地震与地球内部物理实验室

Laboratory of Seismology and Physics of Earth's Interior

Constraining the water content at the top of the mantle transition zone with the elasticity of wadsleyite and olivine

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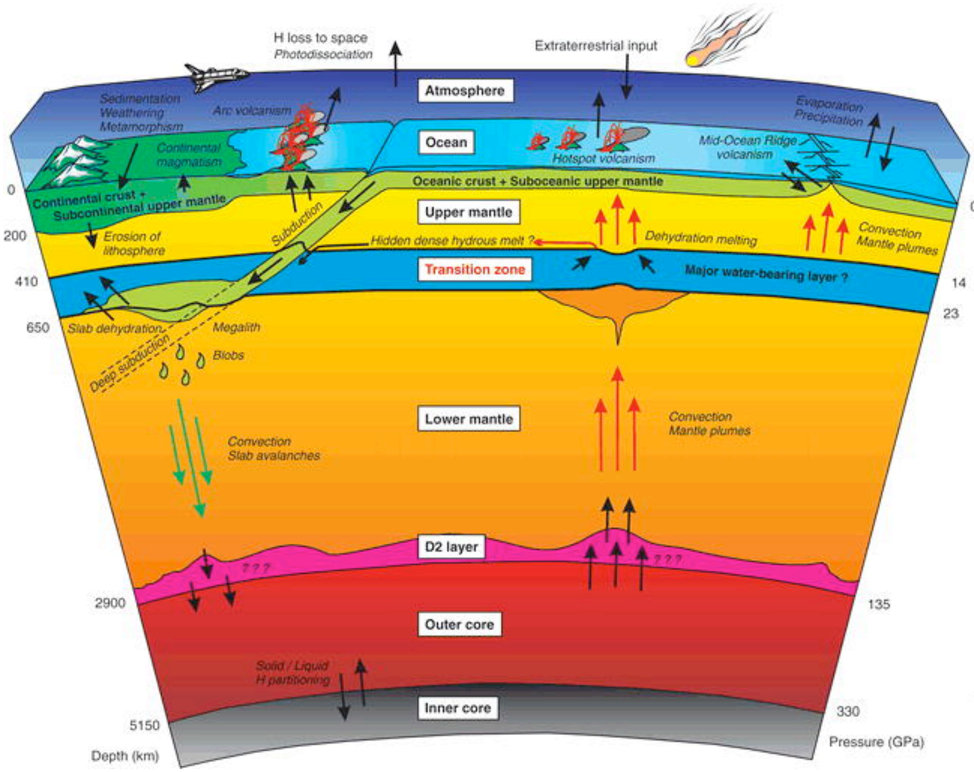
EGU 2020 Vienna

N S F C

先导专项

Deep Water Cycle



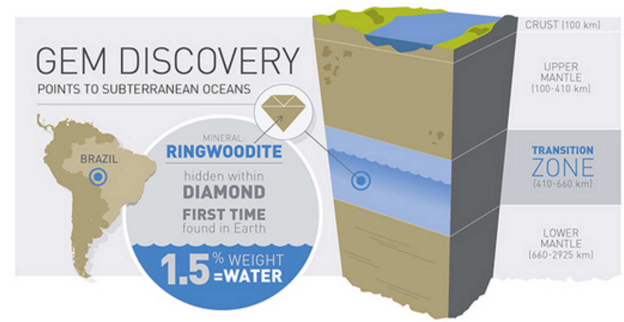
RESEARCH

GEOCHEMISTRY

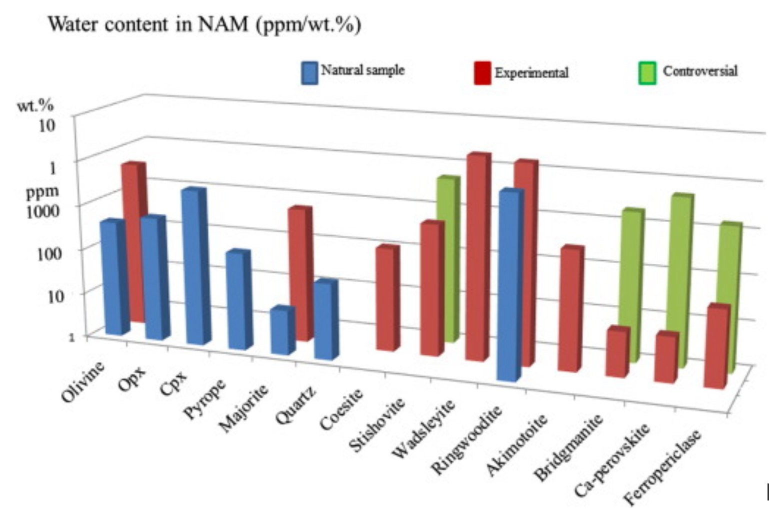
Tschauner et al., 2018 Nature

Ice-VII inclusions in diamonds: Evidence for aqueous fluid in Earth's deep mantle

O. Tschauner,[1*] S. Huang,[1] E. Greenberg,[2] V. B. Prakapenka,[2] C. Ma,[3] G. R. Rossman,[3] A. H. Shen,[4] D. Zhang,[2,5] M. Newville,[2] A. Lanzirotti,[2] K. Tait[6]



(Pearson et al., 2014 Science)



Water-saturated transition zone can contains oceans worth of H_2O

Water content & electrical conductivity

Dry mantle transition zone inferred from the conductivity of wadsleyite and ringwoodite

Takashi Yoshino[1], Geeth Manthilake[1], Takuya Matsuzaki[1] & Tomoo Katsura[1]

Yoshino et al 2008 Nature

Water content in the transition zone from electrical conductivity of wadsleyite and ringwoodite

Xiaoge Huang[1,2], Yousheng Xu[2] & Shun-ichiro Karato[2]

that the water content in the mantle transition zone varies regionally, but that its value in the Pacific is estimated to be ~0.1–0.2 wt%. These values significantly exceed the estimated

Huang et al 2005 Nature

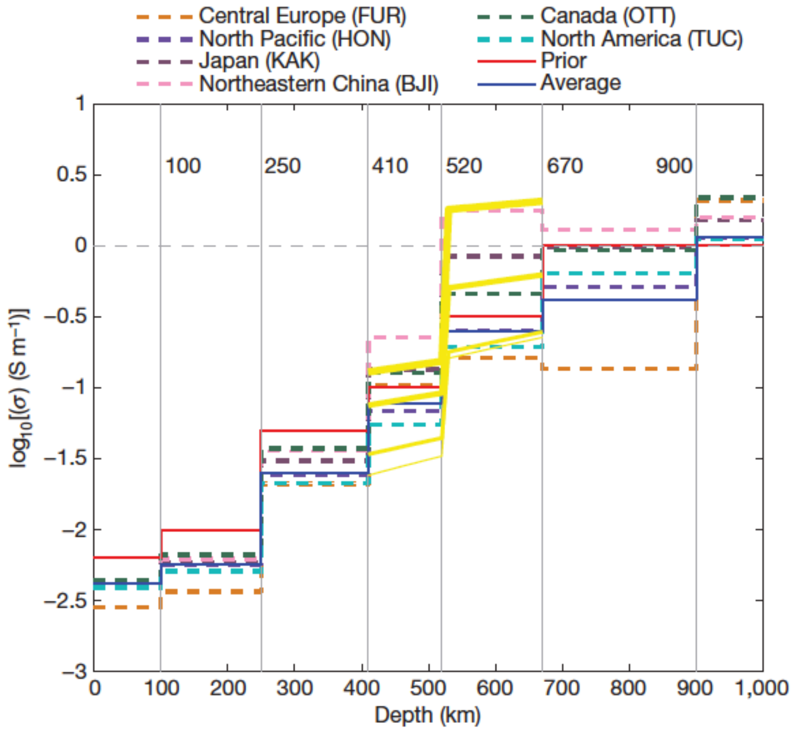
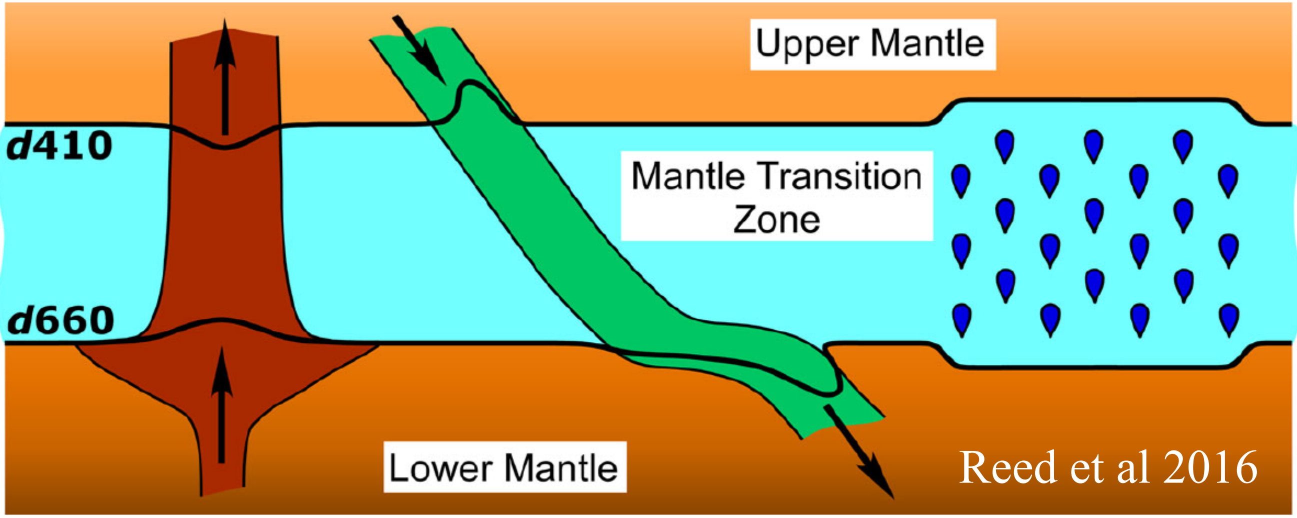


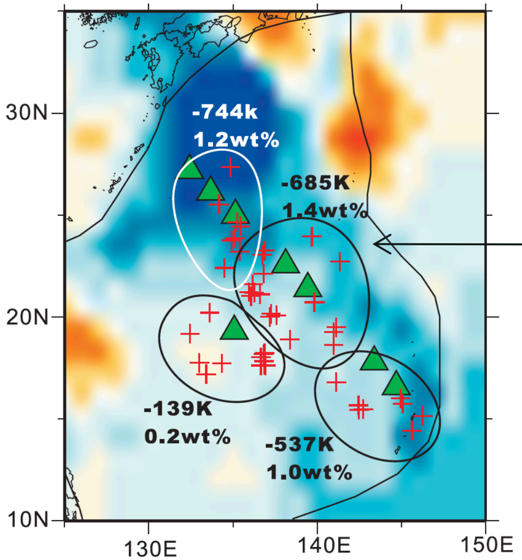
Figure 2 | Global and regional electrical conductivity profiles, based on the three-dimensional inverse solution presented in Fig. 1. The dashed lines correspond to the profiles beneath a set of locations, representative of geographical regions. The blue solid line is the global average. The red solid line represents the prior one-dimensional model used for the inversion[19]. The four yellow lines indicate the existing mineral physics constraints[8] as a function of water content (from the bottom up, in wt%: 0; 0.1, 0.5, 1.0). The three-letter abbreviations refer to the INTERMAGNET geomagnetic observatory codes[27].

~0.5 wt% at 410km

Kelbert et al 2009 Nature

Temperature and water & 410-km 660-km topography



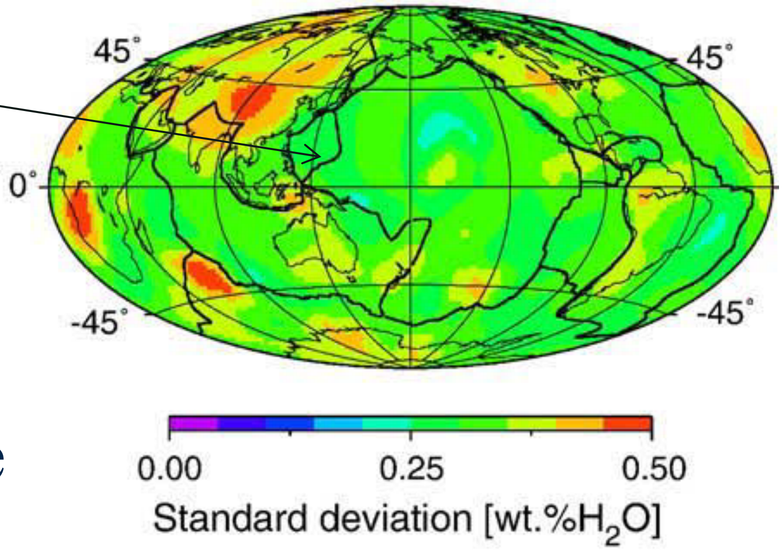


Suetsugu et al 2006

almost dry

very wet

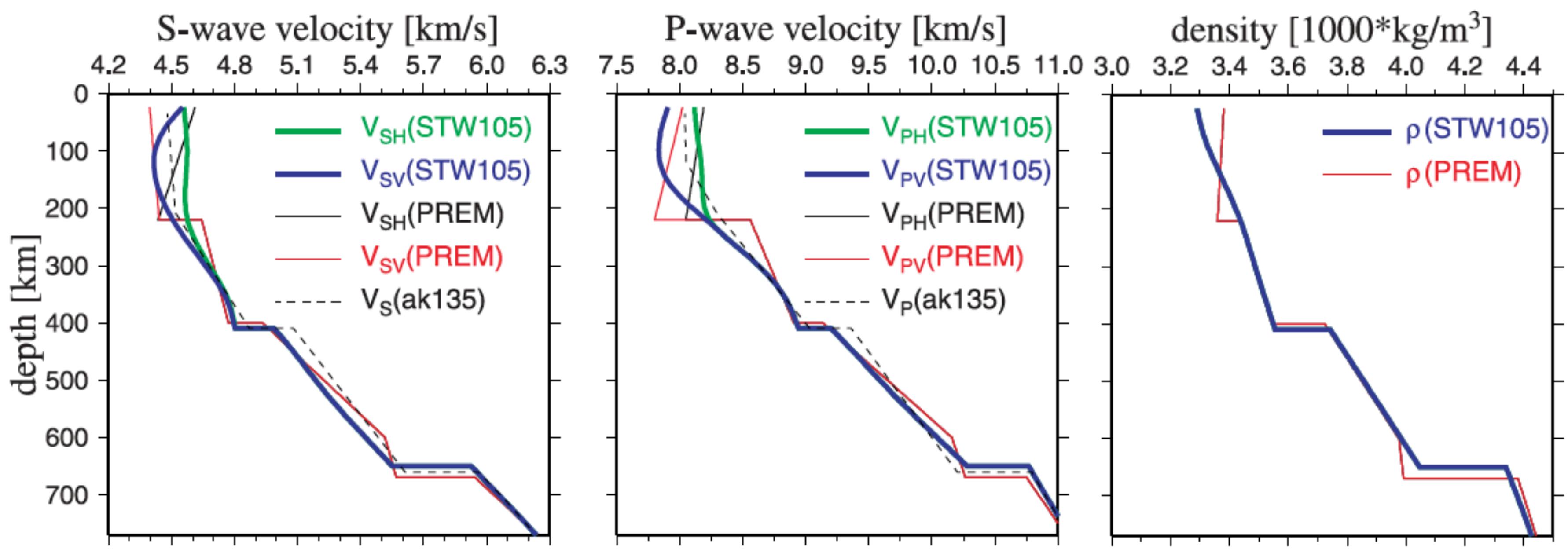
transition zone below Philippine plate



Meier et al 2009

Velocity and density jumps ➡ water content

advantage: jump values are insensitive to the temperature



Require the elastic data at mantle transition conditions

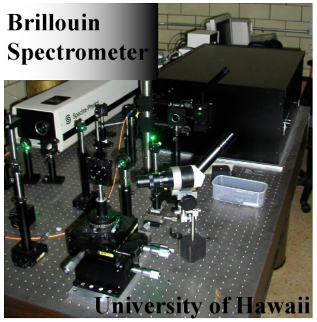
$(Mg_{1-x}Fe_x)_2SiO_4$ → **$(Mg_{1-y-z/4}H_{z/2}Fe_y)_2SiO_4$**

olivine → **Wadsleyite**

obtaining the elasticity

High-pressure experiment:

✚



Theoretical calculations

DFT ✚

obtaining the elasticity at high PT very challenge

First-principles calculations

1.Based on density functional theory
2.Resolve the quantum mechanic equations
3.No empirical parameters
4.Comparable to experimental data
5. P and T are only two parameters
6. Computation is expensive

Walter Kohn

1998 Nobel Laureate

Helmoholtz free energy — vibrational free energy

$$F(V,T) = U(V) + \sum_{qj} \frac{\hbar\omega_{qj}(V)}{2} + K_B T \sum_{qj} \ln(1 - \exp[\frac{\hbar\omega_{qj}(V)}{K_B T}])$$

Ground state energy

Calculating Vibration frequency is 2-3 order more expensive than calculating ground state energy.

Calculating elasticity

$$c_{ijkl}(V,T) = \frac{1}{V}\left(\frac{\partial^2 F(V,T,e_{mn})}{\partial e_{ij}\partial e_{kl}}\right) + \frac{1}{2}P(2\delta_{ij}\delta_{kl} - \delta_{il}\delta_{jk} - \delta_{ik}\delta_{jl})$$

Free energy ←

$$F(V,T,e_{mn}) = U_0(V,e_{mn}) + \frac{1}{2}\sum_{q,j}\hbar\omega_{q,j}(V,e_{mn}) + k_B T\sum_{q,j}\ln\{1-\exp[-\hbar\omega_{q,j}(V,e_{mn})/k_B T]\}$$

Orthorhombic crystal: 15 strained configurations at each volume

15 × 8 volumes =120 Phonon DoS calculations

Usually, calculating elasticity at high PT is extremely expensive

The method developed by Wu & Wentzcovitch (2011)

Only requiring frequencies for one unstrained configuration at each volume

Volume dependence of frequencies ➡ **Strain dependence of frequencies**

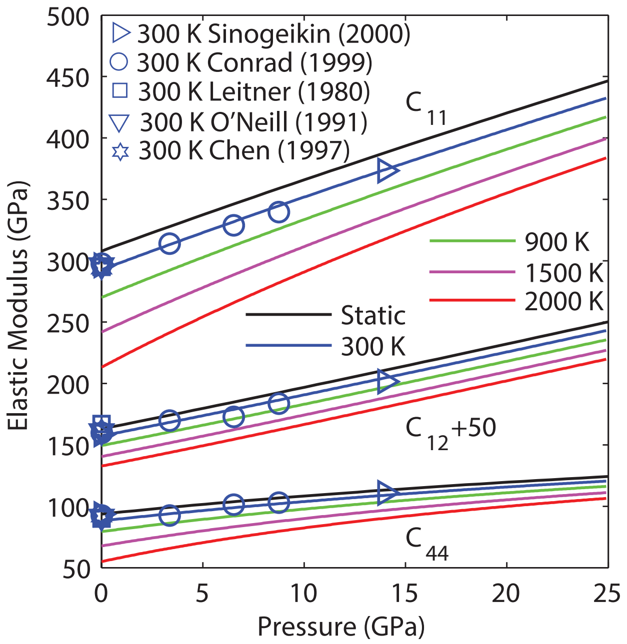
The number of phonon DoS for each volume: 16 ⟶ 1

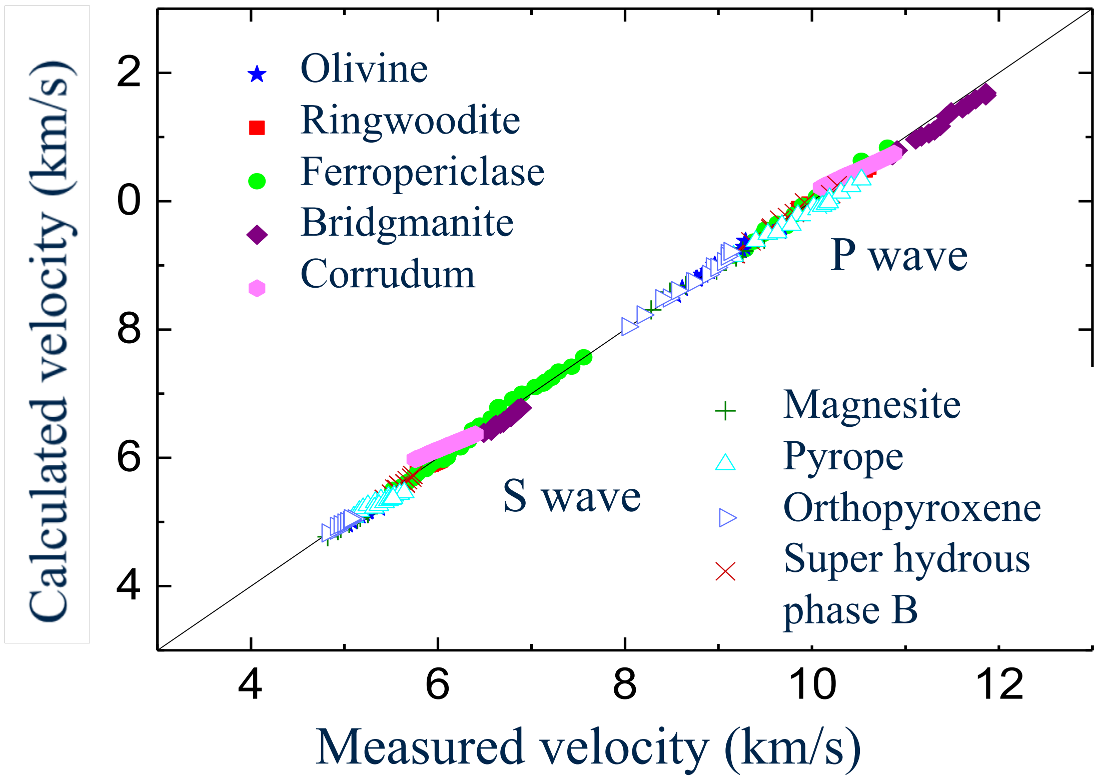
Computational workloads are less than tenth of the usual method

The method's performance

The method can predict precisely elasticity of many minerals at high PT

Wu & Wentzcovitch (2011)

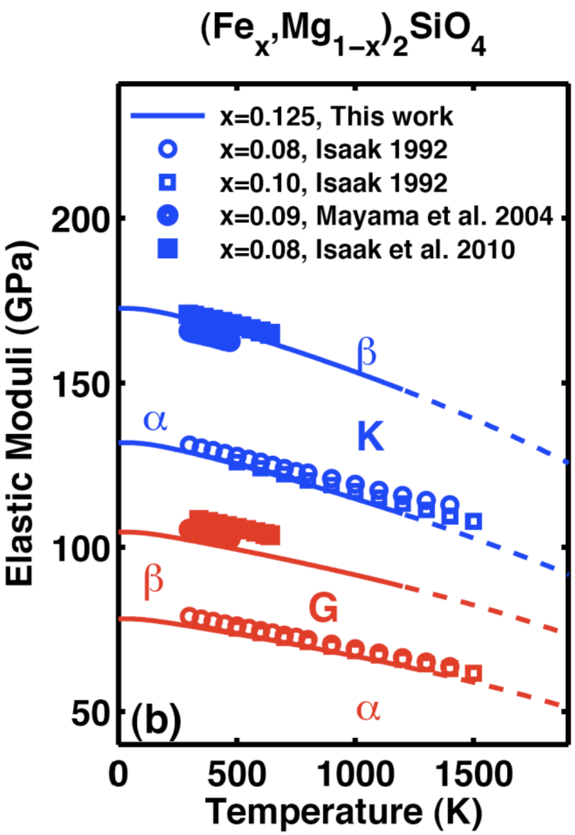


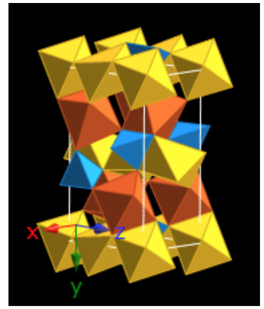


Elasticity of Pyrope

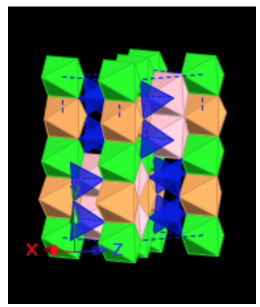
Hu et al., 2016 JGR

Elasticity of $Mg_{1-x}Fe_xSiO_4$

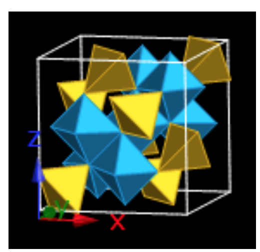




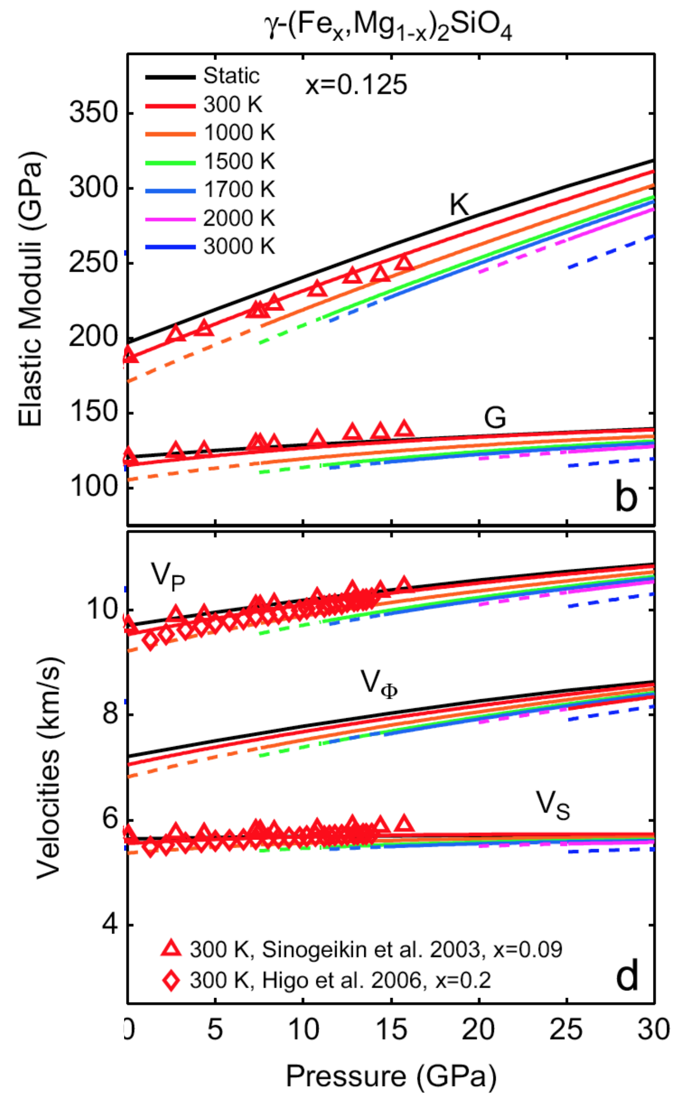
α phase



β phase

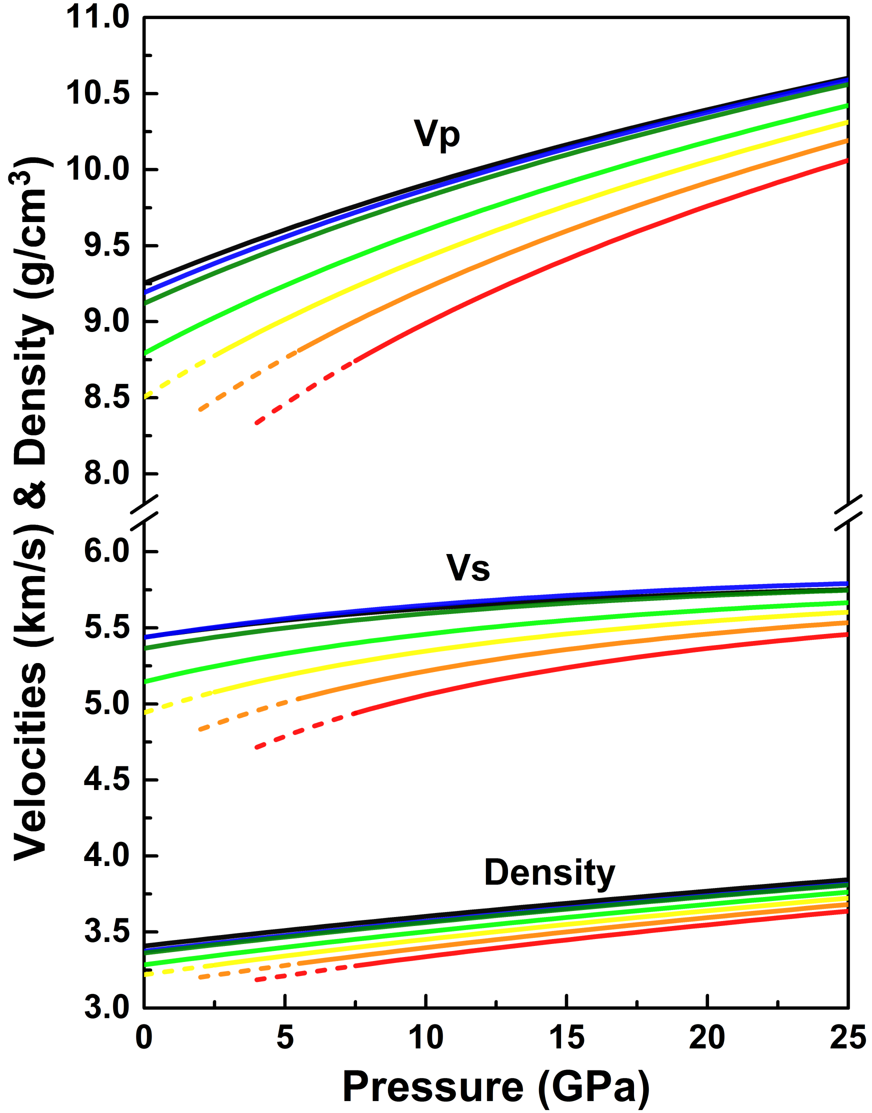


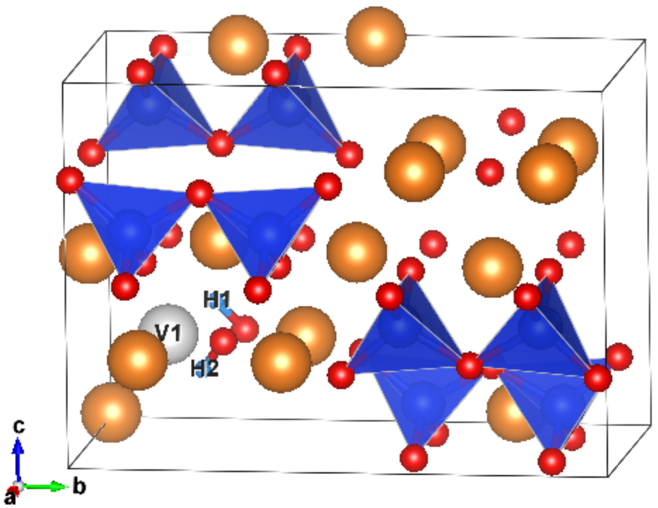
γ phase



Núñez Valdez et al 2012 EPSL; 2013 GRL

Elasticity of hydrous wadsleyite

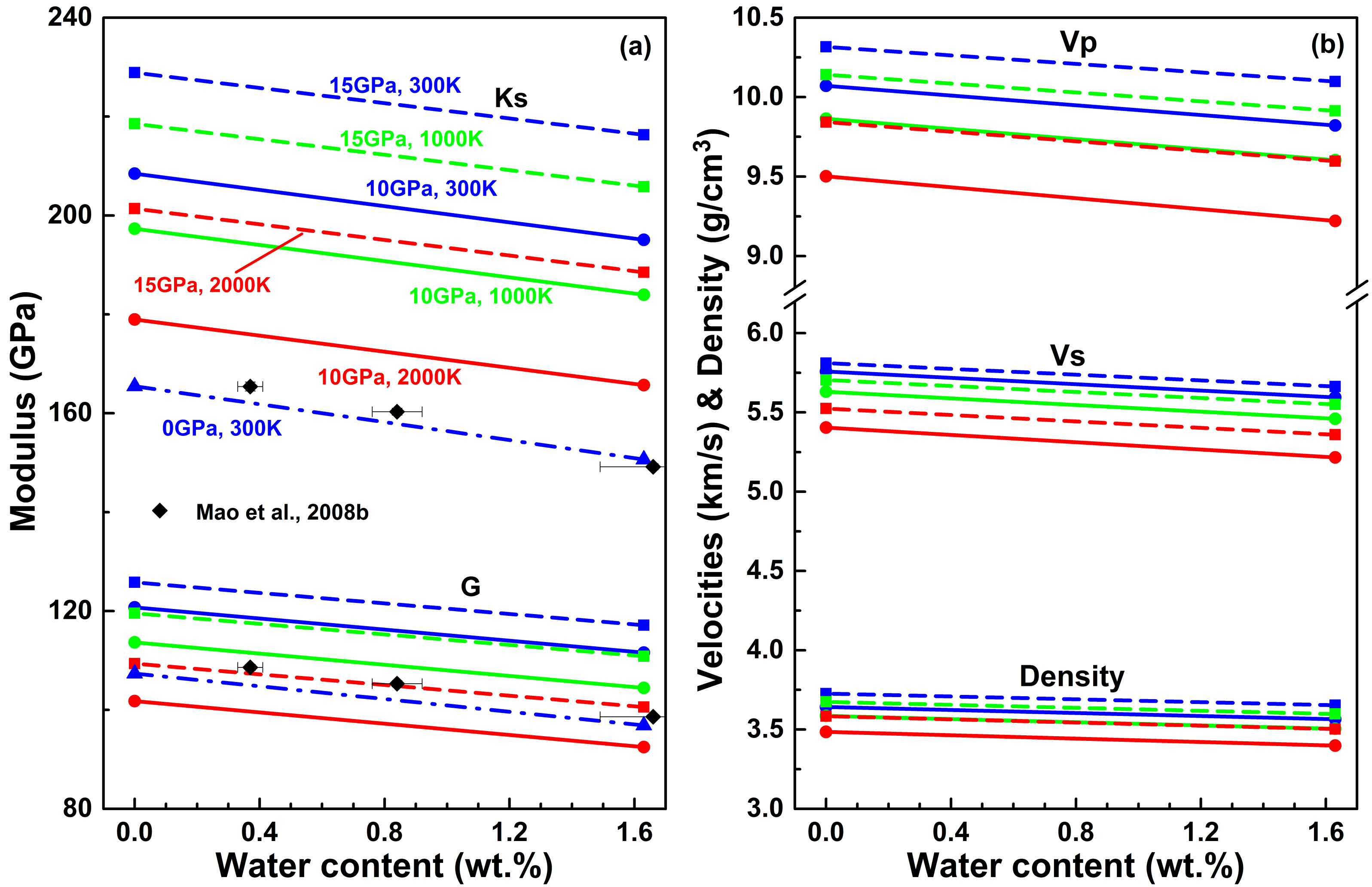




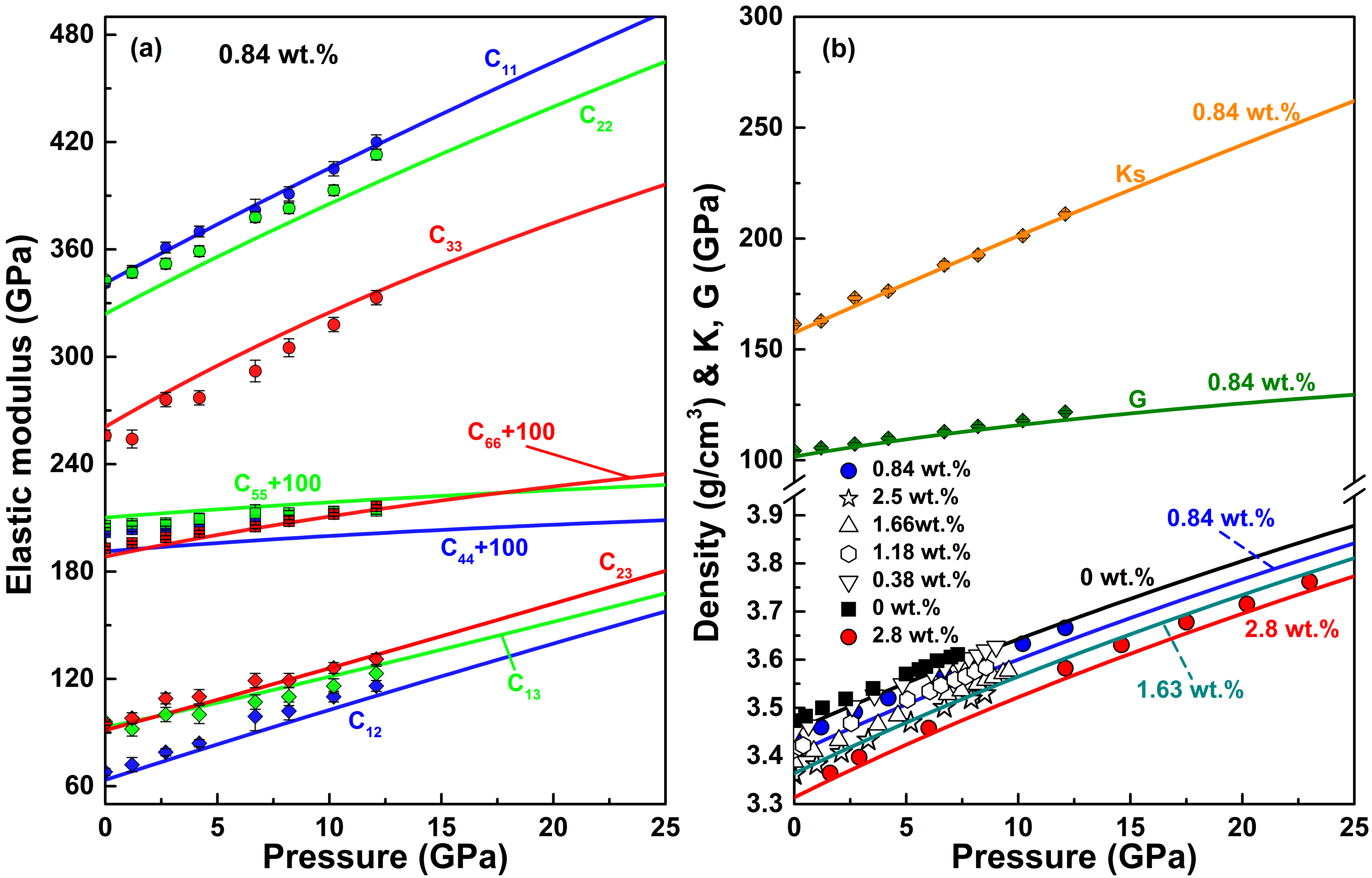
1.65 wt%

Wang et al 2019 EPSL

Water effect on elasticity of wadsleyite

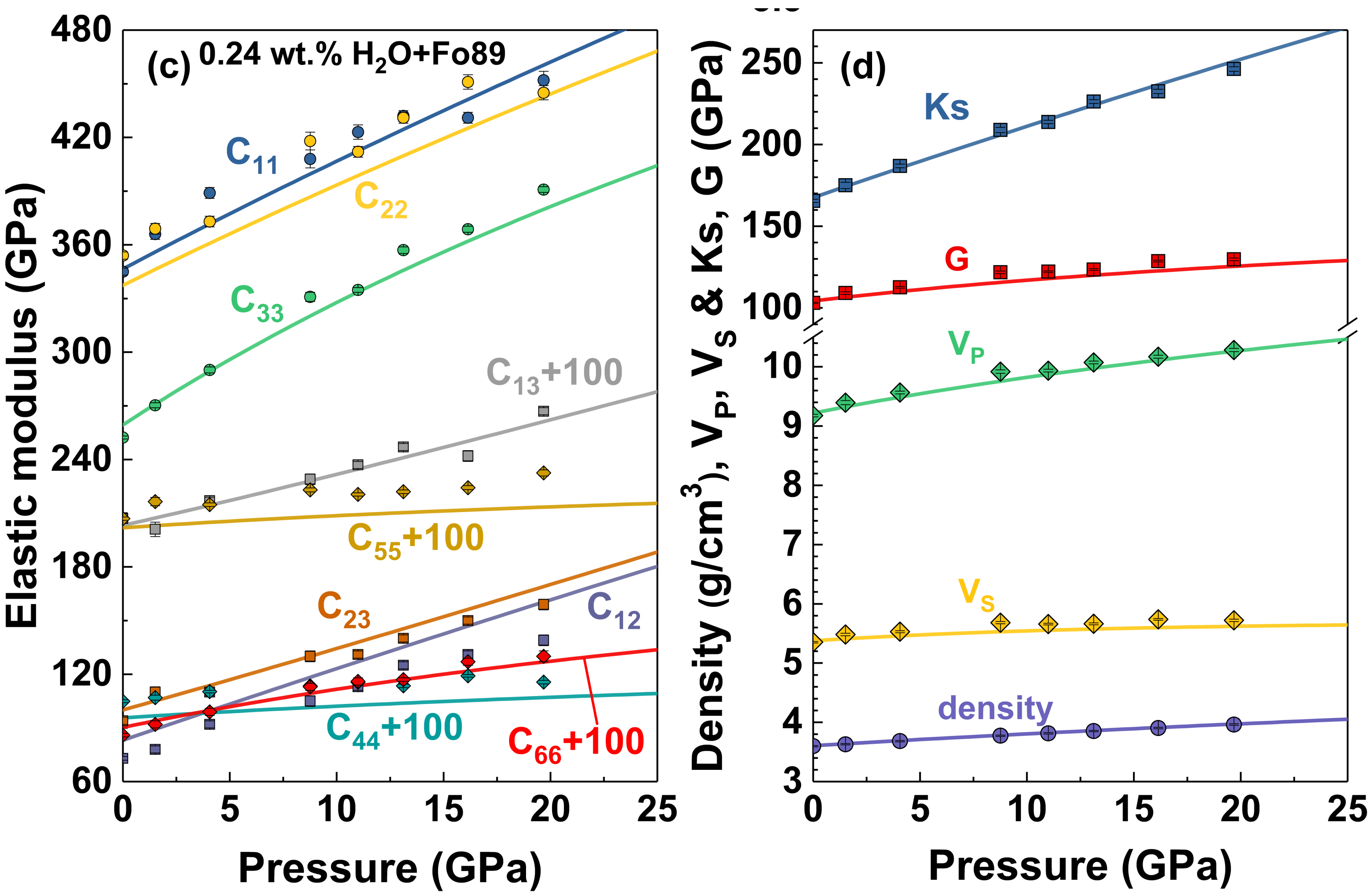


Agree with the experimental data



Exp. Mao et al 2008

Agree with the experimental data



Exp. Buchen et al., 2018

Constrain water content using 410-km jumps

$(Mg_{1-x}Fe_x)_2SiO_4$
olivine

x=0 & 0.125

→

$(Mg_{1-y-z}H_{2z}Fe_y)_2SiO_4$
Wadsleyite

y=0 & 0.125
z= 0.125 at y=0

$$D = \sqrt{\left(\frac{f \cdot \Delta Vp_{model} - \Delta Vp_{obs}}{\Delta Vp_{obs}}\right)^2 + \left(\frac{f \cdot \Delta Vs_{model} - \Delta Vs_{obs}}{\Delta Vs_{obs}}\right)^2 + \left(\frac{f \cdot \Delta \rho_{model} - \Delta \rho_{obs}}{\Delta \rho_{obs}}\right)^2}$$

410-km jumps	ΔV_{Pobs} (km/s)	ΔV_{Sobs} (km/s)	$\Delta \rho_{obs}$ (g/cm^3)
AK135	0.3299	0.2104	0.130
PREM	0.2288	0.1627	0.181

The best–fit results

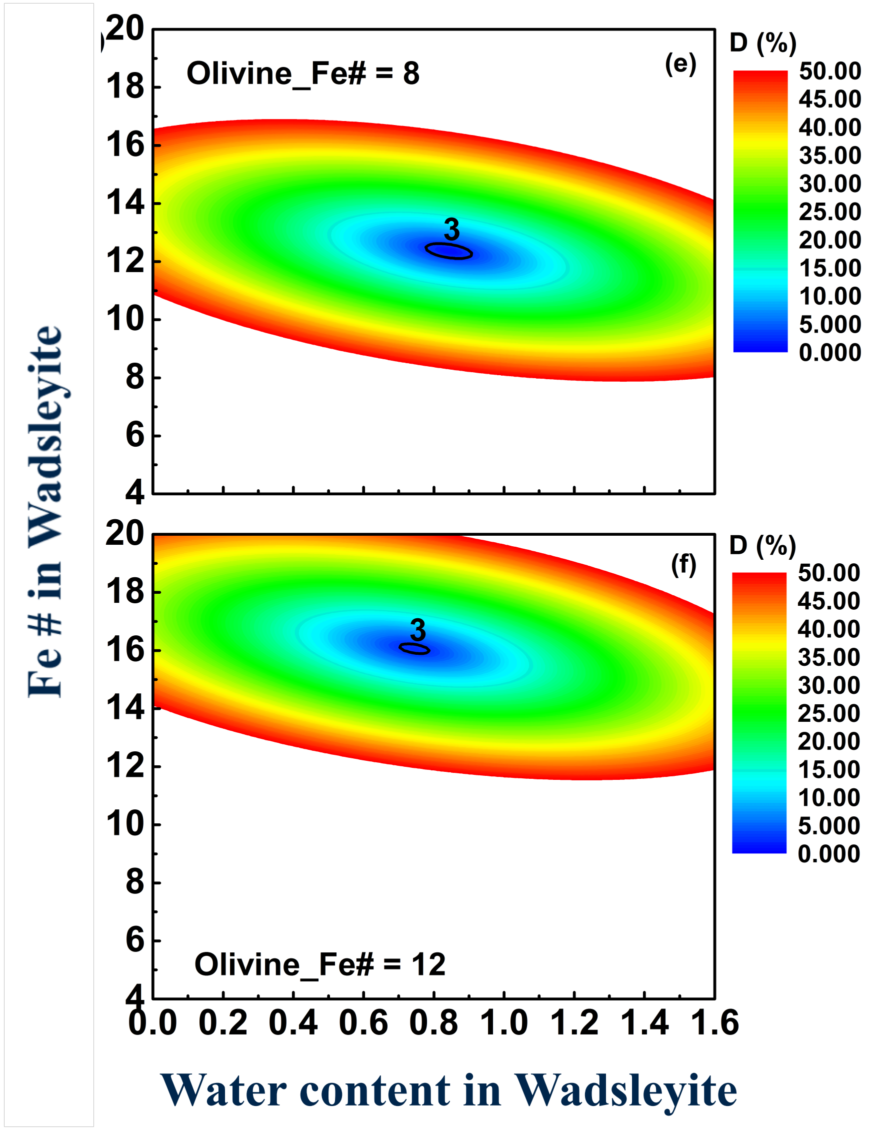
AK135 model

Two conclusions:

- **~0.8 wt % in wadsleyite**
- **Wads_Fe# - Oli_Fe# ≃4**

Fe#=100*x

$(Mg_{1-x}Fe_x)_2SiO_4$



Wang et al 2019 EPSL

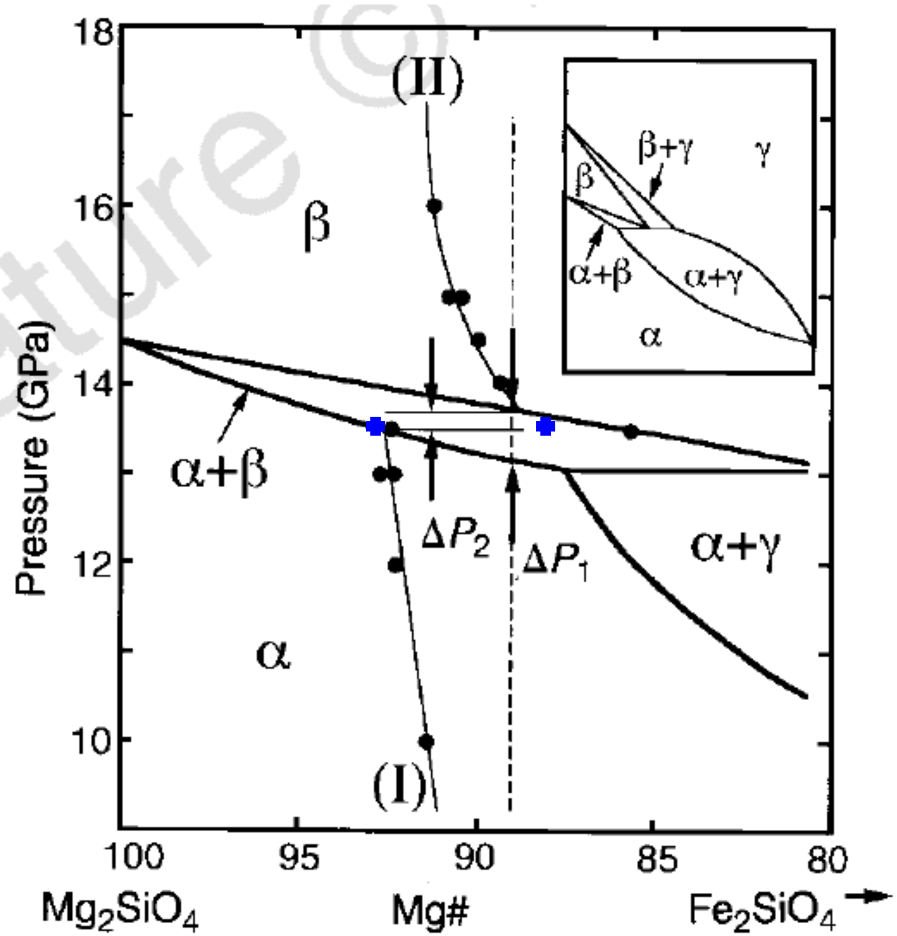
Prediction agrees with high-pressure experiment

More Fe in Wadsleyite

The best-fit result

Olivine_Fe#=7
Wads_Fe# =11.5

Two blue points
in the figure

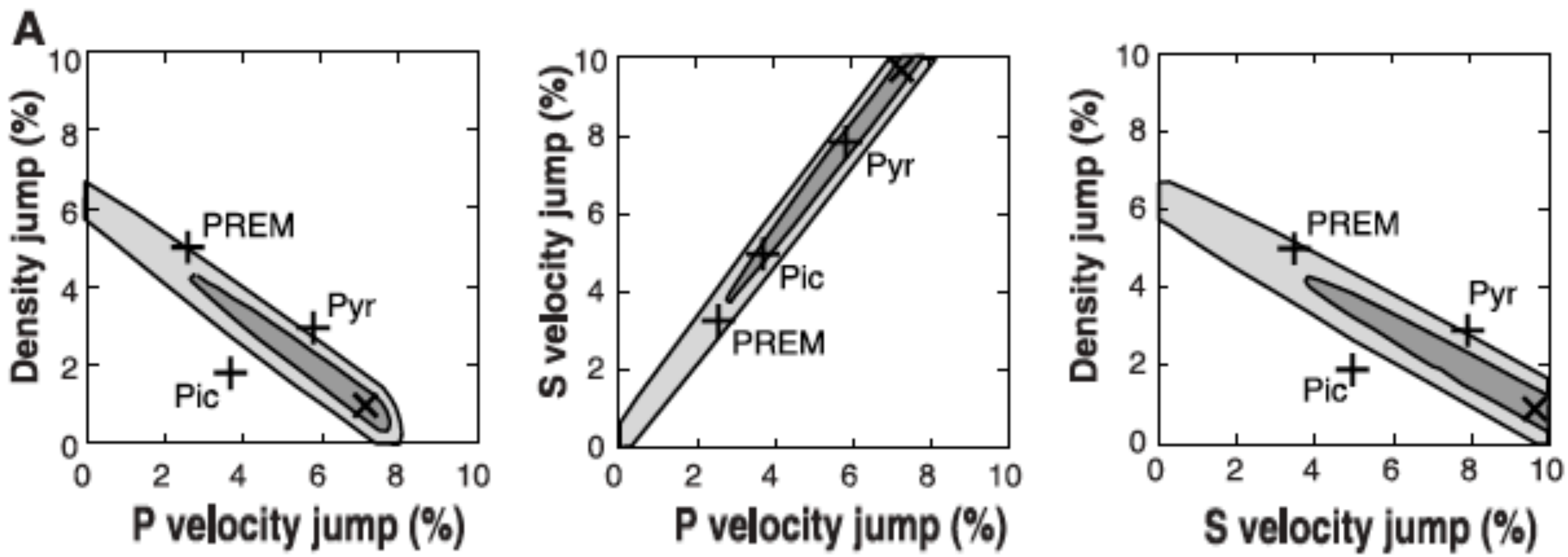


Fe partitioning between wadsleyite and olivine

Irifune and Isshiki 1998

Uncertainty of 410-km jumps

	ΔV_P (km/s)	ΔV_S (km/s)	$\Delta\rho$ (g/cm^3)
AK135	0.3299	0.2104	0.130
PREM	0.2288	0.1627	0.181



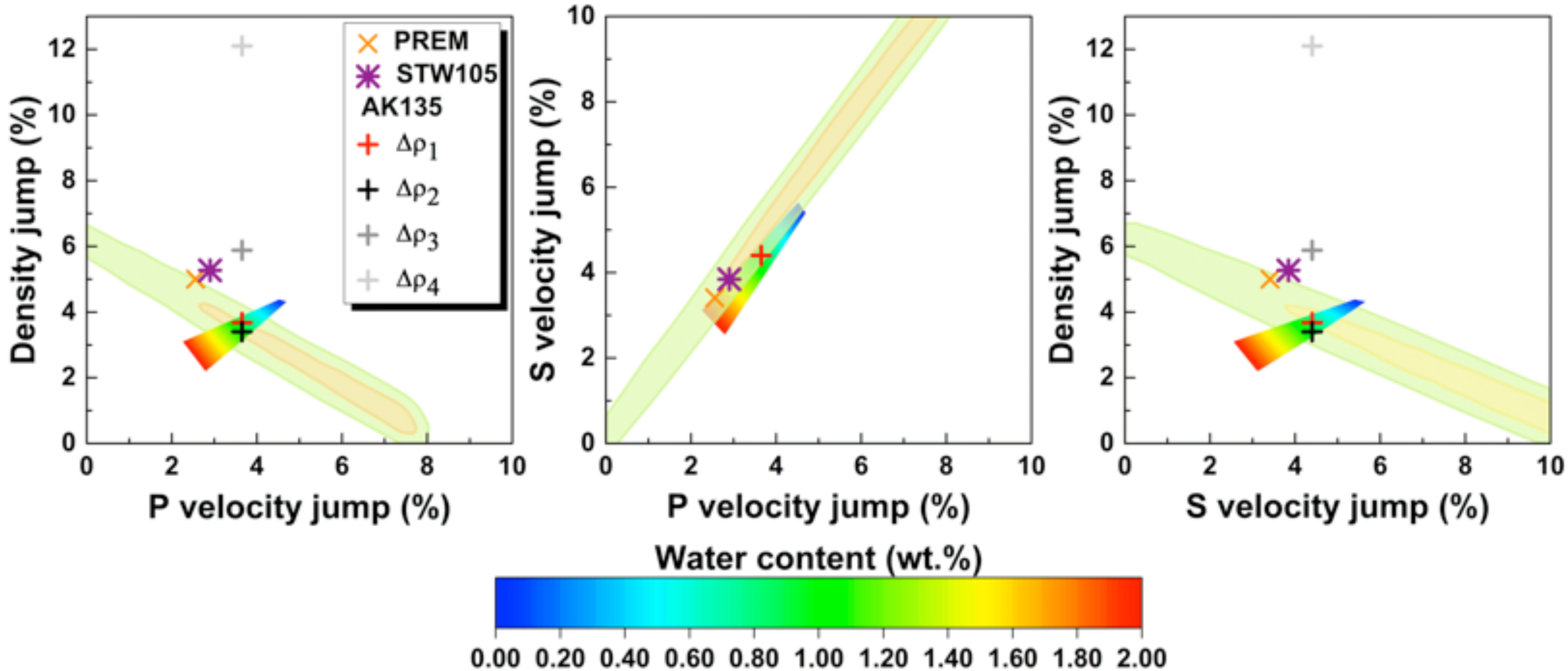
$$\Delta V_S = 1.3\Delta V_P \qquad \Delta\rho = 6.3\% - 0.7\Delta V_P$$

Shearer and Flanagan 1999 Science

410-km jumps & water content

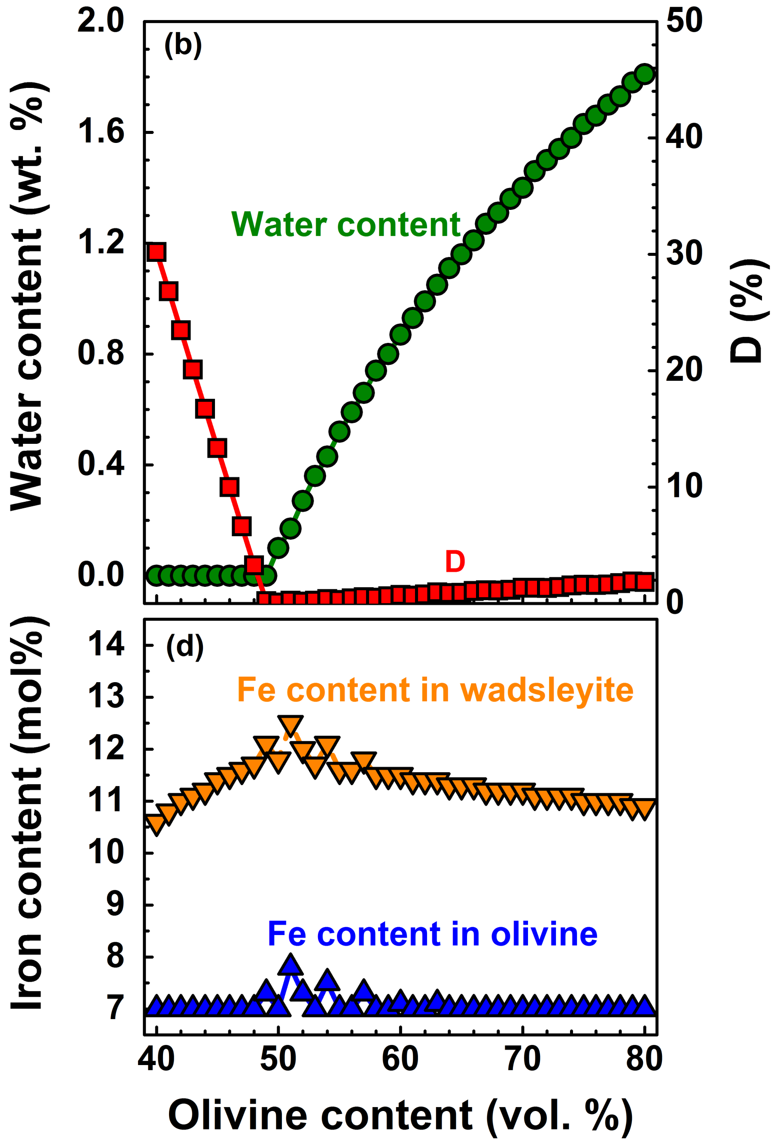
Our results suggest: $\Delta V_P = 3\% \sim 5\%$

0.5 wt% water



60 vol% olivine Olivine_Fe#=8 Wads_Fe# =12

Water content & olivine content



60% olivine → 0.5 wt%

~50% olivine → Dry

Summary

Combing with seismic results, we found that V_P jump at 410 is 3%～5%.

The transition zone is wet at least at its top with 0.5 wt% (0.8 wt% * 60%) water for the pyrolitic mantle.

The transition zone is dry for the mantle with ~ 50% olivine