CIDER 2006 Summer Program

Mineral Physics Component

Min Phys I Thermodynamics (Lars)

Min Phys 2 Mantle Mineralogy (Lars)

Tutorial 1 Constructing Earth Models (Lars)

Tutorial 2 Melts (Marc)

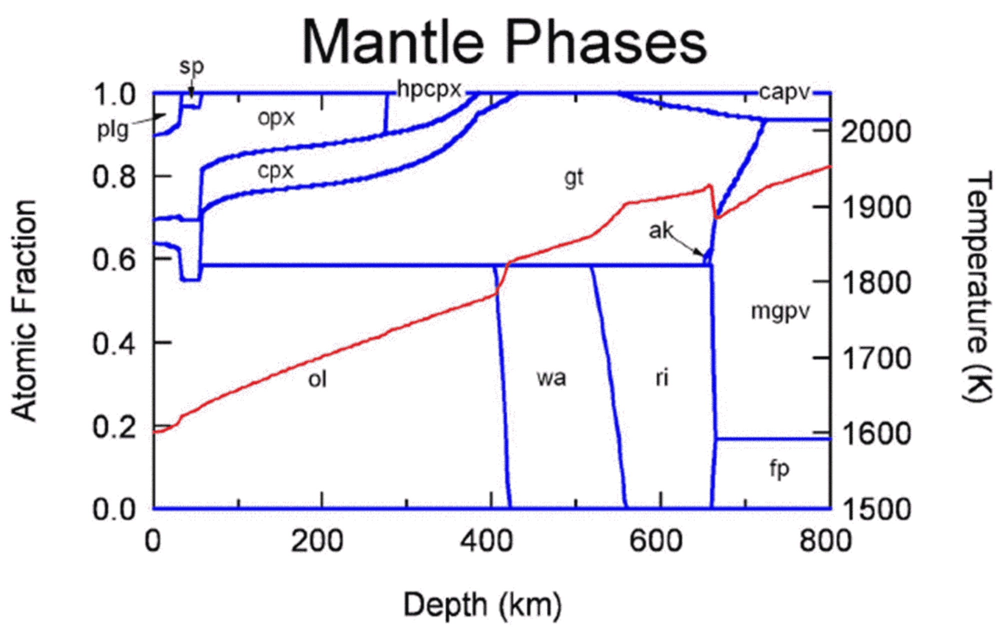
Min Phys 3 Equation of state and Lattice Dynamics (Tom)

→ Min Phys 4 Phase Equilibria (Marc)

Min Phys 5 Elasticity (Tom)

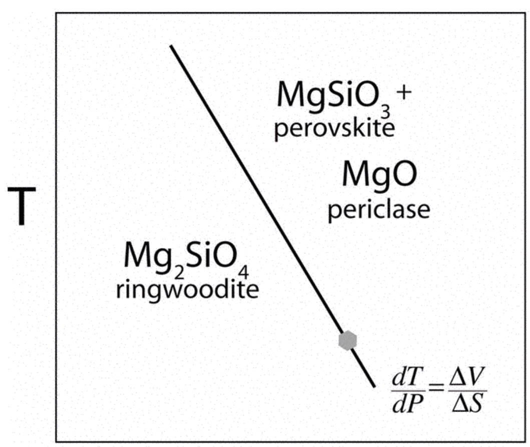
Tutorial 3 Equation of state data analysis (Tom)

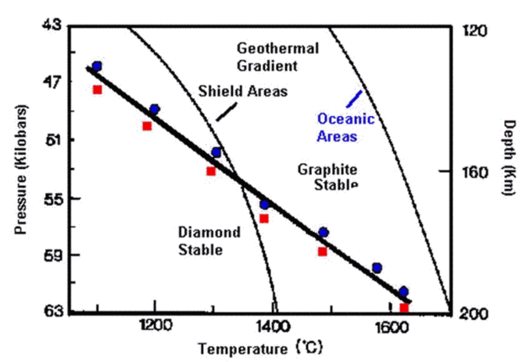
Min Phys 6 Fluids and Melts (Marc)



Wadsleyite (wa); Ringwoodite (ri); akimotoite (ak); Mg-perovskite (mgpv); Ca-perovskite (capv); Ferropericlase (fp)

1. Some simple principles of phase equilibria
2. Some experimental and practical considerations
3. Topical aspects of phase equilbria in and near the transition zone





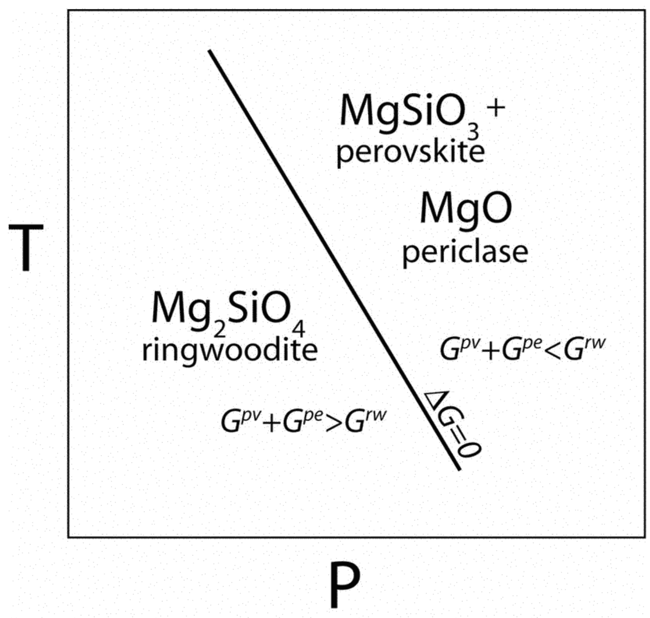
$$S = S^0 + \int_{T^0}^{T} \frac{C_p}{T} dT - \int_{P^0}^{P} V\alpha dP$$

$$V = V(T,P)$$

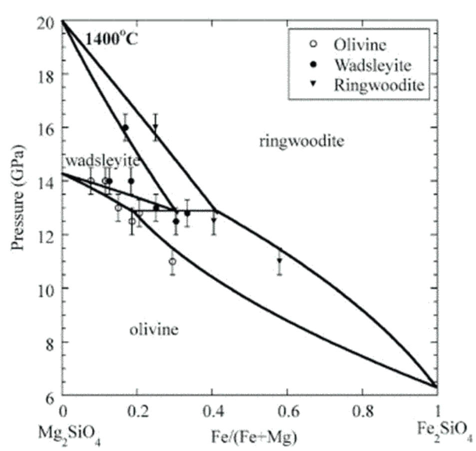
(But beware: simple thermodynamics
Can be inconvenient with some EOS)

$$P = \frac{3}{2}K\left[\left(\frac{V_0}{V}\right)^{7/3} - \left(\frac{V_0}{V}\right)^{5/3}\right]\left\{1 - \frac{3}{4}(4-K')\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]\right\}$$ B-M 3rd order

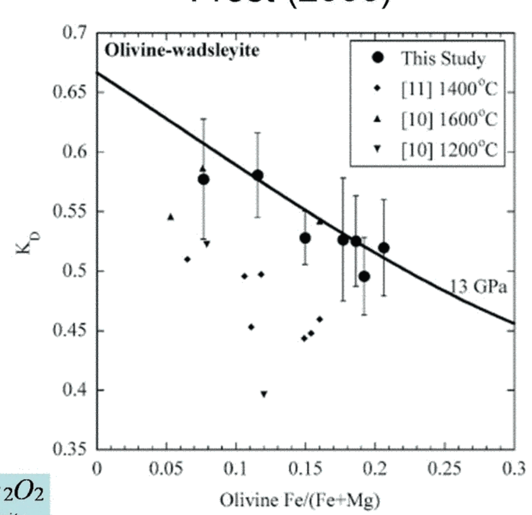
$$V(P,T) = V(1,T)\left(1 + \frac{K'P}{K_T}\right)^{1/K'}$$ Murnaghan EOS



$$0 = \Delta G = \Delta H^0 + \int_{T^0}^{T} \Delta C_p dT - T\left[\Delta S^0 + \int_{T^0}^{T} \frac{\Delta C_p}{T} dT\right] + \int_{P^0}^{P} \Delta V dP$$



Frost (2003)



$$\underset{olivine}{MgSi_{1/2}O_2} + \underset{wadsleyite}{FeSi_{1/2}O_2} \Leftrightarrow \underset{olivine}{FeSi_{1/2}O_2} + \underset{wadsleyite}{MgSi_{1/2}O_2}$$

$$\Delta G = -RT \ln \frac{a_{Mg}^{wd} a_{Fe}^{ol}}{a_{Mg}^{ol} a_{Fe}^{wd}} = -RT \ln \frac{X_{Mg}^{wd} X_{Fe}^{ol}}{X_{Mg}^{ol} X_{Fe}^{wd}} - RT \ln \frac{\gamma_{Mg}^{wd} \gamma_{Fe}^{ol}}{\gamma_{Mg}^{ol} \gamma_{Fe}^{wd}}$$

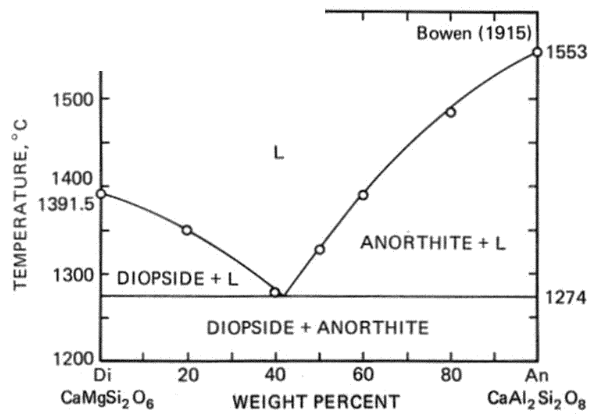
$$\Delta G = -RT \ln K_D - RT \ln \frac{\gamma_{Mg}^{wd} \gamma_{Fe}^{ol}}{\gamma_{Mg}^{ol} \gamma_{Fe}^{wd}}$$

$$a_{Mg}^{wd} = X_{Mg}^{wd} \gamma_{Mg}^{wd}$$

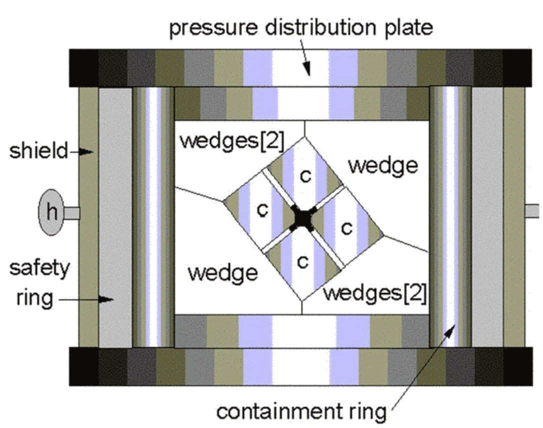
$$a_{Fe}^{wd} = X_{Fe}^{wd} \gamma_{Fe}^{wd}$$

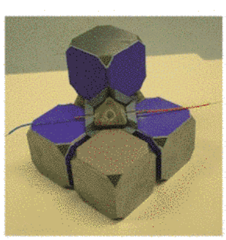
$$RT \ln \gamma_{Mg}^{wd} = W_{FeMg}^{wd} (1 - X_{Mg}^{wd})^2$$

$$RT \ln \gamma_{Fe}^{wd} = W_{FeMg}^{wd} {X_{Mg}^{wd}}^2$$

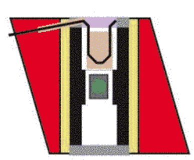


$$G^{Anorthite}_{CaAl_2Si_2O_8} = G^{Liquid}_{CaAl_2Si_2O_8} + RT \ln X^{Liquid}_{CaAl_2Si_2O_8} + RT \ln \gamma^{Liquid}_{CaAl_2Si_2O_8}$$

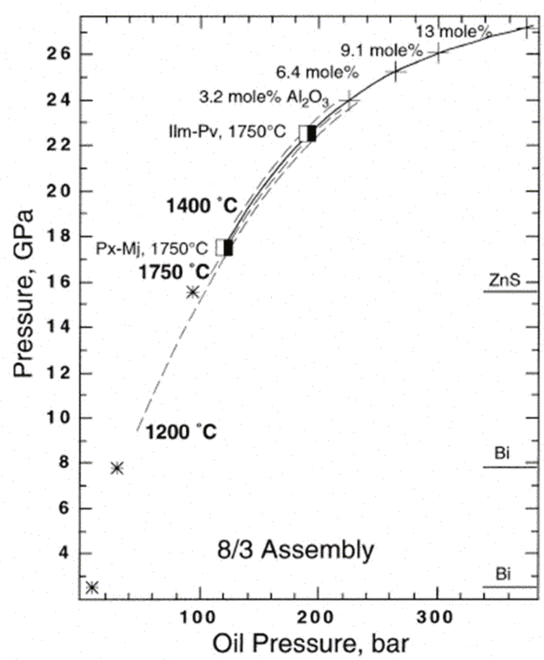


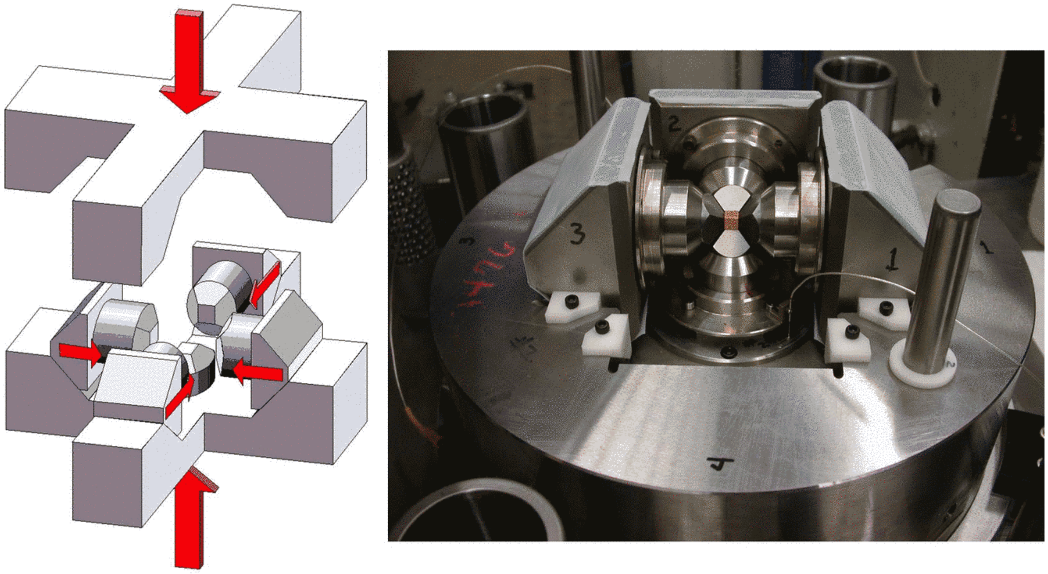


8 cubes (5 shown) press on octahedron
Gaskets are made of pyrophyllite



Cross section of octahedron shows:
MgO pressure medium (red)
ZrO2 insulator (yellow)
stepped LaCrO3 heater (black)
Mo rings (grey)
MgO insulating parts (white)
Sample (grey/green)
Thermocouple wire

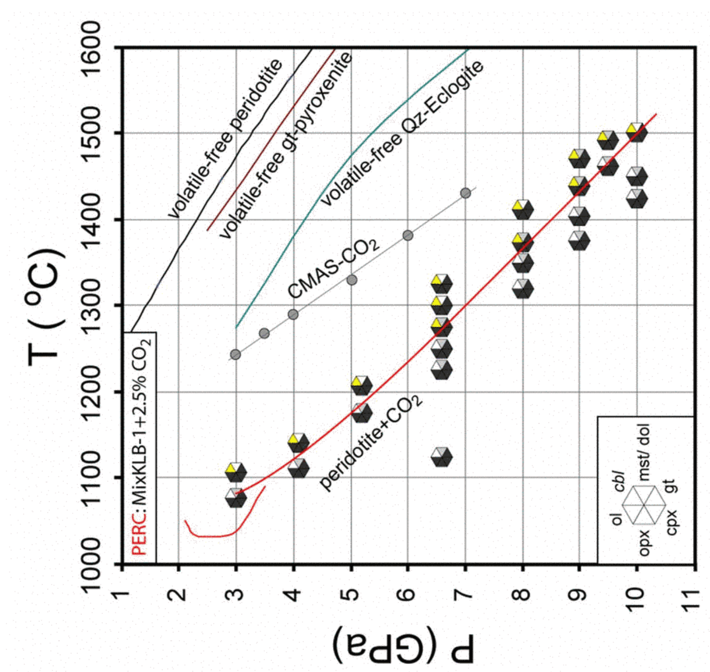




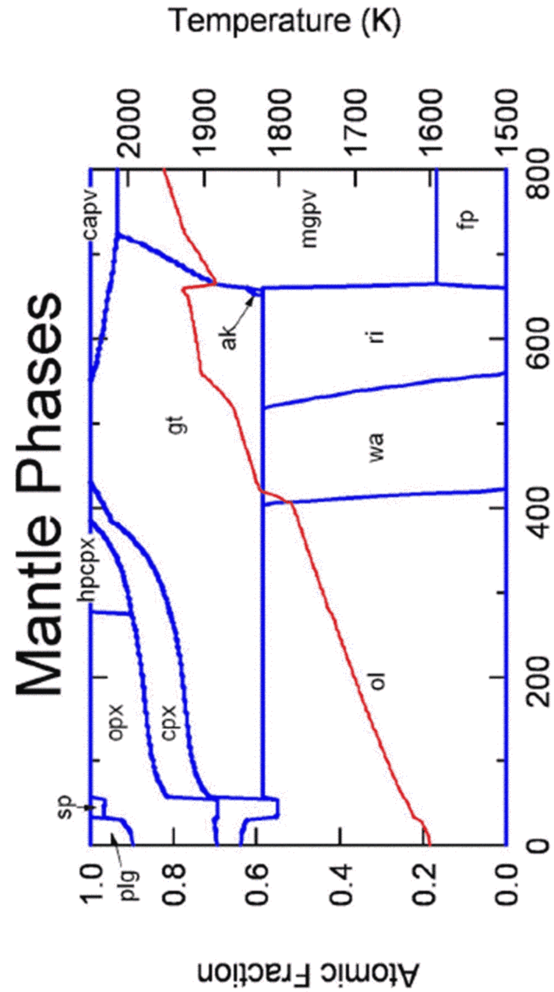
DIA Press

Why use simple or analogue materials in phase equilibria experiments?
(a partial list):

1. To isolate, detect, and characterize the effects of minor phases or components.
2. To reduce problems in experimental design.
3. To obtain results at more tractable temperatures, pressures, etc.
4. To obtain more favorable kinetics.
5. To magnify compositional effects.
6. To reduce the thermodynamic variance of the system.



Dasgupta & Hirschmann (2006)



Wadsleyite (wa); Ringwoodite (ri); akimotoite (ak); Mg-perovskite (mgpv); Ca-perovskite (capv); Ferropericlase (fp)

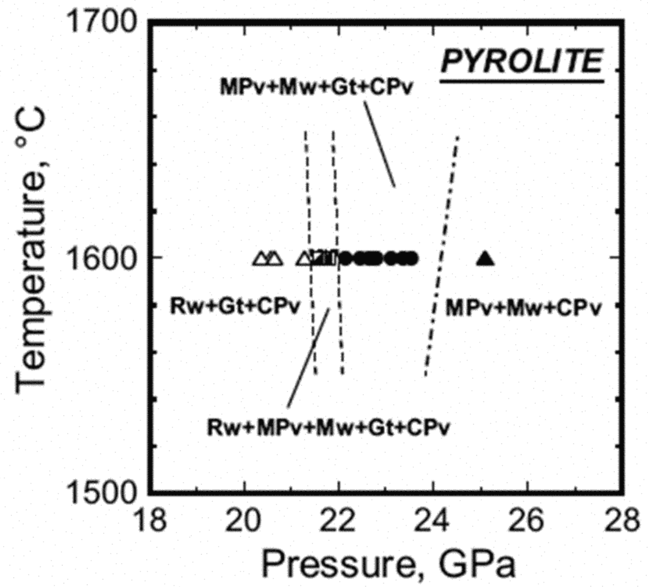
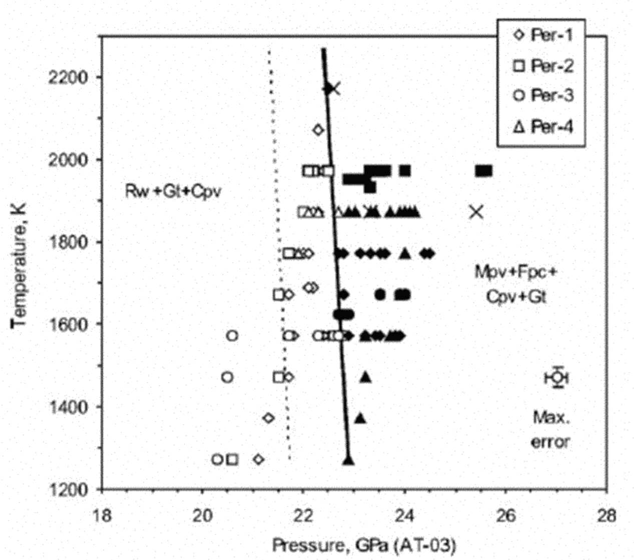
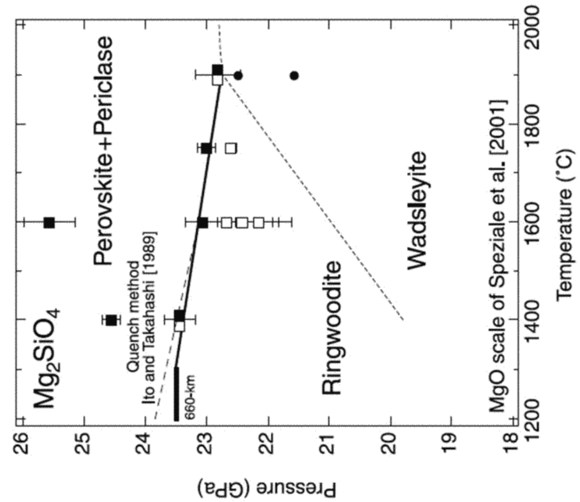


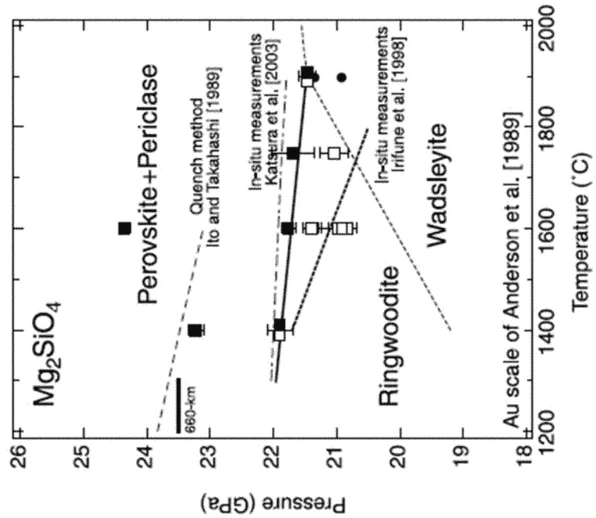
Fig. 4. Phase relations in pyrolite at 1600 °C determined on the basis of the results of in situ X-ray diffraction experiments. Dashed

Nishiyama et al. 2004 -MgO (Matsui) Pressure Scale



Litasov et al. (2004) Au (Tsuchiya, 2003) pressure scale





QuickTime™ and a TIFF (Uncompressed) decompressor are needed to see this picture.

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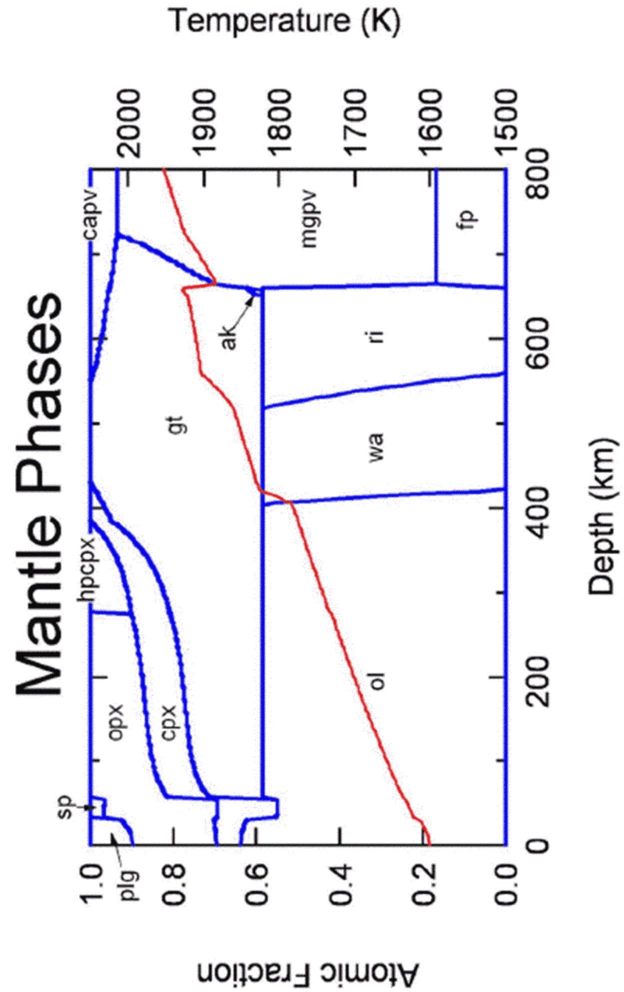
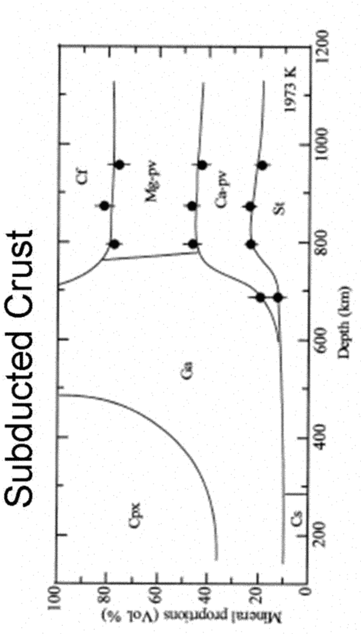
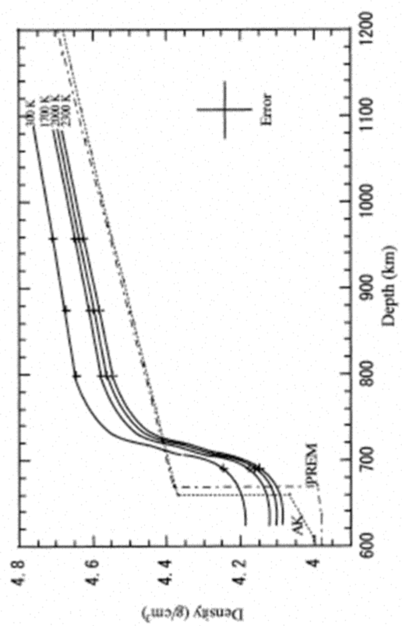
Fei et al. 2004



Wadsleyite (wa); Ringwoodite (ri); akimotoite (ak); Mg-perovskite (mgpv); Ca-perovskite (capv); Ferropericlase (fp)

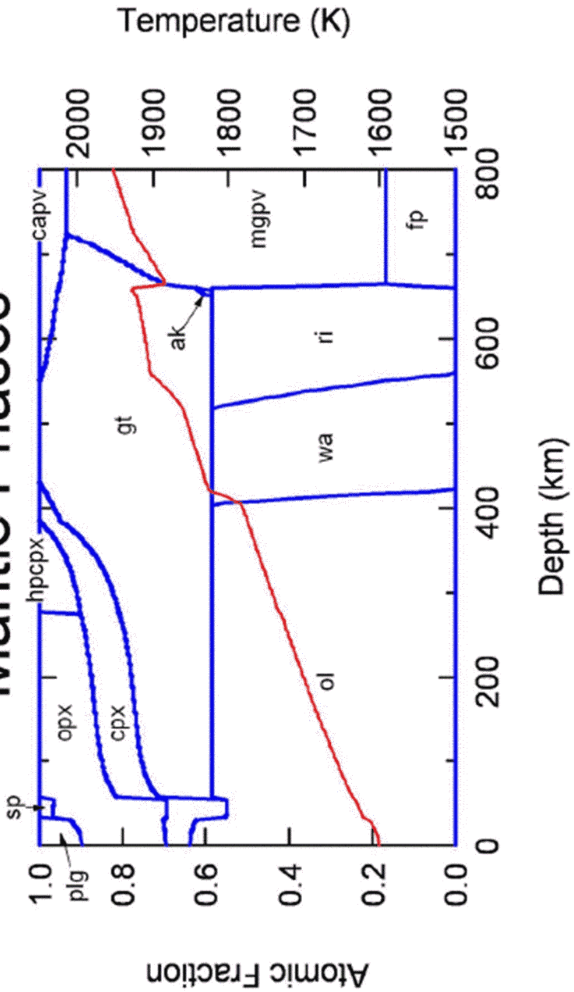
Phase Relations of Subducted Crust



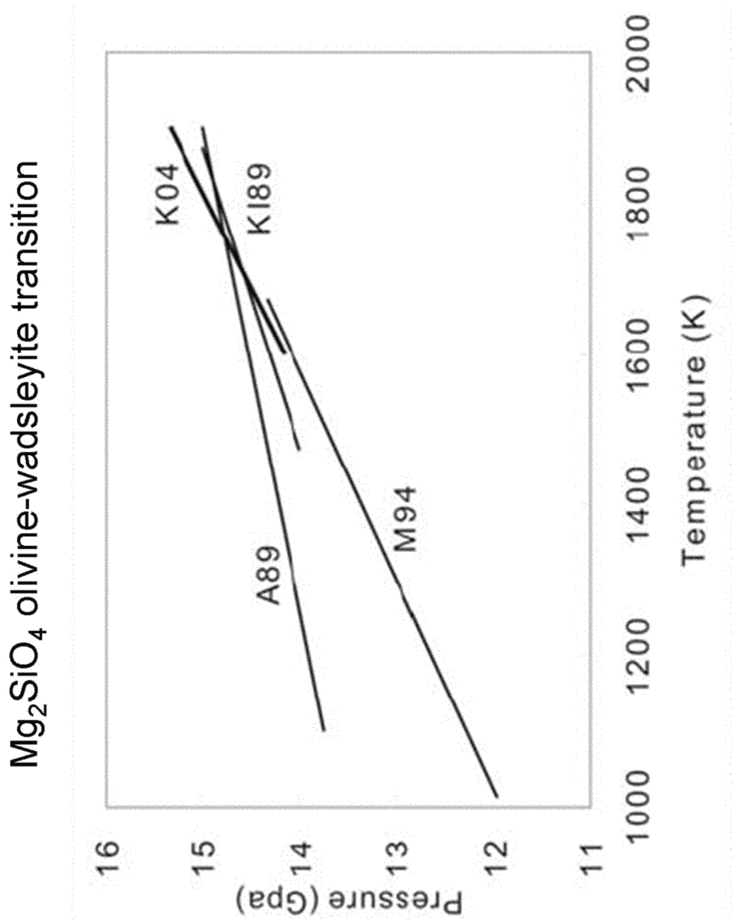


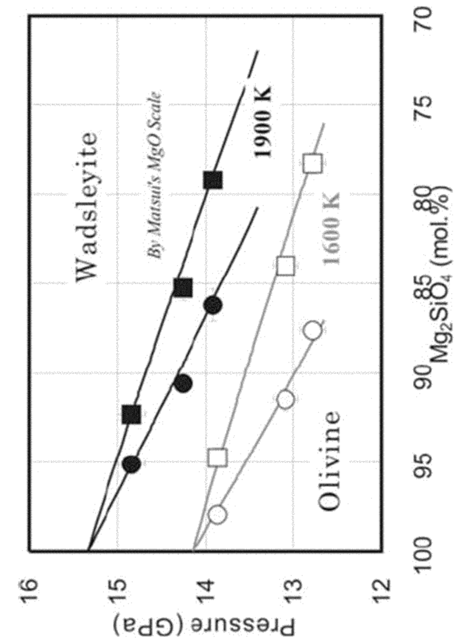
Ono et al. (2001)

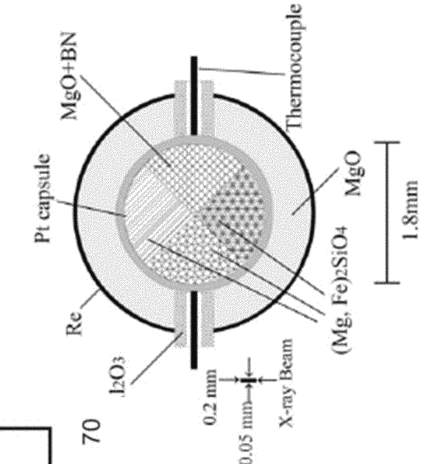
Mantle Phases



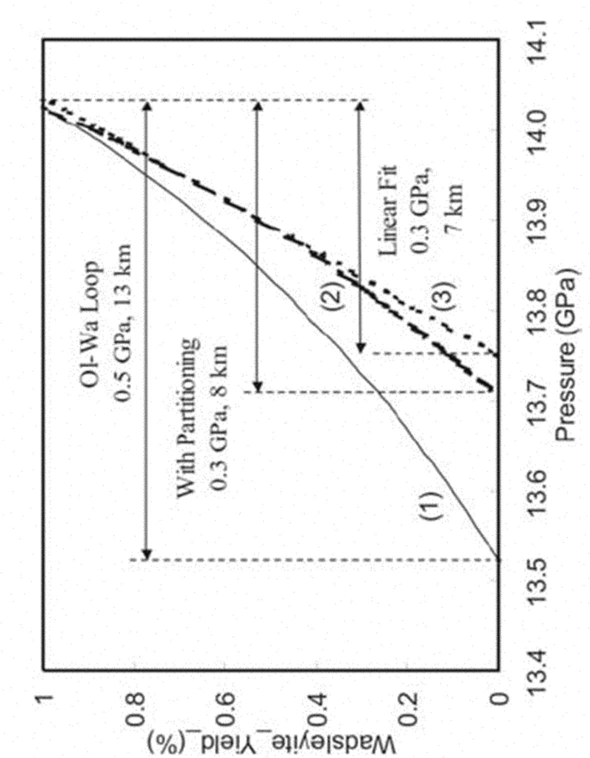
Wadsleyite (wa); Ringwoodite (ri); akimotoite (ak); Mg-perovskite (mgpv); Ca-perovskite (capv); Ferropericlase (fp)



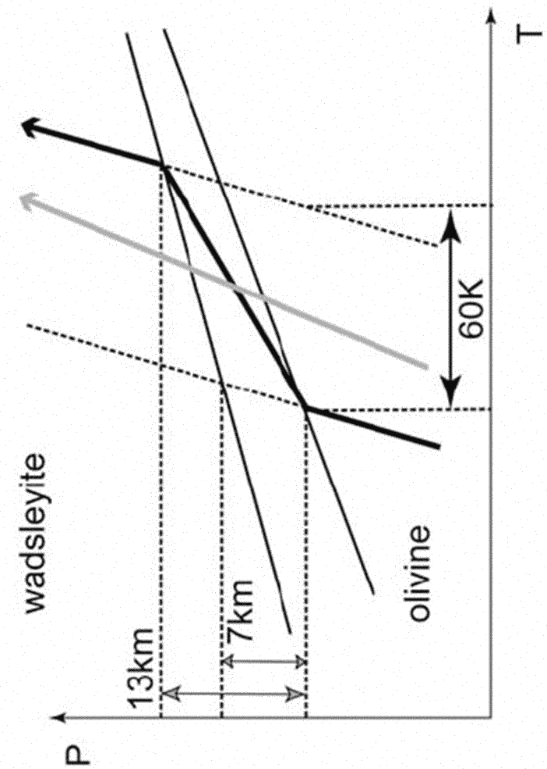




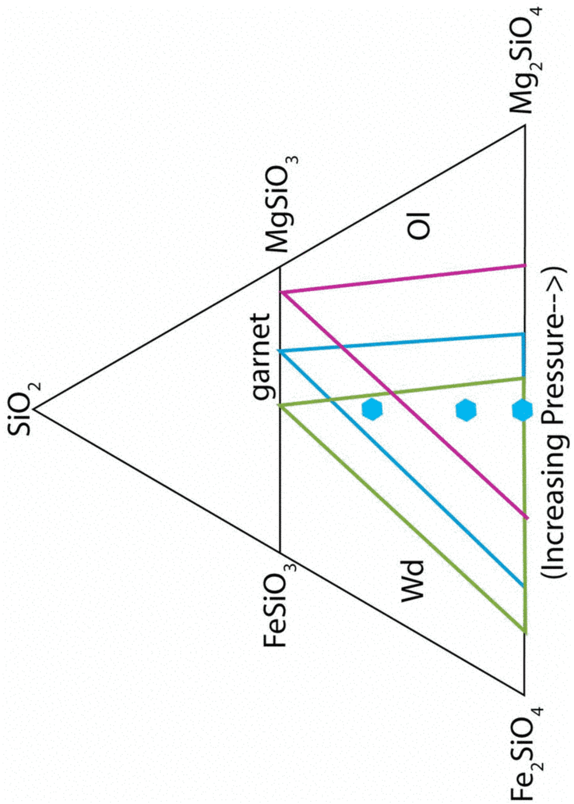
Katsura et al. (2004)



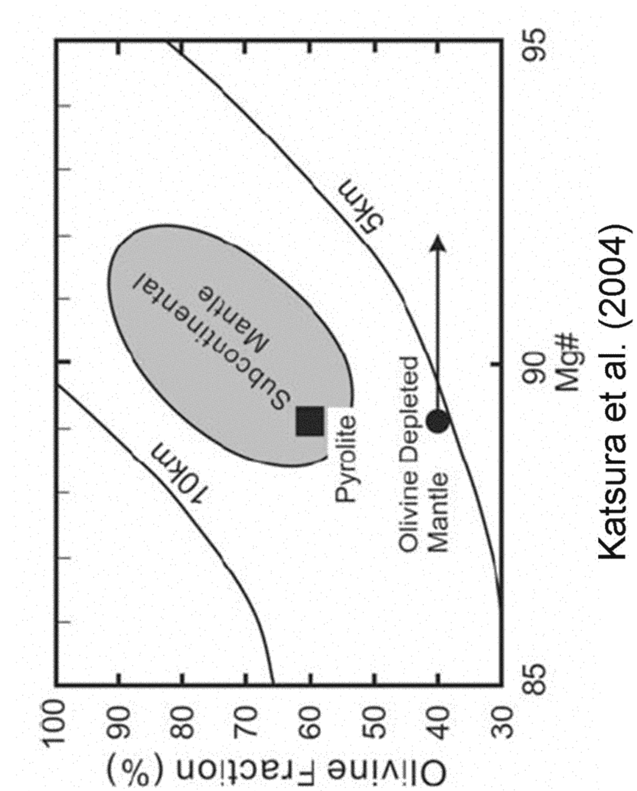
Katsura et al. (2004)



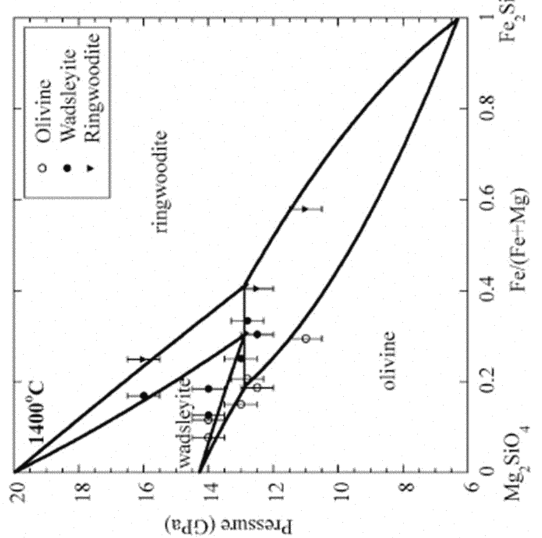
Katsura et al. (2004)

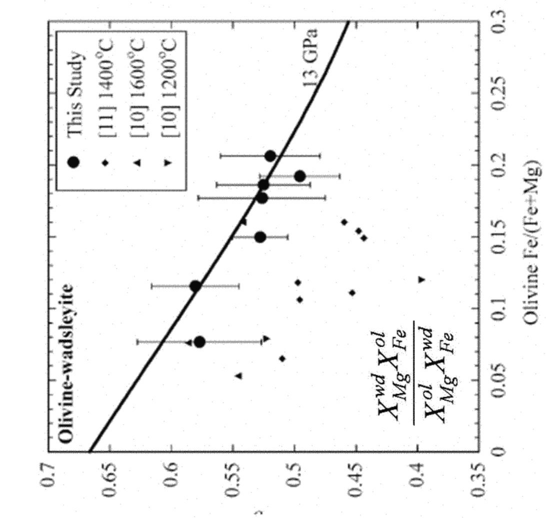


SiO_2
$MgSiO_3$
Mg_2SiO_4
$FeSiO_3$
Fe_2SiO_4
garnet
Ol
Wd
(Increasing Pressure-->)

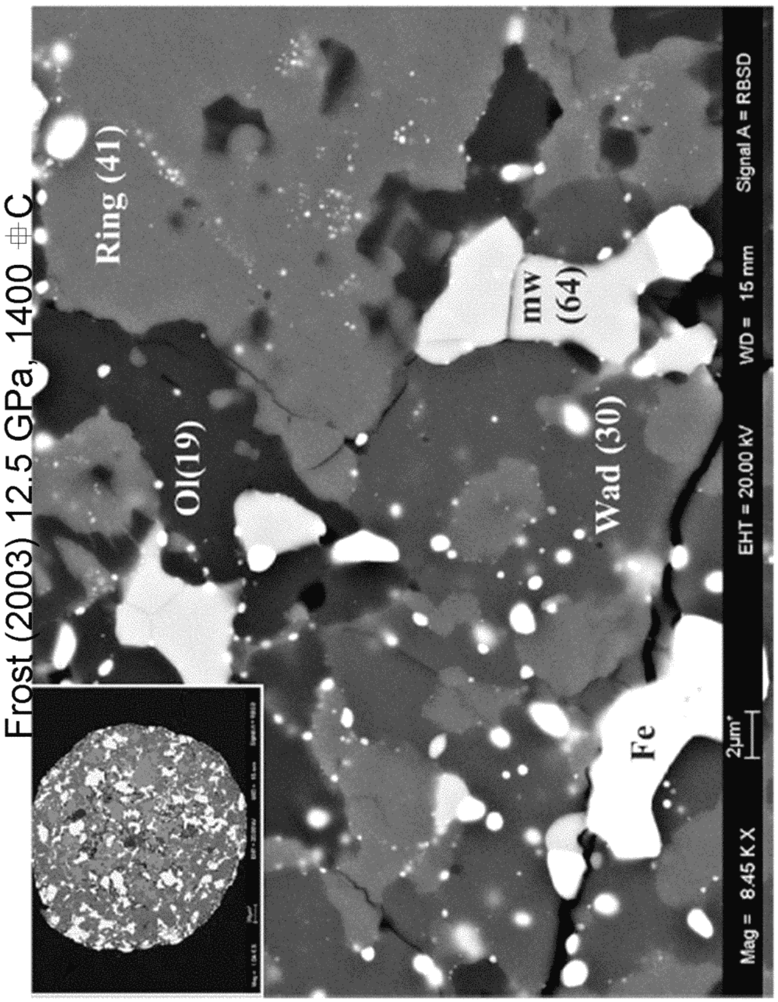


Olivine Fraction (%)
100
90
80
70
60
50
40
30
85
90
95
Mg#
5km
10km
Subcontinental Mantle
Pyrolite
Olivine Depleted Mantle
Katsura et al. (2004)

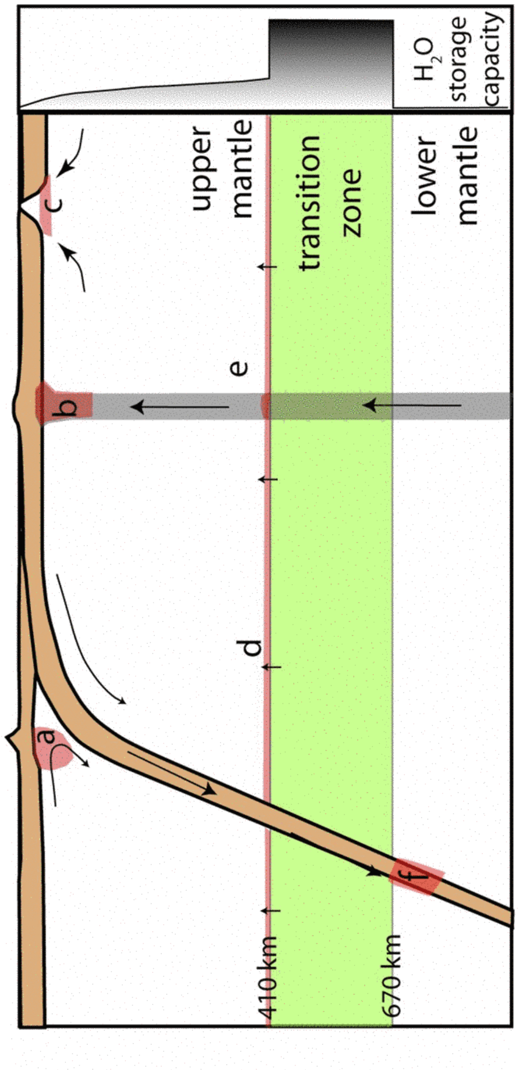


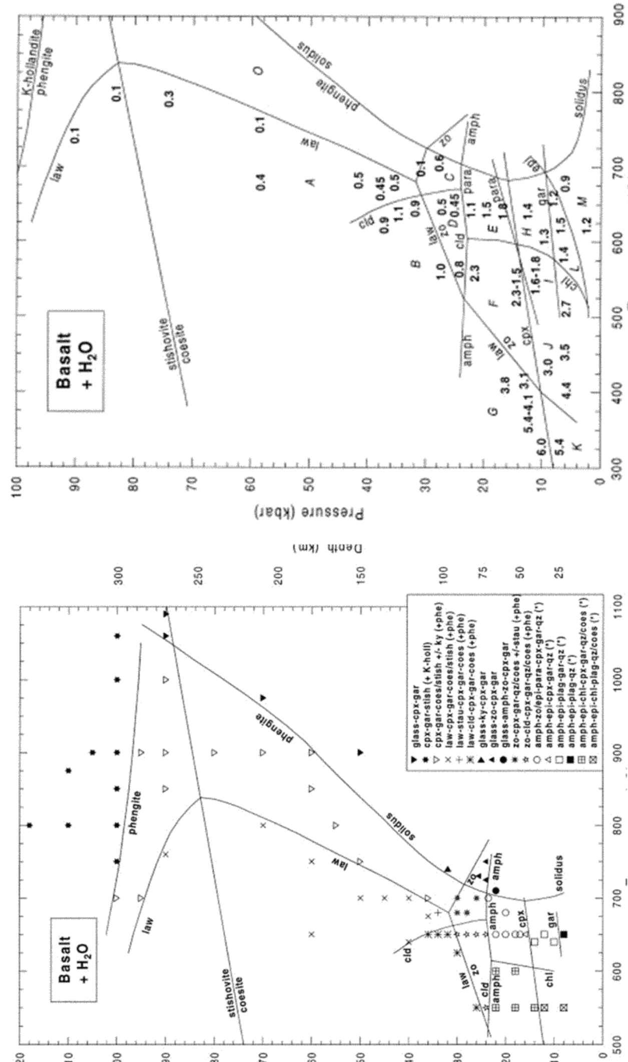


Frost, 2003

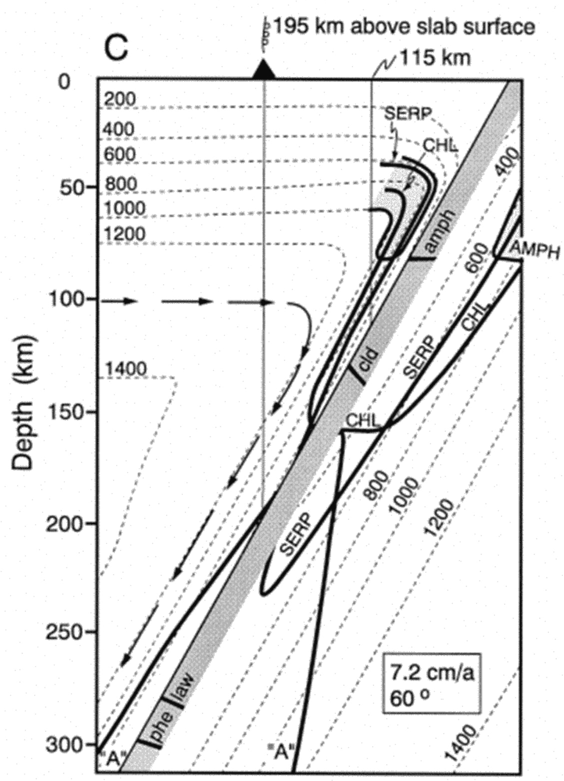


Frost (2003) 12.5 GPa, 1400 °C





Schmidt and Poli (1998)



Dense Hydrous Magnesian Silicates (DHMS)

Minerals	Formula	H_2O (wt.%)
Chlorite	$Mg_5Al_2Si_3O_{10}(OH)_8$	13
Serpentine	$Mg_3Si_2O_5(OH)_4$	4 28
Chondrodite	$Mg_5Si_2O_8(OH)_2$	5.30
Clinohumite	Mg9Si4O16(OH)2	3
10 Å Phase	$Mg_3Si_4O_{14}H_6$	13
Phase A	$Mg_7Si_2O_8(OH)_6$	12
Phase E	$Mg_{2.3}Si_{1.25}H_{2.4}O_6$	11.40
Superhydrous phase B/phase C[a]	$Mg_{10}Si_3O_{14}(OH)_4$	5.80
Phase D(G)[a]	$)_6$	14.5–18

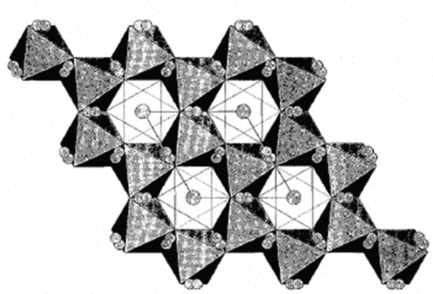
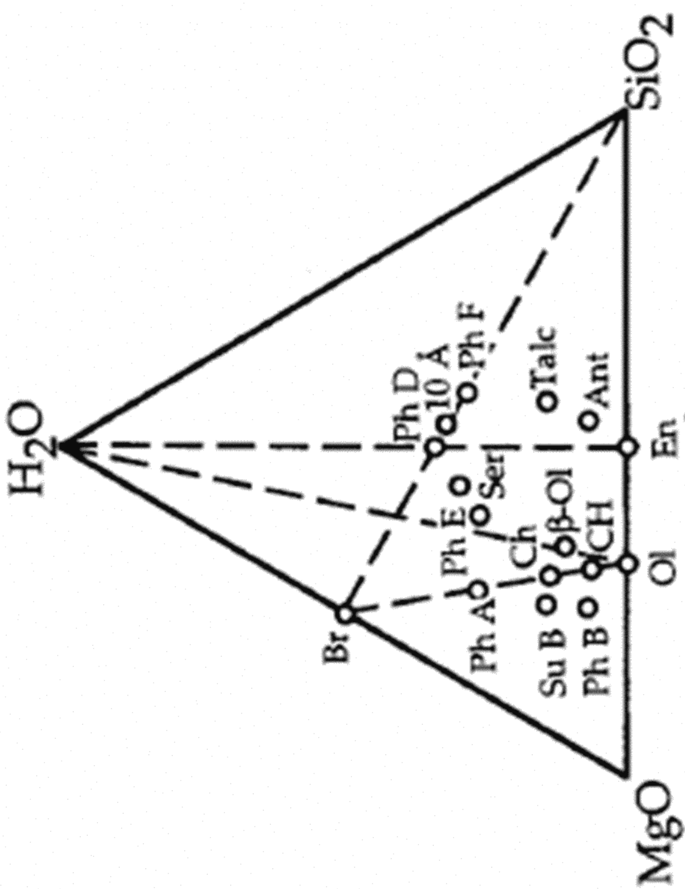
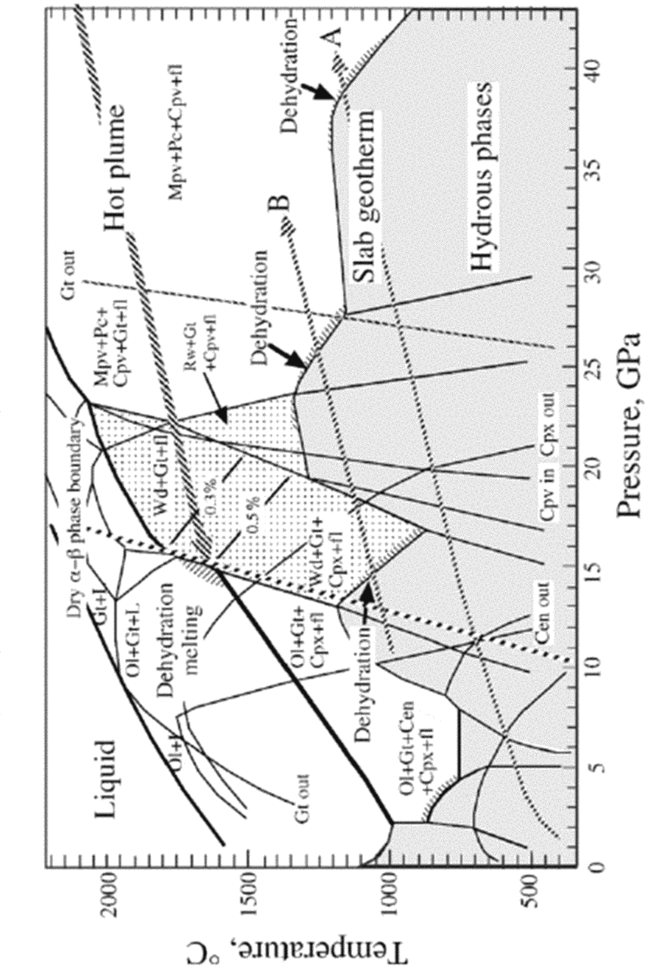


FIGURE 1. Crystal structure of phase D projected along *c*. Shaded and unshaded octahedra represent SiO_6 and MgO_6 octahedra, respectively. Large spheres represent Mg and small ones H.





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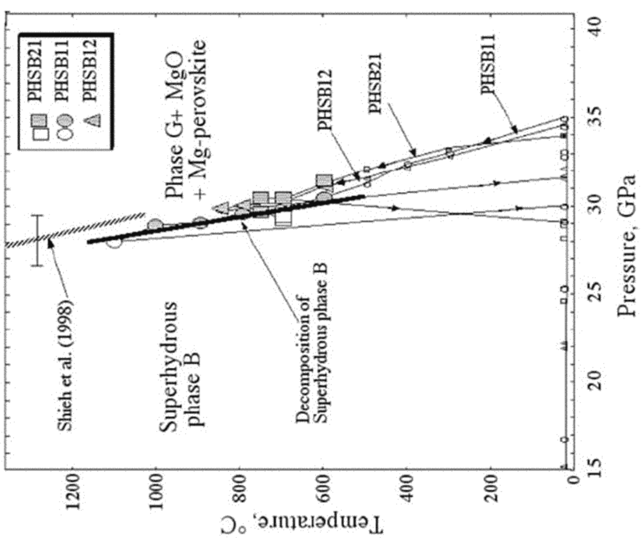


1 - 2 OHTANI ET AL.: IN SITU X-RAY OBSERVATION O

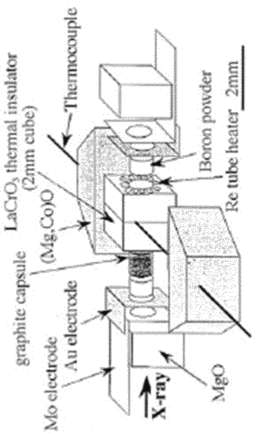
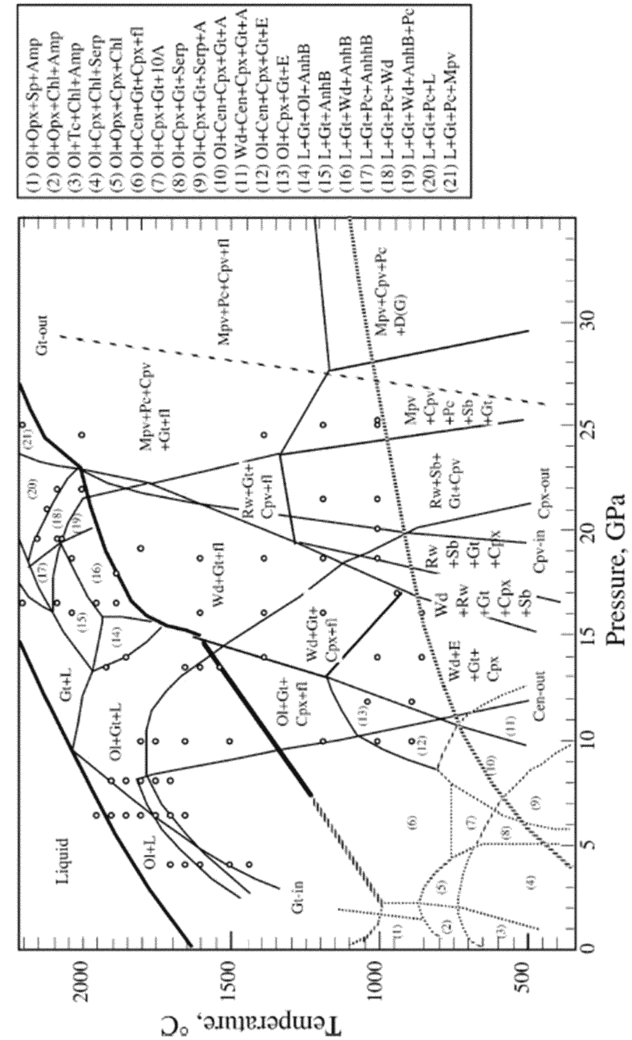
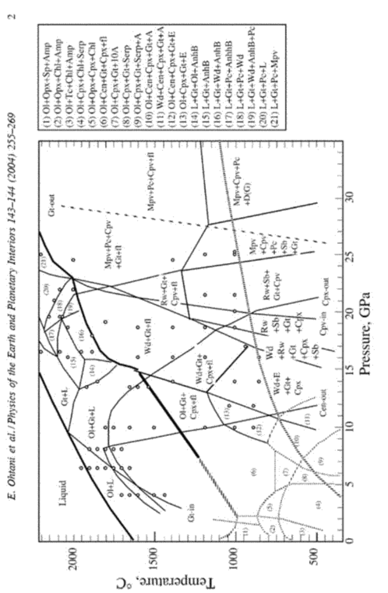
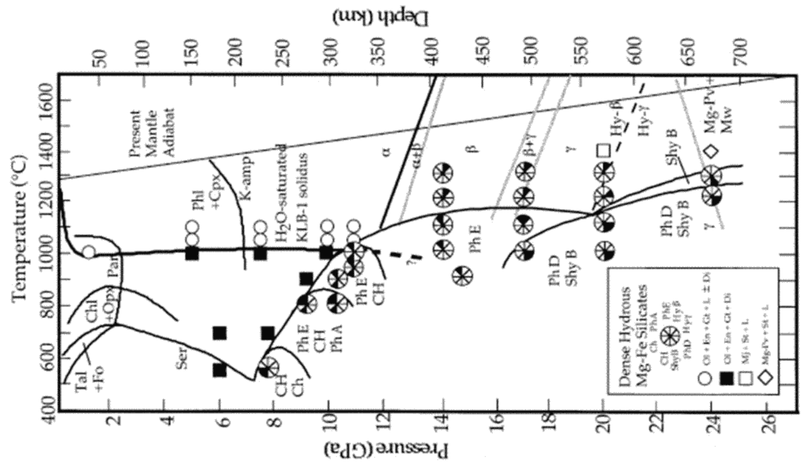


Figure 1. Furnace assembly used for in situ X-ray diffraction at high pressure and temperature.

E. Ohtani et al. / Physics of the Earth and Planetary Interiors 143–144 (2004) 255–269 2







Kawamoto, 2004

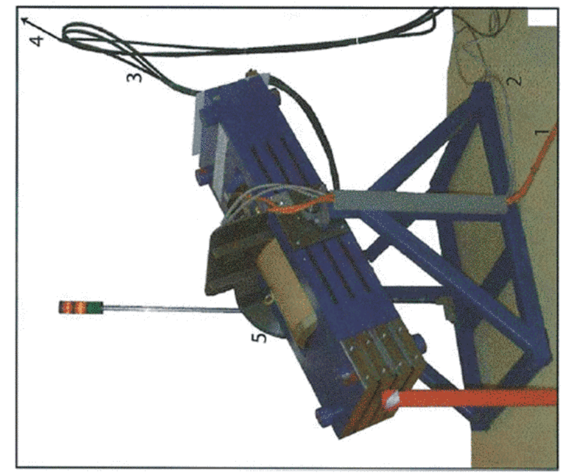
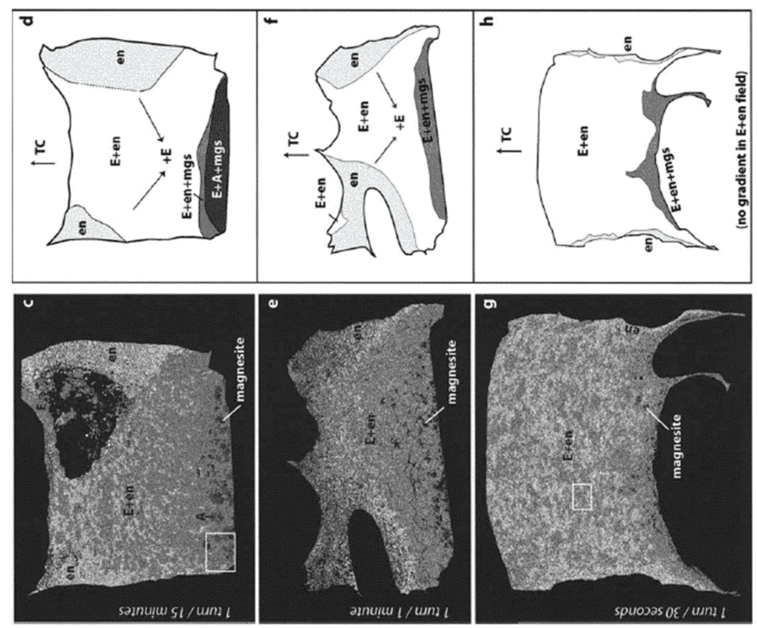
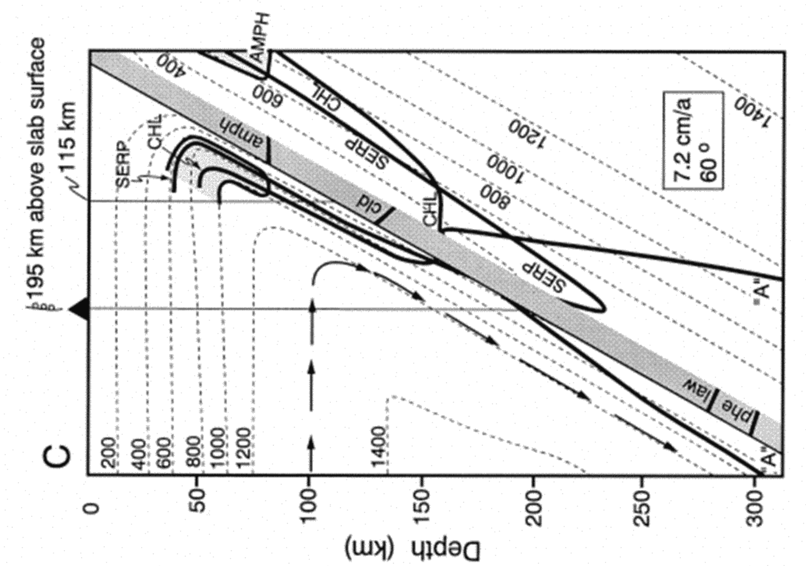
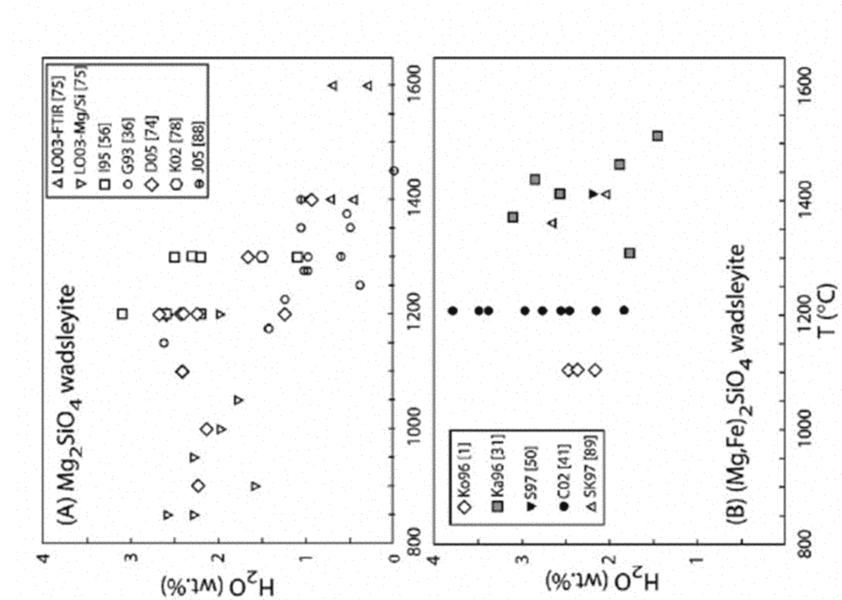


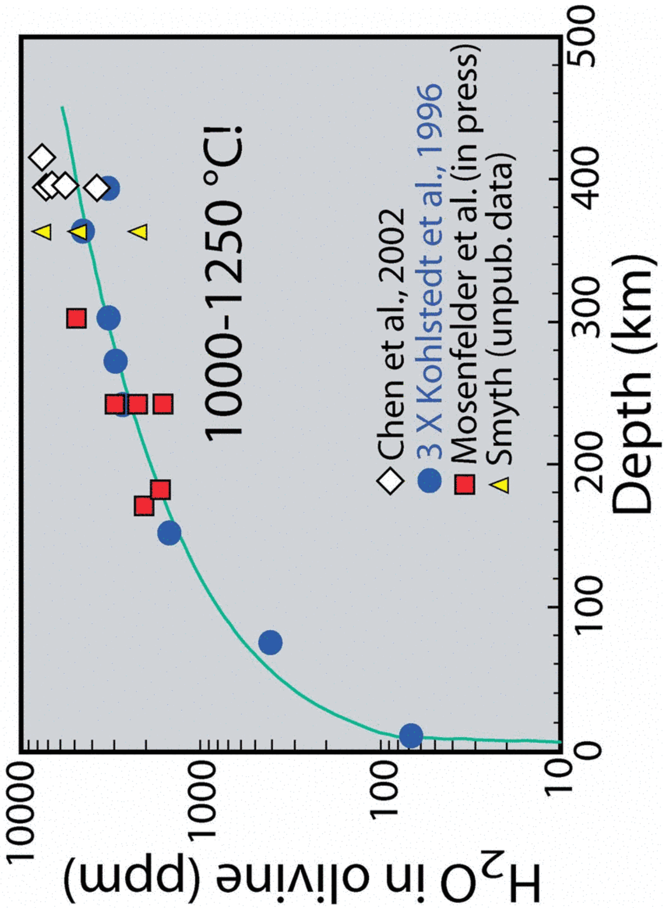
Fig. 2. Rocking multianvil device; 600-ton O-frame press with 6/8 cylindrical multianvil module. 1: Power cables; 2: cooling water hoses; 3: hydraulic pressure hoses; 4: pull-out wire; arrow indicates where fixed to the wall; 5: sprocket wheel.

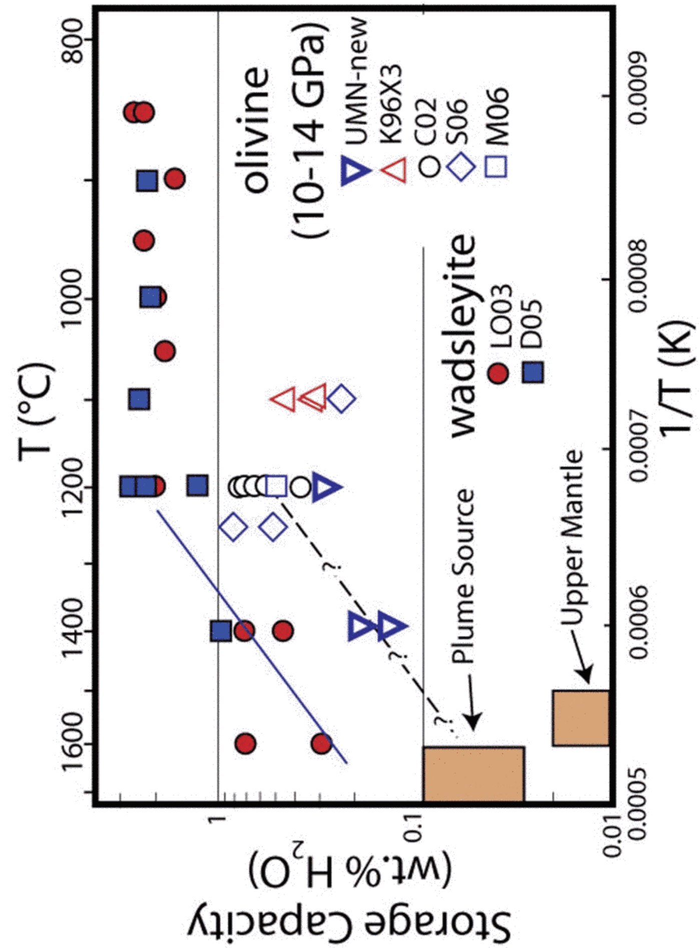
Schmidt+Ulmer, 2004

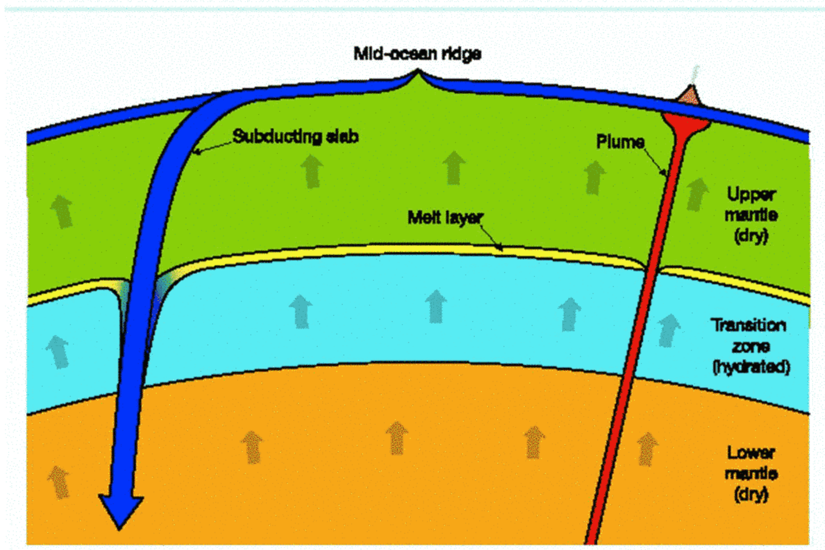



C
195 km above slab surface
115 km
Depth (km)
7.2 cm/a
60 °
SERP
CHL
AMPH
amph
cld
phe
law
"A"
"A'"


(A) Mg_2SiO_4 wadsleyite
(B) $(Mg,Fe)_2SiO_4$ wadsleyite
H_2O (wt.%)
T (°C)
LO03-FTIR [75]
LO03-Mg/Si [75]
I95 [56]
G93 [36]
D05 [74]
K02 [78]
J05 [88]
Ko96 [1]
Ka96 [31]
S97 [50]
C02 [41]
SK97 [89]

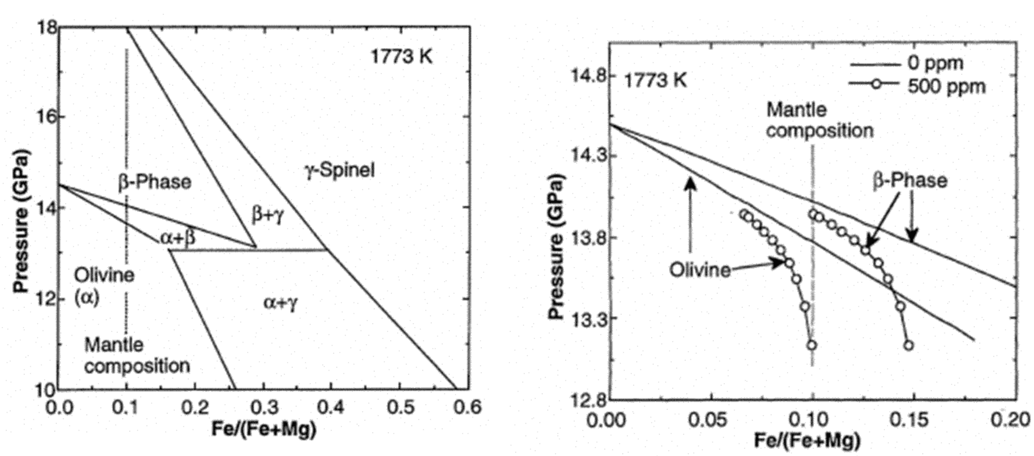

H2O in olivine (ppm)
10000
1000
100
10
0
100
200
300
400
500
Depth (km)
1000-1250 °C!
Chen et al., 2002
3 X Kohlstedt et al., 1996
Mosenfelder et al. (in press)
Smyth (unpub. data)


T (°C)
800
1000
1200
1400
1600
olivine
(10-14 GPa)
UMN-new
K96X3
C02
S06
M06
wadsleyite
LO03
D05
Plume Source
Upper Mantle
Storage Capacity
(wt.% H2O)
1
0.1
0.01
0.0005
0.0006
0.0007
0.0008
0.0009
1/T (K)

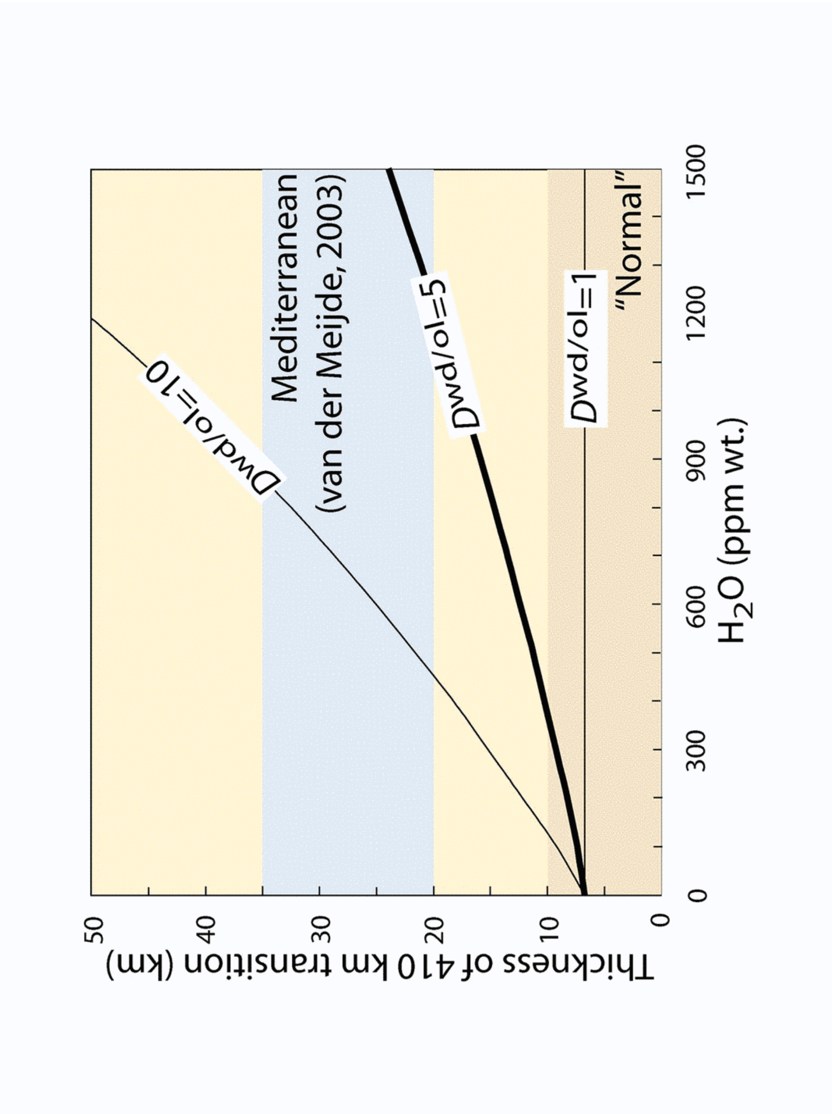


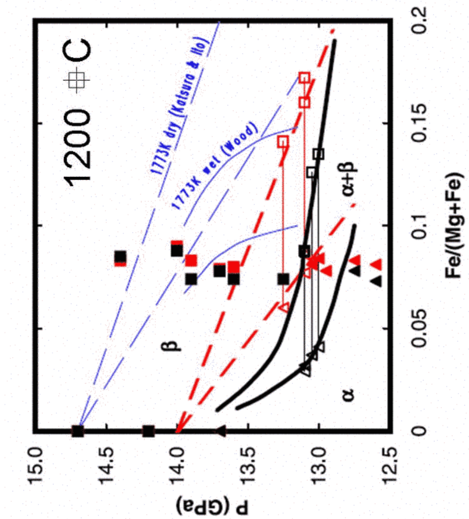
Bercovici and Karato, 2003

H_2O should thicken 410 km discontinuity

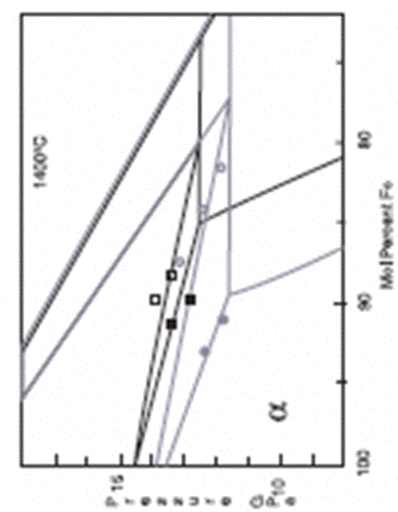


Wood, 1995

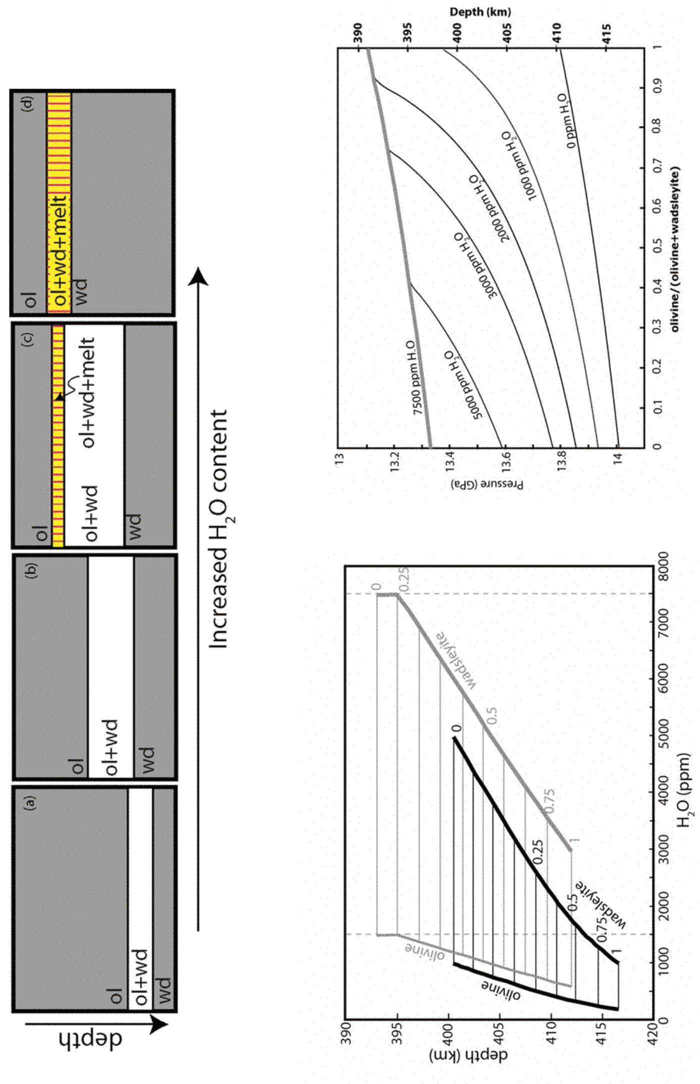




Chen et al. (2002)



Smyth and Frost (2002)


depth
(a)
ol
ol+wd
wd
(b)
(c)
ol+wd+melt
(d)
Increased H_2O content
Depth (km)
Pressure (GPa)
olivine/(olivine+wadsleyite)
0 ppm H_2O
1000 ppm H_2O
2000 ppm H_2O
3000 ppm H_2O
5000 ppm H_2O
7500 ppm H_2O
depth (km)
H_2O (ppm)
olivine
wadsleyite