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

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Deep Water Cycle

Water-saturated transition zone can contains oceans worth of H₂O

(Pearson et al., 2014 Science)
Dry mantle transition zone inferred from the conductivity of wadsleyite and ringwoodite

Takashi Yoshino¹, Geeth Manthilake¹, Takuya Matsuzaki¹ & Tomoo Katsura¹

Yoshino et al 2008 Nature

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

Xiaoge Huang¹,², Yousheng Xu² & Shun-Ichiro Karato²

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

Huang et al 2005 Nature

\(~0.5\) wt% at 410km

Kelbert et al 2009 Nature
Temperature and water & topography

Almost dry

Very wet

Transition zone below Philippine plate

Suetsugu et al. 2006

Meier et al. 2009
Velocity and density jumps \( \rightarrow \) water content

**Advantage:** Jump values are insensitive to the temperature

Require the elastic data at mantle transition conditions

\[(\text{Mg}_{1-x}\text{Fe}_x)_2\text{SiO}_4\] olivine \( \rightarrow \) \[(\text{Mg}_{1-y-z/4}\text{H}_{z/2}\text{Fe}_y)_2\text{SiO}_4\] 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

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

Helmholtz free energy

vibrational free energy

Ground state energy

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

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

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 x 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 \rightarrow Strain dependence of frequencies

The number of phonon DoS for each volume: 16 \rightarrow 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$_x$SiO$_4$

Núñez Valdez et al 2012
EPSL; 2013 GRL
Elasticity of hydrous wadsleyite

$1.65 \text{ wt\%}$

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

\[(\text{Mg}_{1-x}\text{Fe}_x)_2\text{SiO}_4\] olivine
\[x=0 \& 0.125\]

\[(\text{Mg}_{1-y-z}\text{H}_{2z}\text{Fe}_y)_2\text{SiO}_4\] Wadsleyite
\[y=0 \& 0.125\]
\[z=0.125 \text{ at } y=0\]

\[\Delta V = \sqrt{\left(\frac{f \cdot \Delta V_{P_{\text{model}}} - \Delta V_{P_{\text{obs}}}}{\Delta V_{P_{\text{obs}}}}\right)^2 + \left(\frac{f \cdot \Delta V_{S_{\text{model}}} - \Delta V_{S_{\text{obs}}}}{\Delta V_{S_{\text{obs}}}}\right)^2 + \left(\frac{f \cdot \Delta \rho_{\text{model}} - \Delta \rho_{\text{obs}}}{\Delta \rho_{\text{obs}}}\right)^2}\]

<table>
<thead>
<tr>
<th>410-km jumps</th>
<th>$\Delta V_{P_{\text{obs}}}$ (km/s)</th>
<th>$\Delta V_{S_{\text{obs}}}$ (km/s)</th>
<th>$\Delta \rho_{\text{obs}}$ (g/cm$^3$)</th>
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<tr>
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<td>0.3299</td>
<td>0.2104</td>
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<tr>
<td>PREM</td>
<td>0.2288</td>
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The best–fit results

AK135 model

Two conclusions:
• \(~0.8\) wt \% in wadsleyite
• \(\text{Wads}_\text{Fe#} - \text{Oli}_\text{Fe#} \approx 4\)

\[
\text{Fe#} = 100 \times x \\
(\text{Mg}_{1-x}\text{Fe}_x)_2\text{SiO}_4
\]

Wang et al 2019 EPSL
Prediction agrees with high-pressure experiment

More Fe in Wadsleyite

The best-fit result

Olivine$_{\text{Fe\#}}$ = 7
Wads$_{\text{Fe\#}}$ = 11.5

Two blue points in the figure

Fe partitioning between wadsleyite and olivine

Irifune and Isshiki 1998
### Uncertainty of 410-km jumps

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\[
\Delta V_S = 1.3 \Delta V_P \quad \Delta \rho = 6.3\% - 0.7 \Delta V_P
\]

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
Combing with seismic results, we found that $V_p$ jump at 410 is $3\% \sim 5\%$.

The transition zone is wet at least at its top with $0.5 \text{ wt}\%$ ($0.8 \text{ wt}\% \times 60\%$) water for the pyrolitic mantle.

The transition zone is dry for the mantle with $\sim 50\%$ olivine.