

Hydrous silicate melt at high pressure

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First principle molecular dynamics

Up to 135GPa

Motivation

Can conductivity and seismic anomaly near the mantle transition zone be explained by a presence of hydrous partially molten zone?

Water filter model (Bercovici and Karato, 2003)

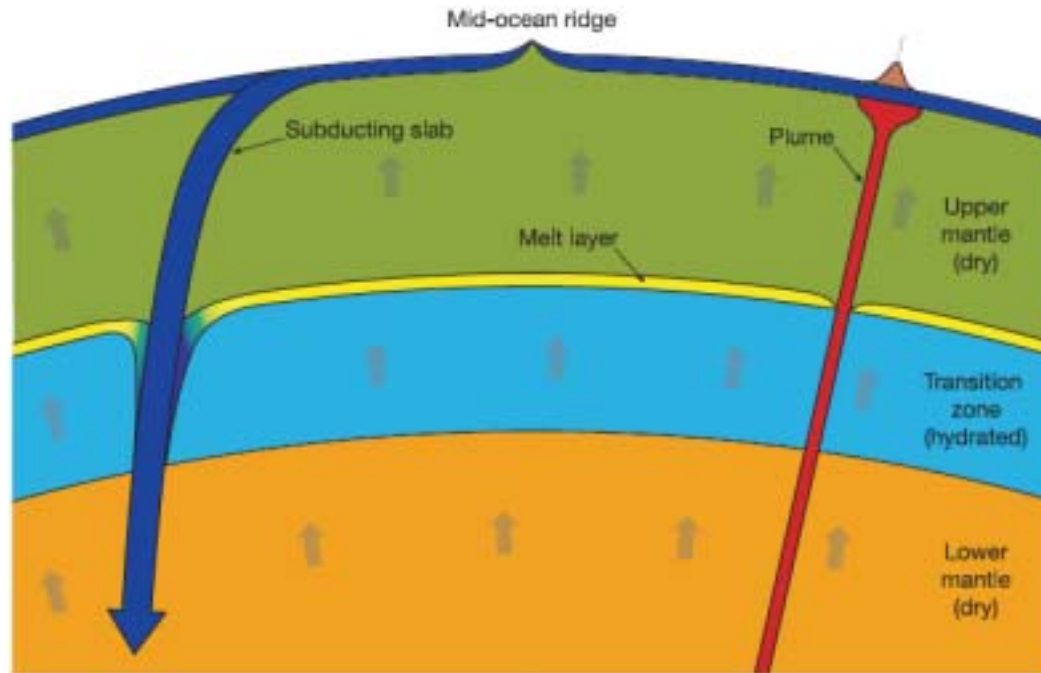


Figure 1 Sketch of the transition-zone water-filter model. Slabs subducting from cold lithosphere (dark blue) force up a broad background of passively upwelling ambient mantle (arrows) that, upon passing through the high-water-solubility transition zone (light blue) gets hydrated. When leaving the transition zone at the 410-km boundary, this ambient mantle becomes low-water solubility olivine and is thus super-saturated, wherein it partially melts, thereby extracting water and filtering off incompatible elements into the melt phase. The wet, enriched melt is likely to be heavy and thus gathers into the high-melt fraction layer trapped above the 410-km boundary (yellow). The residual solid portion of upwelling ambient mantle is buoyant but very dry and

depleted of incompatible elements; it provides the MORB source region (green). The water-filtering mechanism is suppressed in mantle plumes (red) due to the plume material's higher temperatures and velocities which result in reduced water-solubility and shorter residence times in the transition zone, thereby leading to greatly diminished hydration and thus little or no melting upon passing the 410-km boundary. Plumes thus arrive at the surface still relatively wet and enriched in compatible elements, thereby providing the source for enriched OIBs. Slabs efficiently entrain the melted material, returning water to the transition zone and incompatible elements to the deeper mantle.

Molecular Dynamics

Basic: $F=ma$ (equation of motion
Newton mechanics)

$F=d\phi/dr$ (Hellmann-Feynman force)

ϕ : potential energy

Potential function

$$\Phi = \sum_{ij} \sum_{j \neq i} \phi(r_{ij})$$

Initial condition: velocity and position



Calculation force acting on each particle



Update of velocity and position



Calculation of physical parameters

Time step
 Δt (fs)

Simulation

- System

$12\text{MgSiO}_3 + 8\text{H}_2\text{O}$: 10wt.% H_2O

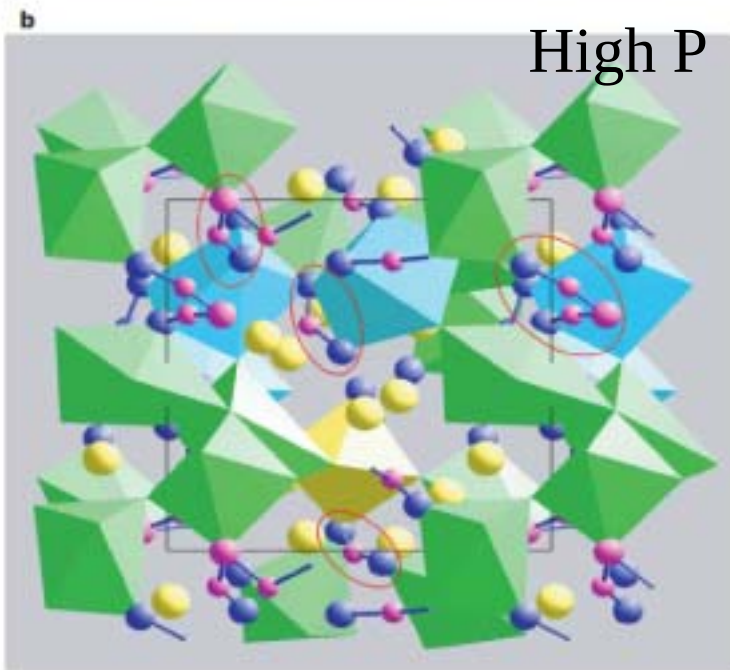
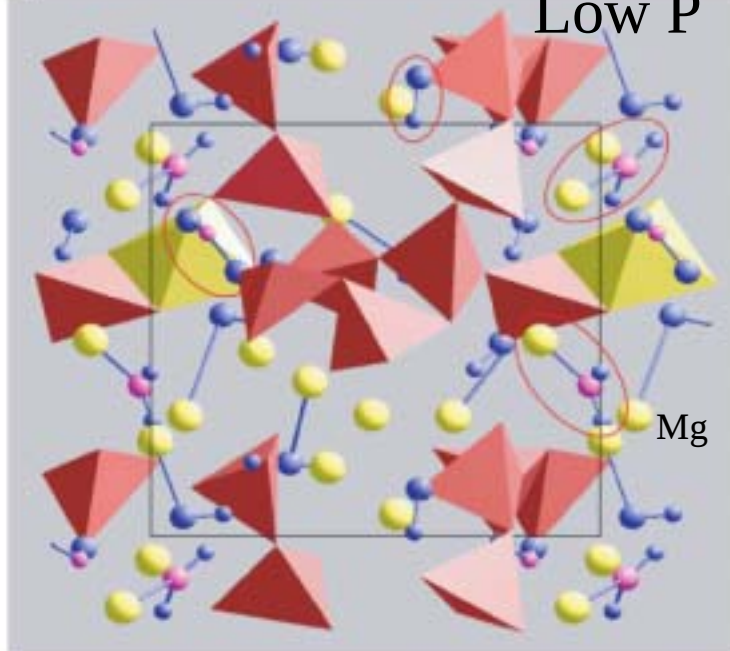
- Initial condition

Pyroxene and water molecule in vacant space

- Periodical boundary condition

- Procedure

Melting at 6000K $\rightarrow$ isochoric cooling



MgSiO₃-H₂O liquid

- At low P

Hydroxyls (OH)

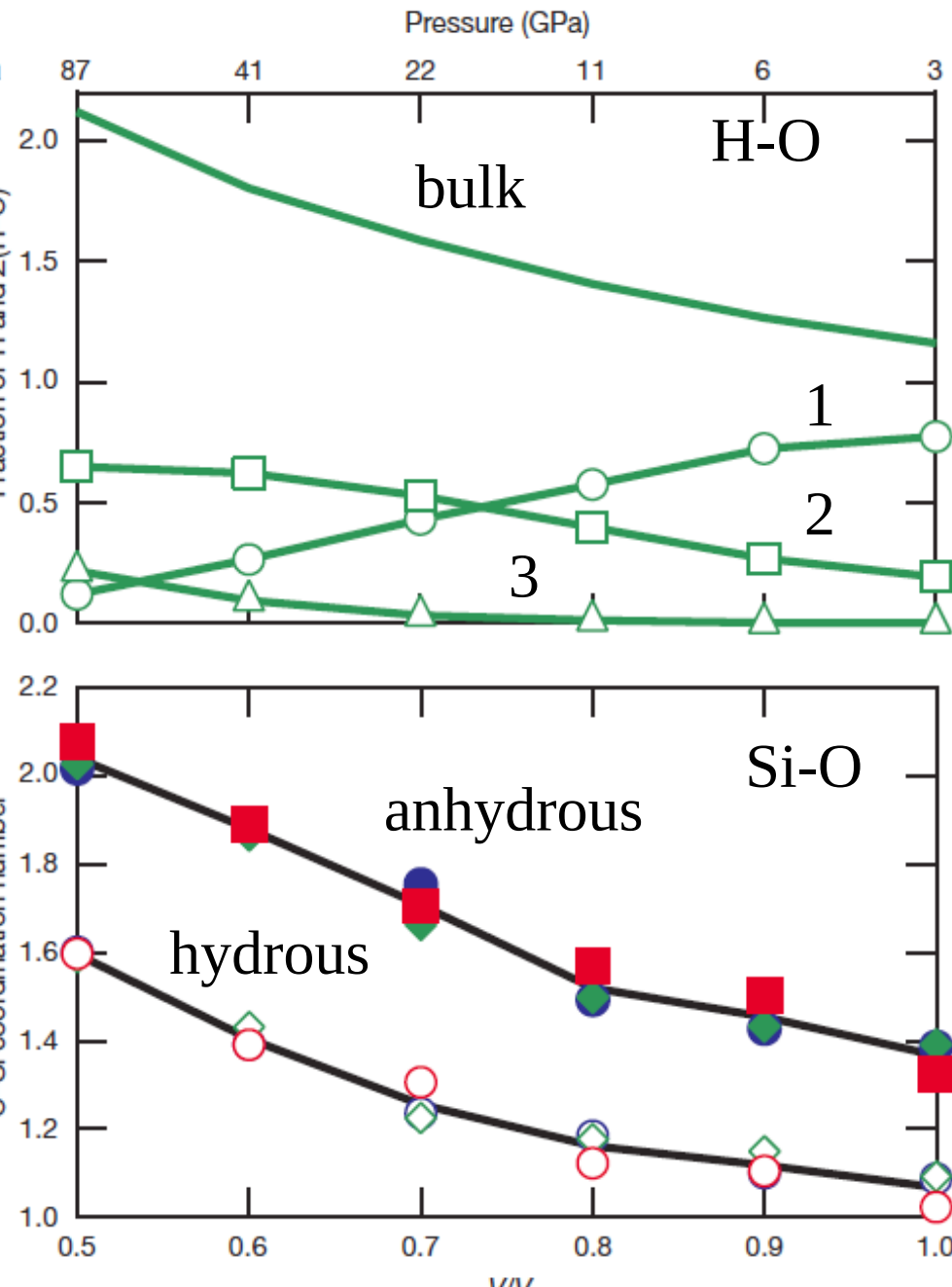
Molecular water (Mg-O-H₂)

- At high P

Si-O-H-O-Si

-O-H-O-H- chain

O-H-O edge decoration of
SiO₆ octahedra



Coordination numbers

- H-O coordination number
1 at low P to 2 at high P
increasing P
more symmetric (ice X)
no molecular water
- Si-O coordination number
Hydrous melt disrupts Si-O
bonds (decrease in viscosity)
- Mg-O coordination number
no water effect >20GPa
CN decreases at low P

Electrical conductivity of silicate melt at 410 km

Diffusivity of hydrogen (Arrhenius relation)

$$D = D_0 \exp\left(-\frac{E^* + PV^*}{kT}\right) \quad (1)$$

Electrical conductivity of hydrogen silicate melt
(Nernst-Einstein relation)

$$\sigma = \frac{Dxq^2}{kTH_R} \quad (2)$$

At 410km, 14GPa and 1800K

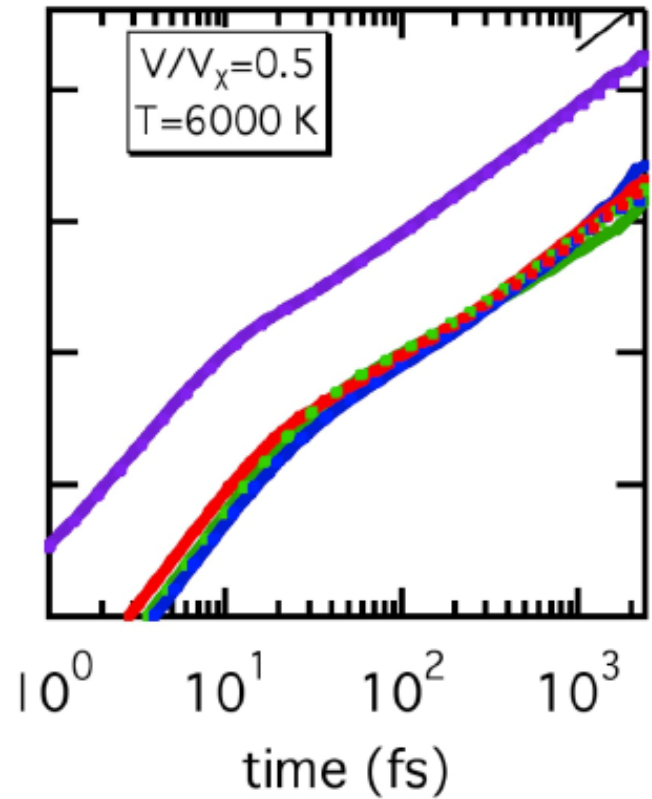
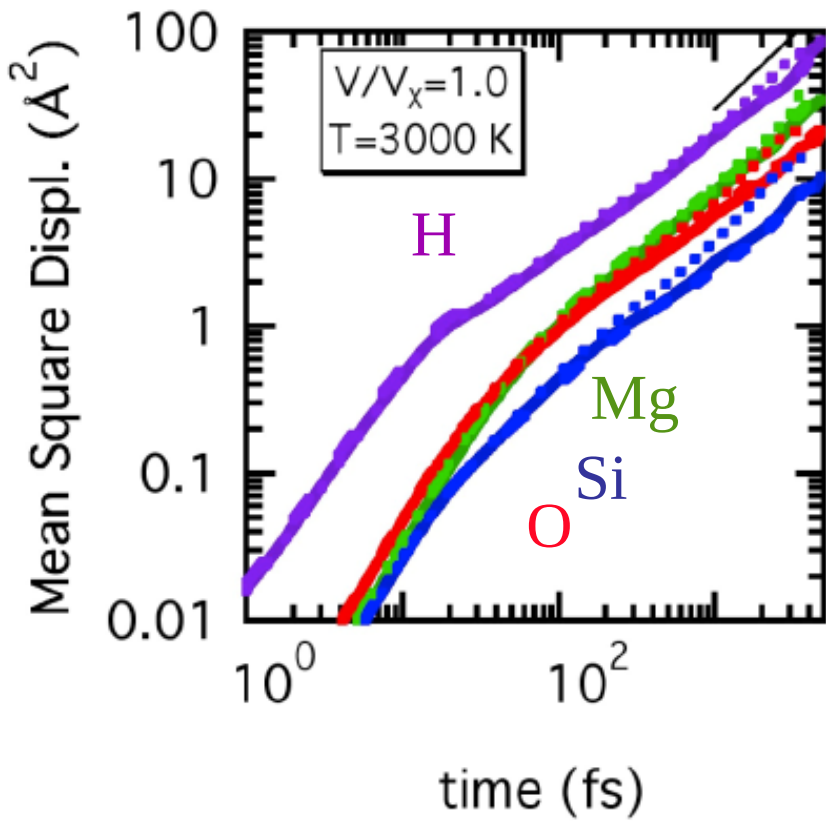
Water content: 3 wt.%

Answer: 18S/m

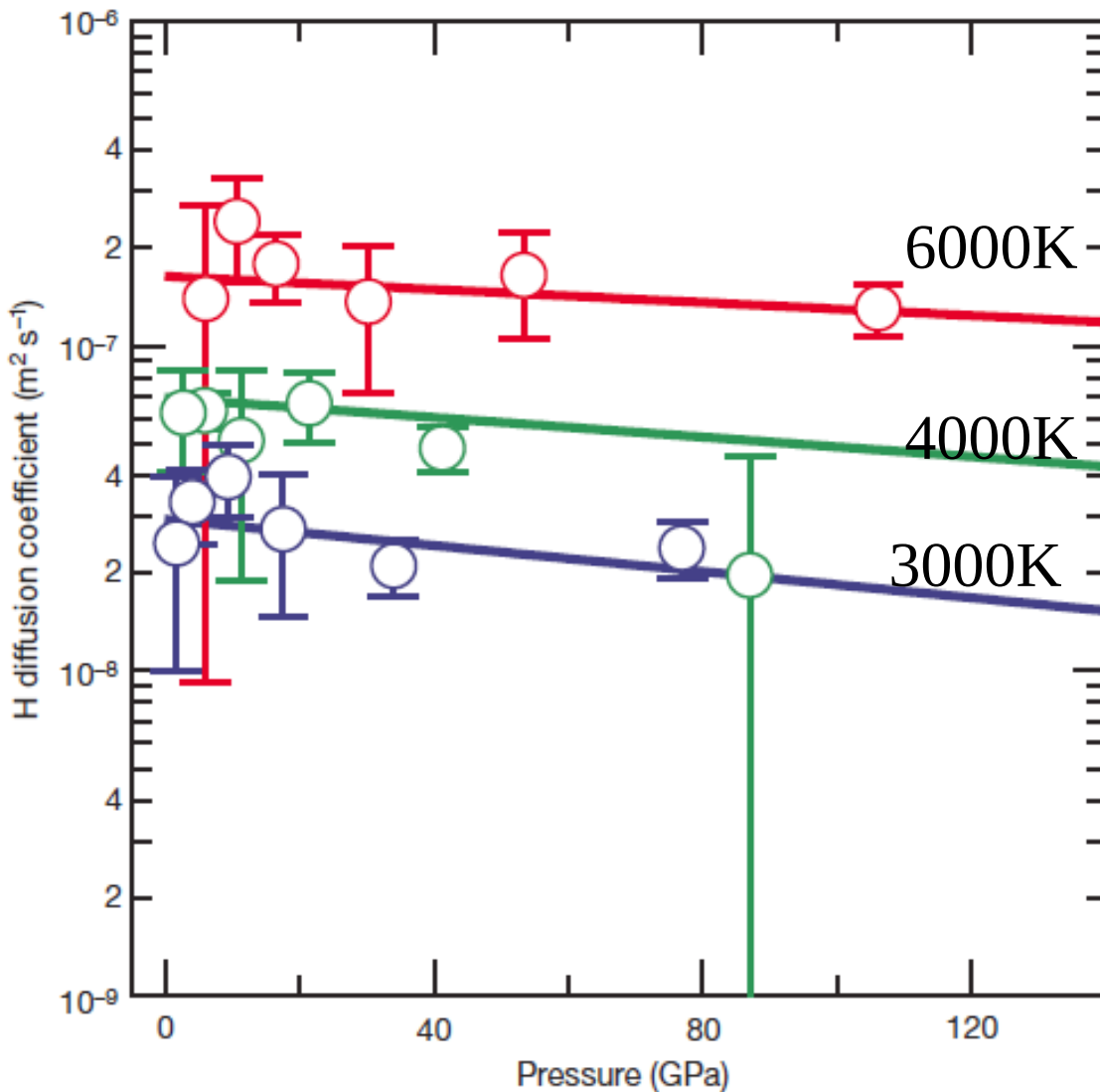
A large conductance anomaly 18000S

5% partial melt and 20km thickness

Self-diffusion coefficient: slope (m^2/s)



Self-diffusion of hydrogen



Activation enthalpy (E^*)

86kJ/mol

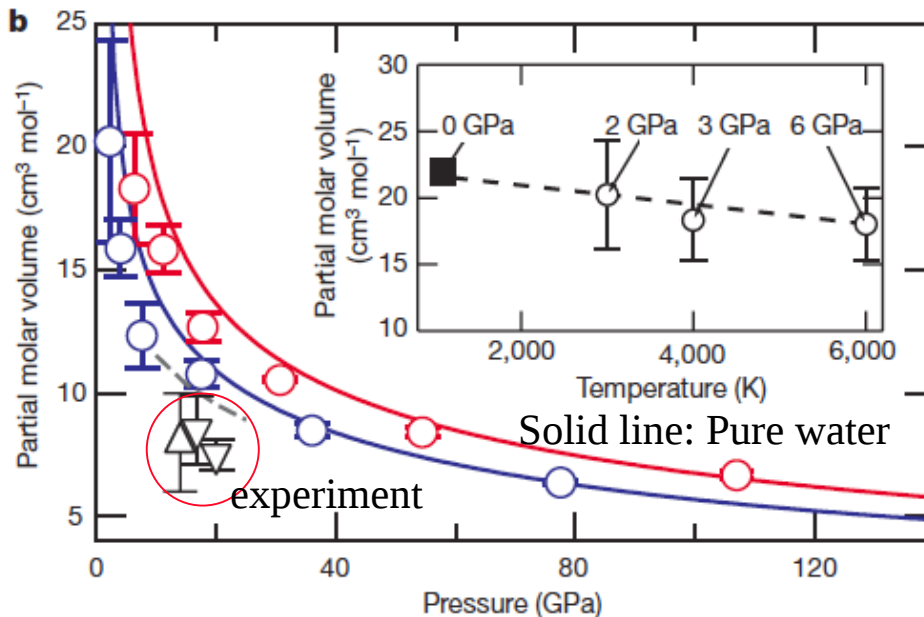
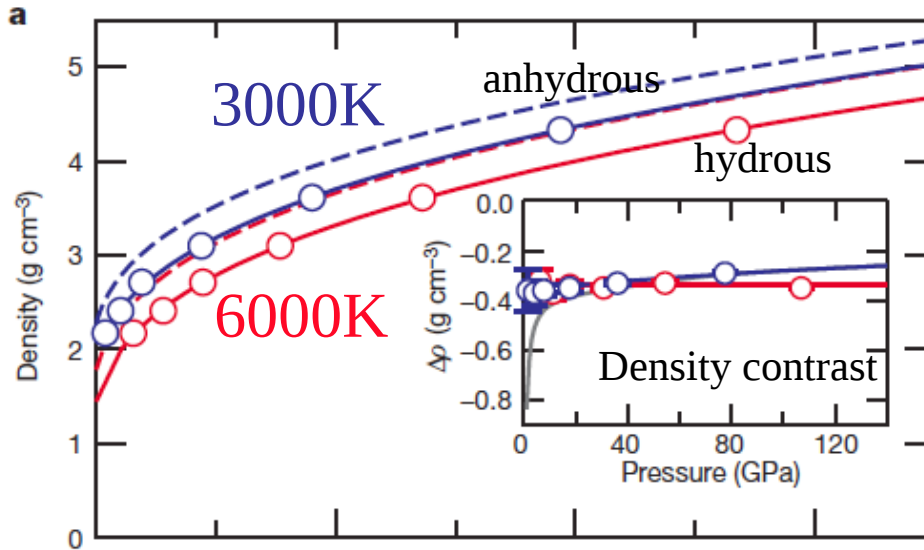
Activation volume (V^*)

0.11 cm^3/mol

Literature value

126kJ/mol (hydrous
basaltic melt)

Density of hydrous silicate melt



Equation of State (Mie-Gruneisen form)

$$P(V, T) = P_c(V, T) + \frac{\gamma}{V} C_v (T - T_0)$$

P_c : reference isotherm, γ : Gruneisen parameter
 C_v increases and γ decreases with P

Thermal pressure increases

Density contrast between dry and wet is very small

Estimated water content at 410km: 3wt.%

$\bar{V}_{\text{H}_2\text{O}}$ Partial molar volume of water in the silicate melt

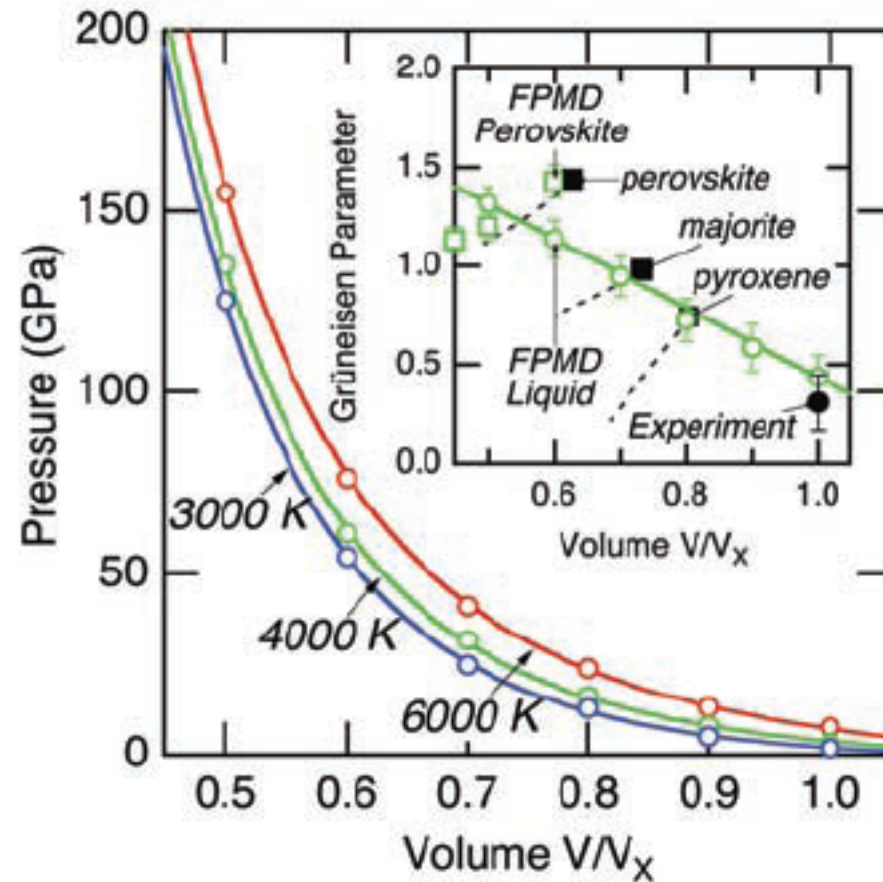
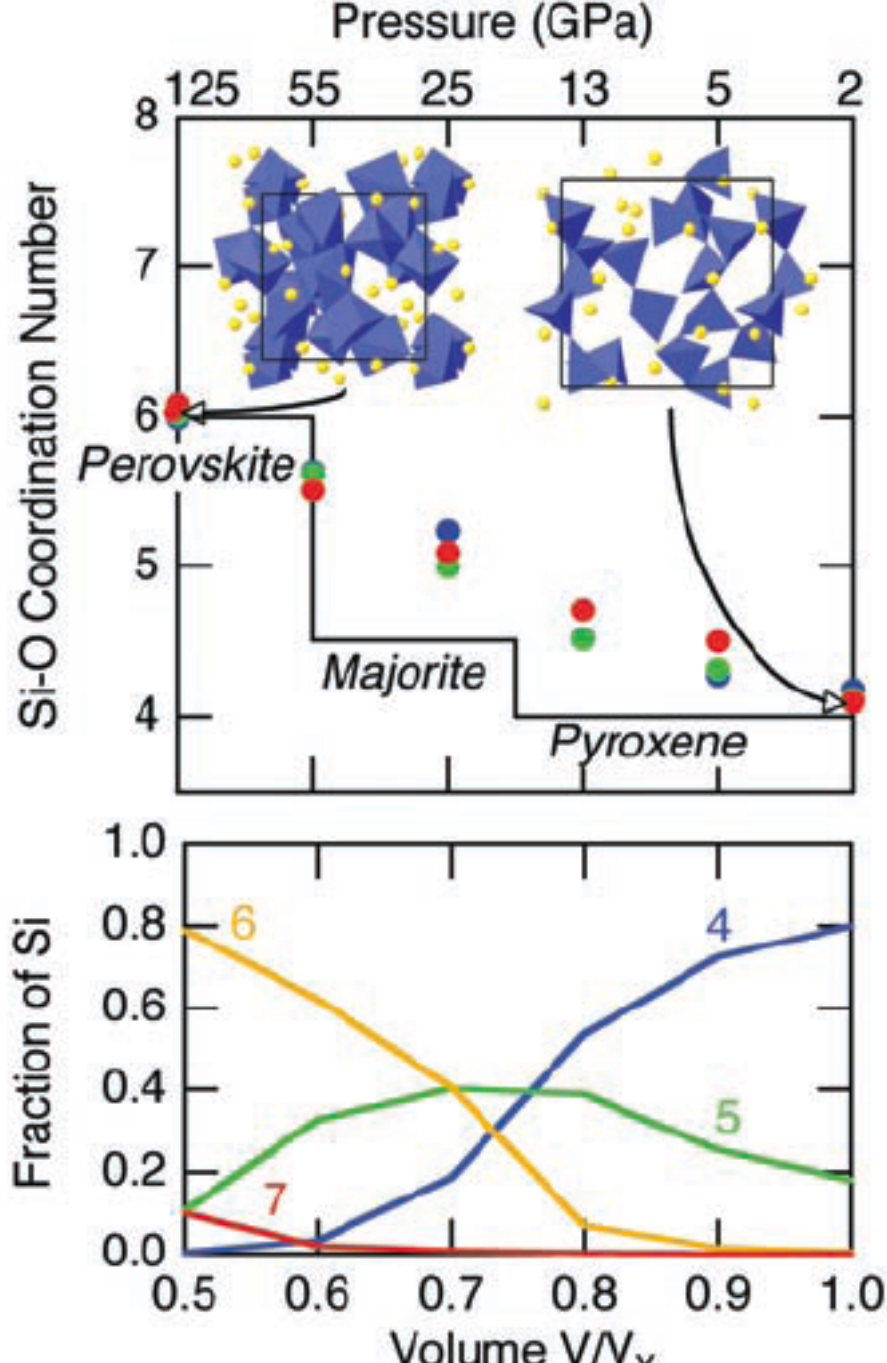
$$\Delta V = V_{\text{H}_2\text{O}} - \bar{V}_{\text{H}_2\text{O}}$$

At low P , ΔV large and negative

At high P , $\Delta V \rightarrow 0$

Ideal mixing (silicate + water)
at high P (no immiscibility)

MgSiO₃ liquid



Stixrude & Karki, 2005
Science