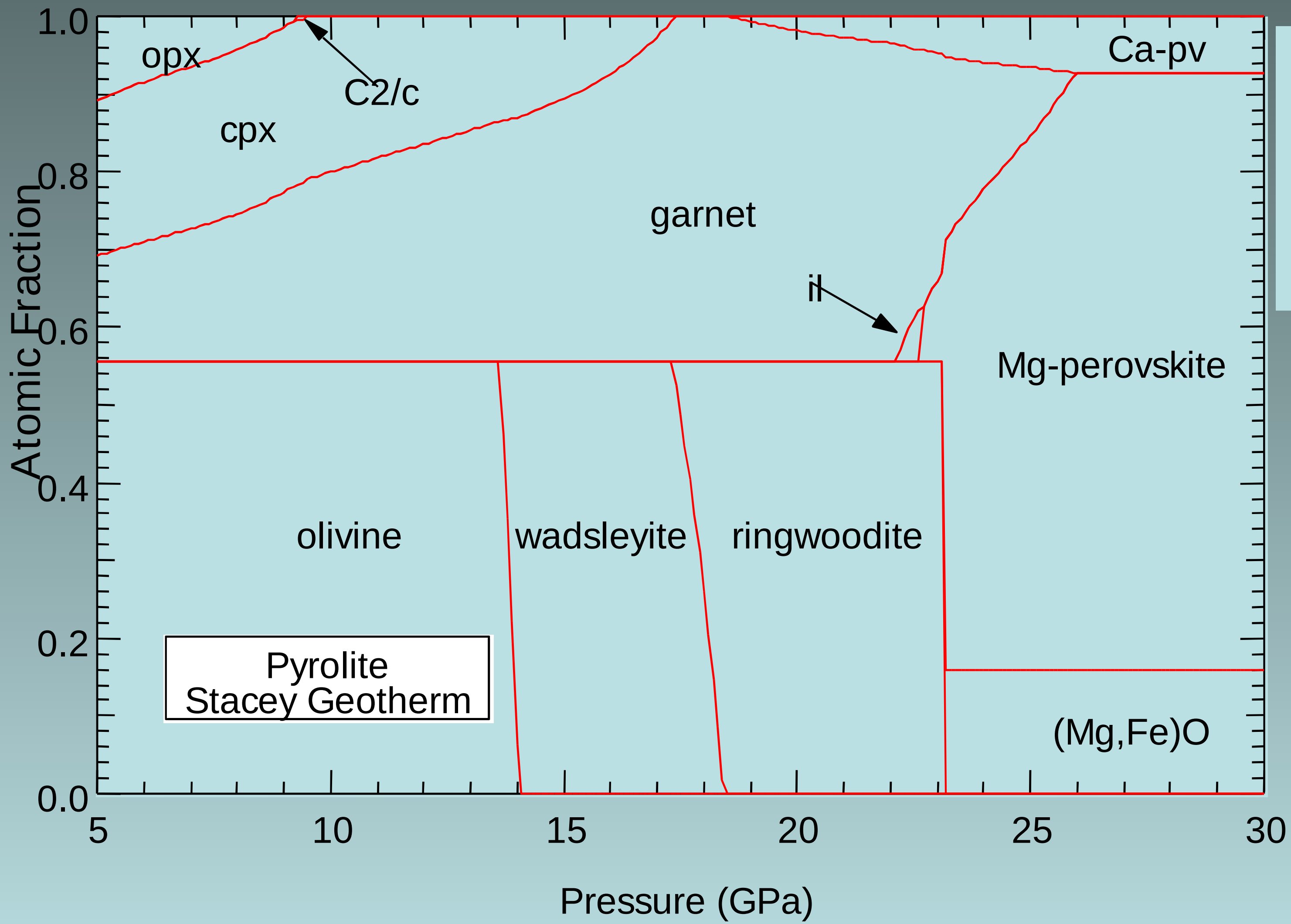
Interpreting Geophysical Data for Mantle Dynamics

Wendy Panero

University of Michigan

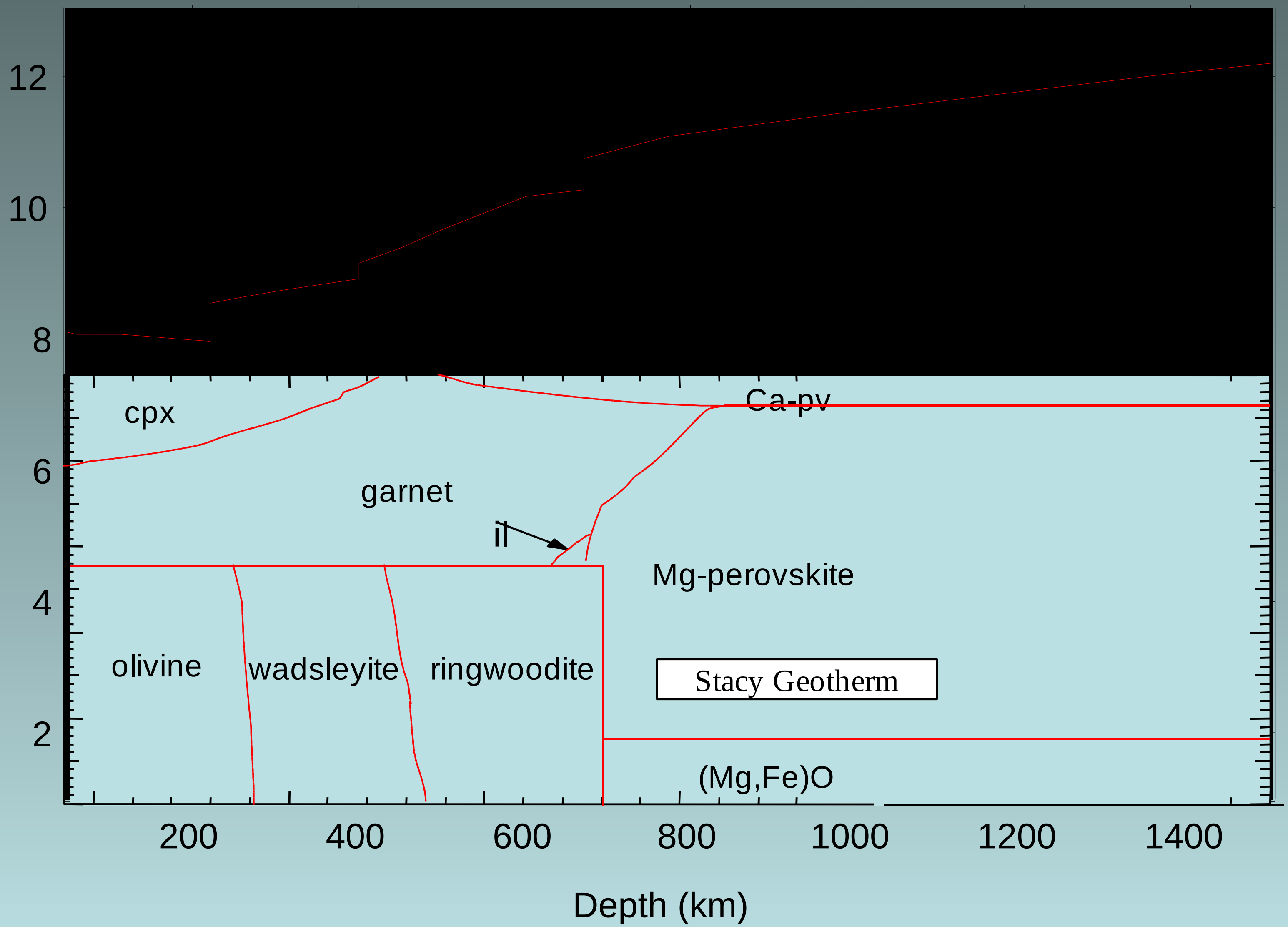
Chemical Constraints on Density Distribution



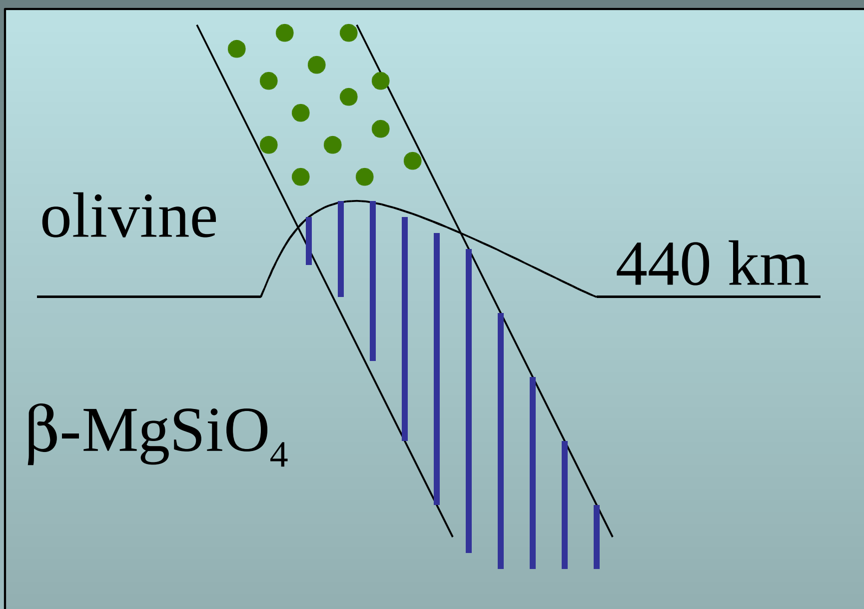
SiO_2	45.4 wt%
MgO	37.1 wt%
FeO	8.3 wt%
Al_2O_3	4.3 wt%
CaO	3.3 wt%

Stixrude, unpublished

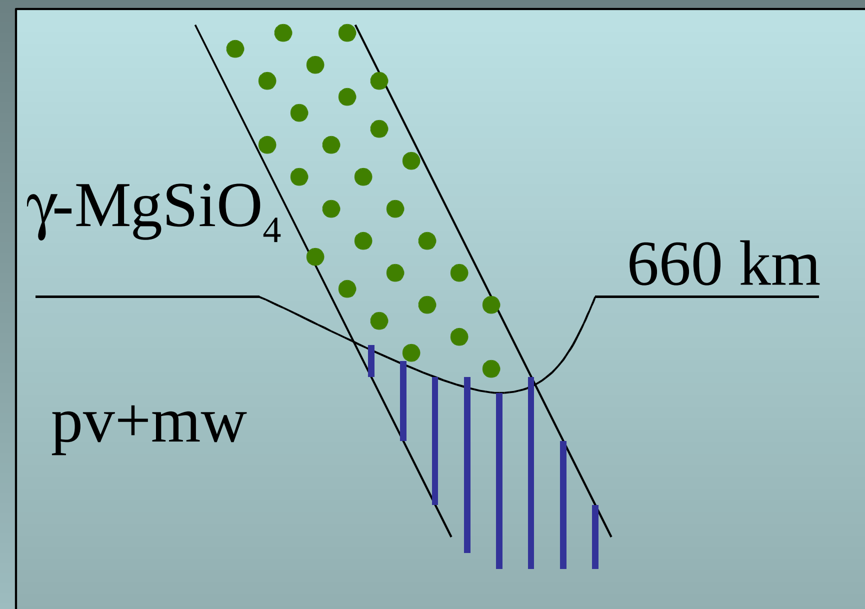
Chemical Constraints on Density Distribution



Cold Slabs, Clapeyron Slopes and Whole Mantle Convection



exothermic reaction

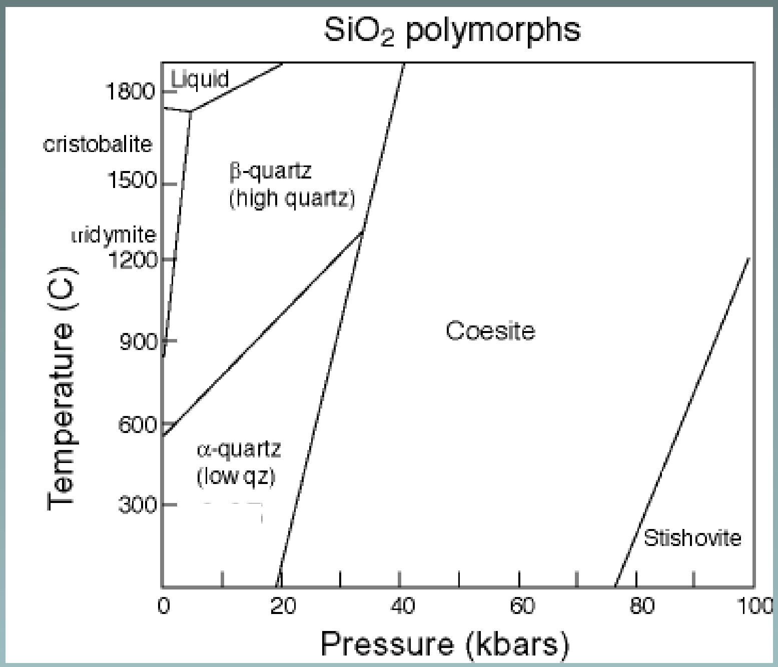


endothermic reaction

$$F_b = - g ? v_i (D r_i)(?z / ?P)(?P / ?T)_i DT$$

Clapeyron Slope

$$dG = VdP - SdT$$



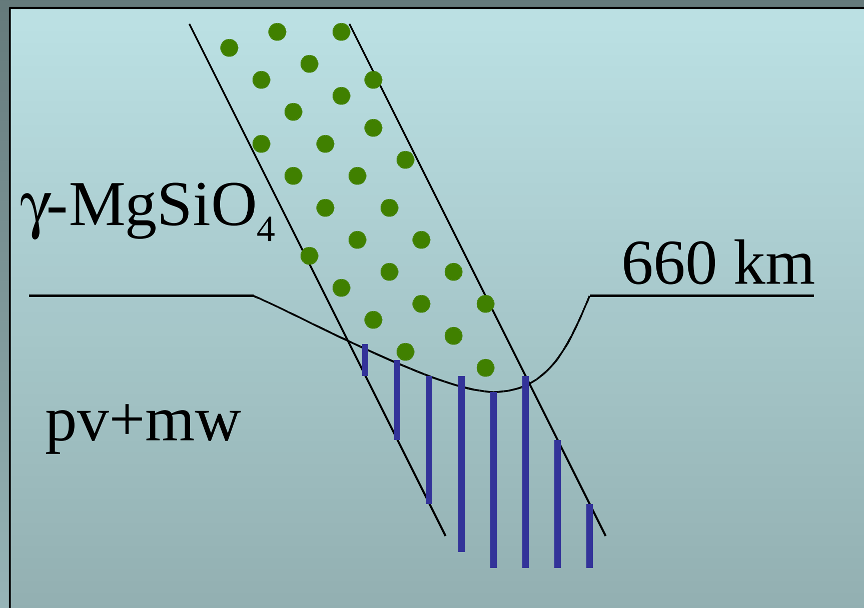
Equilibrium:

$\Delta G_1 = \Delta G_2$

$$V_1 dP - S_1 dT = V_2 dP - S_2 dT$$

$$\frac{dP}{dT} = \frac{\Delta V_{rxn}}{\Delta S_{rxn}}$$

Cold Slabs, Clapeyron Slopes and Whole Mantle Convection



endothermic reaction

$$F_b = - g ? v_i (D r_i)(?z/?P)(?P/?T)_i DT$$

Clapeyron slope must be greater than… ask a geodynamicist

Determination of Clapeyron Slopes

$$\frac{dP}{dT} = \frac{\Delta V_{rxn}}{\Delta S_{rxn}}$$

Phase Equilibria

- ex-situ
- in-situ

Thermodynamic

Determination of Clapeyron Slopes

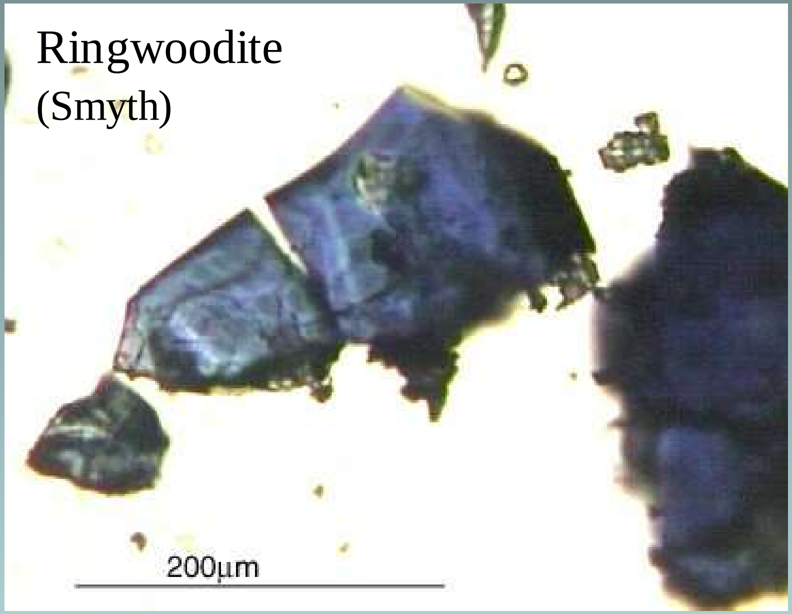
$$\frac{dP}{dT} = \frac{\Delta V_{rxn}}{\Delta S_{rxn}}$$

Phase Equilibria

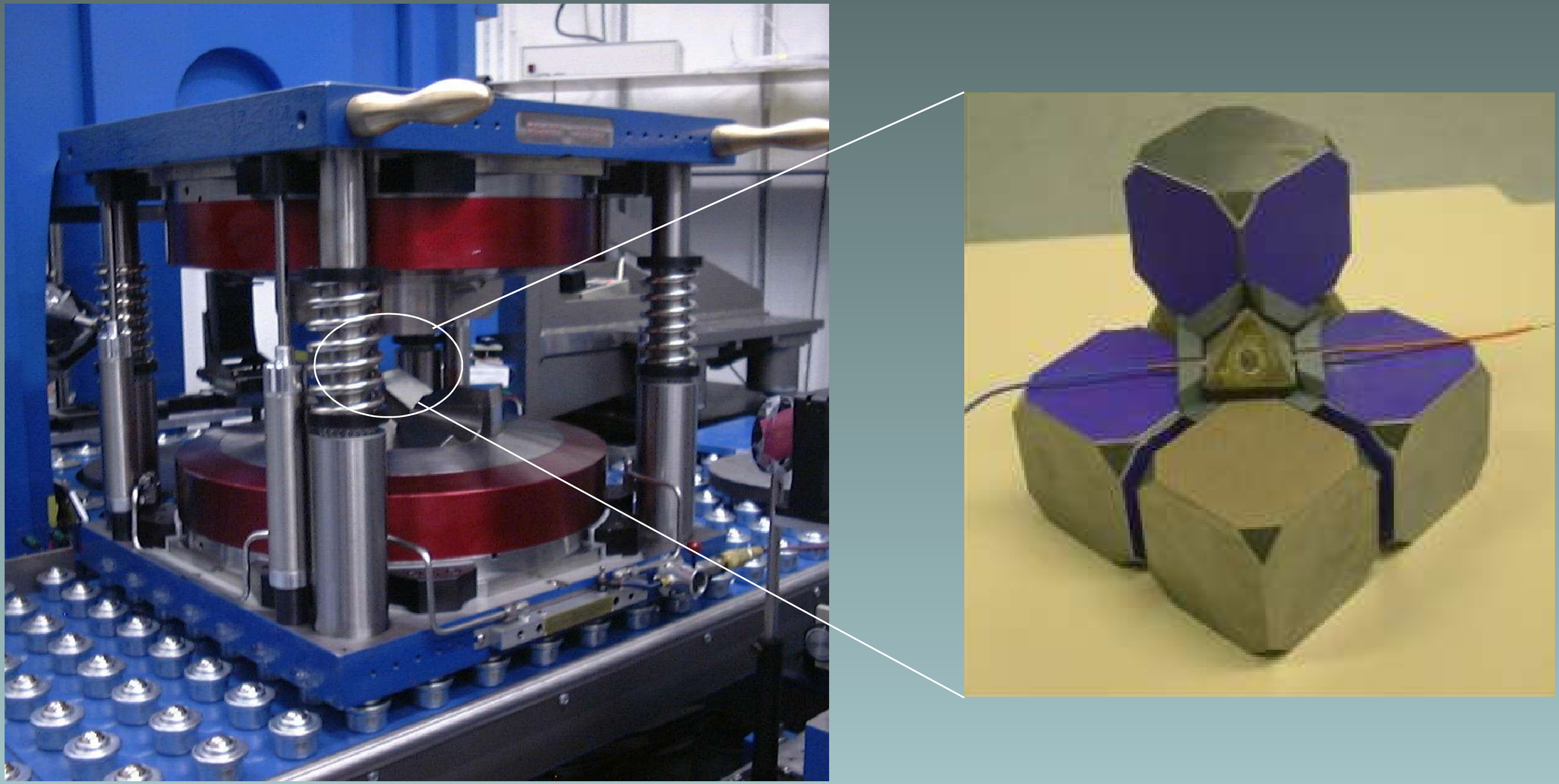
ex-situ

in-situ

Thermodynamic



Multi-Anvil Press



Determination of Clapeyron Slopes

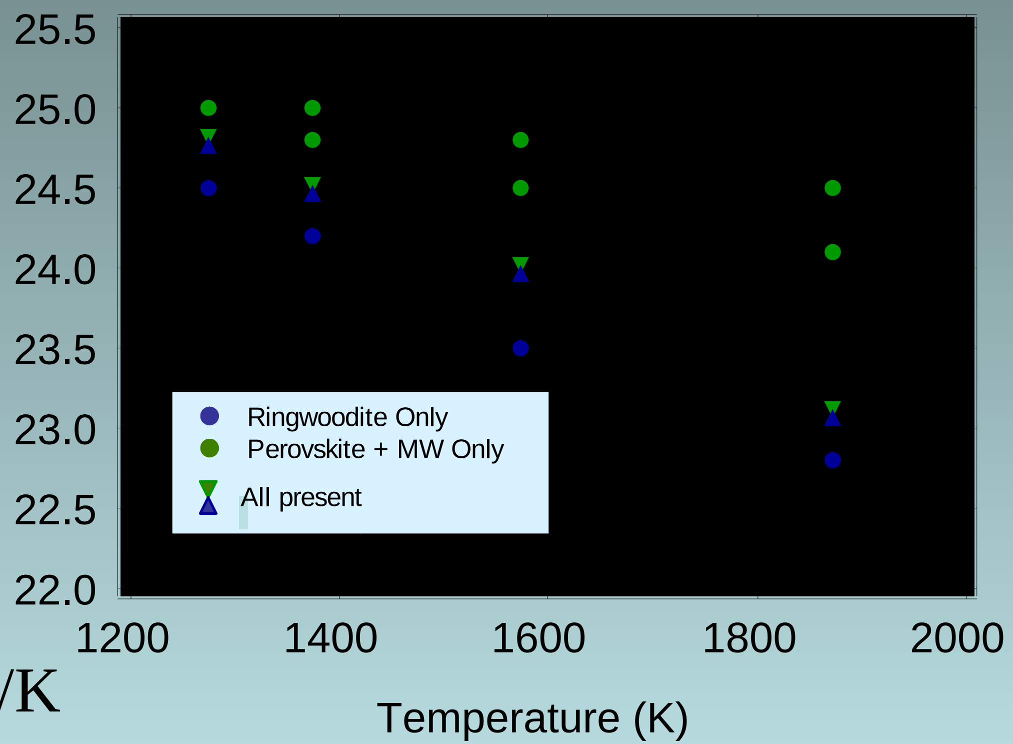
$$\frac{dP}{dT} = \frac{\Delta V_{rxn}}{\Delta S_{rxn}}$$

Phase Equilibria

ex-situ

in-situ

Thermodynamic



Clapeyron slope = -2.8 MPa/K

Determination of Clapeyron Slopes

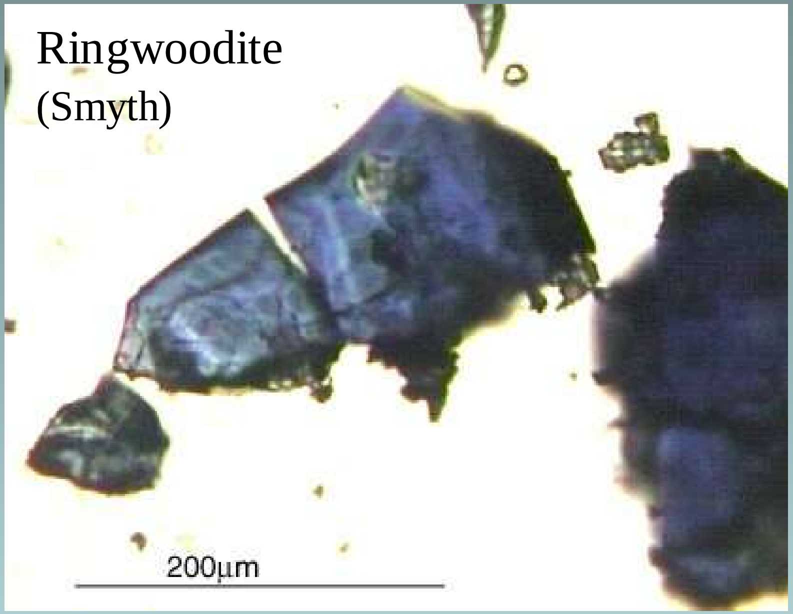
$$\frac{dP}{dT} = \frac{\Delta V_{rxn}}{\Delta S_{rxn}}$$

Phase Equilibria

ex-situ

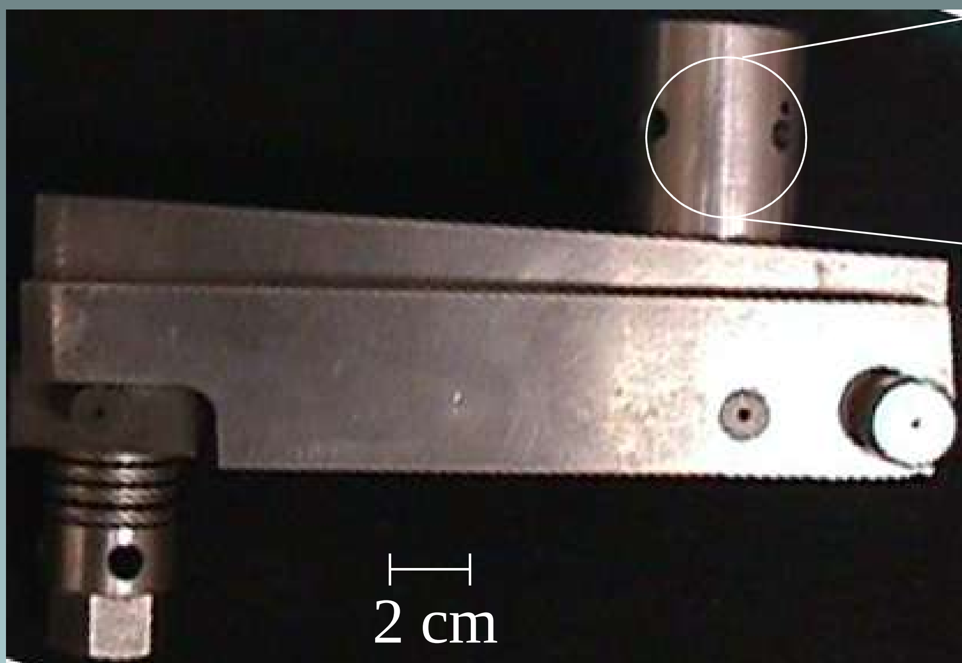
in-situ

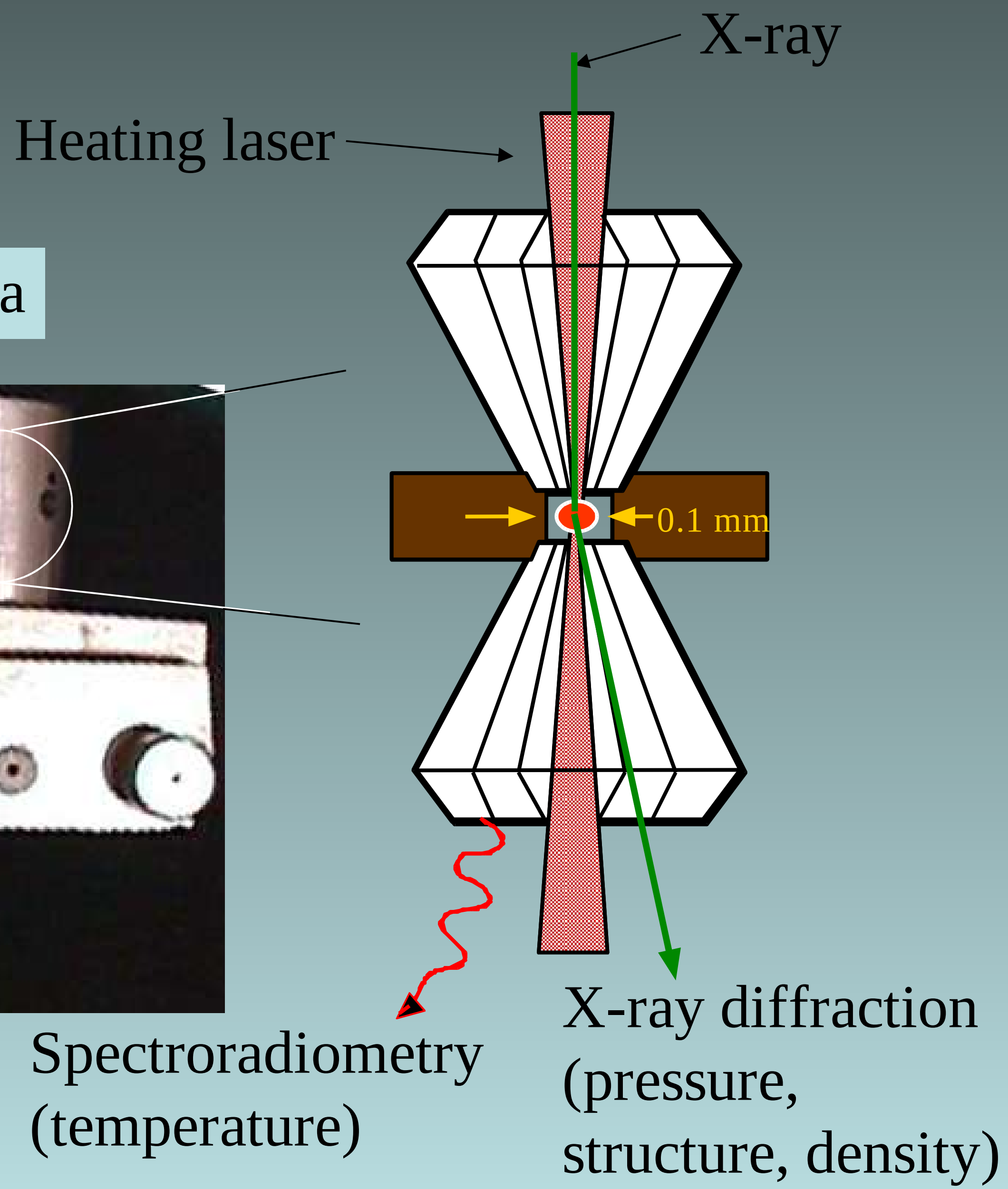
Thermodynamic



The Laser-Heated Diamond Anvil Cell

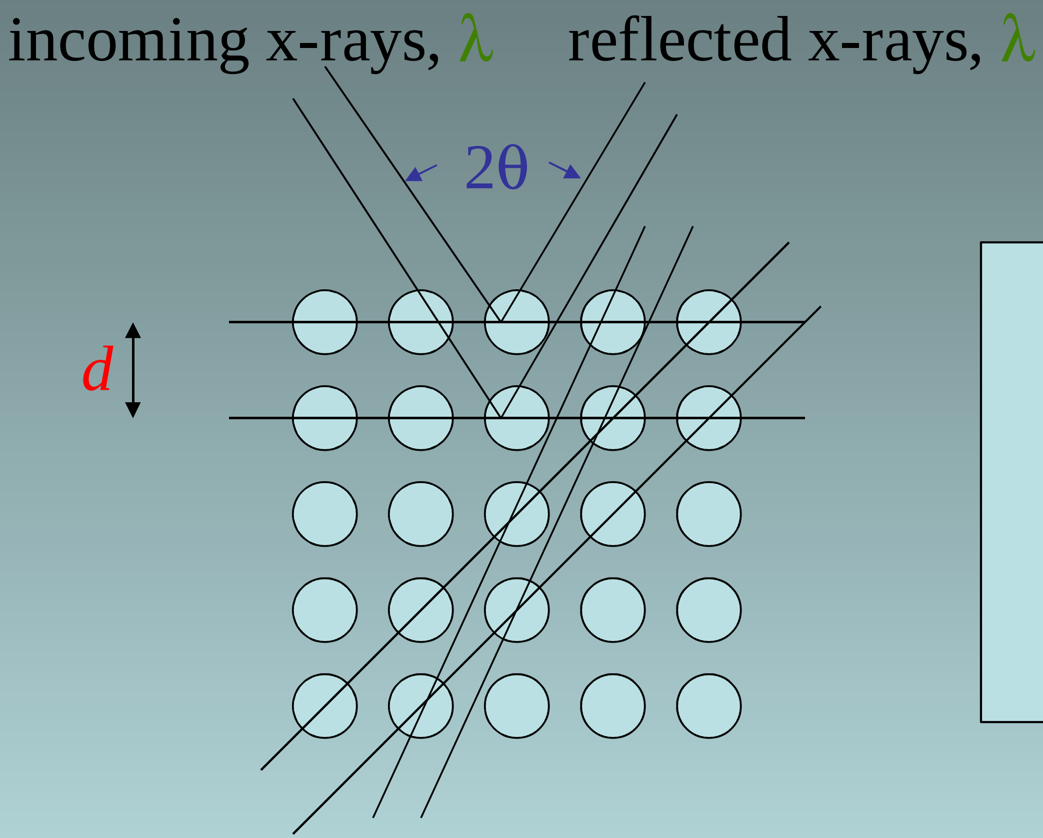
Pressure = Force/Area





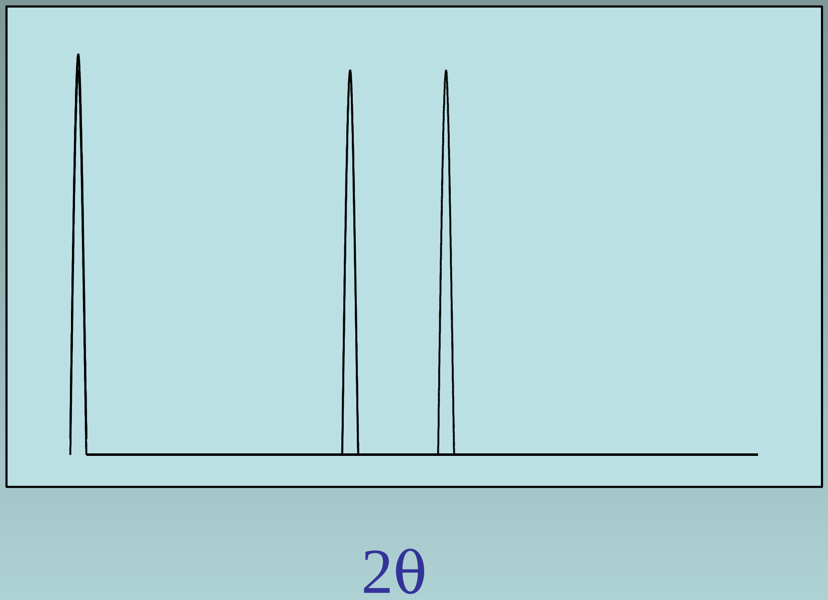
Techniques

X-ray Diffraction



Diffraction condition:

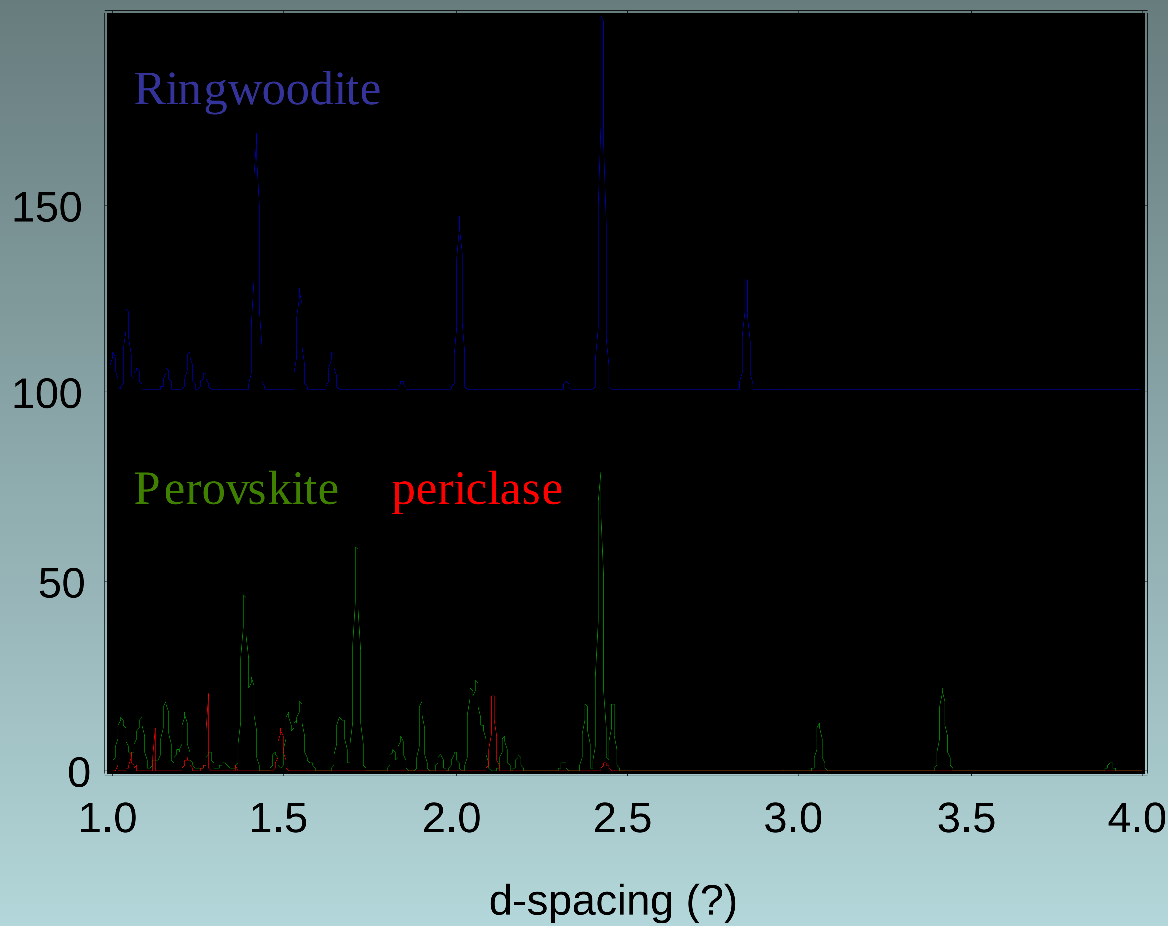
$$\lambda = 2d\sin(2\theta)$$



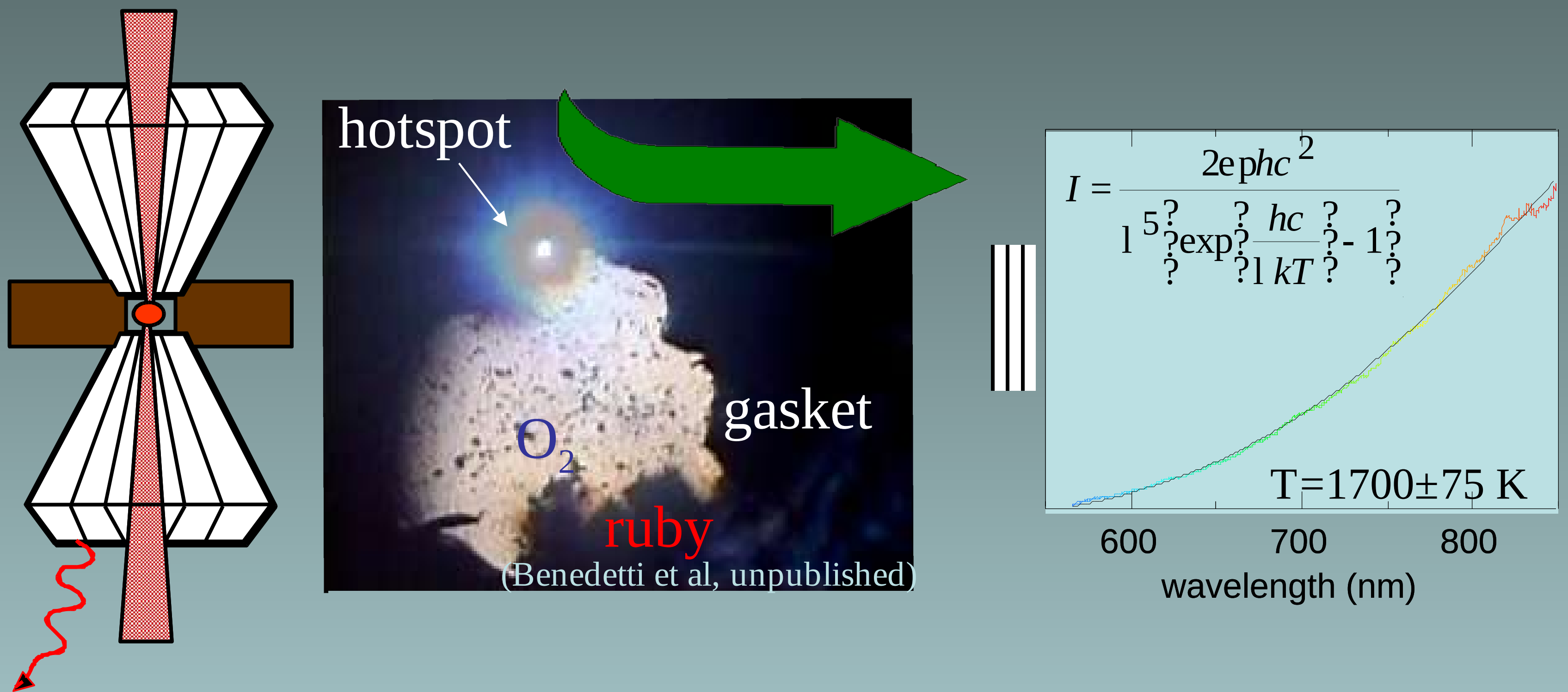
e.g. Cullity

Techniques

X-ray Diffraction



Temperature Measurements

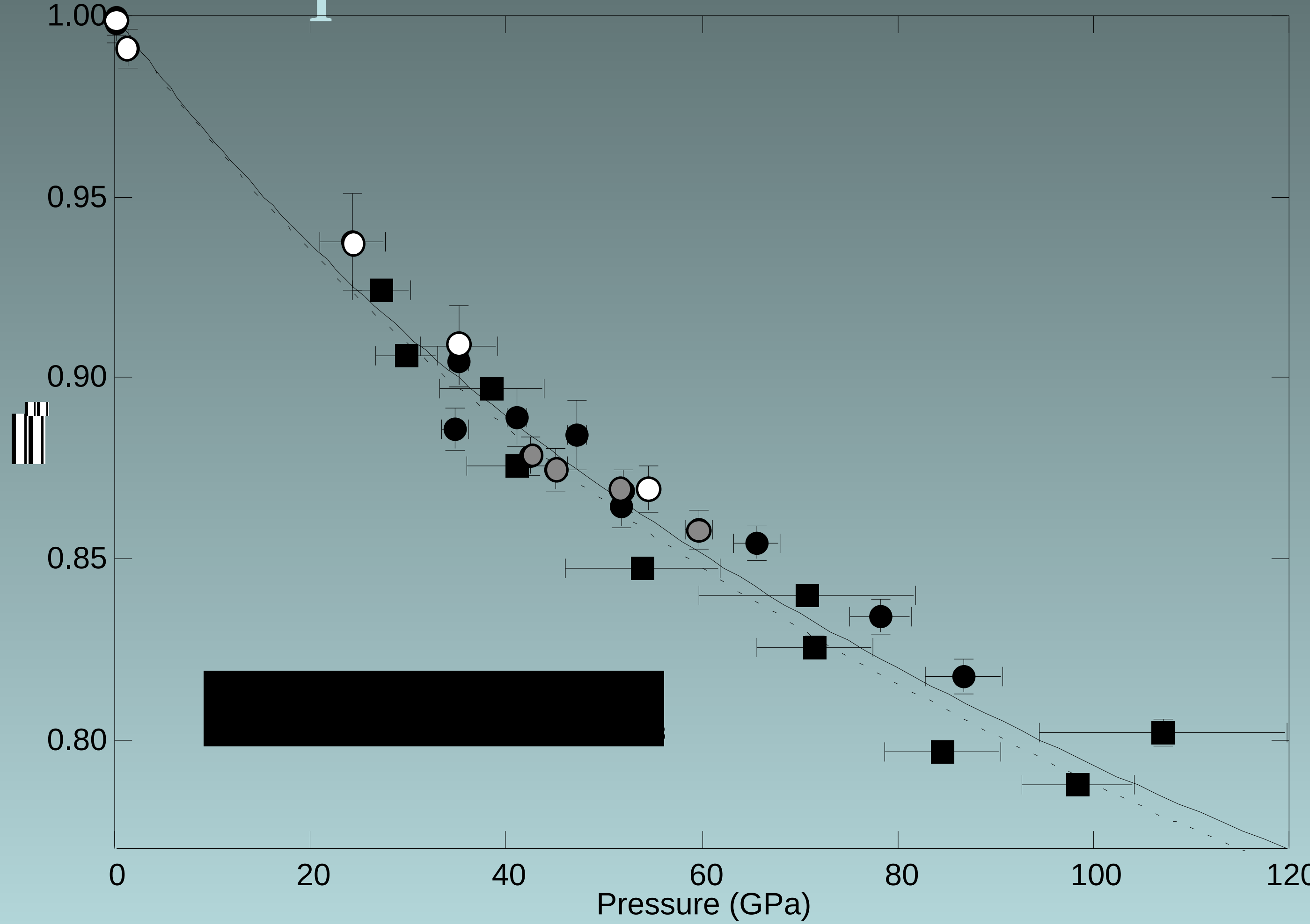


side view

top view

Kavner and Panero, *PEPI* 2004

Pressure Measurements: Equations of State



Lee et al., 2004

Constant Temperature Equations of State

Bulk Modulus $$K_{0T} = \left(\frac{\partial P}{-\partial \ln(V)} \right)_T$$

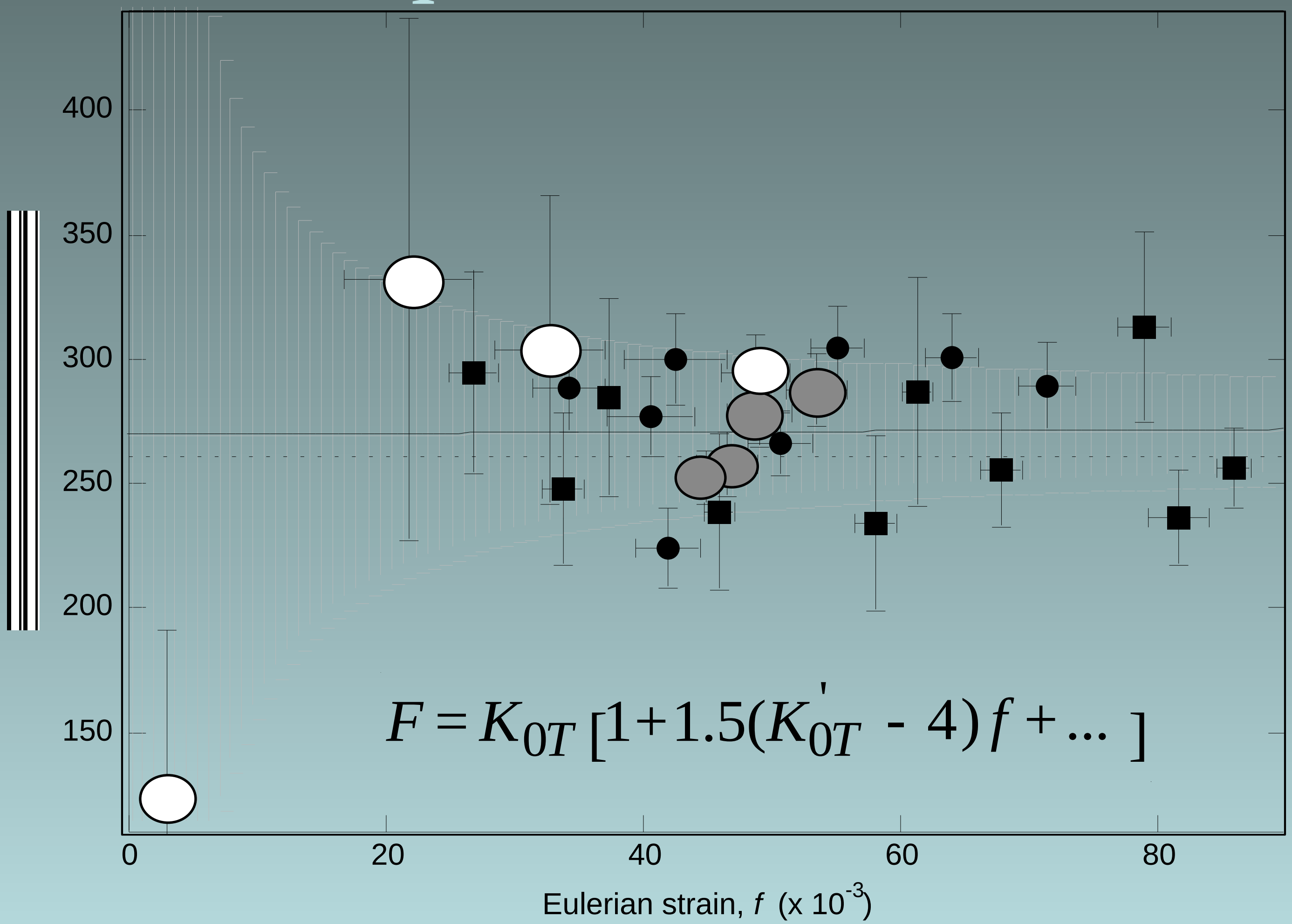
$$f = [(v/v_0)^{-2/3} - 1]/2$$

$$P = 3f(1+2f)^{5/2} K_{0T} [1 + 1.5(K_{0T}^{'} - 4) f + \ldots]$$

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

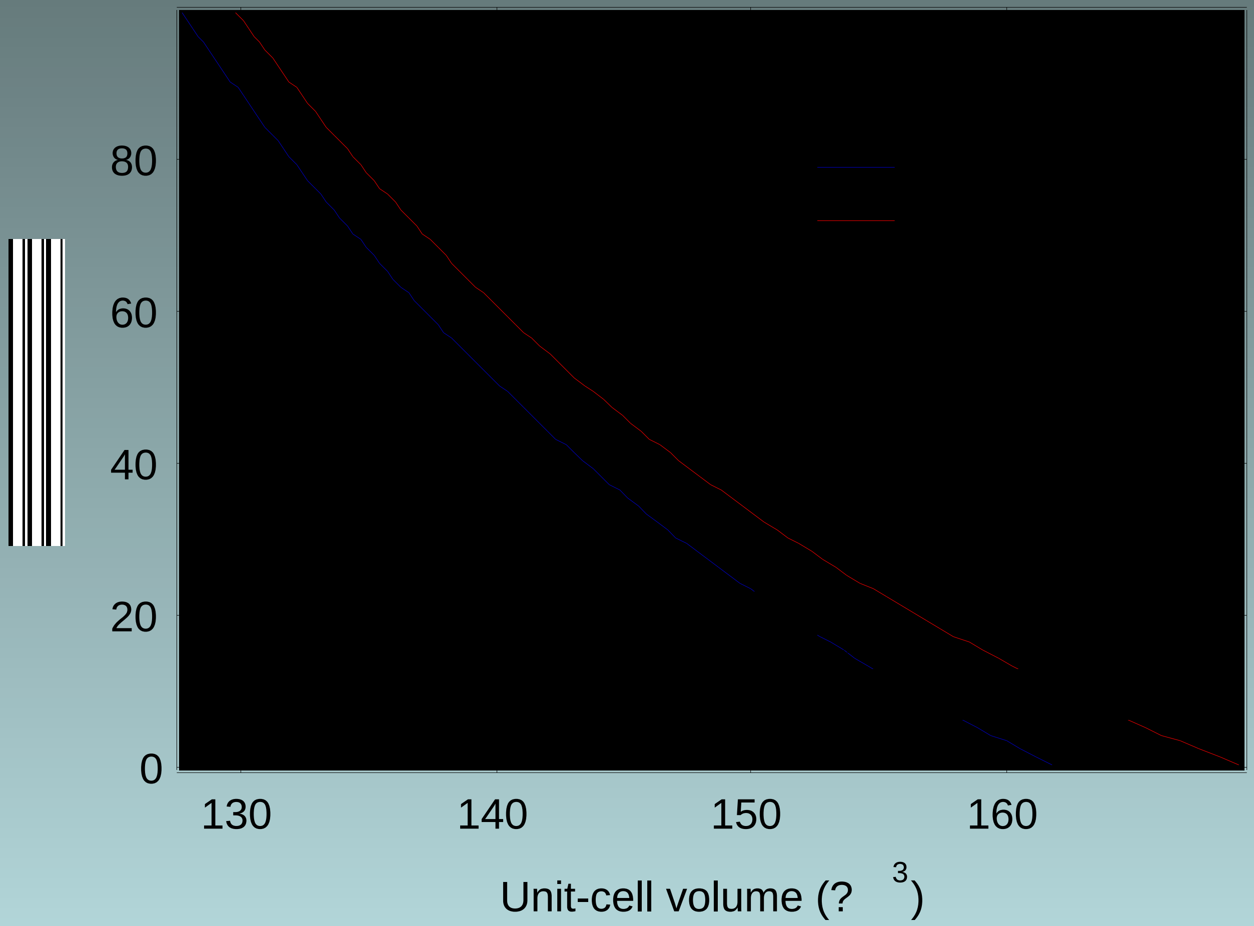
$$F = K_{0T} [1 + 1.5(K_{0T}^{'} - 4) f + \ldots]$$

Constant Temperature Equations of State



Lee et al., 2004

PVT Equations of State



PVT Equations of State

$$P(V,T) = P_{0K}(V) + P_{th}(T)$$

Thermodynamic definition $$-\left(\frac{\partial E}{\partial V}\right)_T = P$$

$$P_{th} = -\left(\frac{\partial E_{th}}{\partial V}\right)_T = \frac{\gamma}{V} E_{th}$$

Model for internal energy:
e.g. Debye

$$E_{th} = 9nk_B T(T/\Theta_D)^3 \int_0^{\Theta_D/T} \frac{x^3}{e^x - 1} dx$$

Determination of Clapeyron Slopes

$$\frac{dP}{dT} = \frac{\Delta V_{rxn}}{\Delta S_{rxn}}$$

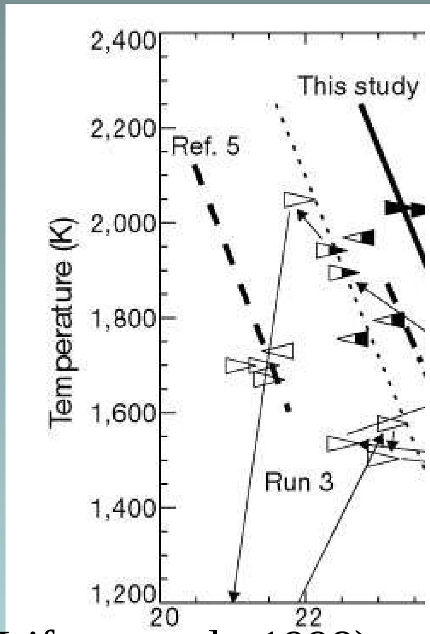
Shim et al., 2001

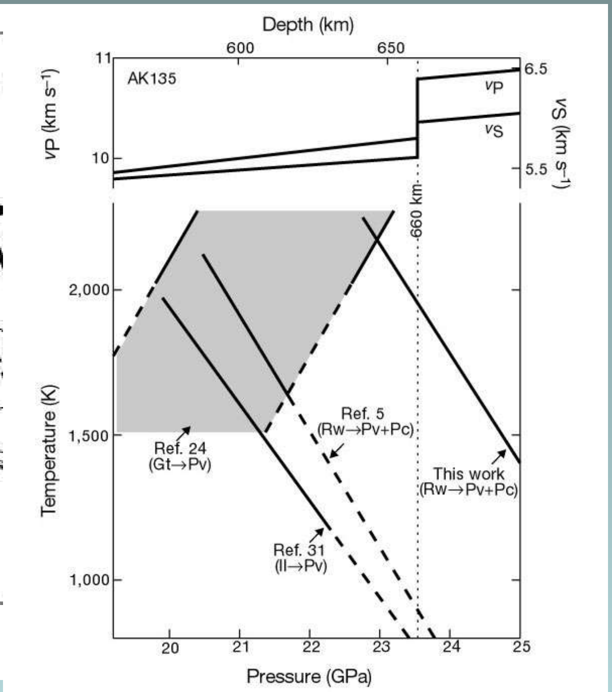
Phase Equilibria

ex-situ

in-situ

Thermodynamic





Clapeyron slope = -3 MPa/K (Irifune et al., 1998)

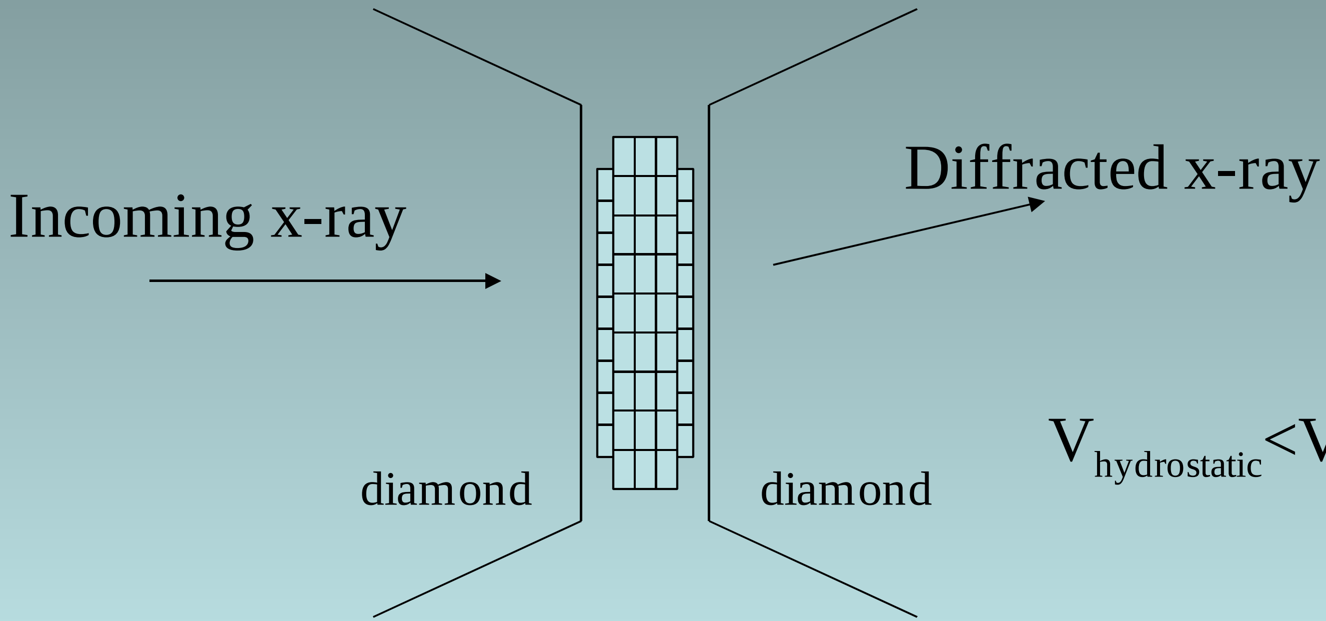
Clapeyron slope = no constraint (Shim et al., 2001; Chudinovskikh et al., 2001)

Sources of Error

Non-hydrostatic stresses

Pressure standards

Temperature and pressure gradients



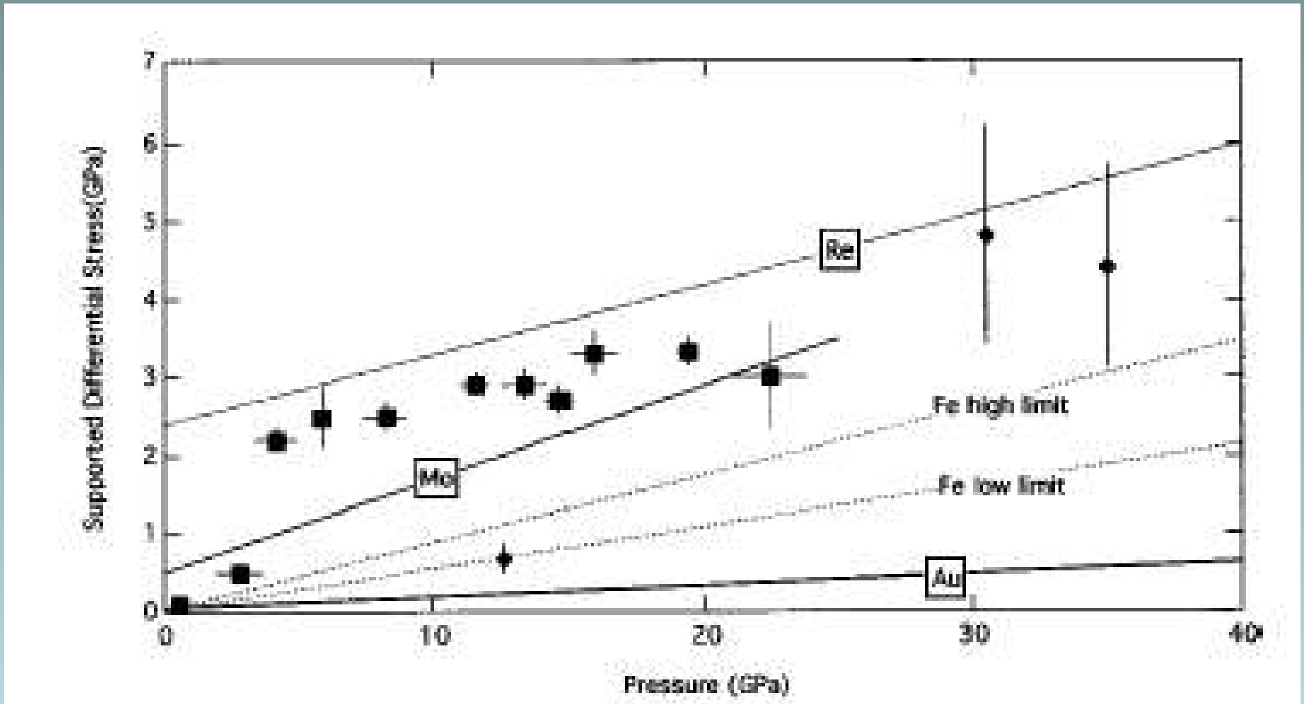
$V_{hydrostatic} < V_{non\text{-}hydrostatic}$

Sources of Error

Non-hydrostatic stresses

Pressure standards

Temperature and pressure gradients



Kavner and Duffy, 2003

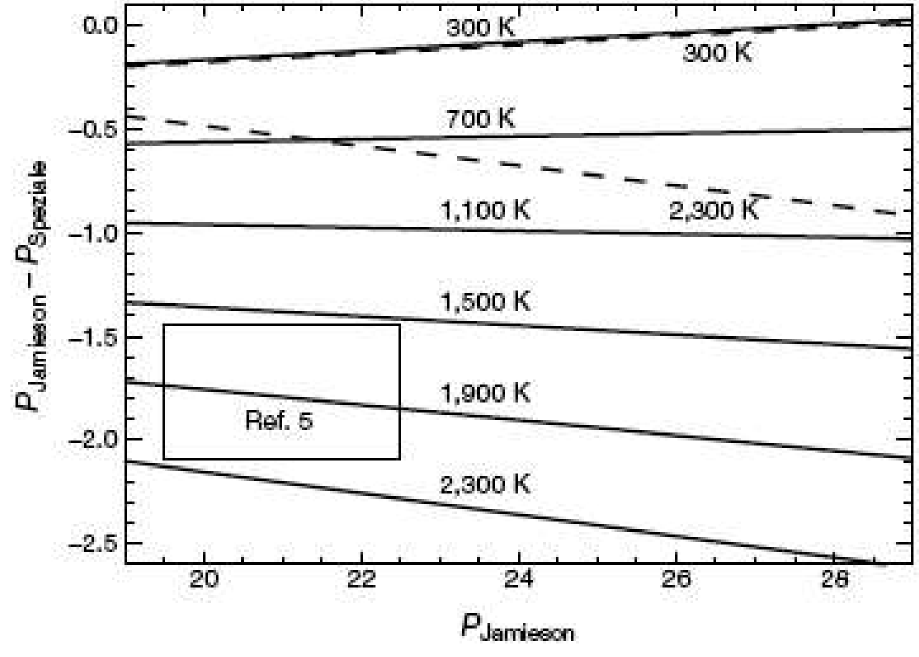
Sources of Error

Non-hydrostatic stresses

Pressure standards

Temperature and pressure gradients

Gold relative to Platinum



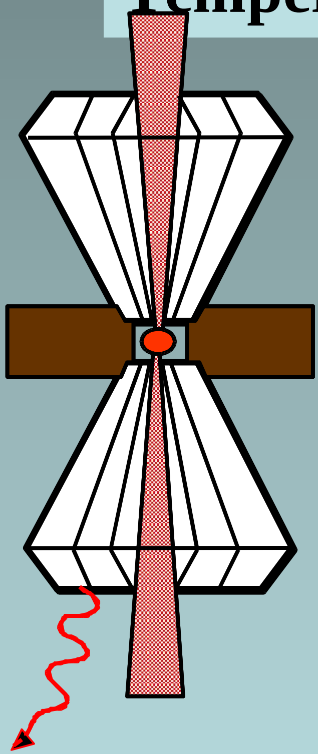
Shim et al., 2001

Sources of Error

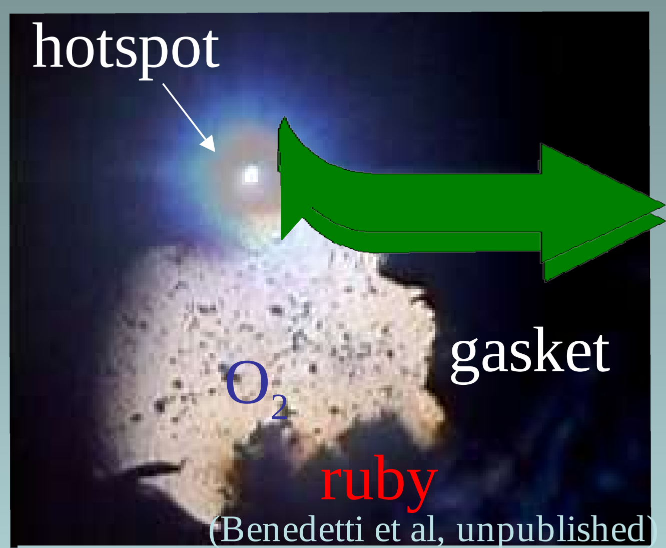
Non-hydrostatic stresses

Pressure standards

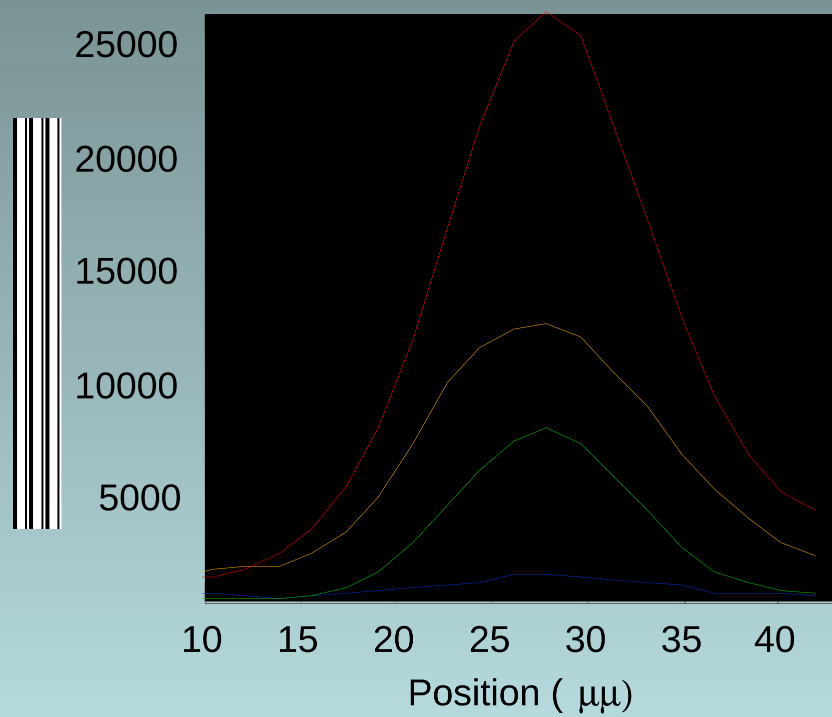
Temperature and pressure gradients



side view



top view



Kavner and Panero, *PEPI* 2004

Determination of Clapeyron Slopes

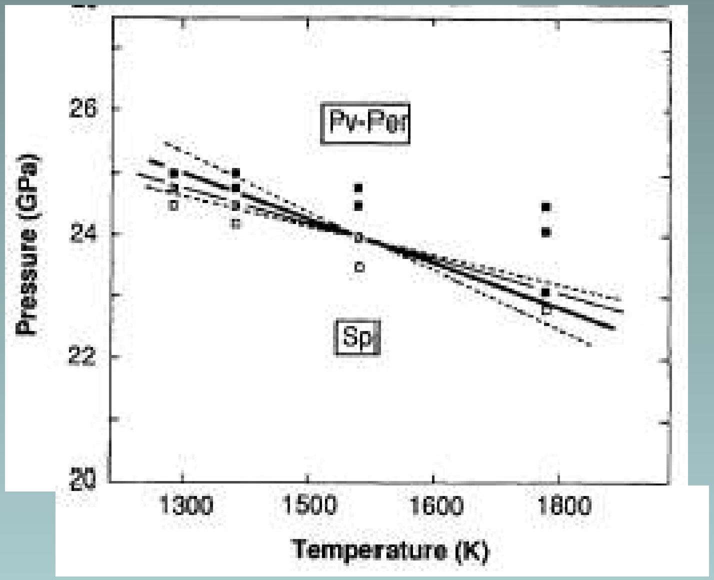
$$\frac{dP}{dT} = \frac{\Delta V_{rxn}}{\Delta S_{rxn}}$$

Phase Equilibria

ex-situ

in-situ

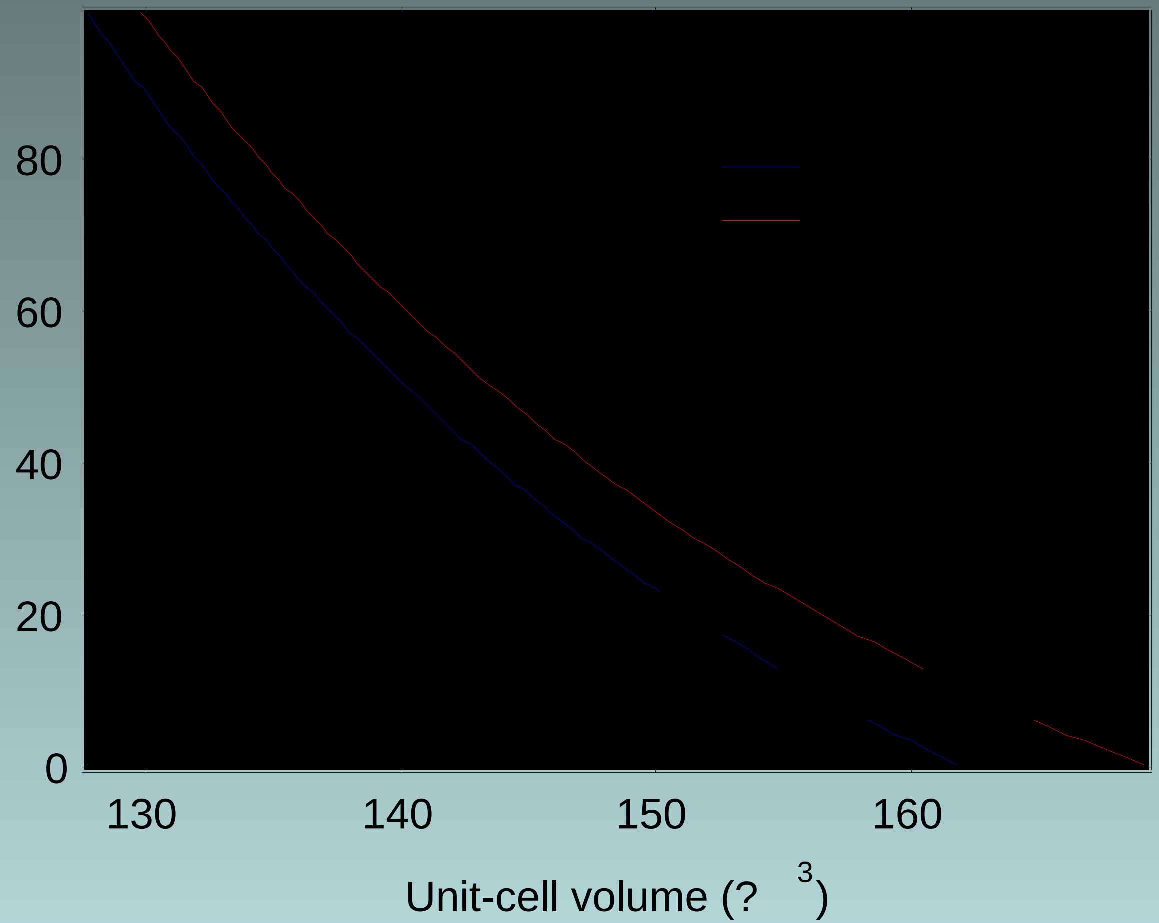
Thermodynamic



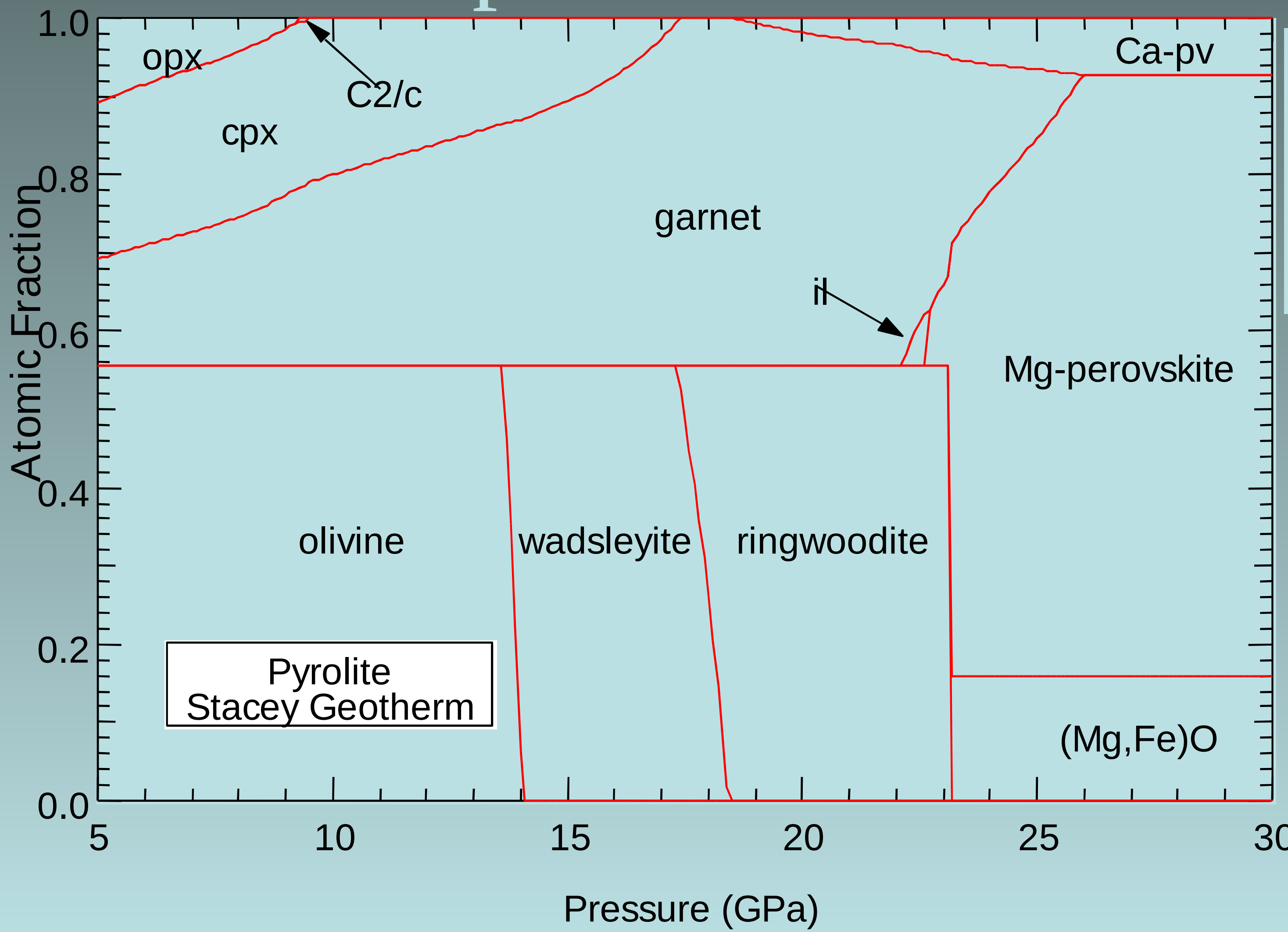
Clapeyron slope = -4±2 MPa/K

Ito et al., 1990

Interpretation of Tomography: Thermal Variations



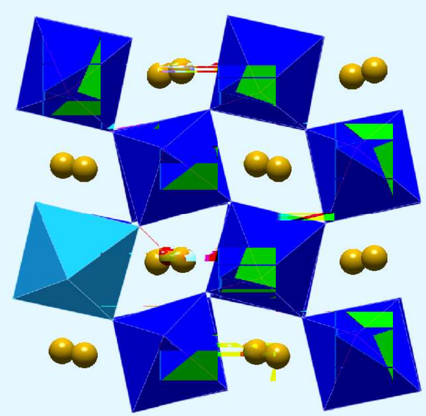
Interpretation of Tomography: Compositional Variations



SiO_2	45.4 wt%
MgO	37.1 wt%
FeO	8.3 wt%
Al_2O_3	4.3 wt%
CaO	3.3 wt%

Interpretation of Tomography: Compositional Variations

Perovskite Composition	K_0 (GPa)	ρ (Mg/m^3)	$\sqrt{K_0/r}$ (km/s)
$MgSiO_3$	262	4.12	7.974
$MgSiO_3$~10% FeO	262	4.25	7.851
$MgSiO_3$ ~3.25% Al_2O_3	261	4.123	7.956
$MgSiO_3$ ~3.25% Al_2O_3+H_2O	256	4.088	7.913



Theory

Quantum mechanical or classical

–effects of *a priori* assumptions

–size of calculation, time for calculation

General approach:

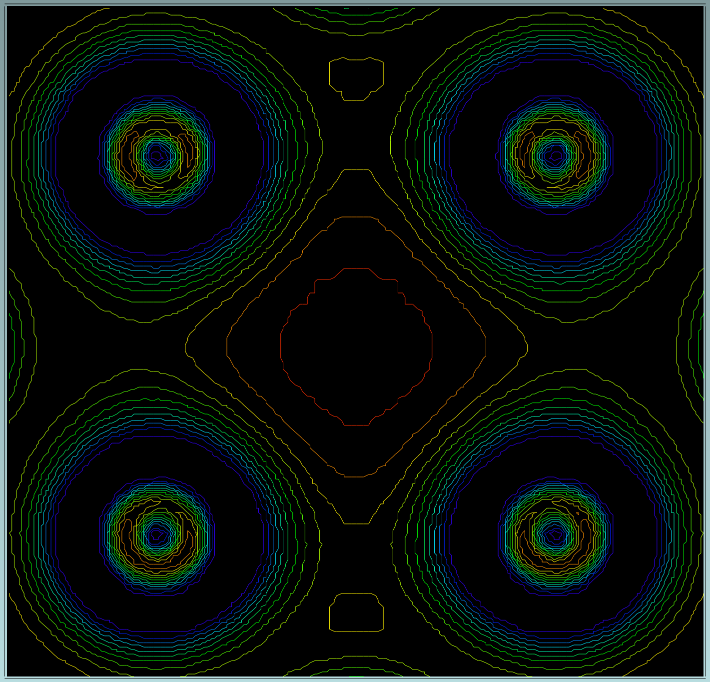
G of each phase

PT-space for lowest energy

Limitations:

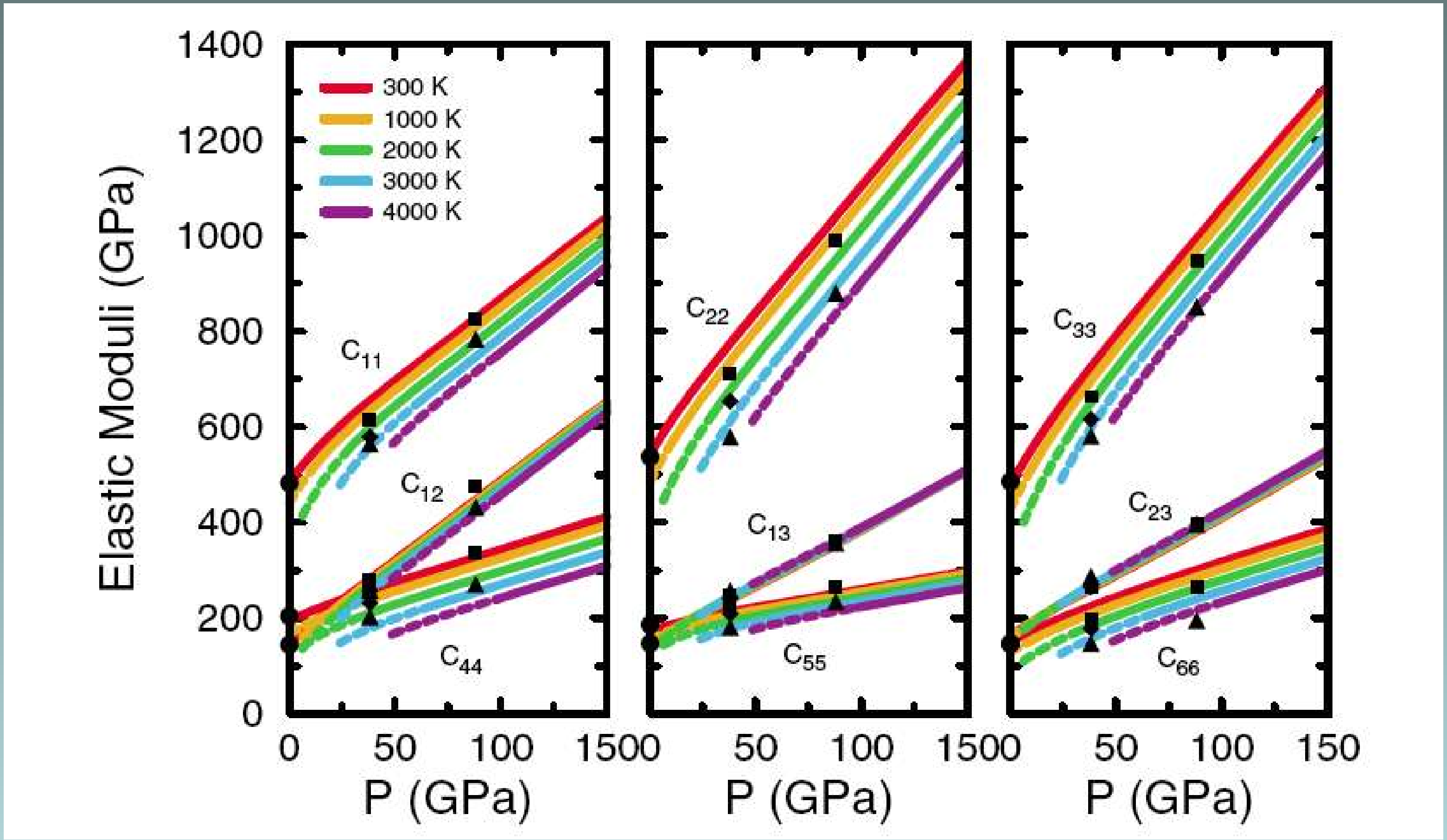
Temperature

Multi-component systems



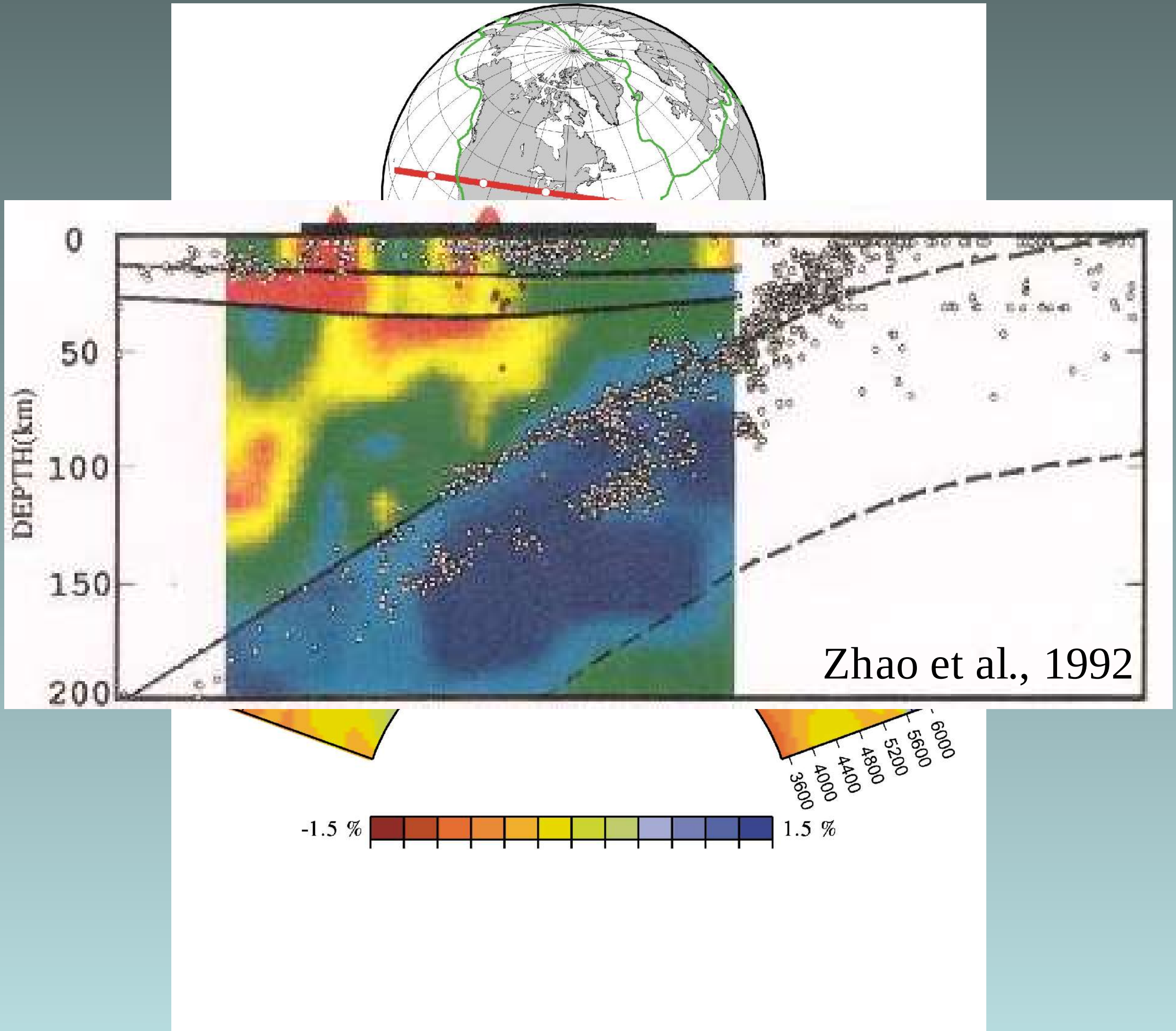
Theory

MgSiO$_3$ perovskite



Wentzcovitch et al., 2004

?



Van Heijst, Ritsema, and Woodhouse [1999]