Interpreting Geophysical Data for Mantle Dynamics

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Chemical Constraints on Density Distribution

Stixrude, unpublished
Chemical Constraints on Density Distribution

Compressional wave speed (km/s)

Depth (km)

Chemical Constraints on Density Distribution

 Olivine

Wadsleyite

Ringwoodite

Garnet

Mg-perovskite

(Mg,Fe)O

Stacy Geotherm
Cold Slabs, Clapeyron Slopes and Whole Mantle Convection

\[ F_b = - g \frac{\partial}{\partial z} \left( \frac{\partial F}{\partial P} \left( \frac{\partial P}{\partial T} \right) \right)_i dT \]
Clapeyron Slope

\[ G = P - T \]

Equilibrium:
\[ \Delta G_1 = \Delta G_2 \]

\[ V_1 dP - S_1 dT = V_2 dP - S_2 dT \]

\[ \frac{dP}{dT} = \frac{DV_{rxn}}{DS_{rxn}} \]
Cold Slabs, Clapeyron Slopes and Whole Mantle Convection

\[ \gamma - \text{MgSiO}_4 \]

660 km

\[ \text{pv+mw} \]

endothermic reaction

\[ F_b = - g \frac{\partial}{\partial \gamma} v_i (\frac{\partial \gamma}{\partial z})\frac{(\frac{\partial z}{\partial P})(\frac{\partial P}{\partial T})_i}{\partial P} DT \]

Clapeyron slope must be greater than… ask a geodynamicist
Determination of Clapeyron Slopes

\[ \frac{dP}{dT} = \frac{DV_{\text{rxn}}}{DS_{\text{rxn}}} \]

Phase Equilibria
- ex-situ
- in-situ

Thermodynamic
Determination of Clapeyron Slopes

\[ \frac{dP}{dT} = \frac{DV_{\text{rxn}}}{DS_{\text{rxn}}} \]

Phase Equilibria
ex-situ
in-situ
Thermodynamic

Ringwoodite
(Smyth)

200µm
Multi-Anvil Press
Determination of Clapeyron Slopes

\[
\frac{dP}{dT} = \frac{DV_{\text{rxn}}}{DS_{\text{rxn}}}
\]

Clapeyron slope = -2.8 MPa/K
Determination of Clapeyron Slopes

Phase Equilibria
- ex-situ
- in-situ

Thermodynamic

\[
\frac{dP}{dT} = \frac{DV_{rxn}}{DS_{rxn}}
\]

Ringwoodite
(Smyth)
The Laser-Heated Diamond Anvil Cell

Pressure = Force/Area

Spectroradiometry (temperature)

X-ray diffraction (pressure, structure, density)
Techniques
X-ray Diffraction

Diffraction condition:
\[ \lambda = 2d \sin(2\theta) \]

e.g. Cullity
Techniques
X-ray Diffraction

![Graph showing X-ray diffraction patterns for Ringwoodite, Perovskite, and periclase. The graph displays intensity on the y-axis and d-spacing on the x-axis.]
Temperature Measurements

hot spot

O$_2$

gasket

ruby

(Benedetti et al, unpublished)

side view  top view

Kavner and Panero, *PEPI* 2004

\[
I = \frac{2e^2 \hbar c}{1 - \exp\left(\frac{\hbar c}{kT}\right)}
\]

\(T = 1700 \pm 75\) K
Pressure Measurements: Equations of State

Lee et al., 2004
Constant Temperature Equations of State

Bulk Modulus \( K_{0T} = \frac{P}{\frac{\ln(V)}{T}} \)

\[ f = \left[ \left( \frac{v}{v_0} \right)^{-2/3} - 1 \right] / 2 \]

\[ P = 3f(1 + 2f)^{5/2} K_{0T} \left[ 1 + 1.5(K_{0T} - 4)f + \ldots \right] \]

\[ F = \frac{P}{3f(1 + 2f)^{5/2}} \]

\[ F = K_{0T} \left[ 1 + 1.5(K_{0T} - 4)f + \ldots \right] \]
Lee et al., 2004

\[ F = K_{0T} \left[ 1 + 1.5(K_{0T}' - 4) f + \ldots \right] \]
PVT Equations of State

![Graph showing the relationship between unit-cell volume and pressure for MgSiO$_3$-perovskite at 300 K and 2000 K. The graph includes lines representing thermal pressure and thermal expansion.]
PVT Equations of State

\[ P(V, T) = P_K(V) + P_{th}(T) \]

Thermodynamic definition
\[ -\frac{\partial E}{\partial V} = P \]

\[ P_{th} = -\frac{\partial E_{th}}{\partial V} = \frac{g}{V} E_{th} \]

Model for internal energy:

E.g. Debye

\[ E_{th} = 9nk_B T(T/Q_D)^3 \frac{Q_D}{T} \int_0^x \frac{x^3}{e^x - 1} dx \]
Determination of Clapeyron Slopes

\[ \frac{dP}{dT} = \frac{DV_{\text{rxn}}}{DS_{\text{rxn}}} \]

Shim et al., 2001

Phase Equilibria
- ex-situ
- in-situ

Thermodynamic

Clapeyron slope = -3 MPa/K (Irifune et al., 1998)
Clapeyron slope = no constraint (Shim et al., 2001; Chudinovskikh et al., 2001)
Sources of Error

Non-hydrostatic stresses
- Pressure standards
- Temperature and pressure gradients

Non-hydrostatic < Non-hydrostatic

Incoming x-ray

Diffracted x-ray

$V_{\text{hydrostatic}} < V_{\text{non-hydrostatic}}$
Sources of Error

Non-hydrostatic stresses
Pressure standards
Temperature and pressure gradients

Kavner and Duffy, 2003
Sources of Error

Non-hydrostatic stresses

Pressure standards

Temperature and pressure gradients

Gold relative to Platinum

Shim et al., 2001
Sources of Error

- Non-hydrostatic stresses
- Pressure standards
- Temperature and pressure gradients

Oxygen

Kavner and Panero, PEPI 2004
Determination of Clapeyron Slopes

\[
\frac{dP}{dT} = \frac{D V_{rxn}}{D S_{rxn}}
\]

Phase Equilibria

- ex-situ
- in-situ

Thermodynamic

Clapeyron slope = -4±2 MPa/K

Ito et al., 1990
Interpretation of Tomography: Thermal Variations

![Graph](image-url)

- Pressure (GPa)
  - 0
  - 20
  - 40
  - 60
  - 80

- Unit-cell volume (Å$^3$)
  - 130
  - 140
  - 150
  - 160

- MgSiO$_3$-perovskite

Thermal Expansion

Thermal Pressure
Interpretation of Tomography: Compositional Variations

- **SiO\textsubscript{2}**: 45.4 wt%
- **MgO**: 37.1 wt%
- **FeO**: 8.3 wt%
- **Al\textsubscript{2}O\textsubscript{3}**: 4.3 wt%
- **CaO**: 3.3 wt%
**Interpretation of Tomography: Compositional Variations**

<table>
<thead>
<tr>
<th>Perovskite Composition</th>
<th>$K_0$ (GPa)</th>
<th>$\rho$ (Mg/m$^3$)</th>
<th>$\sqrt{K_0/r}$ (km/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MgSiO$_3$</td>
<td>262</td>
<td>4.12</td>
<td>7.974</td>
</tr>
<tr>
<td>MgSiO$_3$ ~10% FeO</td>
<td>262</td>
<td>4.25</td>
<td>7.851</td>
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<tr>
<td>MgSiO$_3$ ~3.25% Al$_2$O$_3$</td>
<td>261</td>
<td>4.123</td>
<td>7.956</td>
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<td>MgSiO$_3$ ~3.25% Al$_2$O$_3$+H$_2$O</td>
<td>256</td>
<td>4.088</td>
<td>7.913</td>
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</tbody>
</table>
Theory

Quantum mechanical or classical
  – effects of \emph{a priori} assumptions
  – size of calculation, time for calculation

General approach:
  G of each phase
  PT-space for lowest energy

Limitations:
  Temperature
  Multi-component systems
Theory

MgSiO$_3$ perovskite

Wentzcovitch et al., 2004
Zhao et al., 1992