Elasticity of iron-rich silicate in Earth’s D” layer

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Post-perovskite

- New phase in MgSiO$_3$ at approximately D$''$ discontinuity conditions
  - pv (Pbnm) $\rightarrow$ ppv (Cmcm)

Tsuchiya et al., EPSL 2004

Murakami et al., Science 2004
Post-perovskite

Duffy, Nature 2004

Sidorin et al, Science 1999

Mantle adiabat

Tsuchiya et al, EPSL 2004
What about Fe?

- D” is where the liquid Fe outer core meets the crystalline silicate mantle
  - Fe-richppv
  - ULVZ
  - Seismic anisotropy
Diamond Anvil Cell

Diagram showing the components of a diamond anvil cell: Table, Culet, Gasket, Sample chamber, and applied Force.
Experimental

- Samples
  - Orthopyroxenes: $\text{Fs10 (Mg}_{0.9}\text{Fe}_{0.1})\text{SiO}_3$, Fs20, Fs40, Fs60, Fs80
- Thermal insulation
  - NaCl, SiO$_2$
- Internal pressure standard
  - Pt, NaCl
- Gasket
  - Re, Be + graphite insert

![Diagram of experimental setup]
Synchrotron XRD and laser-heated DAC

13-IDD, GSECARS

16-IDB, HPCAT

- Gasket hole ~ 60 µm (culet = 150 µm, bevel diameter = 300 µm)
- X-ray beam ~ 6 x 7 µm
- Double-sided Nd:YLF laser heating
W. Mao et al. PNAS 2004

Fs$_{20}$, Mg$_{0.8}$Fe$_{0.2}$SiO$_3$

En80, 113 GPa, quenched from 2000 K

Relative intensity

En80, 147 GPa, quenched from 2400 K

beam stop holder
diamond spots
ppv silicate can take a lot of Fe

W. Mao et al, PNAS 2005
Fe-Mg partitioning: unsettled issue

\[ K = \frac{(Fe/Mg)_{\text{silicate}}}{(Fe/Mg)_{\text{nw}}} \]

Kobayashi et al, GRL 2006

Murakami et al, GRL 2005

Mao et al, Science 1997

Andrault et al, JGR 2001

Kessen et al, EPSL 2002
Fe-Mg partitioning: unsettled issue

- Starting composition: Fa30 \((\text{Fe}_{0.3}\text{Mg}_{0.7})_2\text{SiO}_4\), Fa45
- After decompression, recovered mw had lattice constant, \(a_0 = 4.2336\ \text{Å}\) which corresponds to a composition: \(\text{Fe}_{0.23}\text{Mg}_{0.77}\text{O}\)
- For mass balance the ppv phase has a composition: \(\text{Fe}_{0.37}\text{Mg}_{0.63}\text{SiO}_3\)
- Fe partitions strongly into ppv phase?
How does Fe affect $V_S$?

$$K = -V \left( \frac{\partial P}{\partial V} \right)$$

$$\frac{K}{\rho} = v_p^2 - \frac{4}{3} v_s^2 = v_\Phi^2$$

W. Mao et al, Science 2006
Nuclear resonant x-ray spectroscopy (NRXS)

Synchrotron $^{57}$Fe Mössbauer spectroscopy

Nuclear resonant inelastic x-ray spectroscopy

Intensity

Energy

SMS signal

DAC

KB mirrors

HRM

M

APD

APD

NRIXS signal

Anti-stokes

Stokes

Elastic line

150 nsec

XOR, Sector 3, APS, ANL
Phonon density of states

Debye Model

“Real” Crystal

\[ g(\omega) = \frac{V}{2\pi^2 v_D^3} \omega^2 \]

\[ \frac{3}{v_D^3} = \frac{1}{v_p^3} + \frac{2}{v_S^3} \]

<table>
<thead>
<tr>
<th></th>
<th>(V_P, \text{ km/sec})</th>
<th>(V_S, \text{ km/sec})</th>
<th>(\nu)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PREM, mantle side of CMB</td>
<td>13.72</td>
<td>7.26</td>
<td>0.30</td>
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<tr>
<td>ULVZ (Thorne, JGR 2004)</td>
<td>12.35</td>
<td>5.08</td>
<td>0.40</td>
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<tr>
<td>Fs40 ppv at 130 GPa-300 K</td>
<td>12.72</td>
<td>4.86</td>
<td>0.41</td>
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<tr>
<td>Fs40 ppv at 130 GPa-3000 K</td>
<td>11.91</td>
<td>4.05</td>
<td>0.43</td>
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</table>

W. Mao et al, Science 2006
Fe in ULVZ

- Fe-rich ppv has low enough $V_s$ to explain the depression of velocity in ULVZ
- When Fe-poor mantle contacts core, a thin layer of Fe-rich ppv forms
- Mantle convection sweeps the thin layer into a thickened pile to form ULVZ
Radial x-ray diffraction

Magnitude of waviness
-- deviatoric strain & shear strength

Magnitude dependence on $hkl$
-- elasticity tensor

Intensity vs azimuthal angle
-- lattice preferred orientation
Deformation of a germanate analog

In contrast with phenomenological considerations suggesting (010) as a slip plane, lattice planes near (100) became aligned perpendicular to the compression direction, suggesting that slip on (100) or (110) dominated plastic deformation.
Elastic anisotropy of silicate ppv at 140 GPa

W. Mao et al., in prep.
Determination of single-crystal elasticity tensor

\[ \cos \psi = \cos \eta \cdot \cos \theta \cdot \sin \alpha - \sin \theta \cdot \cos \alpha \]

\[ \varepsilon_{\psi}(hkl) = \frac{d_{\psi}(hkl) - d_{p}(hkl)}{d_{p}(hkl)} = (1 - 3\cos^2 \psi) \cdot Q(hkl) \]

\[ [Q(hkl)/<Q>] G^{-1} = \alpha G(hkl) R^{-1} + (1 - \alpha) G^{-1} \]

\[ G(hkl)_R^{-1} = (3H^4 - H^2) s_{11} + (3K^4 - K^2) s_{22} + (3L^4 - L^2) s_{33} + (6H^2K^2 + L^2 - 1) s_{12} + (6H^2L^2 + K^2 - 1) s_{13} + (6K^2L^2 + H^2 - 1) s_{23} + 3K^2L^2 s_{44} + 3H^2L^2 s_{55} + 3H^2K^2 s_{66} \]

\[ H = hdl/a, \ K = kdl/b, \ L = ldl/c \]

Formulism from Singh et al. J. Appl. Phys., 1998
Linear compressibilities of ppv at 140 GPa

\[ \chi_a = s_{11} + s_{12} + s_{13} \]

\[ \chi_b = s_{22} + s_{12} + s_{23} \]

\[ \chi_c = s_{33} + s_{13} + s_{23} \]

<table>
<thead>
<tr>
<th>( c_{11} )</th>
<th>( c_{22} )</th>
<th>( c_{33} )</th>
<th>( c_{12} )</th>
<th>( c_{13} )</th>
<th>( c_{23} )</th>
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<td>1011</td>
<td>1119</td>
<td>814</td>
<td>722</td>
<td>805</td>
<td>97</td>
<td>124</td>
<td>229</td>
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</table>

W. Mao et al, in prep.
Theoretically determined velocity anisotropy

Iitaka et al, Nature 2004

MgSiO$_3$ ppv

Tsuchiya et al, GRL 2004

Stackhouse et al, EPSL 2005
Possible implications

- Very large azimuthal $V_S$ anisotropy, $(V_{S,\text{max}} - V_{S,\text{min}})/V_{S,\text{aggregate}} = 44\%$

- Small azimuthal $V_P$ anisotropy, $(V_{P,\text{max}} - V_{P,\text{min}})/V_{P,\text{aggregate}} = 8\%$

This implies:

- Seismically observable $V_S$ splitting even with the 100 slip plane and low degree of LPO

- No seismically observable $V_P$ anisotropy

W. Mao et al, in prep.
Current/Future work in D”

• Clapeyron slope of pv-ppv
  – Topography of the top of D”
  – Double crossing

• Melting of ppv
  – CMB Temperature

• FTIR and visible spectroscopy
  – Radiative heat transfer in D”

• Brillouin spectroscopy
  – Elasticity of low-Fe ppv

• Element partitioning among pv, ppv, mw, and Fe
  – Geochemistry of D”
Experimentally determined velocity anisotropy

Calculated elastic moduli of post-perovskite phase (GPa), at selected pressures and temperatures

<table>
<thead>
<tr>
<th></th>
<th>P/GPa</th>
<th>T/K</th>
<th>$C_{11}$</th>
<th>$C_{22}$</th>
<th>$C_{33}$</th>
<th>$C_{12}$</th>
<th>$C_{13}$</th>
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<td>604</td>
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- a: Taken from Oganov and Ono [37]—20-atom cell, 6×6×4 Monkhorst–Pack grid and 500 eV cut-off.
- b: Taken from Tsuchiya et al. [39]—20-atom cell, 4×4×2 Monkhorst–Pack grid and 950 eV cut-off.
- c: Taken from Itaki et al. [40]—20-atom cell, 8×2×4 Monkhorst–Pack grid and 800 eV cut-off.
- d: This work-static optimisation using 20-atom cell, 6×6×6 Monkhorst–Pack grid and 600 eV cut-off.
- e: This work-static optimisation using 60-atom cell, only Γ-point considered and 500 eV cut-off.
- f: This work-molecular dynamics using 60-atom cell, only Γ-point considered and 500 eV cut-off.

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