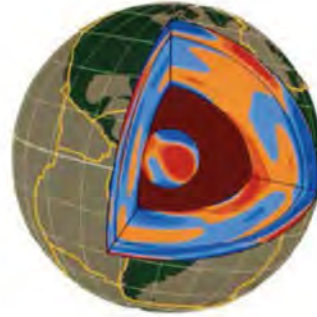


S. Merkel

Université de Lille,
France



CHAIRE DE PHYSIQUE DE L'INTÉRIEUR
DE LA TERRE

Année académique 2019-2020

Pr Barbara ROMANOWICZ

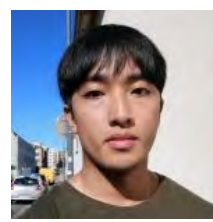
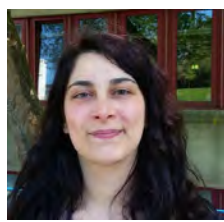
Global Scale Seismic Imaging and
Dynamics of the Earth's Mantle

Colloque en anglais - Workshop in English
co-organised with Nicolas Coltice, ENS de Paris

Thursday October 7 and Friday October 8, 2021

Phase transitions in the mantle: effect on microstructures and seismic observables





S. Merkel C. Thomas

C. Sanchez
Valle

S. Speziale

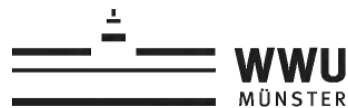
F. Rochira

J. K. Magali

M. Krug

E. Ledoux

J. Gay



GFZ

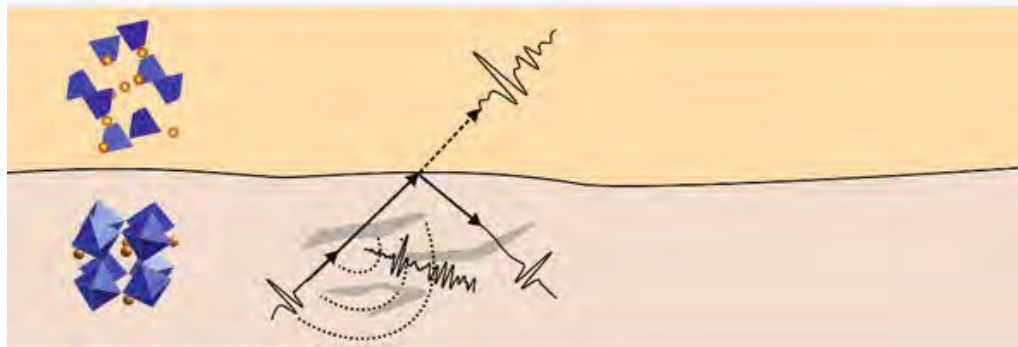
Helmholtz-Zentrum
POTS DAM



 **Université
de Lille**

TIMEleSS

Phase Transformations, MicrostructurEs, and their Seismic Signals from the Earth's mantle



AGENCE NATIONALE DE LA RECHERCHE
ANR

DFG

Deutsche
Forschungsgemeinschaft

In-situ study by multigrains crystallography of deformation of $(\text{Mg,Fe})_2\text{SiO}_4$ wadsleyite at conditions of the 410 km depth discontinuity



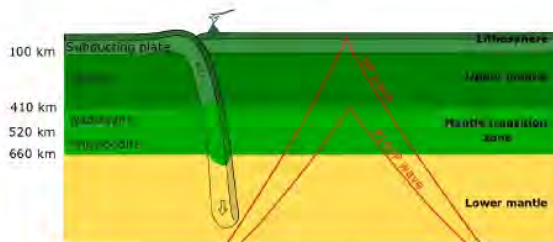
E. Ledoux¹, J. Gay¹, M. Krug², O. Castelnaud³, J. Chantel¹, N. Hilairet¹, A. Fadel¹, M. Bykov⁴, H. Bykova⁴, G. Aprilis⁴, V. Svitlyk⁵, G. Garbarino⁵, C. Sanchez-Valle², C. Thomas⁶, S. Speziale⁷, D. Jacob¹, S. Merkel¹



1. Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France
2. Institute for Mineralogy, WWU Münster, 48149 Münster, Germany
3. Laboratoire PIMM, UMR CNRS 8006, ENSAM, CNAM, 151 Boulevard de l'Hôpital, 75013 Paris, France
4. Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany
5. ESRF, the European synchrotron, 71 Avenue des Martyrs, CS40220, 38043 Grenoble Cedex 9, France
6. Institute of Geophysics, WWU Münster, 48149 Münster, Germany
7. German Research Centre for Geosciences GFZ, 14473 Potsdam, Germany

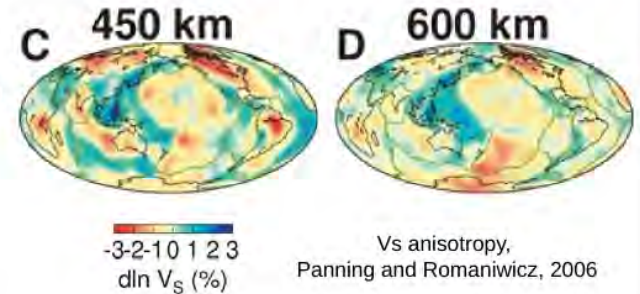


Geological context and topic



Earth's mantle transition zone :

- Dominated by wadsleyite (wd) in its upper part and by ringwoodite (rw) in its lower part
- Controls the sink or the stagnation of subducting slab
- Takes part in the global mantle convection
- Ellusive observations of seismic anisotropy
- Possible sources of anisotropy :
 - deformation-induced LPO of wd and/or rw
 - martensitic transformations of ol > wd > rw



Vs anisotropy, Panning and Romaniwicz, 2006

In this study, we investigate the plastic deformation of wadsleyite to test if it can be source of seismic anisotropy in the mantle transition zone

> first in-situ deformation study on dry wadsleyite at mantle transition zone pressures and temperatures

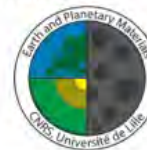
Microstructures Induced by Phase Transformations at the 660km Discontinuity

Jeff Gay¹, Estelle Ledoux¹, Matthias Krug², Anna Pakhomova³, Julien Chantel¹, Carmen Sanchez-Valle², and Sébastien Merkel¹

¹Univ. Lille, CNRS, INRA, ENSCL, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

²Institut für Mineralogie, Westfälische Wilhelms-Universität Münster, Münster, Germany

³Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany



1. Introduction

- Phase transition from ringwoodite to bridgmanite in pyrolytic material responsible for seismic reflectors observed at 660 km depth
- Track mineralogical microstructures in-situ using Multigrain X-ray Diffraction (3D XRD)
 - Texture
 - Grain size distribution
 - Phase transformation
- Combine mineralogical and seismological observations to model deep mantle processes
 - Identify origins of seismic reflectors
 - Effect of phase transitions of bridgmanite on slab subduction
 - Map deformation below 660 km discontinuity



Figure 1. Phase transformation of cubic ringwoodite to orthorhombic bridgmanite.

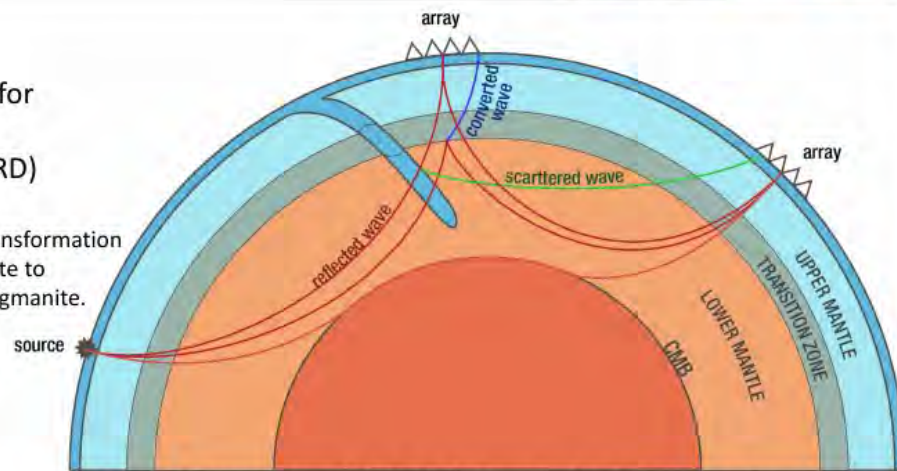
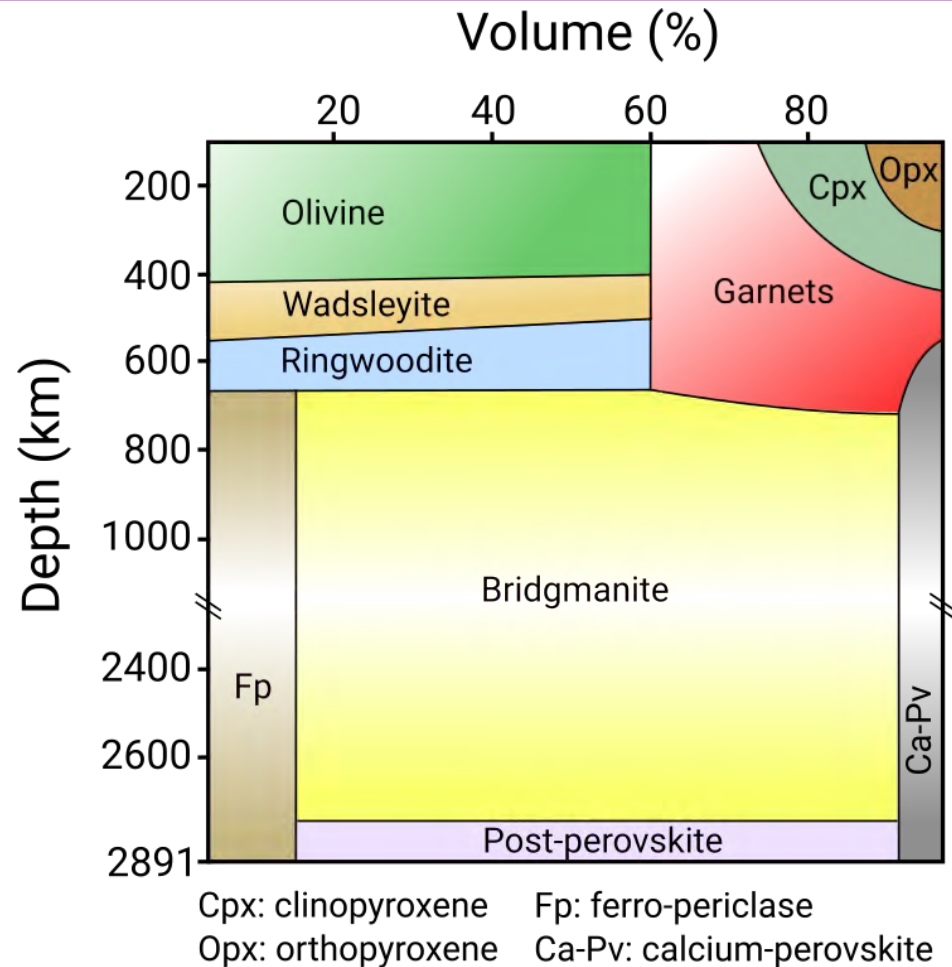


Figure 2. Cross section of Earth displaying seismic reflectors at various depths within the mantle.



Main phase transitions in a pyrolitic composition

410 km: olivine to wadsleyite

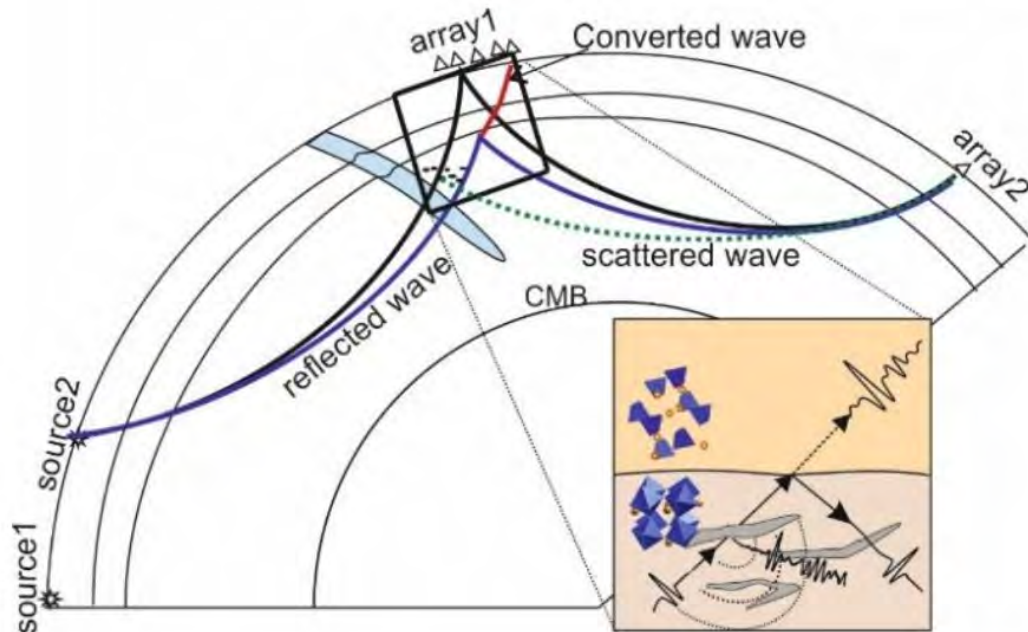
520 km: wadsleyite to ringwoodite

660 km: ringwoodite / garnet to bridgmanite + ferropericlase + Ca-perovskite

D'': bridgmanite to post-perovskite

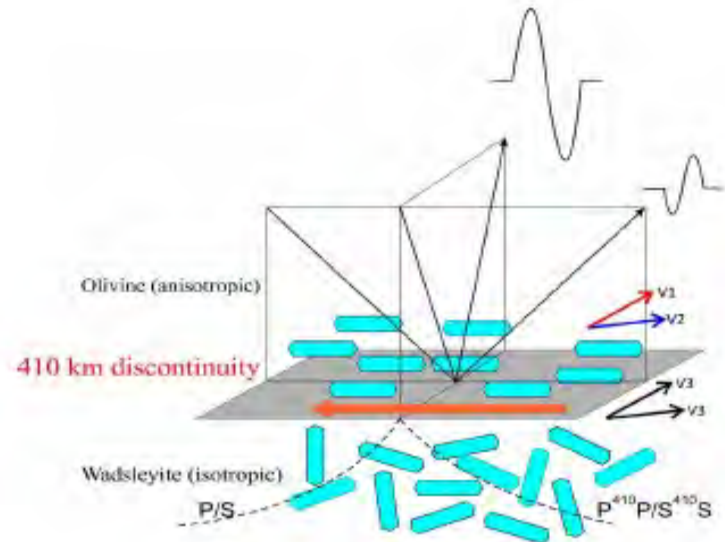
Sharp transition of physical properties

- Reflectors
- Wave conversions

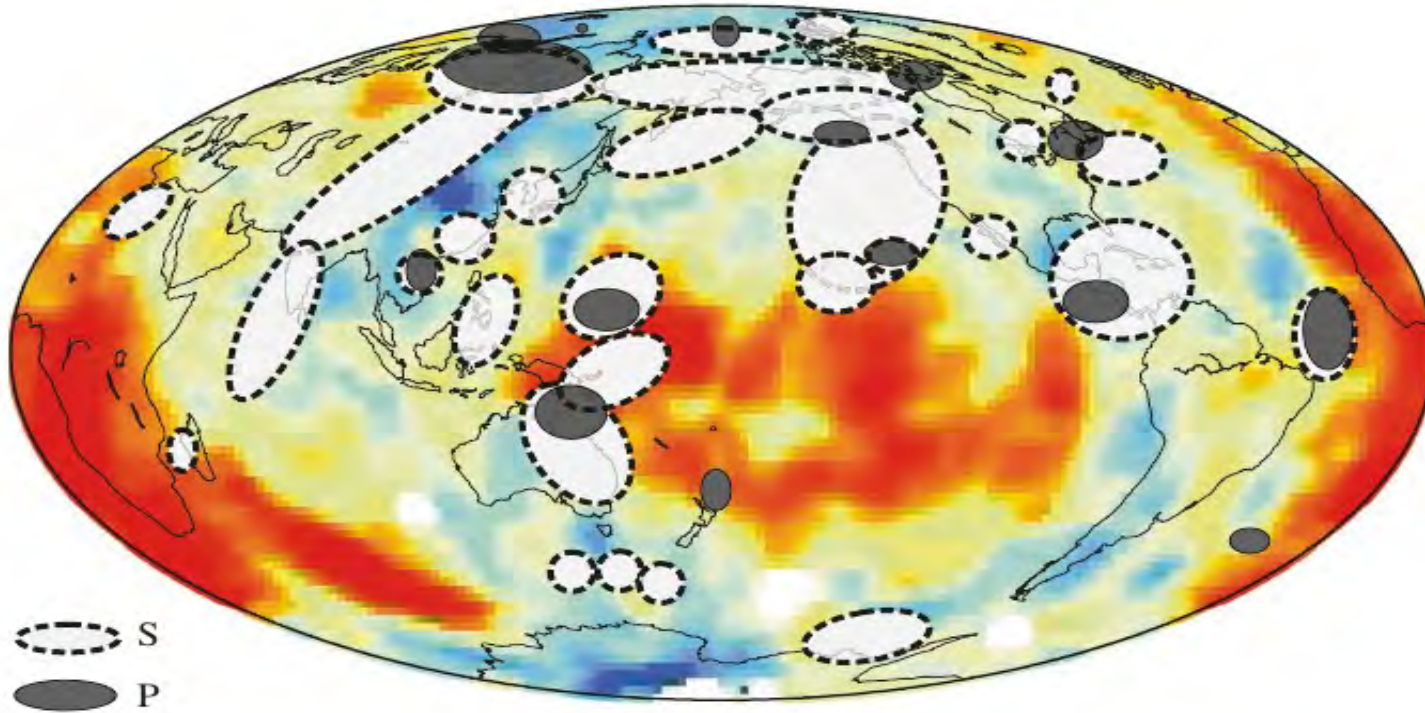


Microstructural imprint


- Anisotropy before and after the phase transformation
- Waveform and polarity of reflected / converted waves

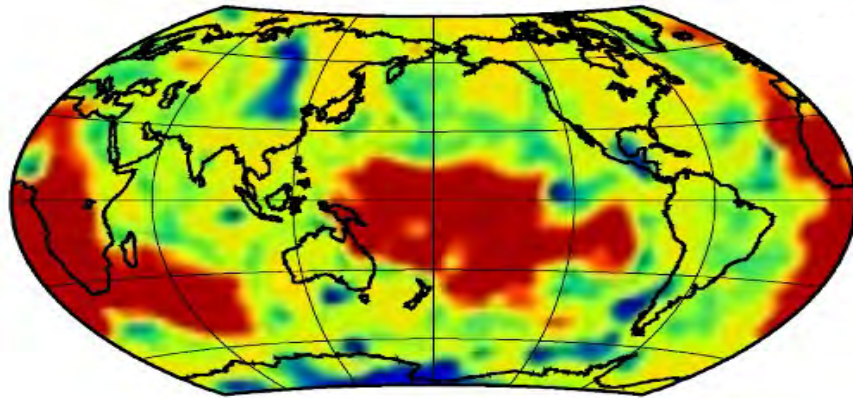


Phase transitions detectability

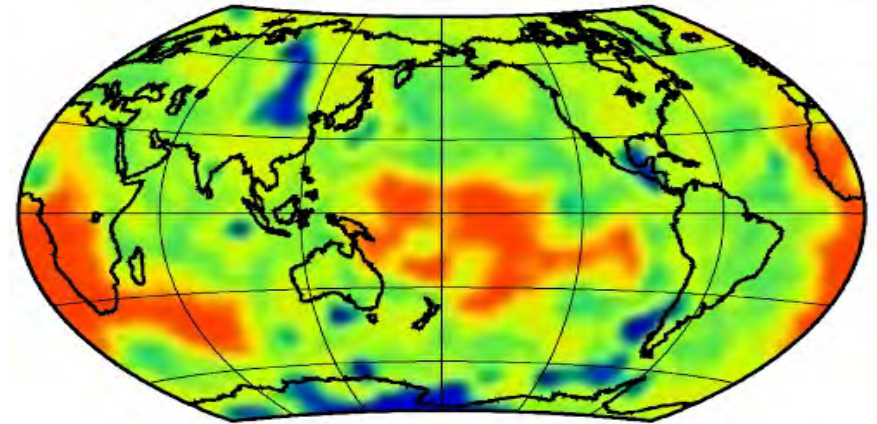


Locations of observations of D'' reflections overlaid on the tomography model of Grand, 2002.


50 100 150 200 250 300
Phase boundary above CMB (km)



$\gamma = 12 \text{ MPa/K}$



$\gamma = 6 \text{ MPa/K}$

Lower mantle tomography and phase change mapping

Daoyuan Sun¹ and Don Helmberger¹

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 113, B10305, doi: 10.1029/2007JB005289, 2008

Mineralogical effects on the detectability of the postperovskite boundary

Brent Grocholski^{a,1}, Krystle Catalli^a, Sang-Heon Shim^a, and Vitali Prakapenka^b

PNAS | February 14, 2012 | vol. 109 | no. 7 | 2277

Experimental evidence for perovskite and post-perovskite coexistence throughout the whole D'' region

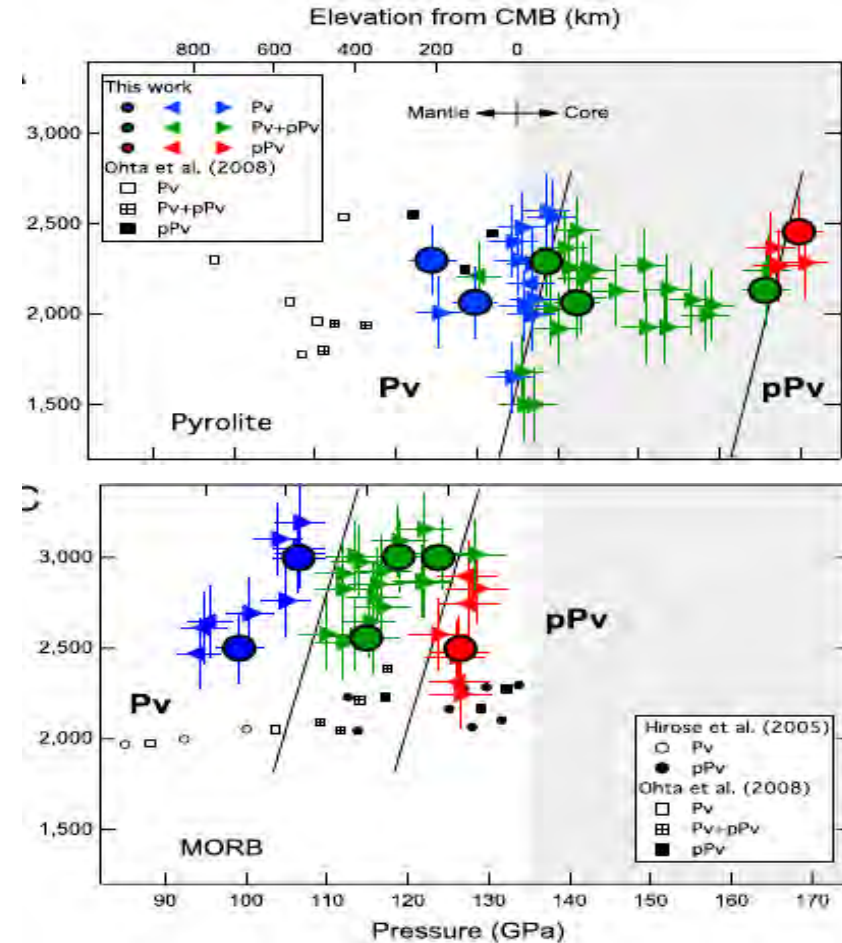
Denis Andrault^{a,*}, Manuel Muñoz^b, Nathalie Bolfan-Casanova^a, Nicolas Guignot^c, Jean-Philippe Perrillat^d, Giuliana Aquilanti^d, Sakura Pascarelli^d

D. Andrault et al. / Earth and Planetary Science Letters 293 (2010) 90–96

Thickness and Clapeyron slope of the post-perovskite boundary

Krystle Catalli¹, Sang-Heon Shim¹ & Vitali Prakapenka²

NATURE | Vol 462 | 10 December 2009



Laser-heated DAC

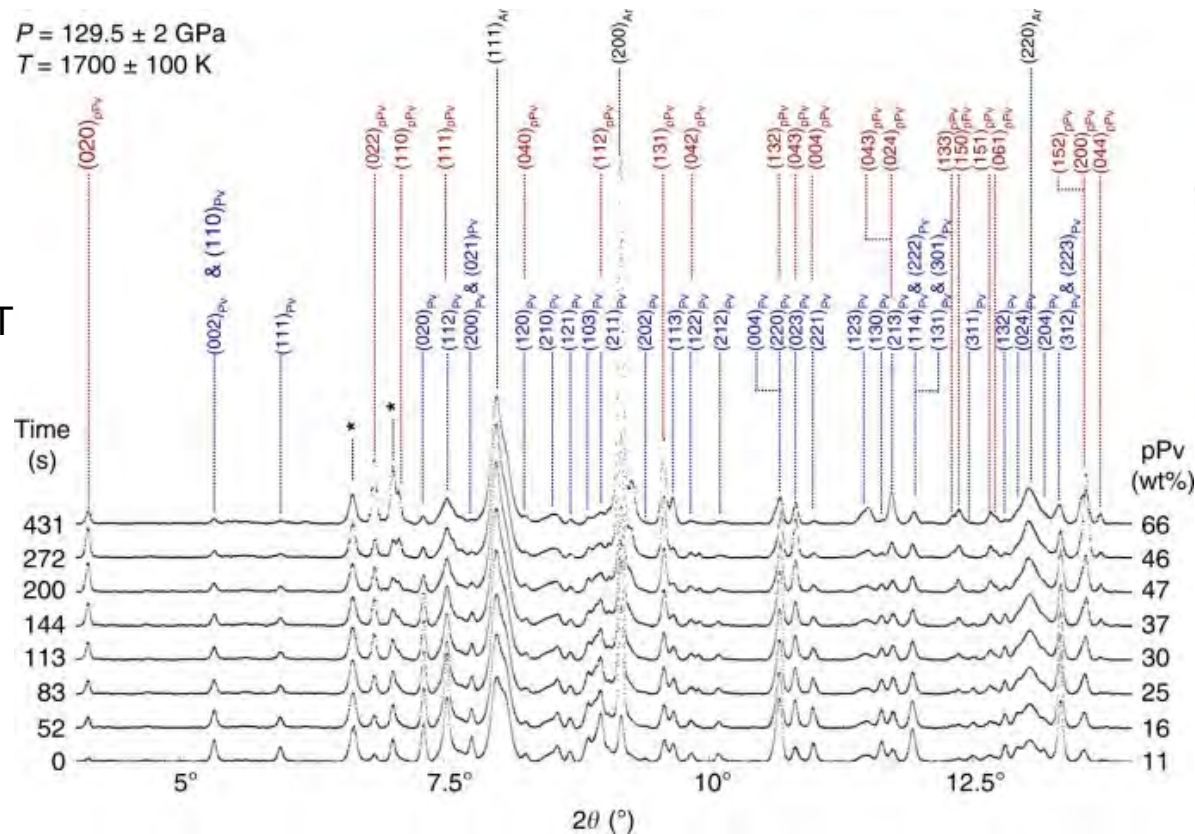
Starting material: Enstatite, 14% Fe

Pressure medium: Argon

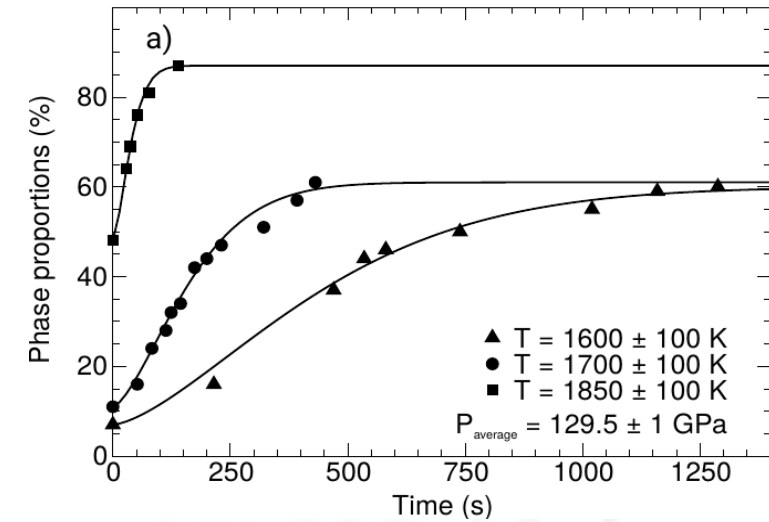
Conversion to Pv at ~90 GPa

Conversion to pPv at various P and T

Continuous monitoring with XRD

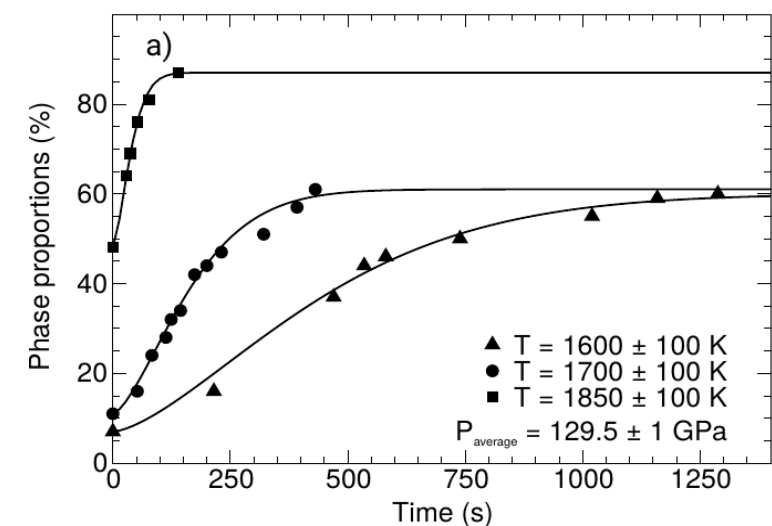


PETRA III
P02.2



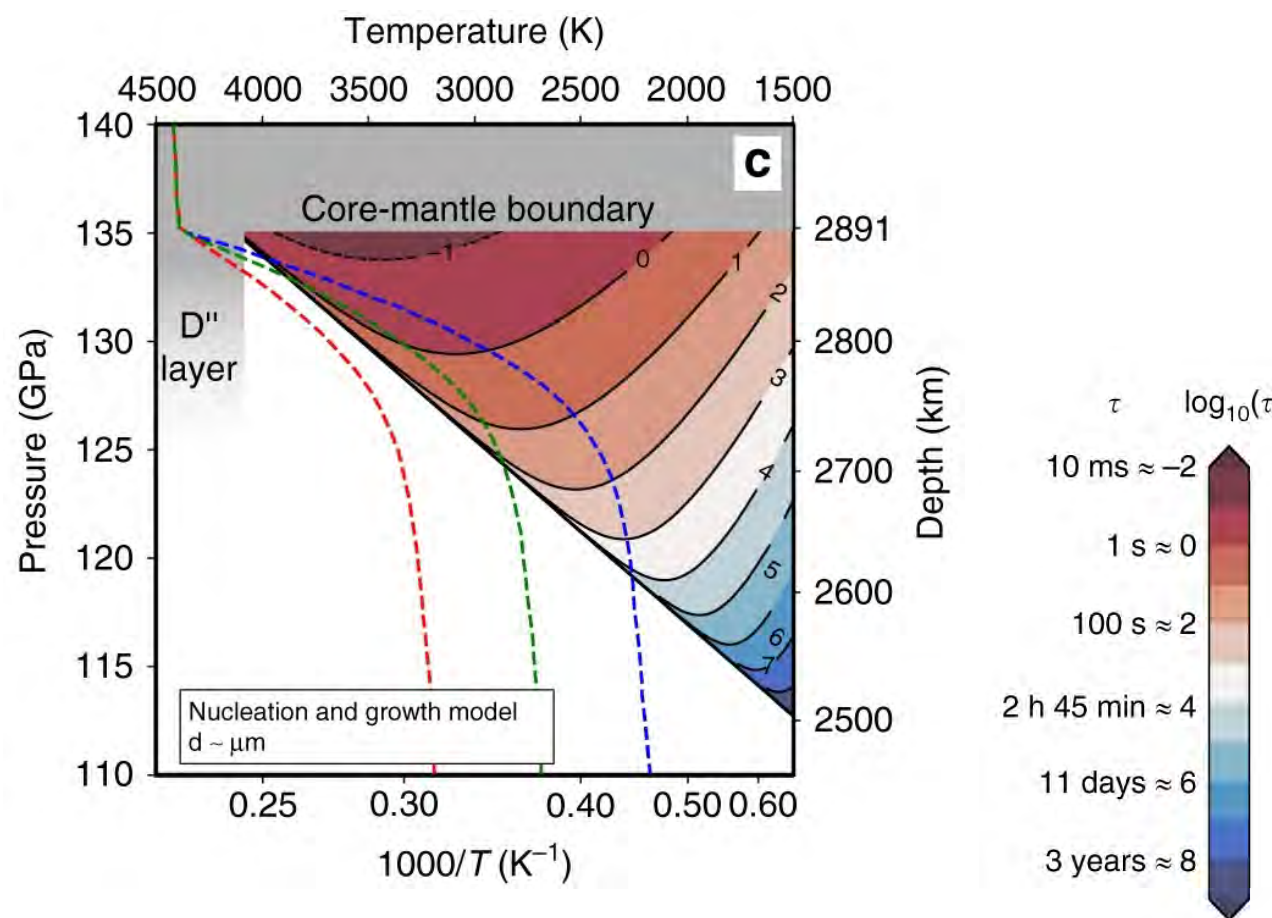
$$\xi(t) = 1 - e^{-\left(\frac{t}{\tau}\right)^n}$$

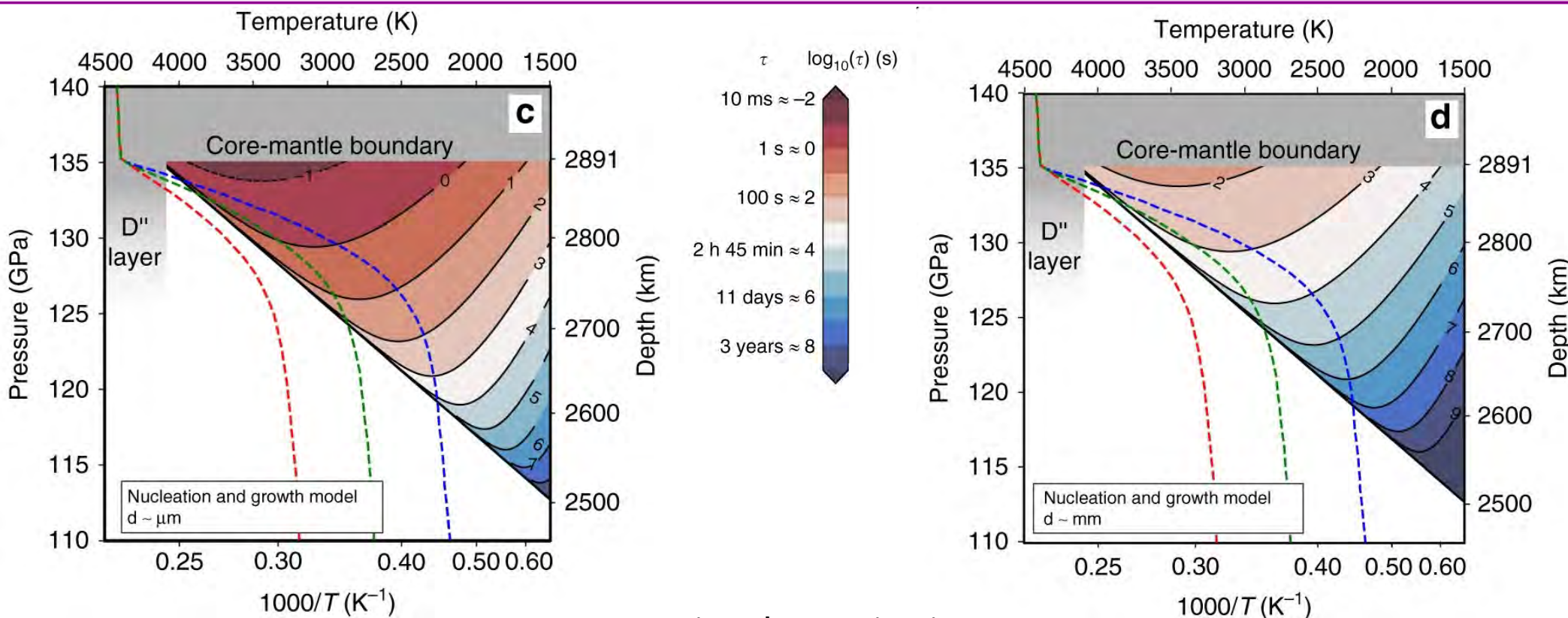
τ : transformation time scale



$$\xi(t) = 1 - e^{-\left(\frac{t}{\tau}\right)^n}$$

τ : transformation time scale

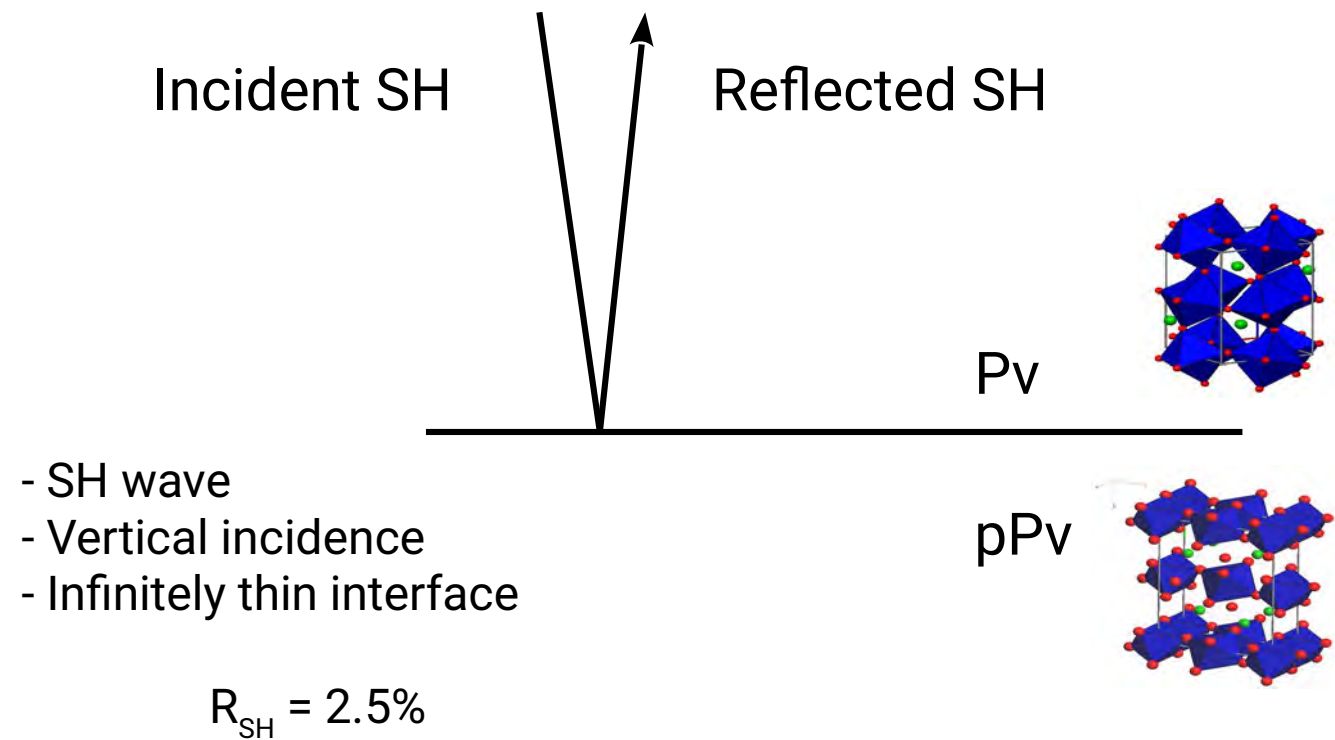
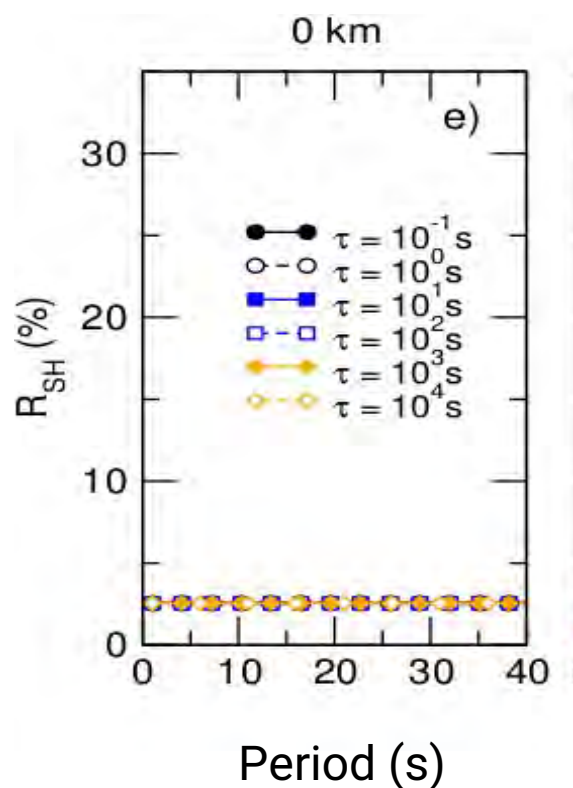




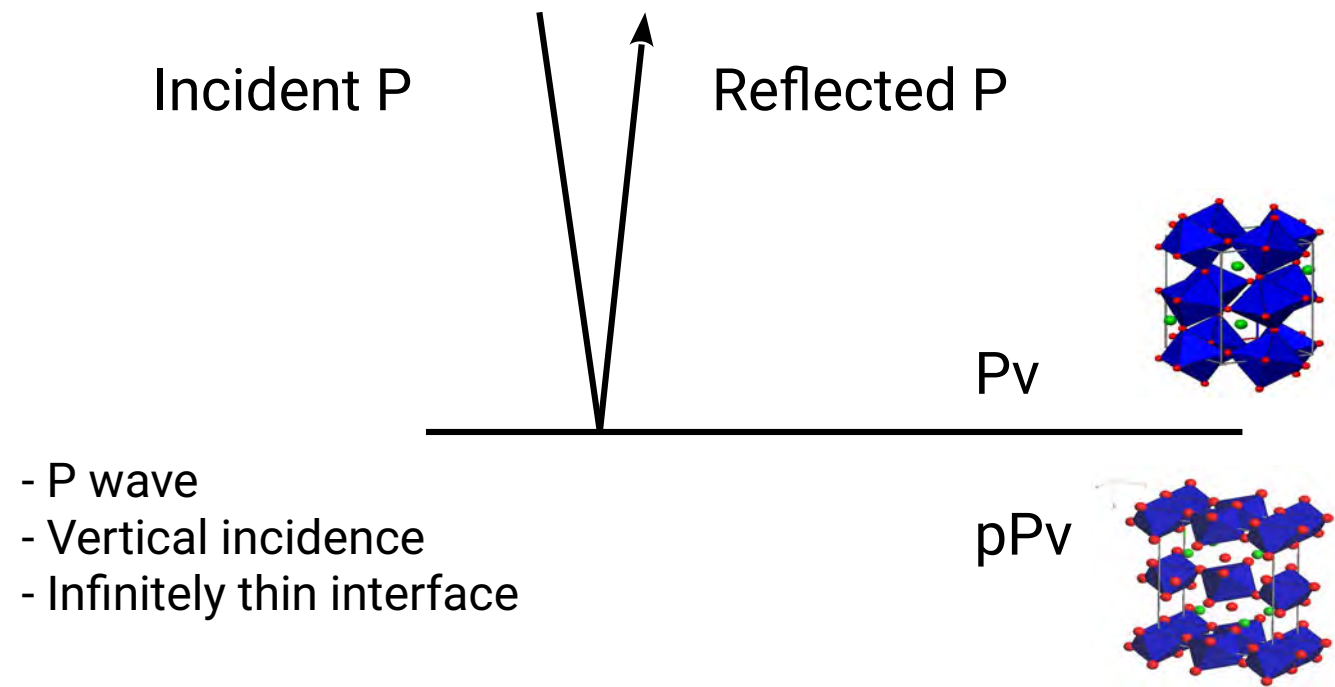
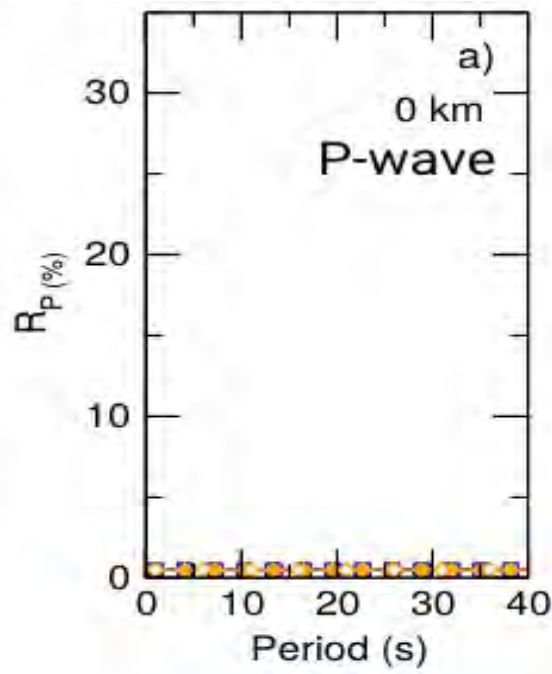
τ : proportional to grain size

Constant product growth rate hypothesis for nucleation and growth model

No effect of grain size in a shear transformation model



Independant of kinetics
 Independant of wave period



- P wave
- Vertical incidence
- Infinitely thin interface

$$R_{SH} = 0.5 \%$$

Independant of kinetics
 Independant of wave period

Seismic attenuation in a phase change coexistence loop

Yanick Ricard*, J. Matas, F. Chambat

Laboratoire des Sciences de la Terre, CNRS, Université de Lyon, Bat Géode, 2 rue Raphael Dubois, 69622, Villeurbanne, 07, France

Physics of the Earth and Planetary Interiors 176 (2009) 124–131

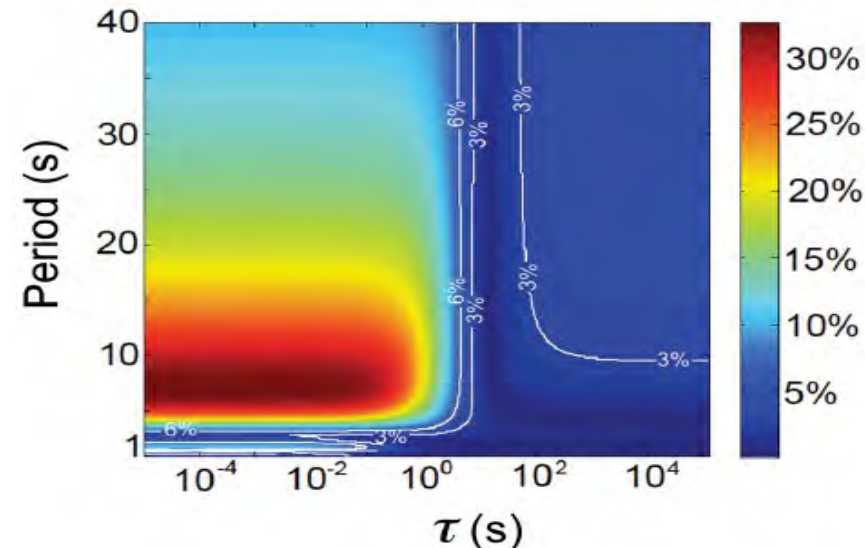
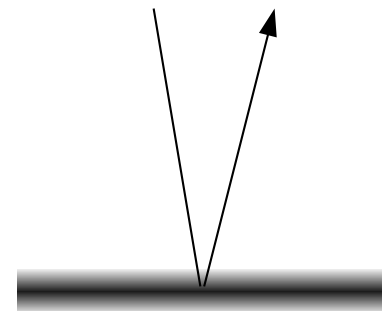
Constraining the kinetics of mantle phase changes with seismic data

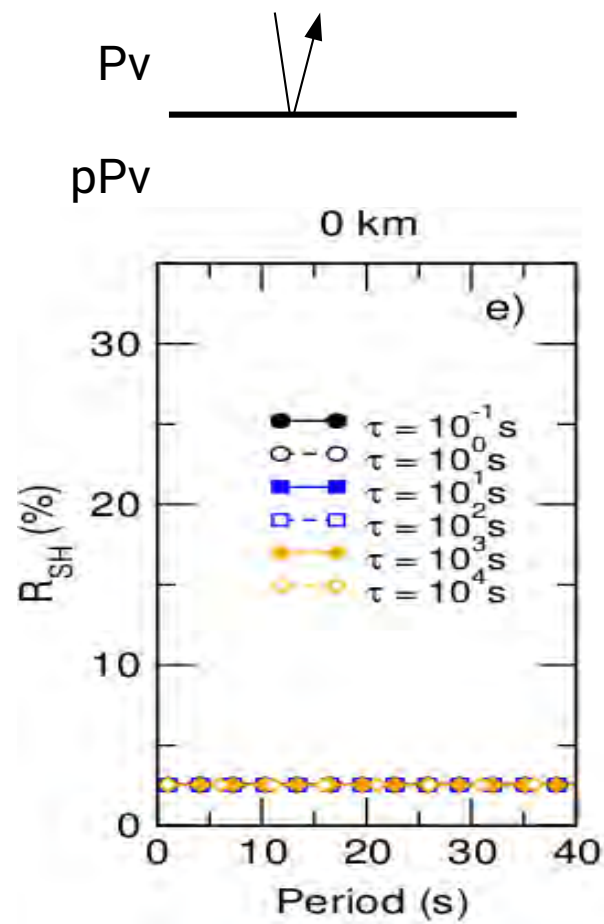
S. Durand, F. Chambat, J. Matas and Y. Ricard

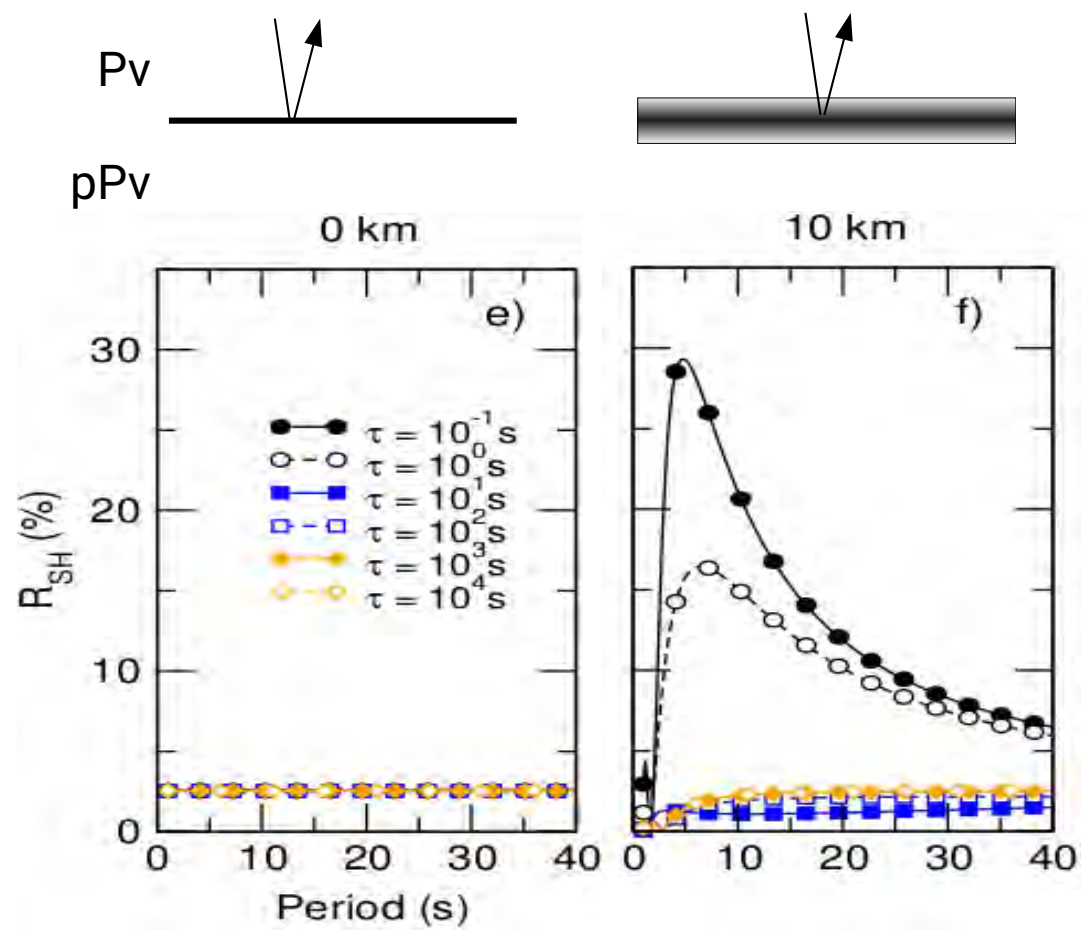
Laboratoire de Sciences de la Terre, CNRS UMR5570, École Normale Supérieure de Lyon, Université de Lyon, Université Claude Bernard Lyon 1, 46 Allée d'Italie, 69364 Lyon Cedex 07, France, E-mail: stephanie.durand@ens-lyon.fr

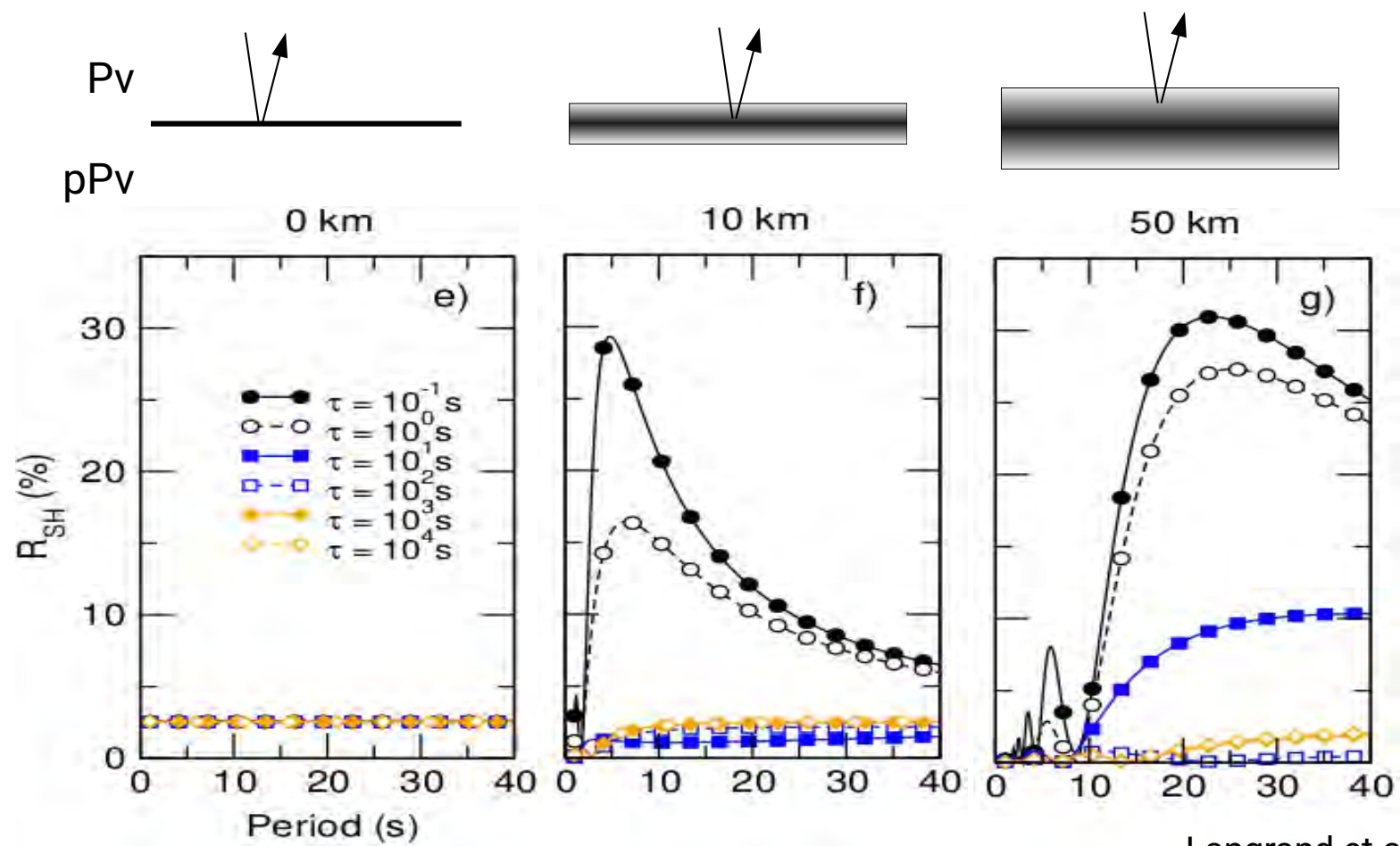
Geophys. J. Int. (2012) 189, 1557–1564

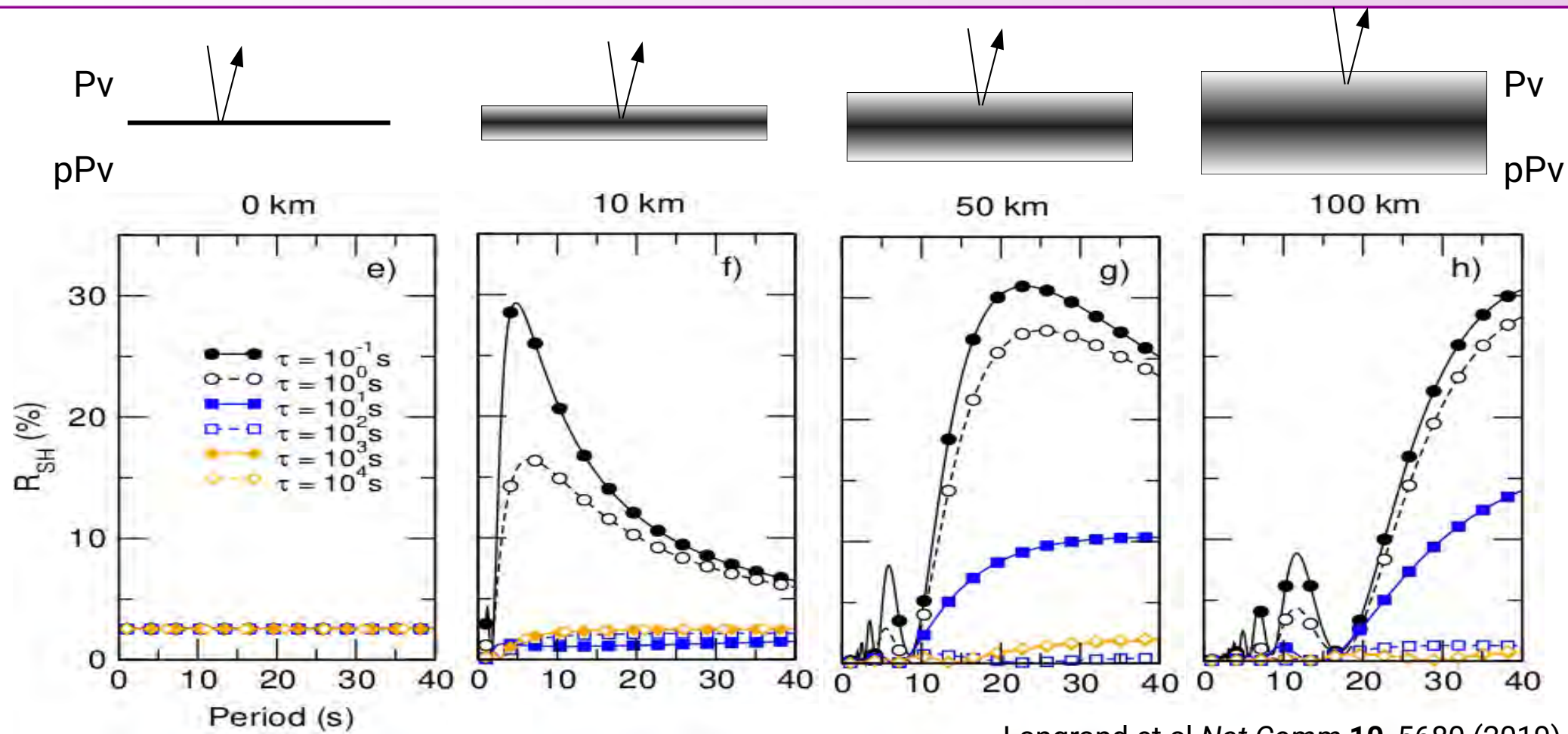
Reflection coefficient at 410 km
vertically incident SH wave
10 km thick olivine-wadsleyite loop
Horizontal axis: transformation kinetics
Vertical axis: wave period

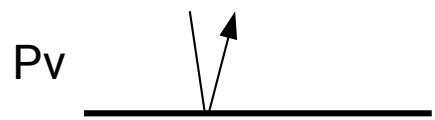




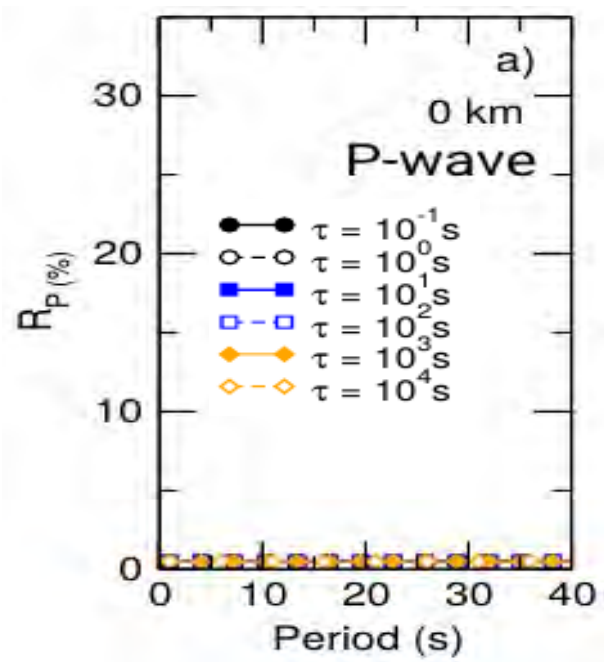


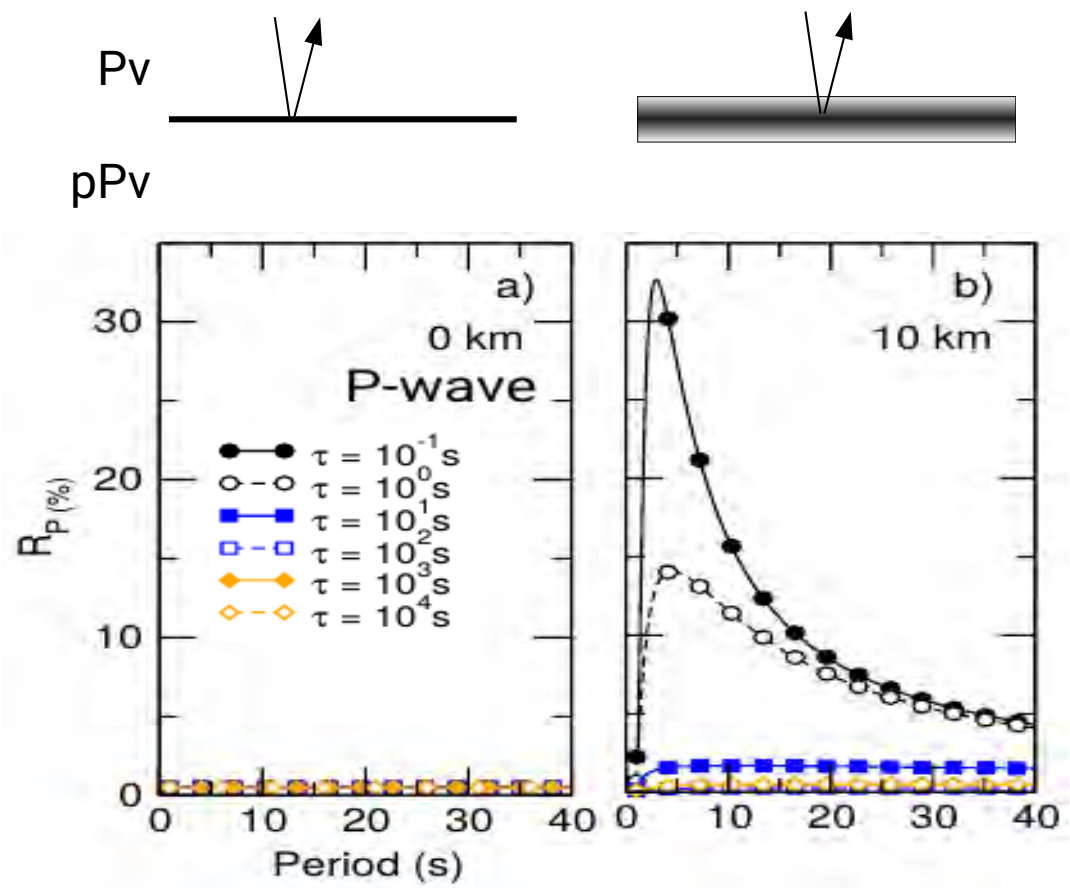


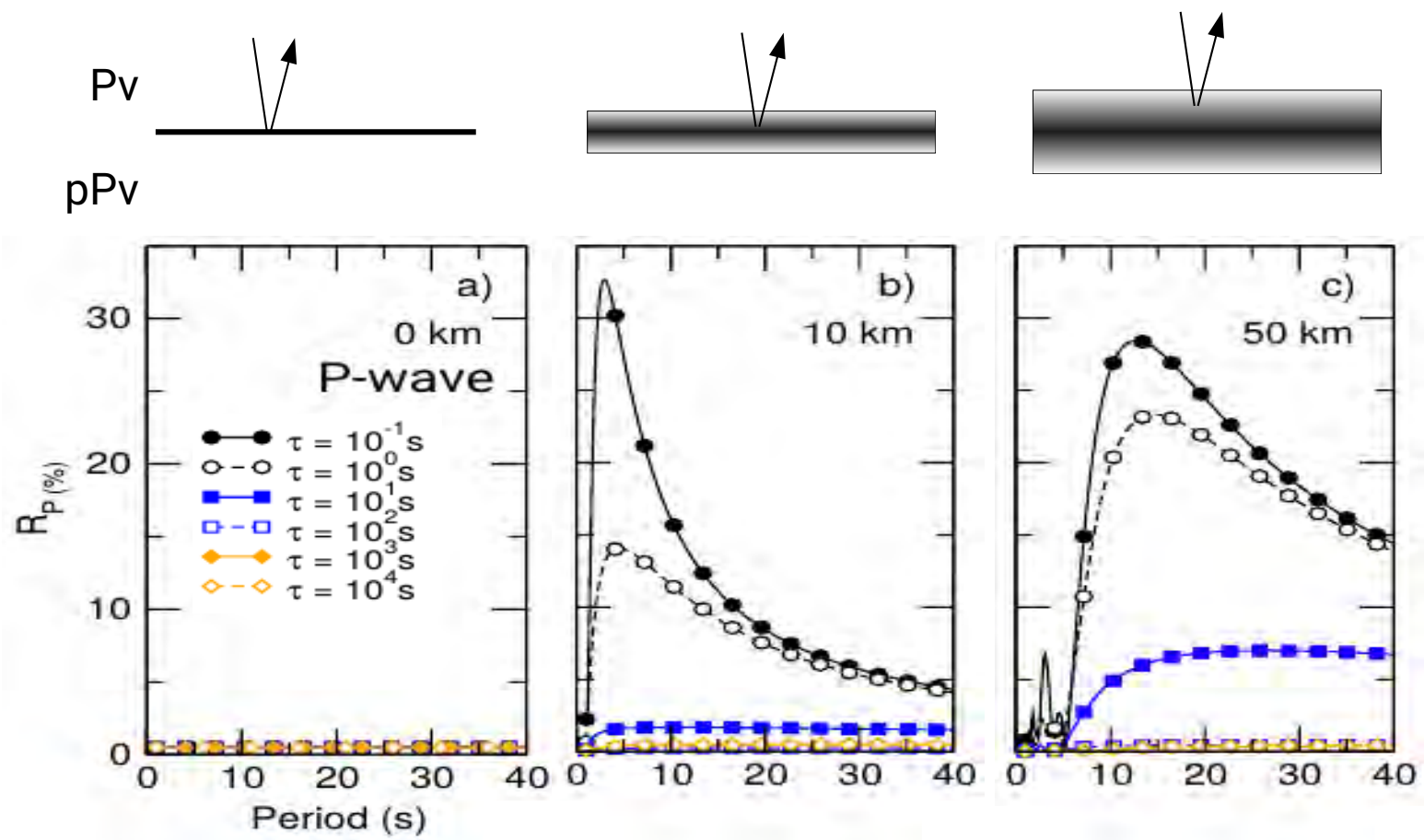


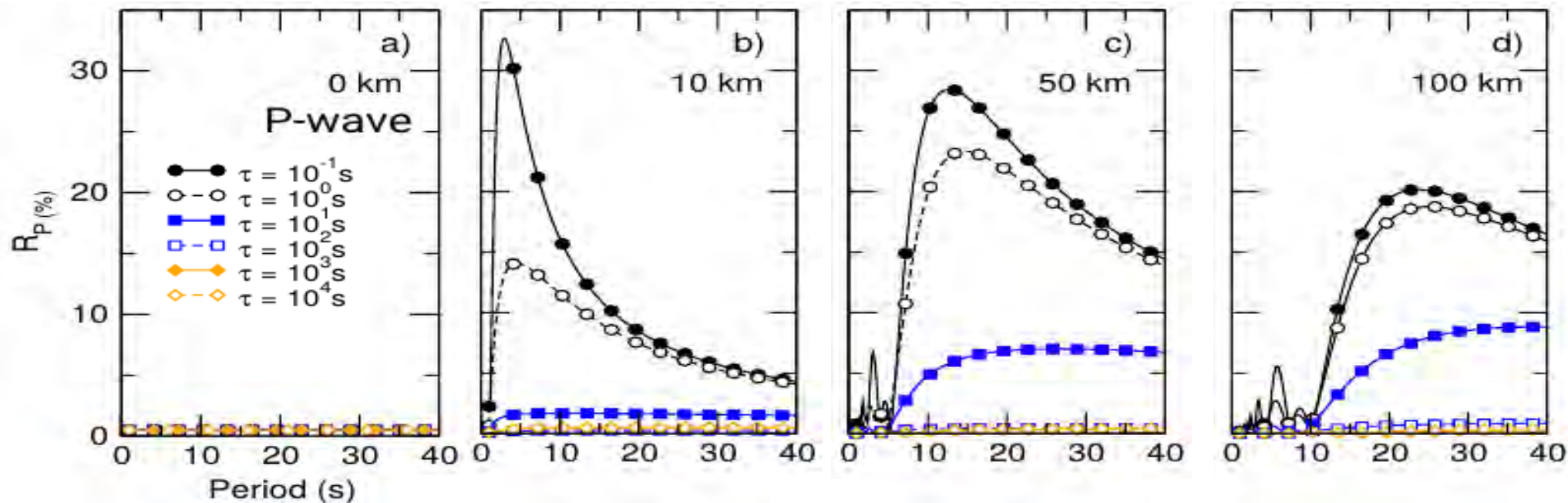
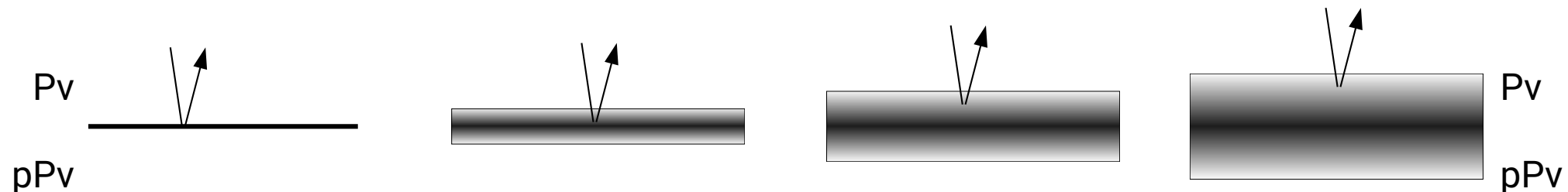


pPv



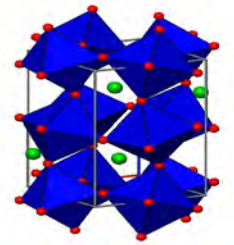




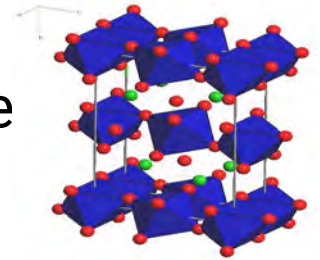


On the detectability of the Pv-pPv transformation

Pure
Pv



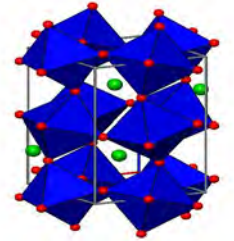
Pure
pPv



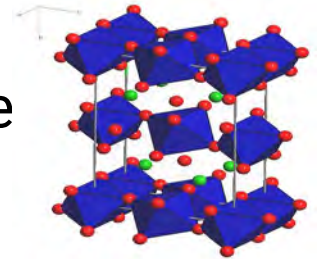
Fast at D'' pressure and temperature conditions

- Experimental (grains $\sim 1 \mu\text{m}$): 10^{-1} à 10^3 s,
- Extrapolation (shear model): no grain size effect
- Extrapolation (nucleation and growth model, grains $\sim 1 \text{ mm}$): 10^2 à 10^6 s (11 days)

Pure
Pv



Pure
pPv



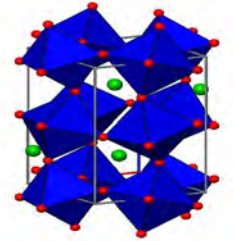
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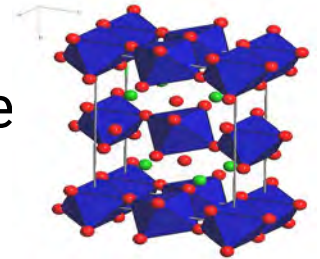
Seismic detectability

- Reflection amplification due to
 - Transformation kinetics
 - Pv / pPv coexistence loop
- Efficient for thick Pv / pPv coexistence layer (up to 100 km)
- Depends on wave period

Pure
Pv



Pure
pPv



Fast at D'' pressure and temperature conditions

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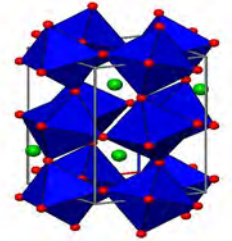
Seismic detectability

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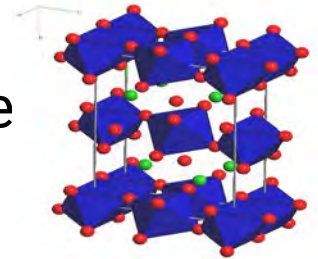
Potential

- Cut-off frequency : thickness of Pv / pPv coexistence layer
- Amplitude measurements : kinetics of phase transformation
→ temperature / grain size

Pure
Pv



Pure
pPv

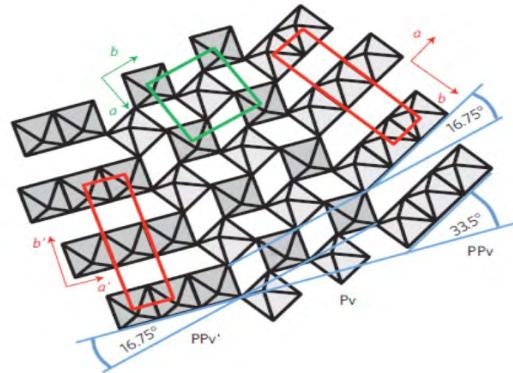
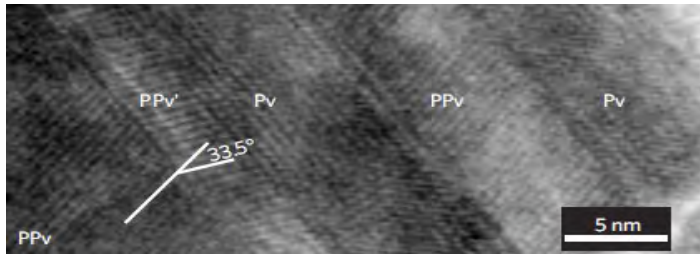


Microstructures

Strong inheritance of texture between perovskite and post-perovskite in the D'' layer

David P. Dobson^{1,2*}, Nobuyoshi Miyajima³, Fabrizio Nestola⁴, Matteo Alvaro⁴, Nicola Casati⁵, Christian Liebske², Ian G. Wood¹ and Andrew M. Walker⁶

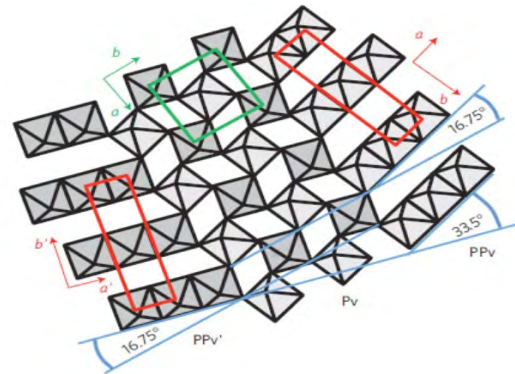
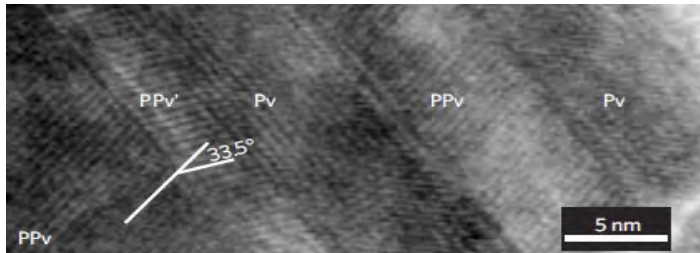
NATURE GEOSCIENCE | VOL 6 | JULY 2013



Strong inheritance of texture between perovskite and post-perovskite in the D'' layer

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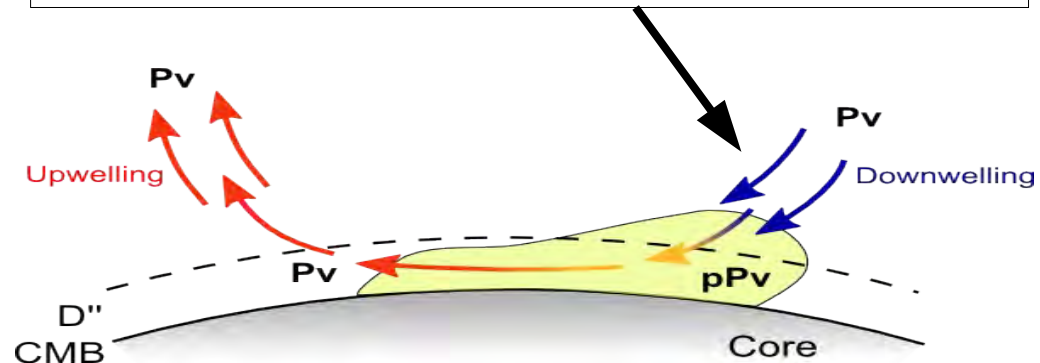


If martensitic (with orientation relationships):

- Texture memory
- Deformation history preserved
- Anisotropy

If no orientation relationships

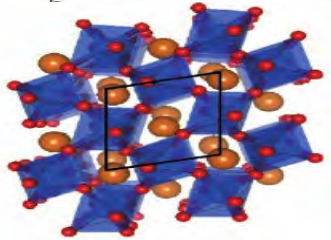
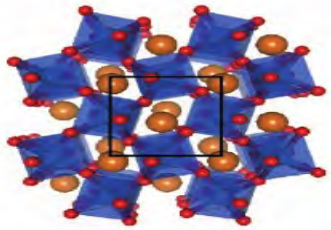
- Loss of memory
- Random texture
- Loss of anisotropy



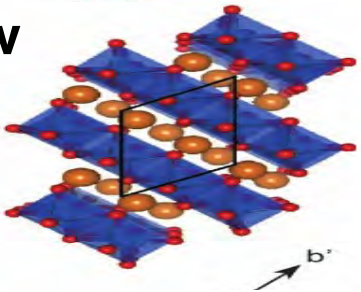
Tsuchiya et al, 2004

simulations MgSiO_3

Pv

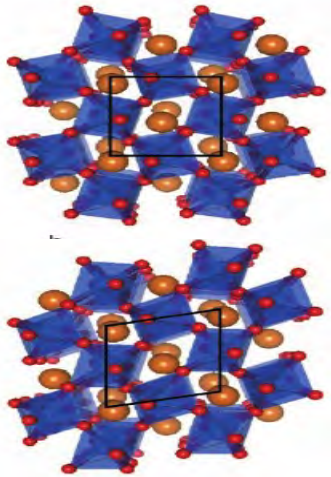


pPv

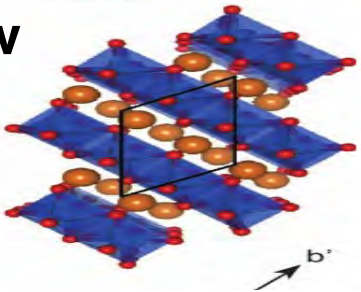


Tsuchiya et al, 2004
simulations MgSiO_3

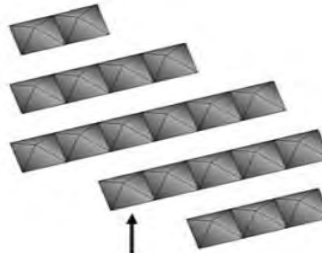
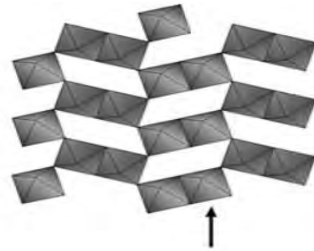
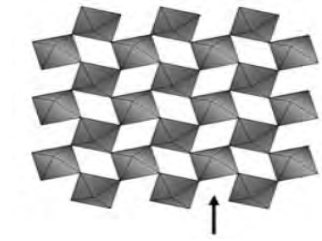
Pv



pPv

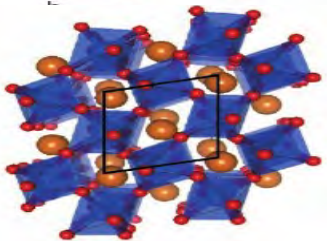
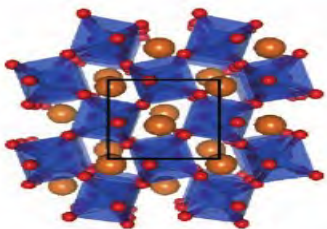


Oganov et al, 2005
simulations MgSiO_3

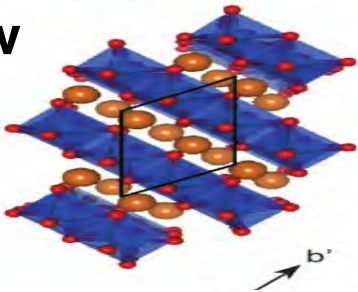


Tsuchiya et al, 2004
simulations MgSiO_3

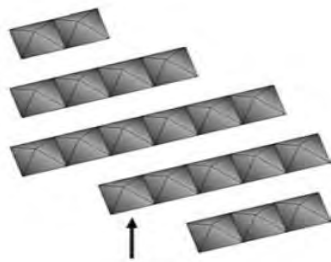
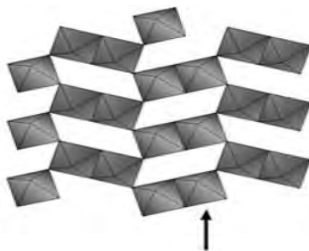
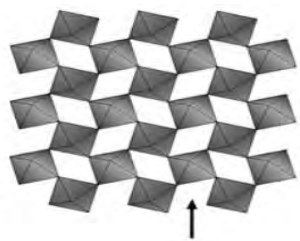
Pv



pPv



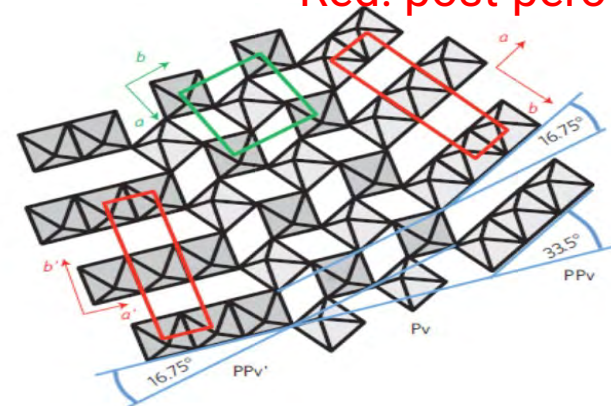
Oganov et al, 2005
simulations MgSiO_3



Dobson et al, 2013
TEM + experiments NaNiF_3

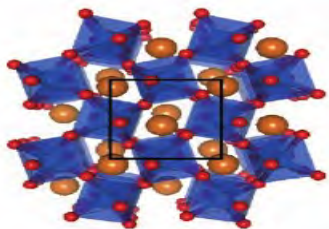


Green: perovskite
 Red: post-perovskite



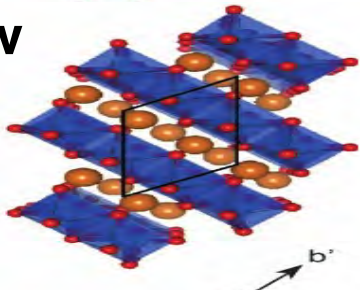
Tsuchiya et al, 2004
simulations MgSiO_3

Pv

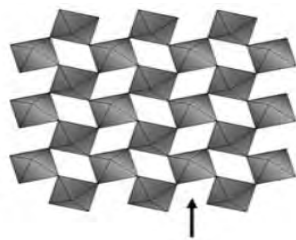


~45°
rotation
around c-axis

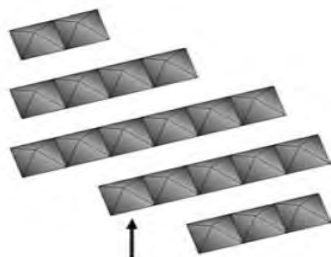
pPv



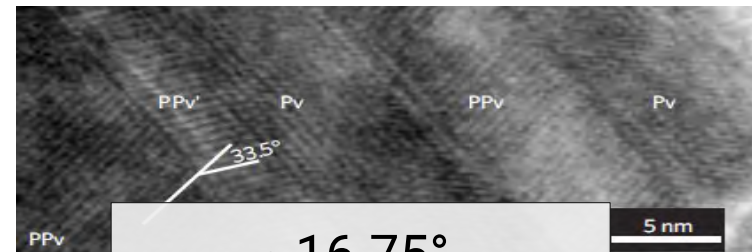
Oganov et al, 2005
simulations MgSiO_3



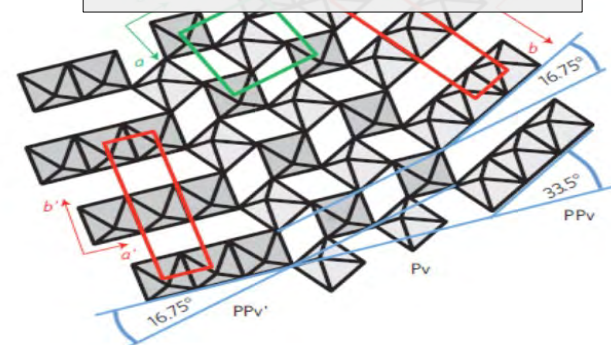
random
rotation
around c-axis



Dobson et al, 2013
TEM + experiments NaNiF_3



~16.75°
rotation
around c-axis



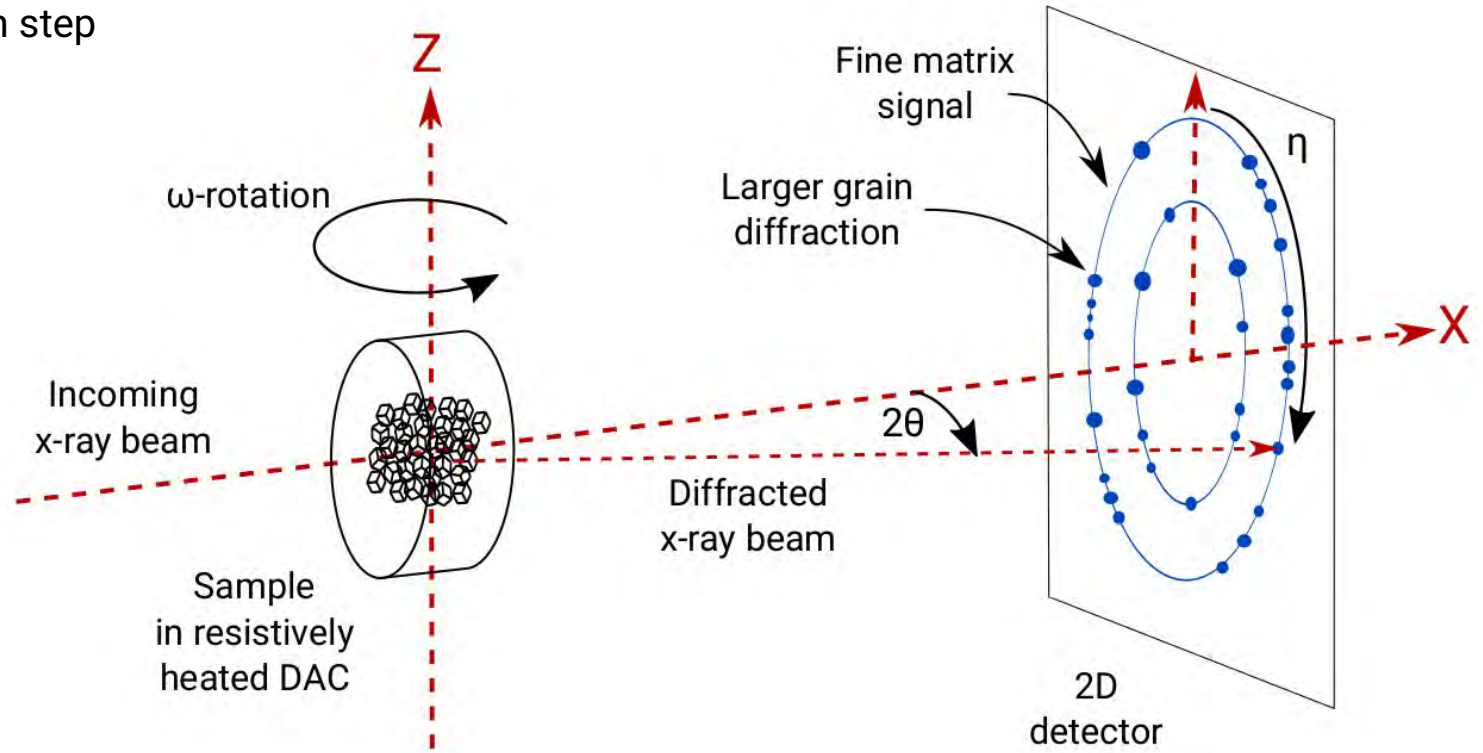
Diamond anvil cell sitting on a rotation stage

Collect images at every rotation step

Typical numbers

- Rotation range: $\Delta\omega = 45^\circ$
- Rotation step: $\delta\omega = 0.5^\circ$
- 90 diffraction images per P/T point

Allows to map orientations of individual grains inside a diamond anvil cell, at mantle P/T conditions.



Typical numbers

- $\sim 10^4$ spots per P/T point
- Random walk through orientation space to identify grains
- $\sim 10^6$ iterations
- $\sim 5 \cdot 10^2$ to $5 \cdot 10^3$ indexed grains per P/T point

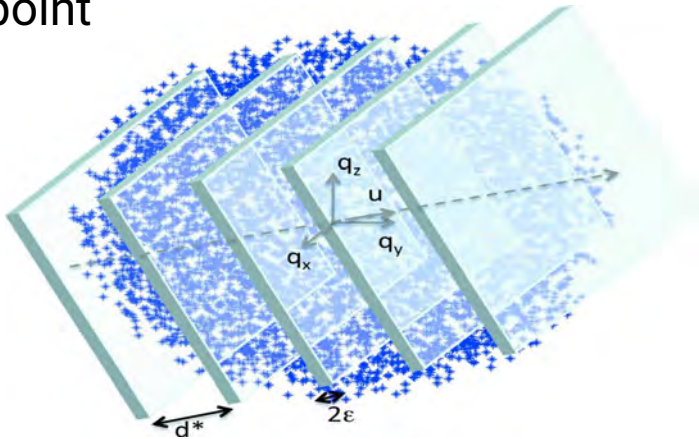


Illustration:
 Wejdemanna and Poulsen,
J. Appl. Cryst. 2016

Results

Average sample

- Fine matrix vs. grains volume ratio
- Phase proportions

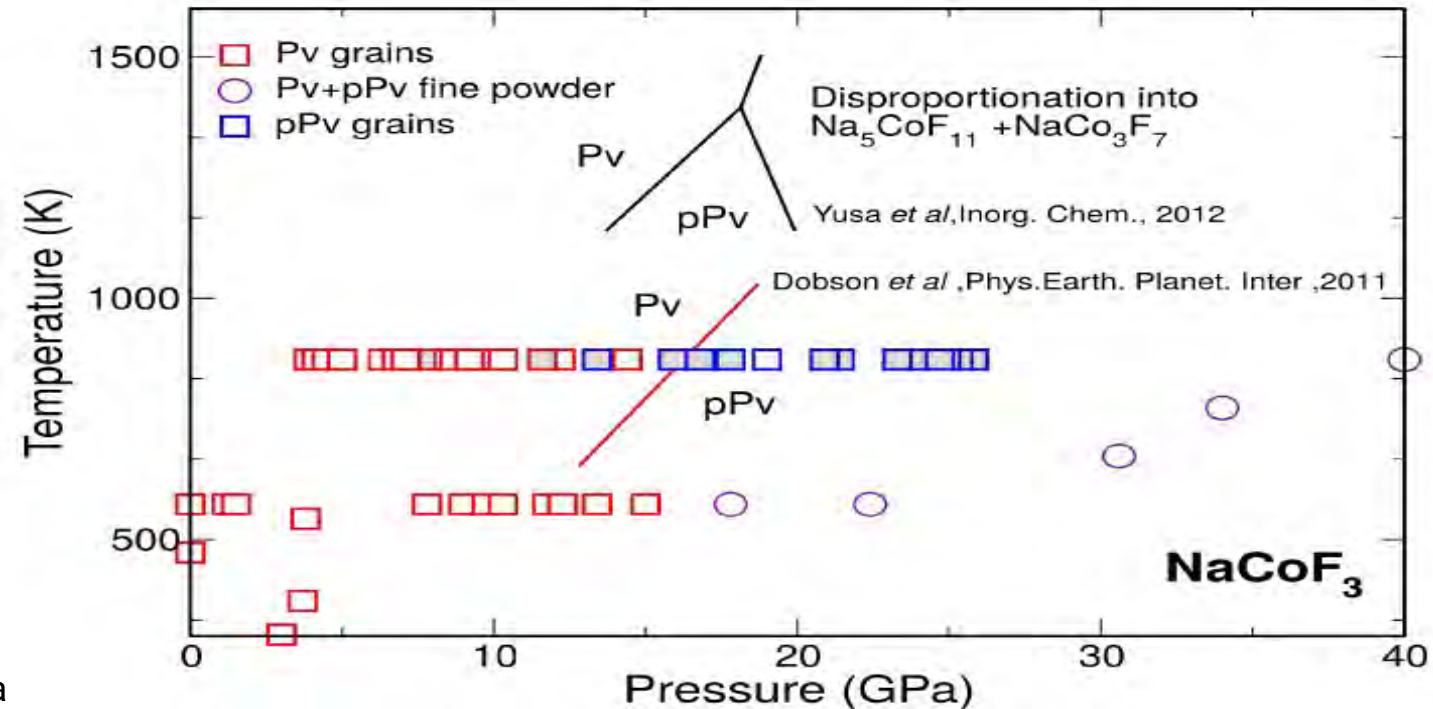
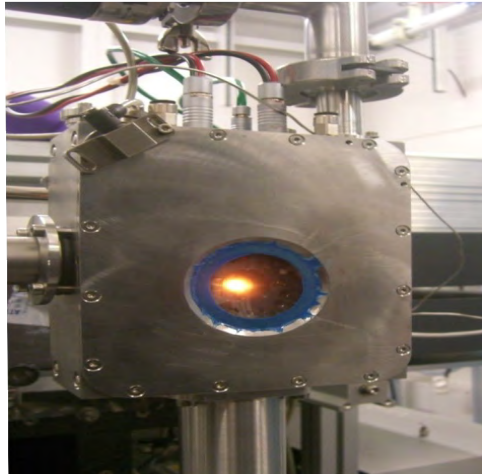
Grain scale, for each indexed grain

- Orientation
- Relative volume

Potential for deep Earth Mineralogy

- Follow mineral microstructures at deep Earth mantle pressure **AND** temperatures

Nisir et al, *J. Geoph Res.* 2012
 Nisir et al, *High Pres. Res.* 2014
 Rosa et al, *J. Appl. Cryst.* 2015
 Rosa et al, *J. Geoph Res.* 2016
 Langrand et al, *J. Appl. Cryst.* 2017



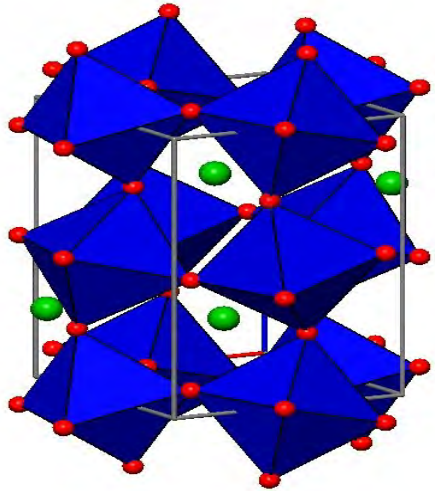
Sample

- NaCoF_3
- Pv to pPv transition at ~15 GPa

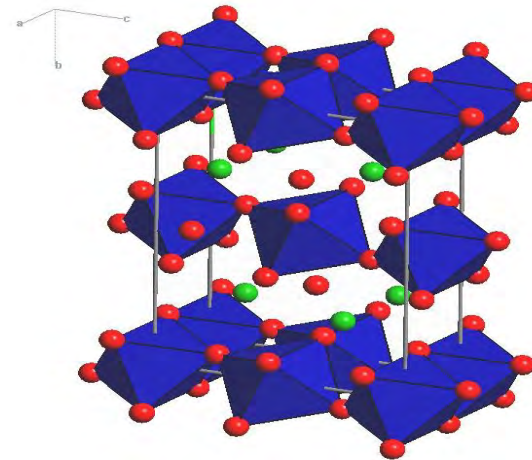
Confinement

- Resistive heating DAC
- Rhenium gasket
- Run duration: ~10s of hours for each T

NaCoF₃ Perovskite
Before Transformation
P = 14.1 GPa – T = 900 K



NaCoF₃ post-Perovskite
After Transformation
P = 17.5 GPa – T = 900 K

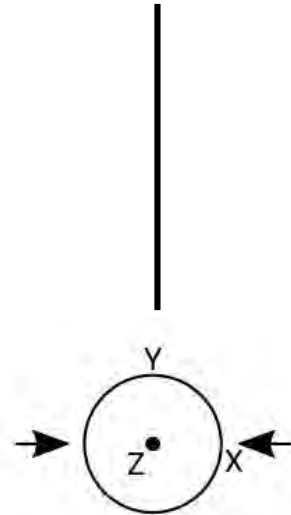


NaCoF₃ Perovskite

Before Transformation

P = 14.1 GPa – T = 900 K

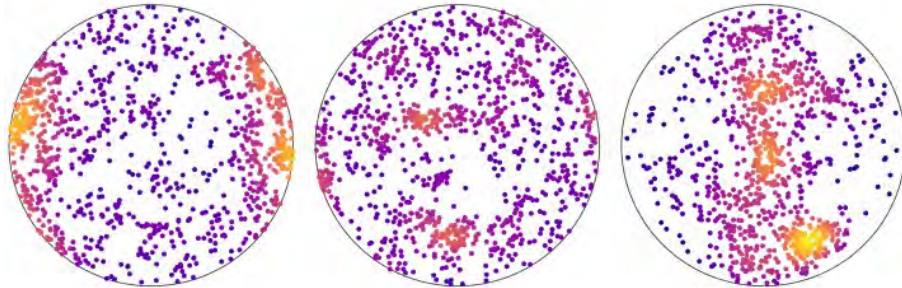
Fine matrix: 47 %
Extracted spots: 62232
Indexed spots: 61 %
Indexed grains: 1028



Pv - 100

Pv - 010

Pv - 001



Indexed Pv grains

NaCoF₃ Perovskite

Before Transformation

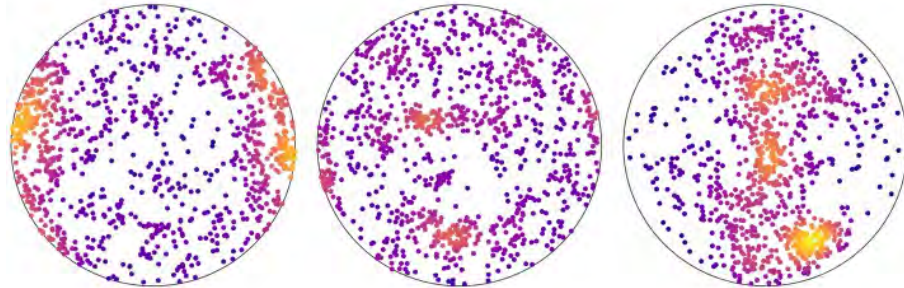
P = 14.1 GPa – T = 900 K

Fine matrix: 47 %
 Extracted spots: 62232
 Indexed spots: 61 %
 Indexed grains: 1028

Pv - 100

Pv - 010

Pv - 001



Indexed Pv grains

NaCoF₃ post-Perovskite

After Transformation

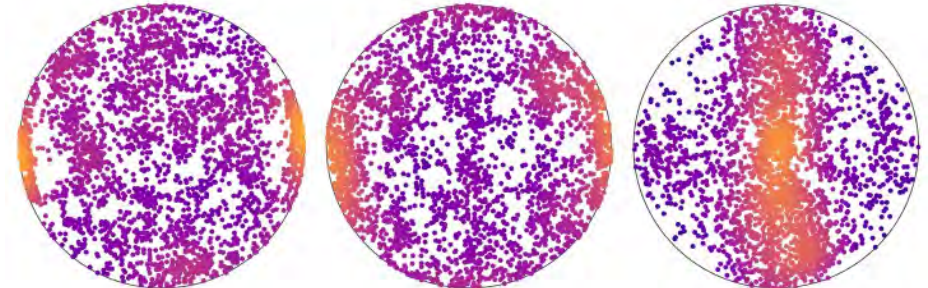
P = 17.5 GPa – T = 900 K

Fine matrix: 22 %
 Extracted spots : 121293
 Indexed spots: 77 %
 Indexed grains: 2946

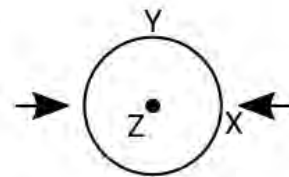
pPv - 100

pPv - 010

pPv - 001



Indexed pPv grains



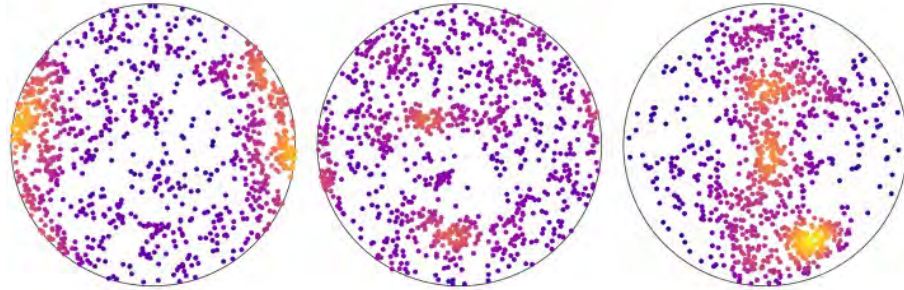
Experiment START

Pv, experimental
1028 grains orientations

Pv - 100

Pv - 010

Pv - 001



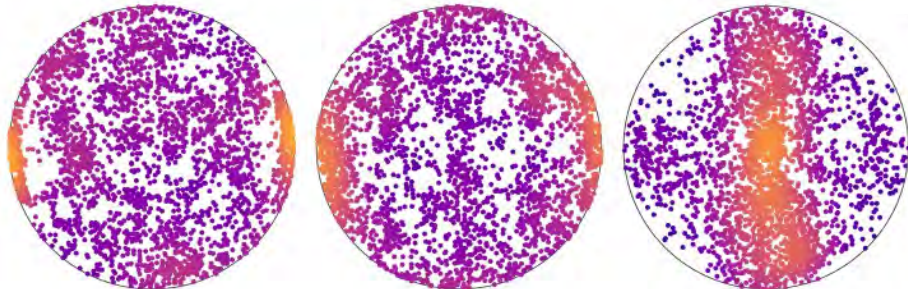
END

pPv, experimental
2946 grain orientations

pPv - 100

pPv - 010

pPv - 001



Number of grains multiplied by 3
Fine matrix: 47% to 22%

Orientation concentrations for $(001)_{Pv}$
~ Orient conc for $(001)_{pPv}$

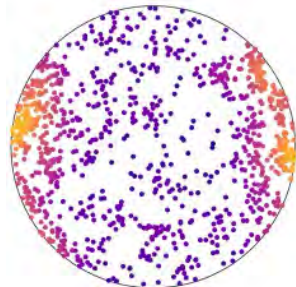
Orientation concentrations for $(100)_{Pv}$
~ Orient conc for $(010)_{pPv}$

In favor of a Dobson-like mechanism

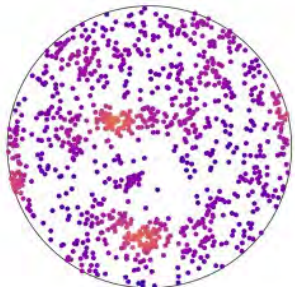
Experiment START

Pv, experimental
1028 grains orientations

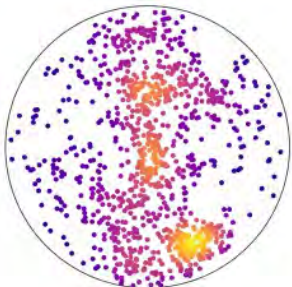
Pv - 100



Pv - 010



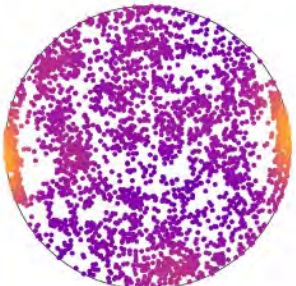
Pv - 001



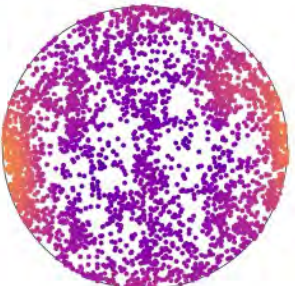
END

pPv, experimental
2946 grain orientations

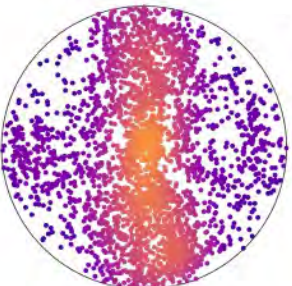
pPv - 100



pPv - 010

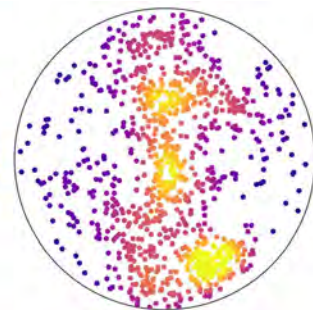
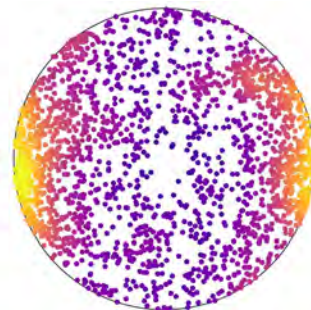
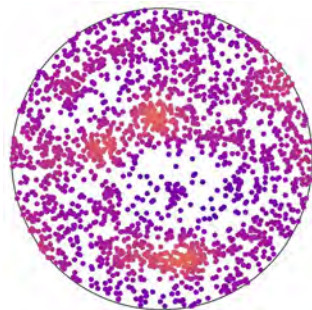


pPv - 001



Simulation

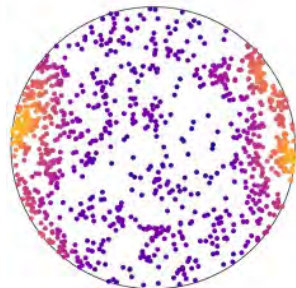
pPv, Dobson orientation relationships
2056 grain orientations



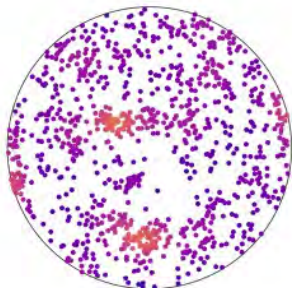
Experiment START

Pv, experimental
1028 grains orientations

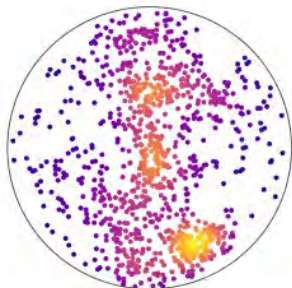
Pv - 100



Pv - 010



Pv - 001



END

pPv, experimental
2946 grain orientations

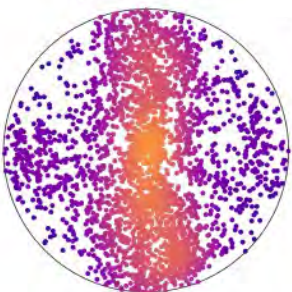
pPv - 100



pPv - 010

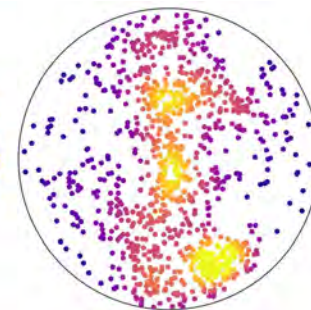
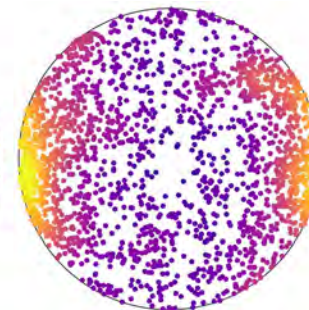
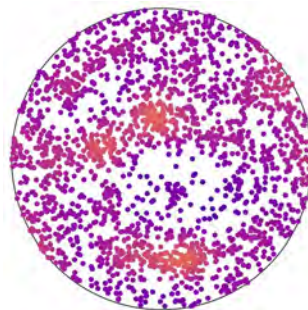


pPv - 001

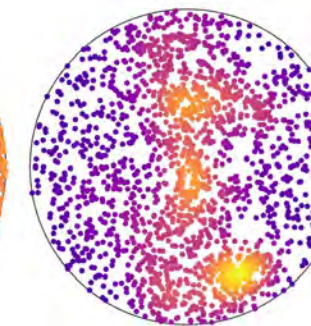
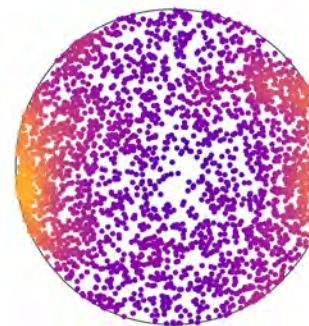
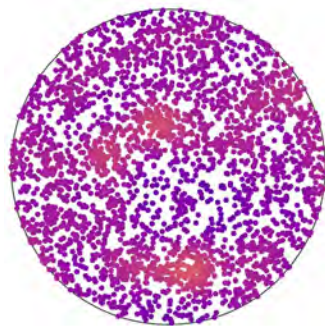


Simulation

pPv, Dobson orientation relationships
2056 grain orientations



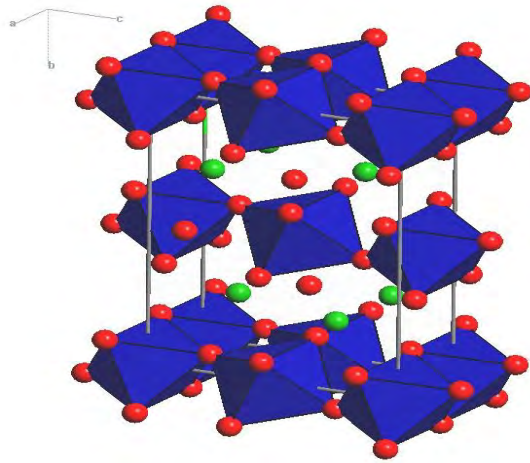
Add random nucleation for the
missing 900 grains



NaCoF₃ post-perovskite

Before Transformation

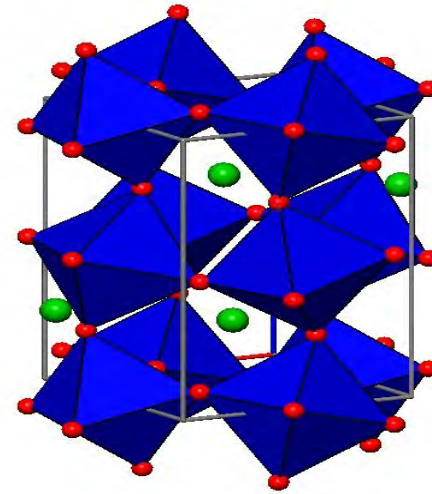
P = 17.8 GPa – T = 900 K



NaCoF₃ Perovskite

After Transformation

P = 13.4 GPa – T = 900 K



NaCoF₃ post-perovskite

Before Transformation

P = 17.5 GPa – T = 900 K

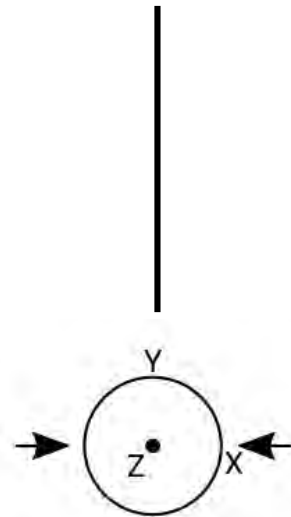
Fine matrix: 68 %
 Extracted spots: 4715
 Indexed spots: 62 %
 Indexed grains: 1317

NaCoF₃ Perovskite

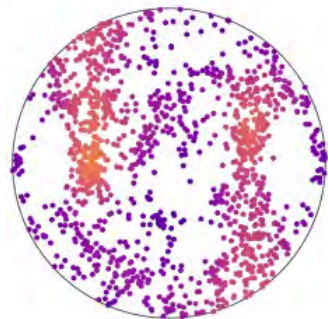
After Transformation

P = 12.5 GPa – T = 900 K

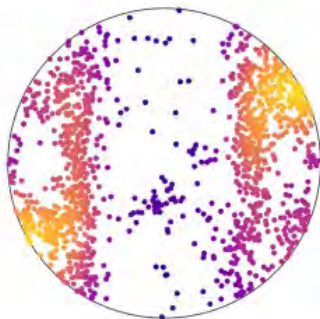
Fine matrix: 4 %
 Extracted spots: 17635
 Indexed spots: 60 %
 Indexed grains: 271



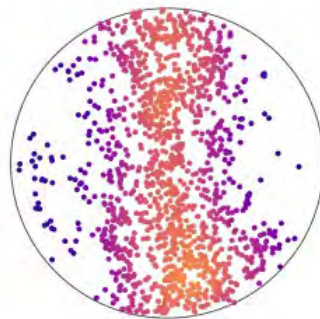
pPv - 100



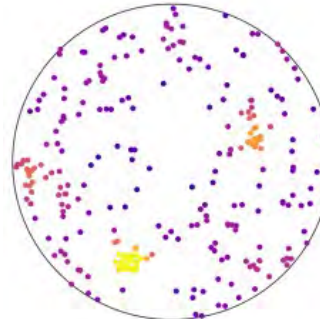
pPv - 010



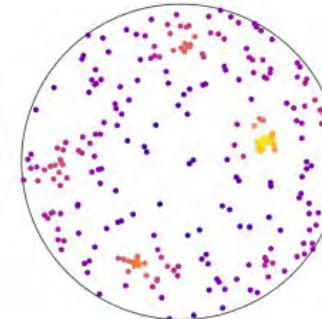
pPv - 001



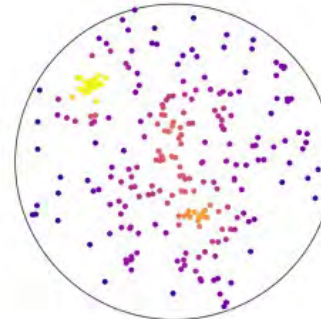
Pv - 100



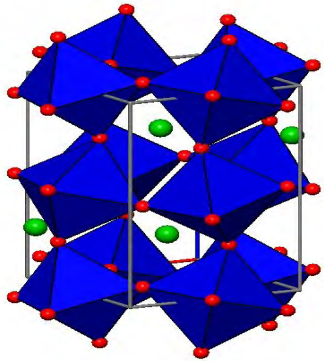
Pv - 010



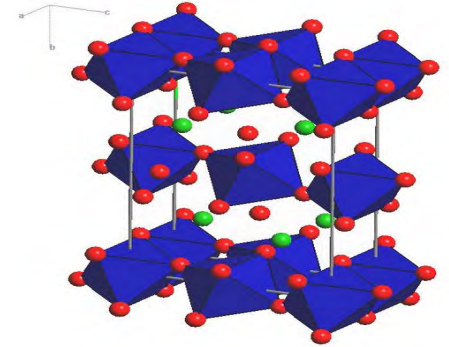
Pv - 001



Orientation memory
Dobson-like mechanism
Grain size divided by ~ 2



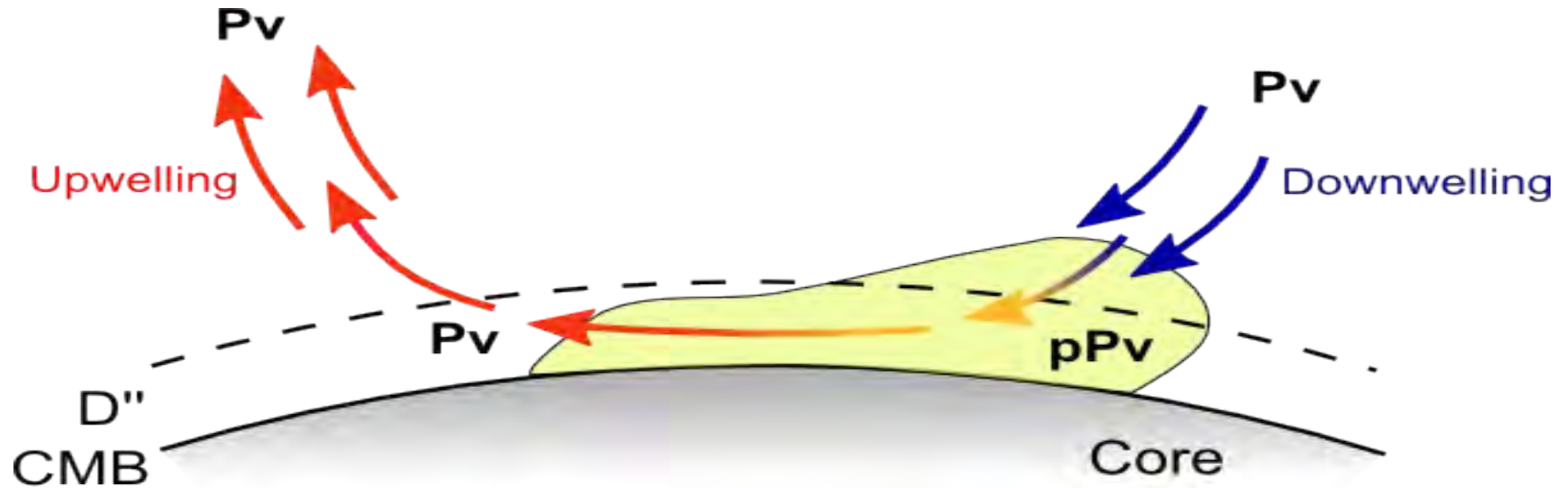
NaCoF₃ Perovskite

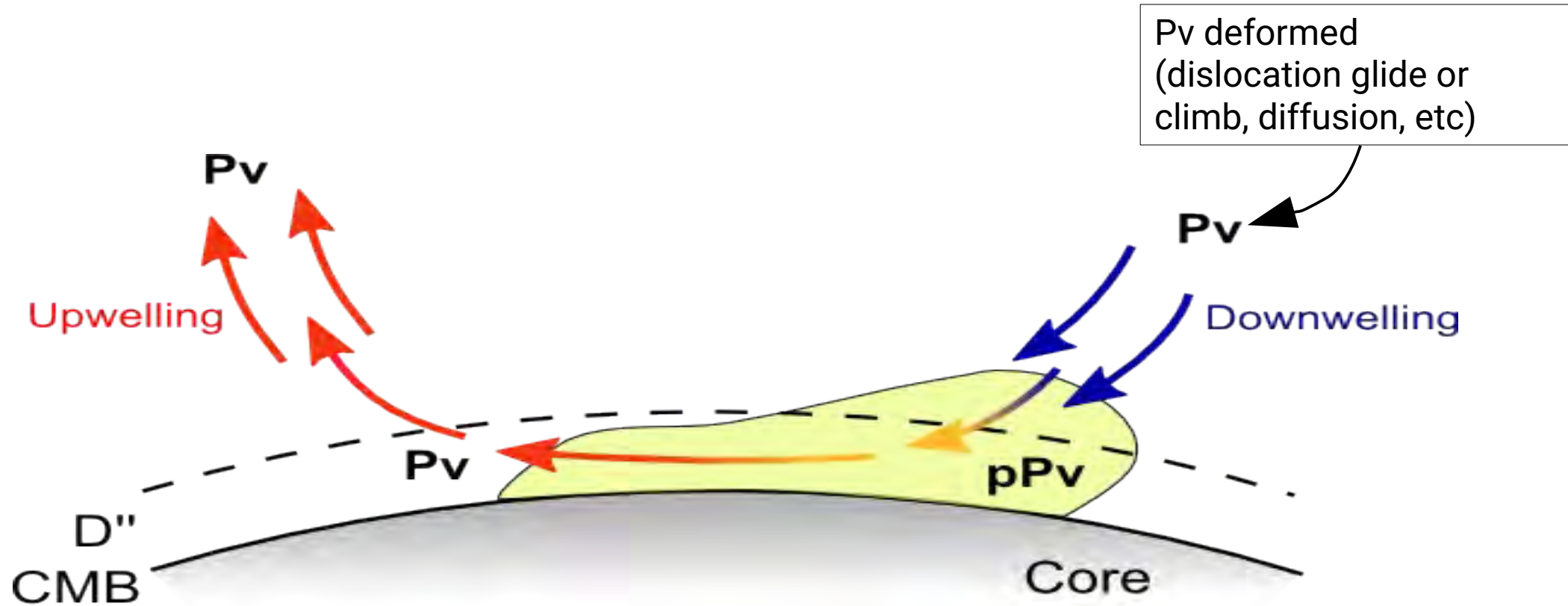


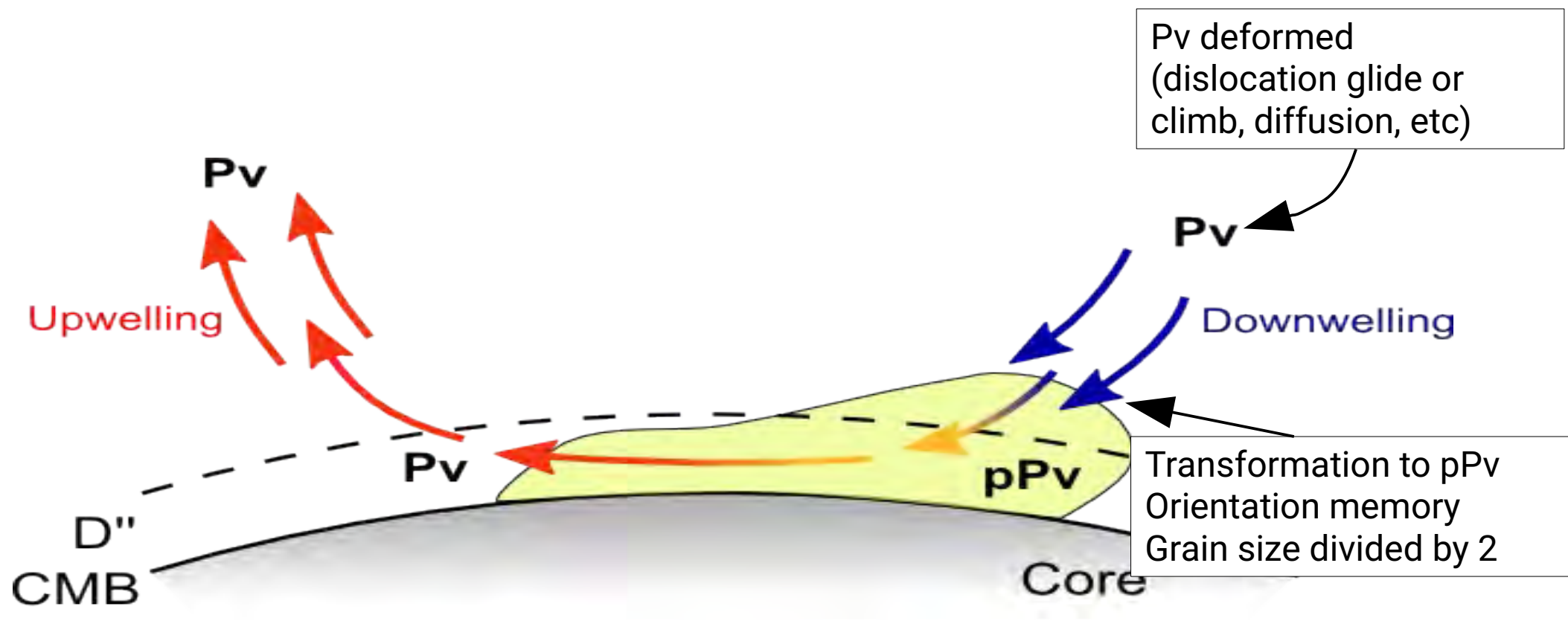
NaCoF₃ post-Perovskite

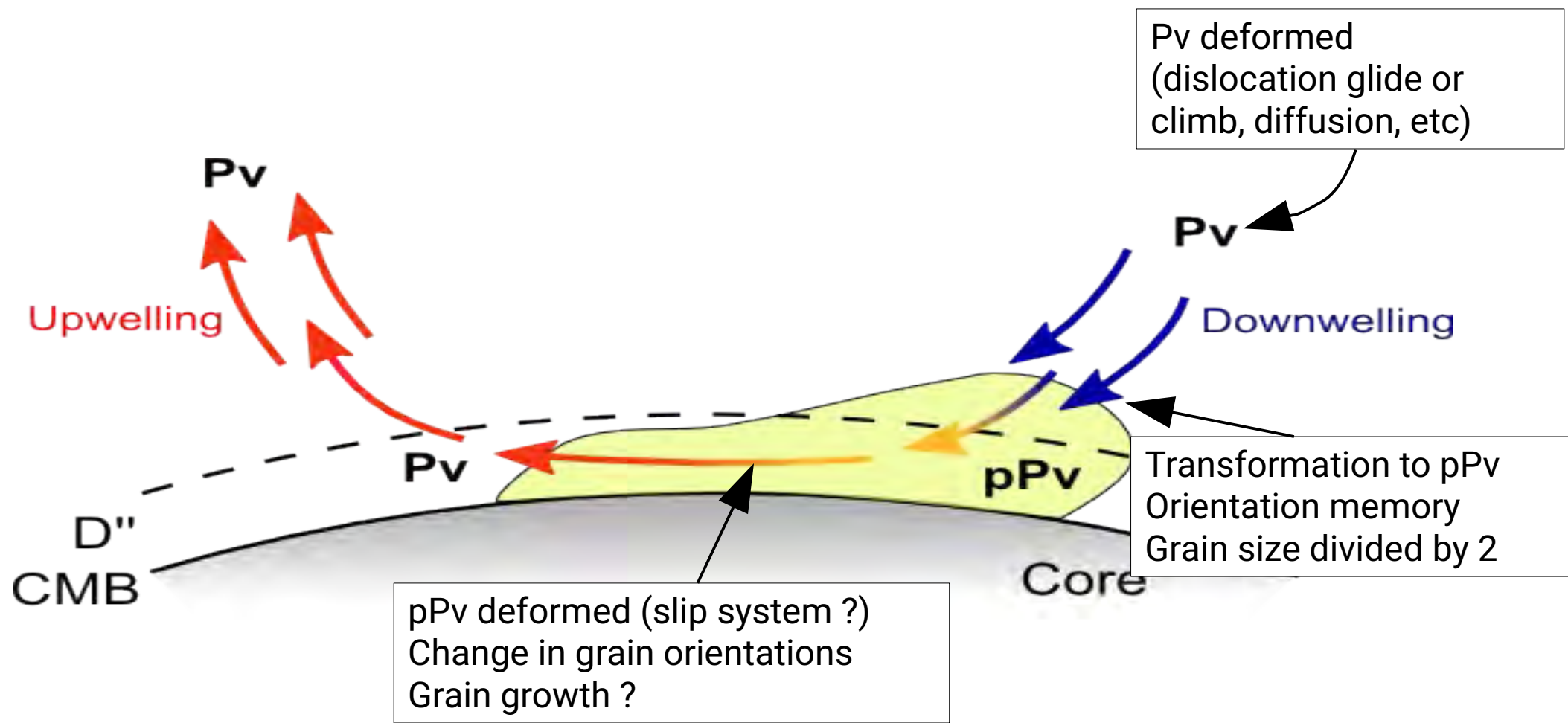


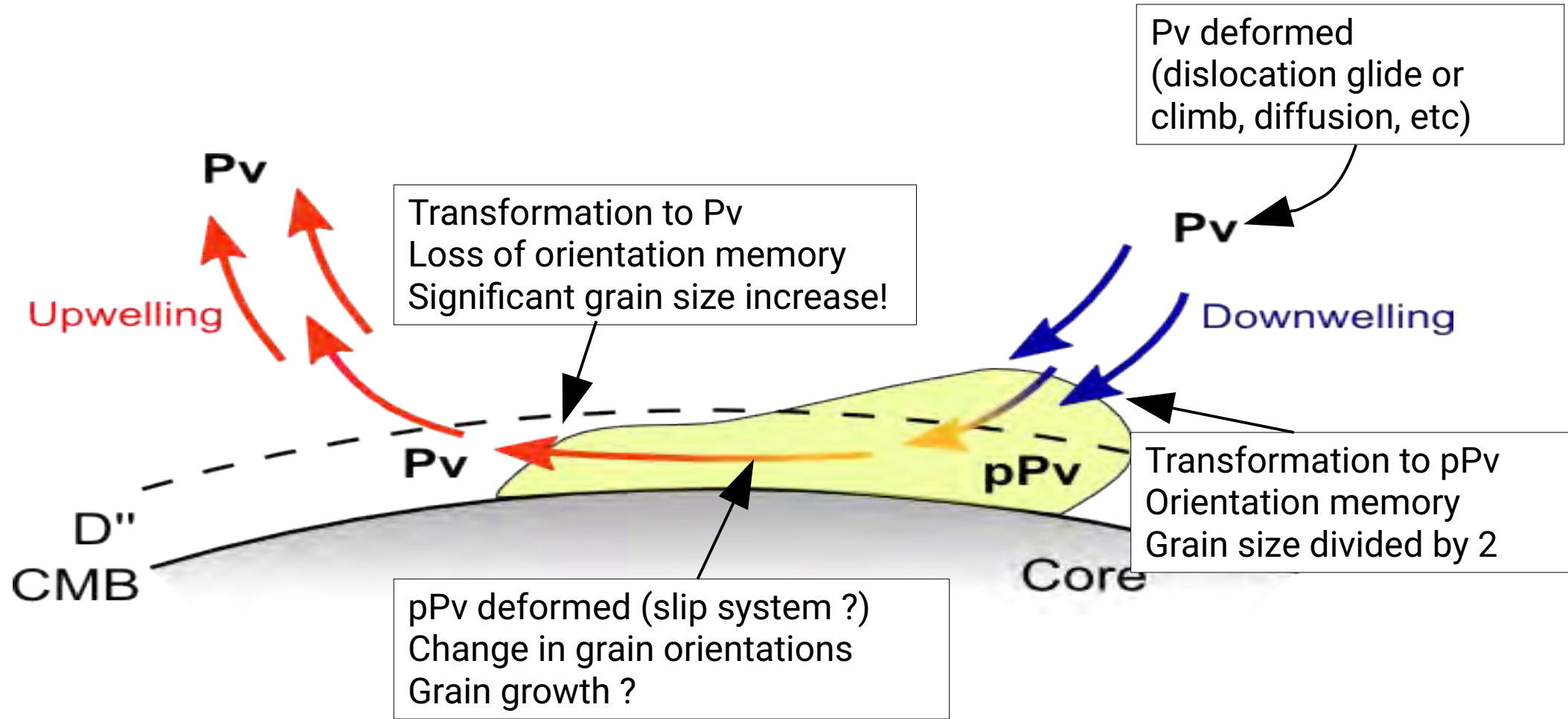
No orientation memory
Nucleation and growth dominated
Grain size multiplication (x10?)

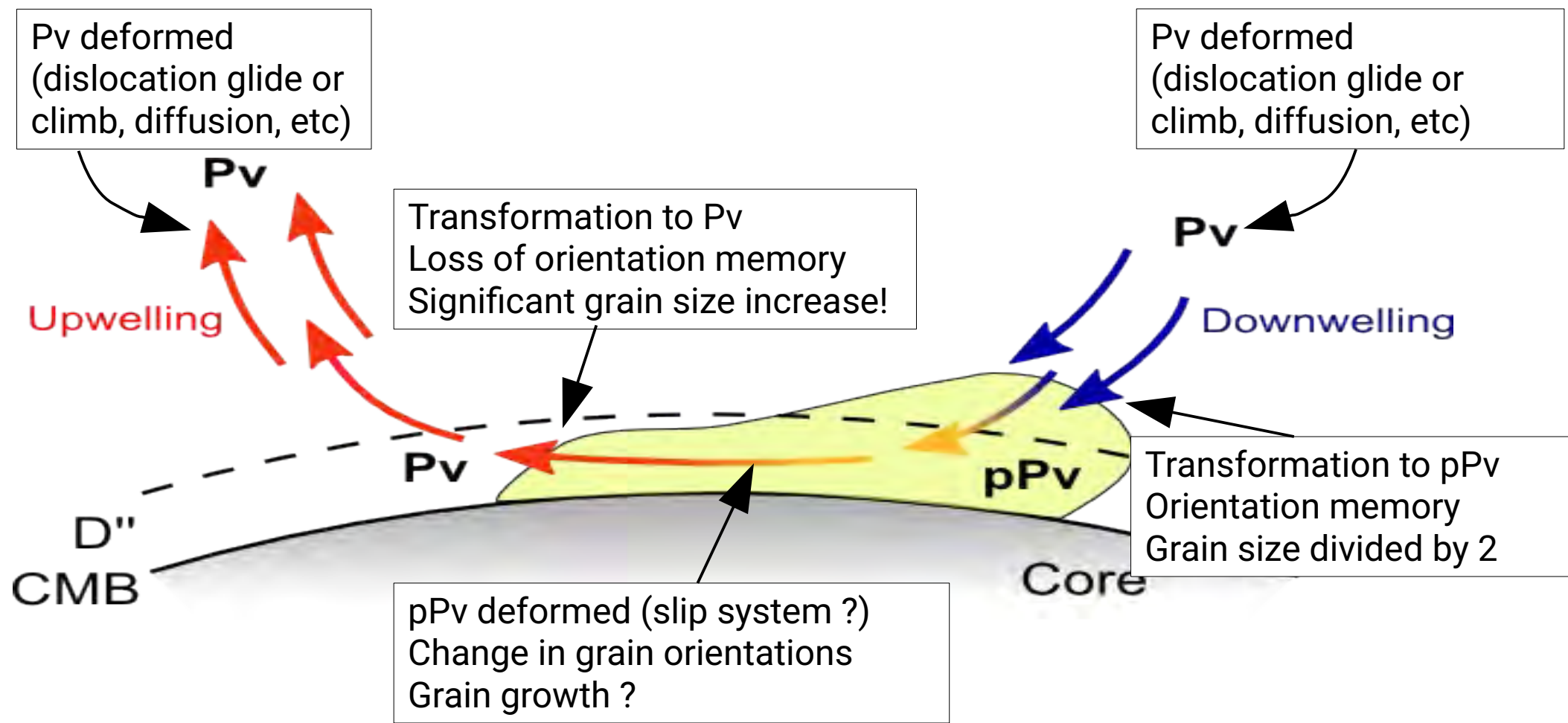


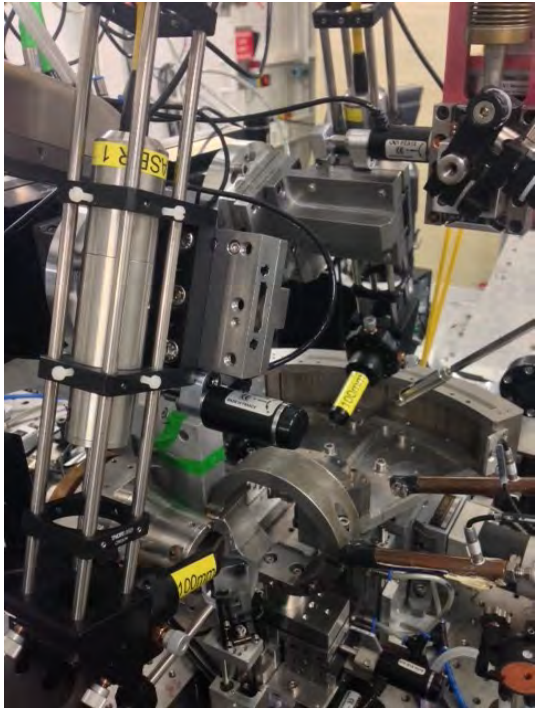




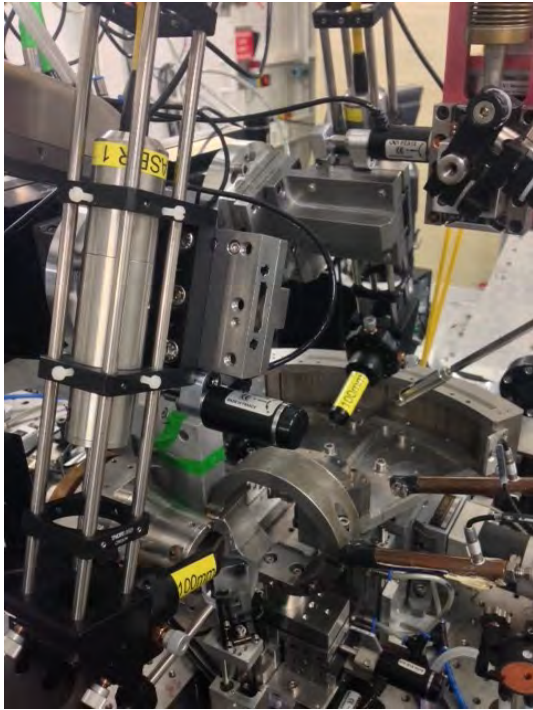




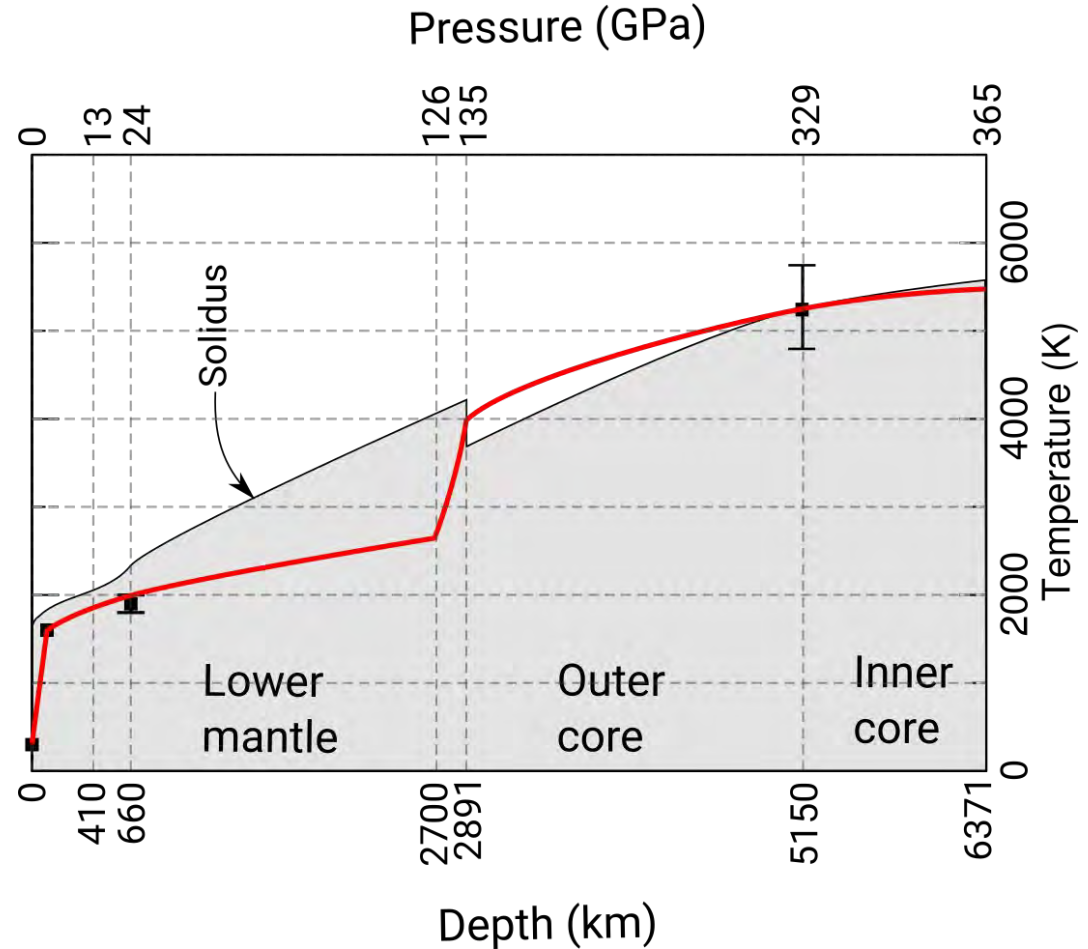


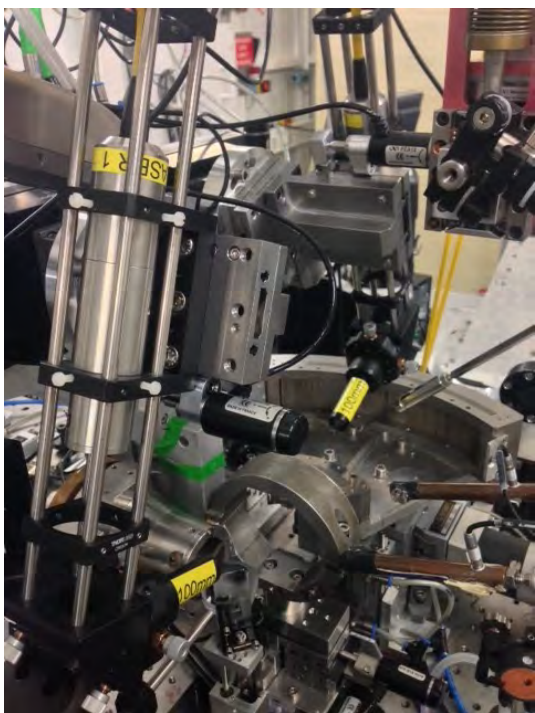


Combining multigrain
crystallography and in-situ
laser-heating in the DAC



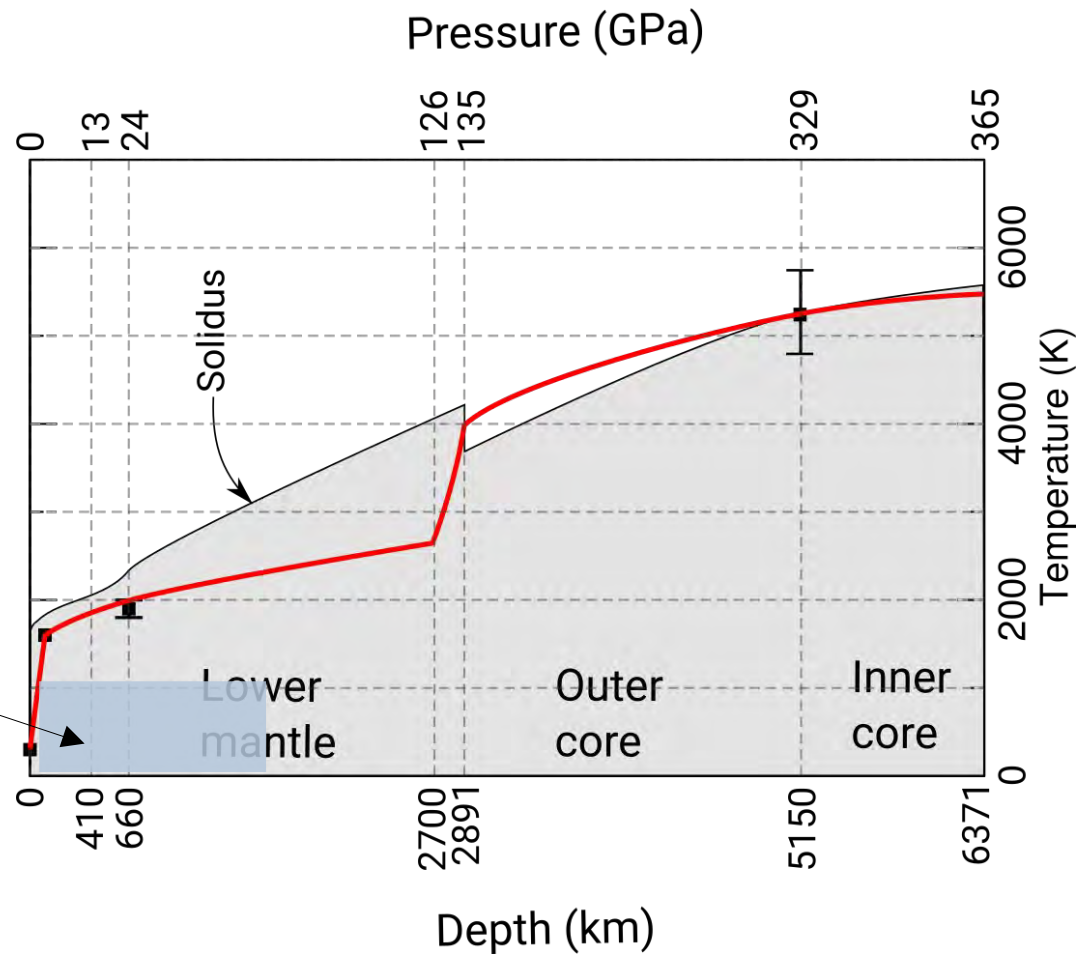
Combining multigrain
crystallography and in-situ
laser-heating in the DAC

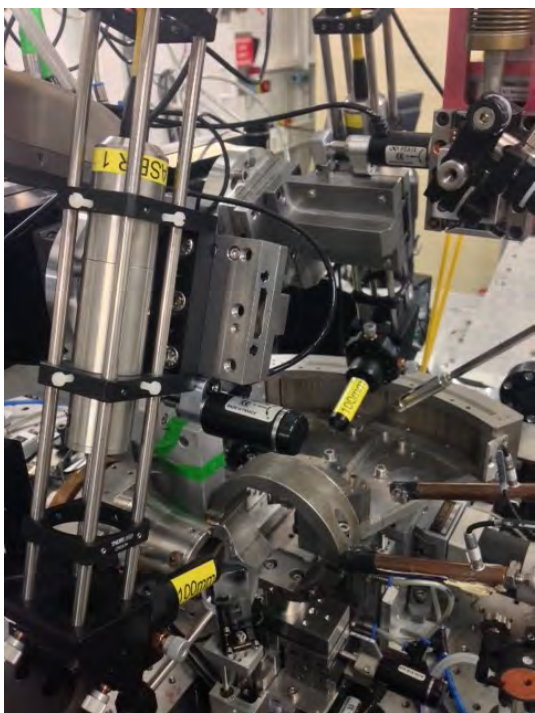




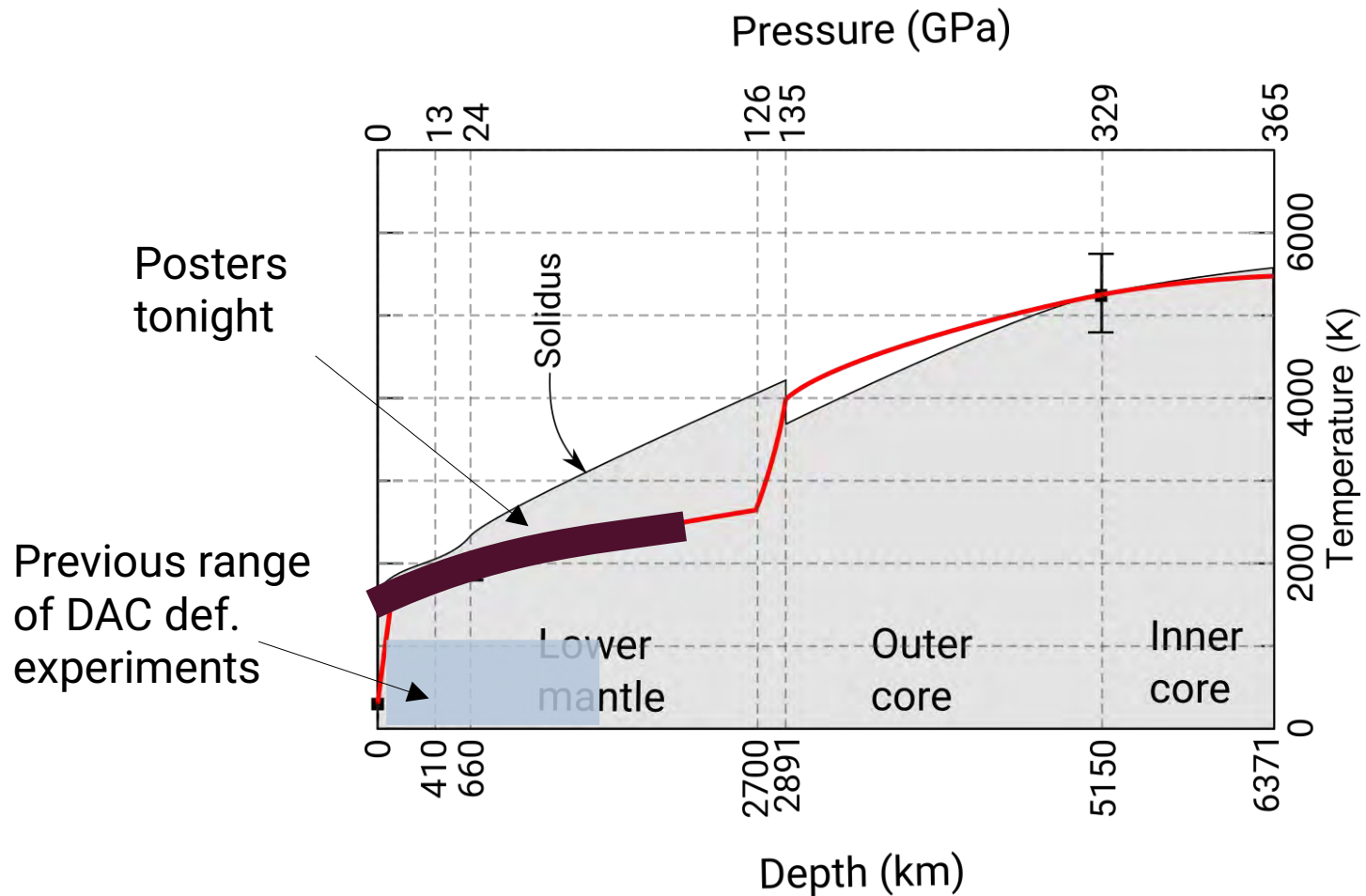
Combining multigrain crystallography and in-situ laser-heating in the DAC

Previous range of DAC def. experiments

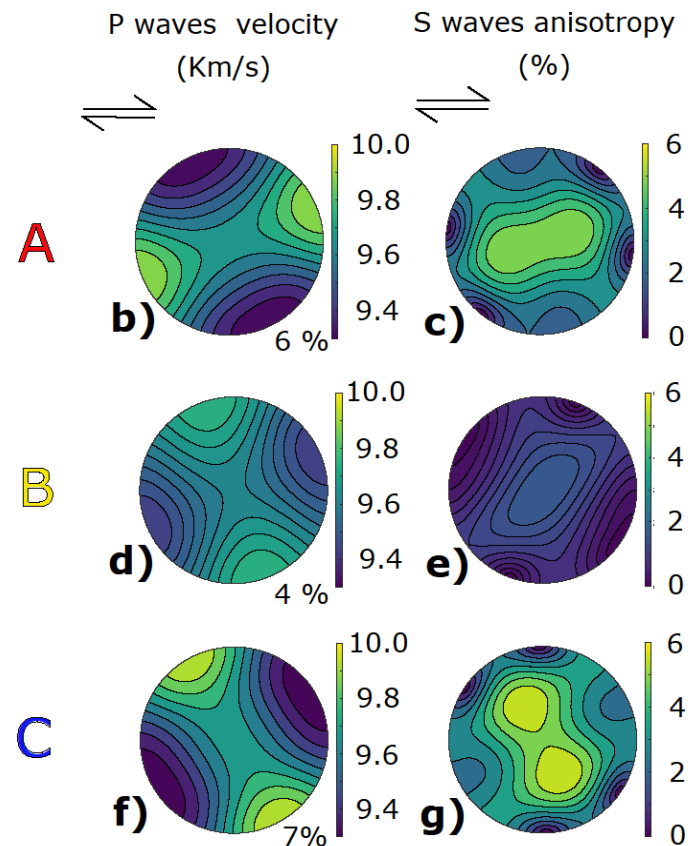
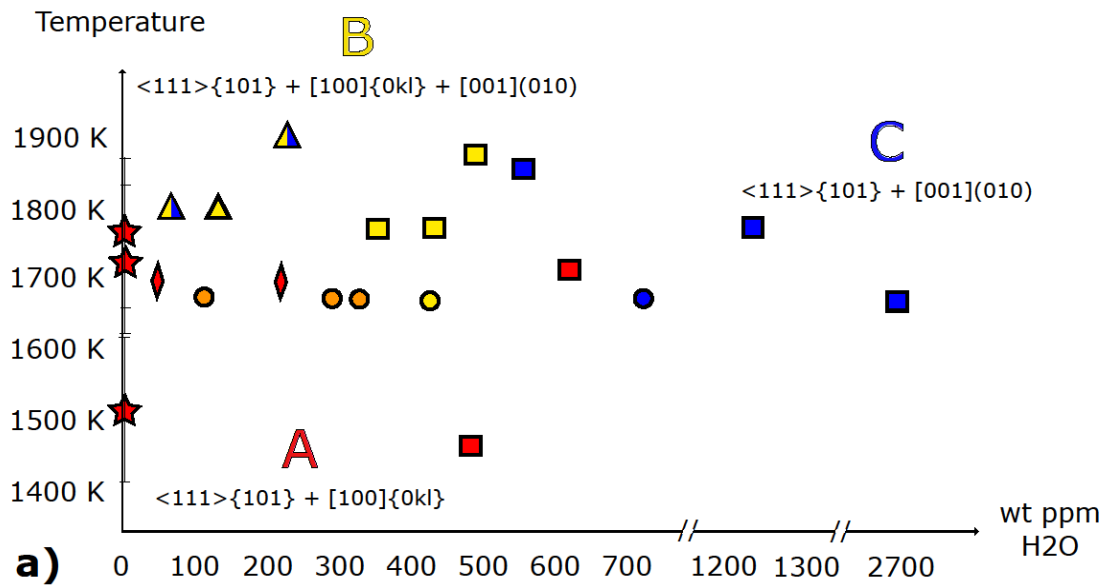




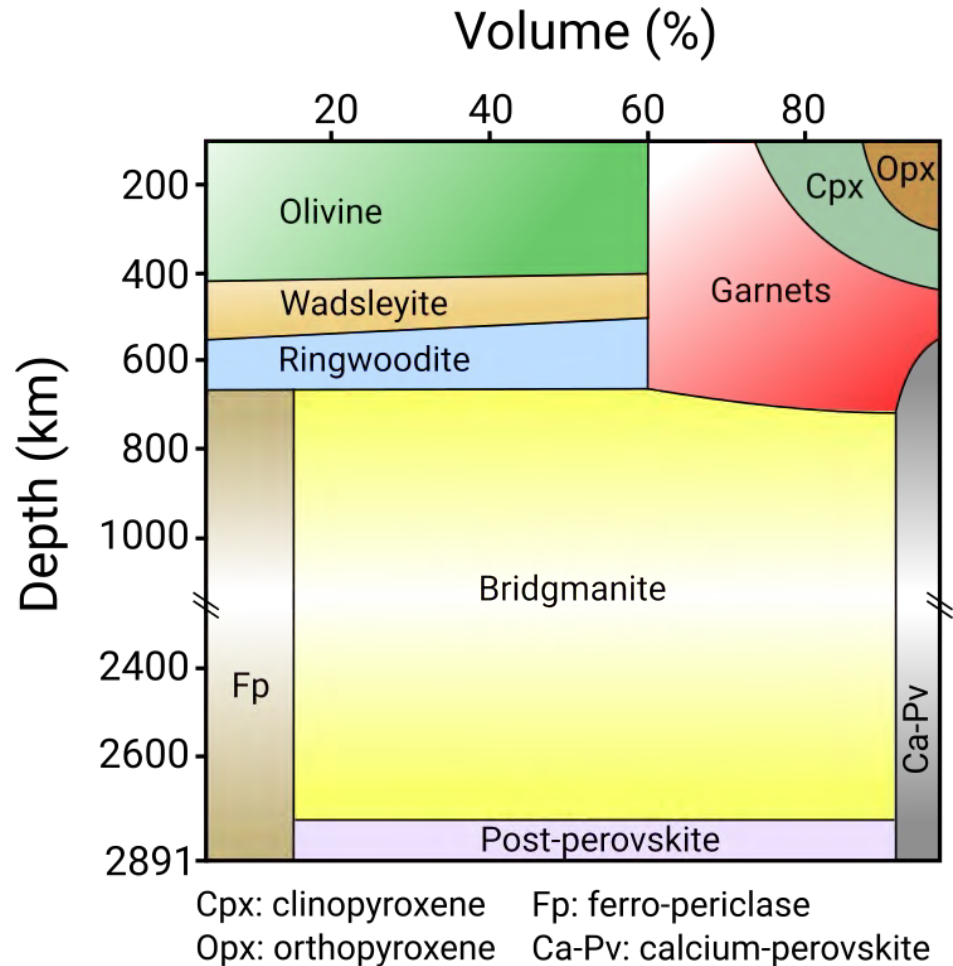
Combining multigrain crystallography and in-situ laser-heating in the DAC

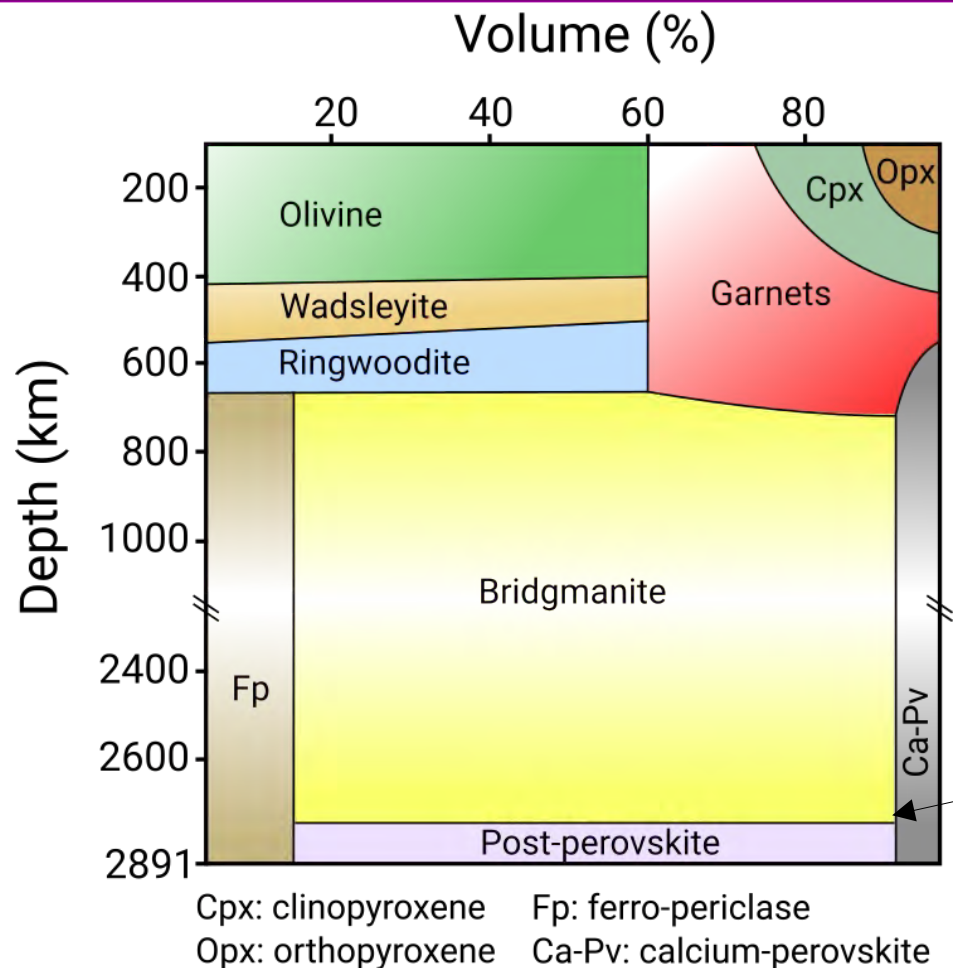


A primer: effect of water and temperature on anisotropy in wadsleyite



Phase transitions in the Earth's mantle



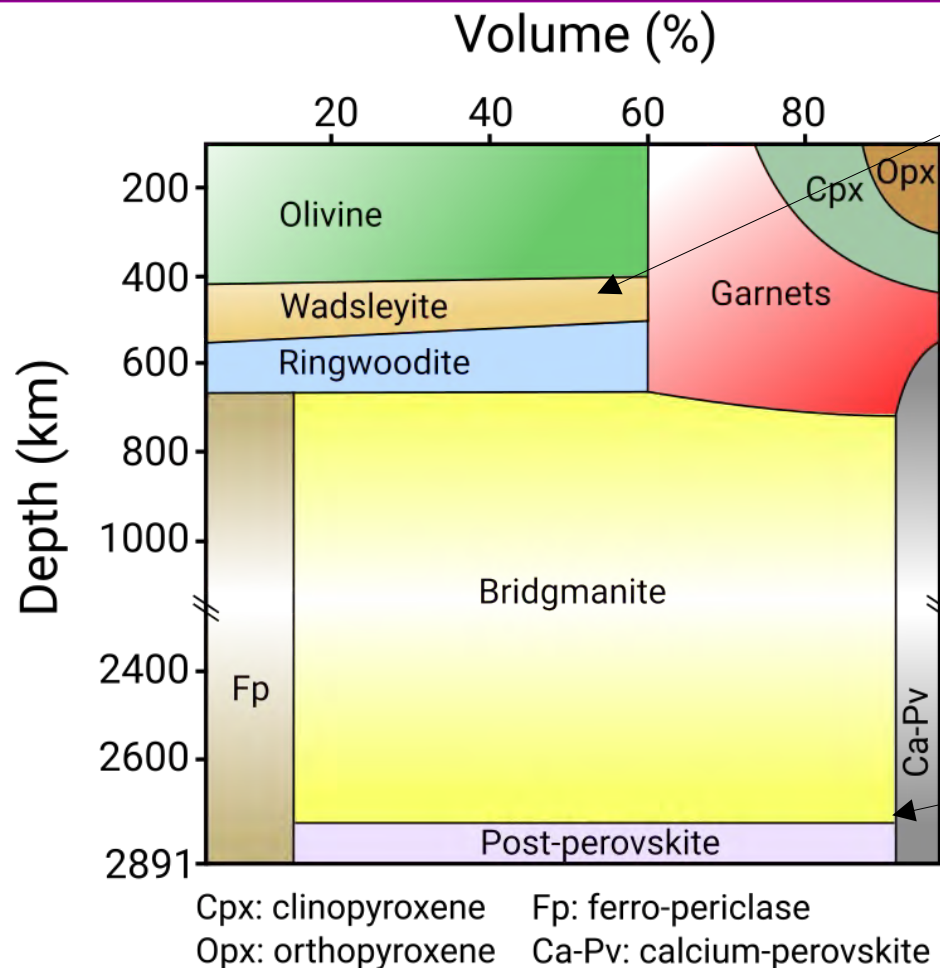


Detectability of the transition

- Effect of kinetics
- Dependence of wave period → thickness of Pv-pPv coexistence
- Amplitude of reflection → kinetics → temperature

Microstructures

- Texture memory at the Pv → pPv transition
- Loss of texture at the pPv → Pv transition



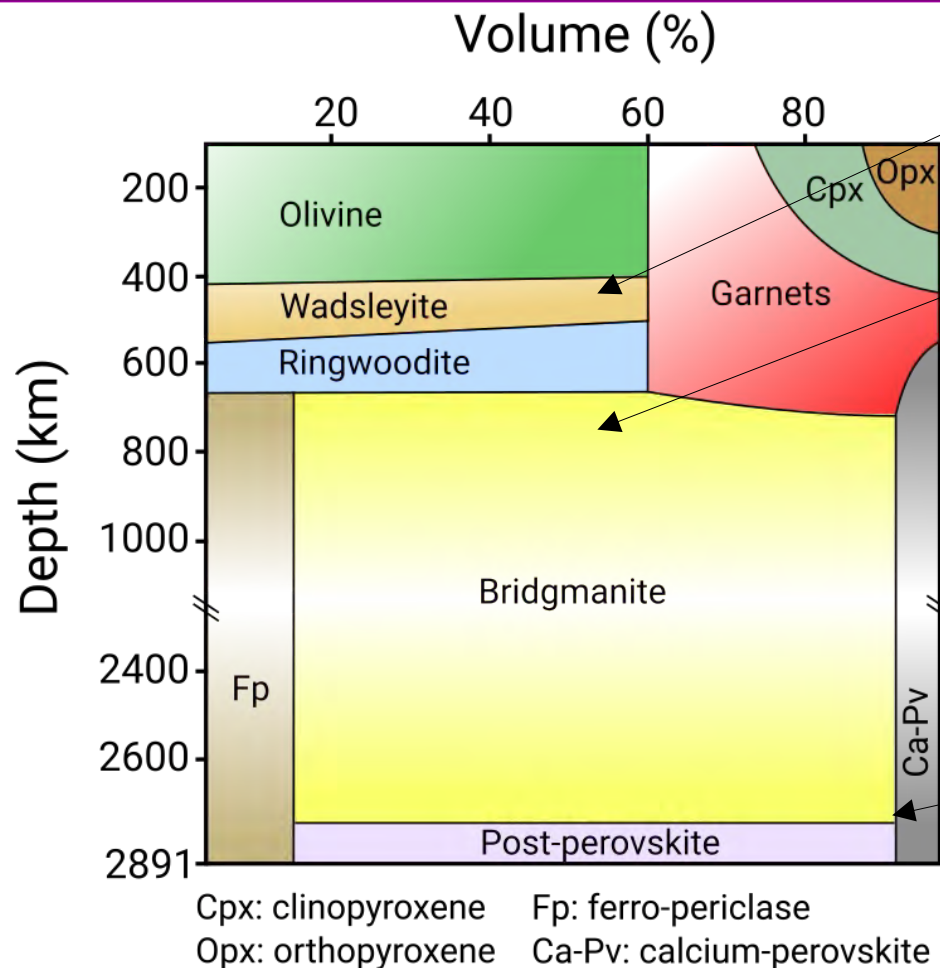
Poster of E. Ledoux later today on wadsleyite and anisotropy in the transition zone

Detectability of the transition

- Effect of kinetics
- Dependence of wave period → thickness of Pv-pPv coexistence
- Amplitude of reflection → kinetics → temperature

Microstructures

- Texture memory at the Pv → pPv transition
- Loss of texture at the pPv → Pv transition



Poster of E. Ledoux later today
on wadsleyite and anisotropy in the transition zone

Poster of J. Gay later today
on bridgmanite and lower mantle

Detectability of the transition

- Effect of kinetics
- Dependence of wave period → thickness of Pv-pPv coexistence
- Amplitude of reflection → kinetics → temperature

Microstructures

- Texture memory at the Pv → pPv transition
- Loss of texture at the pPv → Pv transition