Post-perovskite phase transition and mineral chemistry in the pyrolitic lowermost mantle

Murakami et al., 2005
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This study investigates:

- Pressure and temperature of the post-perovskite phase change
- Iron partitioning between MgPv and Mw and between MgPP (post-perovskite phase) and Mw
- Possible correlation with and implications for the seismic D” layer

Sample set-up

- P-T conditions generated using LHDAC methods
- Starting material was a gel with chemical composition of KLB-1 peridotite (similar to pyrolite)
- Sample plate was about 20 μm, covered with 60 nm thick gold film on both sides as pressure standard, loaded in rhenium gasket
- NaCl insulation layer, except in one experiment where sample was sandwiched by pure KLB-1 gel layers

Experimental procedures

- In situ angle dispersive x-ray diffraction
- ~50 μm area heated using double-side heating, minimizing temperature gradient
- Temperature uncertainty: +/- 200K with NaCl, +/- 400K without
- Ten experiments at P of 38 to 126 GPa and T of 1950 to 2550 K; each run was done for a single P-T of interest
- Recovered samples were trimmed of insulating layers and Ar-ion thinned

Analytical procedures

- Tsuchiya (2003) EOS of gold used– gives higher pressure at lower mantle conditions than other EOS
- Pressure uncertainty derived from temperature error in EOS.
- Chemical analyses of recovered samples made with transmission electron microscope (TEM) at 200 kV
- Composition calculated using experimentally determined K-factor
- Analytical uncertainty less than +/- 10%

Pv and PP stability

- MgPv + Mw + CaPv observed up to 103 GPa; no minor modification of pv seen
- Above 115 GPa, MgPP + Mw + CaPv stable.
- Splitting of CaPv peak observed for quenched samples above 114 GPa, indicating tetragonal structure; upon heating, became sharp single peak.

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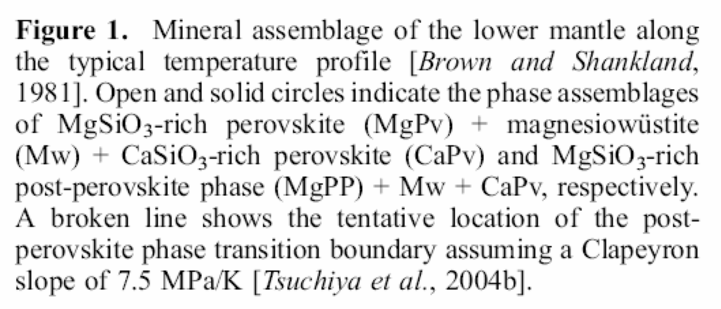

Figure 1. Mineral assemblage of the lower mantle along the typical temperature profile [*Brown and Shankland*, 1981]. Open and solid circles indicate the phase assemblages of $MgSiO_3$-rich perovskite (MgPv) + magnesiowüstite (Mw) + $CaSiO_3$-rich perovskite (CaPv) and $MgSiO_3$-rich post-perovskite phase (MgPP) + Mw + CaPv, respectively. A broken line shows the tentative location of the post-perovskite phase transition boundary assuming a Clapeyron slope of 7.5 MPa/K [*Tsuchiya et al.*, 2004b].

Review for the seismologists

- $2\lambda=2d\sin\theta$
  - For a given wavelength, there is only one angle theta at which the waves will constructively interfere
- Each peak in the diffraction spectrum corresponds to a different hkl plane
- Non-cubic structure will cause splitting of the peaks

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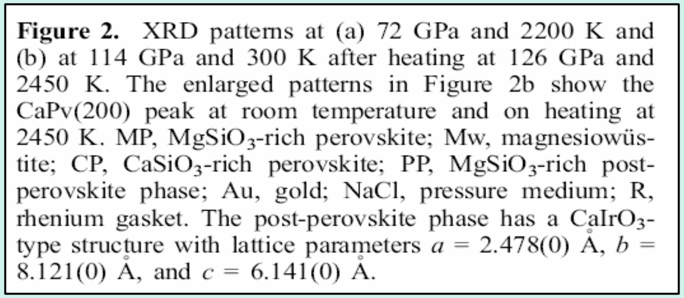

Figure 2. XRD patterns at (a) 72 GPa and 2200 K and (b) at 114 GPa and 300 K after heating at 126 GPa and 2450 K. The enlarged patterns in Figure 2b show the CaPv(200) peak at room temperature and on heating at 2450 K. MP, $MgSiO_3$-rich perovskite; Mw, magnesiowüstite; CP, $CaSiO_3$-rich perovskite; PP, $MgSiO_3$-rich post-perovskite phase; Au, gold; NaCl, pressure medium; R, rhenium gasket. The post-perovskite phase has a $CaIrO_3$-type structure with lattice parameters a = 2.478(0) Å, b = 8.121(0) Å, and c = 6.141(0) Å.

Implications for D” ?

- PP phase change occurs about 113 GPa and 2500K….~2500km depth (400km above CMB)
- If other gold EOSs are used, pressure decreases by 4 to 8 GPa.
- D” is 2600-2700 km depth
- Difference could be due to uncertainty in P
- May be that D” boundary is not a phase change– velocity increase (~3%) is too large compared to theoretical calculations
- Could be onset of strong preferred orientation under the strong shear flow within the MgPP dominant mantle (??)

Iron partitioning

- Iron depletion at heating spot; typical of LHDAC experiments due to large thermal gradient
- Fe-Mg partition coefficient between Mw and MgPv– K(Mw/MgPv)– is 2.0-2.4 at P from 38 to 92 GPa

K(Mw/MgPv) = $(Fe_{Mw}/Mg_{Mw})/(Fe_{MgPv}/Mg_{MgPv})$

- K(Mw/MgPP) is 7.8 (+/- 2.5)– iron partitions strongly into Mw
- “Space for cations” argument: shorter Mg-O distances in MgPP than in MgPv unfavorable for large Fe^{2+} if it is in the high spin state

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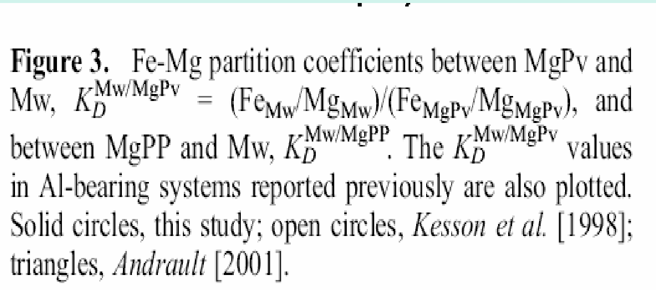

Figure 3. Fe-Mg partition coefficients between MgPv and Mw, $K_D^{Mw/MgPv} = (Fe_{Mw}/Mg_{Mw})/(Fe_{MgPv}/Mg_{MgPv})$, and between MgPP and Mw, $K_D^{Mw/MgPP}$. The $K_D^{Mw/MgPv}$ values in Al-bearing systems reported previously are also plotted. Solid circles, this study; open circles, *Kesson et al.* [1998]; triangles, *Andrault* [2001].

Implications of Fe-partitioning

- Fe affects viscosity, electrical conductivity, radiative heat transfer, and melting reaction
- Suggests Fe-poor MgPP has higher melting T than MgPv, higher viscosity, lower conductivity, whereas Fe-rich Mw has high conductivity, low viscosity
- *Yamazaki and Karato* (2001) suggested Mw occurs as films after large shear strains due to convection– possible that viscosity and conductivity vary dramatically on very small vertical scales in the lowermost mantle

Table 1. Representative Phase Chemistry of the Lower Mantle[a]

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Conclusions

- MgPv – MgPP phase change occurs about 113 GPa and 2500K
- Too shallow for D” – alternative explanation may be preferred orientation due to shear flow
- Fe partitions strongly into Mw from MgPP, much less strongly from MgPv
- Fe partitioning may have dramatic effects on lowermost mantle physical properties and flow