration
HT deformation



mylonitic peridotite, Kapvaal

HT (thermometry)
AND high stress
Why?

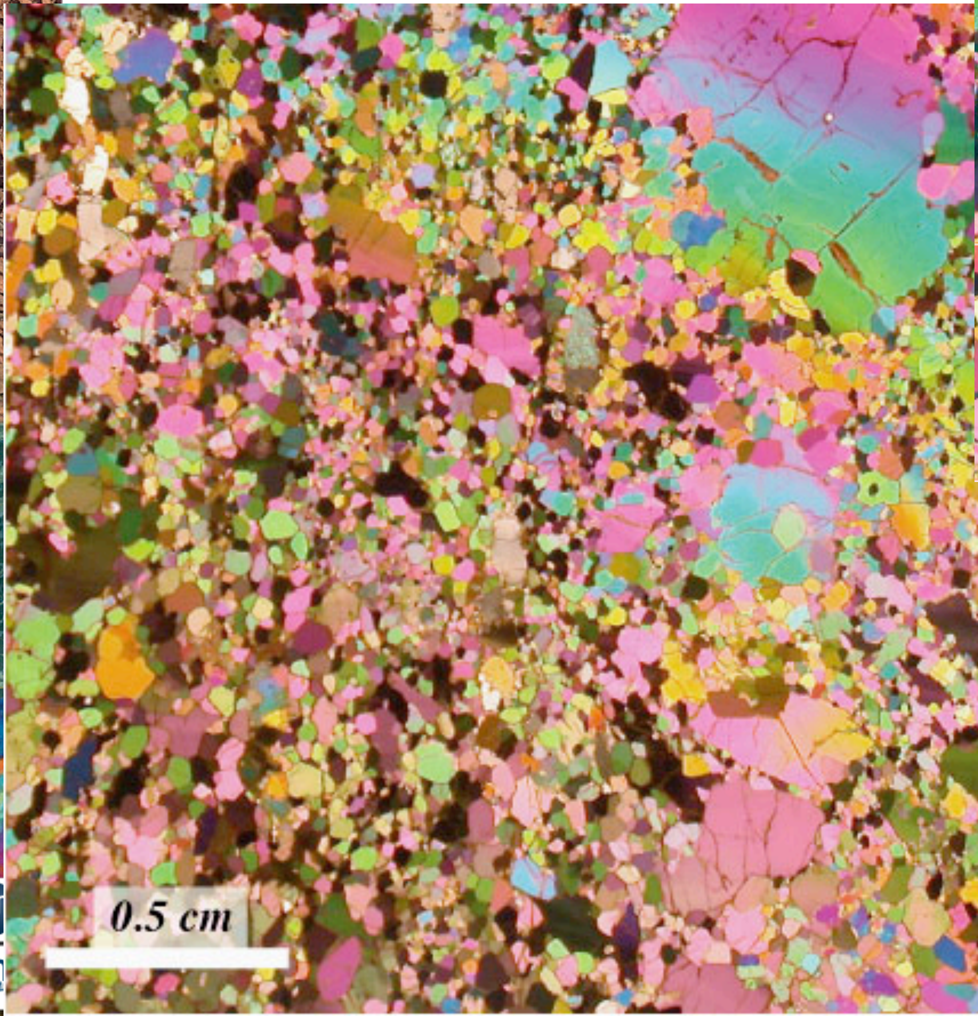


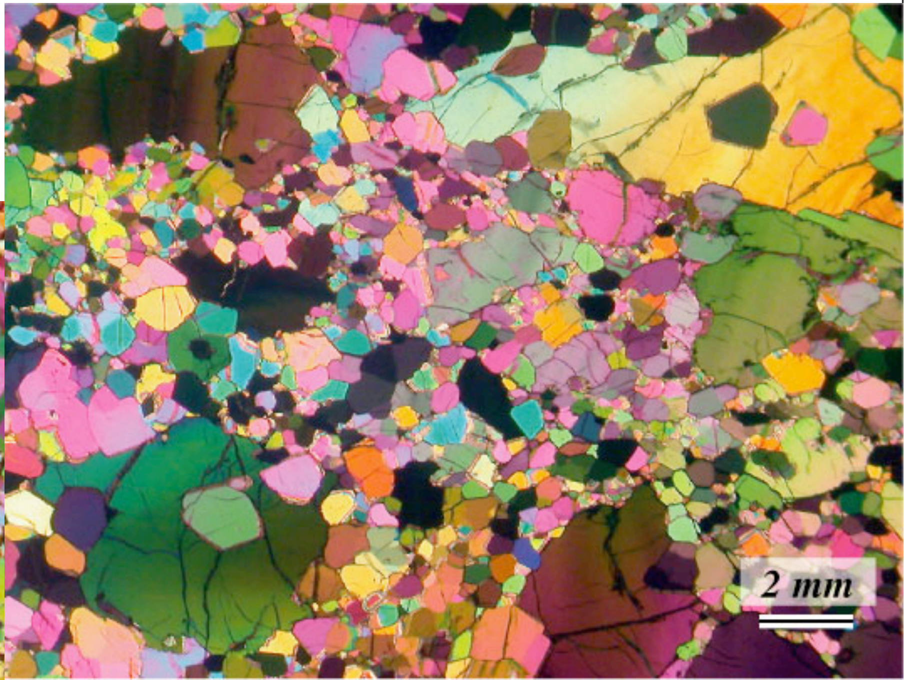
Olivine = strong recrystallization

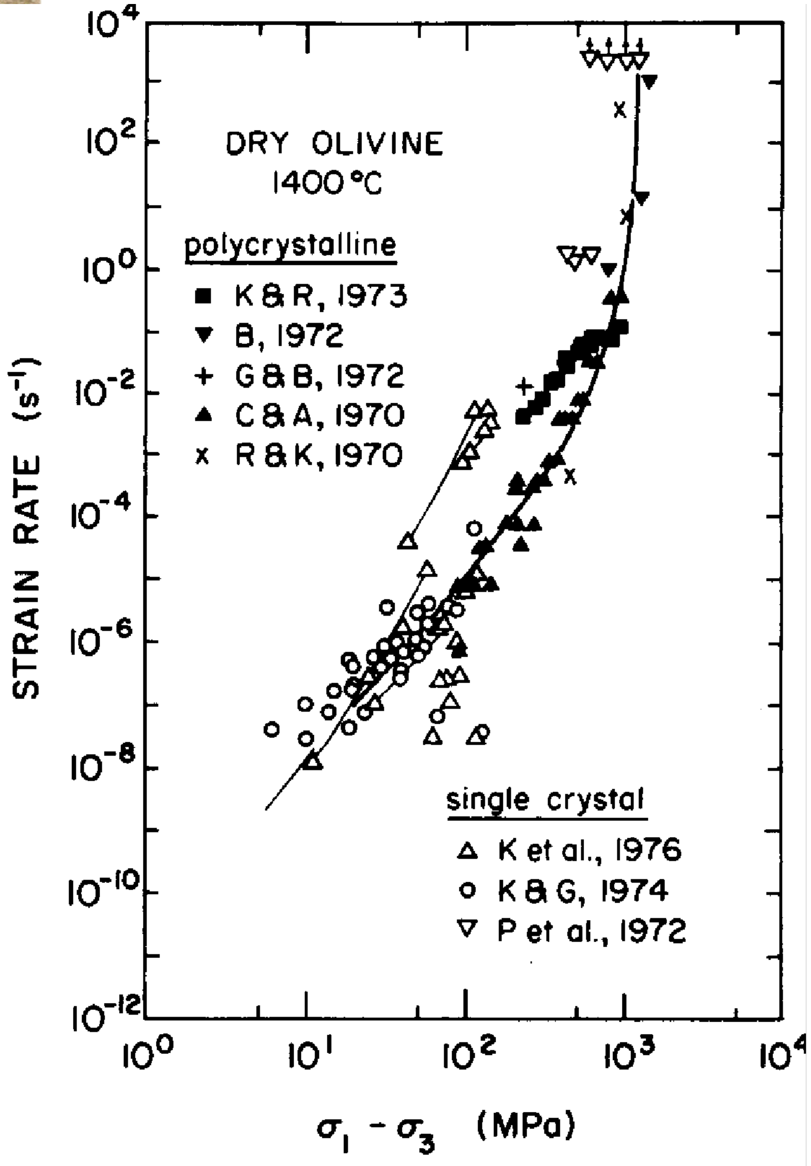
Opx = dislocation glide

Olivine : nucleation recrystallization + grain boundary migration

Very HT (~1400°C thermometry)
Dynamic or static?







Stress – strain rate relation in deformation experiments

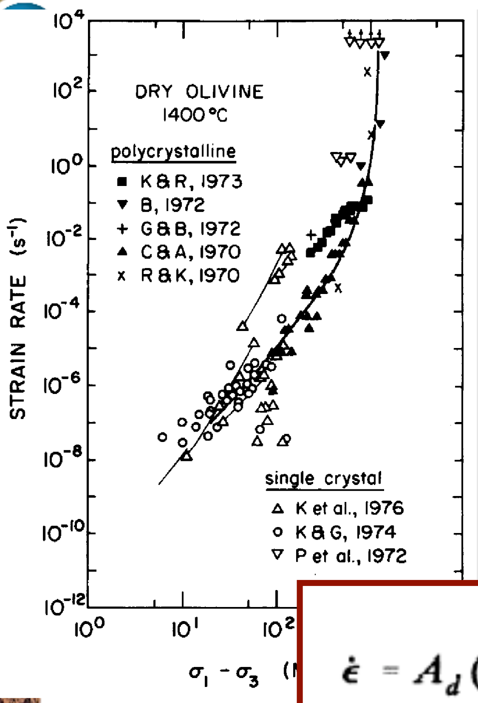
- ➢ *dominant deformation process*

dislocation creep
(glide + climb + reX)

$$\dot{\epsilon} = A_d (\sigma_1 - \sigma_3)^n \exp\left(-\frac{Q_d + PV_d}{RT}\right)$$

diffusion creep
(± grain boundary sliding)

$$\dot{\epsilon} = A_{gb} \frac{(\sigma_1 - \sigma_3)}{d^3} \exp\left(-\frac{Q_{gb} + PV_{gb}}{RT}\right)$$

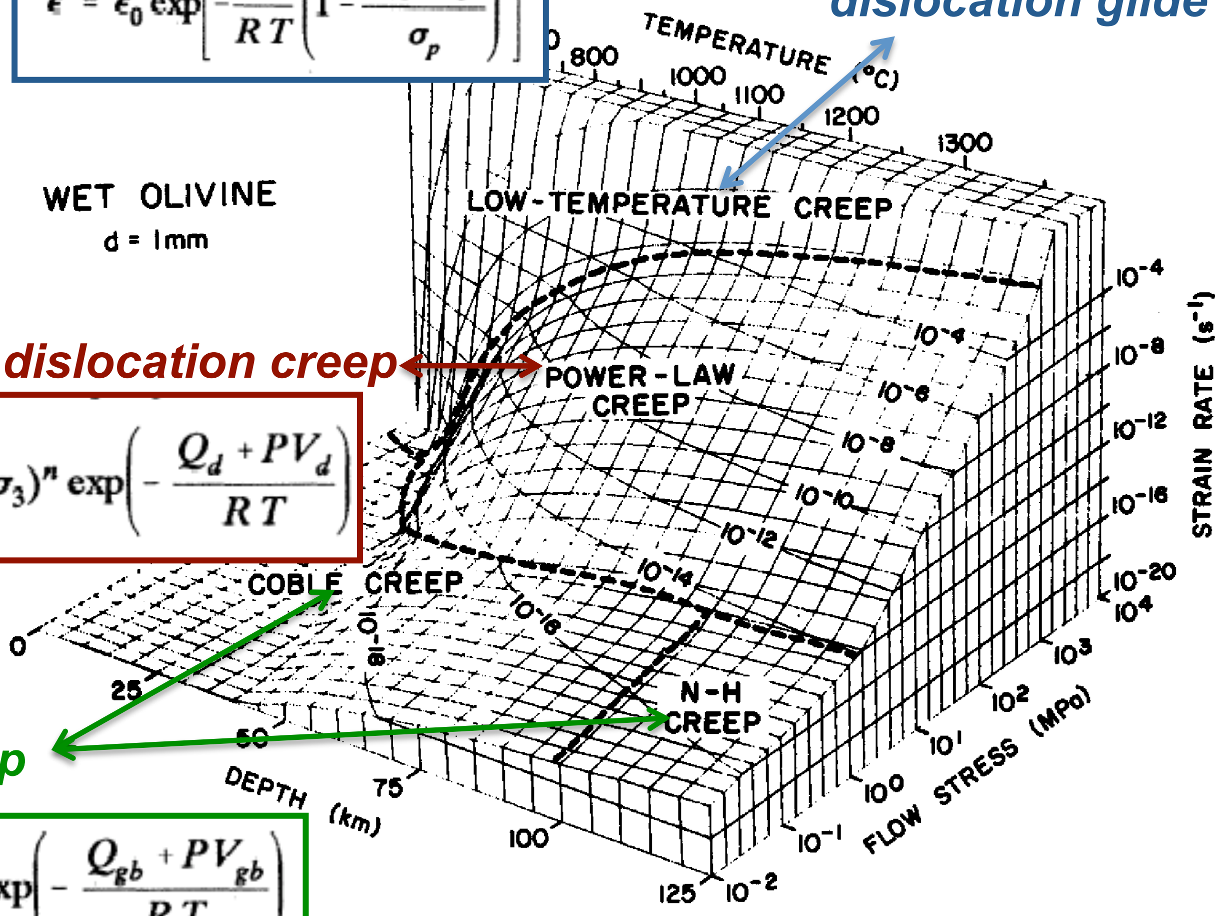


Deformation mechanisms maps

dry olivine polycrystals (dunite)

$$\dot{\epsilon} = \dot{\epsilon}_0 \exp\left[-\frac{Q_d'}{RT}\left(1-\frac{(\sigma_1-\sigma_3)}{\sigma_p}\right)^2\right]$$

dislocation glide



dislocation creep

$$\dot{\epsilon} = A_d(\sigma_1-\sigma_3)^n \exp\left(-\frac{Q_d+PV_d}{RT}\right)$$

diffusion creep

$$\dot{\epsilon} = A_{gb}\frac{(\sigma_1-\sigma_3)}{d^3}\exp\left(-\frac{Q_{gb}+PV_{gb}}{RT}\right)$$

Remember: Experimental points used to define these maps are obtained in a very limited T, strain rate, and grain size range => lots of extrapolation!!!

Dislocation creep - high T/Tm

power-law creep

constant

Burgers vector

Stress exponent
(>2, usually 3)

$$\dot{\varepsilon} = A\, D_{eff}\, \frac{\mu b}{kT}\left(\frac{\sigma}{\mu}\right)^{n}$$

Strain rate

diffusivity

Boltzmann constant
1.32E-23 J/mol

Shear modulus

T in K

$\dot{\varepsilon}\ s^{-1}$

$\sigma\ Pa$

Apparent
(macroscopic)
activation energy

$$\dot{\varepsilon} = A \exp\frac{-Q}{RT}\sigma^{n}$$

Other parameters also affect the mechanical behavior...

from Hirth and Kohlstedt, 2004

melt fraction
$\dot{\varepsilon} \propto e^{-\alpha\phi}$

grain size
$\dot{\varepsilon} \propto d^{0\text{-}3}$

stress
$\dot{\varepsilon} \propto \sigma^{1\text{-}3.5}$