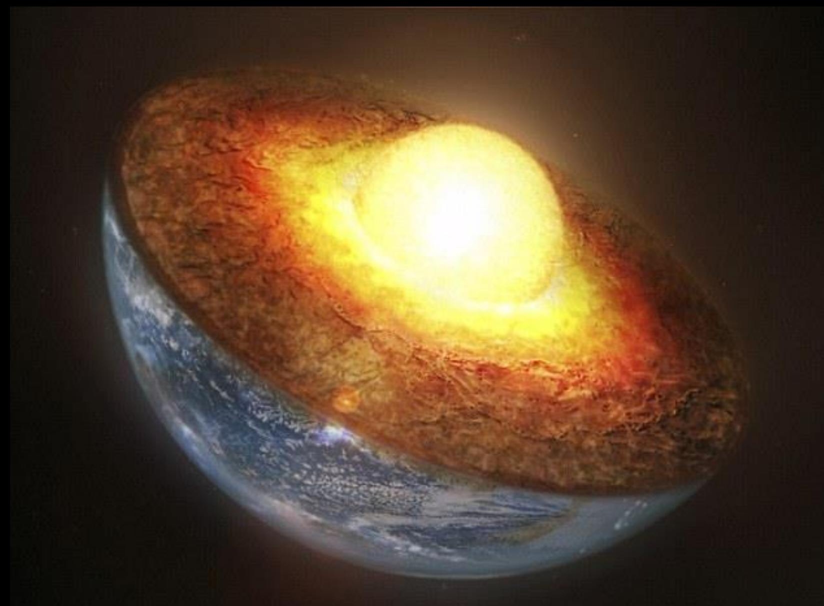
Earth mineralogy and its phase transition



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EHIME UNIVERSITY GRC GEODYNAMICS RESEARCH CENTER

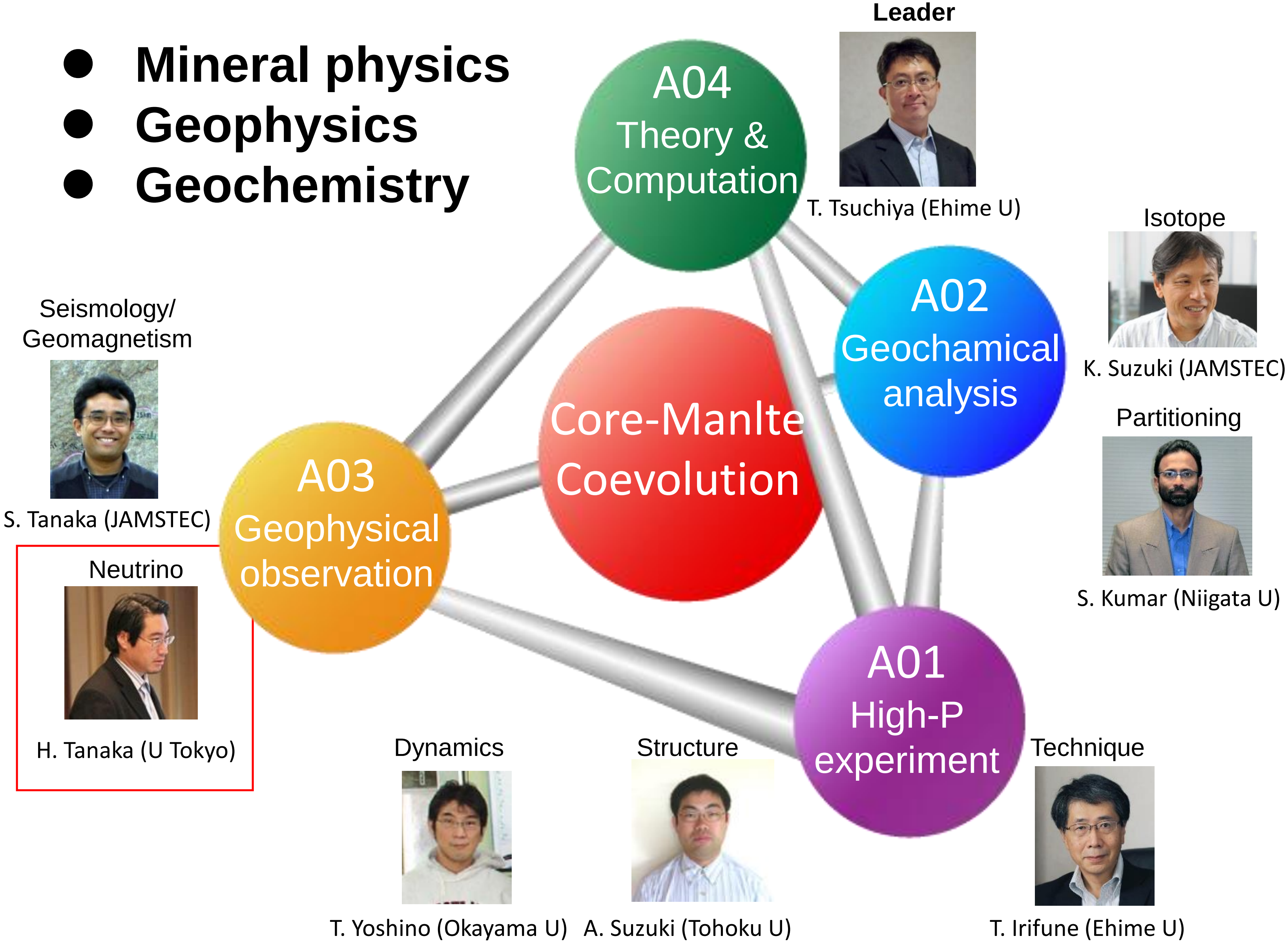
CoreMantle evolution 文部科学省 科学研究費助成事業 新学術領域研究（研究領域提案型）

JSPS Grant for Innovative Research

Core-Mantle Interaction and Coevolution

http://core-mantle.jp/

- **Mineral physics**
- **Geophysics**
- **Geochemistry**



Institutions

Tohoku U
Niigata U
U Tokyo
Tokyo Tech
Kyoto U
Osaka U
Okayama U
Hiroshima U
Ehime U
Kyushu U
JAMSTEC

Facilities

SPring-8
J-PARC
KEK
KamLAND

1. Basics of silicate crystallography
2. High-pressure mineralogy
3. Earth’s compositional model
4. Earth’s interior dynamics from mineral physics

1. Basics of silicate crystallography
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Rock-forming minerals

Minerals forming igneous, sedimentary, or metamorphic rocks

Silicates (> 90% of the Earth's crust)

- Quartz
  SiO_2

- Feldspar
  Alkali metal + Al

- Mica
  Hydrous
  Sheet structure

- Amphibole
  Hydrous
  Metamorphic rock

- Pyroxene
  Chain structure
  Mafic
  $(Mg,Ca)SiO_3$

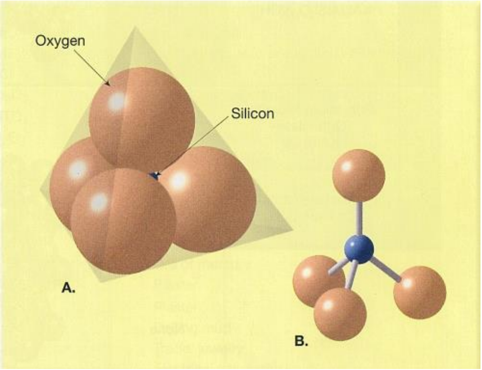
- Olivine
  Mafic
  $(Mg,Fe)SiO_4$

Others

- Calcite
  Carbonate

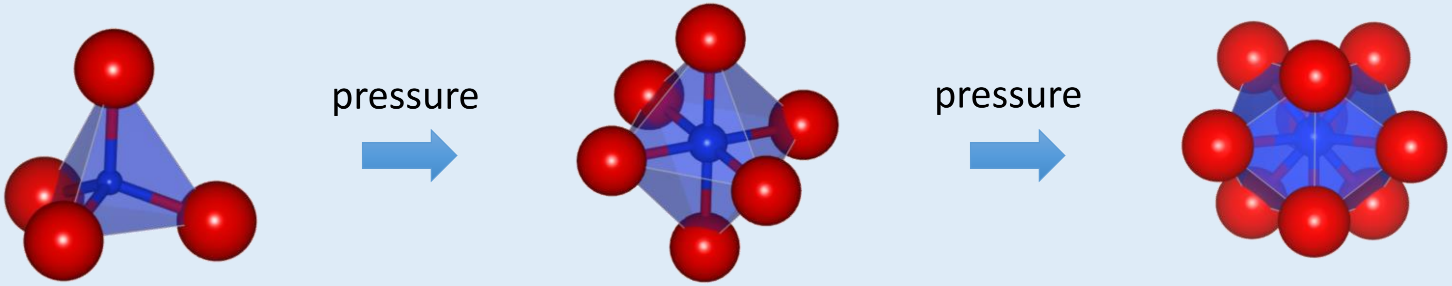
- Pyrite
  Sulfide

Silicate minerals



Fundamental block of SiO_4 tetrahedron in low-pressure silicate minerals

The coordination number of silicon (cation atoms) generally increases with pressure.



4-fold (tetrahedron) quartz | 6-fold (octahedron) stishovite | 9-fold (3-capped prism) Fe_2P-type

Gibbs

$$G(P,T) = F(V,T) + P(V,T)V$$

Helmholtz

$$F(V,T) = E(V,T) - TS(V,T)$$

Cation coordination change:

- V reduces (by 5~10 %)
- S (phonon) increases (generally)

Crystal structure frameworks of silicates in terms of SiO_4 connectivity

- Independent
- Chain
- Double chain
- Sheet
- 3D

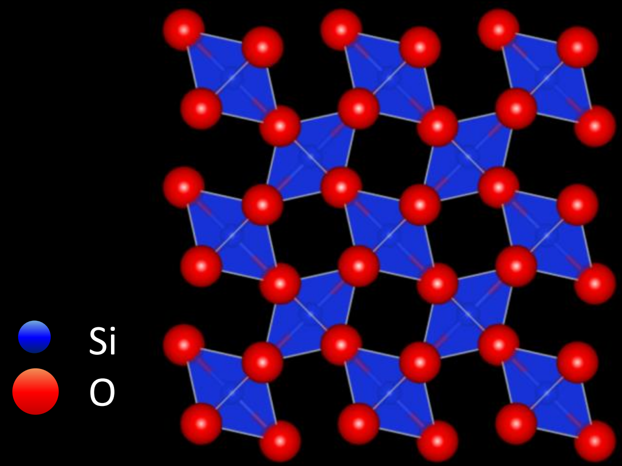
Each structure is defined crystallographycally (X-ray diffraction).

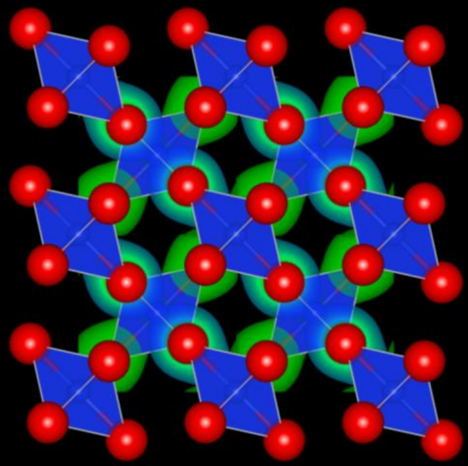
Mineral/Formula	Cleavage	Silicate Structure	Example
Olivine group $(Mg, Fe)_2SiO_4$	None	Independent tetrahedron	Olivine
Pyroxene group (Augite) $(Mg,Fe)SiO_3$	Two planes at right angles	Single chains	Augite
Amphibole group (Hornblende) $Ca_2(Fe,Mg)_5Si_8O_{22}(OH)_2$	Two planes at 60° and 120°	Double chains	Hornblend
Micas: Biotite $K(Mg,Fe)_3AlSi_3O_{10}(OH)_2$	One plane	Sheets	Biotite
Micas: Muscovite $KAl_2(AlSi_3O_{10})(OH)_2$			Muscovite
Feldspars: Potassium feldspar (Orthoclase) $KAlSi_3O_8$	Two planes at 90°	Three-dimensional networks	Potassium feldspar
Feldspars: Plagioclase feldspar $(Ca,Na)AlSi_3O_8$			
Quartz SiO_2	None		Quartz

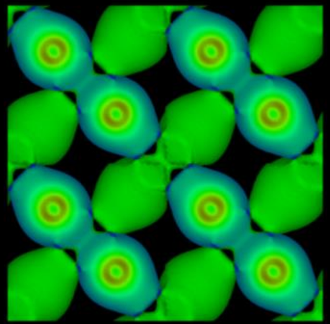
Si-O bonding

Crystal structure

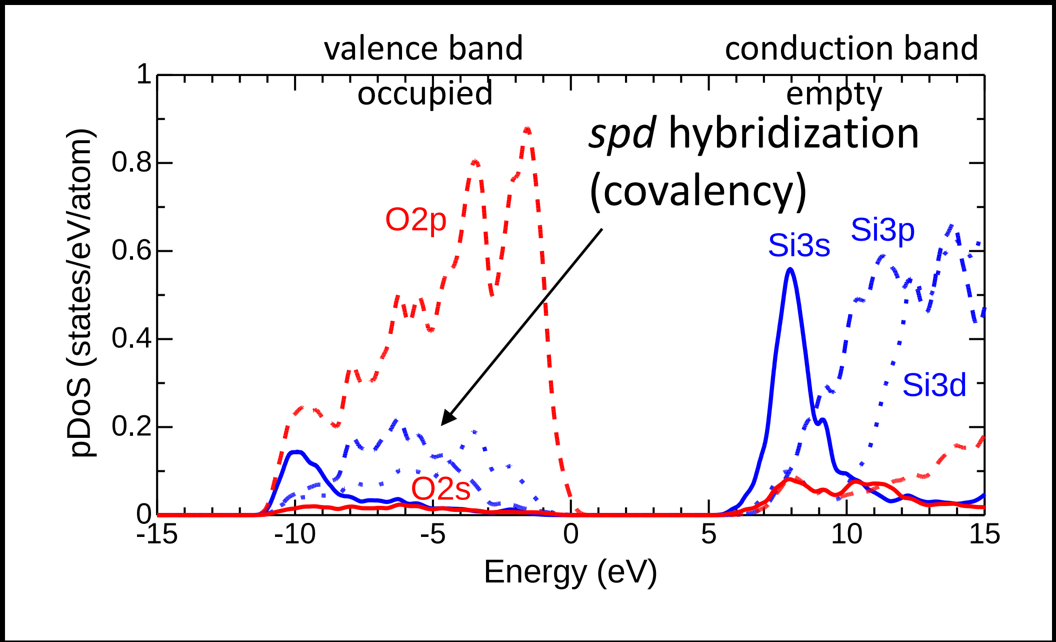
Electron density



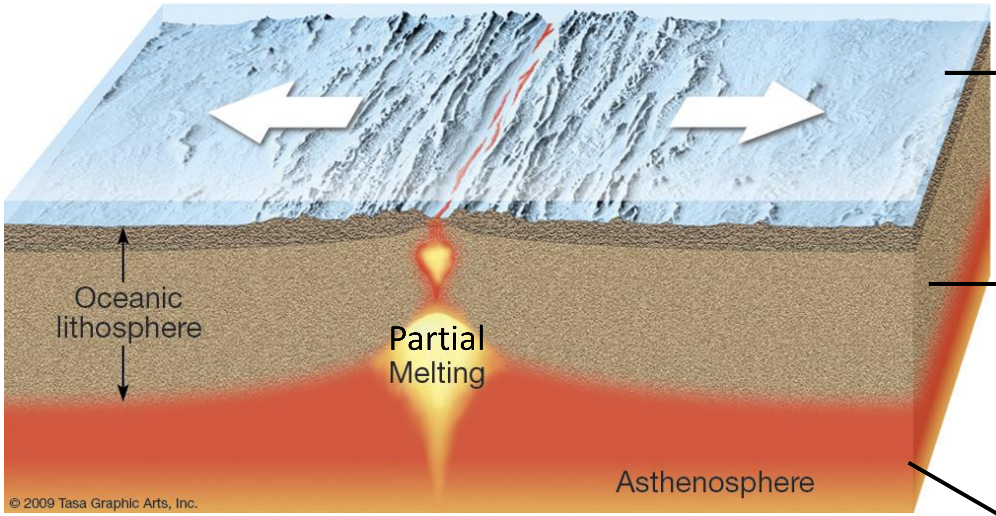




Electronic structure of stishovite



Mantle petrology



Mid-Ocean Ridge
(partial melting)

Mid-Ocean Ridge Basalt (MORB)
Solidified magma
Uppermost ~5 km (Oceanic crust)
Concentration of incompatible elements
(K, Na, U, Th, etc)

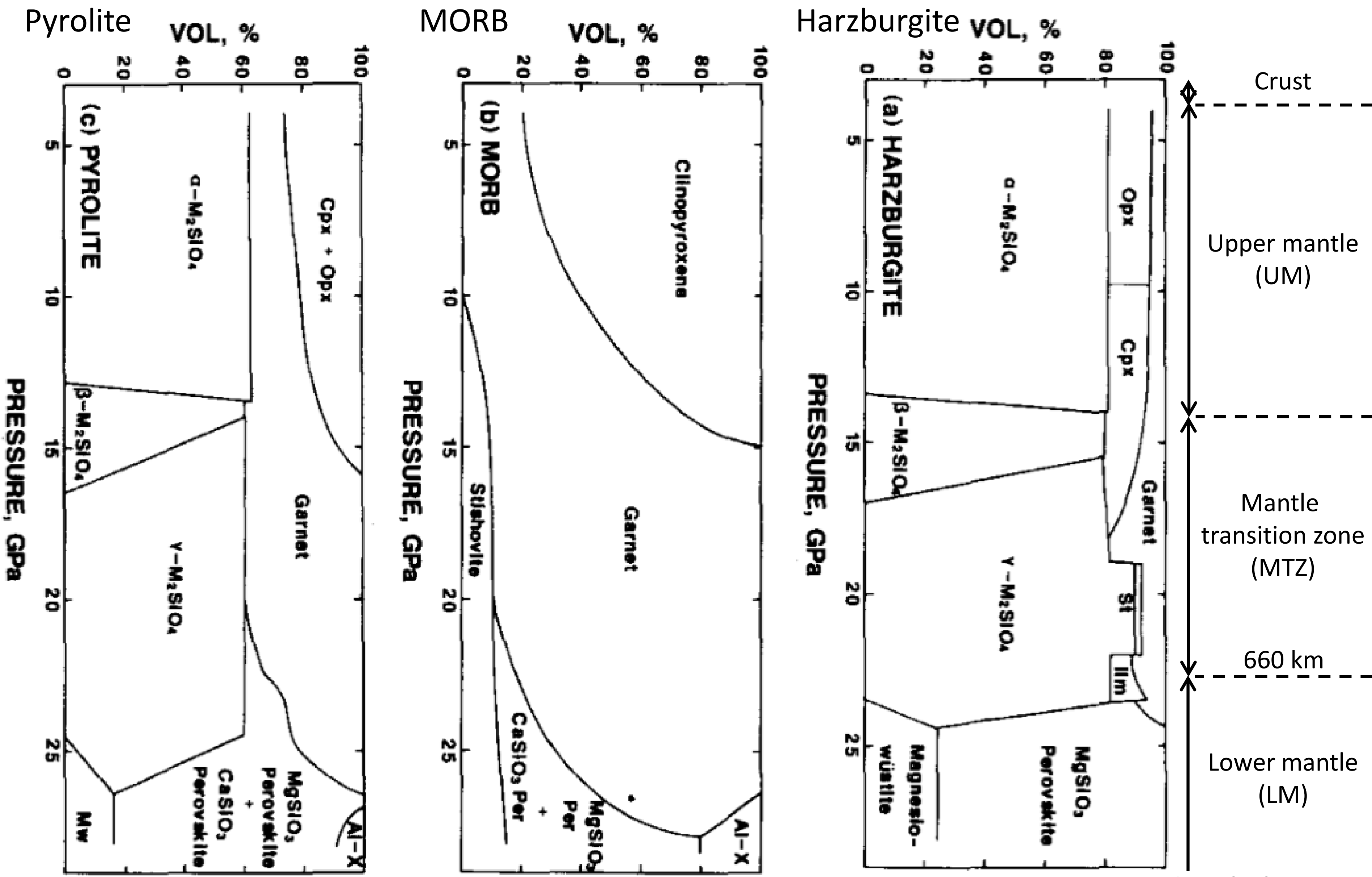
Harzburgite
Residual of partial melting
80~90 km

Pyrolite (Lherzolite)
Upper mantle rock,
which could produce MORB
through partial melting

Lower mantle???

Pyrolite (Pyroxene + Olivine) **= 1/4 Basalt** + **3/4 Dunite** (Olivine-rich peridotite)
Green & Ringwood (1963)

Representative lithology in the upper mantle condition



Irifune (87) EPSL

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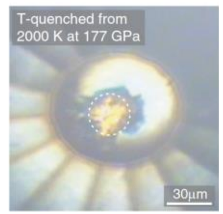
Methods to study materials under high-*P*,*T*

(1) High-P,T experiment

Pressure is generated by pressing hard anvils



Technically difficult

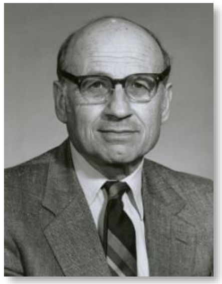
(2) Theory & computation (Ab initio method)

Prediction of material properties based on quantum mechanics and condensed-matter theory

Density functional theory (DFT) (Nobel prize in chemistry in 1988)

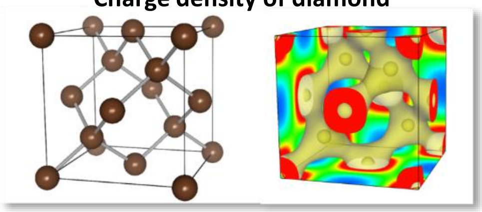
$$\left[-\frac{\hbar^2}{2m}\Delta-\sum_I\frac{Z_I}{|\mathbf{r}-\mathbf{R}_I|}+e^2\int\frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}'+V_{XC}[n(\mathbf{r})]\right]\varphi_i(\mathbf{r})=\epsilon_i\varphi_i(\mathbf{r})$$

$$n(\mathbf{r})=\sum_i|\varphi_i(\mathbf{r})|^2$$

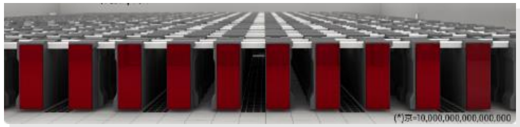


Walter Kohn
April 19, this year (93 old)

Charge density of diamond

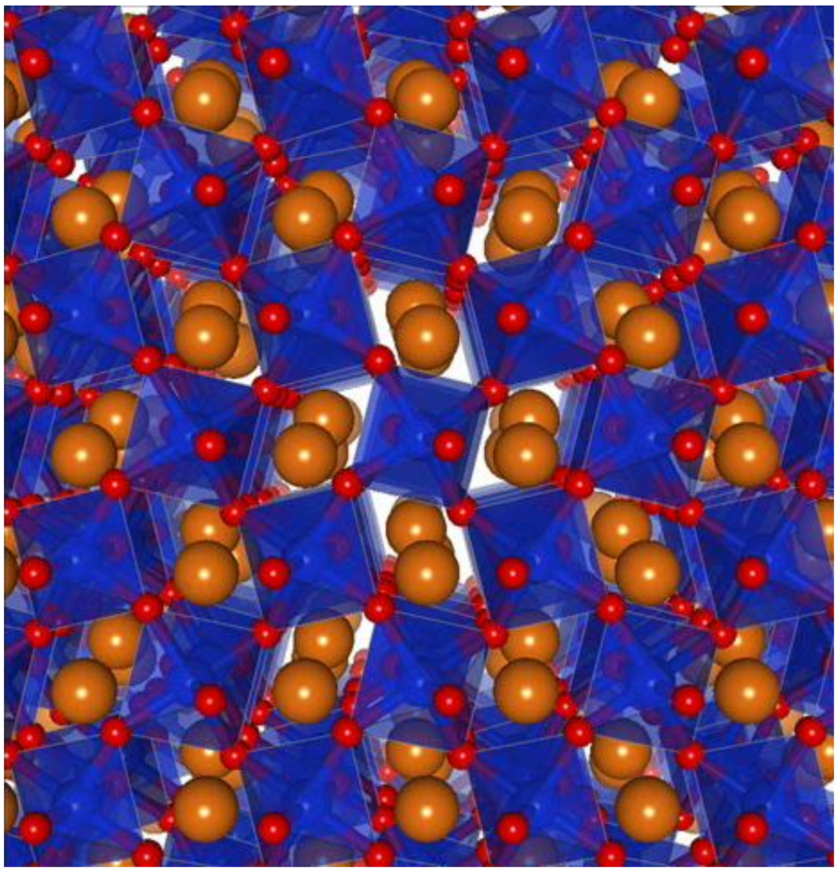


Super computer



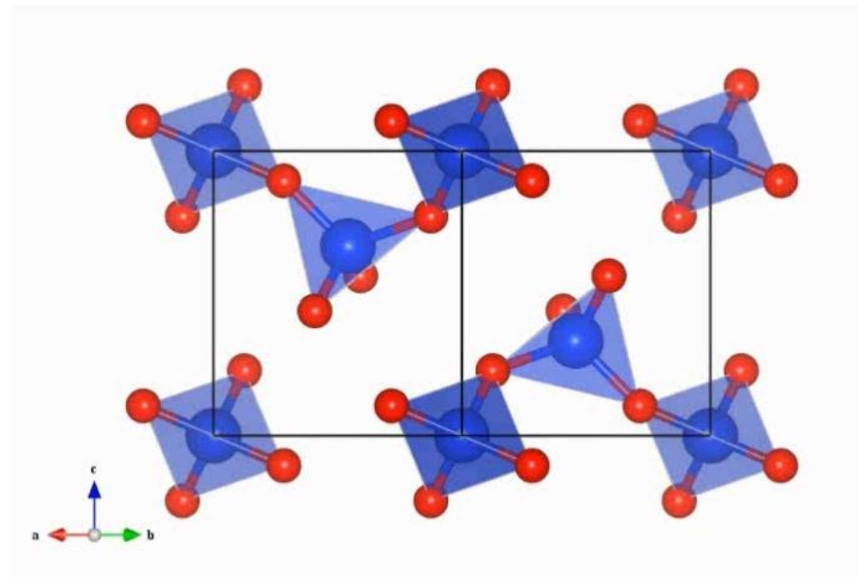
Structure search by ab initio molecular dynamics

$MgSiO_3$ Bridgmanite



~100 GPa

SiO_2 α-Quartz



~700 GPa

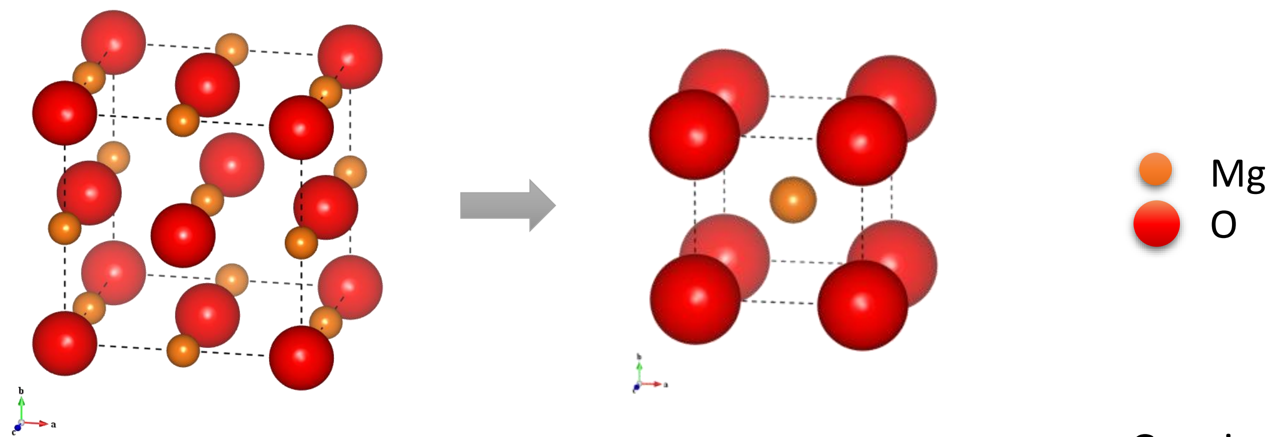
Mg

Si

O

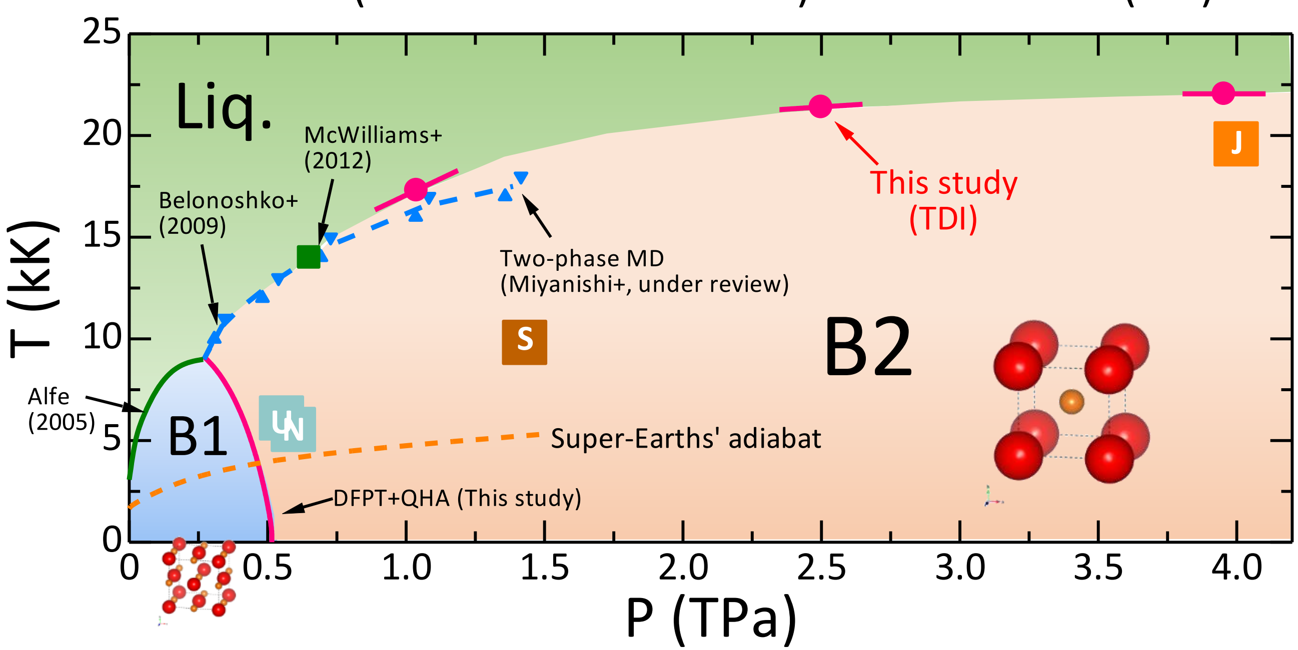
Structure evolution under pressure

MgO

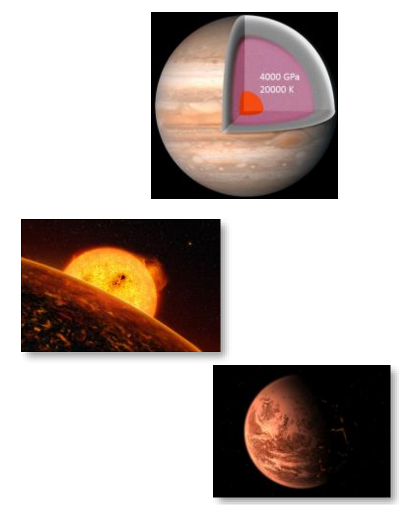


B1 (NaCl) Low-P
(cation coordination VI)

B2 (CsCl) High-P
(VIII)



Gas giant or
super-Earth

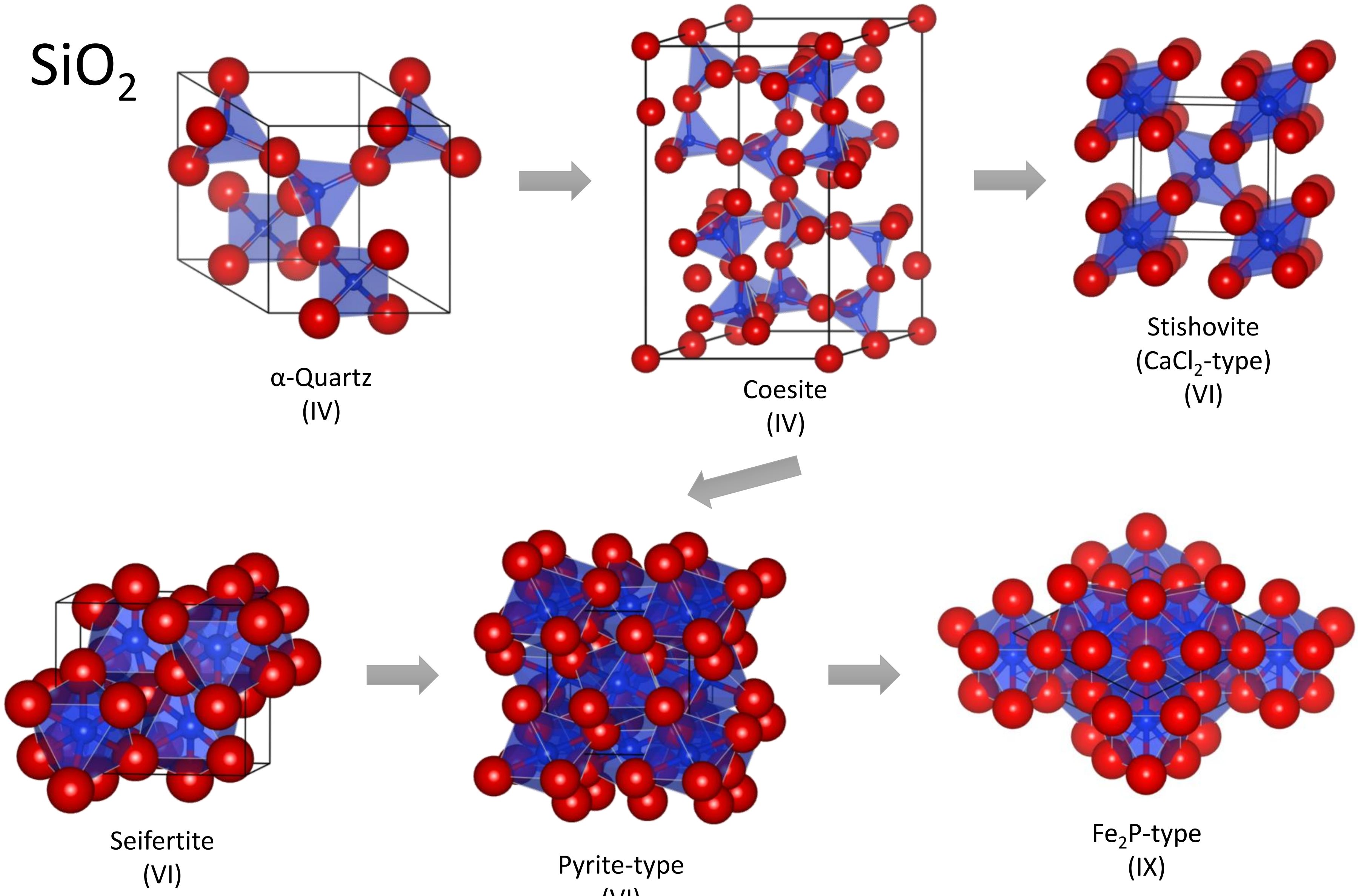


1 TPa = 1000 GPa

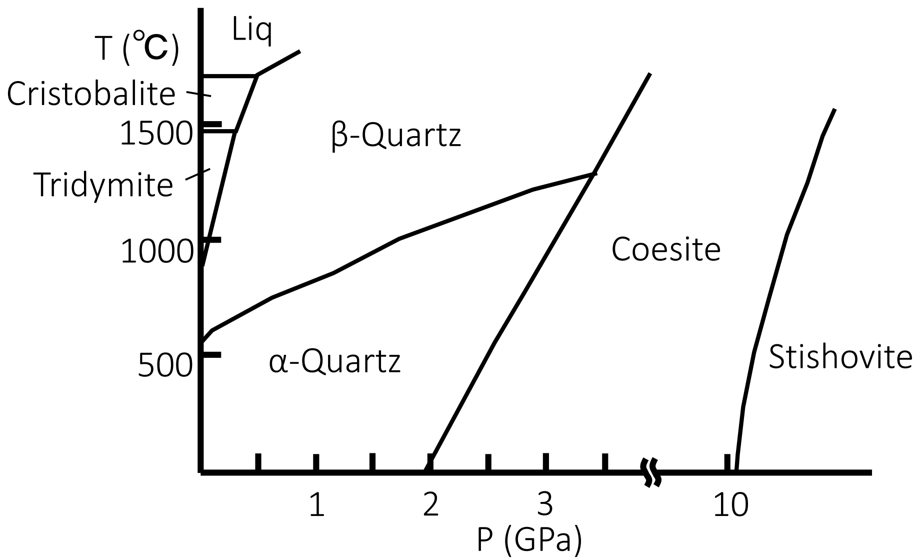
CoE = 364 GPa

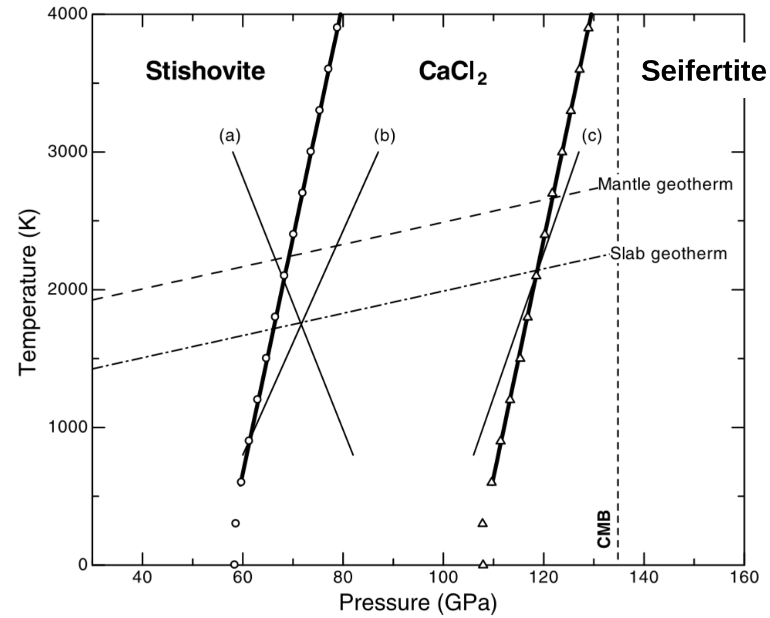
Structure evolution under pressure

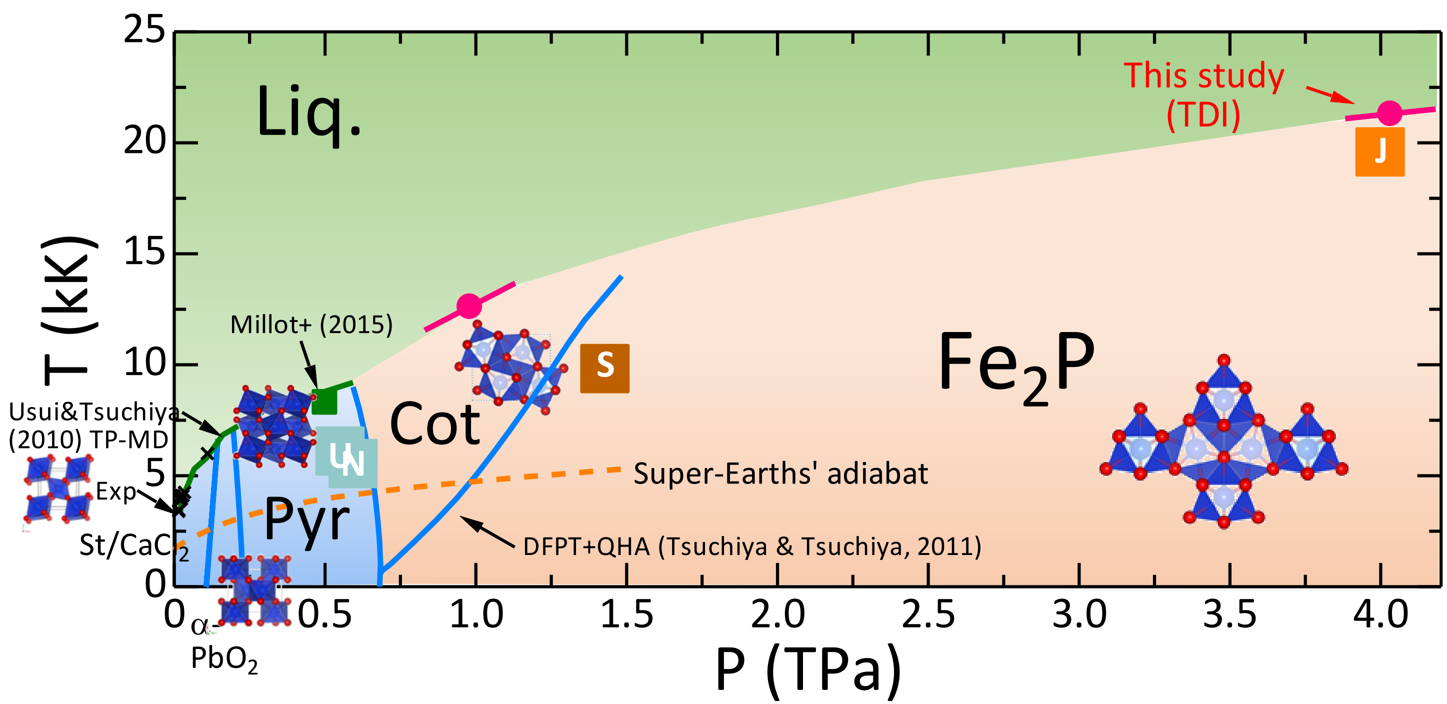
Si
O



Tsuchiya & Tsuchiya (11) PNAS

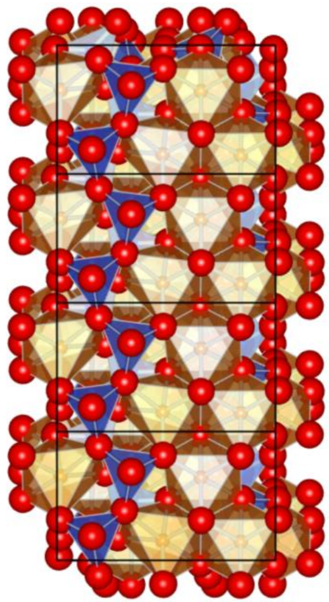

T (°C)
Liq
Cristobalite
1500
Tridymite
1000
500
β-Quartz
α-Quartz
Coesite
Stishovite
1
2
3
10
P (GPa)


Stishovite
CaCl2
Seifertite
(a)
(b)
(c)
Mantle geotherm
Slab geotherm
CMB
Temperature (K)
4000
3000
2000
1000
0
40
60
80
100
120
140
160
Pressure (GPa)

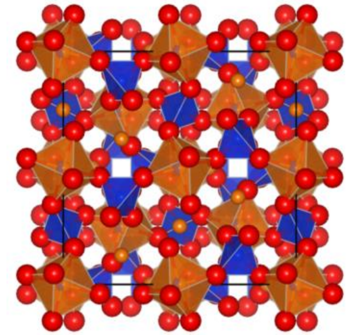

25
20
15
10
5
0
T (kK)
Liq.
This study
(TDI)
J
Millot+ (2015)
Cot
S
Fe2P
Usui&Tsuchiya
(2010) TP-MD
Exp
St/CaCl2
Pyr
Super-Earths' adiabat
DFPT+QHA (Tsuchiya & Tsuchiya, 2011)
0
α-
PbO2
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
P (TPa)

Structure evolution under pressure

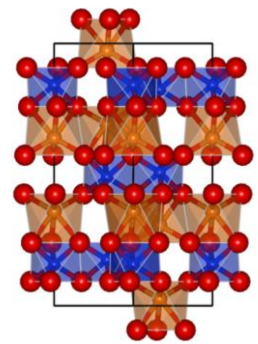
$MgSiO_3$



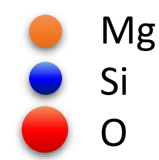
Orthoenstatite
(Mg-VI, Si-IV)

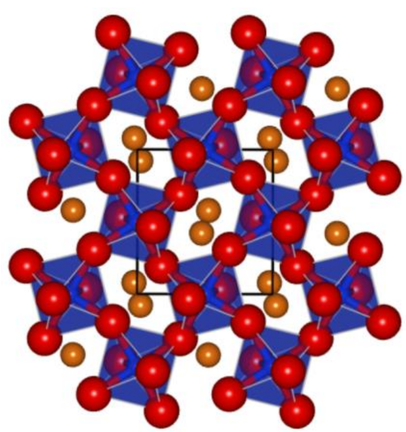


Majorite (High-T)

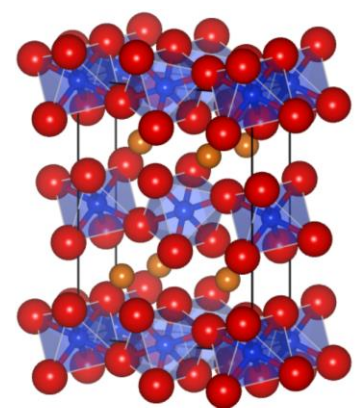


Akimotoite (Lpw-T)
(Mg-VI, Si-VI)





Bridgmanite
(Mg-VIII, Si-IV)



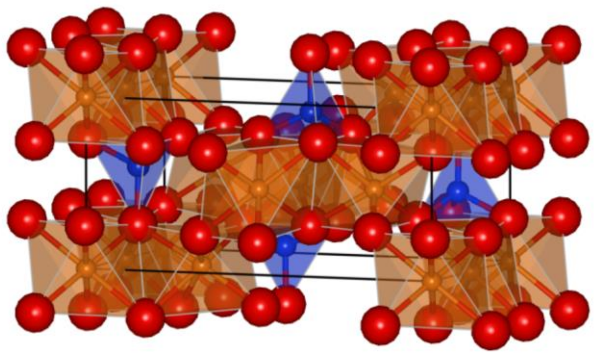
Post-perovskite
(Mg-VIII, Si-IV)

Murakami+ (04) Science
Tsuchiya+ (04) EPSL
etc

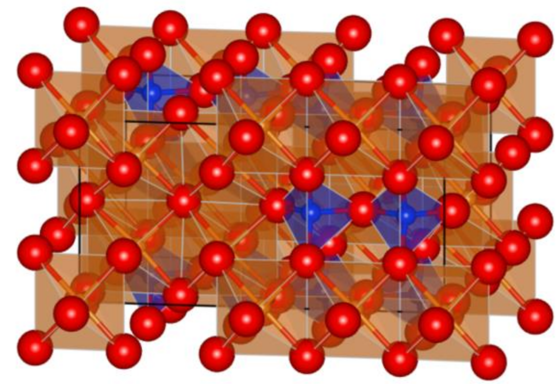
Structure evolution under pressure

Mg
Si
O

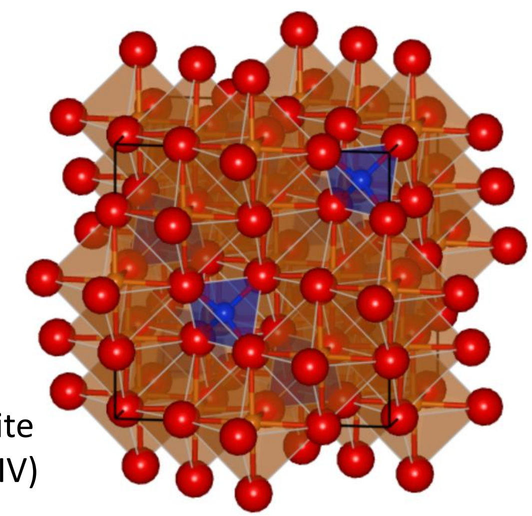
Mg_2SiO_4



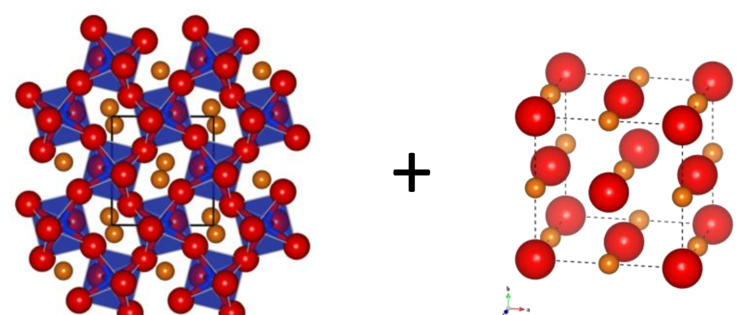
Olivine
(Mg-VI, Si-IV)



Wadsleyite
(Mg-VI, Si-IV)

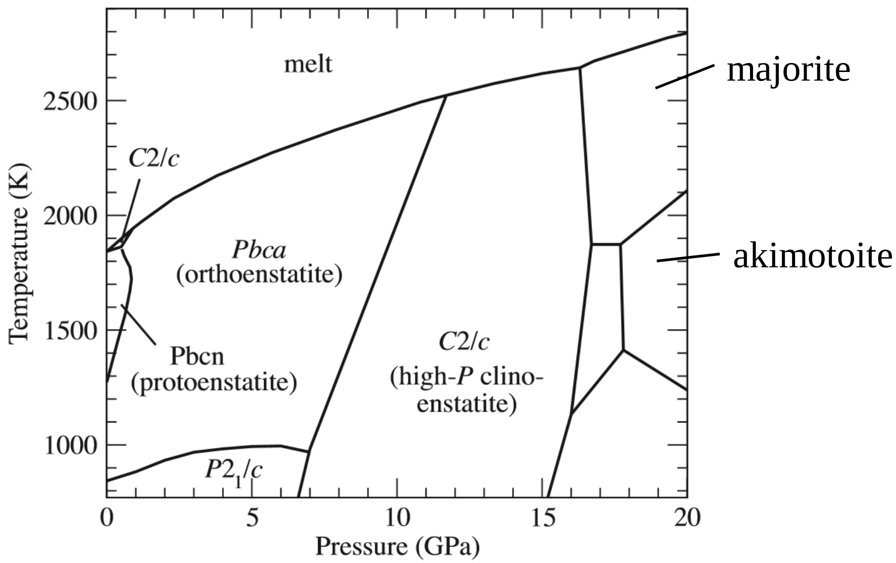


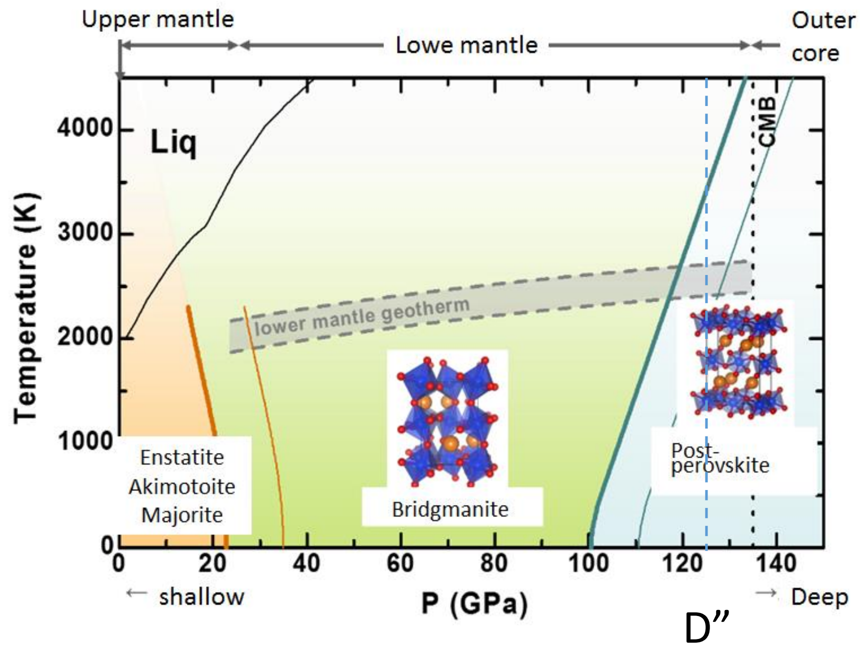
Ringwoodite
(Mg-VI, Si-IV)



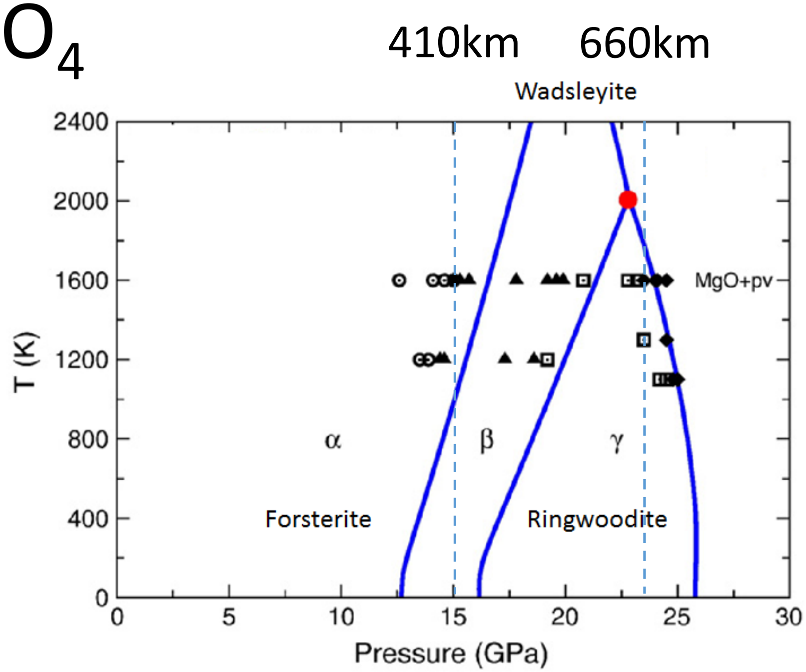
Bridgmanite + Periclase

$MgSiO_3$ ($CaSiO_3$ also similar)



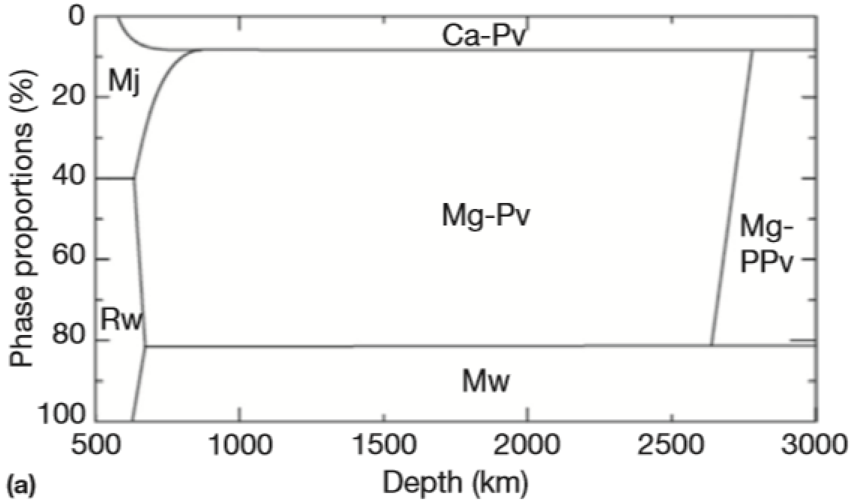


Mg_2SiO_4

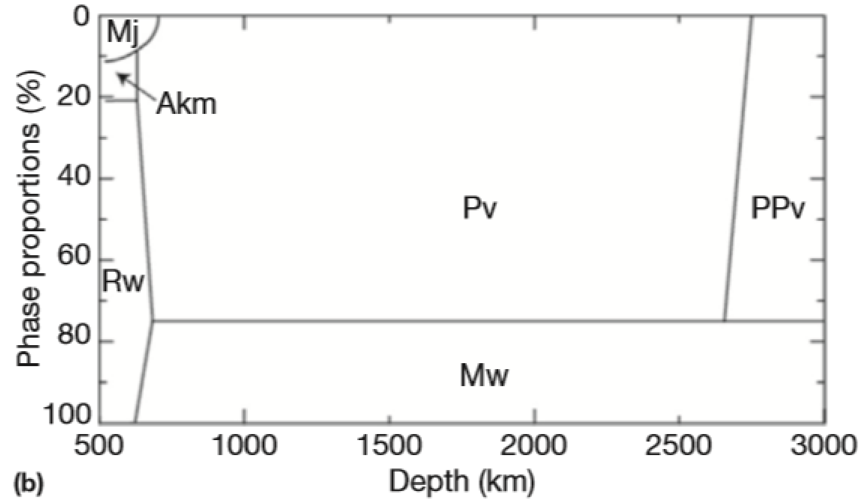


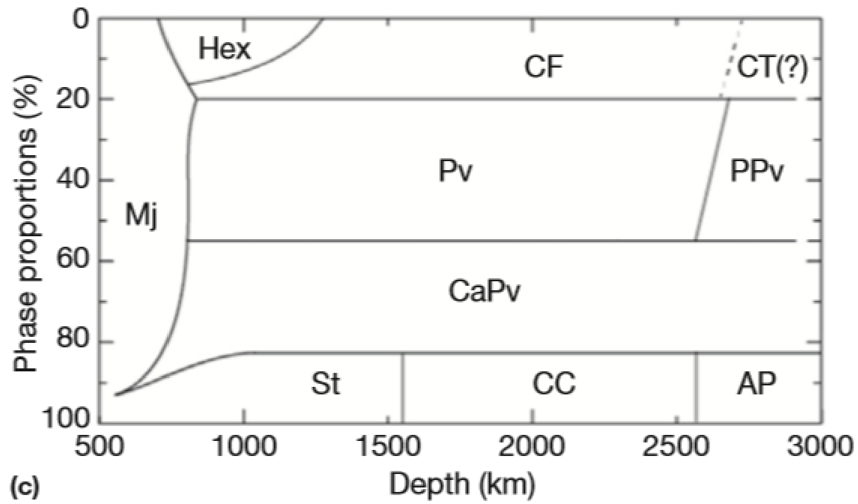
Representative lithology in the lower mantle condition

Pyrolite (olivine rich)



Harzburgite





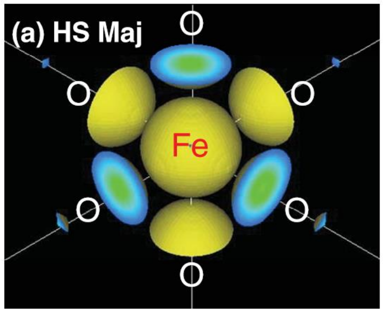
MORB (silica rich)

- Phase diagrams of major silicate and oxide phases are now almost clarified in the Earth's mantle *P*,*T*.
- Lithology is still under debate.

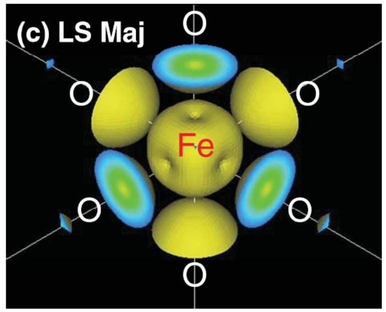
Irifune & Tsuchiya (07) Treatise on Geophysics

Spin crossover in Fe-bearing solid solution

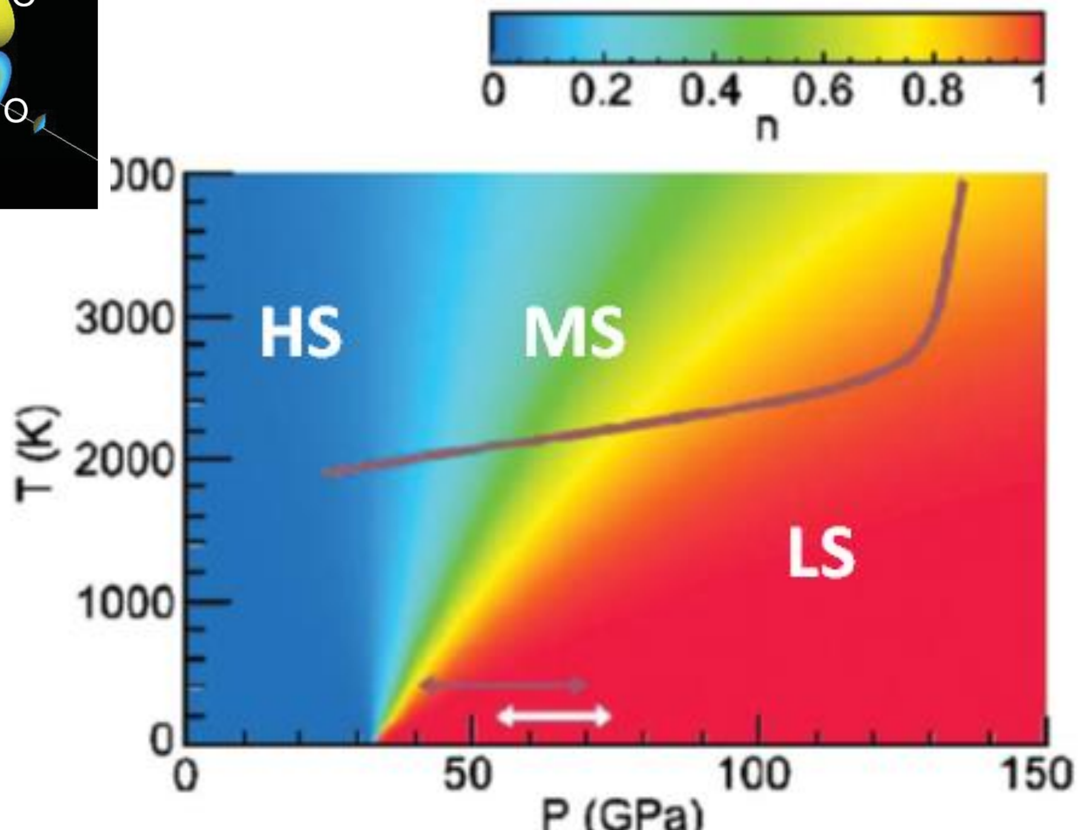
(Mg,Fe)O Ferropericlase



High-spin
(S=2)



Low-spin
(S=0)

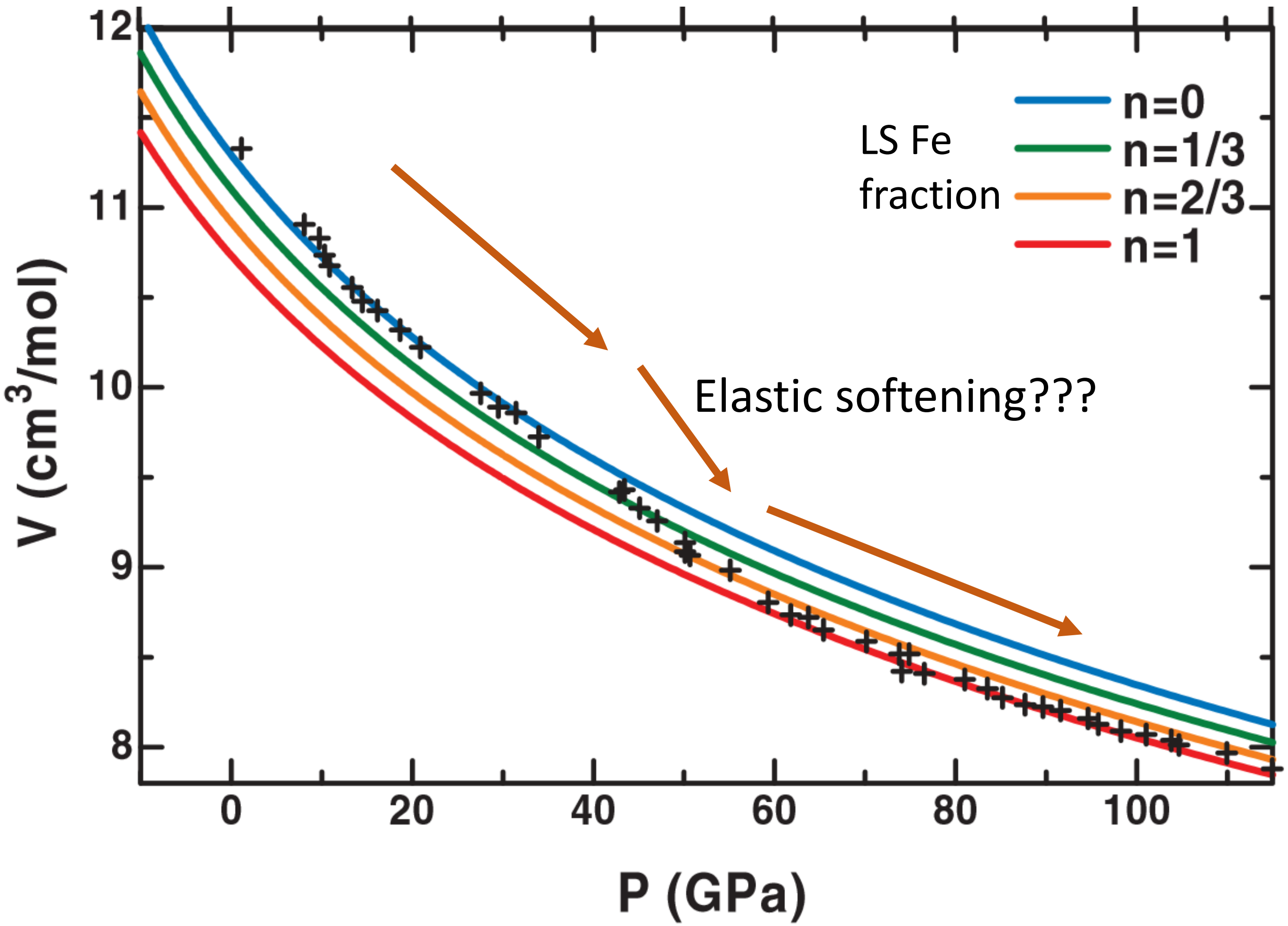


Spin transition

- Decrease volume
- Decrease elastic wave velocity(?)
- Reduce thermal conductivity(?)

Tsuchiya+ (06) Phys Rev Lett
Lin+ (07) Science

Compression across a spin transition

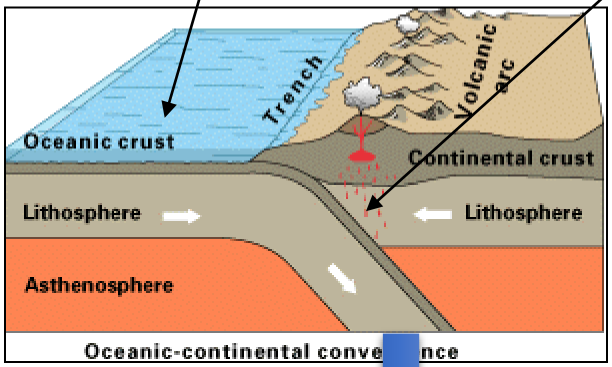


A spin transition affects seismic wave speeds and it is seismologically detectable?

Dense Hydrous Magnesium Silicate (DHMS) phases

Hydration of oceanic crust

Serpentinization of olivine (antigorite)



H_2O in DHMS

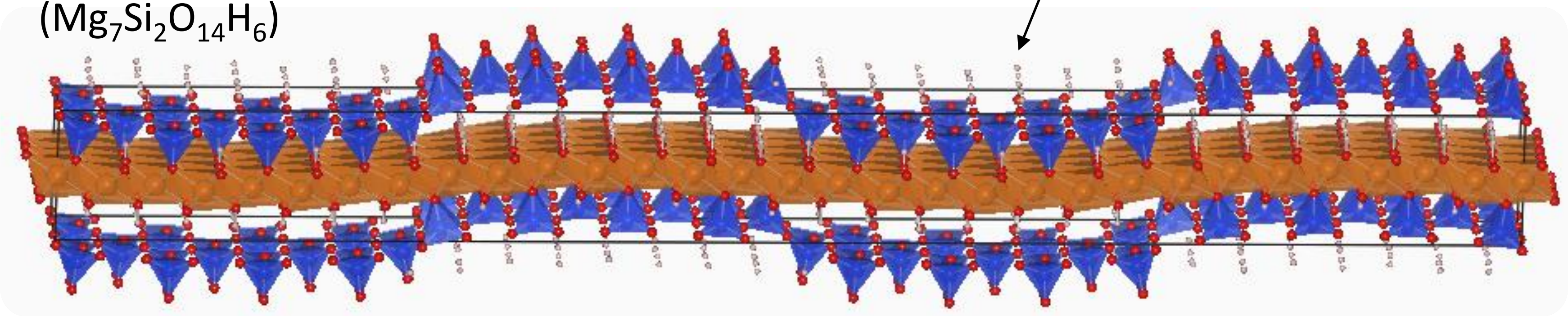
Water (volatile components)

- Reduce melting temperature (magmatism)
- Reduce yield strength and viscosity (seismicity)
- How much and where are still unclear.

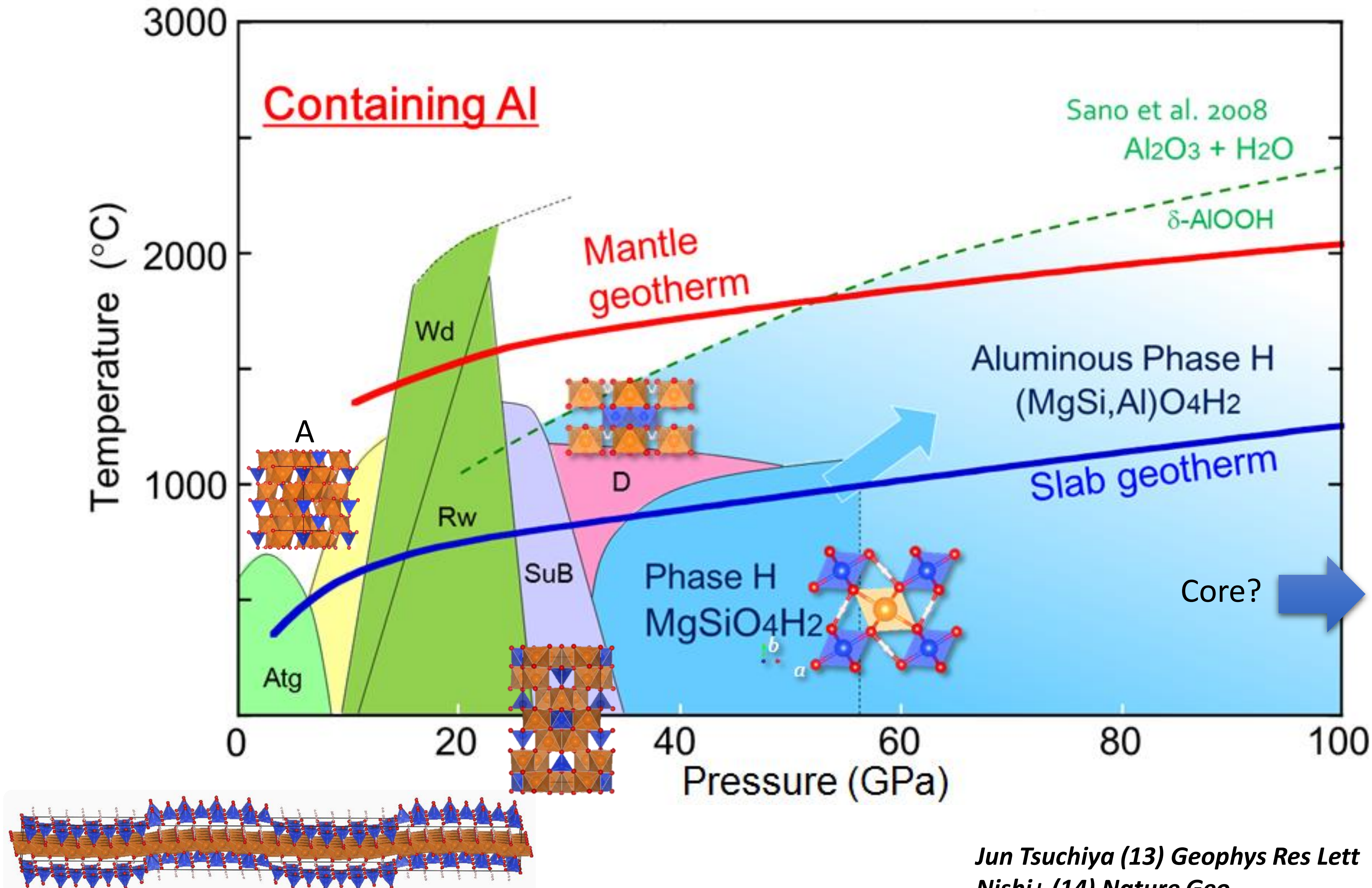
Hydrous minerals have totally different phase relations.

Serpentine ($Mg_7Si_2O_{14}H_6$)

OH



Dense Hydrous Magnesium Silicate (DHMS) phases



Jun Tsuchiya (13) Geophys Res Lett
Nishi+ (14) Nature Geo

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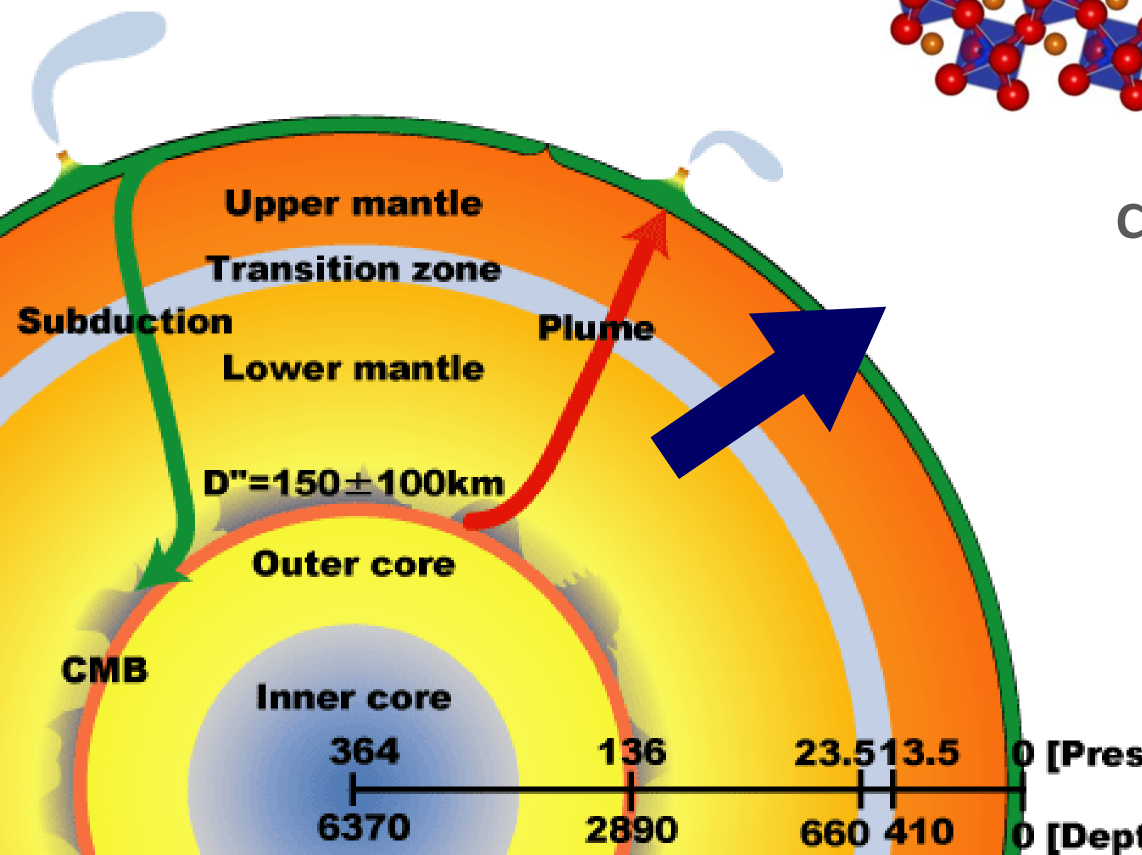
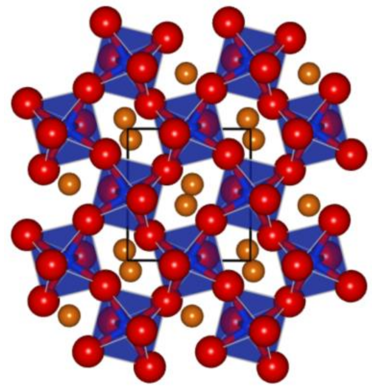
Earth's lower mantle

- *More than 50% of Earth's entire volume*
- *Chemical composition still under debate*

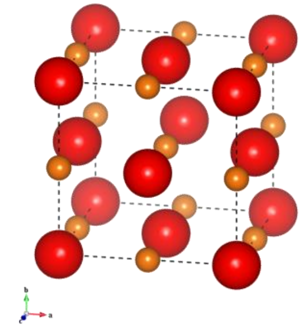


$Fe^{2+,3+}$-bearing $MgSiO_3$
Bridgmanite

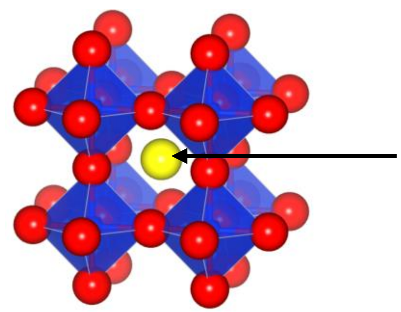


+

Fe^{2+}-bearing MgO
Ferropericlase



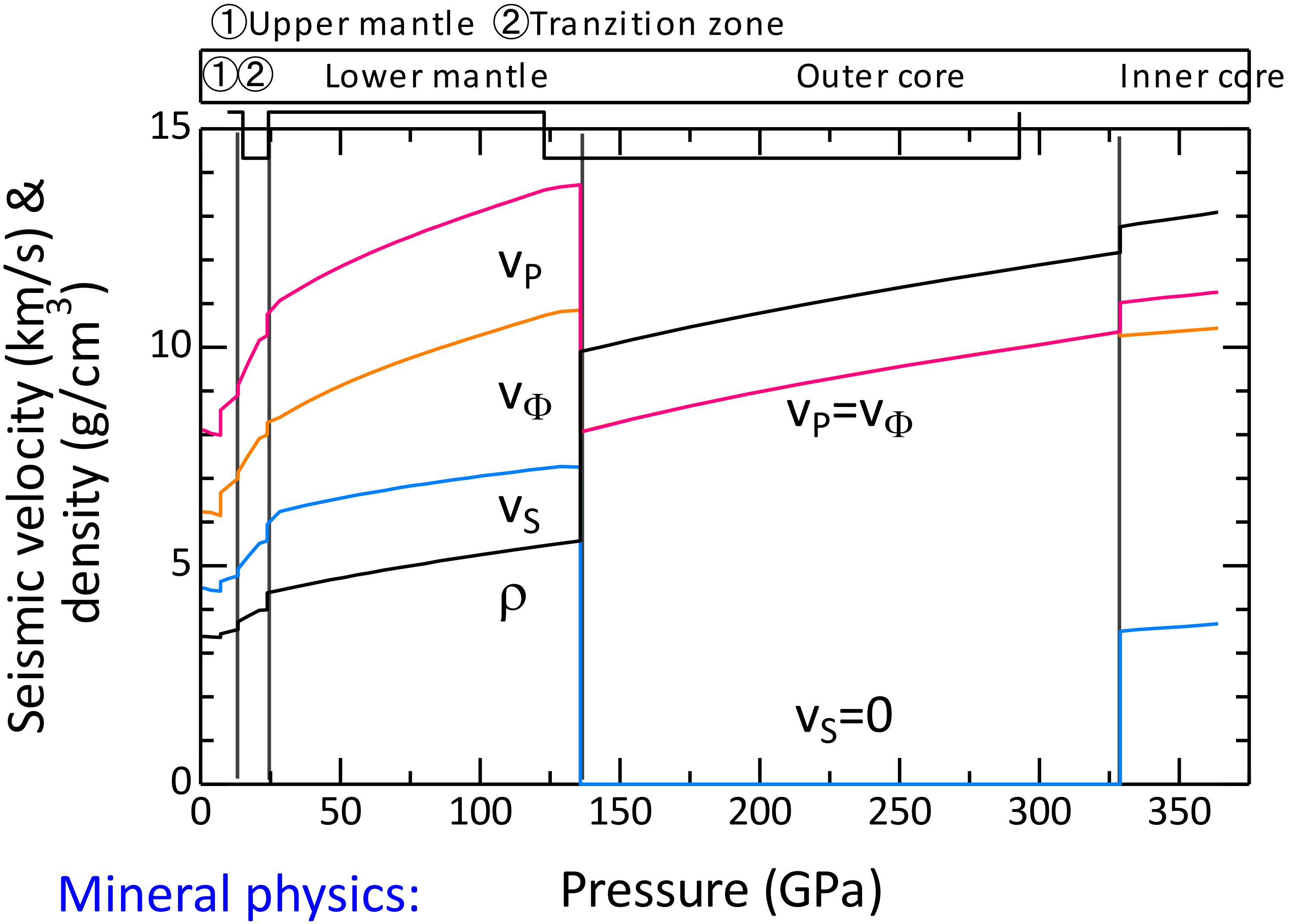
$CaSiO_3$ Perovskite
(minor, ~5%)



Ca
(potential host of large cations, U, Th)

Seismological reference model

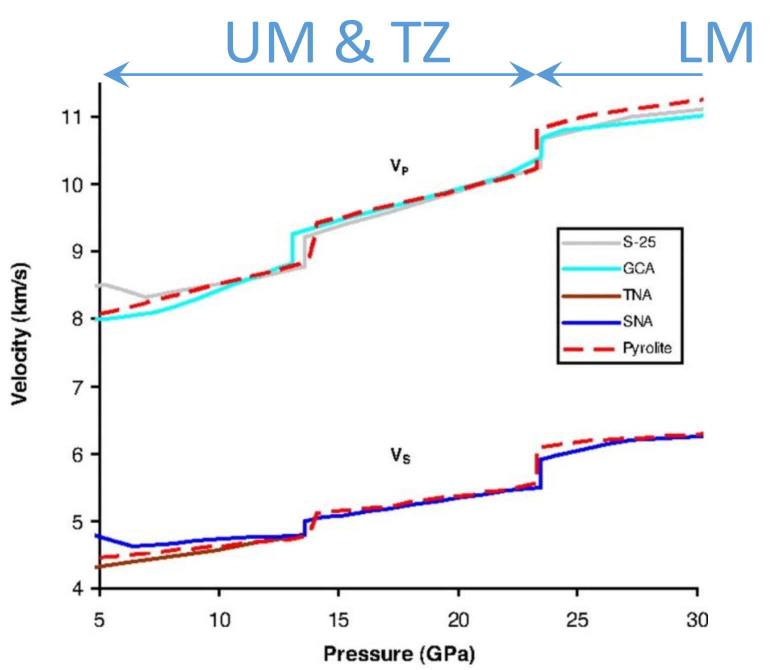
PREM (*Dziewonski & Anderson 81*)



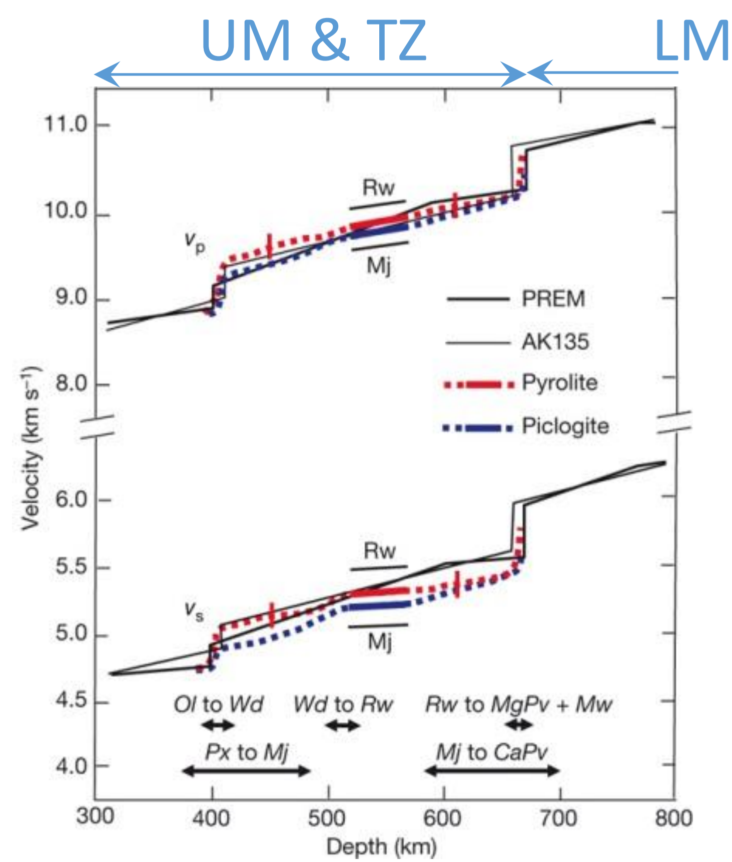
Mineral physics:

Search for lithology which can reproduce these references

Mineralogical model of the upper mantle



Li & Leibermann (07)



Irifune+ (08)

- UM = Pyrolitic
- **LM … measurement still difficult**

Mineralogical model of the lower mantle

◆Chondrite (0.95Pv + 0.05Fp) SiO_2-rich

Vs only measured by DAC + Brillouin scattering at limited *P*,*T*

Murakami+ (12) Nature

◆Pyrolite (0.65Pv + 0.35Fp in mole)

Density only measured by multianvil press just at the top of the LM *P*,*T*

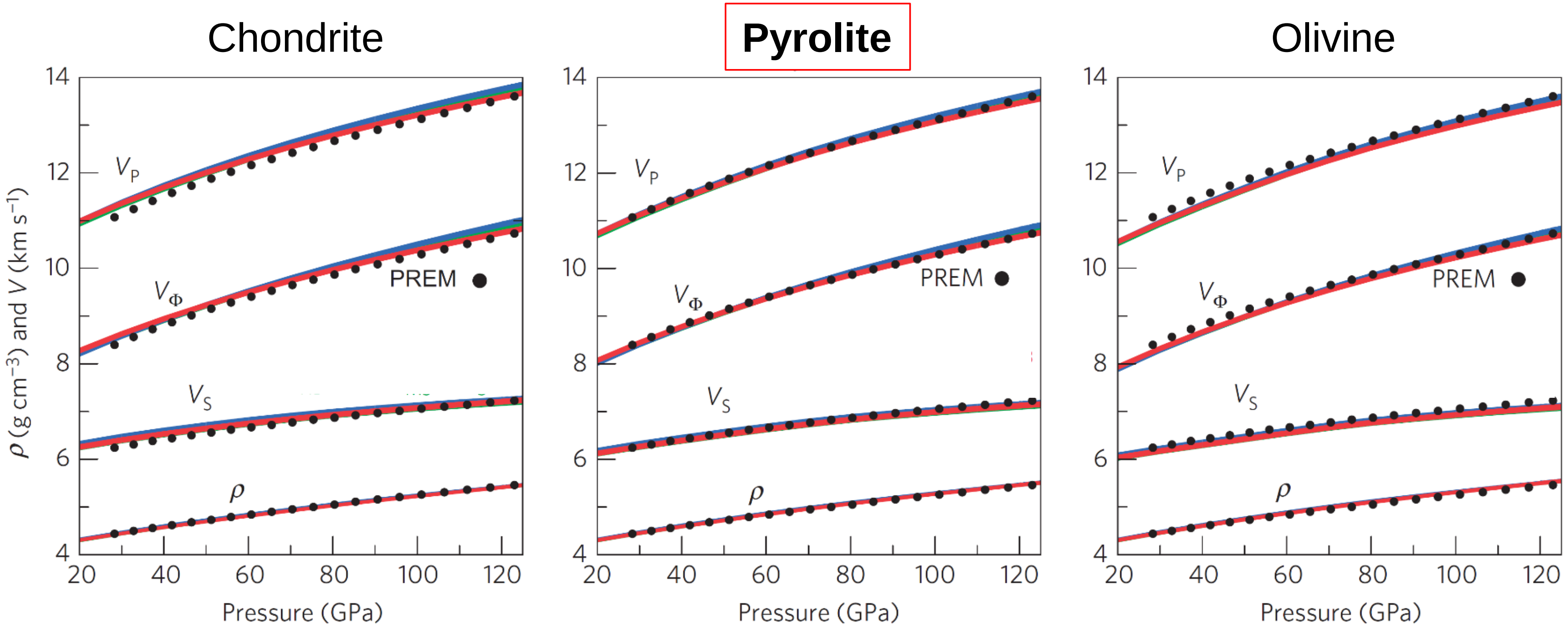
Irifune+ (10) Science

◆Olivine (0.5Pv + 0.5Fp)   Mg,Fe-rich

Bulk modulus only by EoS modeling *Tange+ (12) JGR*

Simultaneous experimental measurements of V_P, V_S, and ρ in the while LM *P*,*T* still impossible

Representative lithology for the lower mantle



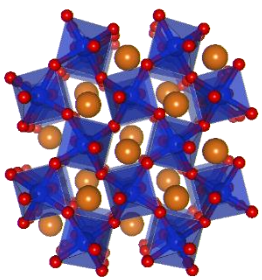
Pyrolite model agrees best with PREM in the whole LM *P* range

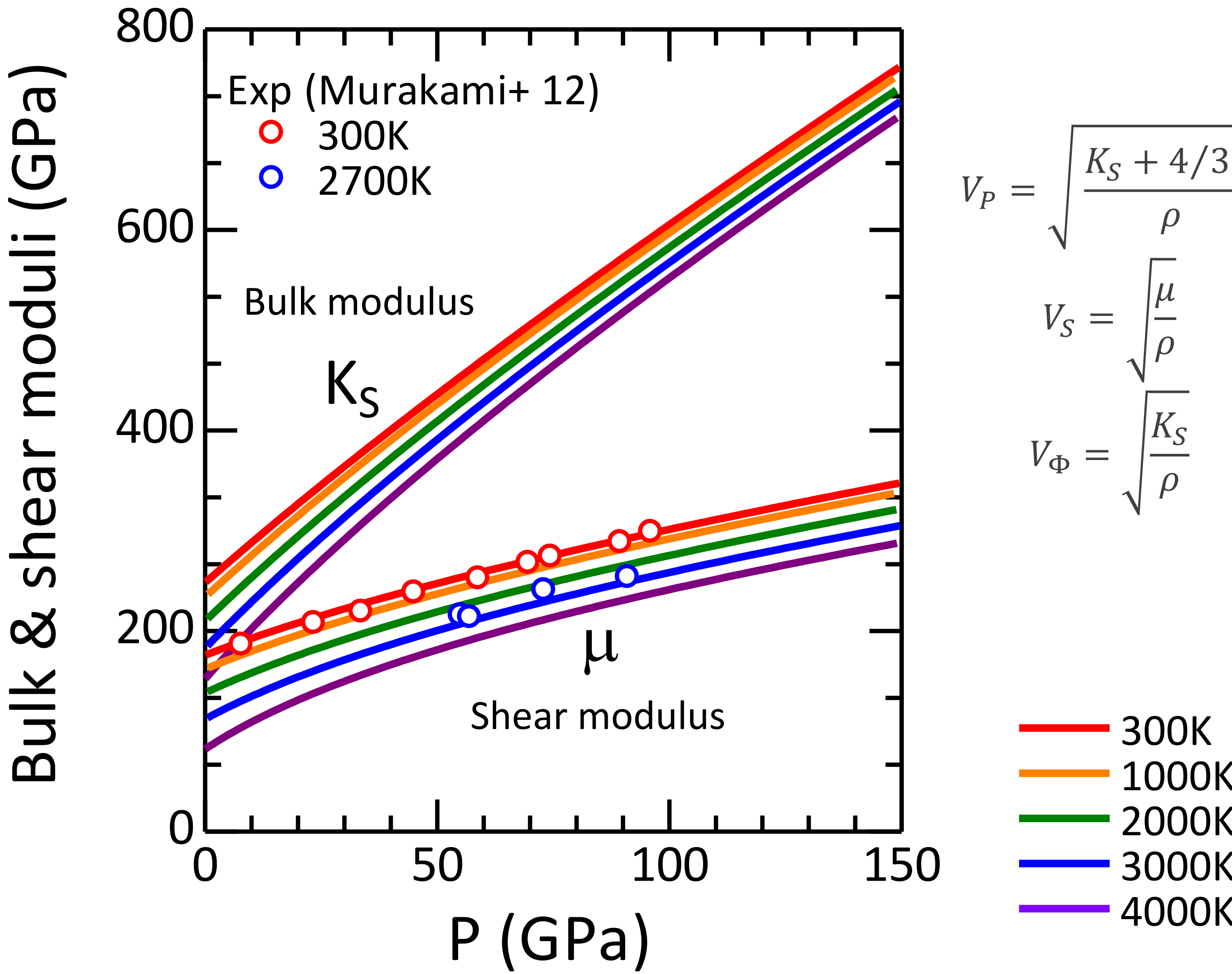
Along an adiabatic *T* profile with T_P =1600 K

Blue: Fe^{2+}-bearing
Green ： Fe^{3+}-bearing
Red ： Fe^{3+}+Al-bearing

Wang, Tsuchiya & Hase (15) Nature Geo

DFT calculations of elastic moduli ($MgSiO_3$ bridgmanite)





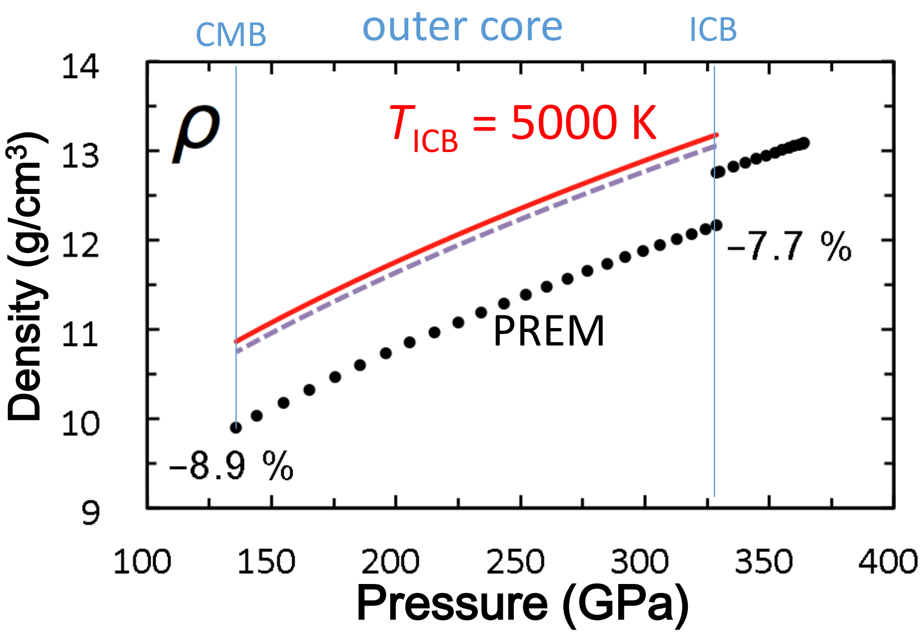
$$V_P = \sqrt{\frac{K_S + 4/3\,\mu}{\rho}}$$

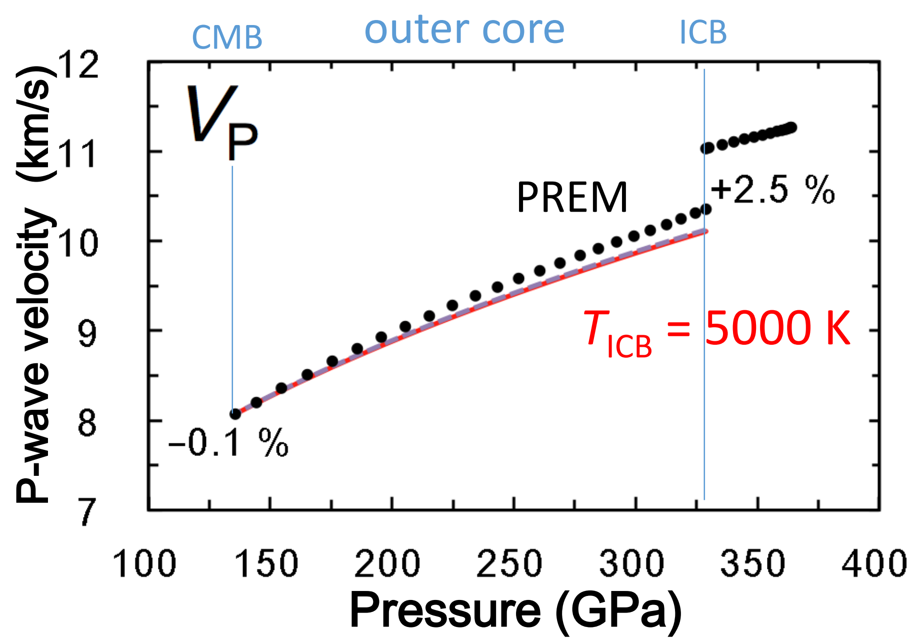
$$V_S = \sqrt{\frac{\mu}{\rho}}$$

$$V_\Phi = \sqrt{\frac{K_S}{\rho}}$$

Liquid iron alloys in the outer core

Fe-Ni + ~10 wt% light elements (O, S, Si, C, H…)   (e.g., Birch 64)



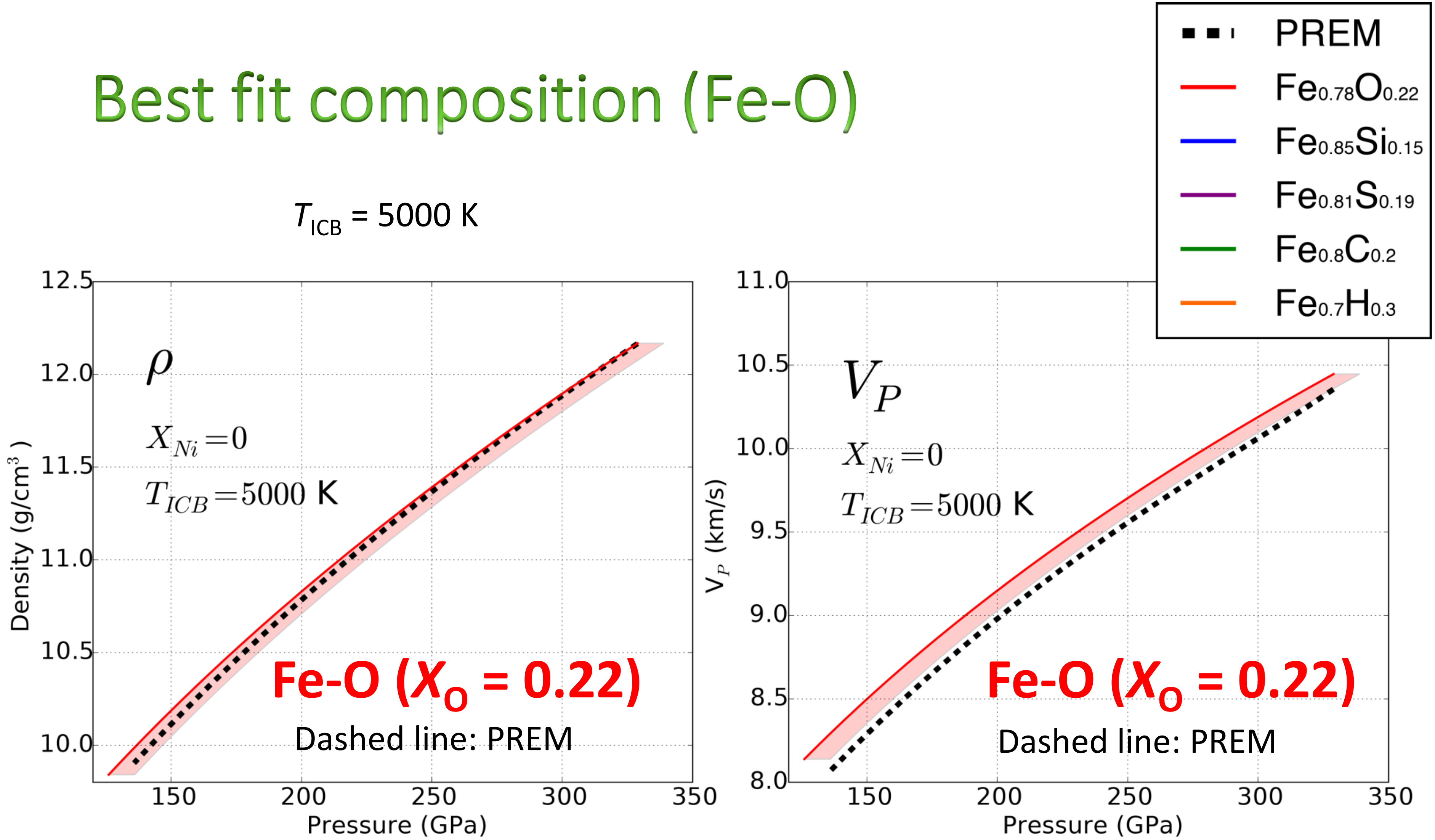


Pure Fe

- **8~9% denser than PREM**
- **Already comparable V_P**

Pozzo+ (13) PRB
Ichikawa, Tsuchiya+ (14) JGR

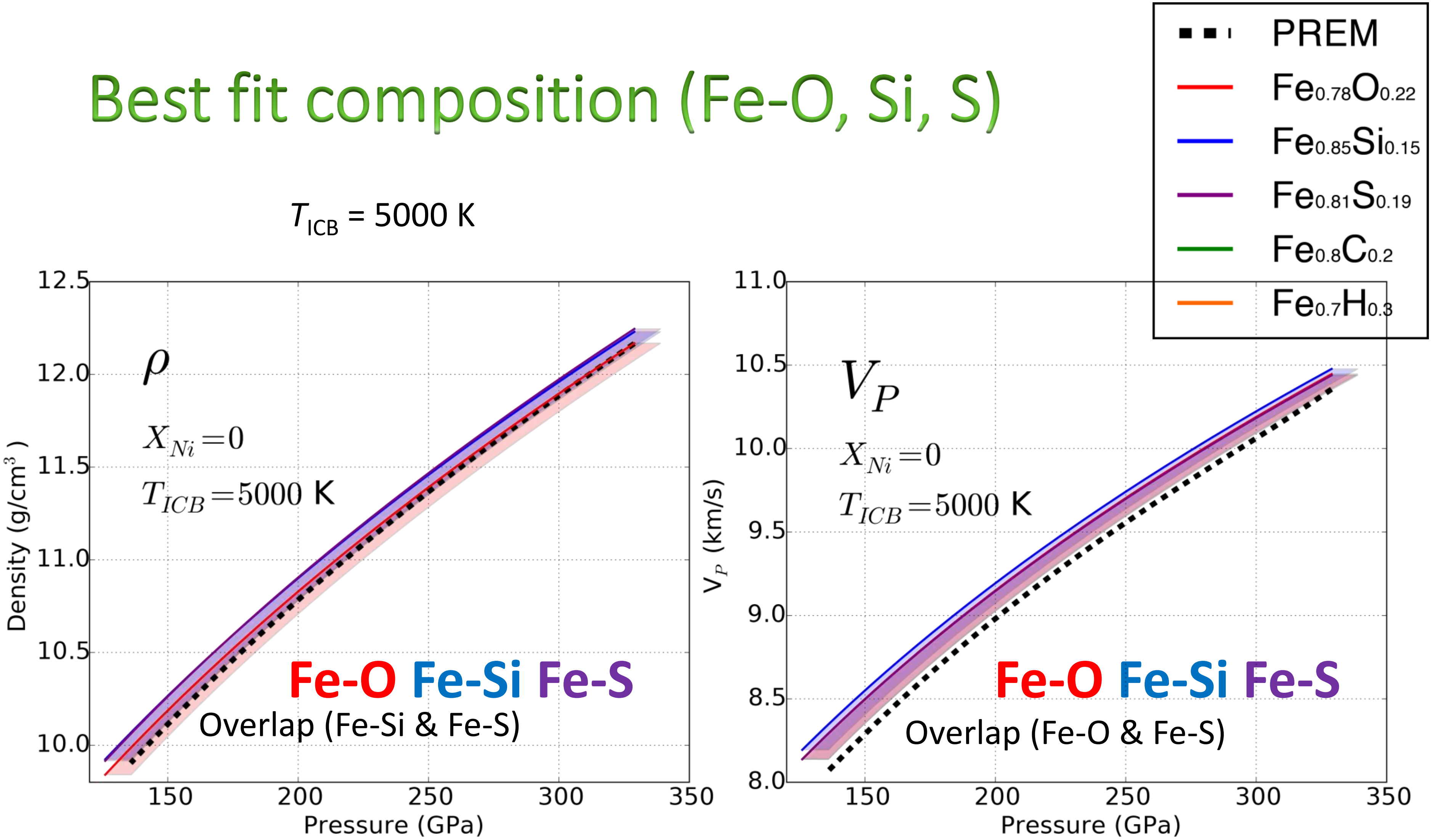
Best fit composition (Fe-O)



Ichikawa+ under review

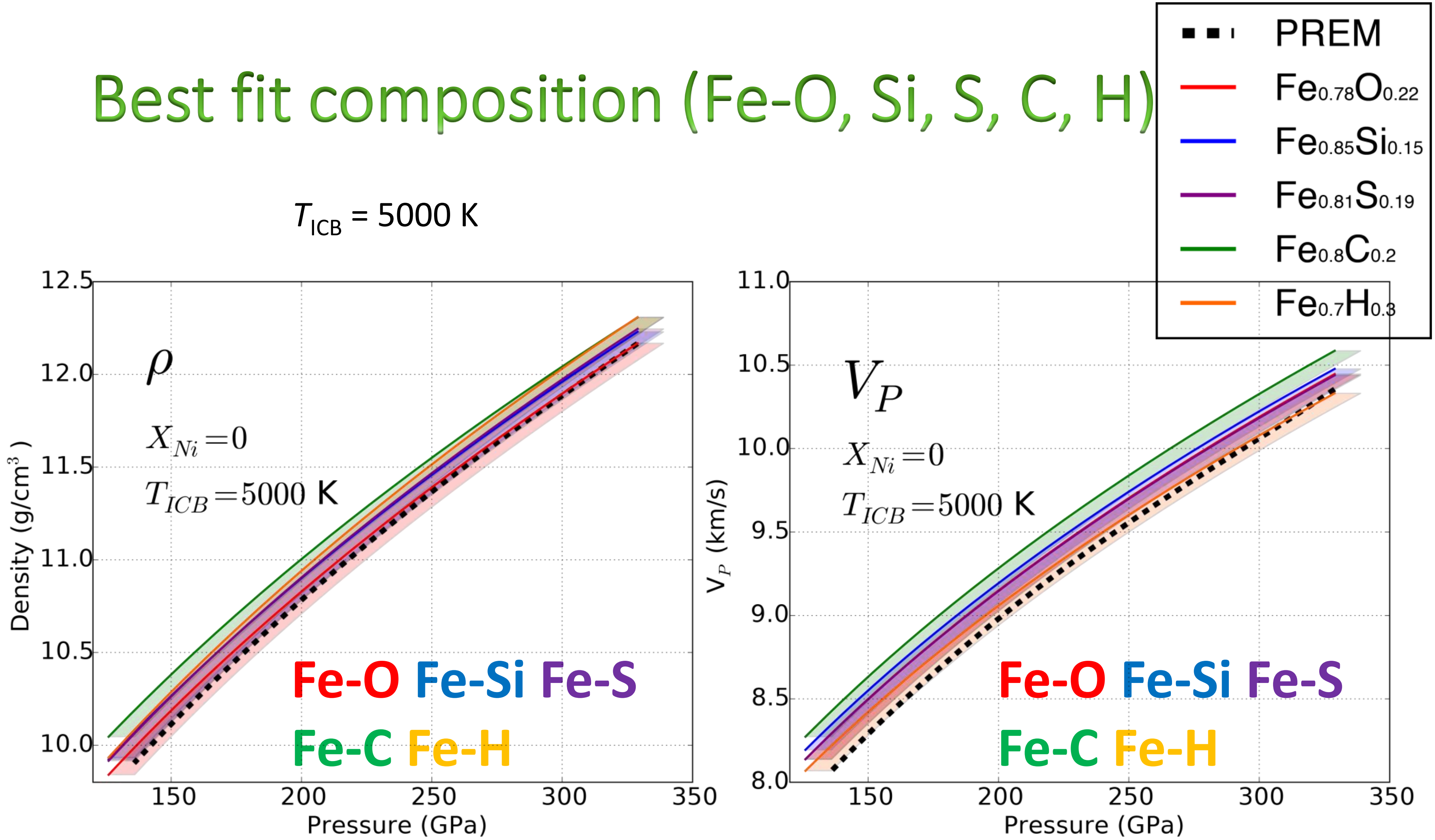
Best fit composition (Fe-O, Si, S)

T_{ICB} = 5000 K



Ichikawa+ under review

Best fit composition (Fe-O, Si, S, C, H)

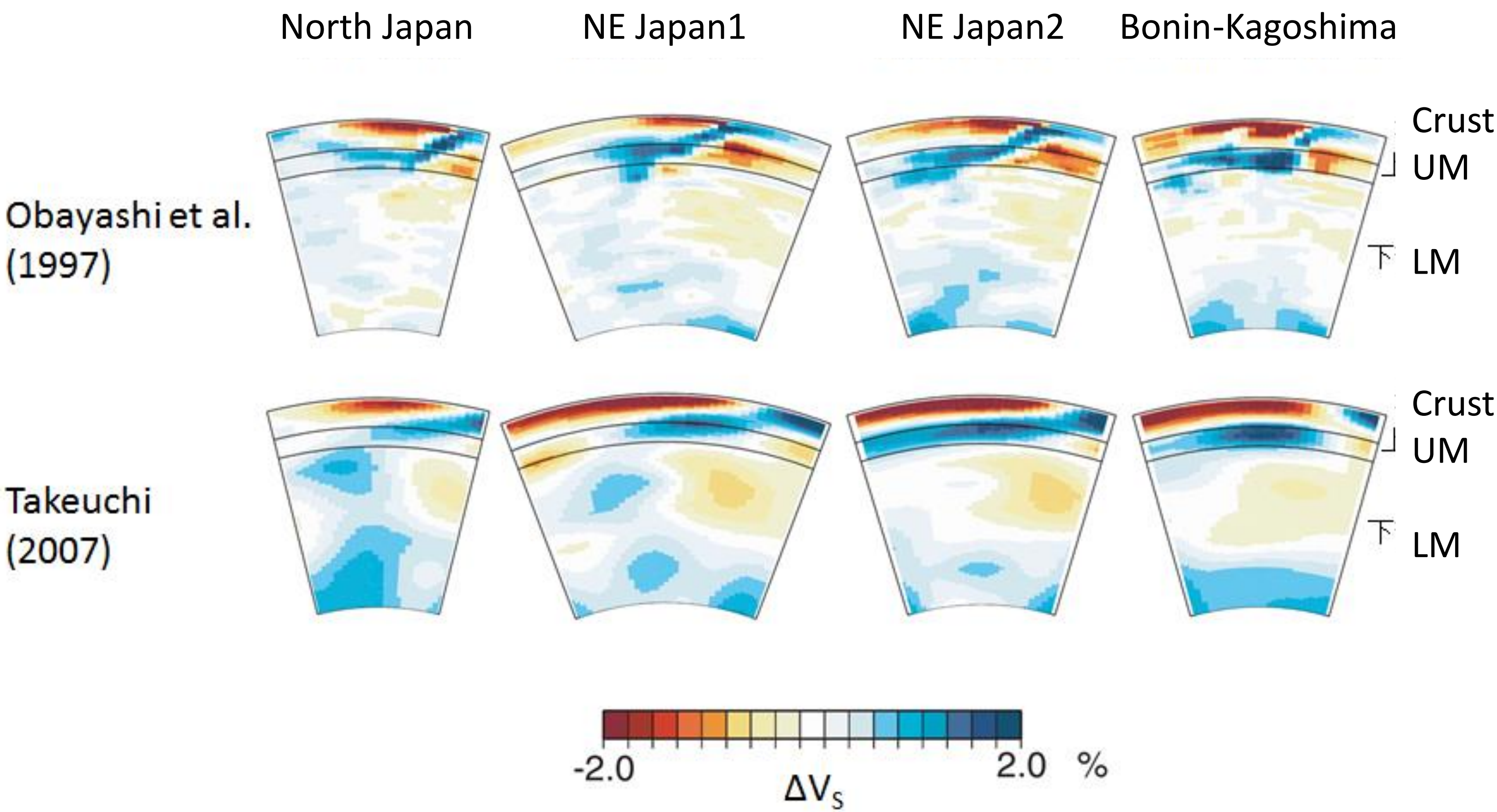


- **Fe-C only shows distinct deviation.**
- **Difficult to distinguish from each other except for Fe-C**
- **Some other independent information required for further constraint**

Ichikawa+ under review

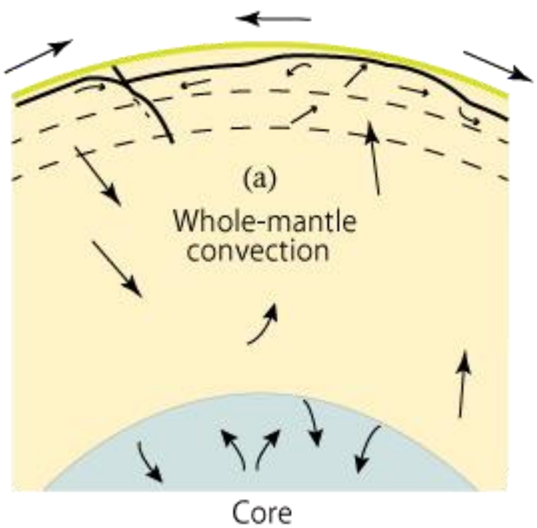
1. Basics of silicate crystallography
2. High-pressure mineralogy
3. Earth’s compositional model
4. Earth’s interior dynamics from mineral physics

Seismic tomography (3D image of seismic wave speeds)

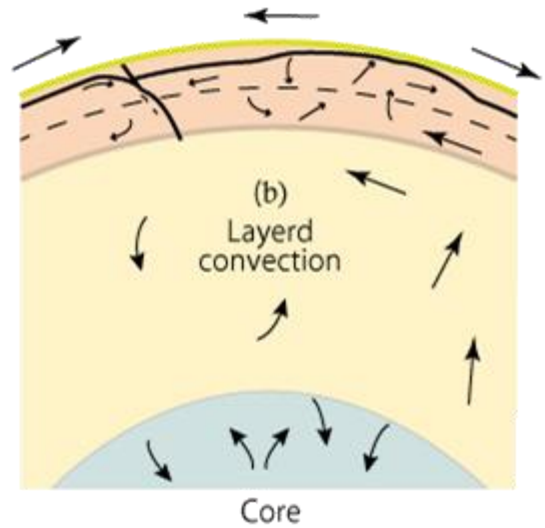


Whole mantle convection or separate convections in UM and LM?

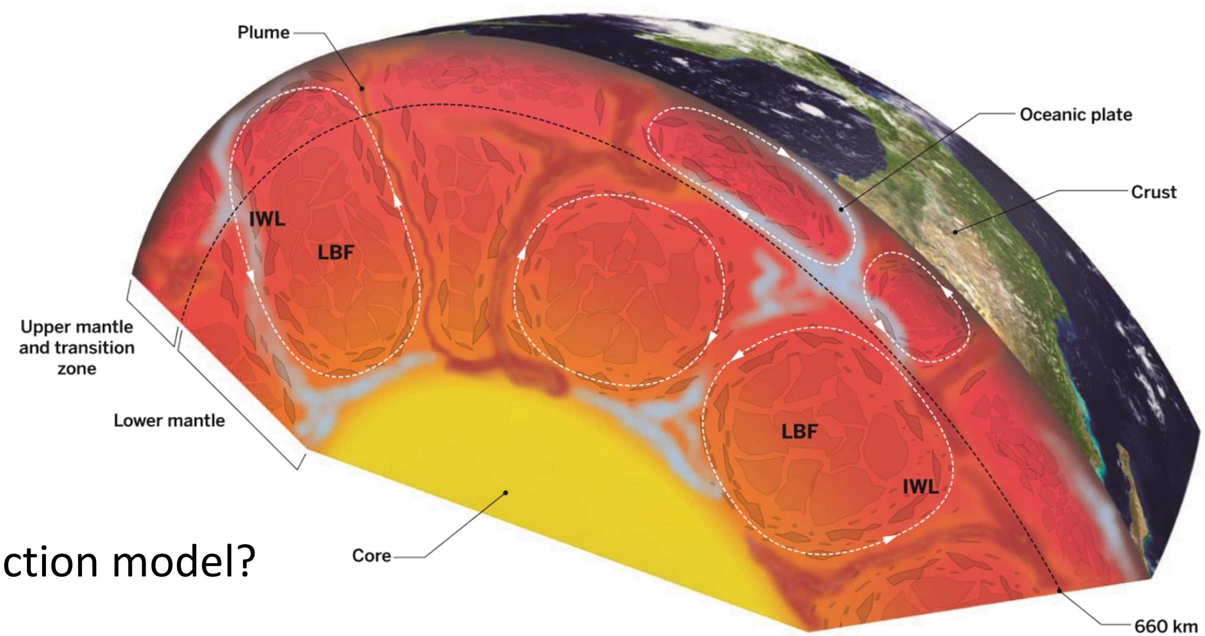
Mantle convection style



UM = LM

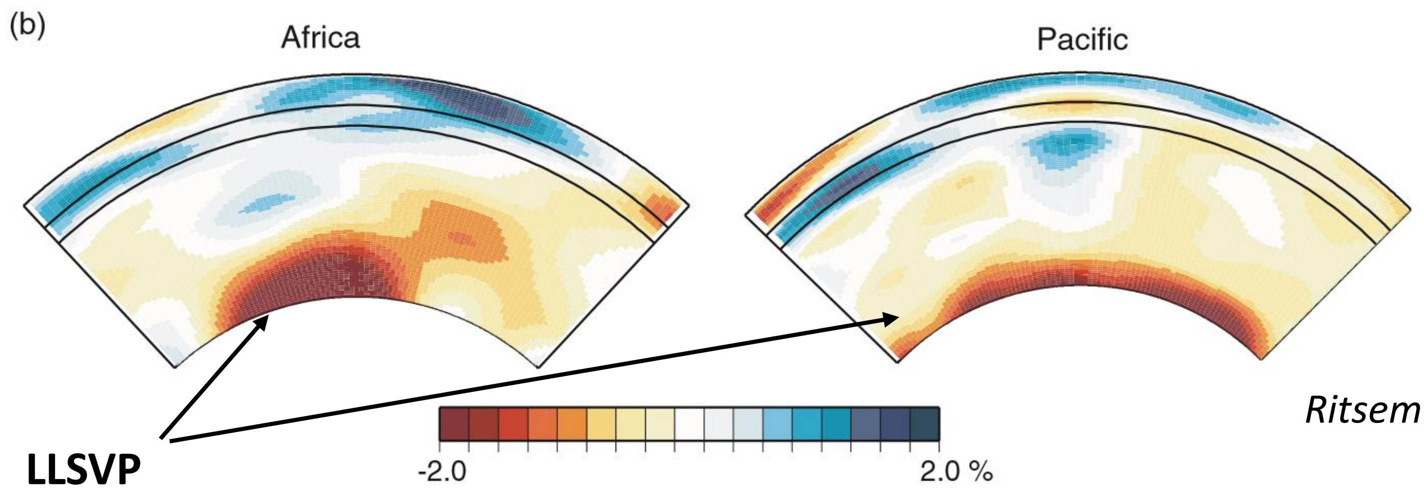


UM ≠ LM



Hybrid convection model?

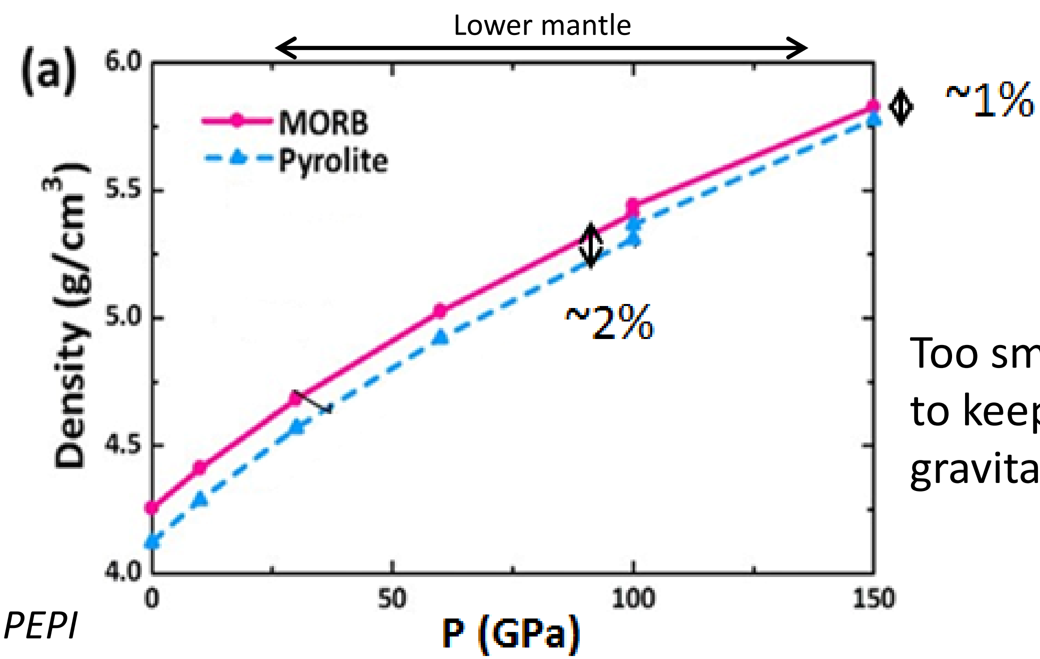
Vigorous mantle convection → Homogeneous mantle?



LLSVP
(Large Low S Velocity Province)

Ritsema (97) JGR
(98) GRL
Takeuchi (08) GRL
etc

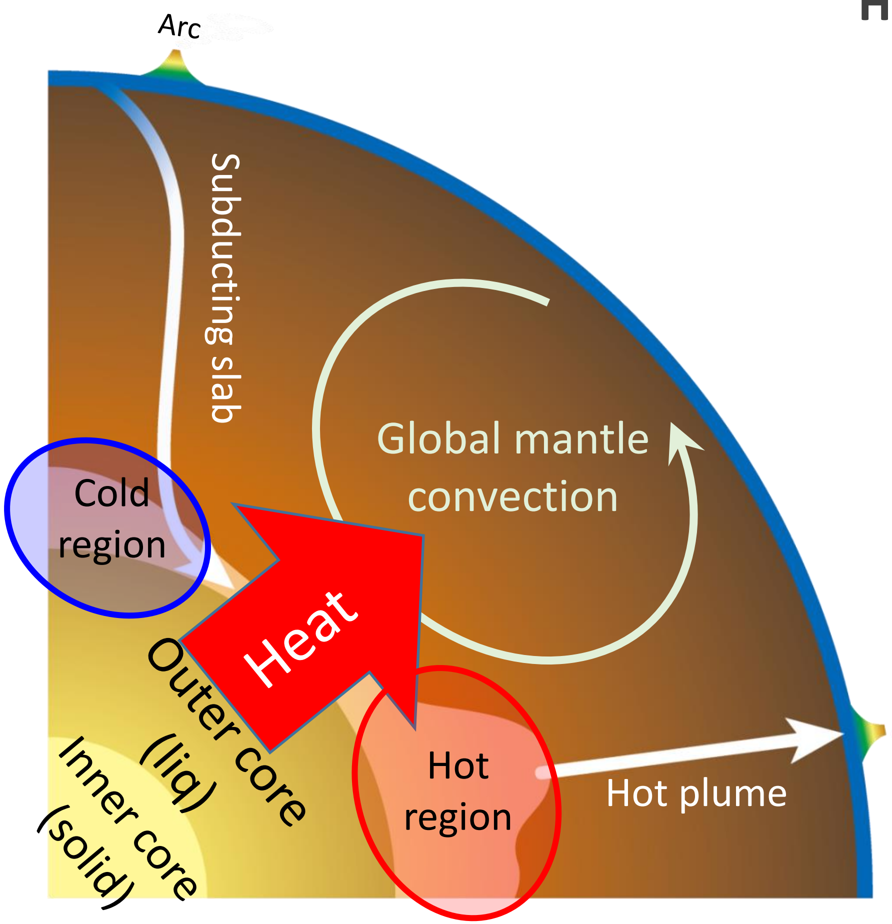
- Chemically distinct dense layer?
- Slab graveyard?
- Remnant of basal magma ocean?
- K, U, Th reservoir?



Too small excess density to keep a long-term gravitational stability

Tsuchiya (11) PEPI

Core-mantle boundary heat flow (J_{CMB})



- Mantle convection strength
- Core cooling rate

Heat flow

$$J_{\mathrm{CMB}} = \int \kappa_{\mathrm{TBL}} \frac{\Delta T_{\mathrm{TBL}}}{d_{\mathrm{TBL}}} dS$$

Thermal boundary layer

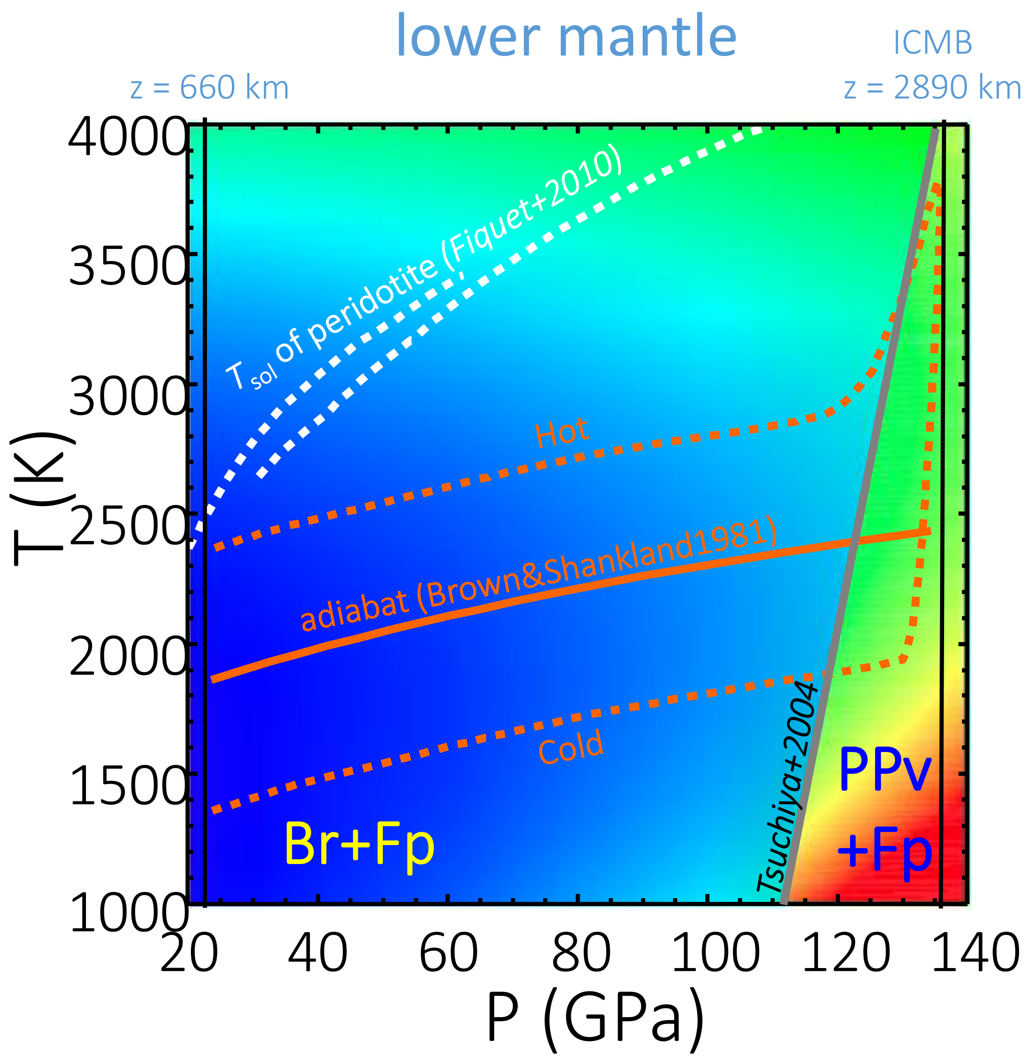
$$\Delta T_{\mathrm{TBL}} \sim 1300 \text{ K}$$
$$d_{\mathrm{TBL}} \sim 100 - 300 \text{ km}$$

Lattice thermal conductivity

$$\kappa_{\mathrm{lat}} = \frac{1}{3} \sum_{s}^{3n} \int \mathbf{v}_{\mathbf{q},s}^{2} c_{\mathbf{q},s} \tau_{\mathbf{q},s} d\mathbf{q}$$

Anharmonic lattice dynamics theory: Phonon group velocity, Mode heat capacity, Phonon lifetime

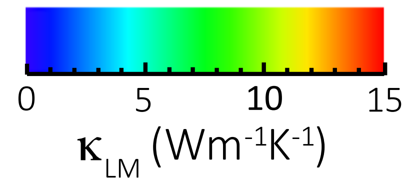
Thermal conductivity of the lower mantle



$\Rightarrow \quad J_{\mathrm{CMB}} \sim 3 - 6\ \mathrm{TW}$

Dekura, Tsuchiya+ (13) Phys Rev Lett

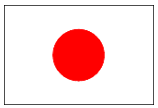
- ~10% of surface heat flow
- Substantial internal heating
- Enough to sustain geodynamo
- Leading to an inner core age of ~2.5 Ga



CMB heat flow can also be guessed from the core side, but
two latest DAC experiments on the core conductivity are ***totally incompatible!***

LETTER

doi:10.1038/nature17957



Experimental determination of the electrical resistivity of iron at Earth's core conditions

Kenji Ohta[1], Yasuhiro Kuwayama[2], Kei Hirose[3,4], Katsuya Shimizu[5] & Yasuo Ohishi[6]

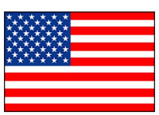
Vol. 534, p. 95-98 (2016)

About 3 times higher than previous estimates

- leading to a younger IC age ~1.2 Ga
- additional heat source required to maintain geodynamo

LETTER

doi:10.1038/nature18009



Direct measurement of thermal conductivity in solid iron at planetary core conditions

Zuzana Konôpková[1]†, R. Stewart McWilliams[2], Natalia Gómez-Pérez[2,3] & Alexander F. Goncharov[4,5]

Vol. 534, p. 99-101 (2016)

Close to the previous estimates

- leading to an older IC age ~4.2 Ga

Mineral

Mineral is a naturally occurring substance, representable by a chemical formula, that is usually solid and inorganic, and has a crystal structure.

It is different from a rock, which is an aggregate of minerals or non-minerals and does not have a specific chemical composition.

The scientific study of minerals is called mineralogy, which is an essential component of geology.

Rock

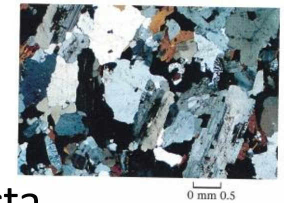
Rock or stone is a naturally occurring solid aggregate of one or more minerals. For example, the common rock granite is a combination of quartz, feldspar and biotite.

Three major groups of rocks are defined: igneous, sedimentary, and metamorphic. The scientific study of rocks is called petrology.

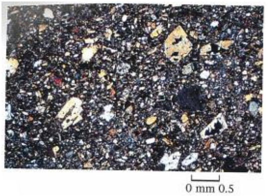
Igneous rocks

They form through the cooling and solidification of magma or lava. This magma can be derived from partial melts of pre-existing rocks in either a planet's mantle or crust.

Plutonic rocks
They result when magma cools and crystallizes slowly within the Earth's crust. A common example is granite.



Volcanic rocks
They result from magma reaching the surface either as lava or fragmental ejecta, forming minerals such as pumice or basalt.



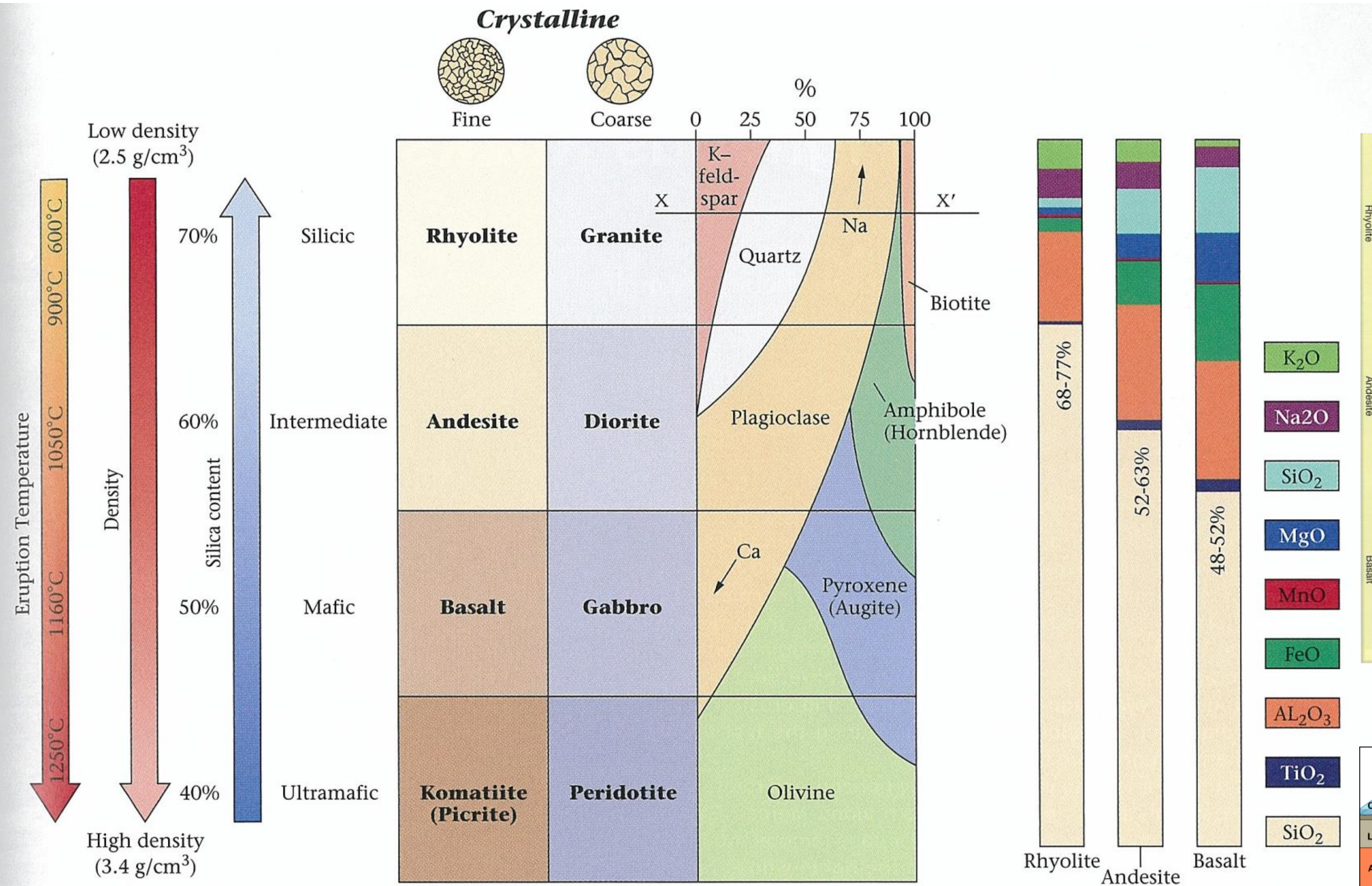
Sedimentary rocks

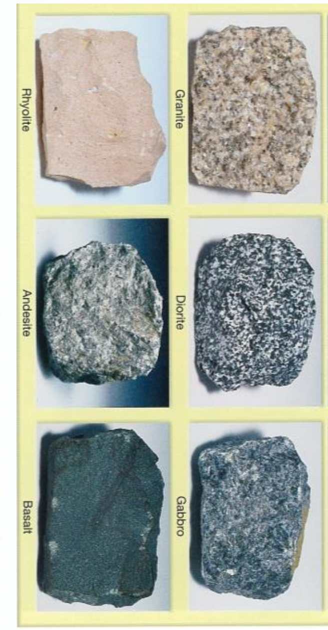
They are types of rock that are formed by the deposition and subsequent cementation of that material at the Earth's surface and within bodies of water.

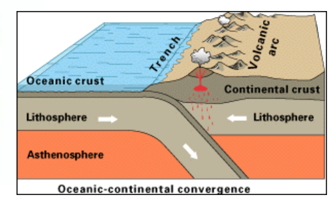
Metamorphic rocks

They arise from the transformation of existing rock types, in a process called metamorphism, by heat and/or pressure.

Classification of igneous rocks







Felsic (white, less dense) ⇔ Mafic (black, denser) ⇔ Ultramafic

Upper continental crust **Oceanic crust** **Upper mantle**

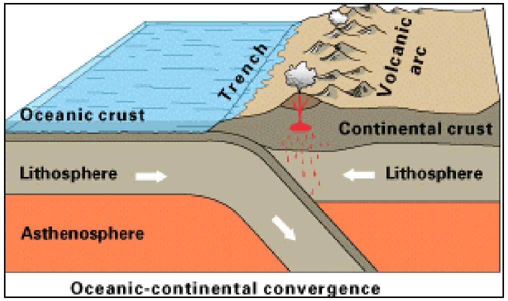
~2.7 g/cm^3 **~2.9 g/cm^3** **~3.3 g/cm^3**

Continental crust (felsic)

The continental crust is the layer of igneous, sedimentary, and metamorphic rocks that forms the continents and the areas of shallow seabed close to their shores, known as continental shelves.

The upper part consists of felsic rocks such as granite, while the lower part consists of mafic rocks such as gabbro.

The average density of the continental crust is about 2.7 g/cm^3.



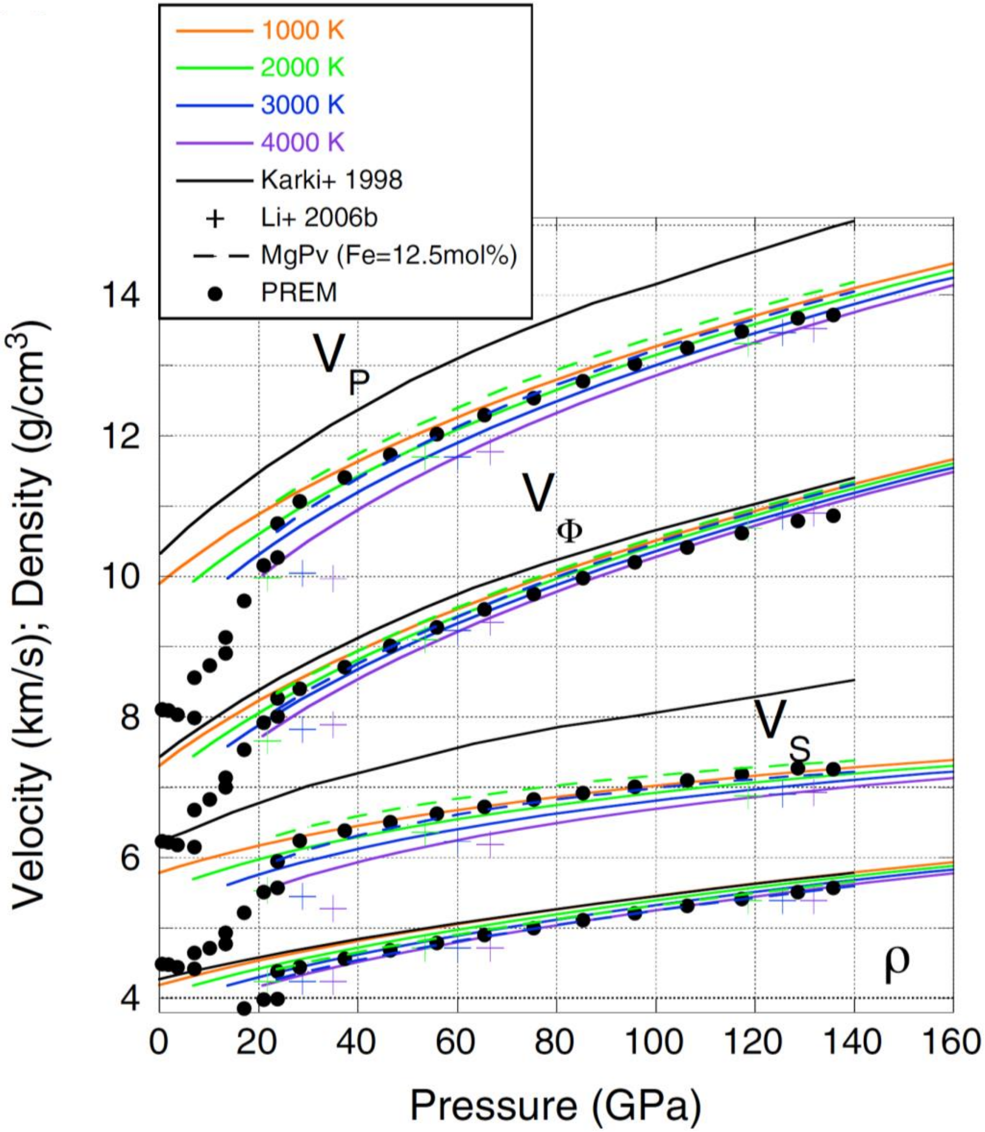
Oceanic crust (mafic)

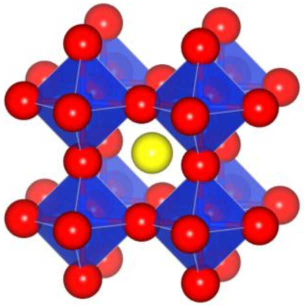
Oceanic crust is the uppermost layer of the oceanic plate. The crust overlies the uppermost layer of the mantle.

Oceanic crust is the result of erupted mantle material originating from below the plate. This occurs mostly at mid-ocean ridges, but also at scattered hotspots, and also in rare but powerful occurrences known as flood basalt eruptions. It is primarily composed of mafic rocks such as basalt.

The average density of the continental crust is about 2.9 g/cm^3.

$CaSiO_3$-perovskite, possible U, Th host phase



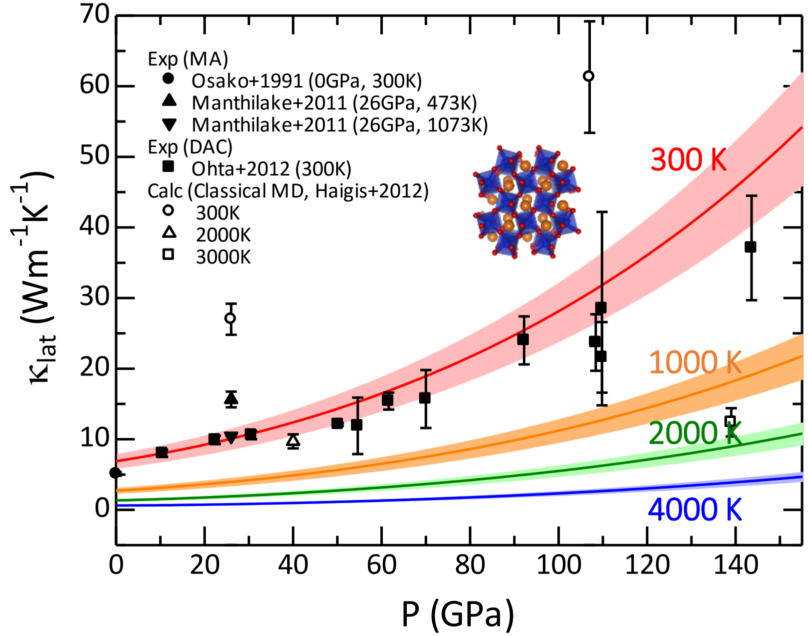


- Quite comparable to the PREM values
- Indicating Ca-Pv is seismologically invisible

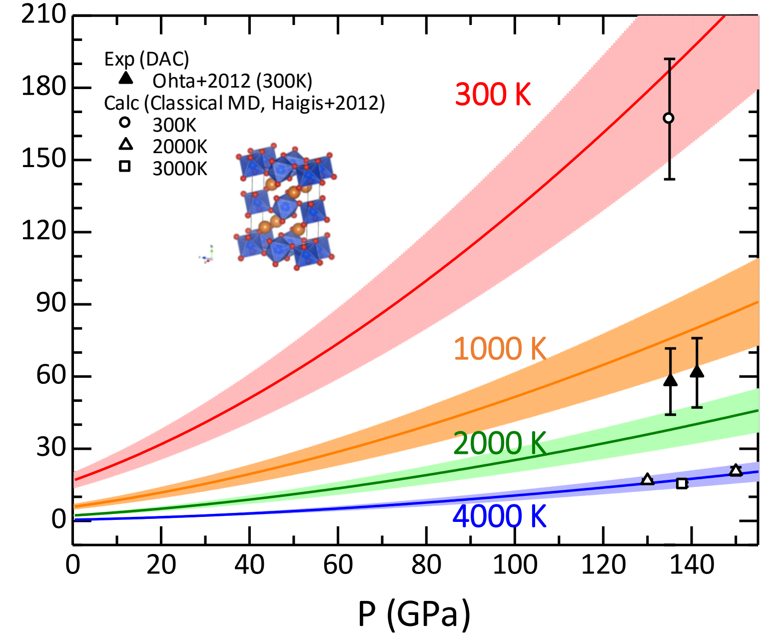
Kawai & Tsuchiya (2015) GRL

Lattice thermal conductivity

MgBr



MgPPv



Dekura, Tsuchiya, Tsuchiya (13) Phys Rev Lett