

## Summary of Dan Shim's lecture on 3/1/05

### Phase transitions in the Earth's mantle

In this lecture, we focused on phase transitions associated with the transition zone

1. 410 km alpha "olivine" → beta "wadsleyite"
2. 660 km gamma "ringwoodite" → perovskite
3. D'' perovskite → post perovskite

PREM → the large velocity jump at ~ 3000 km depth corresponds to the CMB. This is the most significant discontinuity, because it is a chemical transition, not isochemical. Smaller jumps at 410 and 660 km are associated with phase changes in the olivine [(Mg,Fe)<sub>2</sub>SiO<sub>4</sub>] system

NAME	STRUCTURE	A.K.A.
Olivine		α phase
Wadselyite	modified spinel	β phase
Ringwoodite	true spinel	γ phase
* + Periclase	Perovskite + NaCl	

- = perovskite doesn't have a name because it hasn't been observed in nature

In the lower mantle, dominant mineralogy is perovskite [(Mg,Fe)SiO<sub>3</sub>]  
The pyrolite mantle consists of: 60% olivine and 40% pyroxene.

Why do we have phase transitions at high P, T?

### **CRYSTALLOGRAPHY REVIEW**

Highest efficient packing = Hexagonal Close Packed

Close Packed structure has three sites:

Tetrahedral Site: cation surrounded by 4 oxygen (CN=4)

Octahedral Site: " " " 6 " (CN=6)

Dodecahedral " " 12 " (CN=12)

CN= coordination number ≡ number of anions surrounding particular cation and can be 2 – 3 – 4 – 6 – 8 – 12. The available site volume increases with increasing coordination number; distance between cation & anion also increases

Interstitial sites

T (tetrahedral) → coordinated by 4 O's (SMALLEST interstitial site)

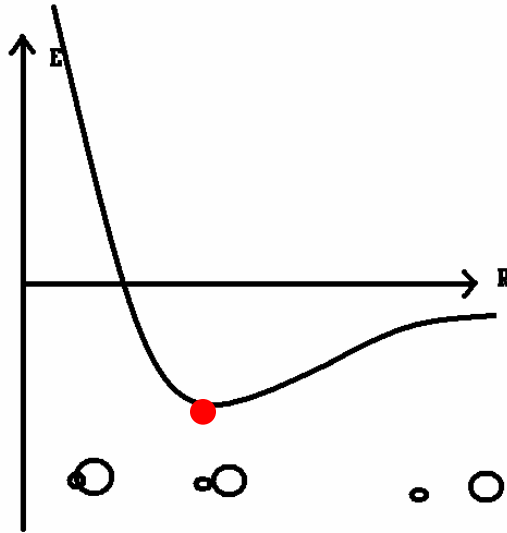
O (octahedral) → coordinated by 6 O's

(dodecahedral) → coordinated by 12 O's (LARGER interstitial site)  
Comparative size of ions →  $O^{2-} \gg Ca^{+2} > Mg^{+2} > Fe^{+2} > Fe^{+3} > Al^{+3} > Si^{+4}$

For typical silicate minerals:

- Si, Al = tetrahedral site (smallest ion)
- Mg, Fe = octahedral site (intermediate sized ion)
- Ca, O = dodecahedral site (largest ion)

Inter-atomic potential



Red dot represents the lowest energy = two hard spheres in contact.

Other crystallographic considerations are:

Corner sharing (more favorable), edge sharing, face sharing (less favorable)

### ***PHASE TRANSITIONS:***

Two major types:

CN number change (atomic arrangement)

Structural change (bond lengths)

Examples:

**Olivine – Wadsleyite (410 km):**

Oxygen lattice changes from HCP (hexagonal close packed) to FCC (face centered cubic)

**Wadsleyite – Ringwoodite (520 km):**

Redistribution of Si

**Pyroxene – Garnet**

CN # change

**Ringwoodite & Garnet – Perovskite (660 km):**

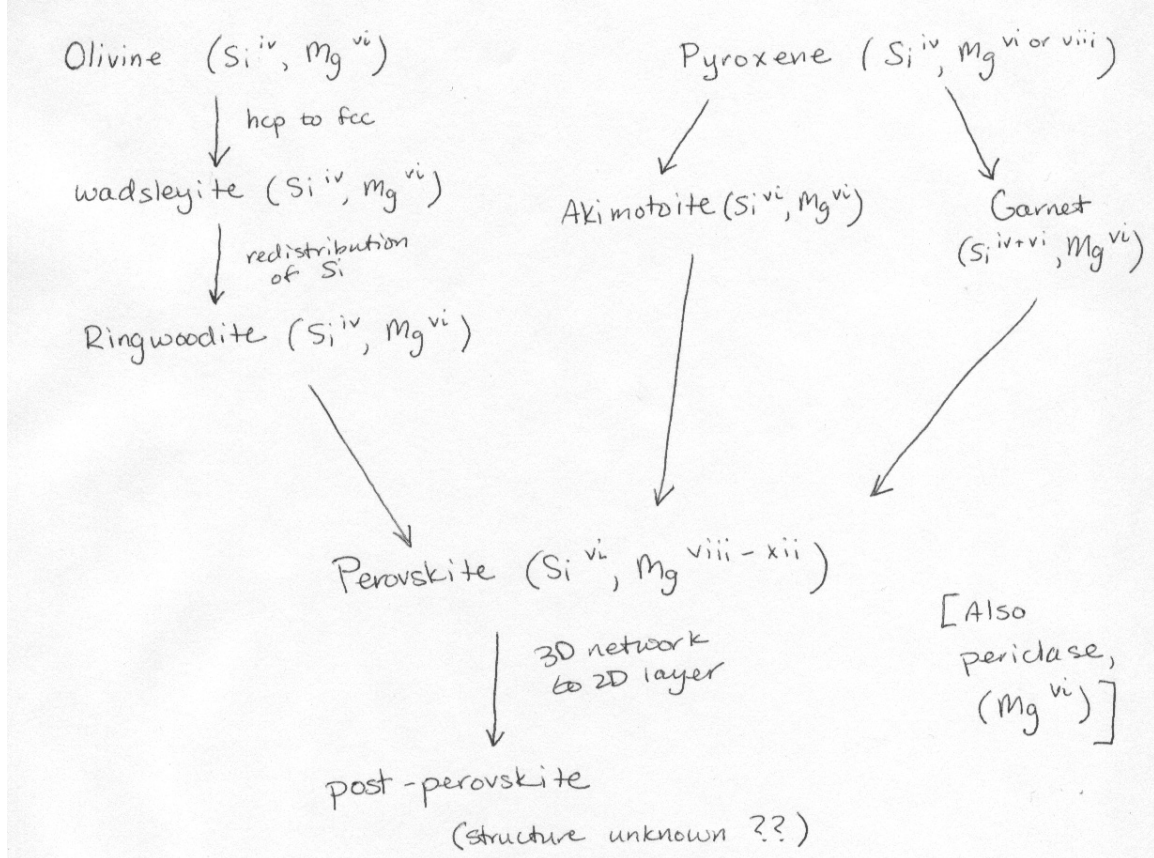
CN # change

**Perovskite – Post Perovskite (~2900 km)**

PPv structure unknown

Transition thought to be Mg CN# change

Chart of phase changes in the mantle



perovskite 10% Fe  
magnesiowüstite 20-30% Fe

Experimental Techniques

A comparative chart:

Technique	P, GPa	$\sigma(P)$ , GPa	T, K	$\sigma(T)$ , K	sample
MA	< 30	1	< 2500	50	high volume
LHDAC	< 150	5	1500-4000	100-200	low volume

*Pressure Measurement Methods*

Oil (limited at high pressure)

Calibration curve (using phase transitions)

Equation of state (standard material (gold))  
*Temperature Measurement Methods*  
 Thermocouple (ex. K type) (Voltage-Temperature calibration is done at 0 GPa (at high pressure this relationship is unknown))  
 Radiometry

Transition Zone Phase Transitions

Phase diagram for  $(\text{Mg,Fe})_2\text{SiO}_4$

Image removed due to copyright considerations.

Please see:

Ahrens, T. J. *Mineral Physics & Crystallography: A Handbook of Physical Constants*. Washington, DC: American Geophysical Union, 1995.

**Clapeyron Slope:** (dP/dT of phase transition boundary)

$\alpha - \beta$  +2.5 - 4.0

$\beta - \gamma$  + 5.0 - 6.9 (topography will be higher induced by thermal anomaly)

post-spinel -2.5 - 3.0

post-ilmenite -2.5 - 3.0

post-garnet +2.4



Near 660 km

Implications of Clapeyron slopes for mantle transitions

Hot upwellings vs. cold downwellings → dynamics considerations

**Discrepancies between experimental mineral physics and seismology that have not been resolved**

Transition intervals for experimentally determined phase transitions

410 km -  $\Delta Z$  13 km

520 km -  $\Delta Z$  40 km

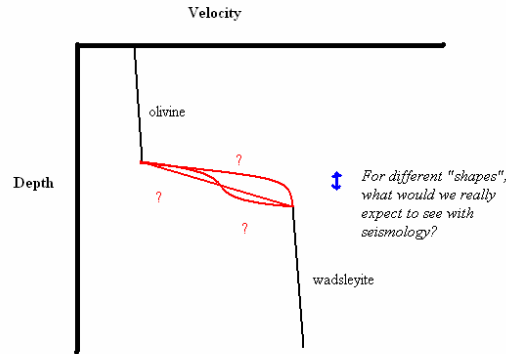
660 km -  $\Delta Z$  3 km

Thickness of 410 km:

Looks like ~ 5km from seismology; smaller than predicted by mineral physics (~ 13 km)

This could be due to:

1. the effects of iron (partitioning between different phases)
2. the effects of water
3. or the seismic signal may not record the entire transition zone. For example, if we look at the details of the olivine-wadsleyite phase transition, the volume fraction of the coexisting phases that exist through the transition interval may not be linear with depth; therefore the density contrast may not be linear with depth as well.



What is the “shape” of the transition, and which part of it would we expect to be sensitive to with seismology?

At what pressure (depth) does the post-spinel boundary occur?

Irifune et al. 1998 → ~600 km ???

How explain this?

T = 1200°?!?!? NO!

Different composition?

Incorrect pressure scale in experiment?

### Post Perovskite:

MgSiO<sub>3</sub> perovskite (orthorhombic, pbnm, 2D) → MgSiO<sub>3</sub> post-perovskite (orthorhombic, cmcm, 3D)

- Pressure ambiguity results in a poorly constrained pressure and temperature of the phase transformation.
- Clapeyron slope is not constrained experimentally
  - Seismic ~6 MPa/K
  - Ab initio +9.56 – 9.85 MPa/K
  - +7.5 ± 0.3 MPa/K
- Change in bulk/shear moduli?
  - ΔV<sub>P</sub> = ~ 0.3%
  - ΔV<sub>S</sub> = ~ 1.5% (larger change in shear velocity...)

- Density increase  $\sim 1 - 1.5\%$
- Elastic anisotropy?
- Contamination of Fe in perovskite results in a shallower transition (1% Fe increase can change the elevation 30-50 km)

Potential Implications for PPv transition with a large clapeyron slope:

Decrease T by 500 K may effect elevation discontinuity by 100 km

**Dynamical models** → what are the implications of the post-perovskite transition?

Nakagama & Tackley (2004) → implications for plume generation?

Depth variations of the post-perovskite boundary

Large Clapeyron slope →  $\sim 100$ km of topography on phase boundary possible?

Composition effects?

What is the temperature gradient at the CMB?

Heat from the core?

(Experimental constraints: melting curve of iron, melting curve of lower mantle silicates...)

What are the implications for D''? Anisotropy?