Deformation and anisotropy of physical properties: From the crystal to the rock and plate scale - 1

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Internal Geophysics School
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What will we talk about?

- Many physical properties, not only seismics, are anisotropic
- Physical causes of anisotropy at:
  - the crystal scale? The crystals structure!
  - at larger scales? Deformation!
- How rocks deform ductilely and why they become anisotropic (in short)
- Using forward models to constrain the interpretation of flow patterns from seismic anisotropy : the D'' example
- Why inversing flow patterns from seismic data is not possible?
- Viscous anisotropy: the memory of deformation

How will we work?

- Course = 1h (questions welcome @ anytime)
- 15 minutes of discussion in groups of 5-6 on what was clear / not clear (take notes!)
- 15 minutes plenary discussion of the not clear points

Anisotropy - variation of a physical property depending on the direction in which it is measured

Oxford Dictionary

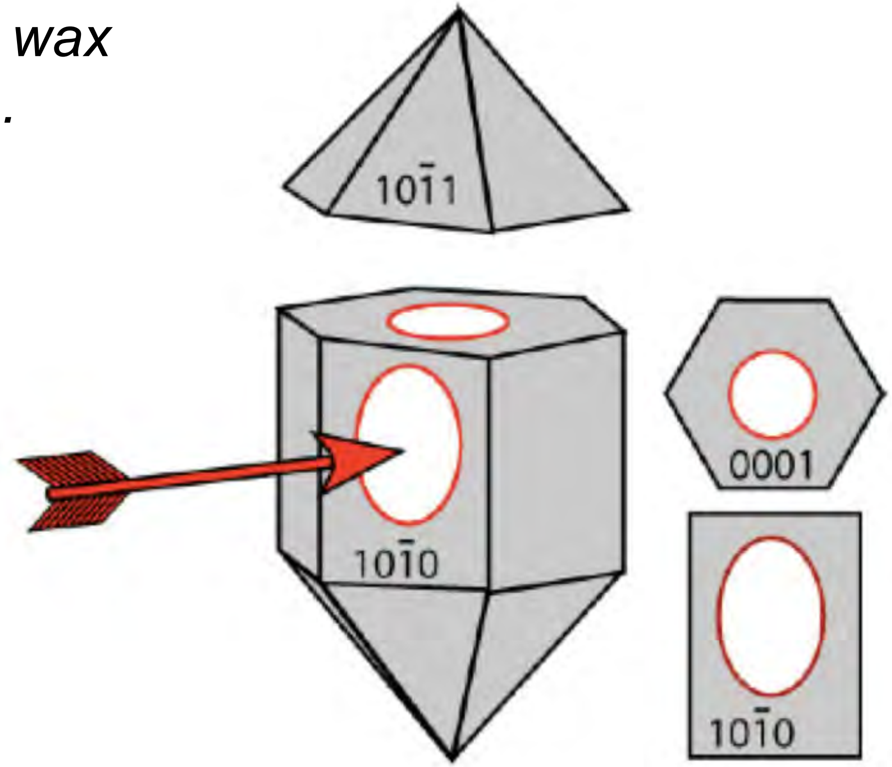
Physical properties

- *Elasticity : seismic wave propagation*
- *Electrical/Magnetic/Thermal Conductivity*
- *Optical properties*
- *Strength/viscosity*

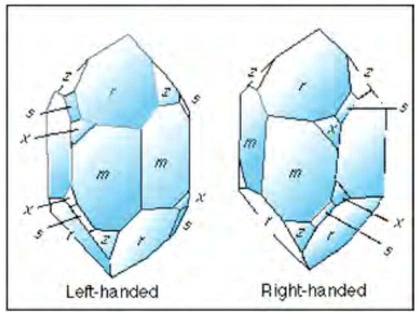
Heat diffusion in a quartz crystal

If we cover a quartz crystal with wax and touch it with a hot needle …

Radial heat flux (q) (controlled by crystal properties not boundary conditions)

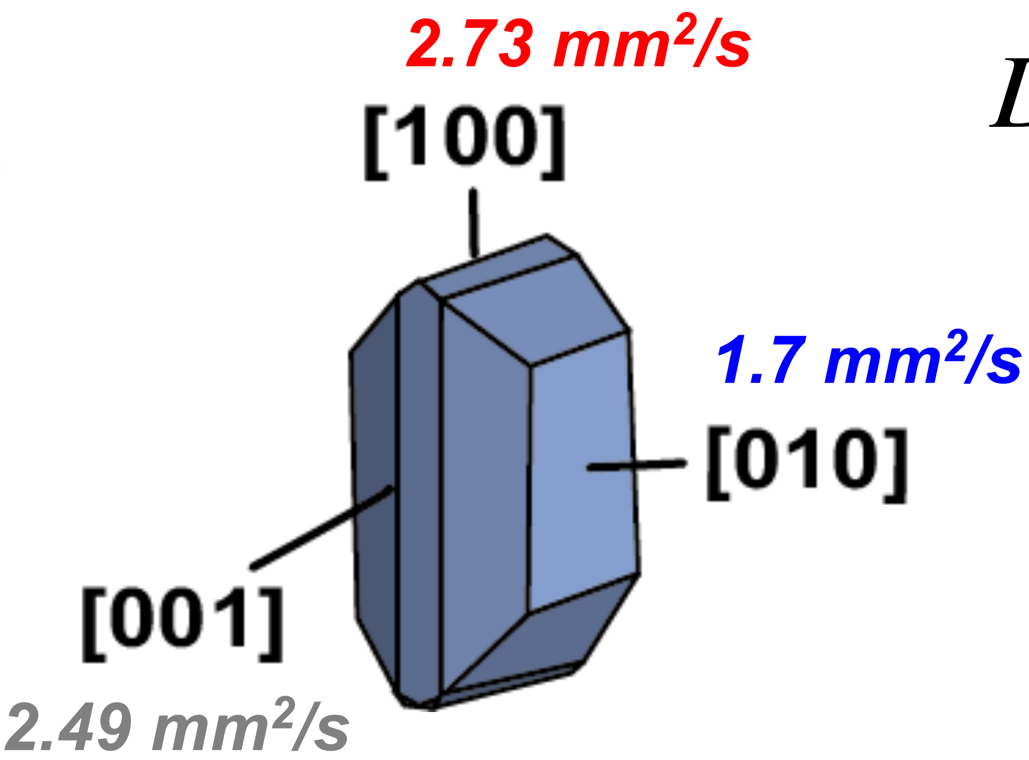


Melting figures are ≠ in ≠ crystallographic faces!



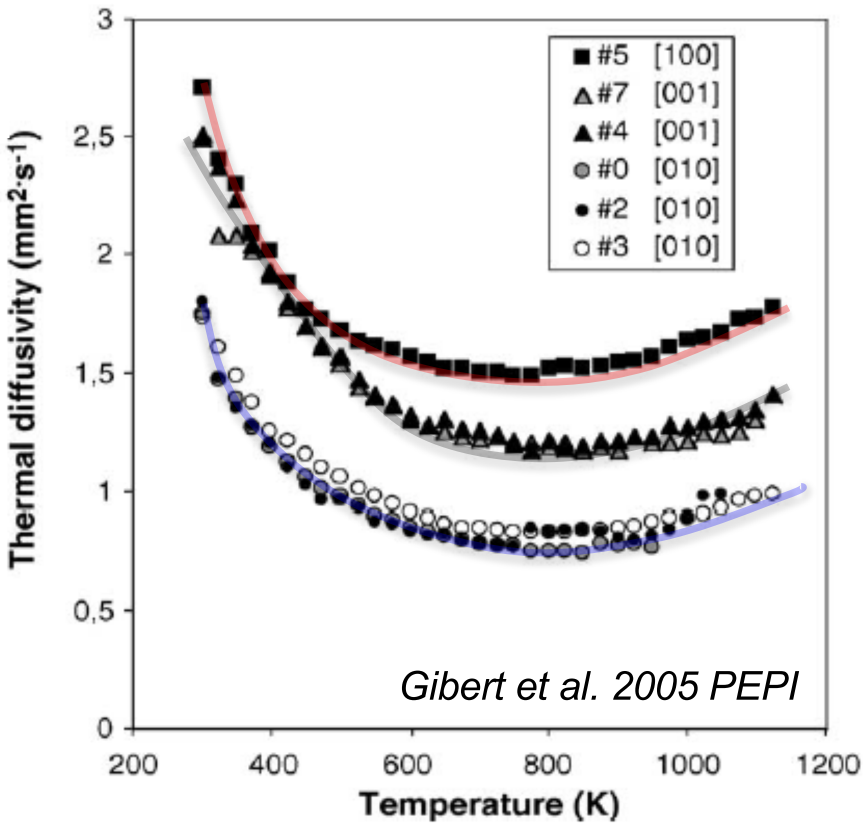
Heat diffusion in an olivine crystal

$$D_{[100]} = 1.6 * D_{[010]}$$



ambient P,T

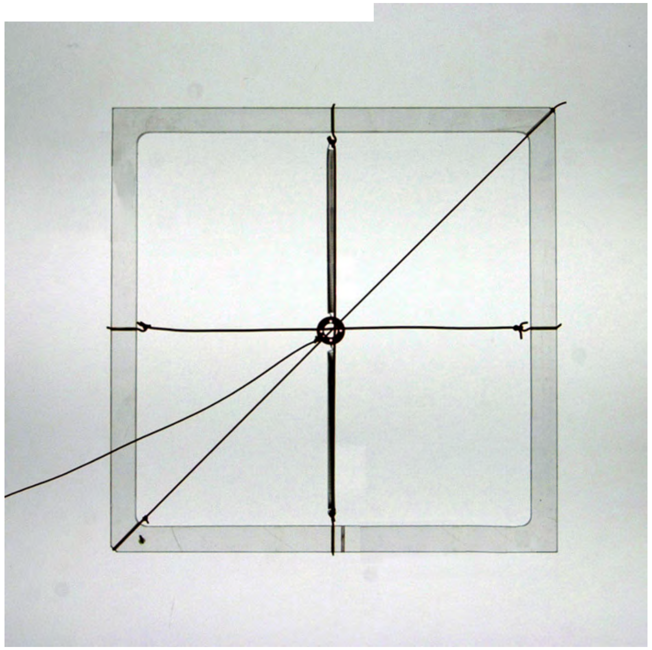
Gibert et al. 2003 GRL



Gibert et al. 2005 PEPI

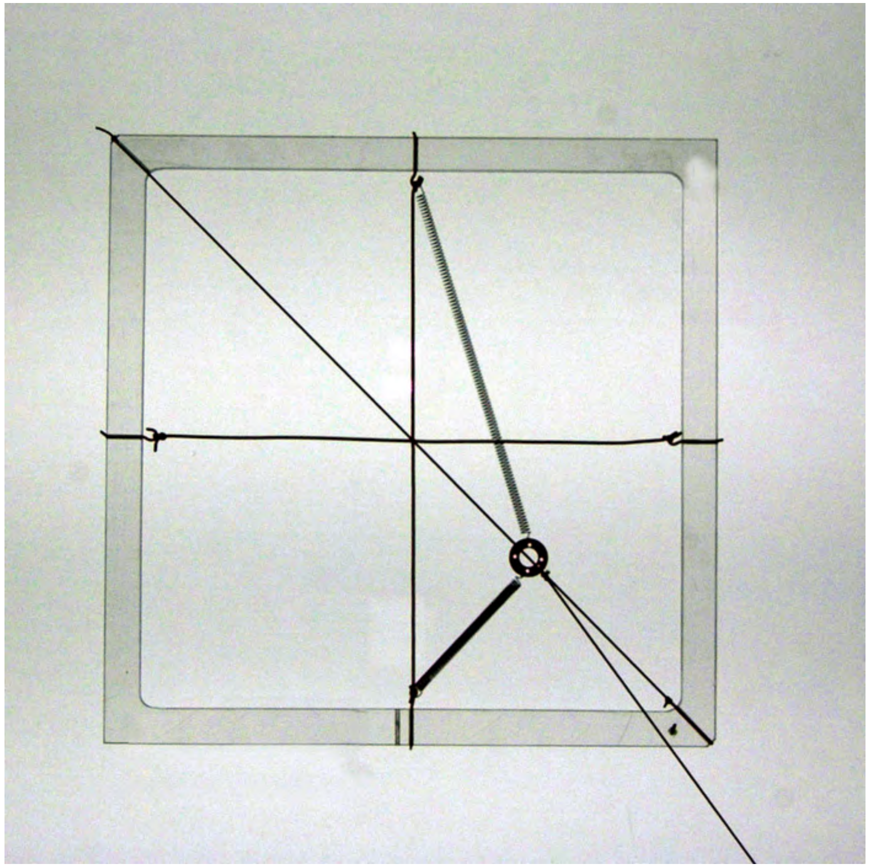
Mechanical anisotropy – elastic behaviour

initial state



Springs with different strengths

How does this affect the displacement of the ring?

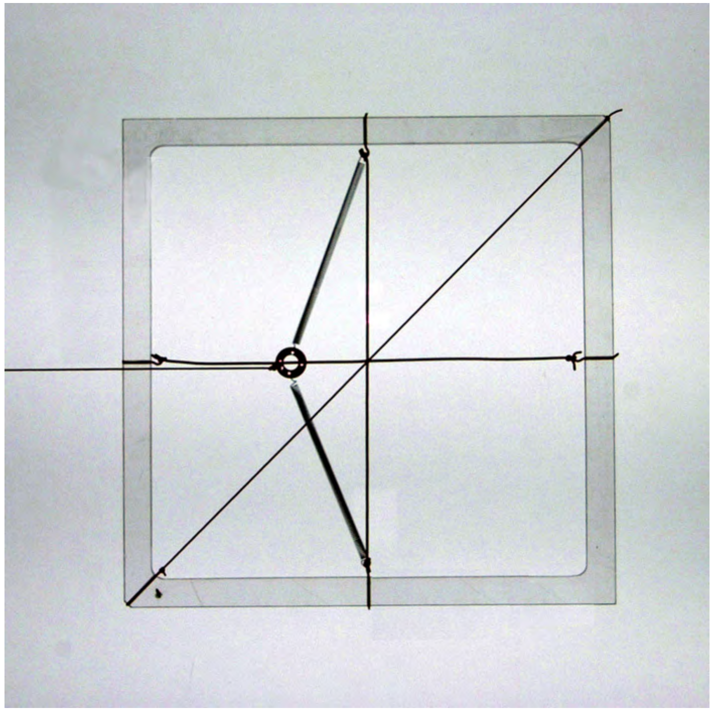


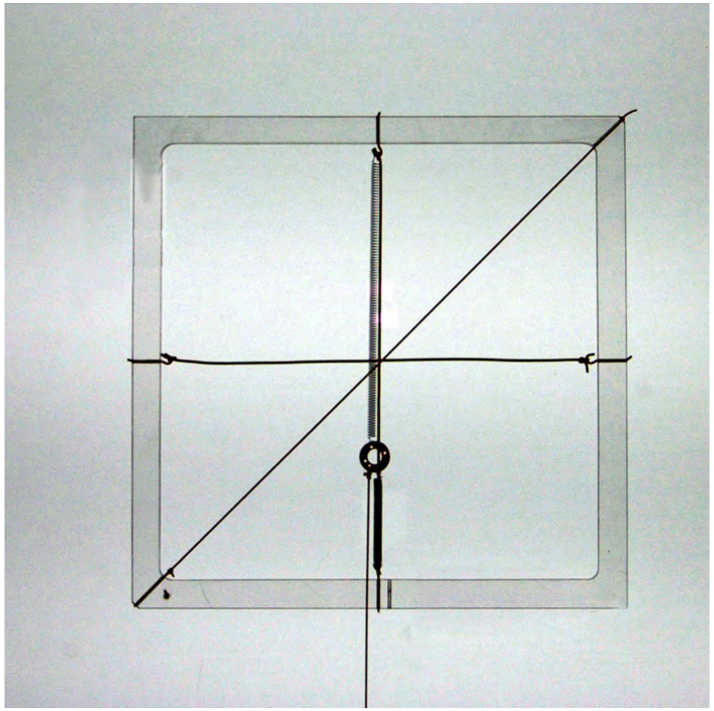
To displace the ring at 45º, the force must be applied with an angle ≠ 45˚

- ***Displacement not necessarily parallel to applied stress***

Mechanical anisotropy – elastic behaviour

Springs with different strengths





Principal directions *(eigen directions of the tensor):*

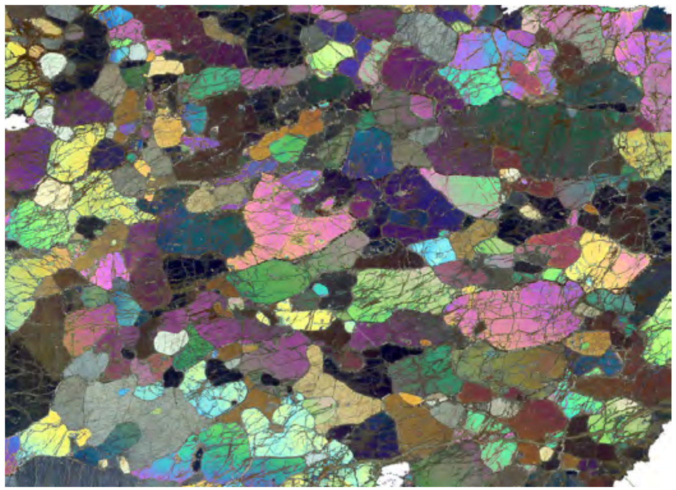
Displacement // applied force, BUT the force needed to obtain the same displacement is ≠

An example of anisotropy well know by geology students …

Optical birrefringence

In a crystal, an EM wave is decomposed in 2 waves polarized in orthogonal directions, which are function of the crystal structure.
The 2 waves propagate at ≠ velocities.

Polarization colors: function of the anisotropy (difference in velocity) & path length



Anisotropic physical properties

2^{nd} rank tensor (properties that relate 2 scalars)

- *Thermal diffusivity and conductivity*
- *Electrical conductivity…*

Variation of the property is function of the sampling direction

4^{th} rank tensor (properties that relate 2 tensors)

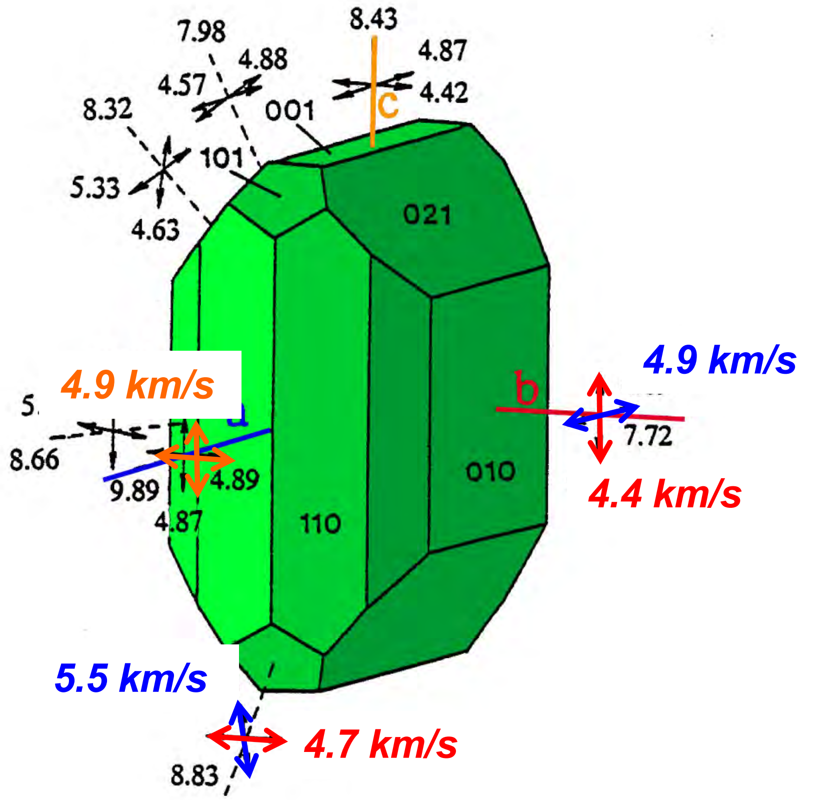
- *Elasticity : Variation of the seismic velocities function of the sampling direction AND of the polarisation of the waves (also EM waves)*
- *Viscosity*

What produces anisotropy?

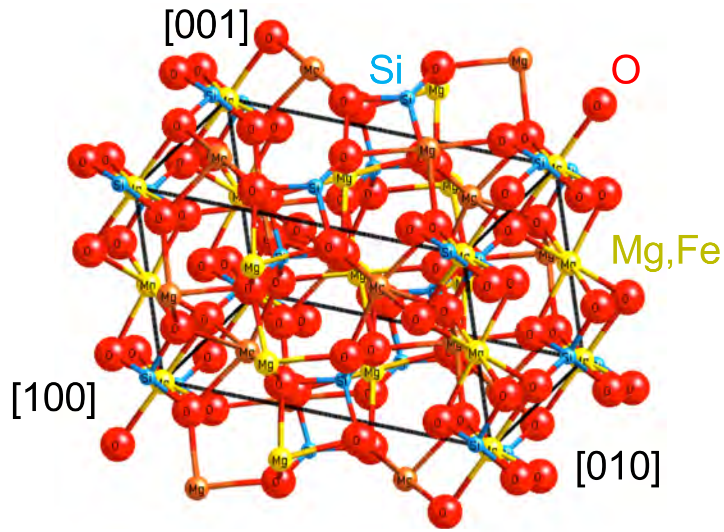
1- In a grain (crystal)

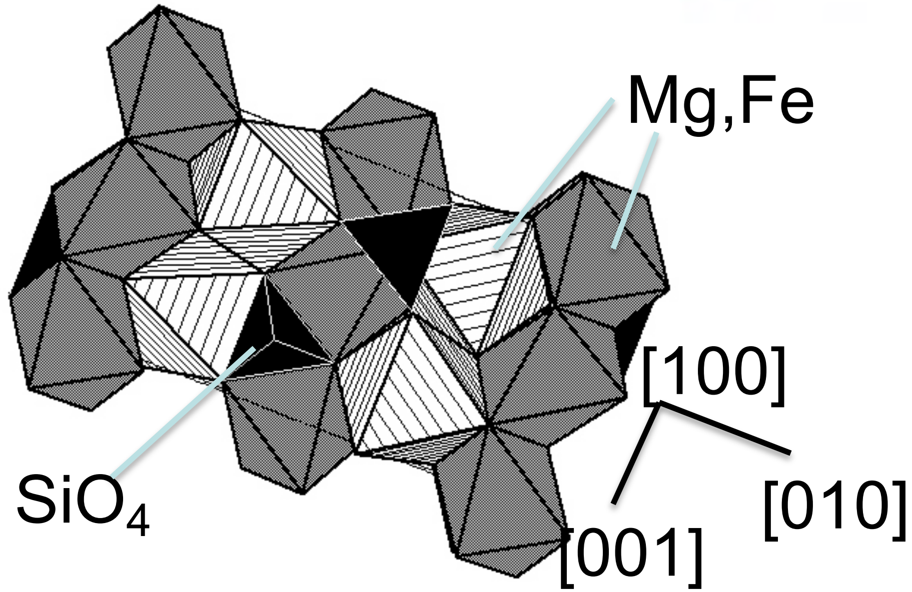
(crystals = bricks that compose the rocks)

Olivine = (Mg,Fe)SiO_4



Seismic velocities





Why is a crystal anisotropic?

Periodic atomic arrangement with ≠ liaisons in ≠ directions

Symmetry of the crystal structure controls the anisotropy

What produces anisotropy?

1- In a crystal

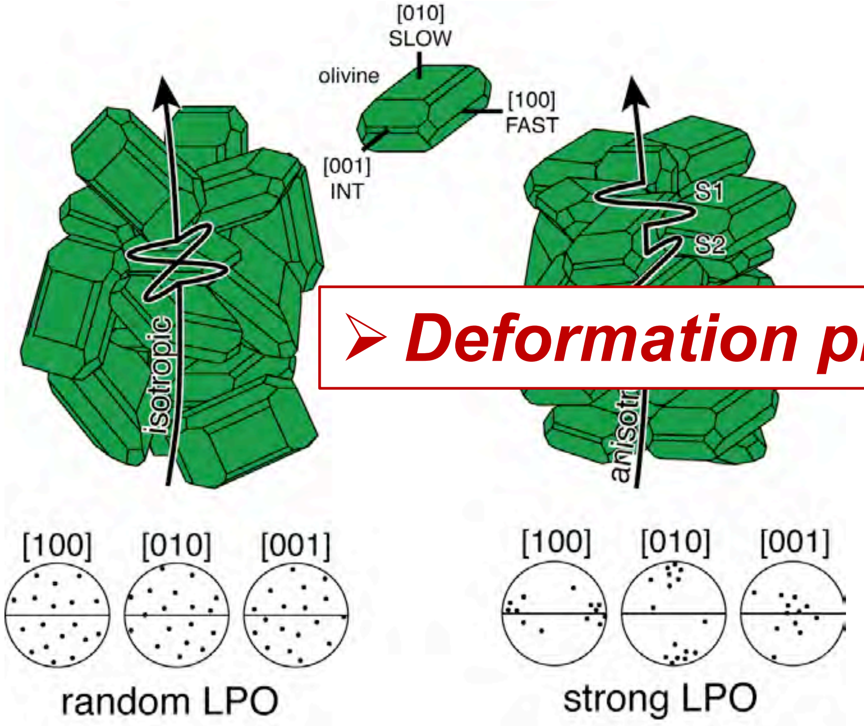
2- In a rock (sample scale = cm to m)

3- At the scale of geophysical observations (10s to 100s of km)

Rock-scale anisotropy results from

Intrinsic anisotropy

Crystal or Lattice Preferred Orientation (CPO or LPO) of anisotropic minerals :



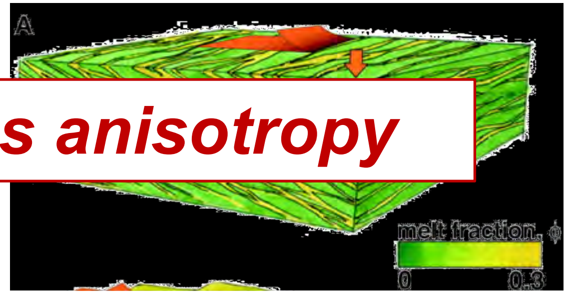
drawing by Luc Mehl

➢ ***Deformation produces anisotropy***

Extrinsic anisotropy

Organized intercalation of materials with
very ≠ properties
@ scale << observation one

Oriented melt/fluid inclusions



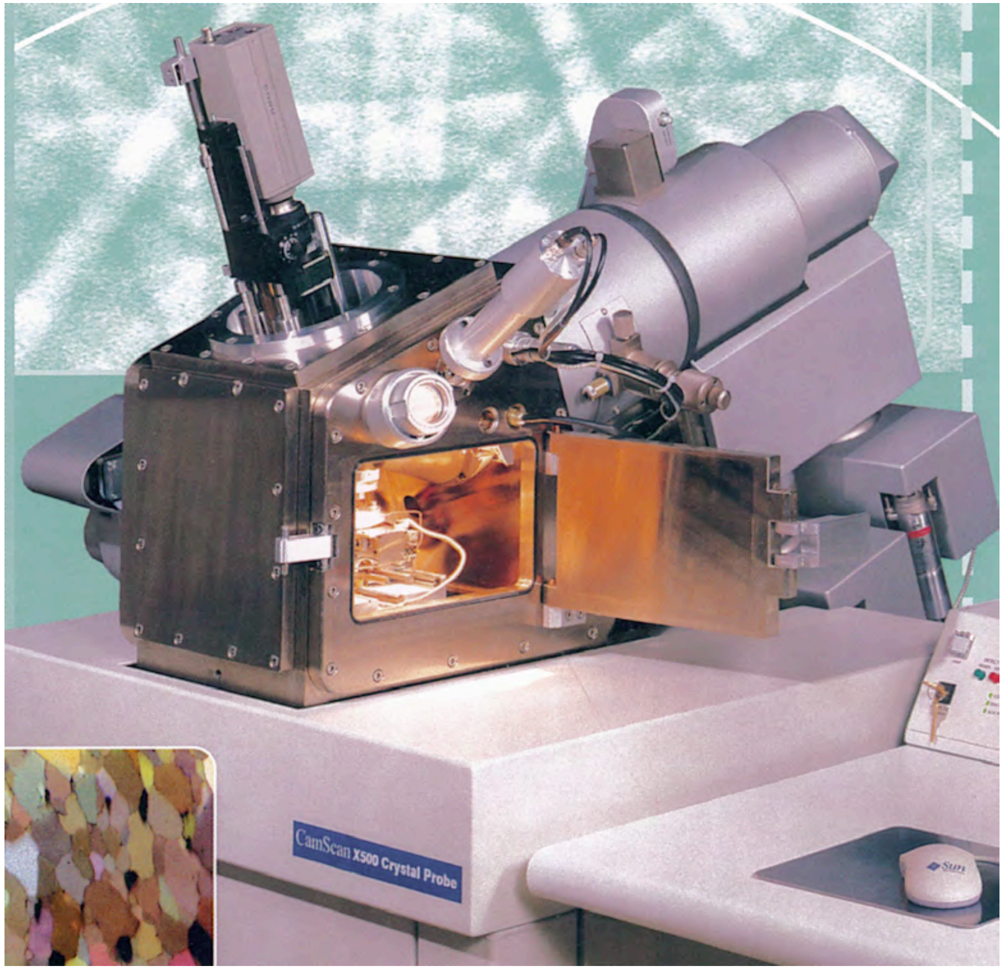
© B. Holtzman

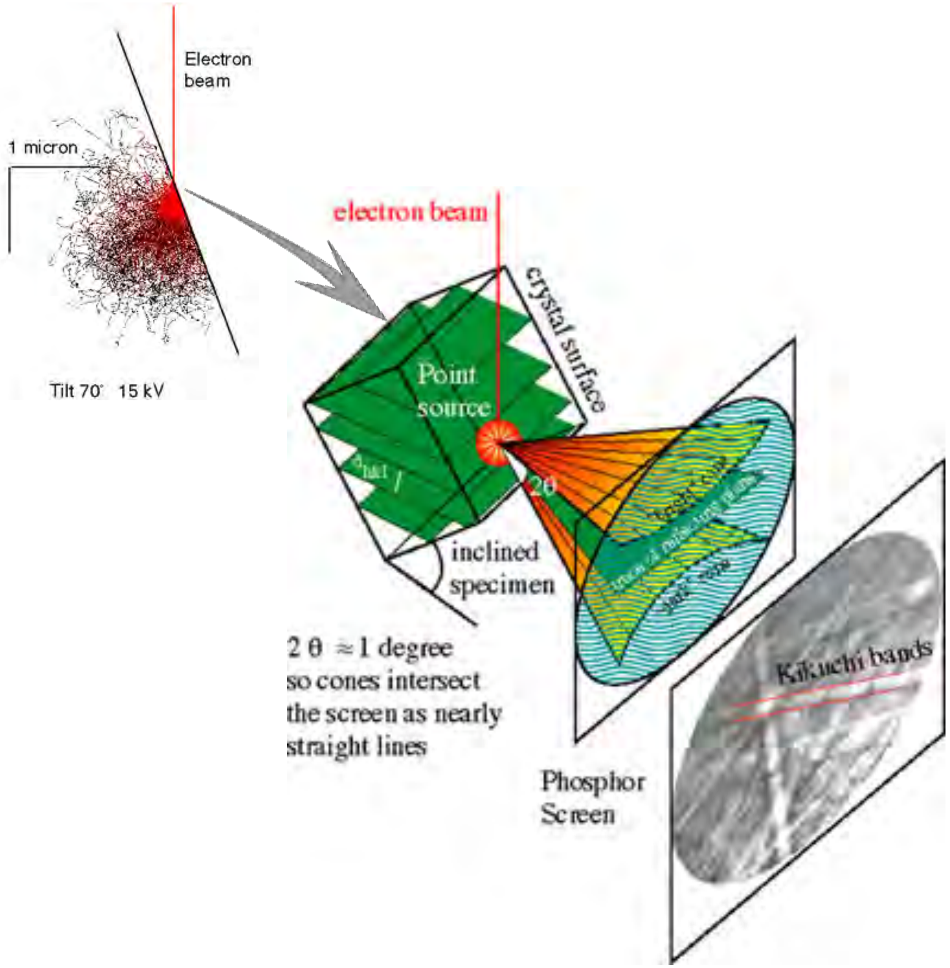
Open fractures
Compositional layering…

Intrinsic @ extrinsic anisotropy may coexist (and interfere constructively or destructively)

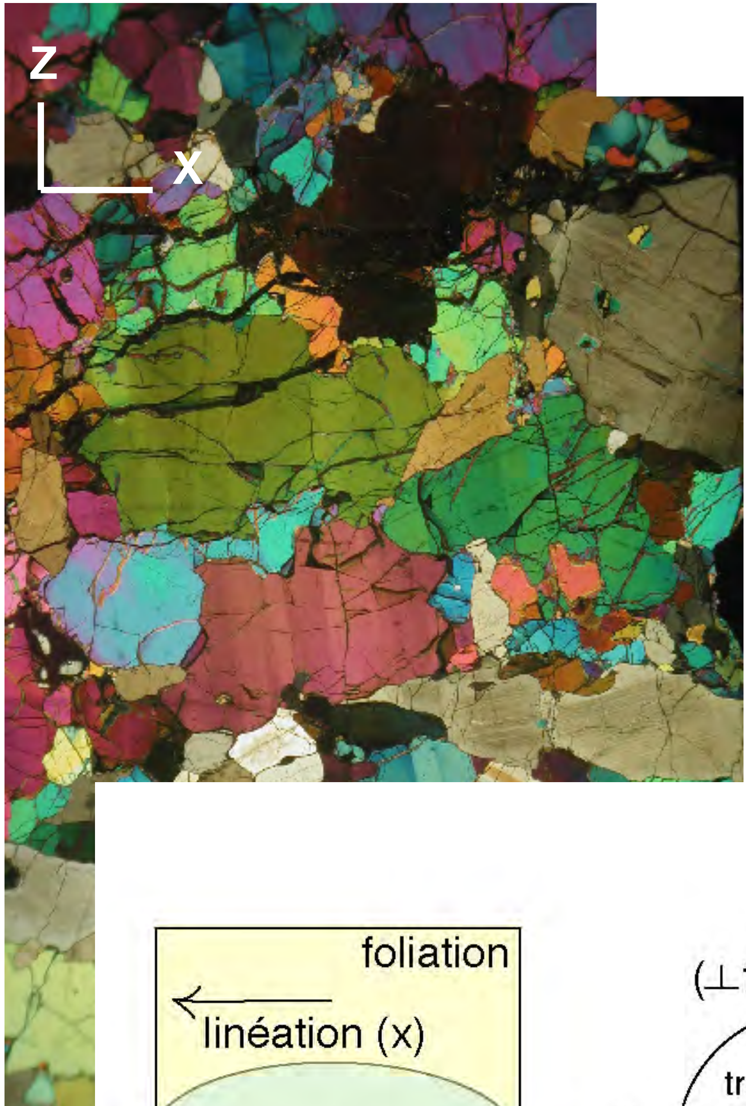
Crystal preferred orientations can be measured

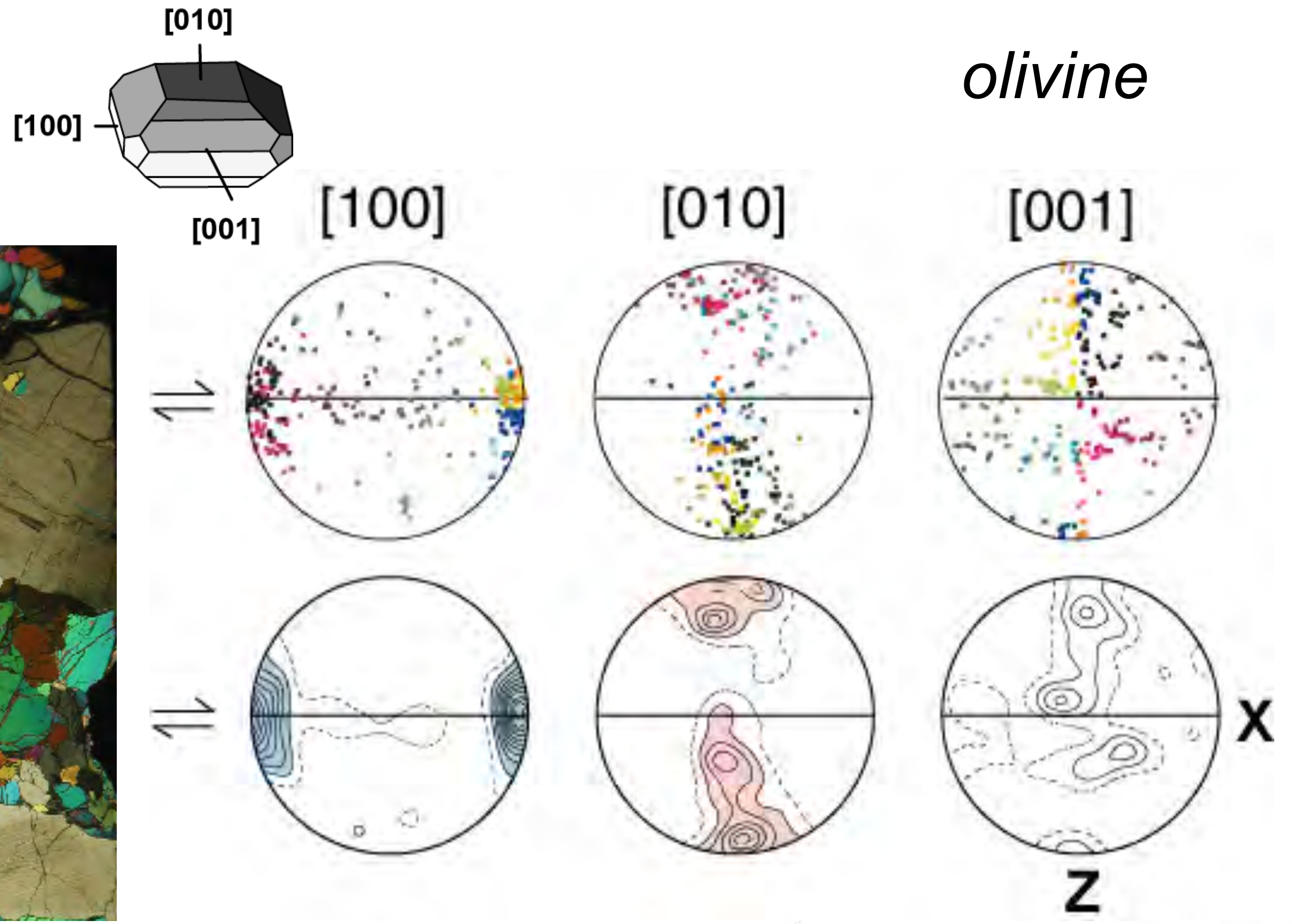
In a SEM by the analysis of electron backscatered diffraction patterns (EBSD)

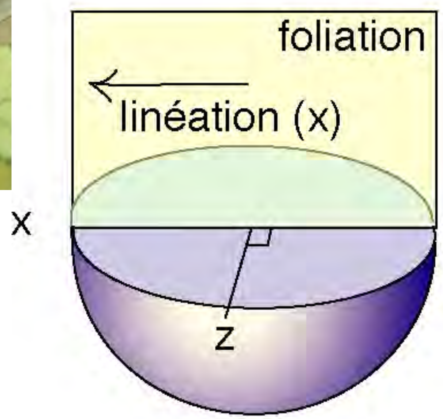


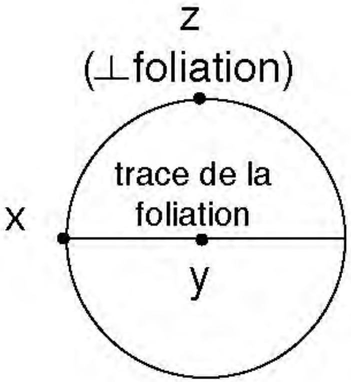


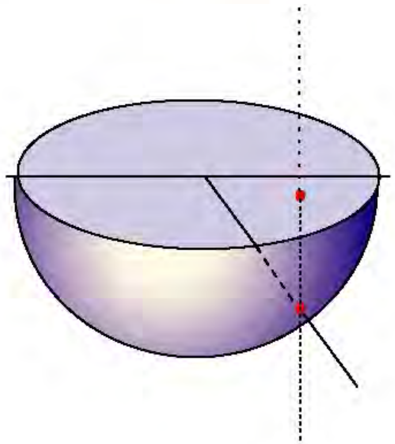
olivine

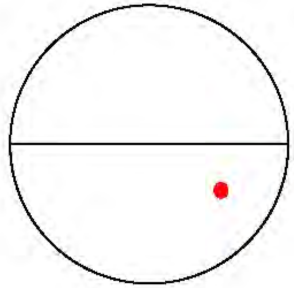

Z
X


[010]
[100]
[001]
[100]
[010]
[001]
X
Z


foliation
linéation (x)
x
z

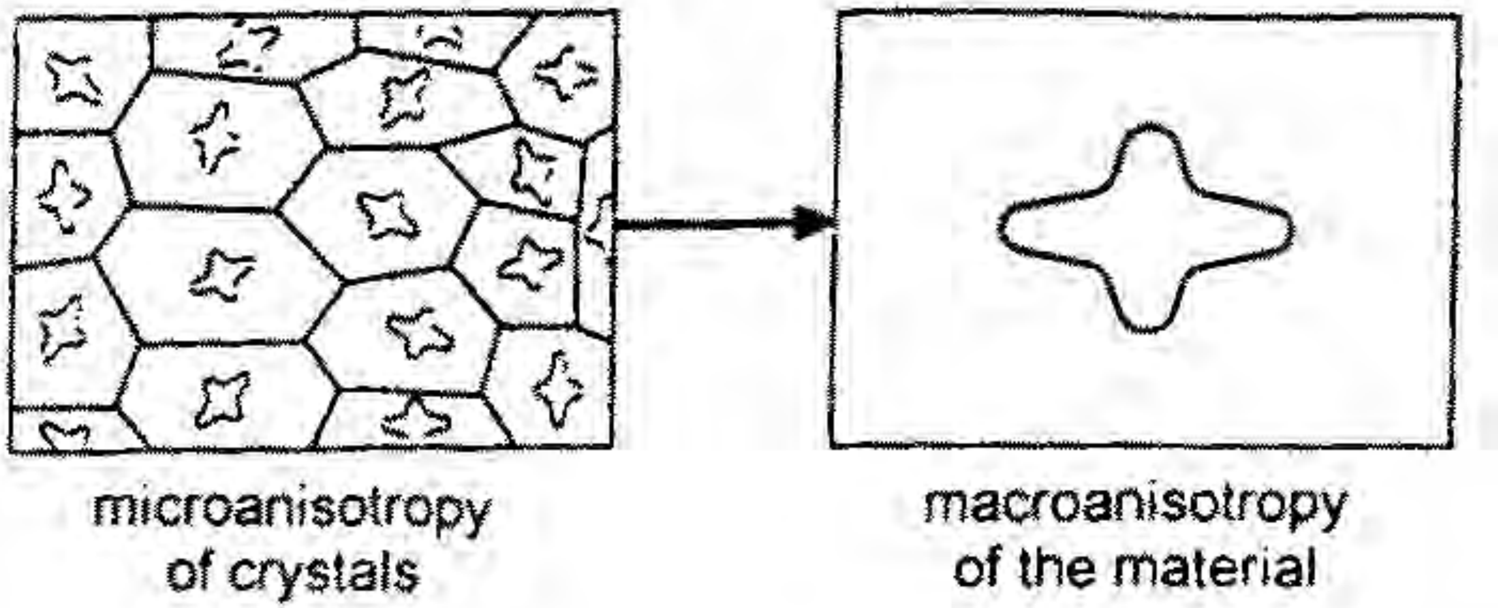

z
(⊥foliation)
trace de la
foliation
x
y





How to determine anisotropic properties at the rock scale?

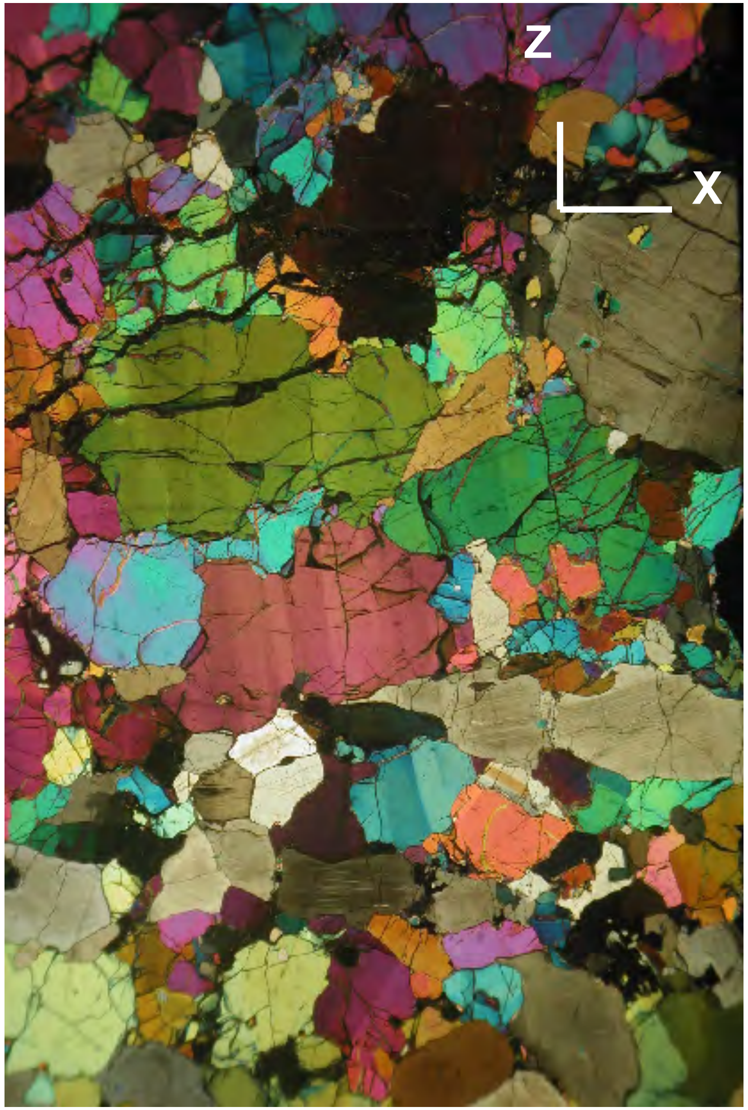
rock = aggregate of anisotropic crystals



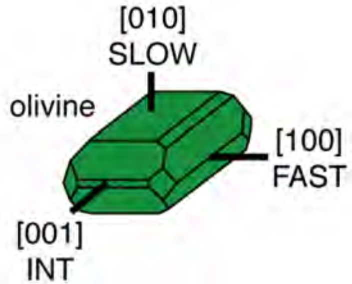
volumetric averaging as function of:

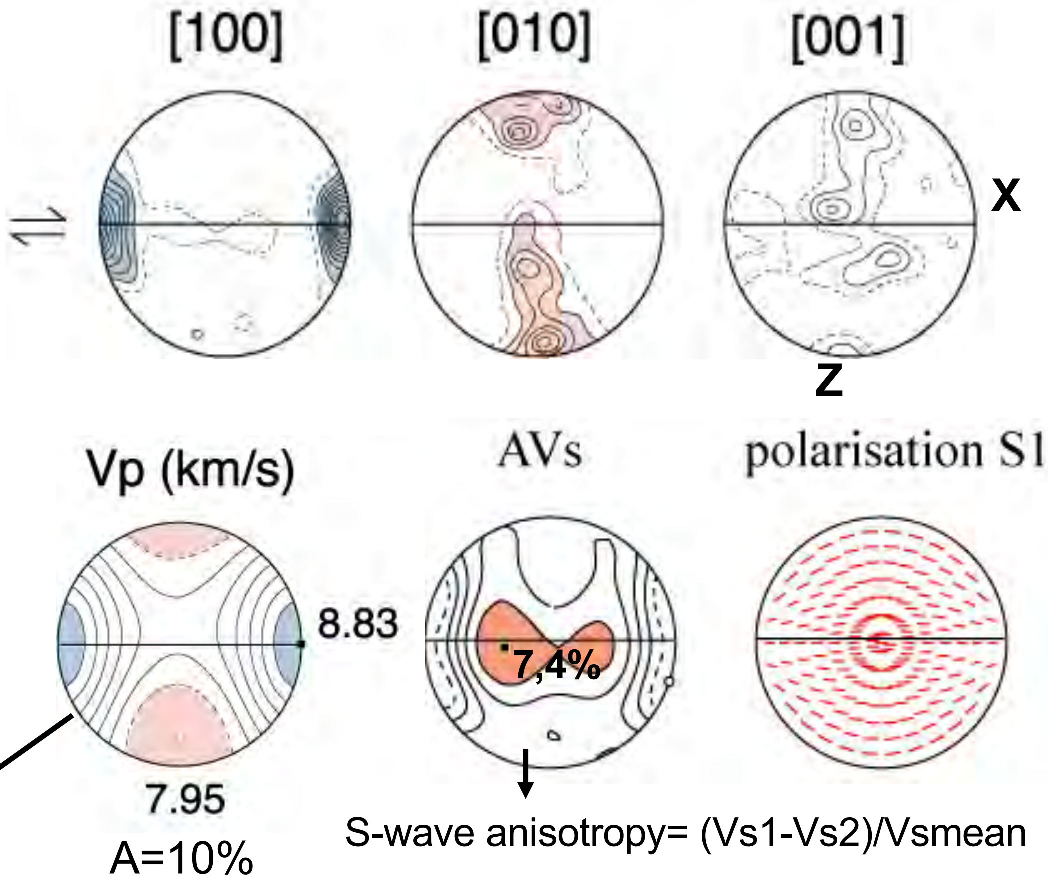
- ***mineralogical composition***
- ***orientation of the crystals***

Simplest approach – works fine for thermal and elastic anisotropy



In the upper mantle, olivine (≥60% vol.) controls the anisotropy





P-wave velocity: F(propagation direction)

S-wave anisotropy= (Vs1-Vs2)/Vsmean

The orientation of the crystals is the key factor for transferring anisotropy to large scales

How do crystal preferred orientations form and evolve?

Relation between flow patterns and CPO

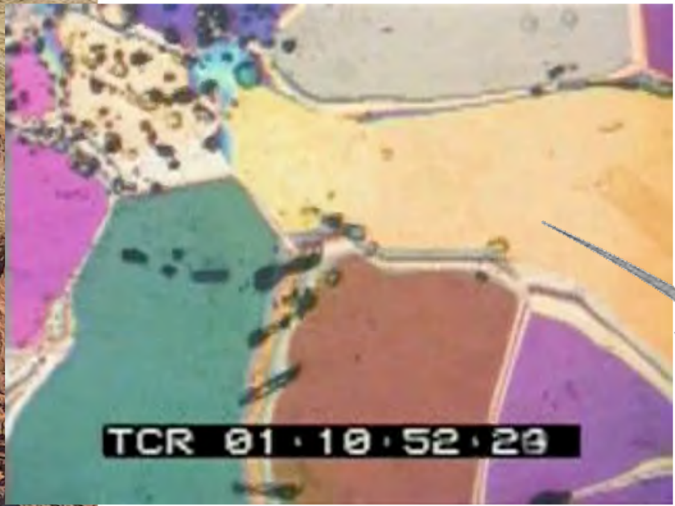
Deformation (flow) of ice Ih (the ice we see on the Mt Blanc)

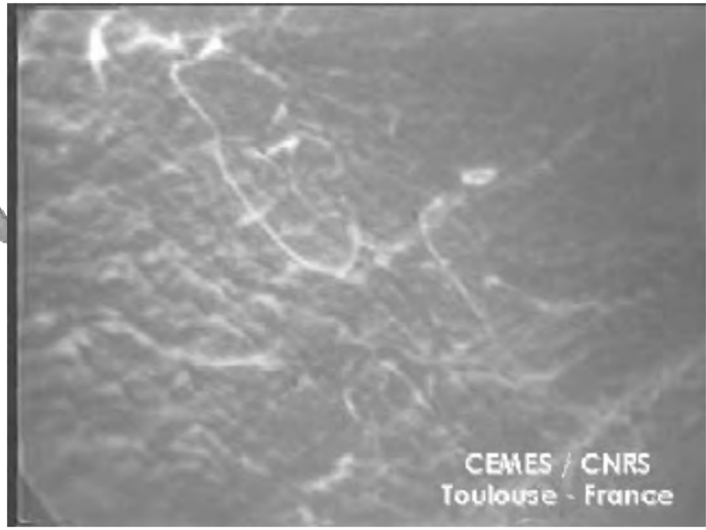
≠ colors : ≠ crystal orientations

Polycrystalline ice
Optical microscope – cross-polarized light
C. Wilson - Univ. Melbourne, Australia

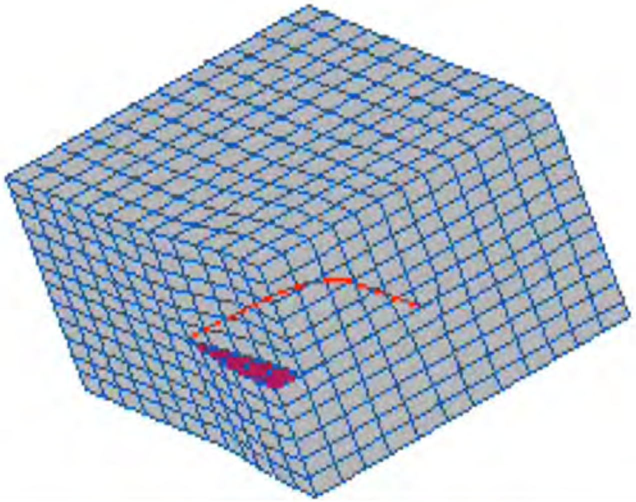
Ductile deformation (flow) of crystalline solids (rocks, but also ice, metals…)

Dislocation creep

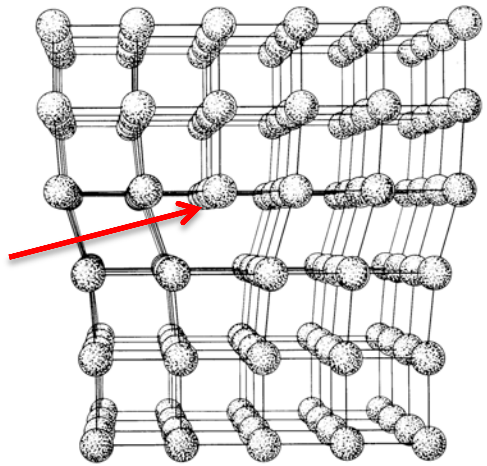




Multiplication & glide of dislocations in a Ti alloy Transmission electron microscopy



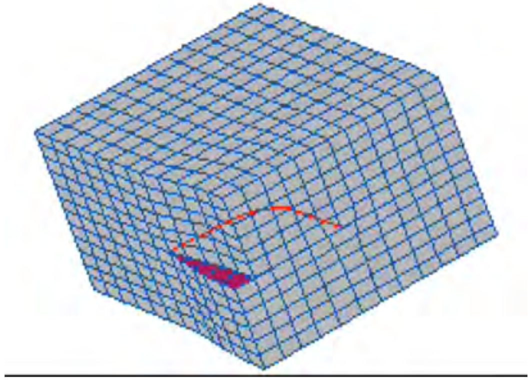
Motion (glide) of dislocations
= shear deformation of the crystal



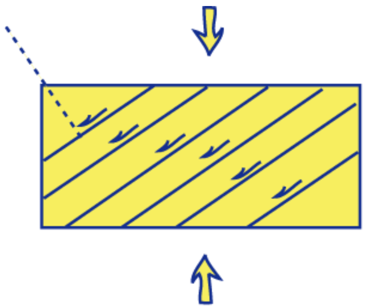
Dislocation = defect in the atomic arrangement in a crystal
= line of atoms not fully connected

How to form crystal preferred orientations by deformation
(dislocation creep)

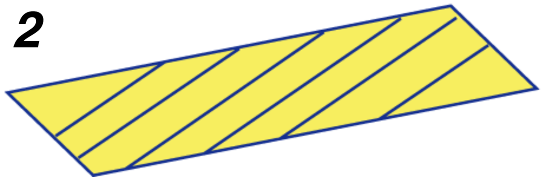
within a grain (crystal):



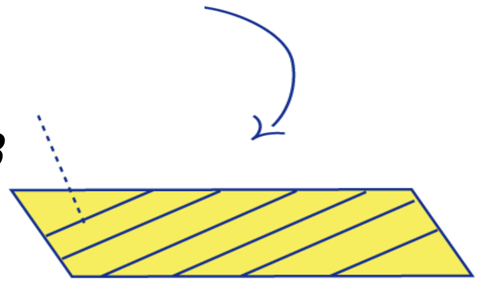
1



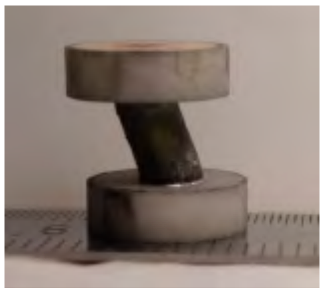
2



3

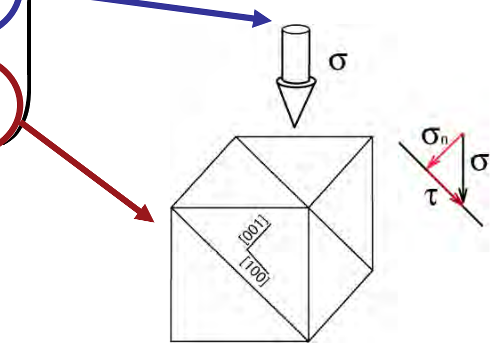


Not always compatible with boundary conditions



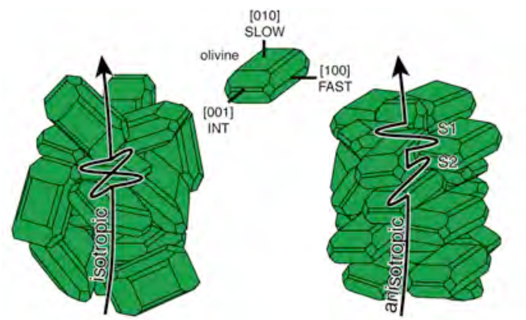
strain = motion of dislocations on well-defined crystal planes & directions

$$\dot{\gamma}^s = \left(\frac{\tau_r^s}{\tau_0^s} \right)^n$$



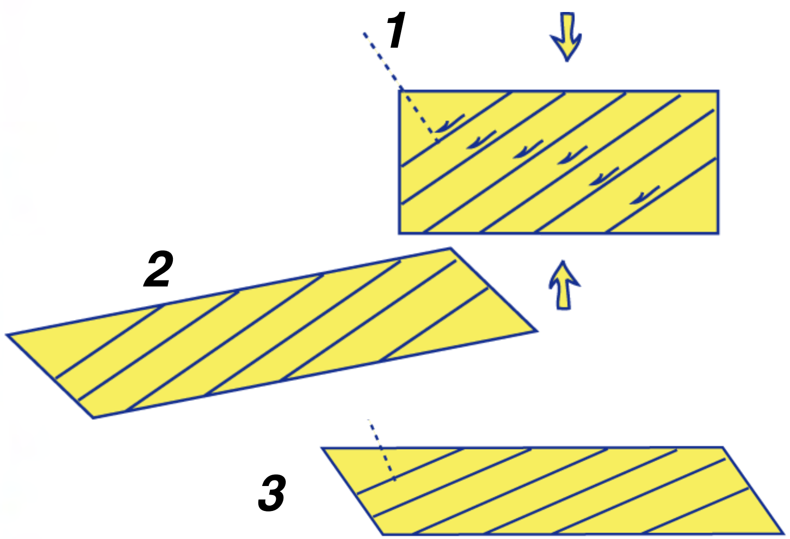
Shape change is constrained by the crystal structure

rock (polycrystal) : interaction with neighbours



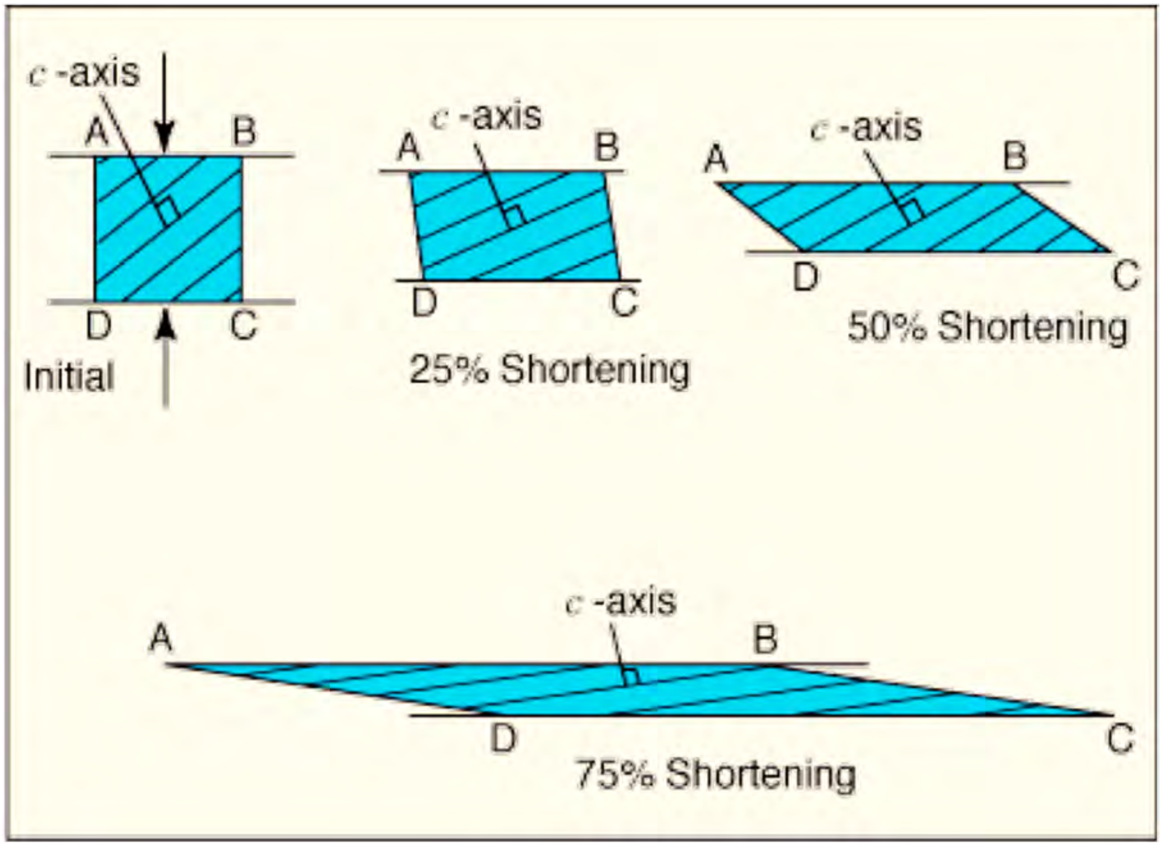
strain compatibility = rotation of the crystal

Why does dislocation glide produce crystal preferred orientations?



motion of dislocations on a small number of crystal planes & directions (weaker bonds)
= crystal deformation has limited degrees of freedom

strain compatibility ➔ rotation of the crystal
- *development of a crystal preferred orientation*
  = all crystals tend to a common orientation



• *parameters controlling CPO evolution during deformation by dislocation creep*

✓ *active slip systems, which depend on the crystal structure and on:*
- *temperature*
- *deviatoric stress (or strain rate)*
- *pressure*
- *water*
- *melt*

✓ *deformation geometry*

✓ *dynamic recrystallisation*

• *preservation / destruction of CPO & anisotropy?*

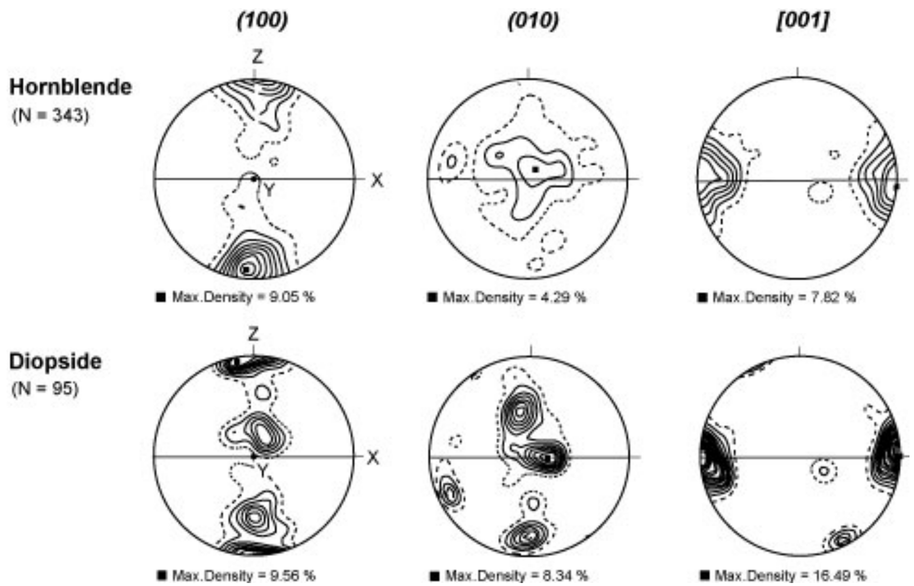
↓ *annealing / static grain growth*

↘ *reactions / crystallization of new minerals under static conditions*

Dislocation glide is not the sole process producing crystal preferred orientations, but it is the most important

Magmatic flow:
Deformation of a crystal mush

Oriented crystallization during reactions & phase transformations:
Inheritance of the orientation of the parent mineral

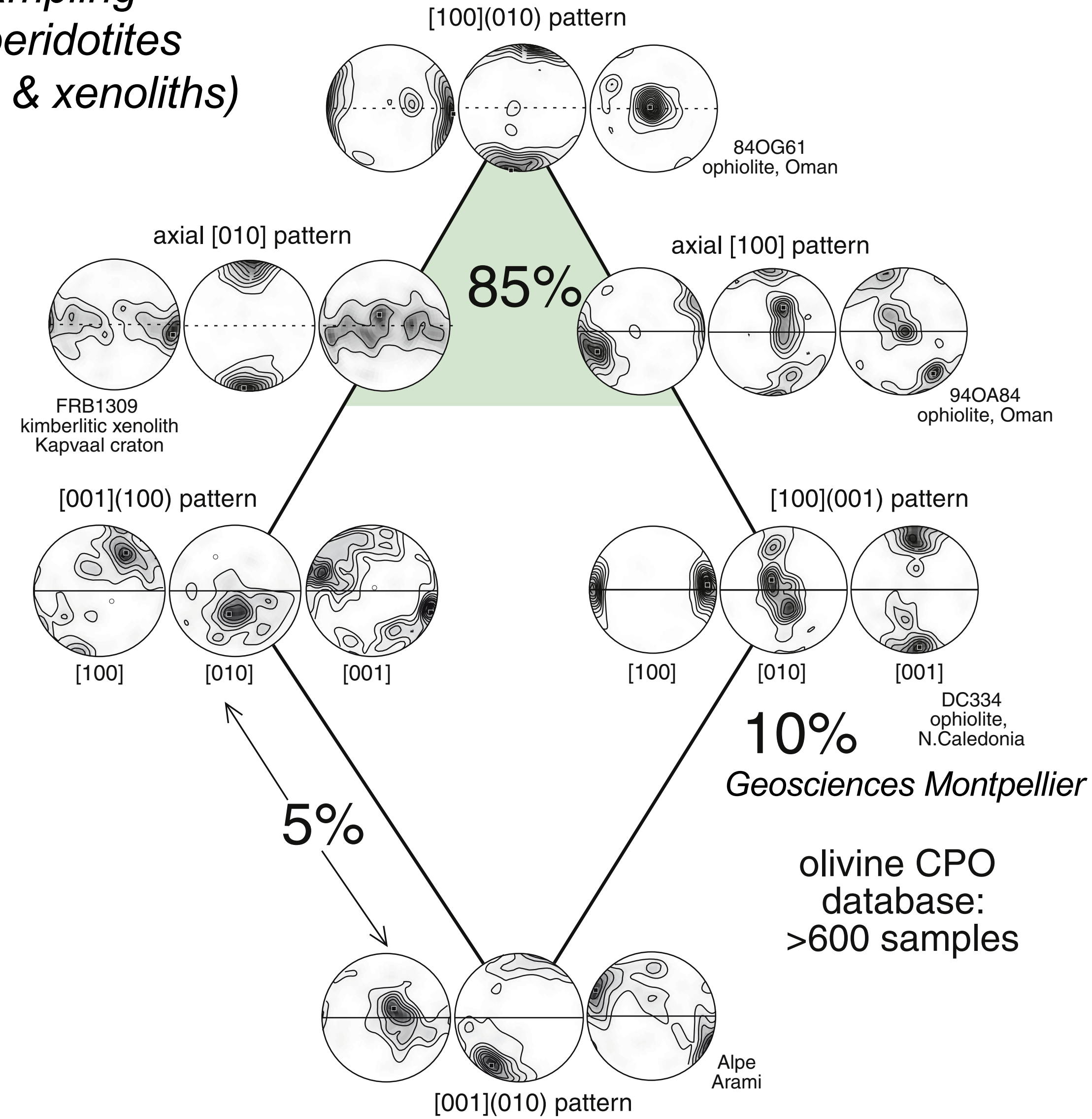


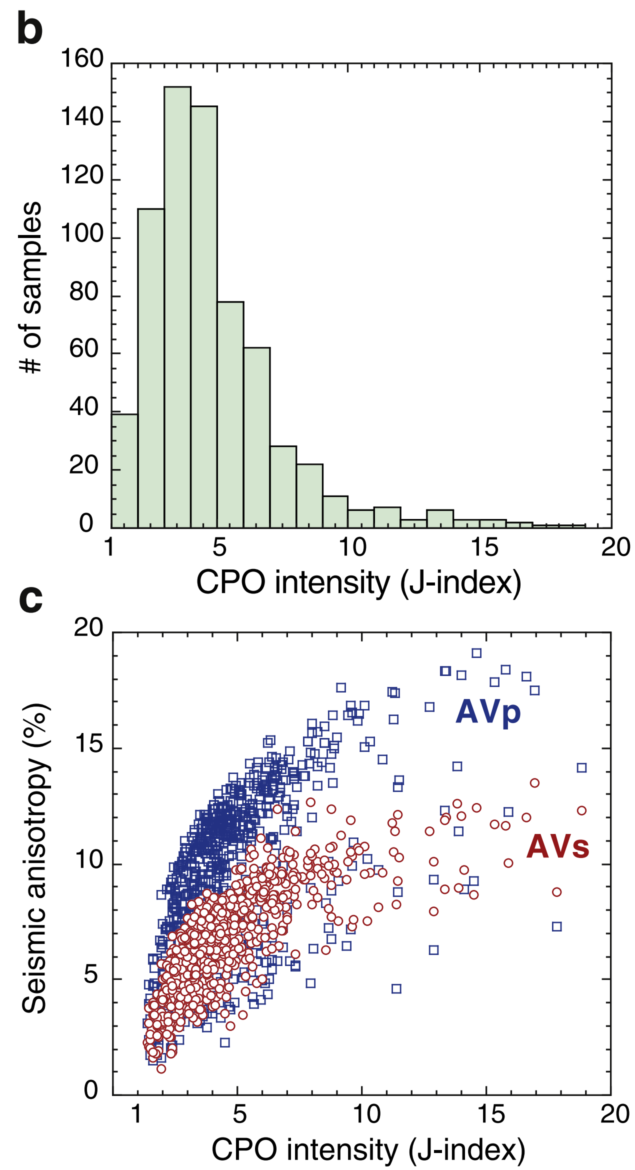
hornblende + plg = magma + diopside
(amphibolite 80% hb)

Diffusion creep with anisotropic diffusivity / crystal growth

✓ *Strain-induced olivine crystal preferred orientations & anisotropy are ubiquitous in the upper 200 km mantle*

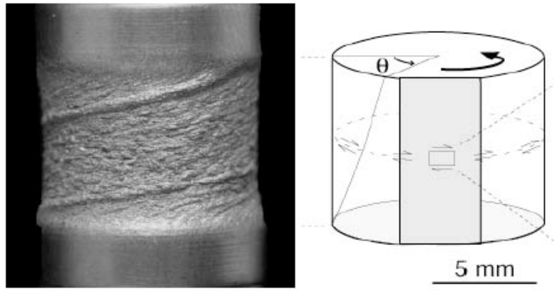
Direct sampling mantle peridotites (massifs & xenoliths)

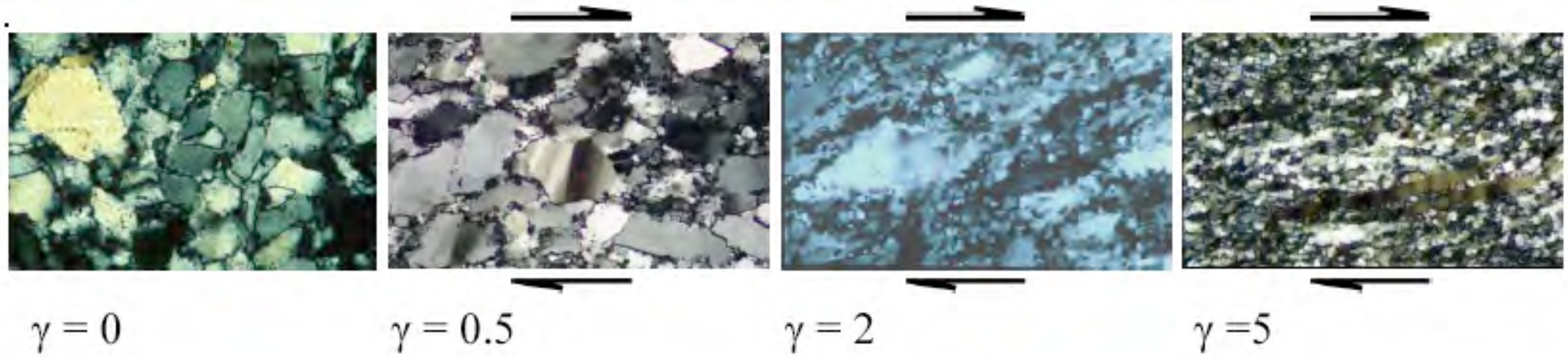


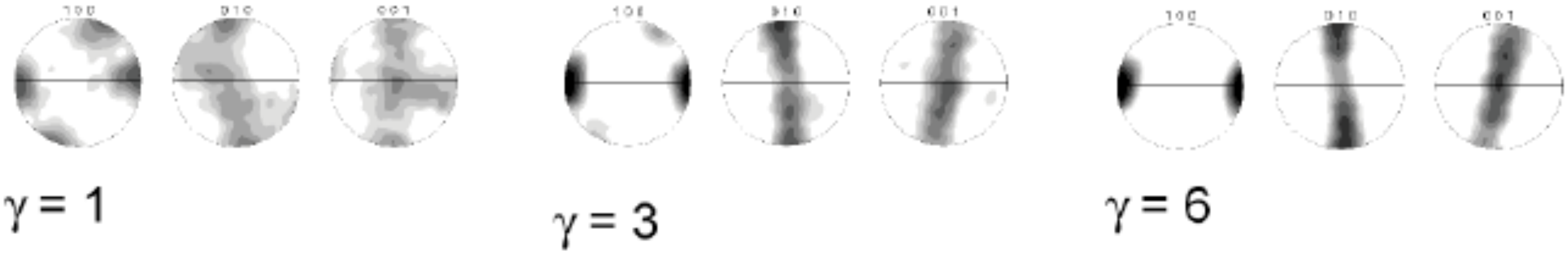


Torsion experiments: Olivine HT-MP

- ***Simple Shear deformation***
- ***evolution CPO = F(strain)***





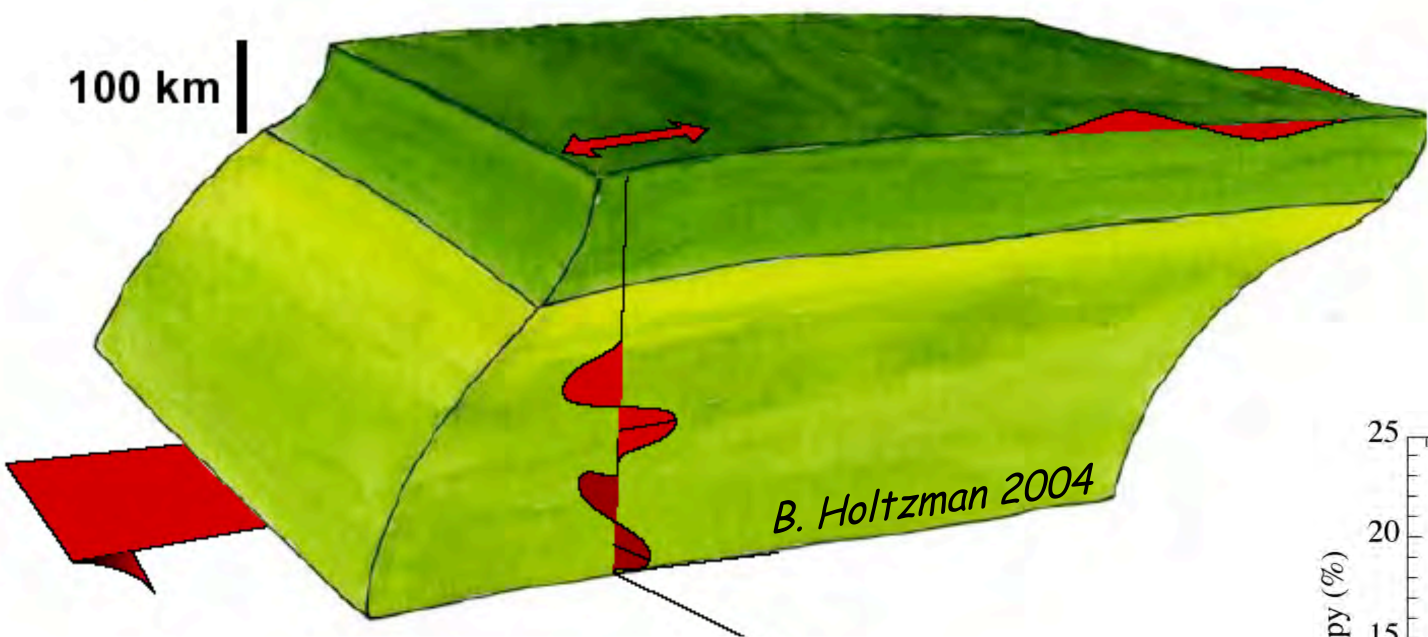


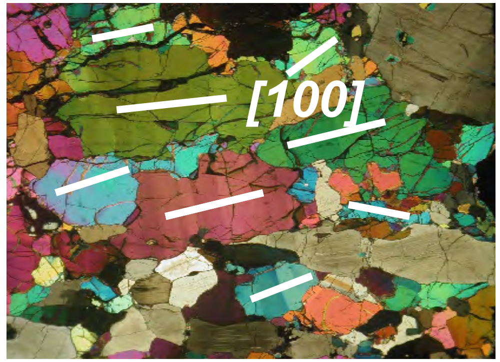
Low strain: γ = 1 to 3
Fast evolution of CPO
[100] ➔ shear direction

High strain: γ > 3
Slow evolution of CPO
[100] // shear direction

Bystricky et al. Science 2003

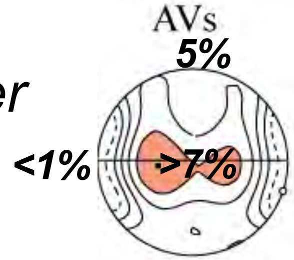
Simple key to qualitatively "read" seismic anisotropy observations in the SHALLOW MANTLE (>250 km):

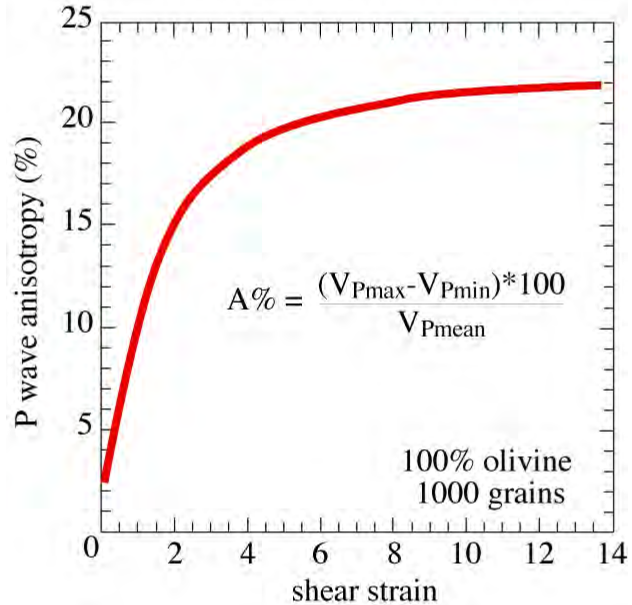




Fast direction of P & Rayleigh propagation, polarisation fast S-wave = flow direction

delay time ~ thickness of the anisotropic layer and orientation of the flow plane



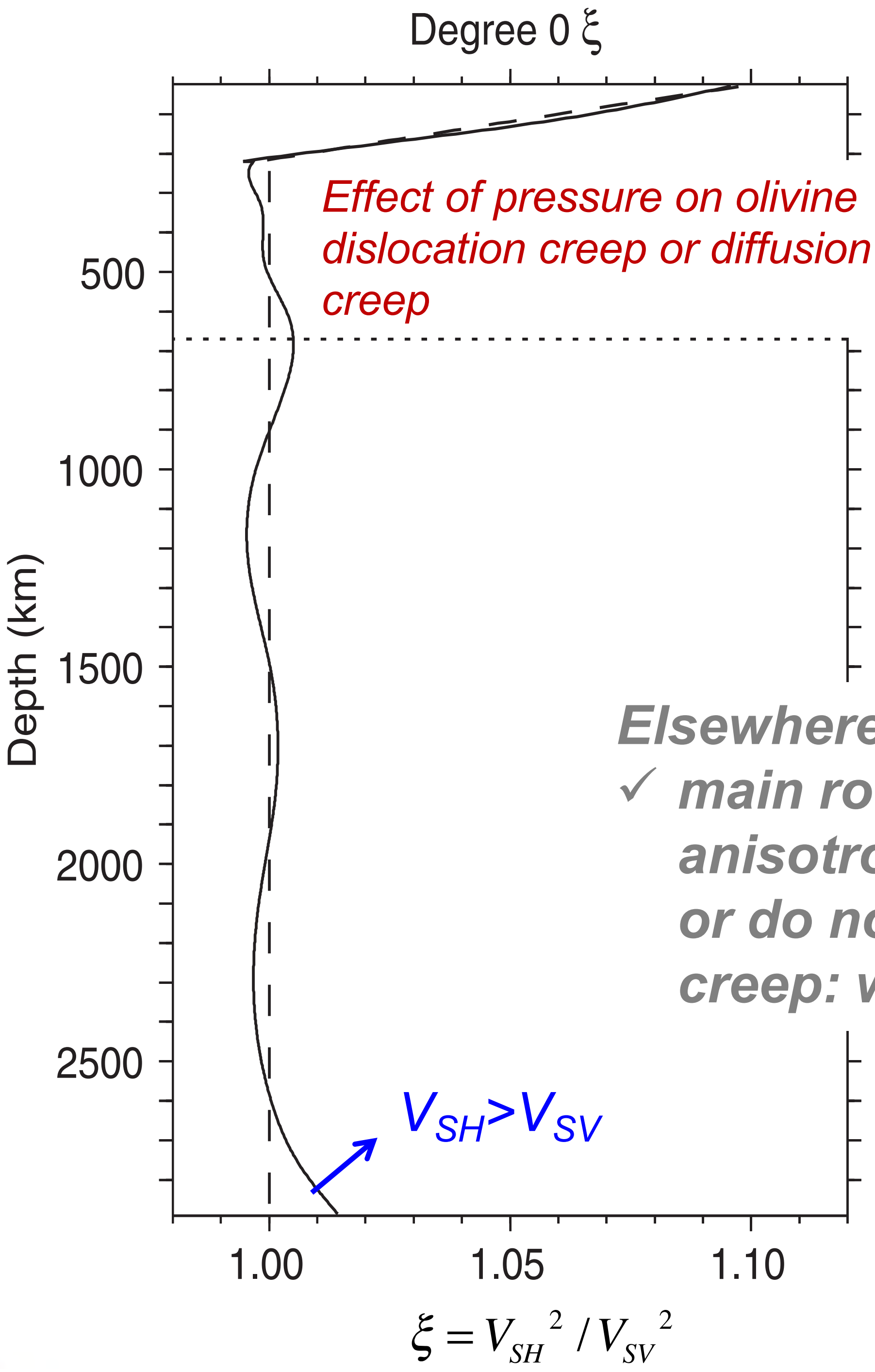


May not work for deformation in presence of melt or water : subduction zones

Does not work at high pressure (below 250 km) : change in dominant slip system

➢ ≠ olivine crystal preferred orientations

Global 1D radial anisotropy



The upper 200-250 km of the Earth is highly anisotropic

Crust

Open fractures, melt, compositional layering…

CPO of micas, amphibole

Upper mantle

CPO of olivine

Aligned melt pockets (asthenosphere)

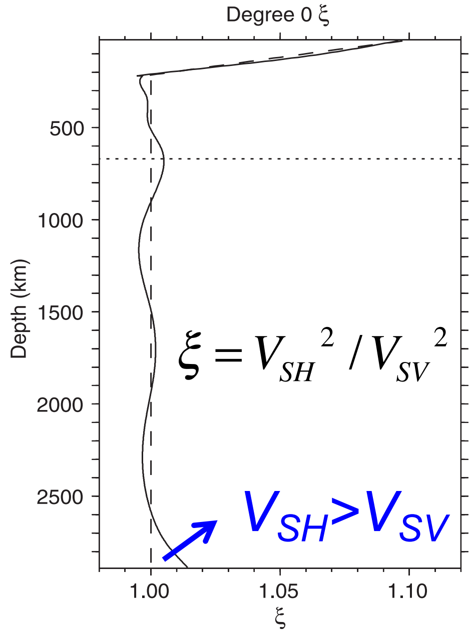
Elsewhere in the mantle?

- ✓ ***main rock-forming minerals less anisotropic (cubic): ringwoodite or do not deform by dislocation creep: wadsleyite, bridgemanite***

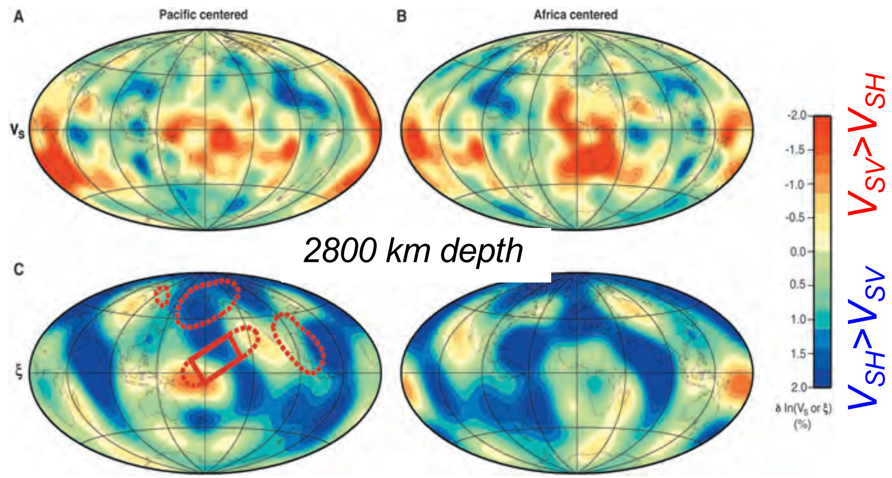
Clear anisotropy also in D"

CPO of postperovskite & ferropericlase *+ layering?*

Seismic anisotropy in D”: observations

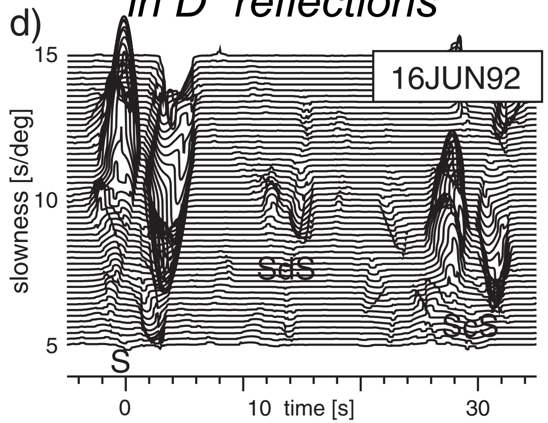


Global tomography



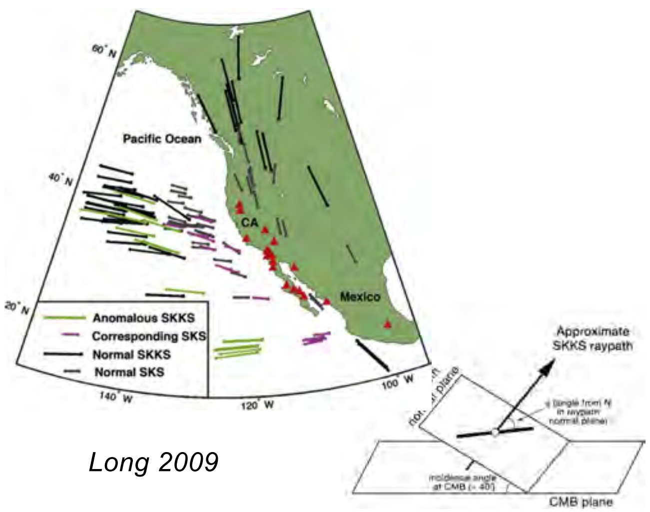
Panning & Romanowicz 2004

Polarity reversals in D” reflections

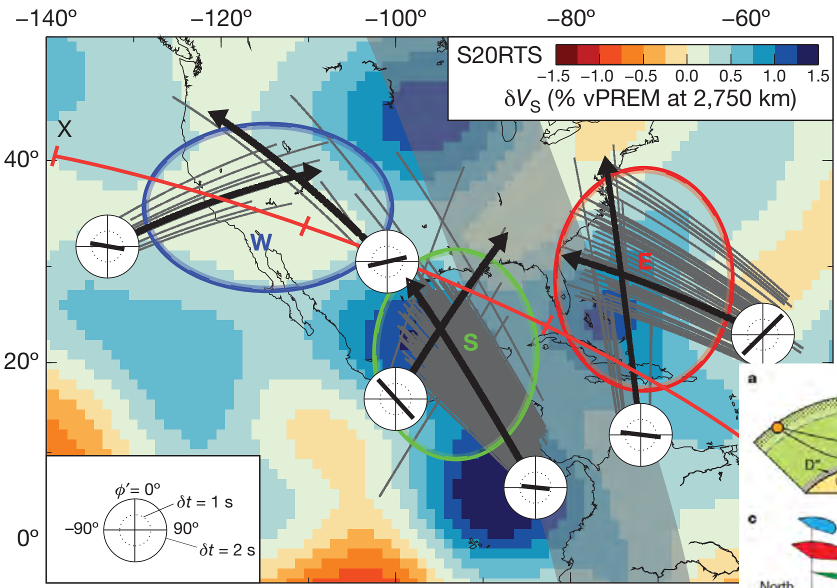


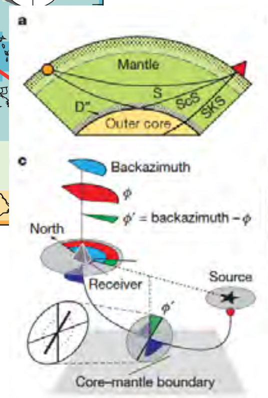
Thomas et al. 2011

Discrepancy in SKS - SKKS splitting



Long 2009





Nowacki et al. 2010

Differential S-ScS splitting

What do we need for using these data to "map" deformation in D"?

- ***Forward models of deformation and seismic anisotropy***

1. *Knowledge on the constitutive minerals deformation:*
   at the crystal scale : which deformation mechanisms?
   at the rock scale : crystal preferred orientation as a function of strain

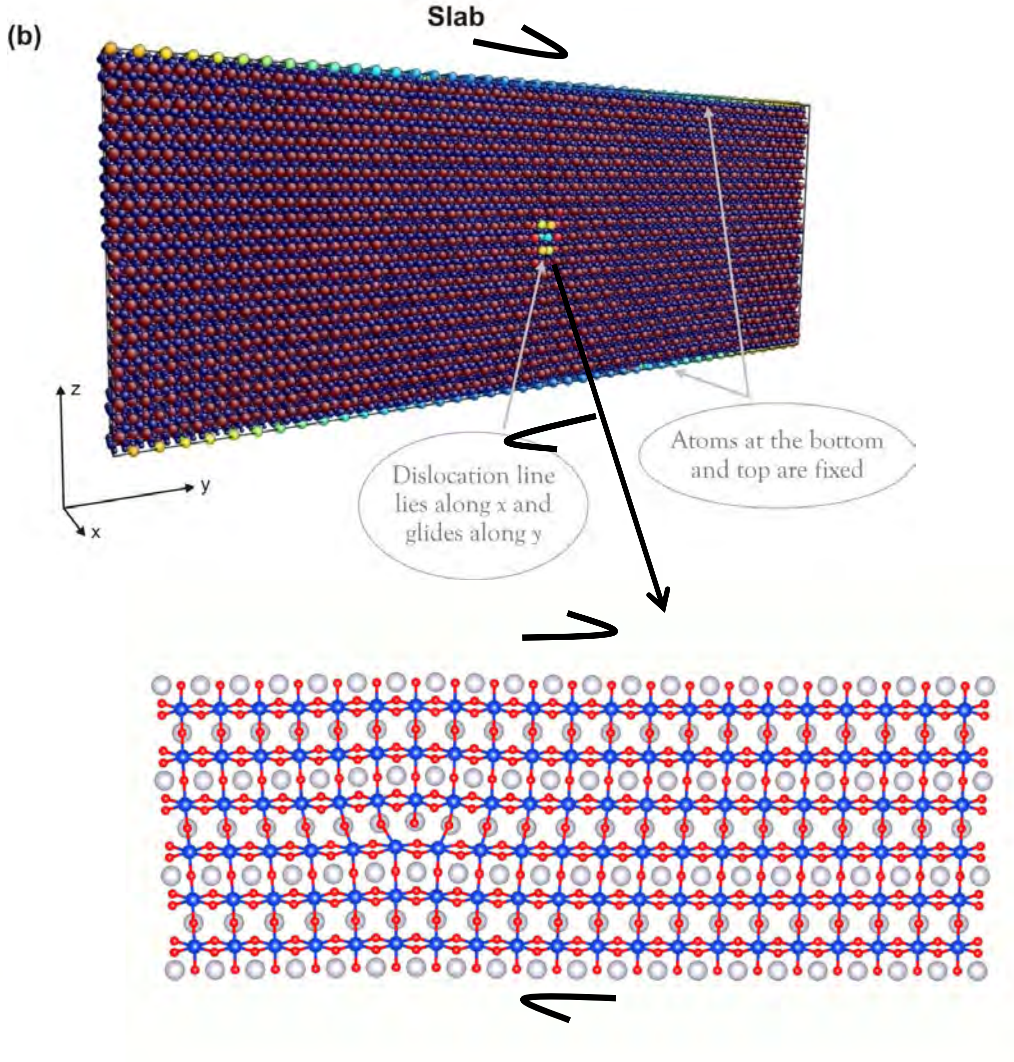
2. *Knowledge on the minerals' seismic properties at high T & P*

3. *Calculation of the resulting seismic anisotropy*

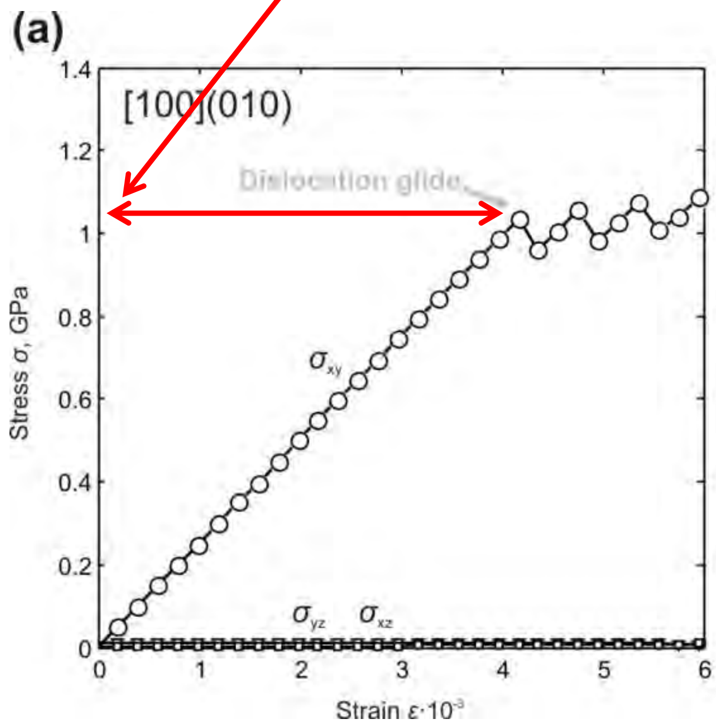
4. *Finite-frequency modelling of wave propagation in an anisotropic Earth*

How does PPV deform?

1. Atomic-scale modeling of dislocations structure & glide at 0 K, 120GPa



Peierls stress ~ critical resolved shear stress for dislocation glide



A. Goryaeva, PhD 2016, Goryaeva et al. PCM 2015a,b, 2017

Alexandra Goryaeva
Philippe Carrez
Patrick Cordier

erc
RheoMan
UMET
Unité Matériaux Et Transformations

How does PPV deform?

➢ *Atomic-scale modeling of dislocations glide at D" temperatures, pressures & strain rates*

Anisotropic Lattice Friction of PPV

@ 0 K & 120 GPa

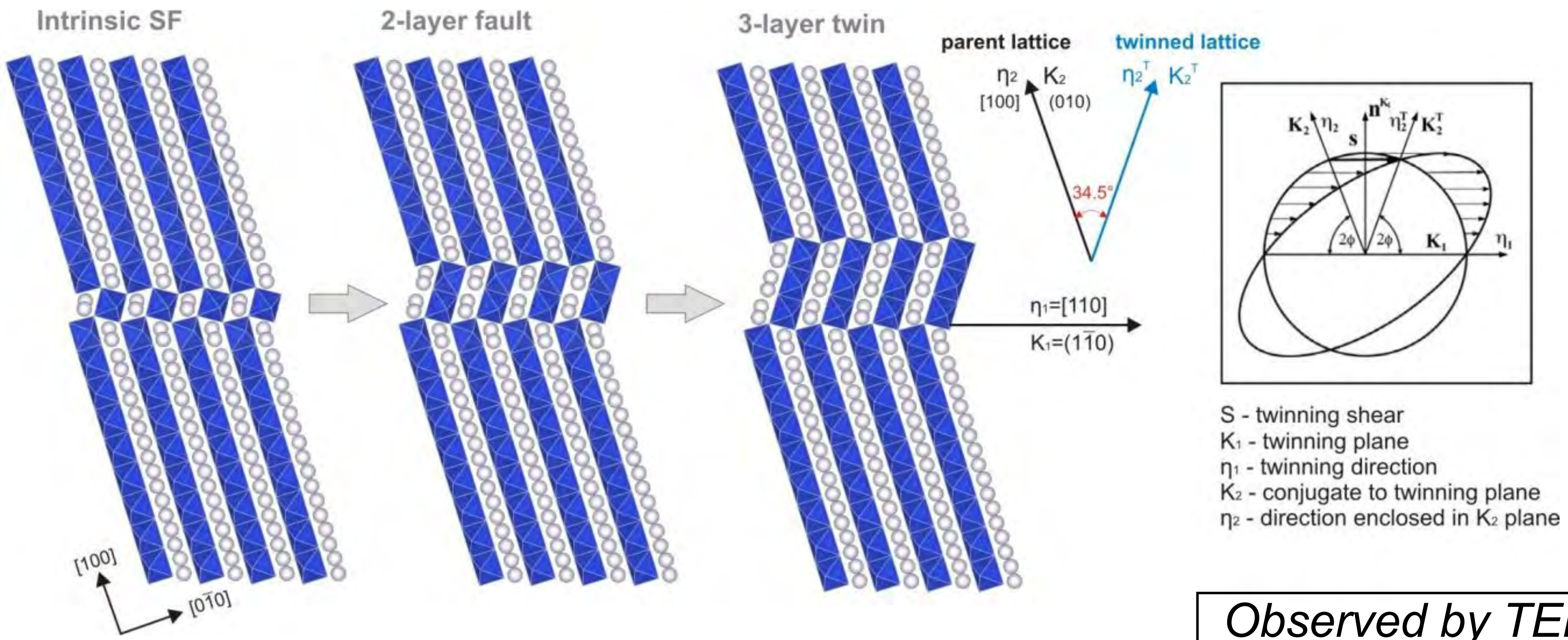
System	Edge σ_p (GPa)	Screw σ_p (GPa)
[100](010)	< 0.1	**1**
[100](011)	~0.12	> 11
[100](001)	~0.1	17.5
[001](010)	2	**3**
½<110>{110}	**2.8 → twinning**	0.7

NEW!

A. Goryaeva, PhD 2016, Goryaeva et al. PCM 2015a,b, 2017

How does PPV deform? Twinning

<110>{110} twinning: rotation by 34.5° around [001]
Abrupt change of orientation = effect on texture evolution

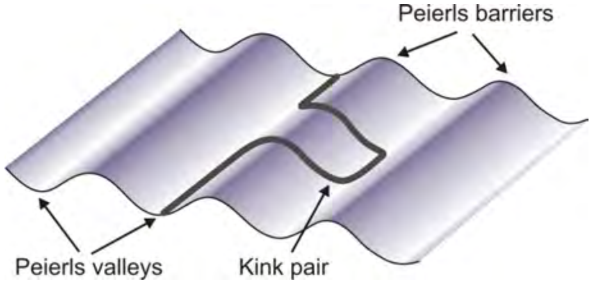


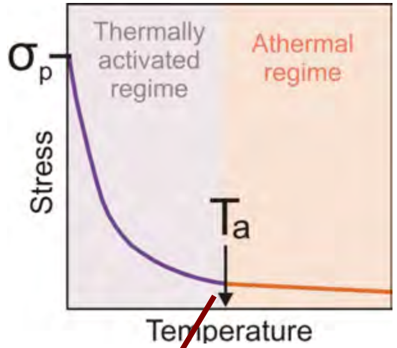
➢ *Accommodates strains // [100] & [010]*

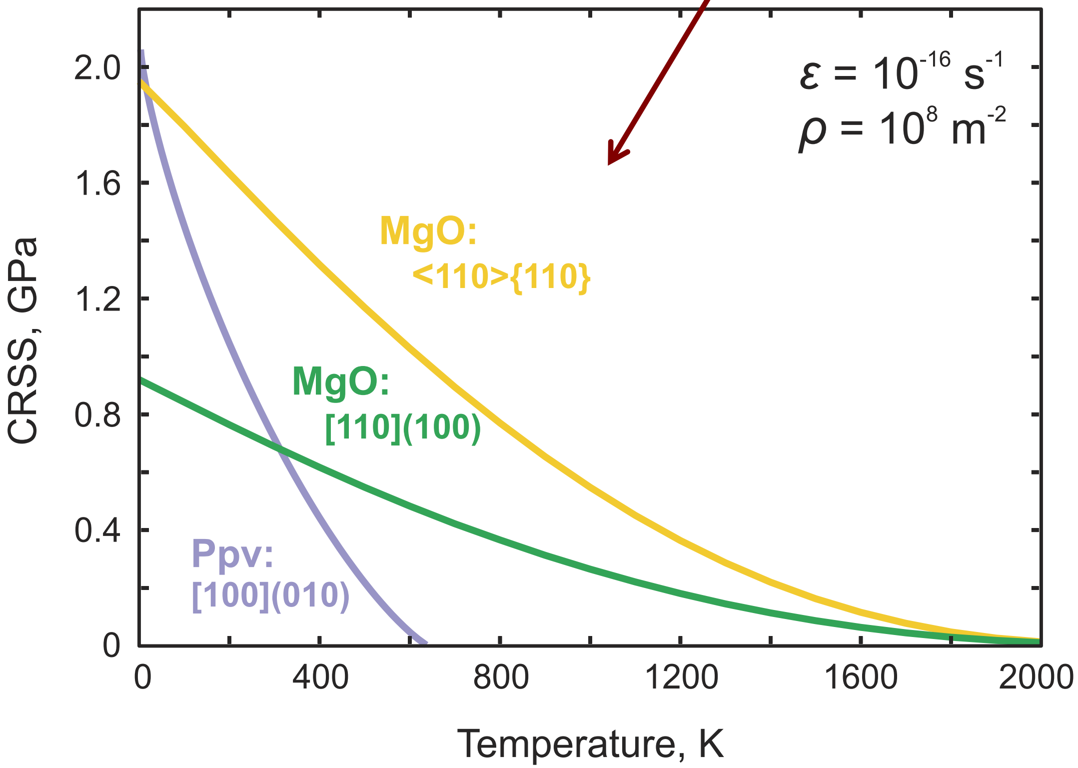
Observed by TEM in $CaIrO_3$ PPV
(Miyajima et al. 2010; Niwa et al. 2012)

How does PPV & MgO deform under D" conditions?

Atomic-scale modeling of dislocation glide @ ***high T (≥2000K)***
high P (120GPa)
low strain rates (10^{-16} s^{-1})







At D" temperatures (>2000K):

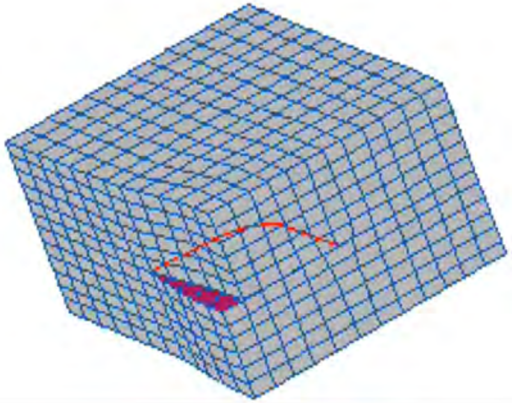
Dislocation glide is easy
(requires low stresses)
&
independent on T
for both PPv and MgO

Cordier et al. Nature 2012 , Goryaeva – PhD 2016; Goryaeva et al. Science Reports 2016; Goryaeva et al. PCM 2017

Modelling the deformation of a rock = polycrystalline aggregate
Viscoplastic self-consistent models (VPSC)

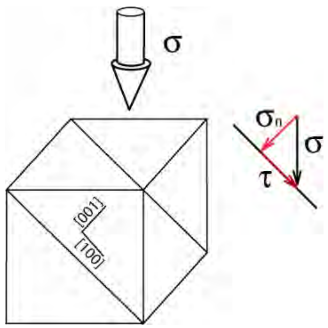
Lebensohn & Tomé 1993

within a grain (crystal):

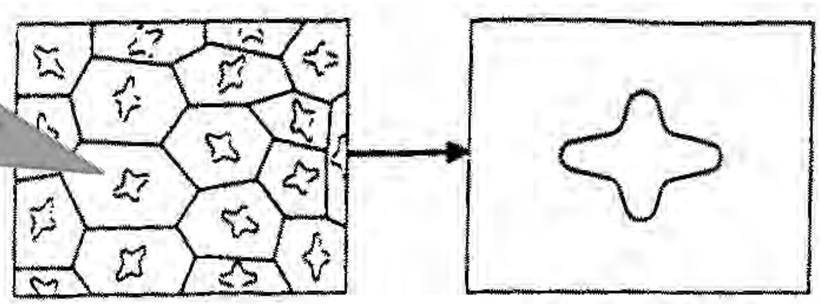


strain = motion of dislocations on well-defined crystal planes & directions

$$\dot{\gamma}^s = \left(\frac{\tau_r^s}{\tau_0^s}\right)^n$$



rock (polycrystal) deformation:



behavior of the aggregate (rock) = average of crystals' behaviors

$$\dot{E}_{ij} = \langle \dot{\varepsilon}_{ij} \rangle \qquad \Sigma_{ij} = \langle \sigma_{ij} \rangle$$

$$\dot{\varepsilon}_{kl} - \dot{E}_{kl} = -M_{ijkl} : (\sigma_{ij} - \Sigma_{ij})$$

Input : ***slip systems' strength, initial texture & mechanical solicitation*** *(stress or velocity gradient tensor)*

→

Output: ***evolution of crystal orientations*** *& mechanical response (strain rate or stress tensor)*

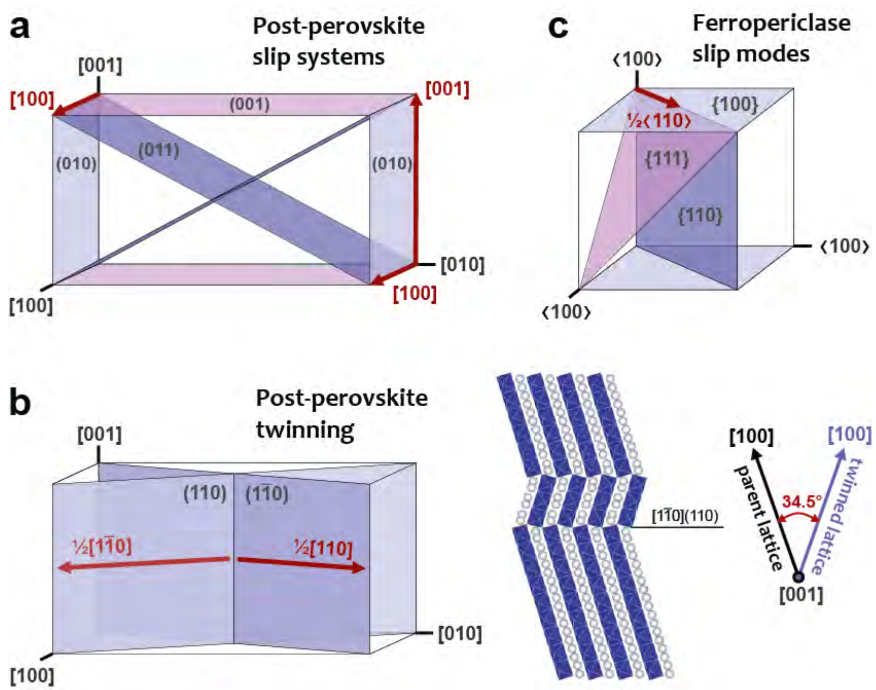
Modelling the deformation of a D" rock
~ aggregate of 70% $MgSiO_3$ PPV + 30% MgO crystals

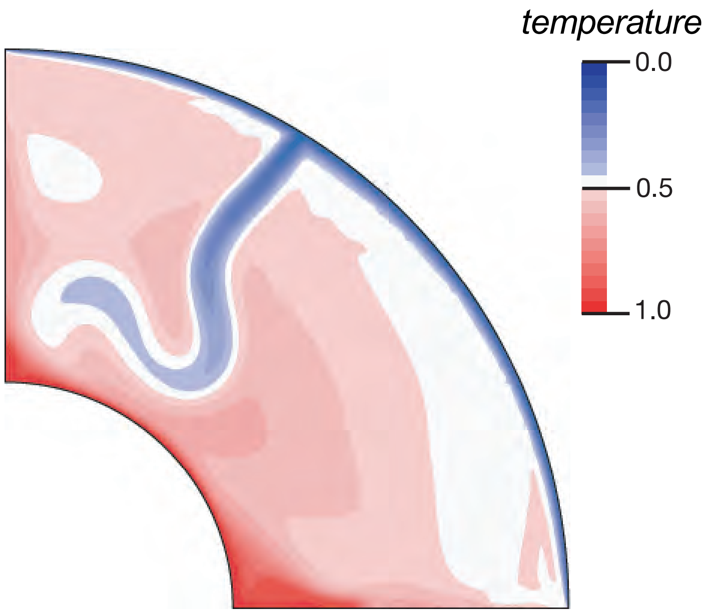
$MgSiO_3$ PPV

Slip system	*CRSS*
[100](010)	*1*
[100](011)	*10*
[100](001)	*20*
[001](010)	***1** / 3*
½ <110>{110} twinning	***3** / not active*

MgO

Slip system	*CRSS*
<110>{110}	*1*
<110>{111}	*5*
[100]{110}	*1*

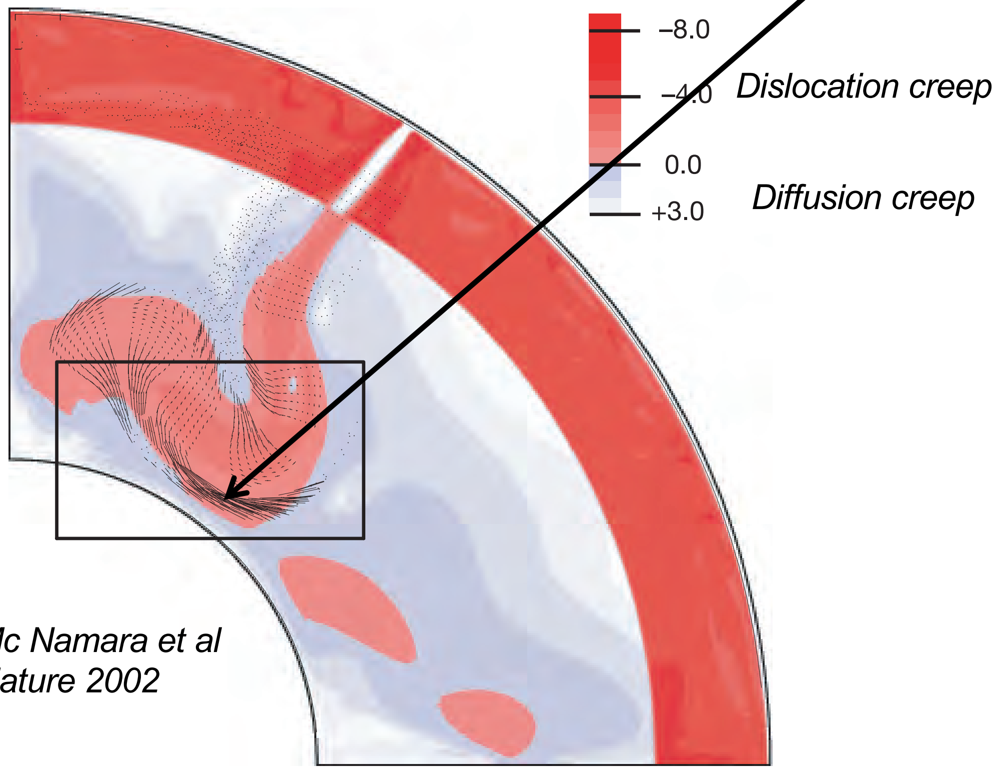




Which deformation in D”?

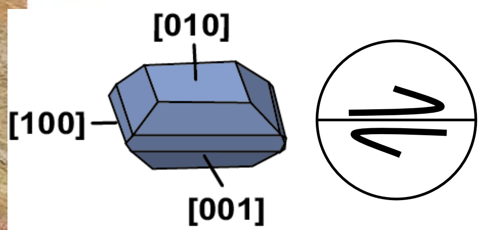
- *Flow patterns can be very complex:*
  - *folding of the slabs…*

  BUT the highest strain domains:
  stretching subparallel to CMB



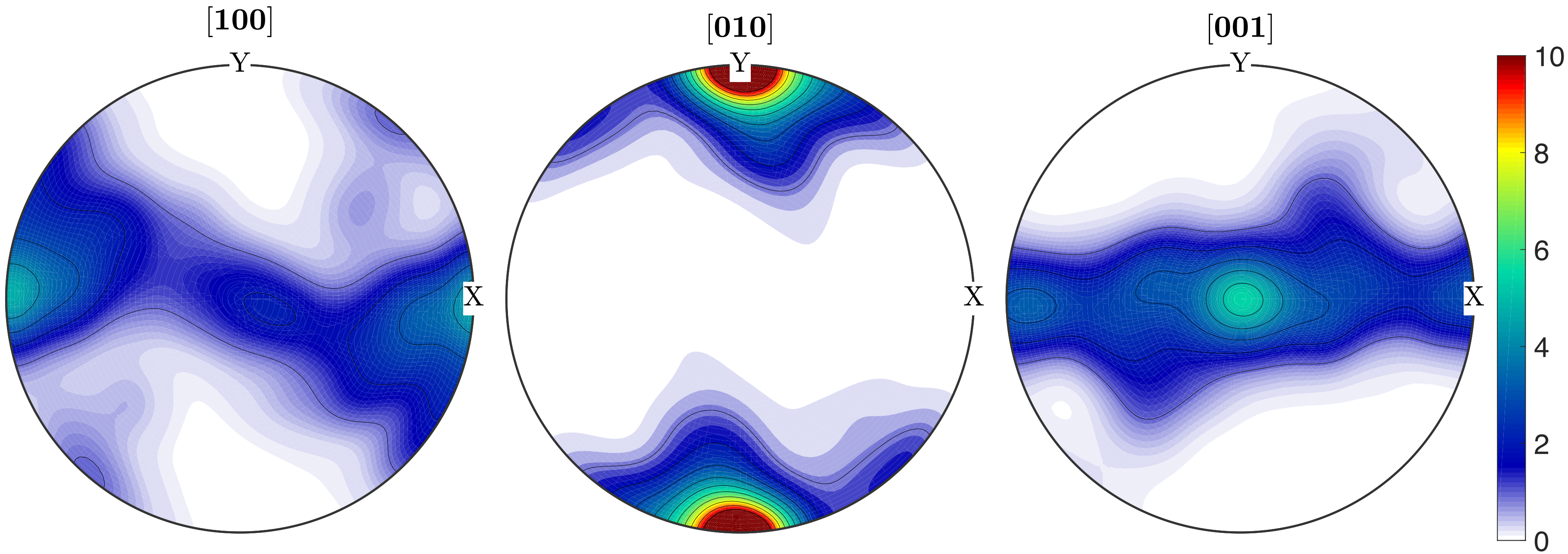
Mc Namara et al
Nature 2002

Modelling the deformation of a 70% PPV – 30% MgO aggregate

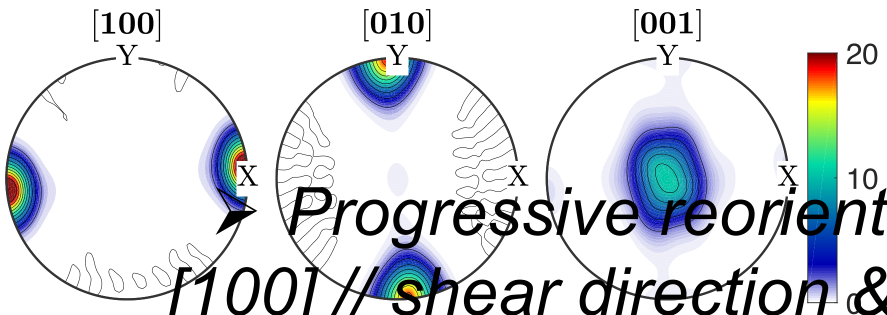


PPV texture evolution with increasing strain
twinning active

Tommasi et al. EPSL 2018



Shear strain of 10

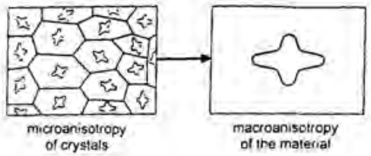


→ *No twinning – shear strain of 10*

- *Progressive reorientation of the crystal leading to [100] // shear direction & [010] // normal to shear plane*
- *Twinning = faster rotation but slower intensification of the CPO dispersion of [100] & [010] = rotation by 34° around [001]*

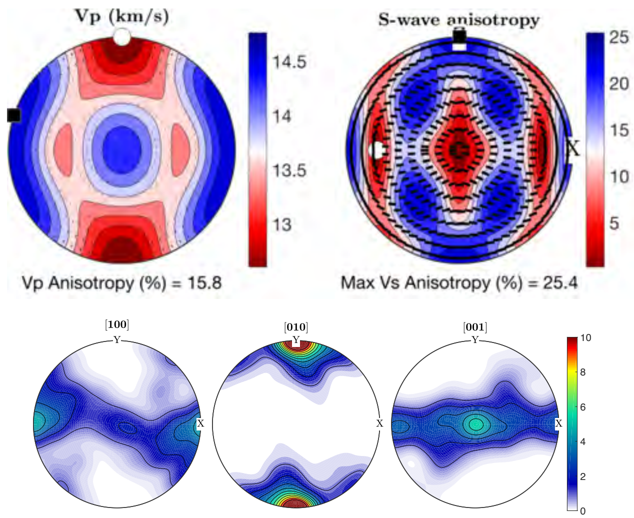
Seismic anisotropy at the rock scale

rock = aggregate of anisotropic crystals



Zhang et al. 2015

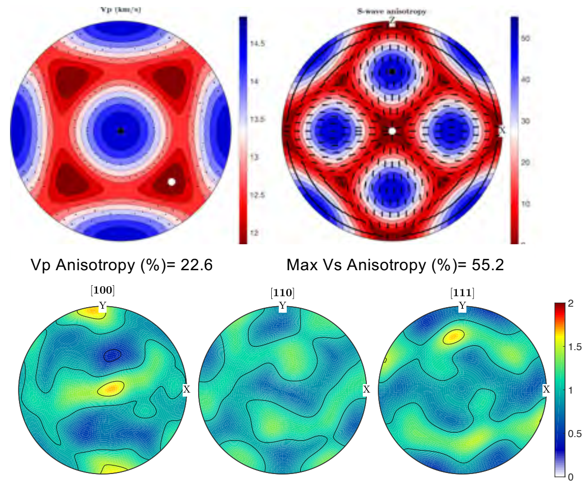
70% $(Fe,Mg)SiO_3$ PPV

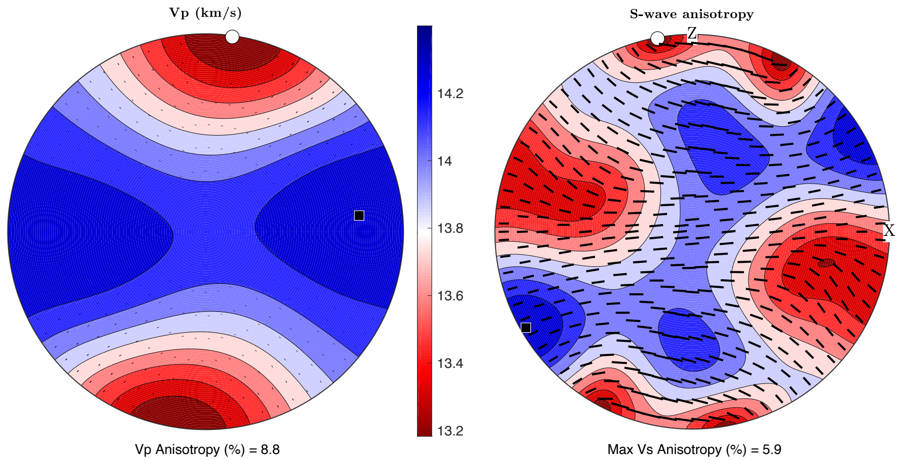


2000 K
125 GPa

+

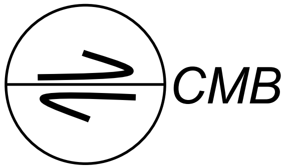
30% (Fe,Mg)O

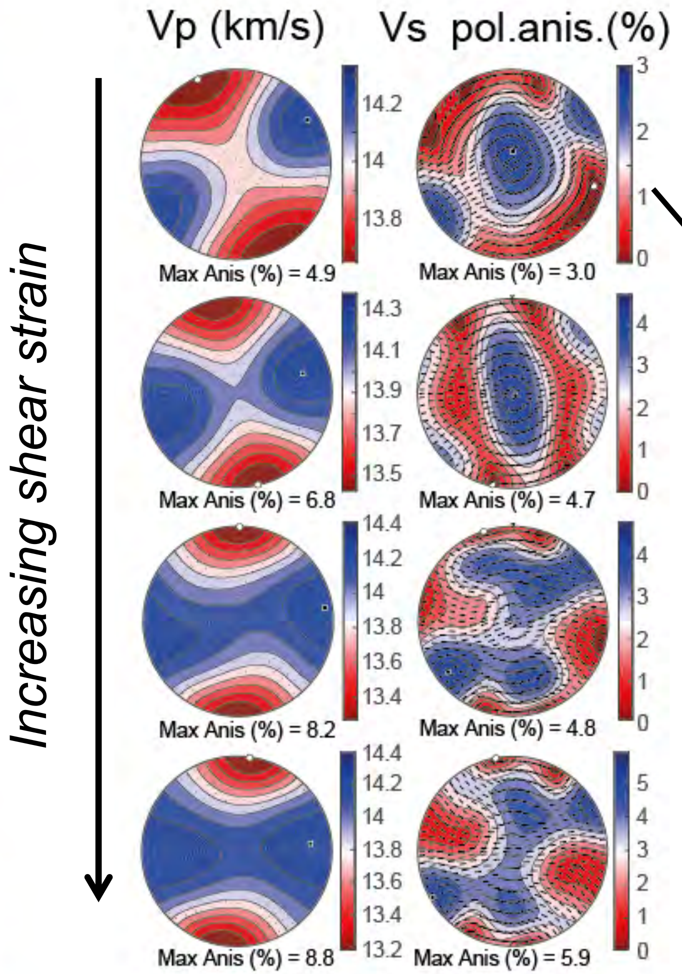


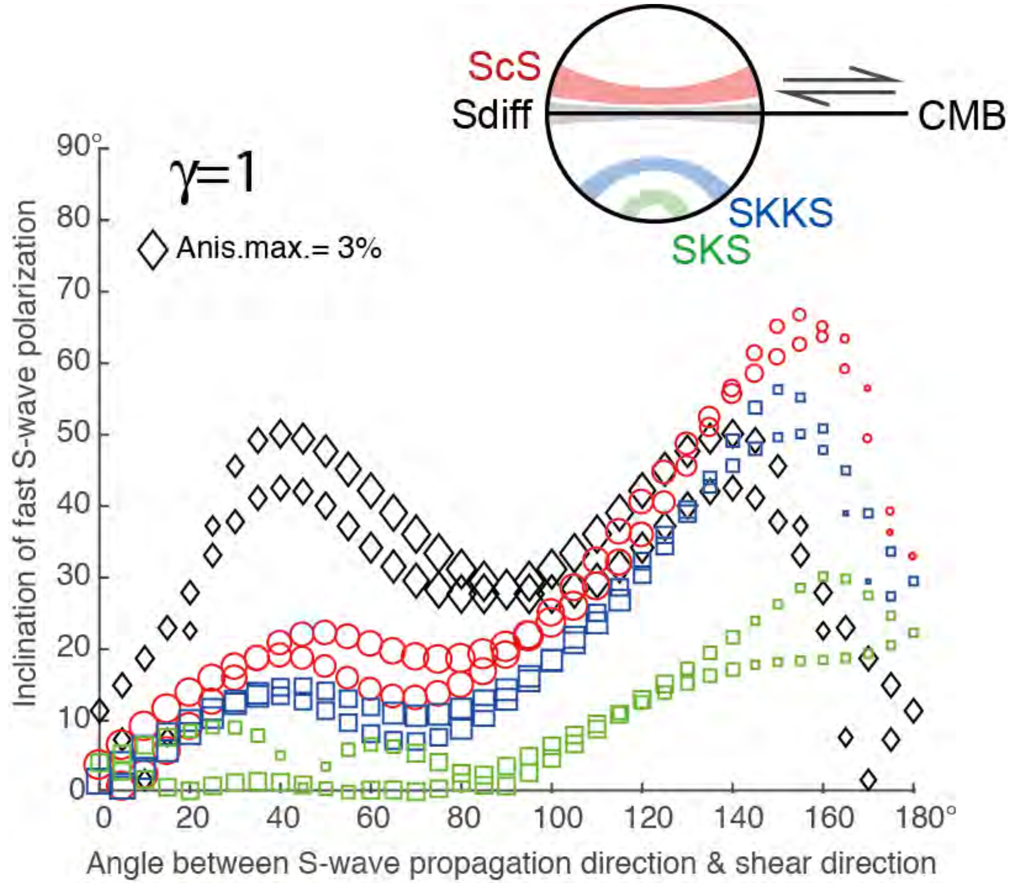


volumetric averaging of the single crystal properties function of:
- mineralogical composition
- orientation of the crystals

Seismic anisotropy of a PPV+MgO aggregate deformed in simple shear parallel to the CMB at 2000 K, 125 GPa

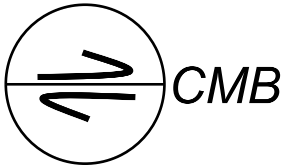




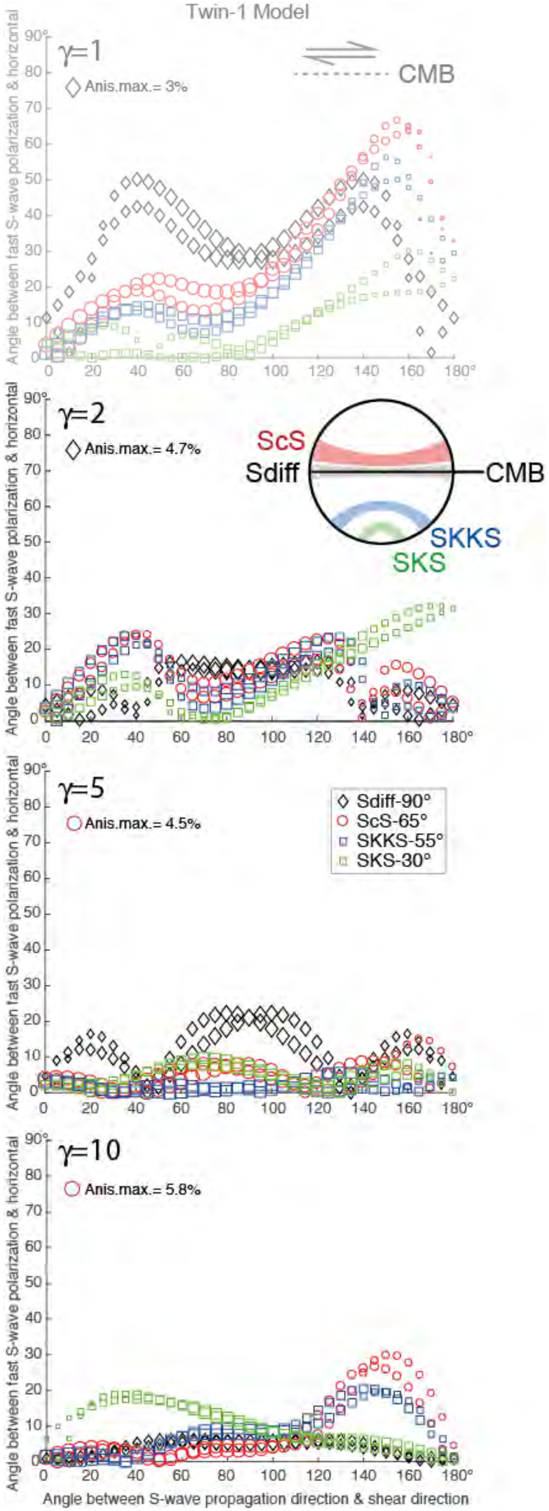


At low shear strains:
fast polarization & birrefringence depend strongly on propagation direction
Sdiff, ScS, SKKS fast polarization may be inclined by up to 50-60° to relatively to the horizontal

Tommasi et al.
EPSL 2018



Increasing shear strain



Tommasi et al.
EPSL 2018

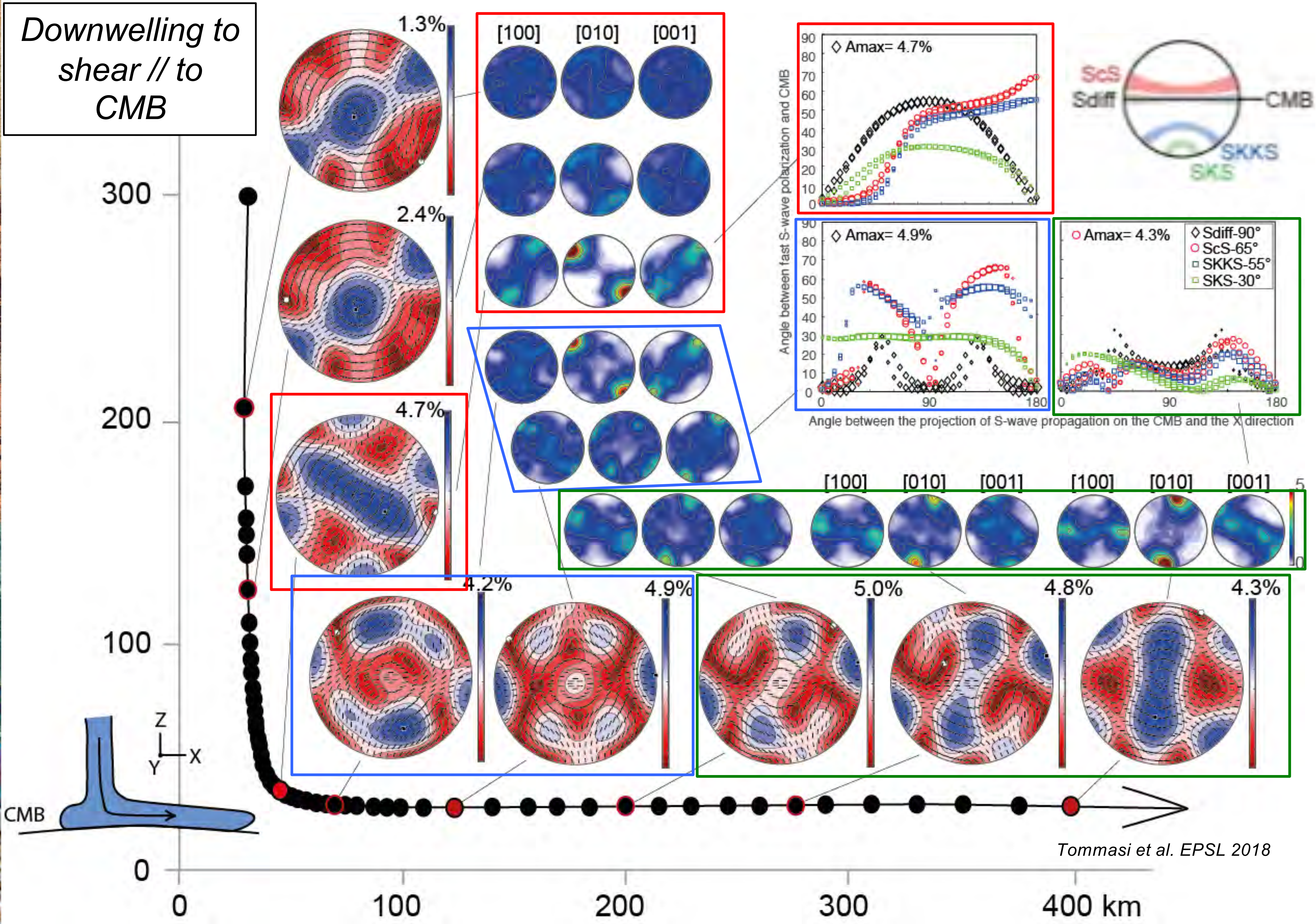
Seismic anisotropy of a PPV+MgO aggregate deformed in simple shear parallel to the CMB at 2000 K & 125 GPa

At low shear strains:
fast polarization & birrefringence depend strongly on propagation direction
Sdiff, ScS, SKKS fast polarization inclined by up to 50-60°

Max inclination of fast polarization decreases with increasing shear strain

At high shear strains:
Fast polarizations mainly subhorizontal, but birrefringence still depends on propagation direction

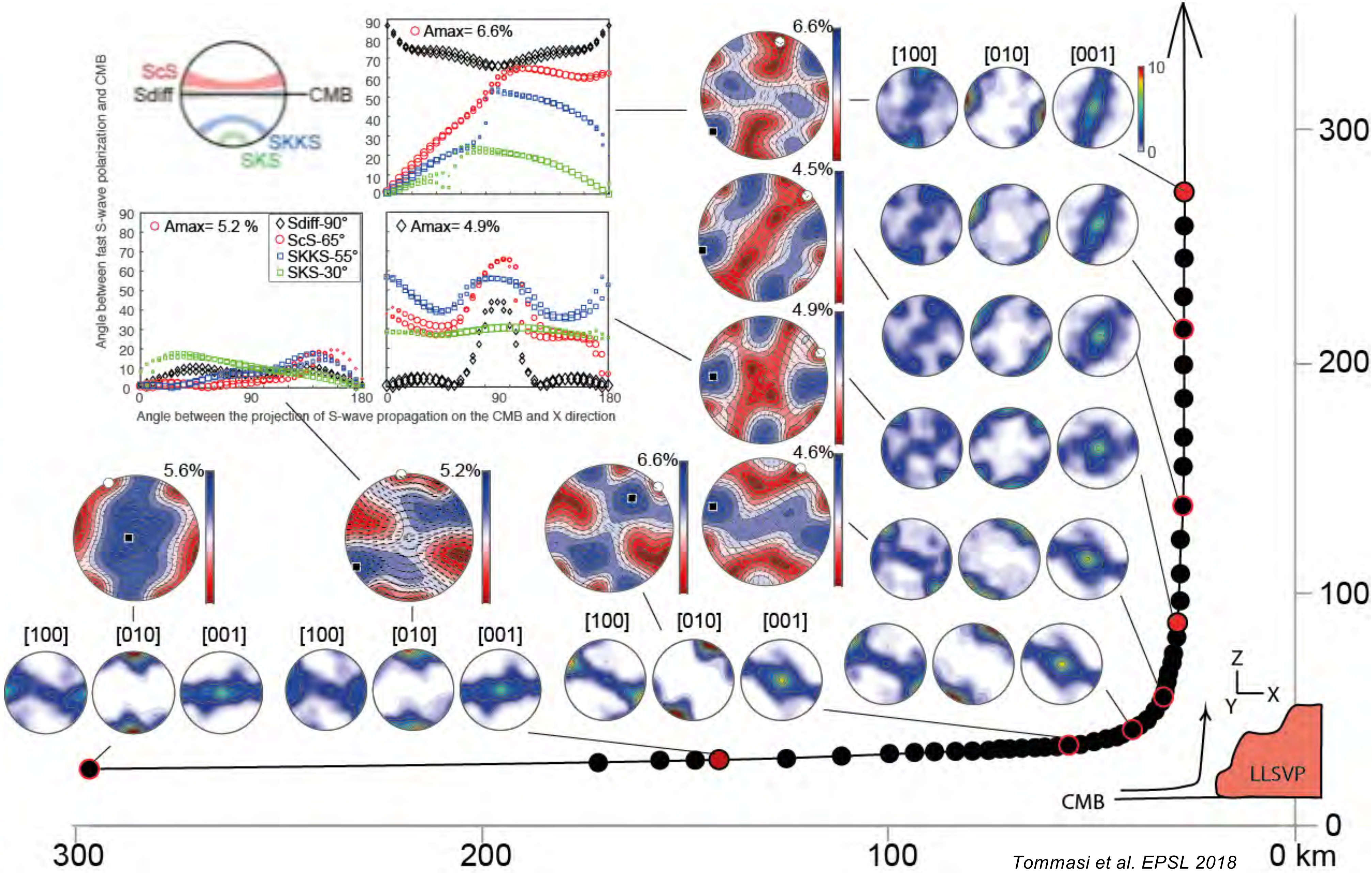
CPO and seismic anisotropy evolution in response to a change in flow direction



Tommasi et al. EPSL 2018

CPO and seismic anisotropy evolution in response to a change in flow direction

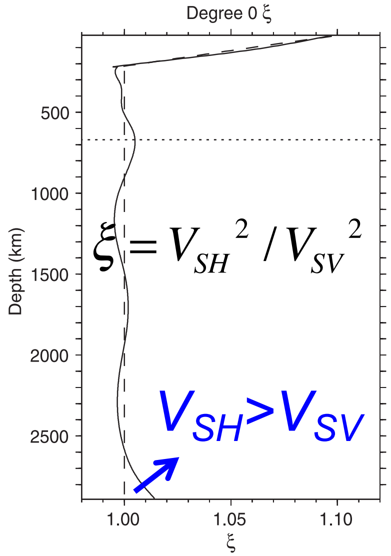
Shear // to CMB to upwelling at the border of a Low Shear Velocity Province



Tommasi et al. EPSL 2018

Seismic anisotropy in D”: Observations vs. model predictions

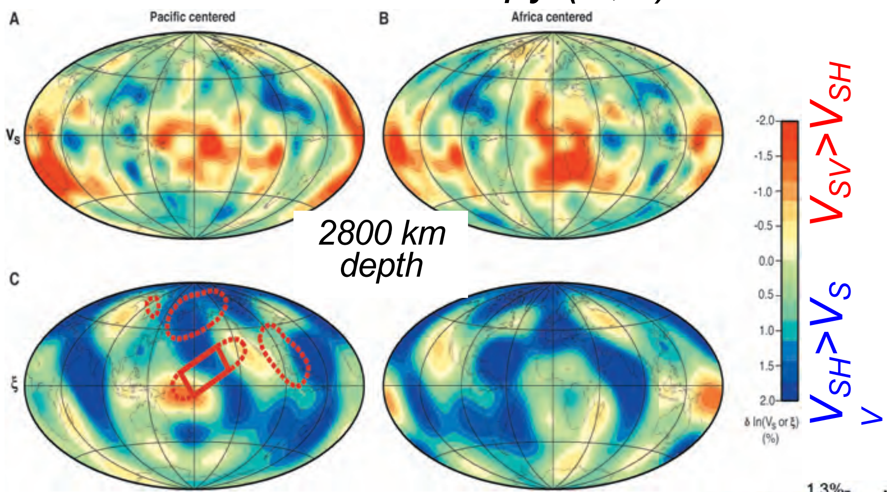
1D global average



Panning & Romanowicz Science 2004

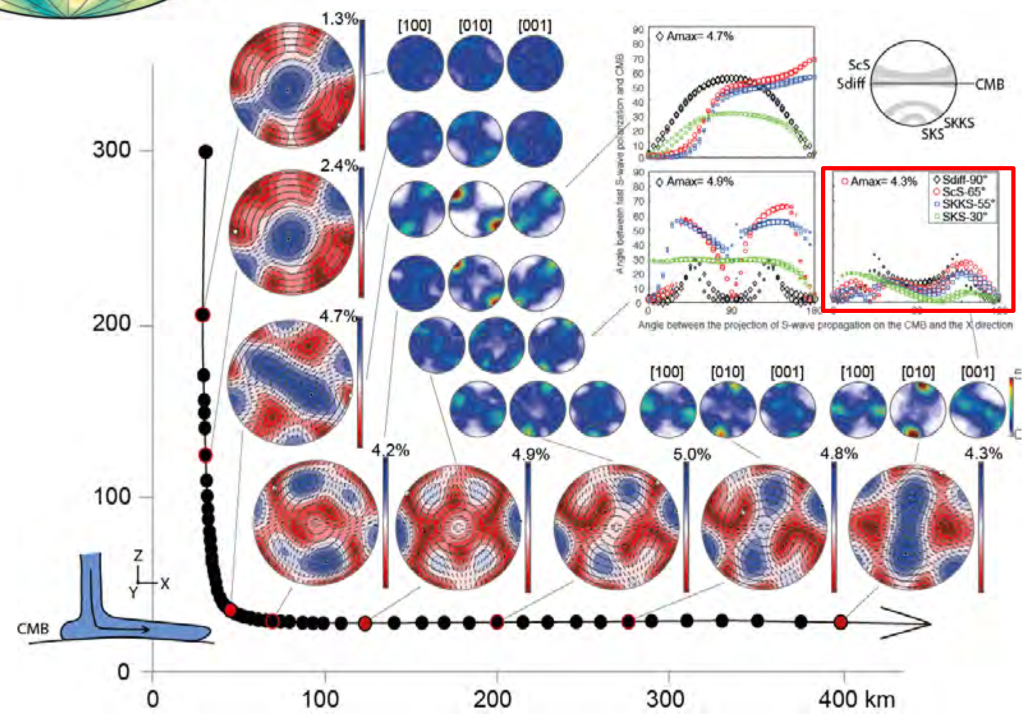
Anisotropic tomography

S-wave velocity anomalies (A,B) and radial anisotropy (C,D)



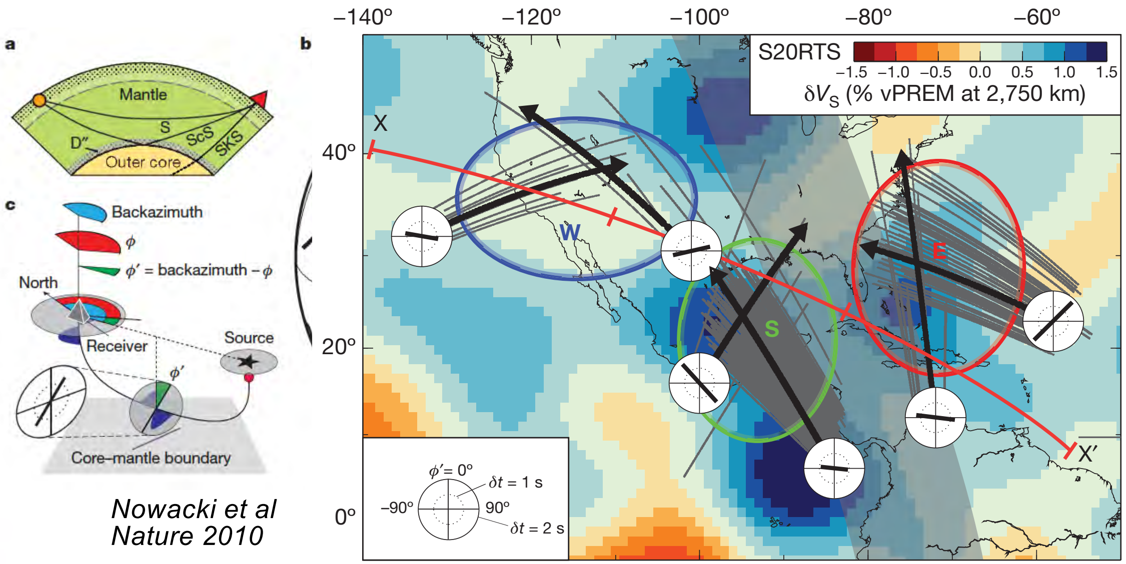
- *Predominance of $V_{SH} > V_{SV}$*
- *Strong $V_{SH} > V_{SV}$ anisotropy mainly in high velocity domains*
- *$V_{SV} > V_{SH}$ = smaller areas, mainly low velocity domains*

- *Shear parallel to the CMB dominates the average flow pattern in D”*



Seismic anisotropy in D”: Observations vs. model predictions

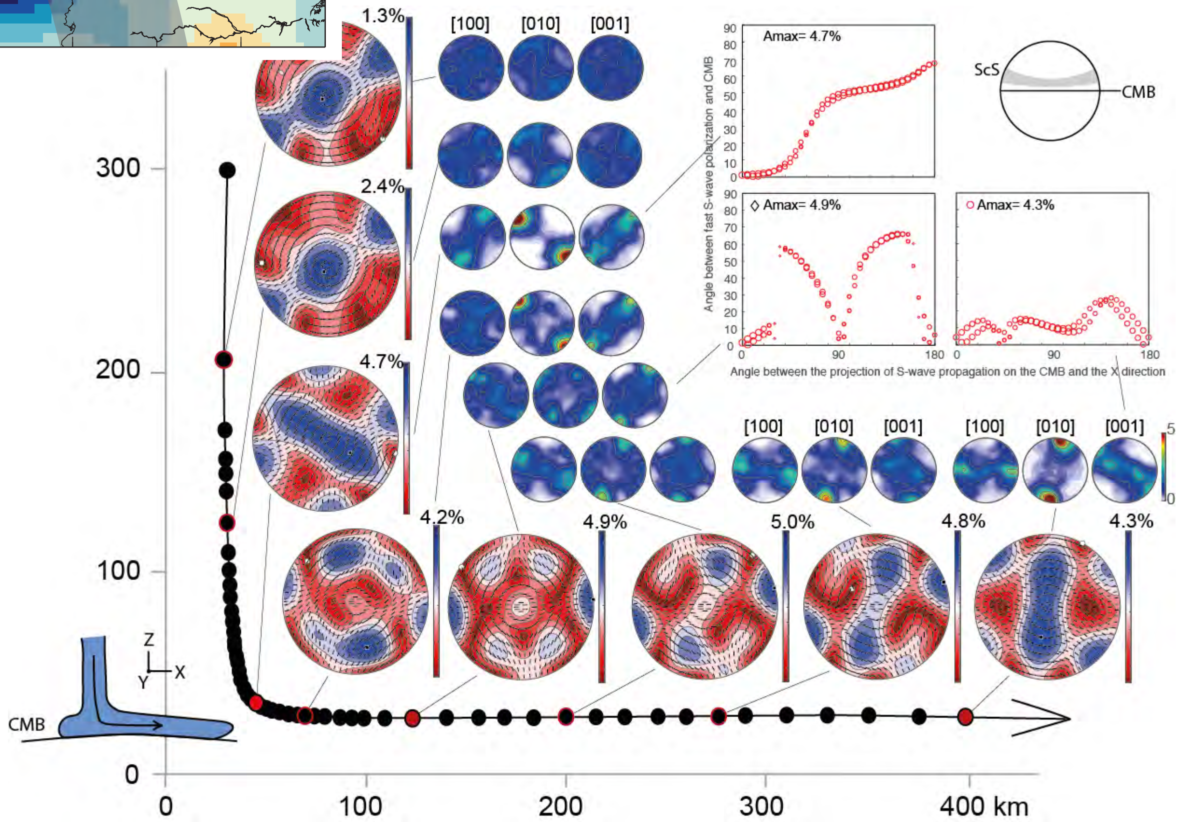
Differential S-ScS splitting



Nowacki et al Nature 2010

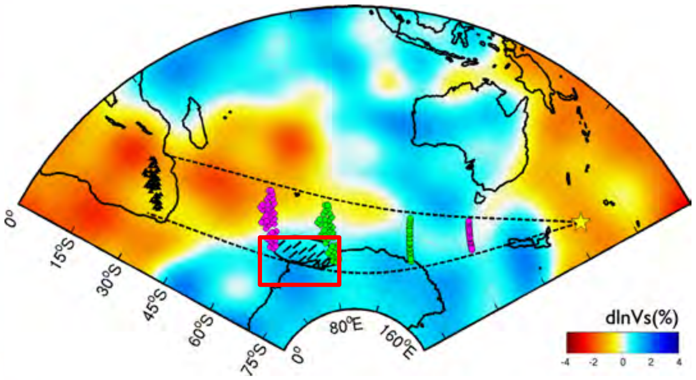
- *Different splitting in cross-cutting ray paths = anisotropy depends on propagation direction*
- *Fast polarizations either sub-parallel or inclined relatively to CMB*

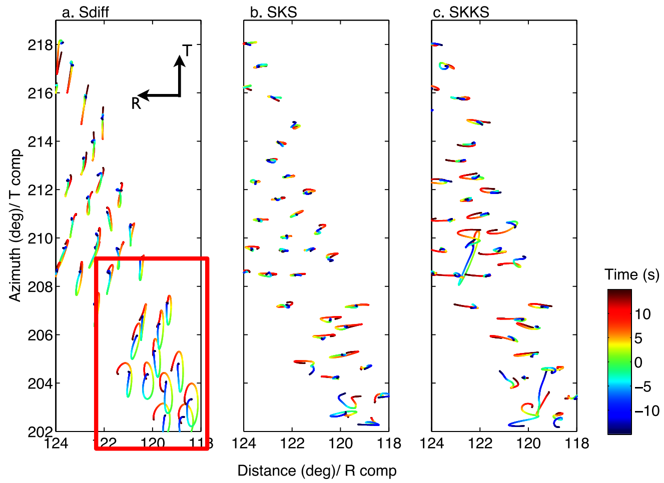
- *Fast ScS polarizations inclined by >30 ° to CMB only observed in or near vertical flow domains*
- *Consistent with the observations = paths sampling high velocity regions (downwellings)*
- *Predicted (local) anisotropy >> measured values : integration of spatially Δ signal*

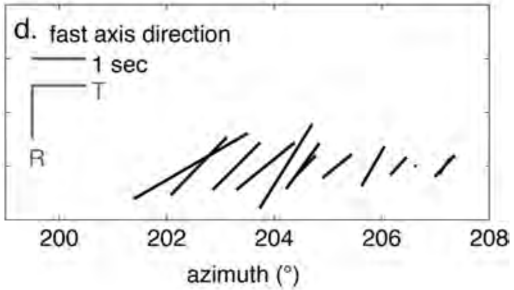


Seismic anisotropy in D": Observations vs. model predictions

Sdiff splitting – 3D waveform modeling

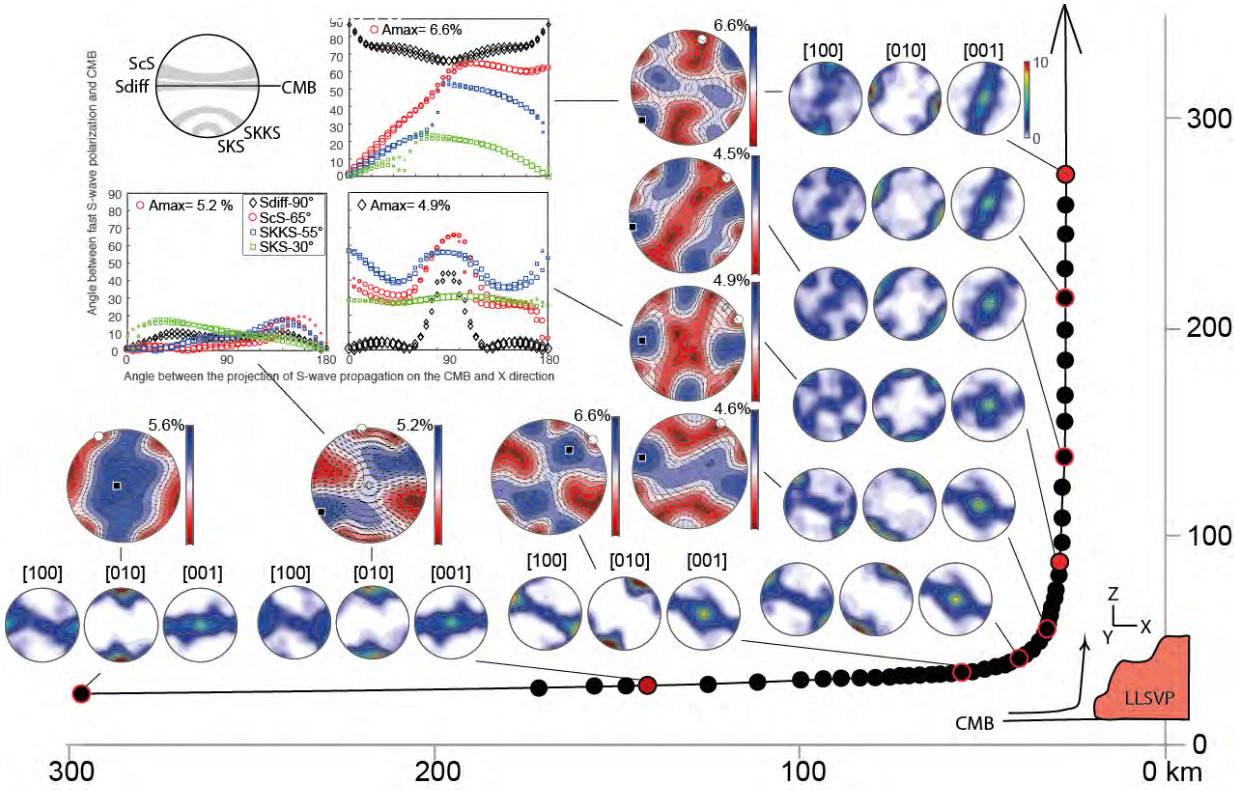






Cottaar & Romanowicz GJI 2013

- *Fast Sdiff polarizations inclined by 45° to CMB observed at southern border of the African LLSVP*
- *No clear SKS or SKKS anisotropy signal*

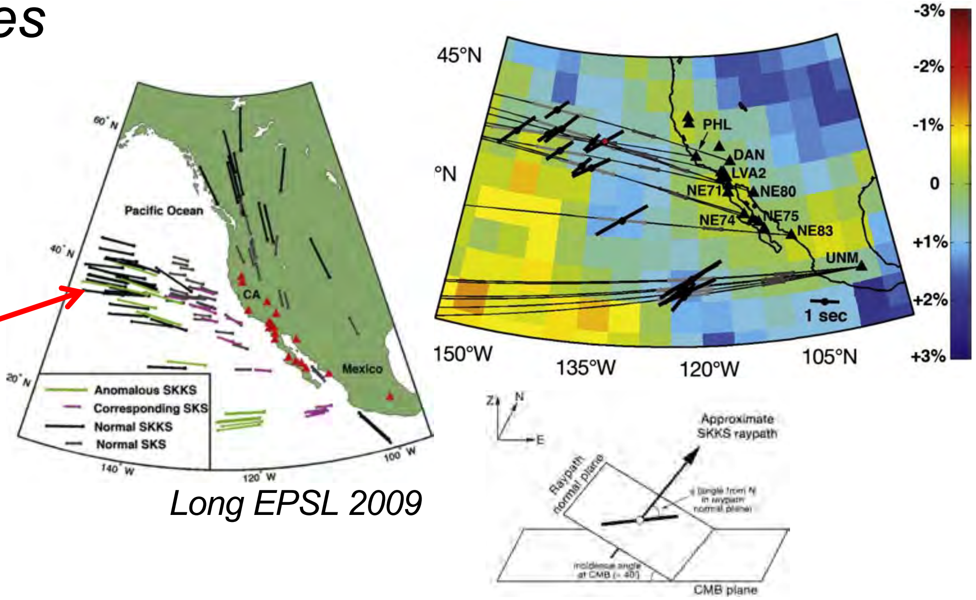


- *Fast Sdiff polarizations inclined relatively to CMB predicted in the upwelling path*

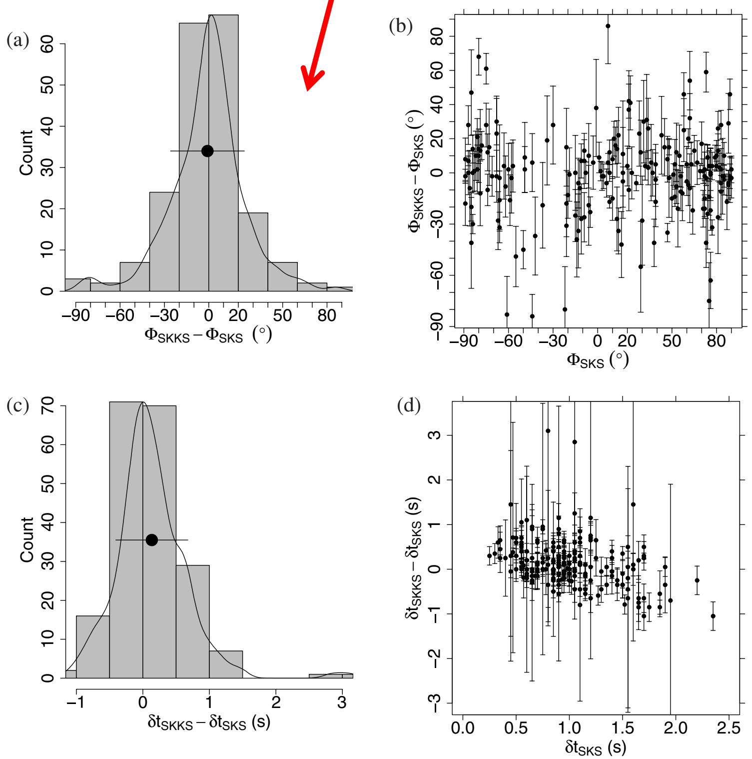
Seismic anisotropy in D”: Observations vs. model predictions

SKKS-SKS splitting discrepancies

- *Similar paths in the upper mantle, but different ones in D”*
- *BUT rare observations & often consistent & discrepant observations overlap*

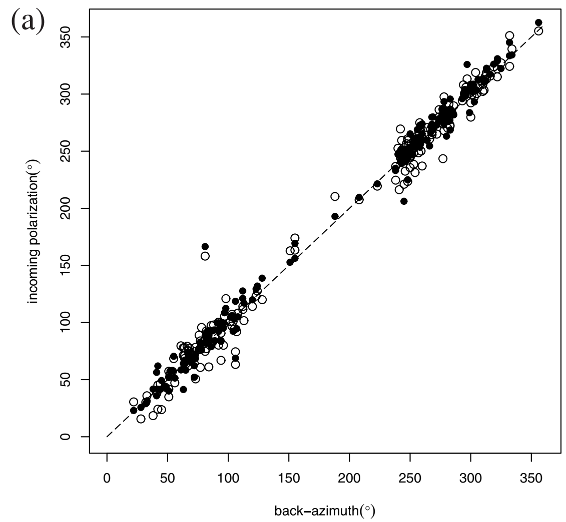


Long EPSL 2009



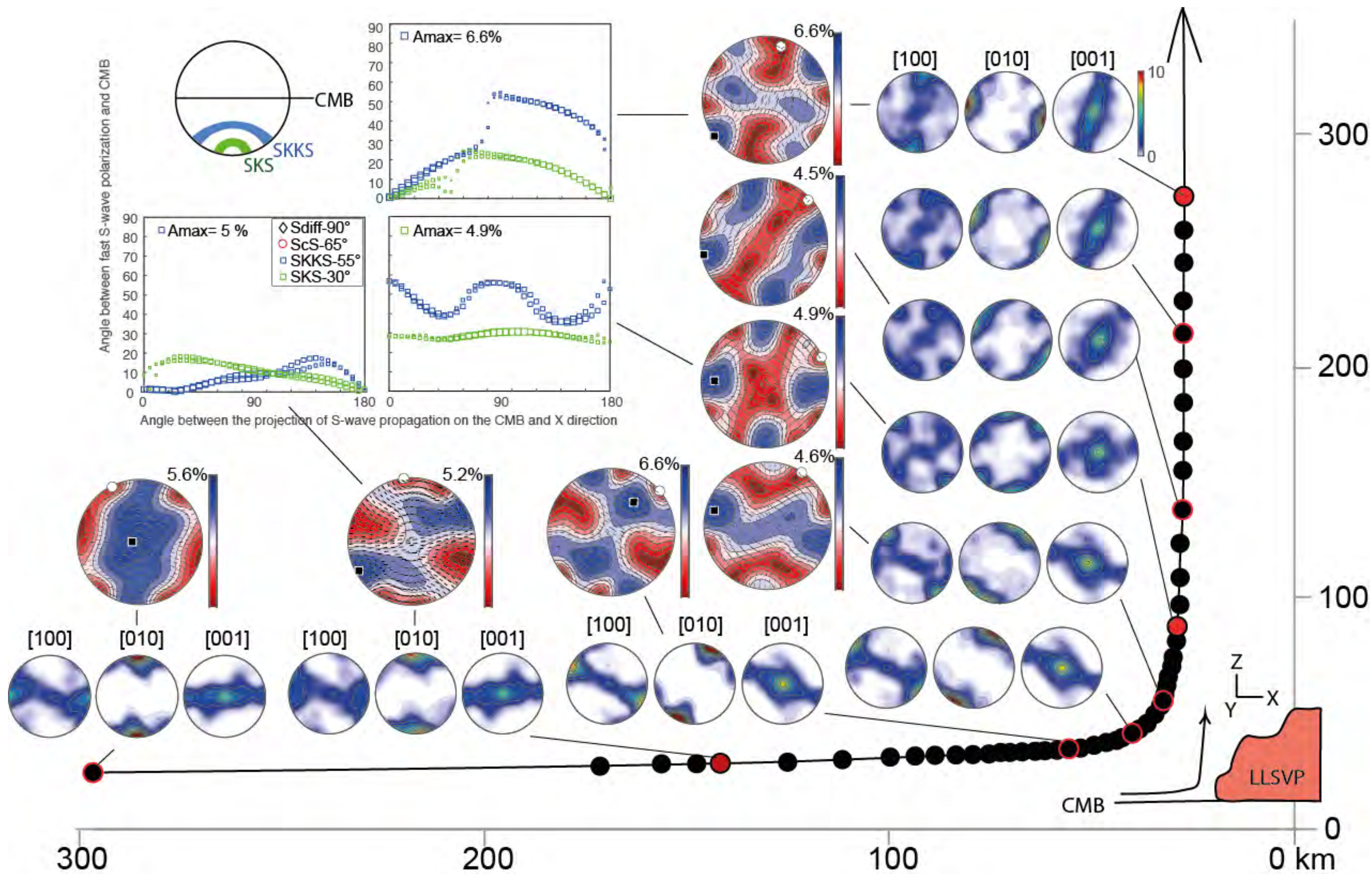
Restivo & Helffrich GJI 2006

- *Also, splitting in D” should deviate the initial polarization of SKS & SKKS from the back-azimuth : rarely observed!*



Seismic anisotropy in D”: *Observations vs.* ***model predictions***

SKKS-SKS splitting



➢ *Clear SKS & SKKS birefringence for most propagation directions for both horizontal shearing & vertical flows. SKS & SKKS signals often ≠.*

➢ *Why this anisotropy is not “seen” by most SKS & SKKS waves? Hypothesis : Finite-frequency effects – averaging of the signal over large volumes with lateral variations in the flow pattern*

Atomic scale models of the deformation of PPV & MgO + VPSC models : ***prediction of the evolution of CPO as a function of strain****, which can be translated into seismic anisotropy patterns.*

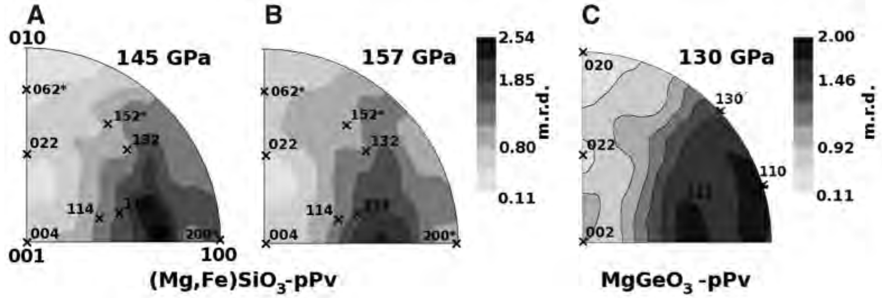
Most ***observations of seismic anisotropy in D" might be explained by an anisotropic PPV-rich D" deforming by dislocation creep with dominant activation of [100](010) & [001](001) slip + twinning****.*
Inclined fast polarizations imply departures from flow // to CMB.
Low observed delay times imply heterogeneity of flow at scales < 1000 km

BUT: Seismic waves integrate the signal over large volumes in D".
No simple key for the interpretation of the observations.

Open question: ≠ between model predictions & experiments

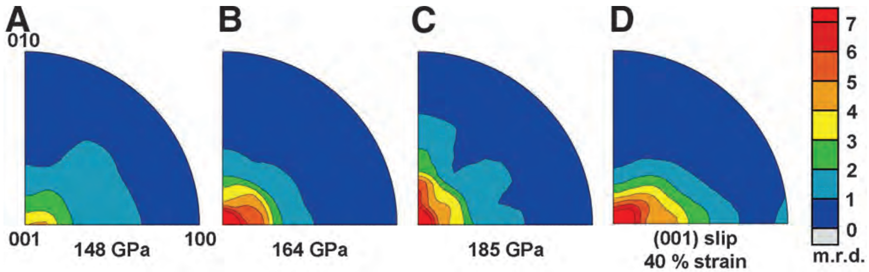
Diamond anvil cell experiments on $MgSiO_3$ PPV at D" p,T conditions
In situ texture measurements by X-ray diffraction; stresses 5-10 GPa

145-157 GPa, 1700-2000 K
stresses 7.2-8.5 GPa



Merkel et al. 2007 Science

148-185 GPa, 3500 K
stresses 5-10 GPa

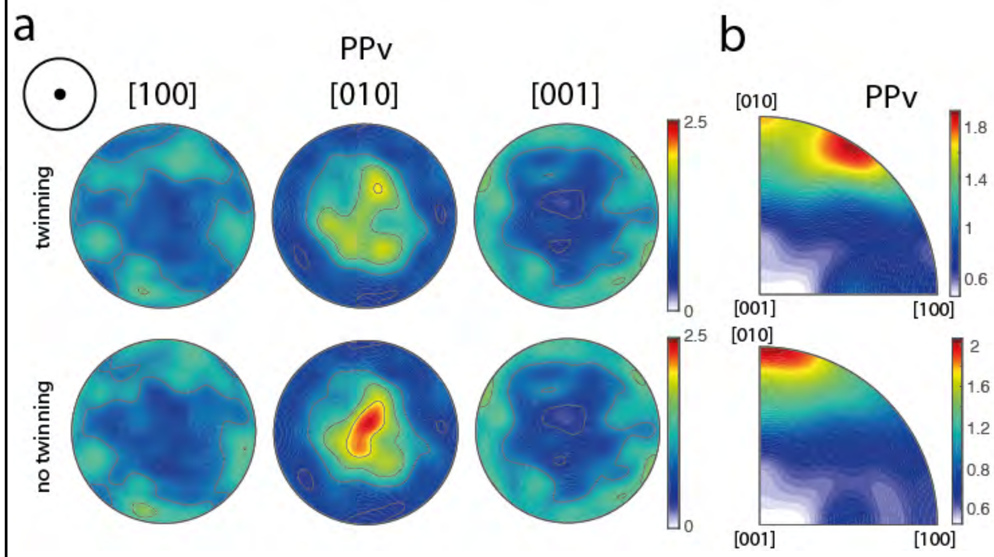


Miyagi et al. 2010 Science

Textures inherited at phase change + glide on (001) & {110} planes?

VPSC simulations based on atomic scale modeling of dislocation glide

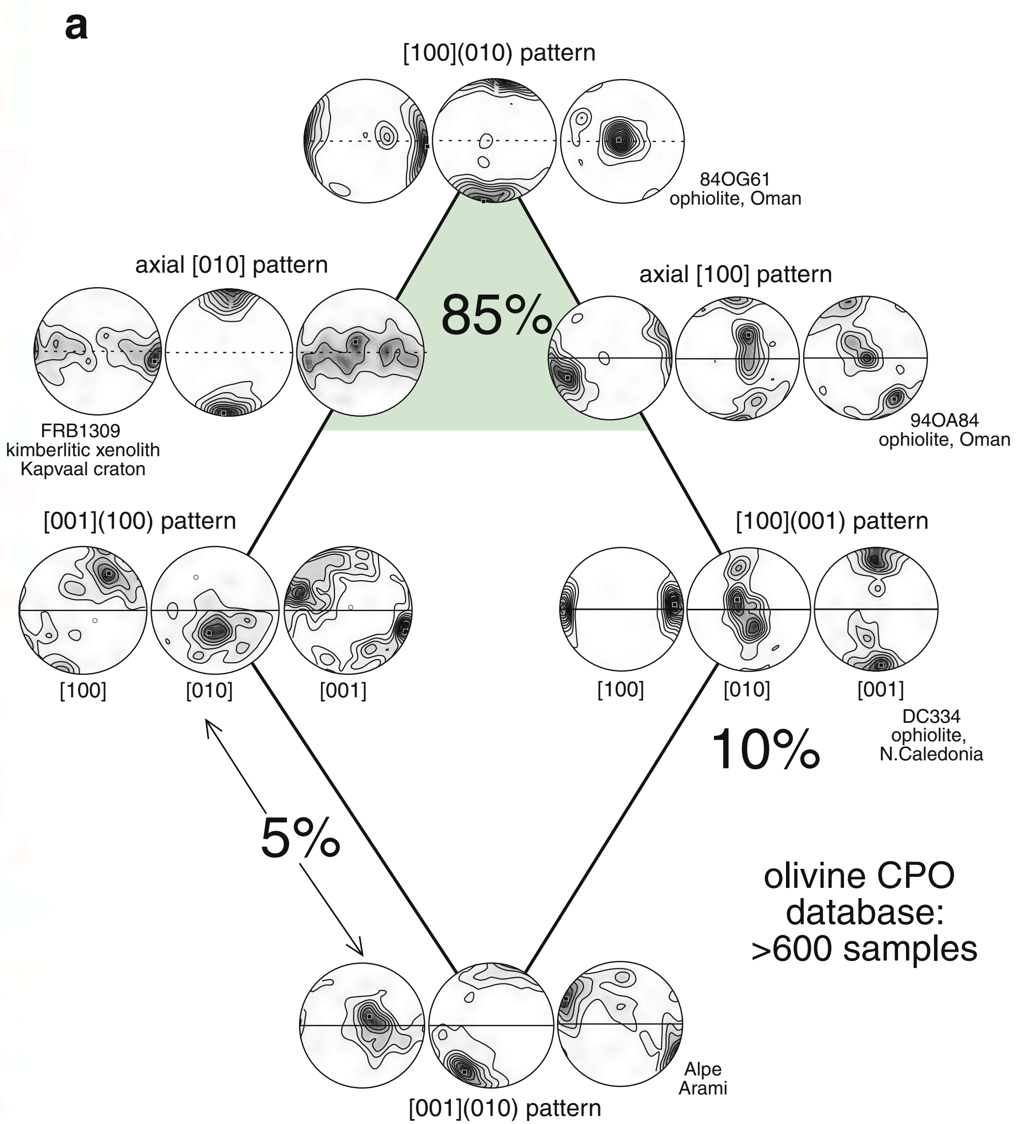
20% shortening



Dominant glide on [100](010) & [001](010)

➢ ***Texture inheritance + stresses in experiments >> mantle stresses?***

Why even for the upper mantle inversing deformation patterns from seismic anisotropy is not possible?



- *Incomplete seismological sampling … full anisotropy tensor is never sampled*
- *Splitting data integrates the anisotropy along the path; discrimination of different contributions only possible by differential analysis*

> *Different processes / flow geometries produce similar olivine CPO*
>
> *Olivine CPO produced under ≠ conditions have ≠ orientations relation to flow pattern, but may only be discriminated in the deformation reference frame, which is not known!*