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From Core to Crust: Towards an Integrated Vision of Earth's Interior

20 - 24 July 2009

Molten Earth: Magma in the Deep Mantle

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MOLTEN EARTH: MAGMA IN THE DEEP MANTLE

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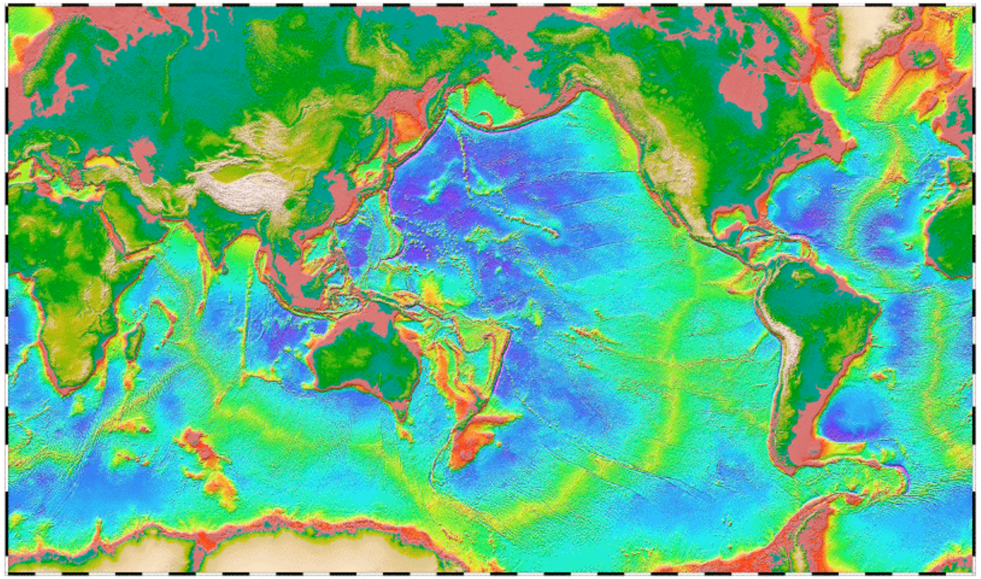
Molten Earth

- Very little of it is molten today
- Melt produced in shallow mantle escapes rapidly to the surface
- Responsible for formation of crust
- Long-term evolution of atmosphere, ocean
- Deep Earth?
- Early Earth?



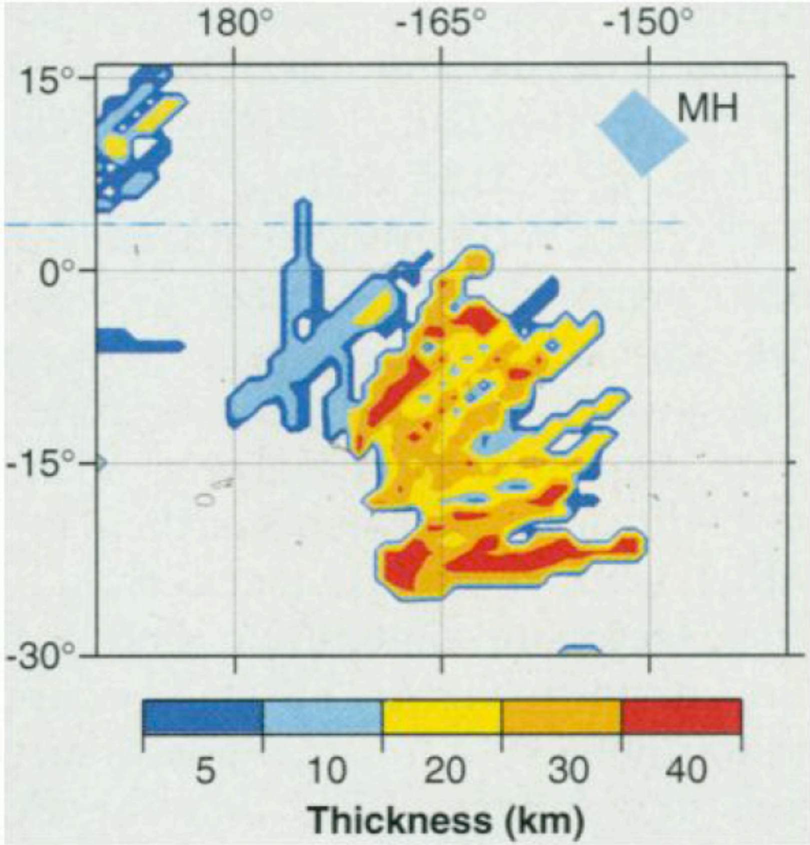
Early Earth

- May have been completely molten
  - Kinetic energy of accretion
  - Core formation
- Archean Lavas
  - Hotter
  - Melting at great depth

Canup (2004) Icarus

Deep Earth

- Ultra Low Velocity Zones
  - Located at core-mantle boundary (2890 km depth)
  - ~10 km thick
  - Collosal velocity anomaly (>20 % in V_S)
  - Possibly partial melts
- Lateral heterogeneity in the deep mantle



Williams & Garnero (1996) Science

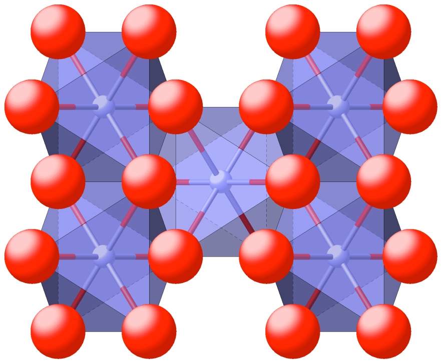
Magma Dynamics Today

- Mostly in upper 100 km
- Large volume contrast
  - ~10 % between liquid and coexisting solids
  - Liquid and crystalline structures differ
- Consequences:
  - Buoyancy
  - Steep melting slope
  - (Clapeyron Equation)
- Higher Pressure?

Structure of Silicates

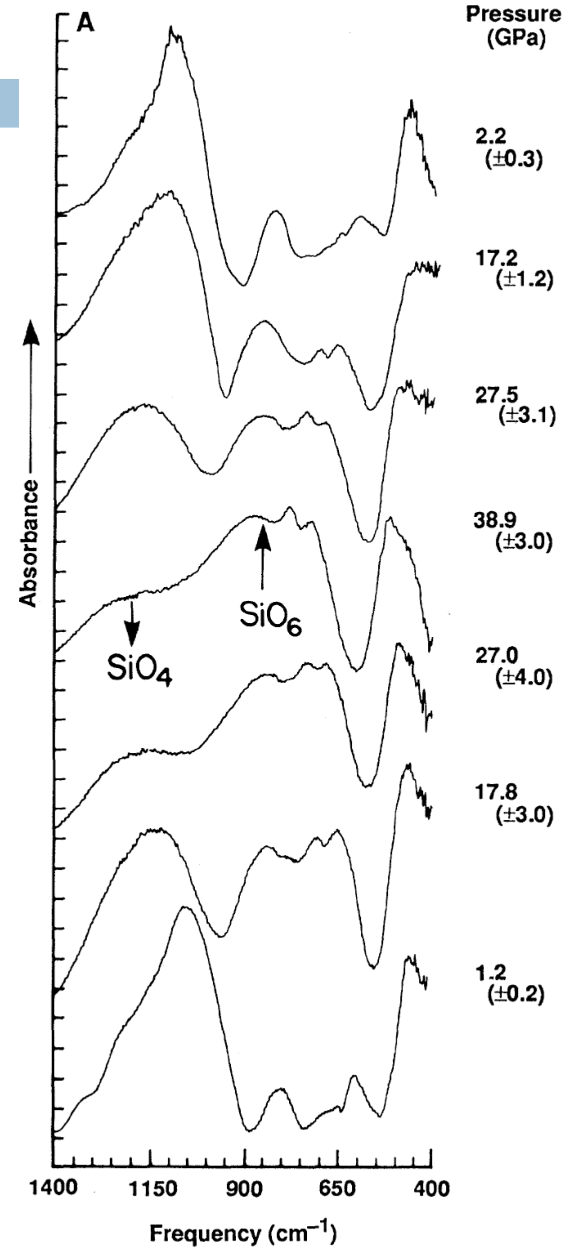
- Tetrahedrally coordinated
  - SiO_4 tetrahedra
  - Most abundant minerals in Earth's crust
- Octahedrally coordinated
  - SiO_6 octahedra
  - Stabilized by elevated pressure (P>10 GPa)
  - Much denser than tetrahedrally coordinated silicates
  - Most abundant "minerals" in mantle ($MgSiO_3$ perovskite)
- Liquids?
  - Can silicate liquids exhibit octahedral coordination?

Chao et al. (1962) JGR



Silicate Liquid Structure?

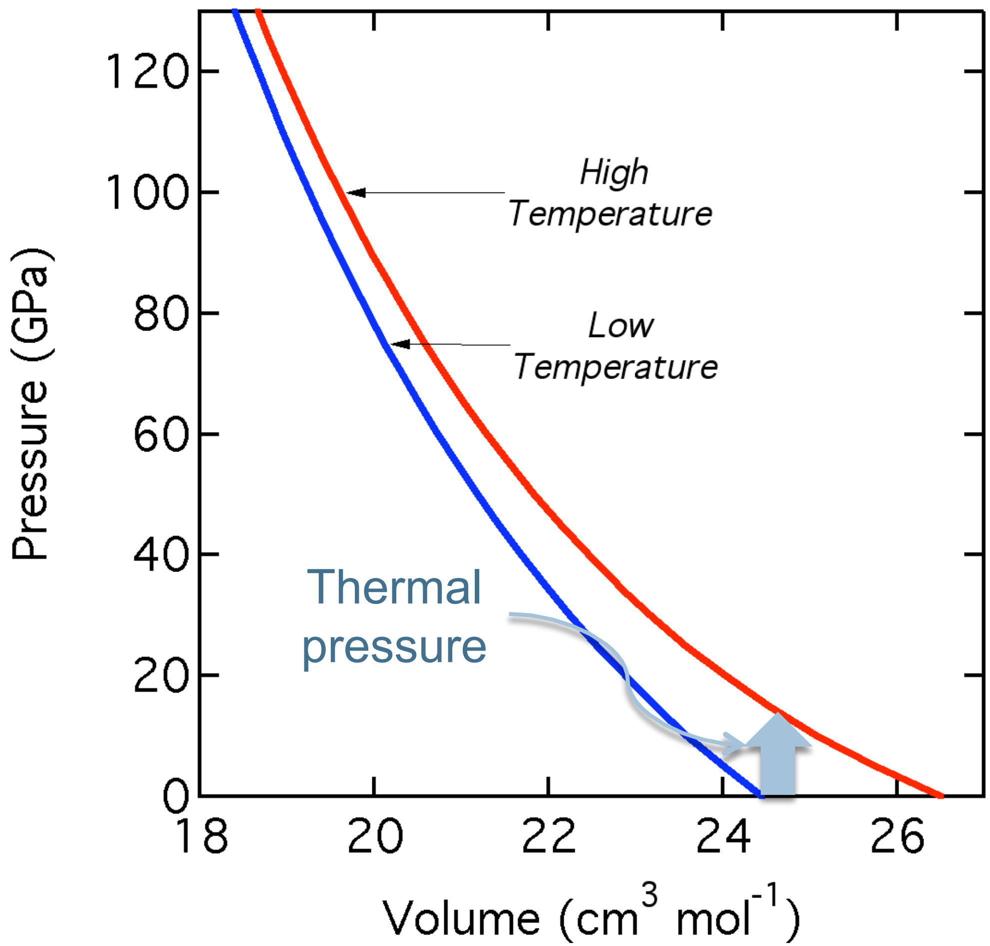
- Low pressure experiment reveals tetrahedral coordination
- No experimental data above a few GPa
- Previous studies on glasses
- Suggest gradual transition from dominantly tetrahedral to dominantly octahedral over several tens of GPa
- Liquids?

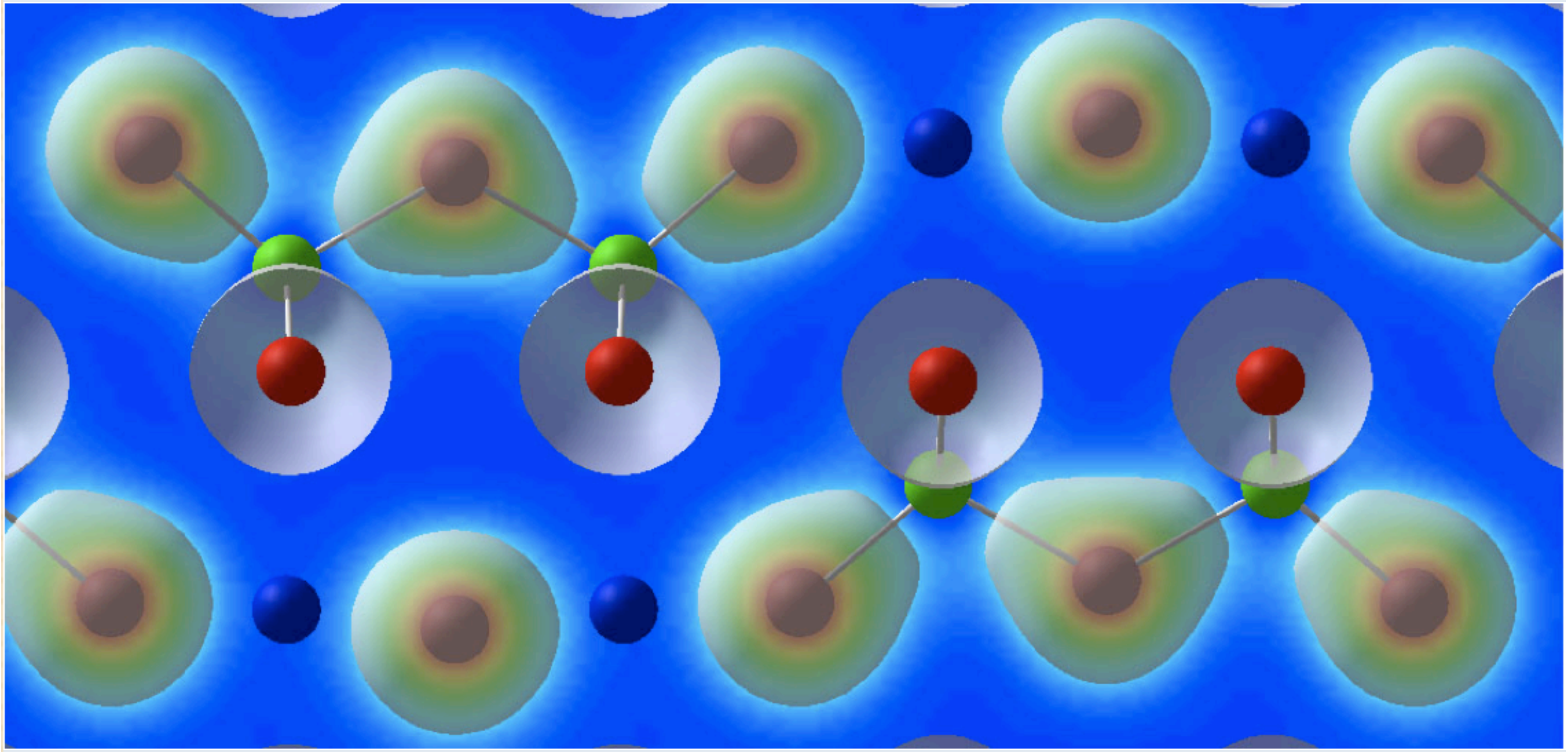


Williams & Jeanloz (1988) Science

Equation of State of Mantle Solids

- Thermal pressure
  - Decreases on compression
  - Thermal effects "squeezed out"
  - $P_{TH} \sim \gamma 3 N k_B T/V$
- Grüneisen parameter γ
  - Decreases on compression
  - Controls magnitude of thermal pressure
  - Controls adiabatic gradient
  - $\gamma = (d\ln T/d\ln V)_S$
- Liquids? Virtually unknown at lower mantle conditions





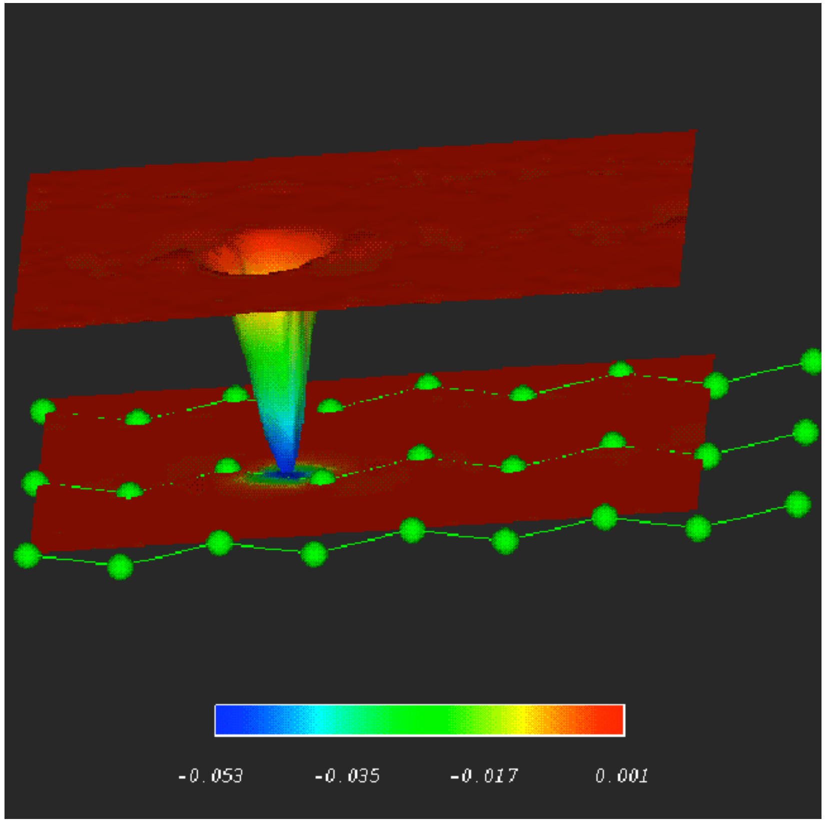
N. de Koker, Bayreuth

Density Functional Theory

Charge density in Mg_2SiO_4 wadsleyite

Density Functional Theory

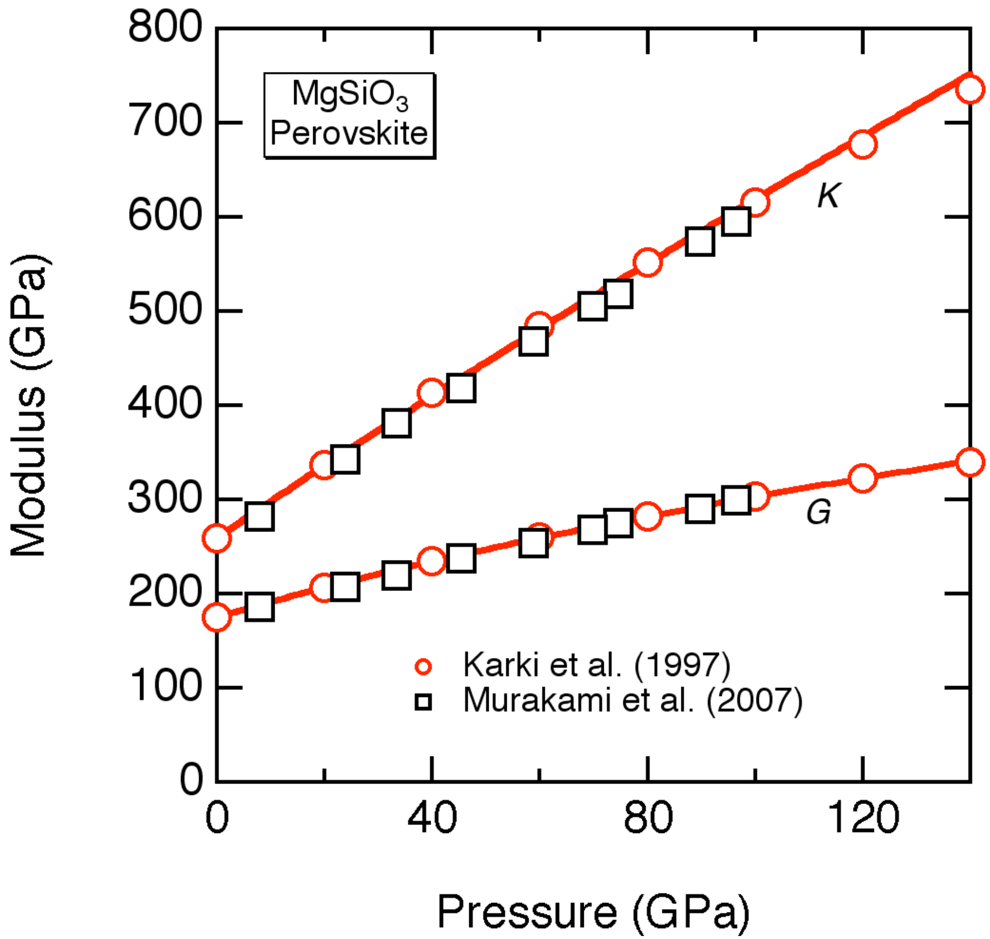
- Schrödinger Equation
  - Exact but insoluble
  - Central quantity: many electron wave function
- Kohn-Sham Equations
  - Exact and an excellent starting point for approximation
  - Central quantity: charge density
- Exchange-correlation hole
  - e^- digs a hole of reduced charge density about itself
  - Approximate form of this interaction
  - Local Density Approximation (LDA)



R. Q. Hood, Cambridge

Density Functional Theory

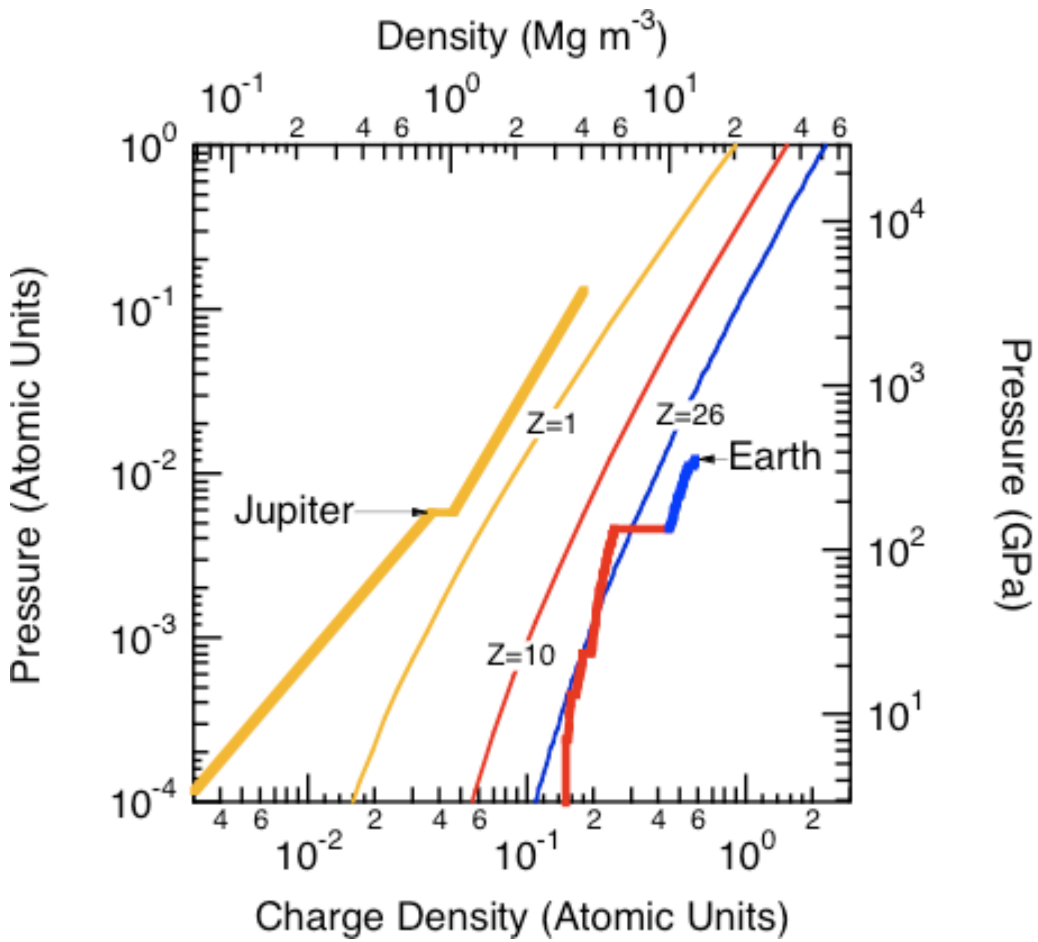
- Predictive power
  - No free parameters
  - No *a priori* assumptions regarding shape of charge density or nature of bonding
- Scope
  - Entire pressure-temperature range of planets (and stars)
  - Entire periodic table
- Accuracy
  - Tested via comparison with experimental data

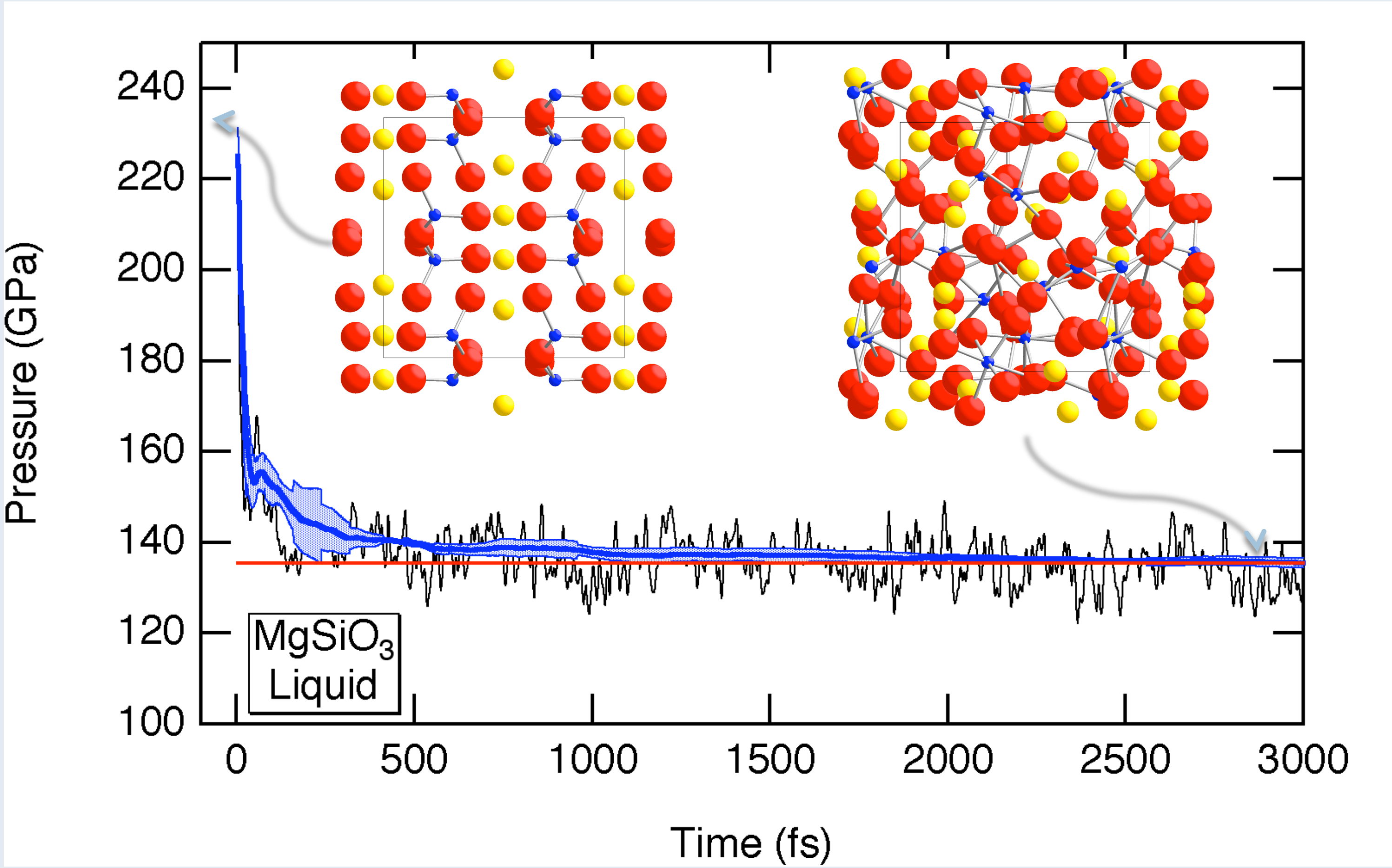


Circles: Karki et al., 1997, Am. Min.
Squares: Murakami et al., 2006, EPSL

Theory of Planetary Materials

- Earth occupies an intermediate regime pressure-temperature regime in which material behavior is remarkably rich
- Pressure is large ~1 Mbar
  - Bond deformation pressure: 1 eV/Å^3~1.6 Mbar
  - Bulk Modulus ~ 1.5 Mbar
- But not so large that simple theories apply, e.g. for stars:
  - Thomas-Fermi
  - Ideal gas law





First Principles Molecular Dynamics

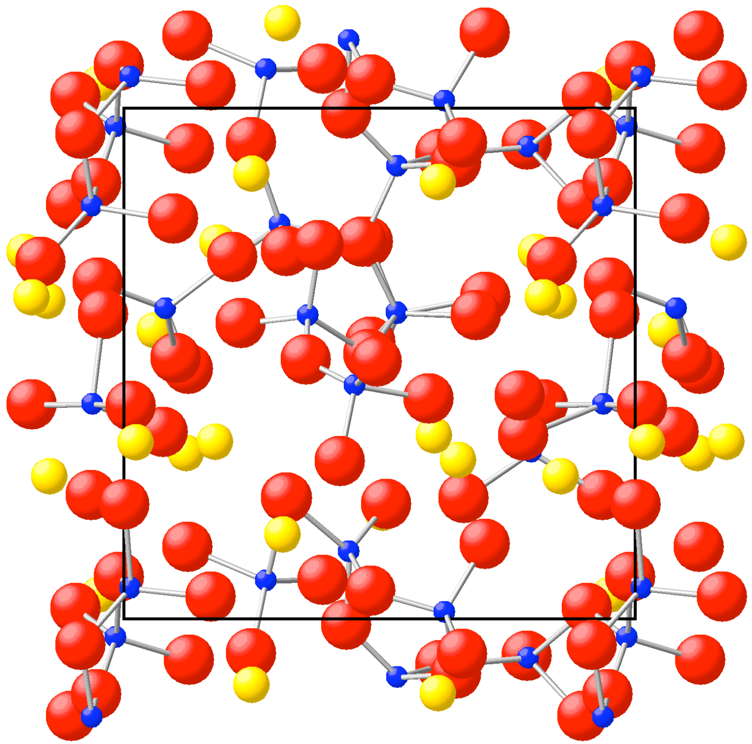
Example: $MgSiO_3$; Two-fold compression: V/V_X=0.5; 6000 K

Initial condition: pyroxene structure, Maxwellian velocities

First Principles Molecular Dynamics

- Dynamics
  - Newtonian trajectory
  - Forces on nuclei from density functional theory
  - Born-Oppenheimer limit
  - Efficient solution of electronic problem
- Statistical mechanics
  - Thermodynamic properties via ergodic hypothesis
  - Nosé Thermostat (*NVT*)
- Computation
  - Plane-wave pseudopotential method
  - VASP: Kresse, Hafner, Furthmüller
- Systems:

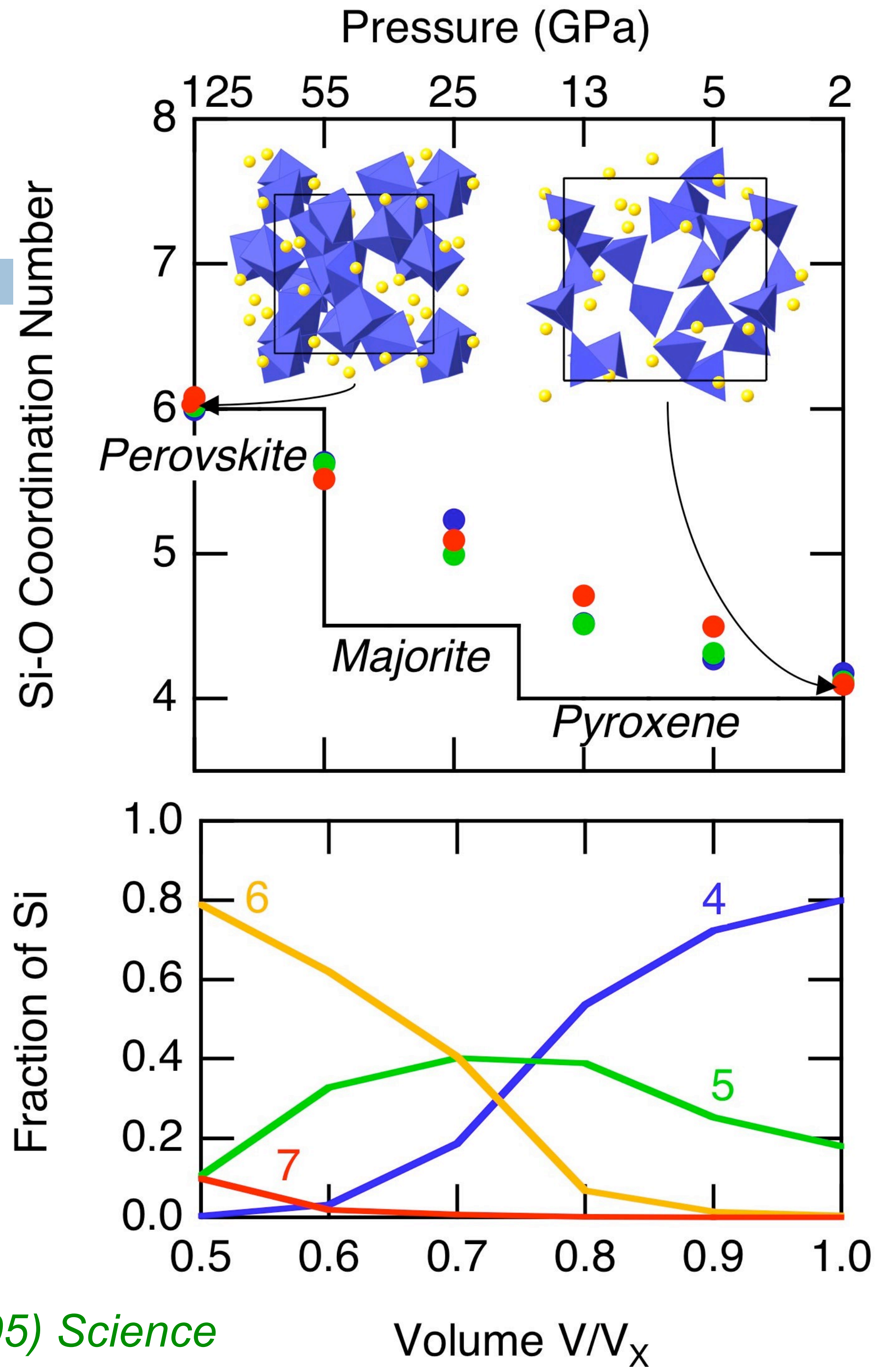
$MgSiO_3$, Mg_2SiO_4, $MgSiO_3$-H_2O
MgO-SiO_2, Fe_2SiO_4



$MgSiO_3$; P~0 GPa; 3000 K

Liquid Structure

- Octahedral coordination at base of mantle
- Gradual change in mean coordination number
- Nearly linear in volume
- Five-fold most abundant at intermediate compression

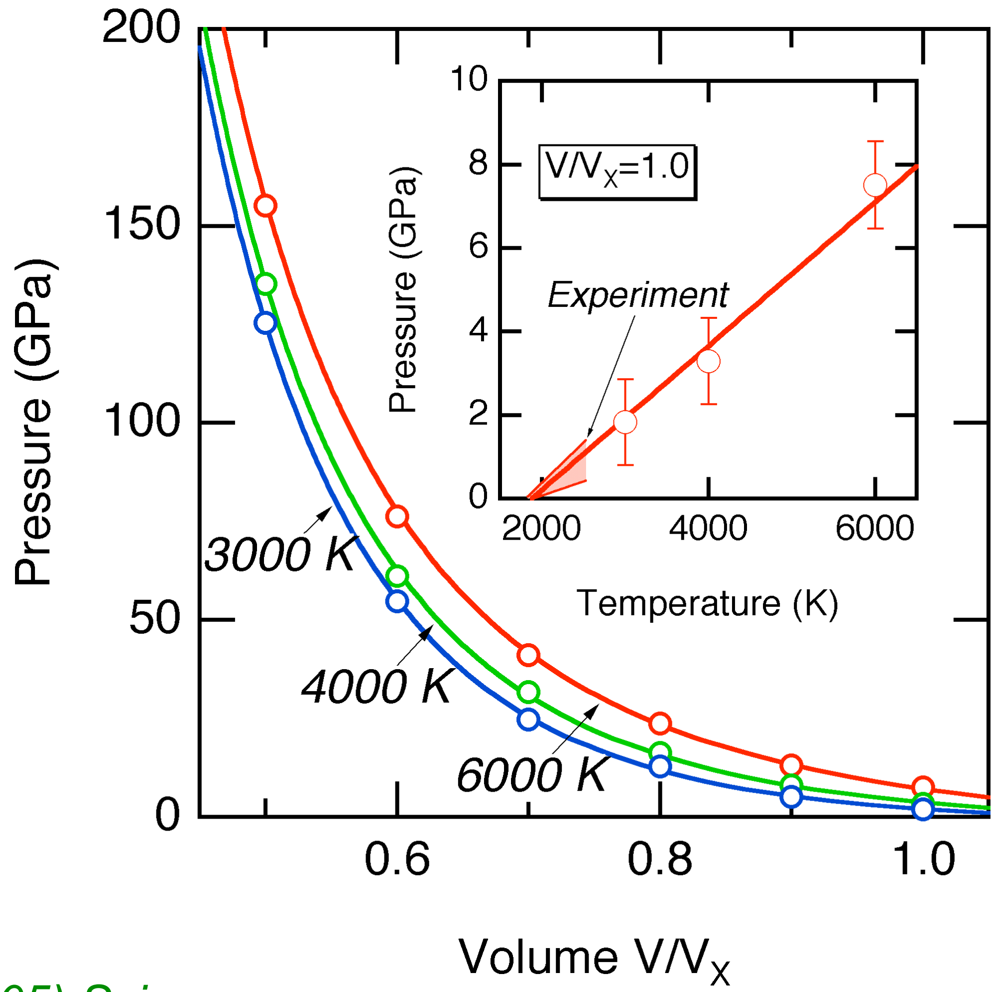


$MgSiO_3$

Stixrude & Karki (2005) Science

Equation of State

- Differs fundamentally from solid equation of state
- Isotherms diverge on compression
- Smooth function
- Excellent agreement with available experimental data

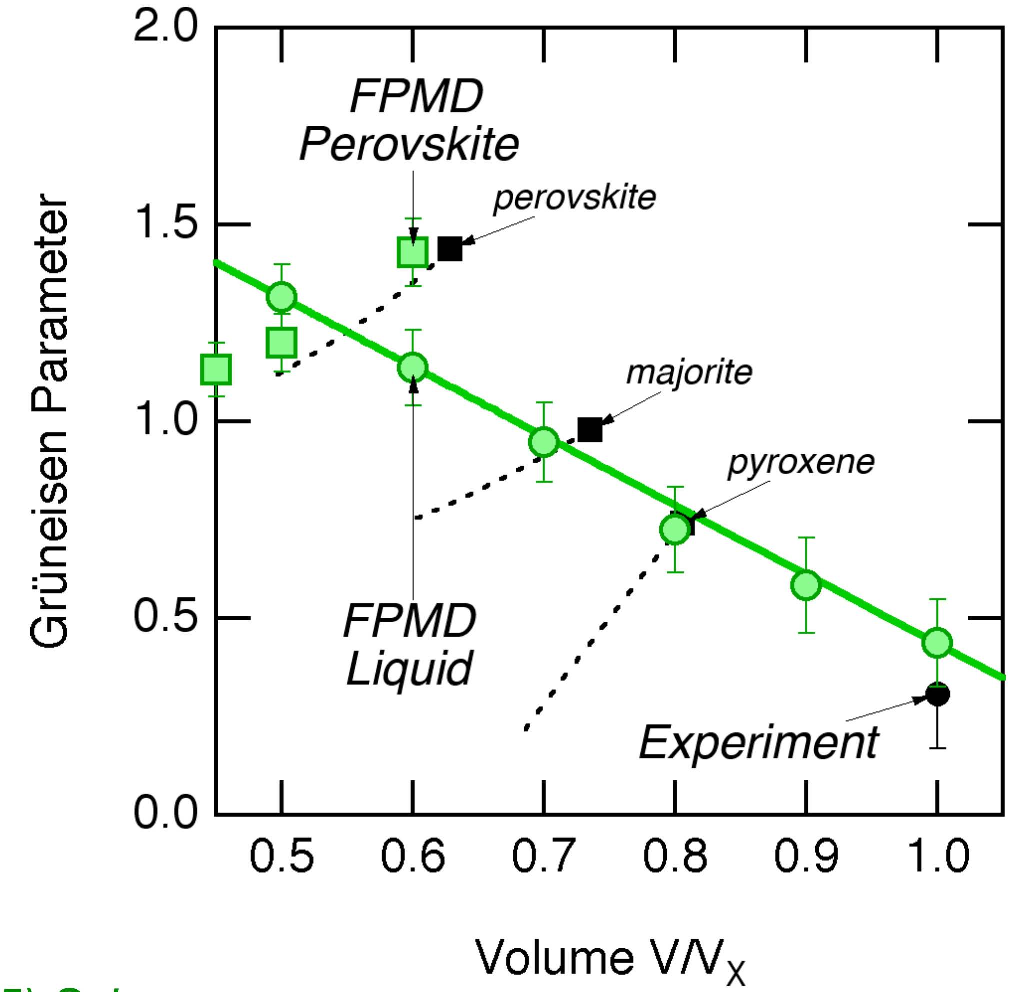


MgSiO$_3$

Stixrude & Karki (2005) Science

Grünseisen Parameter

- Increases on compression
- Differs from all mantle crystalline phases
- Caused by change in liquid structure on compression
- Excellent agreement with available experimental data

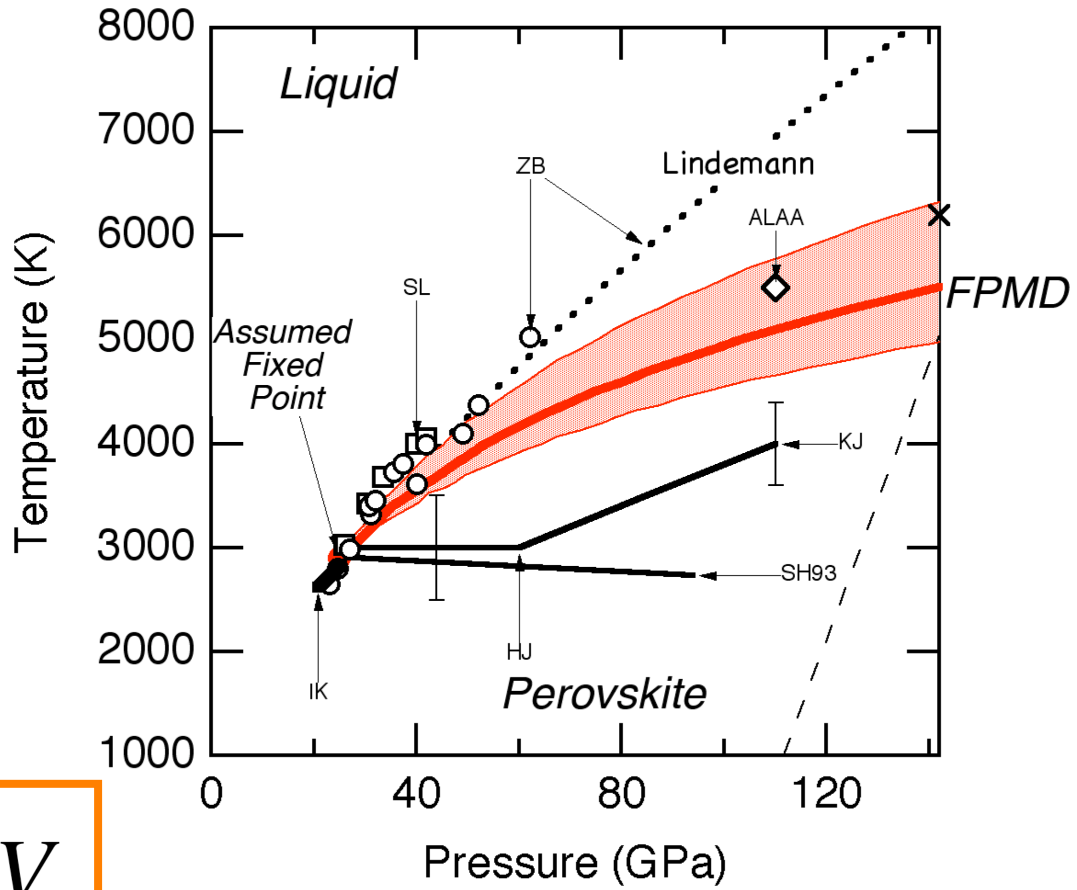


$MgSiO_3$

Stixrude & Karki (2005) Science

Melting Curve

- Integrate Clapeyron equation using FPMD results
- $MgSiO_3$ melts at 5400±600 K at mantle's base
- Agrees with Hugoniot datum
- Disagrees with previous studies based on the laser-heated diamond anvil cell
  - Detection of melt
- Disagrees with Lindemann Law
  - Liquid structure changes on compression



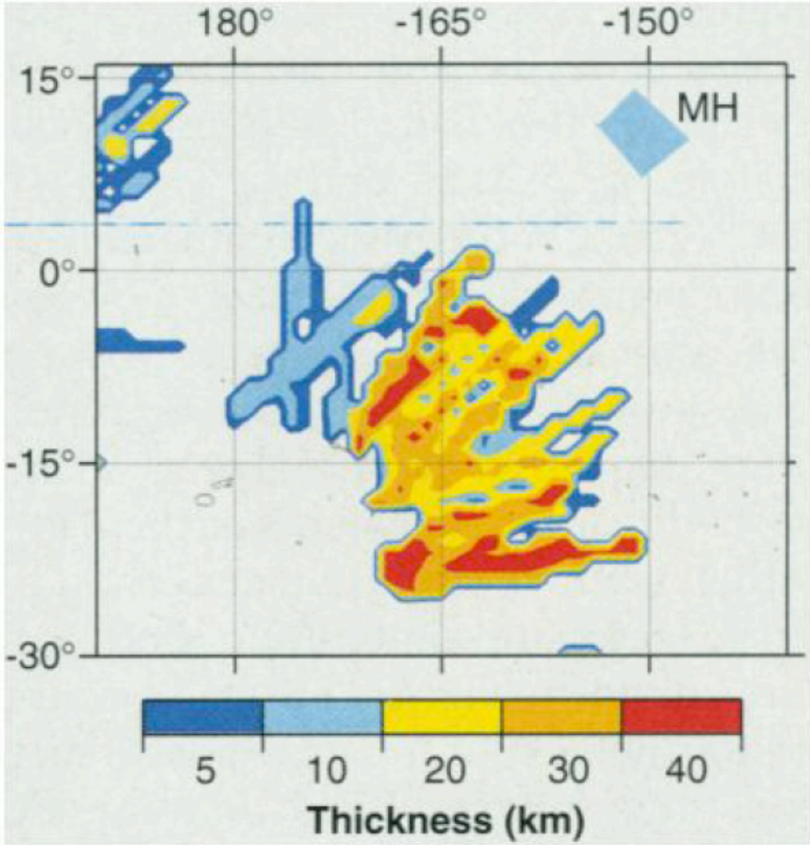
$MgSiO_3$

$$\boxed{\left(\frac{\partial \ln T_M}{\partial P}\right) = \frac{\Delta V}{\Delta H}}$$

Stixrude & Karki (2005) Science

Origin of ULVZ

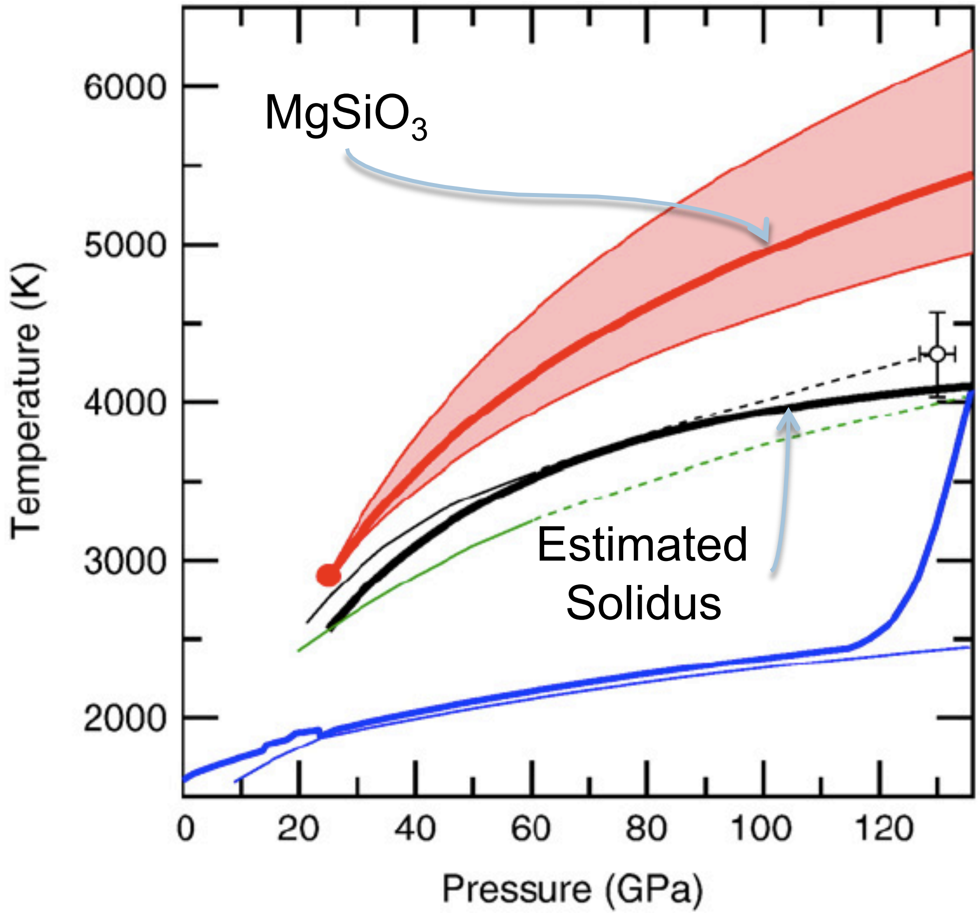
- Ultra Low Velocity Zones
  - Located at core-mantle boundary (136 GPa)
  - ~10 km thick
  - Colossal shear velocity anomaly (ΔV_S>20 %)
  - Large longitudinal velocity anomaly (ΔV_P~10 %)
- Partial Melt
  - Thermodynamically stable
  - Denser than surroundings
  - Satisfy seismic observations



Williams & Garnero (1996) Science

Origin of ULVZ

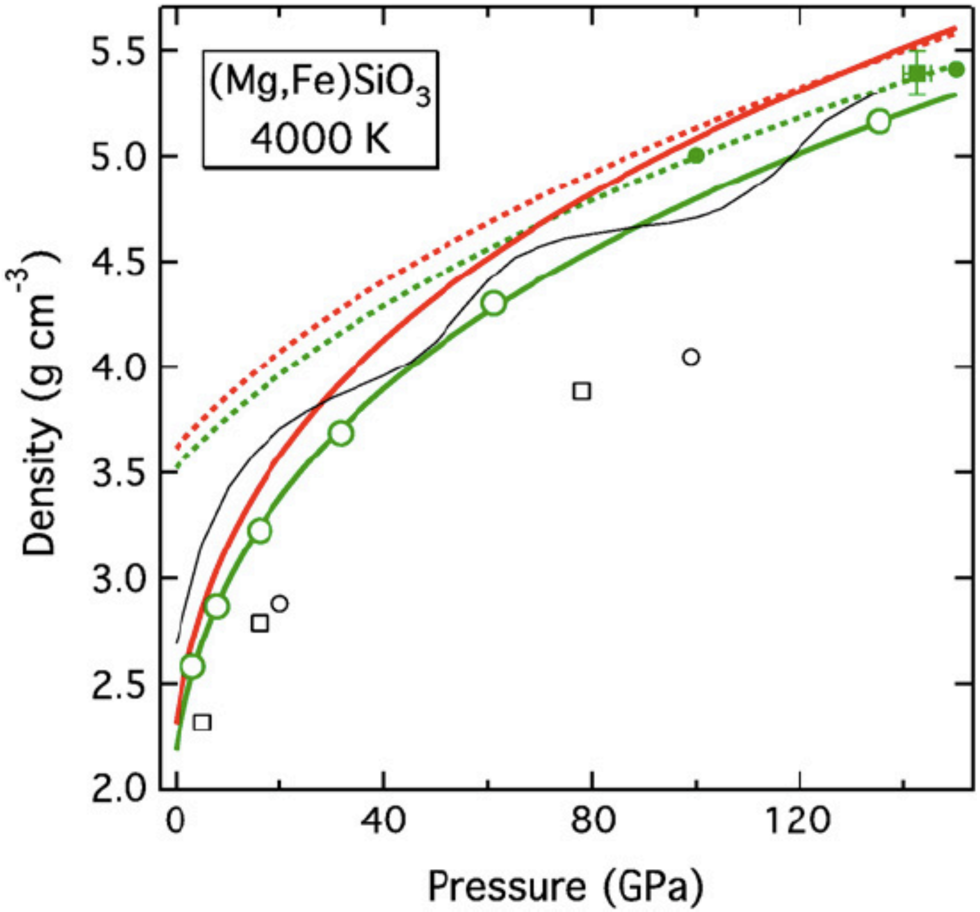
- Base of mantle may be molten
- Assume freezing point depression of 1300 K
- Based on ionic MD (Zhou & Miller, 1997). Water not considered
- Solidus at 4100 K
- Identical to modern estimates of temperature at core-mantle boundary
- Agrees with previous experimentally based extrapolations



Stixrude et al. (2009) EPSL

Origin of ULVZ

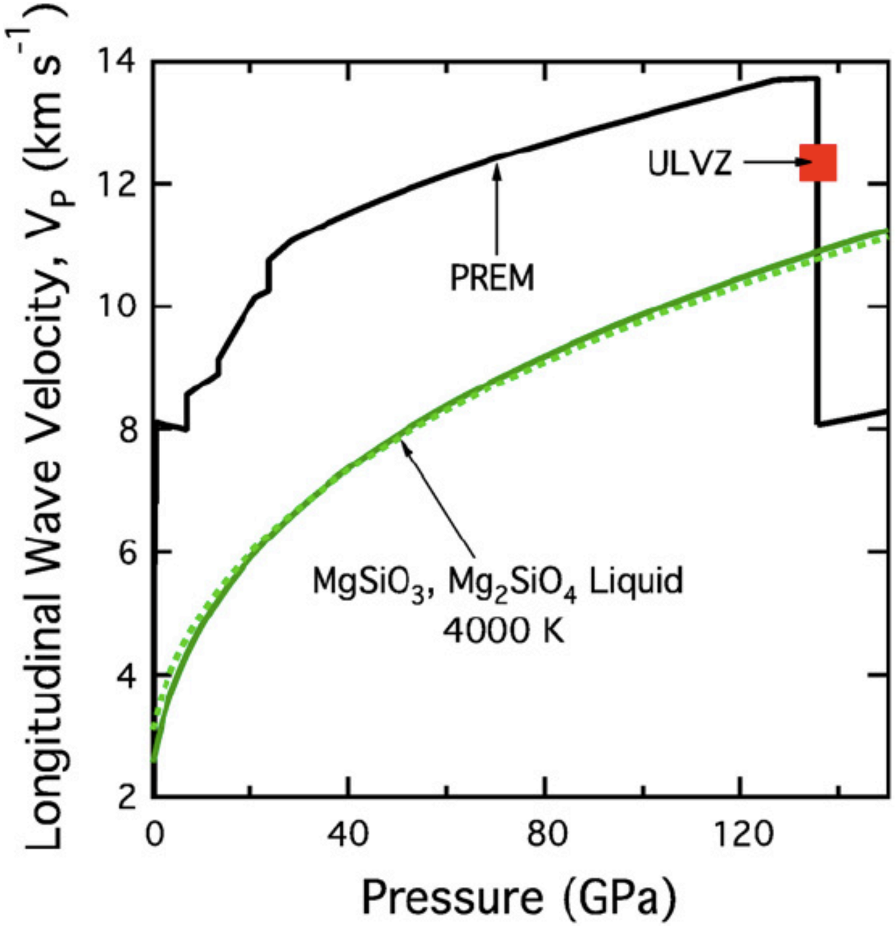
- Liquid likely denser than coexisting solids at base of mantle
- Small volume contrast
- Sensible iron partitioning
- DFT level of theory essential
- Excellent agreement with available shock wave data



Stixrude & Karki (2005) Science
Stixrude et al. (2009) EPSL

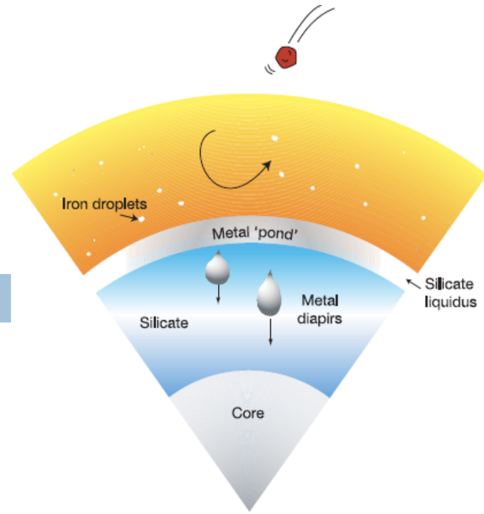
Origin of ULVZ

- Partial melt
- Wave velocity of silicate liquids ~20 % lower than that at mantle's base
- Seismological observation finds ULVZ ~10 % slower
- Precise amount of partial melt required depends sensitively on texture

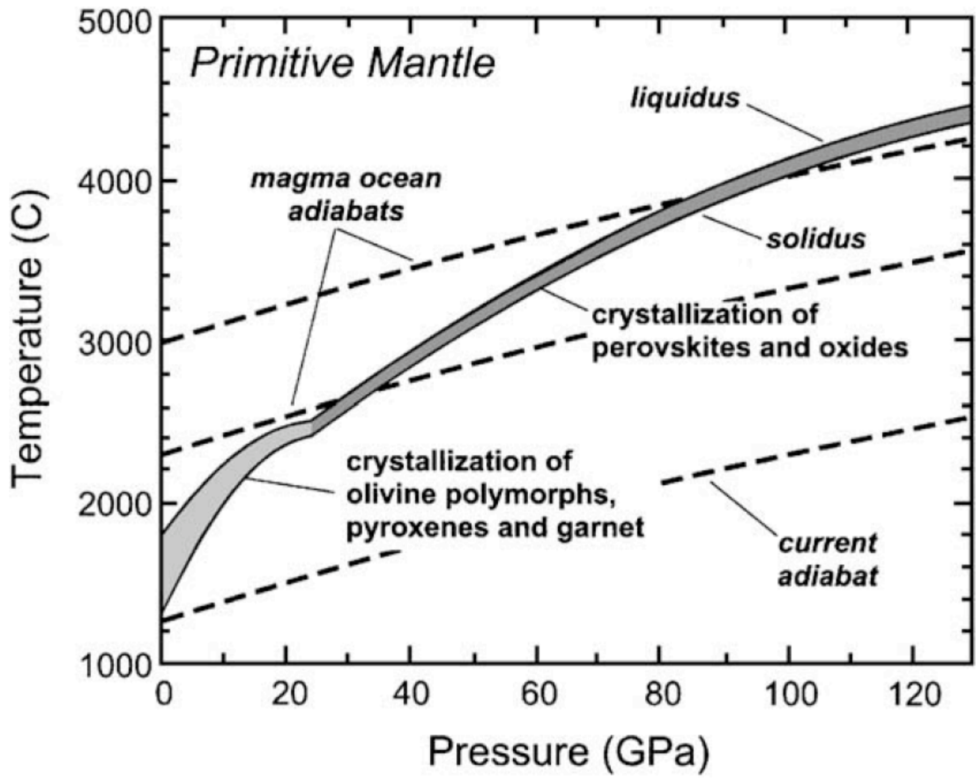


Stixrude & Karki (2005) Science
Stixrude et al. (2009) EPSL

Was the Earth Molten? Previous Studies



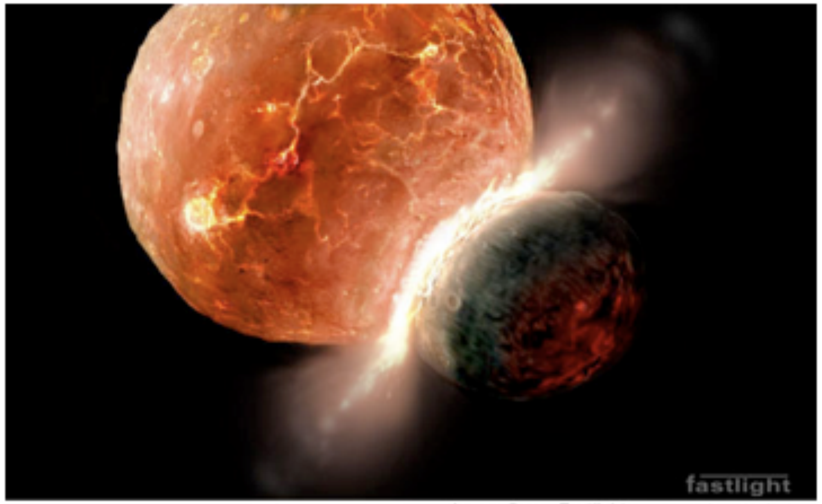
- Concept of magma "ocean" with a crystalline silicate floor comes from studies of moon
- Magma ocean adiabat roughly parallel to that of present mantle
- Shallower than solidus
- Very high potential temperatures required for complete melting
- Crystallization begins at base



Wood et al. (2006) Nature   *Walter & Tronnes (2004) EPSL*

Was the Earth Molten?

- Deep turbulent convection
- Isentropic (adiabatic) temperature gradient
- Much higher than thought because γ is much larger than previously assumed
- Adiabat steeper than melting curve at depth
- *Complete* melting much easier than previously thought

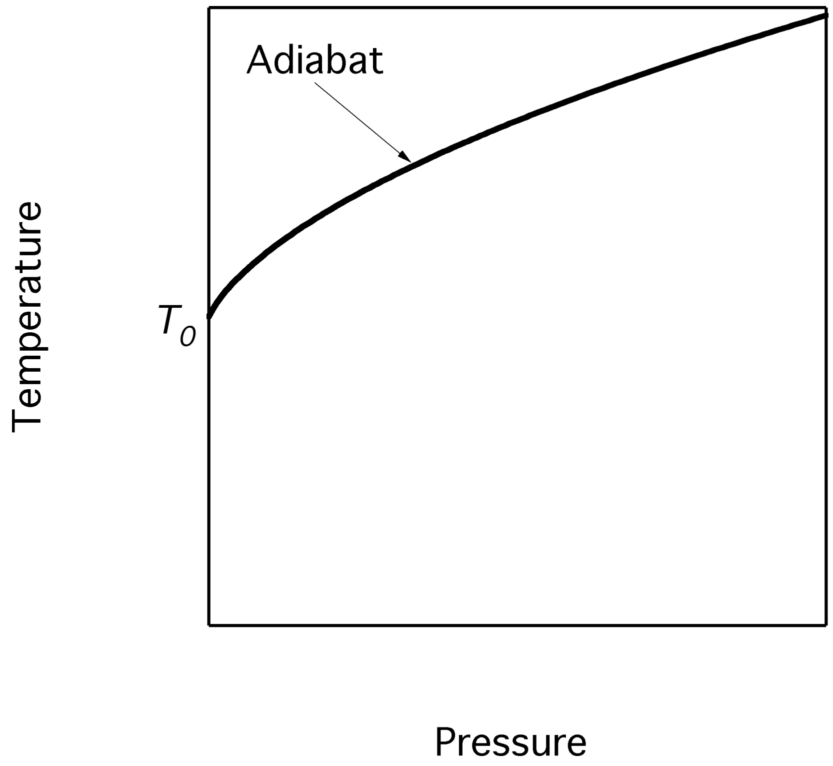


$$\boxed{\left(\frac{\partial \ln T}{\partial P}\right)_S = \frac{\gamma}{K_S}}$$

Was the Earth Molten?

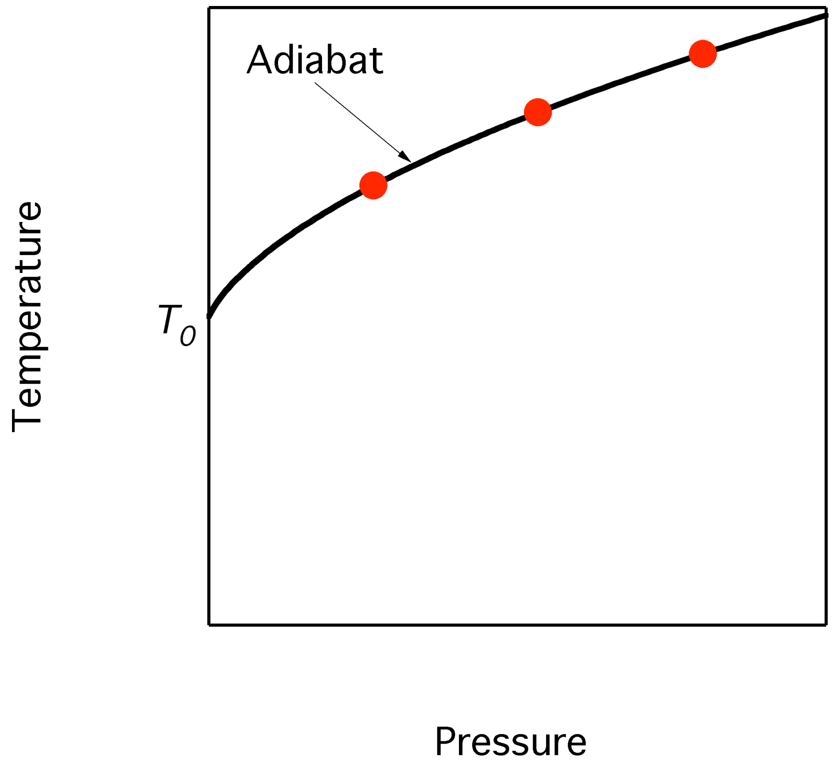
$$\left(\frac{\partial \ln T}{\partial P}\right)_S = \frac{\gamma}{K_S}$$

- Compare temperature at depth $T_{ad}(P)$ to melting temperature $T_M(P)$
- Adiabatic gradient is a material property
- Particular adiabat $T_{ad}(P)$ is specified by temperature at the surface
- Potential temperature T_0
- Increase in temperature originates in gravitational self-compression



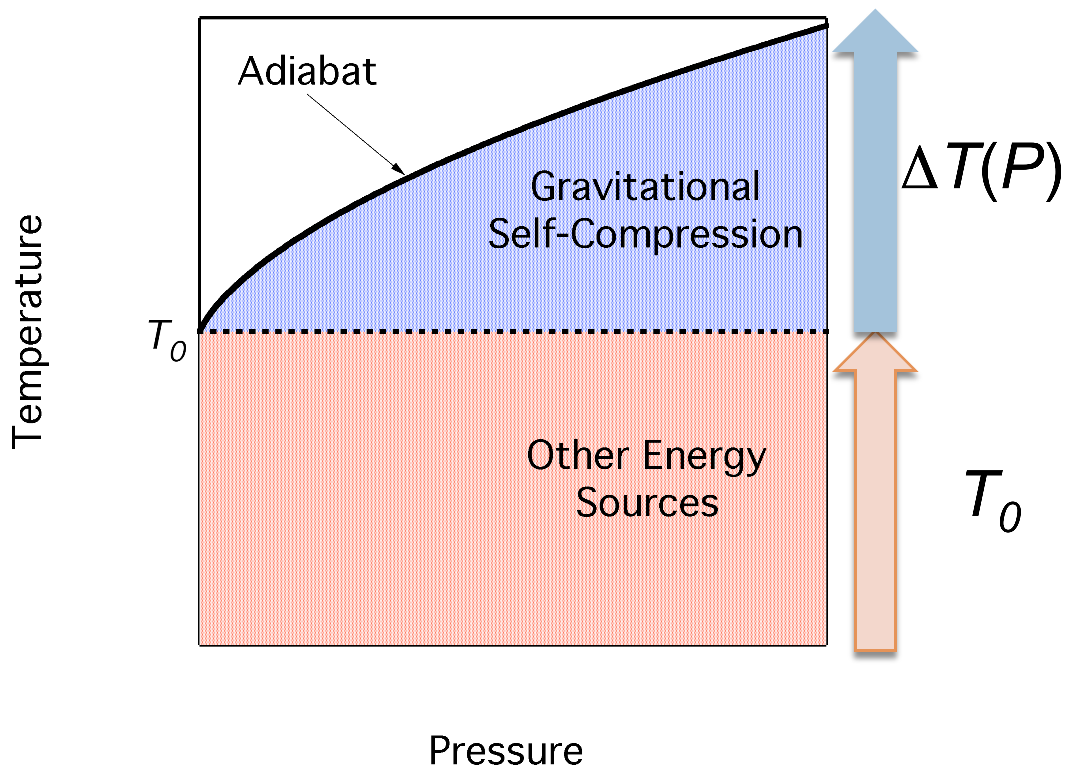
Was the Earth Molten?

- Potential temperature is also the temperature that any parcel of the interior would cool to on adiabatic ascent
- The temperature increment due to gravitational self -compression: $\Delta T(P) = T_{ad}(P) - T_0$



Was the Earth Molten?

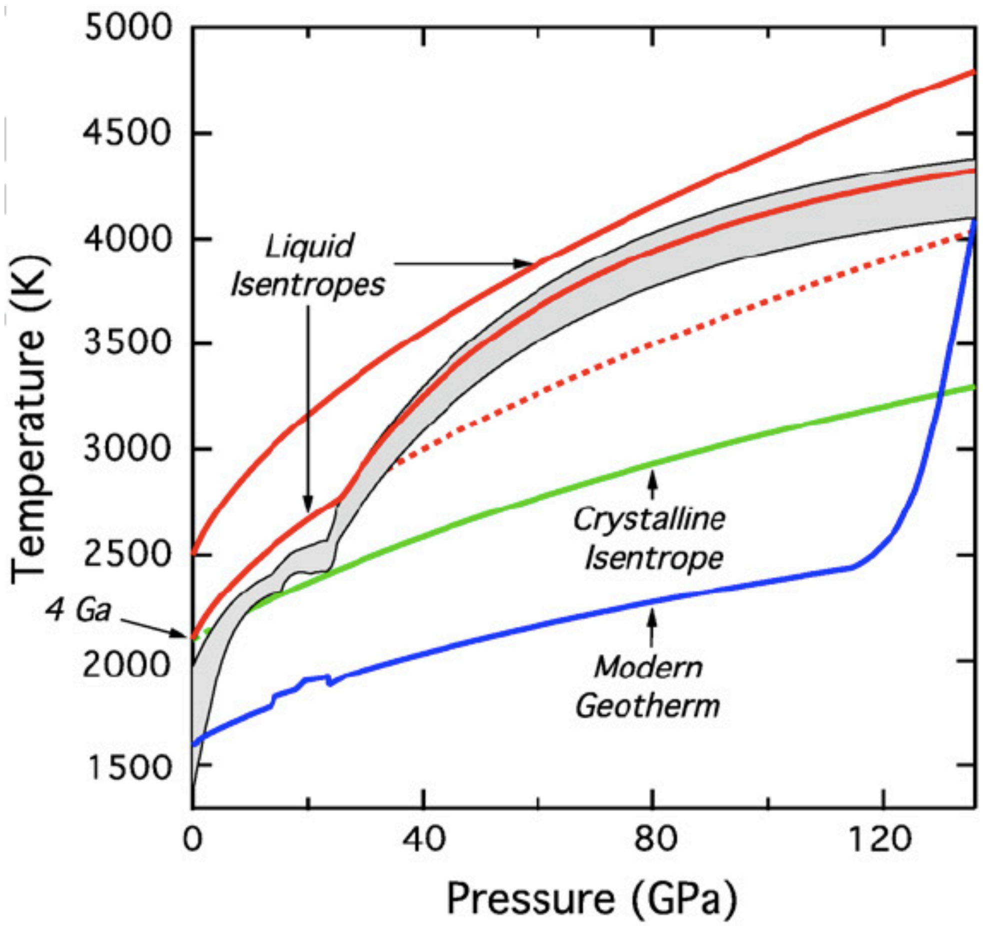
- Temperature $T_{ad}(P)$ is the sum of two energy sources
- Gravitational self -compression sets $\Delta T(P)$
- Other energy sources set T_0
  - Accretional Energy
  - Core Formation
  - Radioactive decay



$$T_{ad}(P) = \Delta T(P) + T_0$$

Was the Earth Molten?

- Complete melting much easier than previously thought
- $\Delta T(P)$ much greater than previously thought
  - Steep liquid-state adiabats (large γ)
- T_0~2450 K sufficient to melt entire mantle
- T_0~2000 K (Archean plumes?) produces melt in lower mantle
- Crystallization of magma ocean begins at mid-mantle depths



Stixrude et al. (2009) EPSL

Molten Earth

Lower Magma Layer

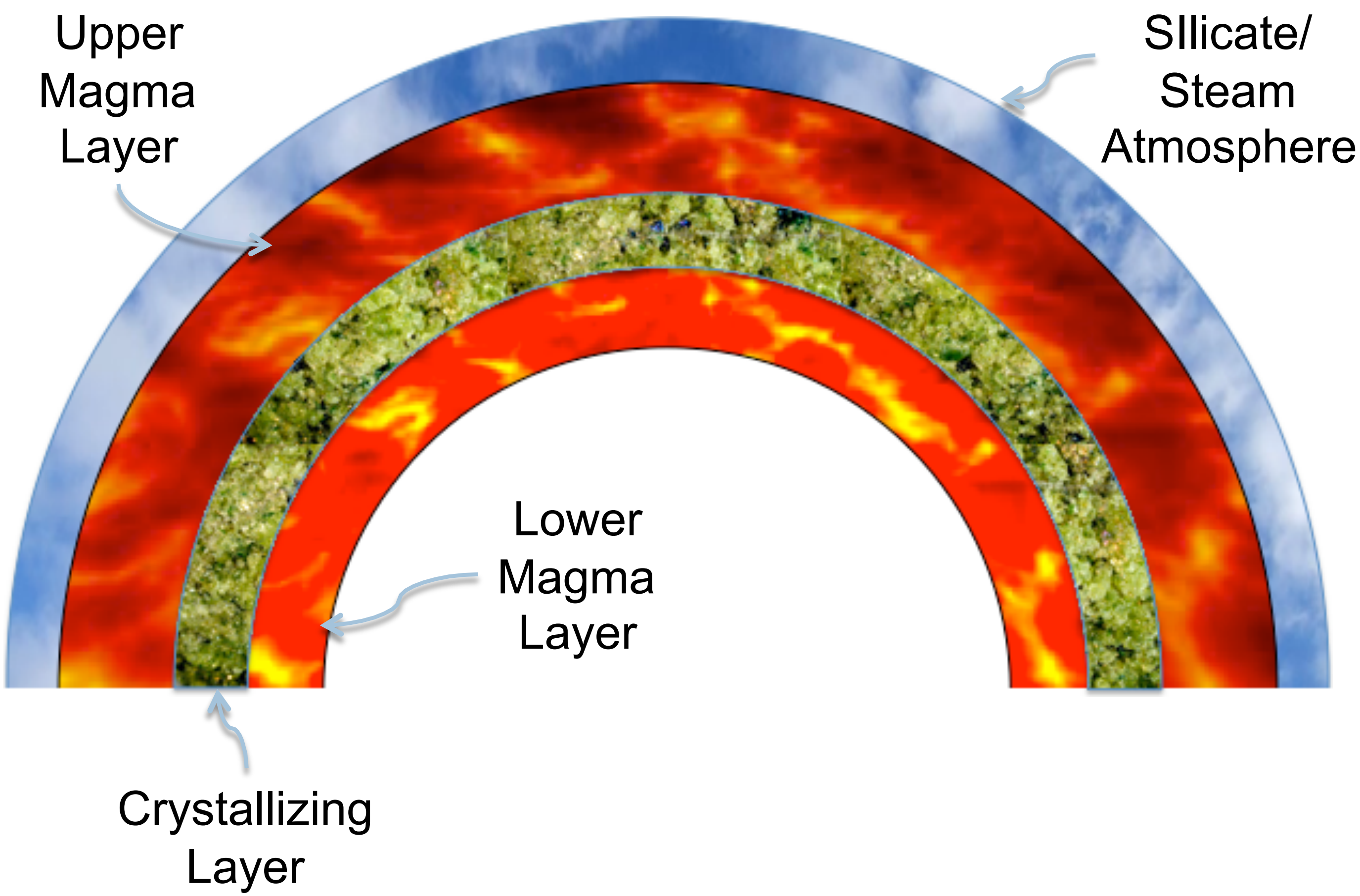
ULVZ a remnant?

Source of chondritic complement?

Source of lower mantle chemical heterogeneity?

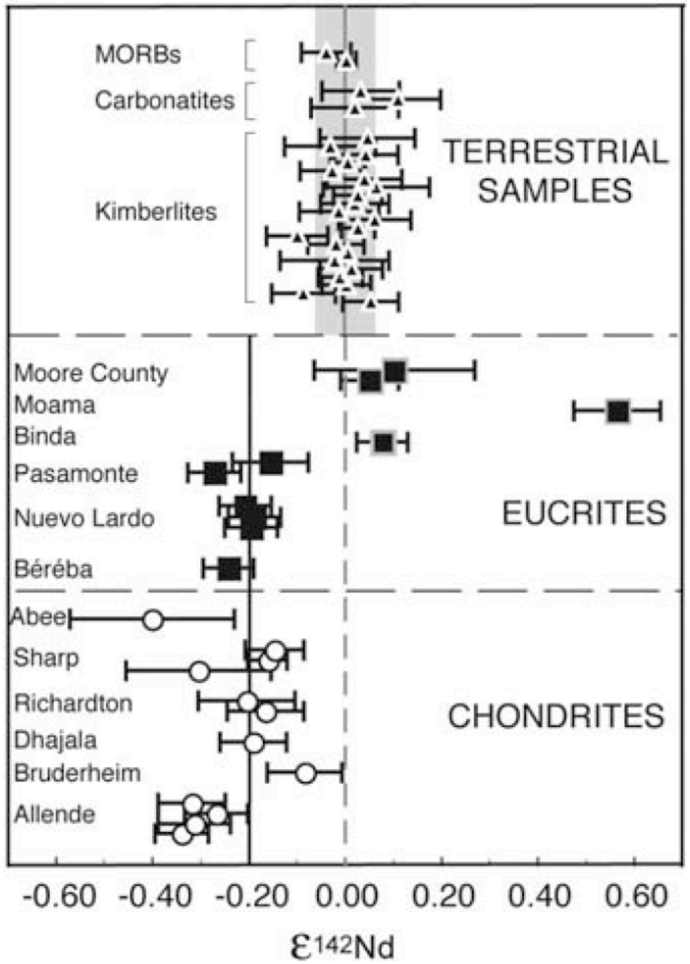
Volatile reservoir?

Reaction with core?



Fossils of Molten Earth?

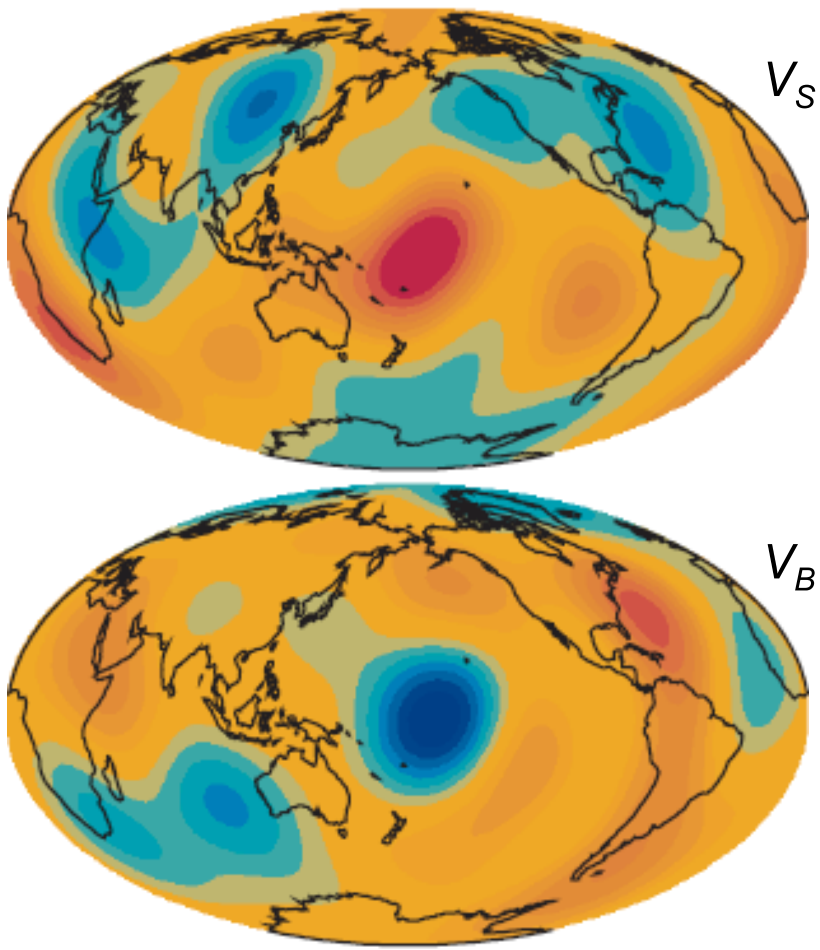
- Geochemically observable Earth, i.e. lavas, not chondritic after all
- Hidden non-chondritic reservoir?
- Possible remnant of lower magma layer



Boyet & Carlson. (2005) Science

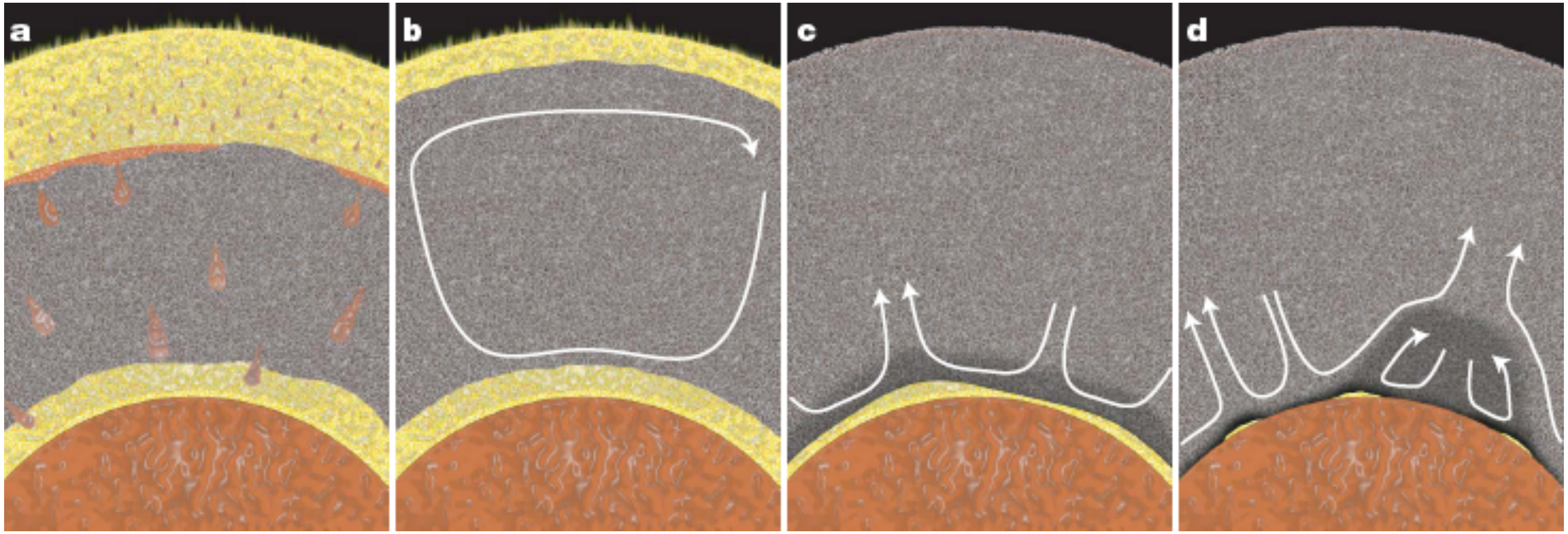
Fossils of Molten Earth

- Lateral variations in shear and bulk sound velocity may be anti-correlated in the lowermost mantle
- Some anomalies have sharp edges
- This cannot be caused by lateral variations in temperature alone
- Lateral variations in composition seem to be required
- Melting processes a natural way to produce compositional heterogeneity
- Lower magma layer may be the source



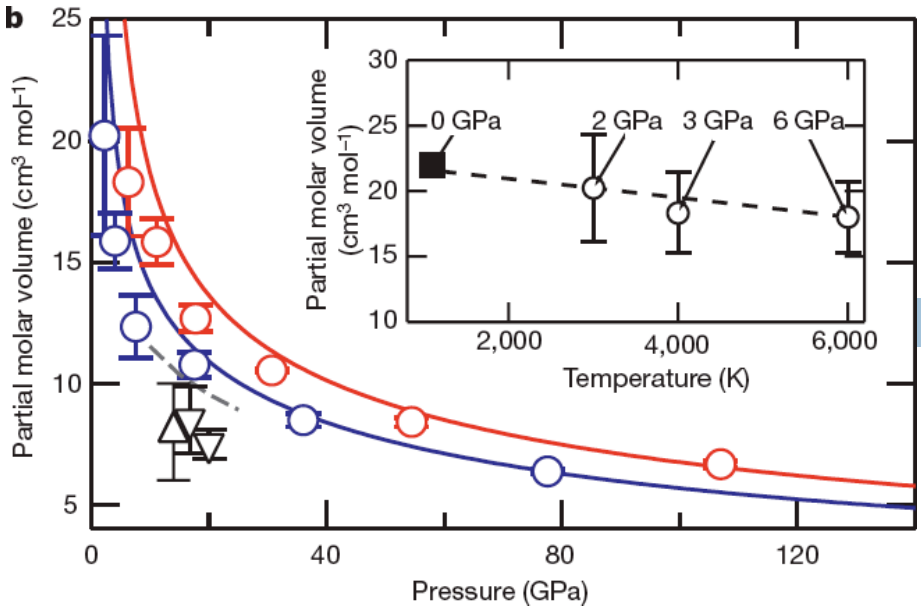
Ishii & Tromp (1999) Science

Molten Earth



Labrosse et al. (2007) Nature

Influence of Water on Melts

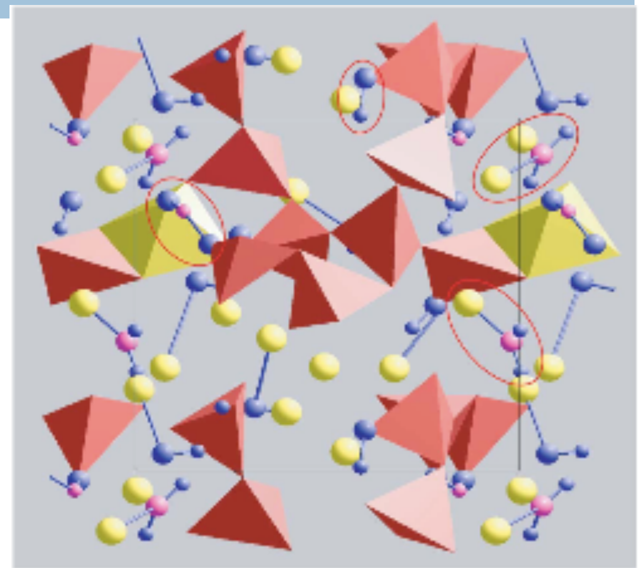


- Large at low pressure
- H_2O in melt is denser and less compressible than pure H_2O
- Volume of solution ≤0 at all pressures
- Solution behaves nearly ideally at high pressure

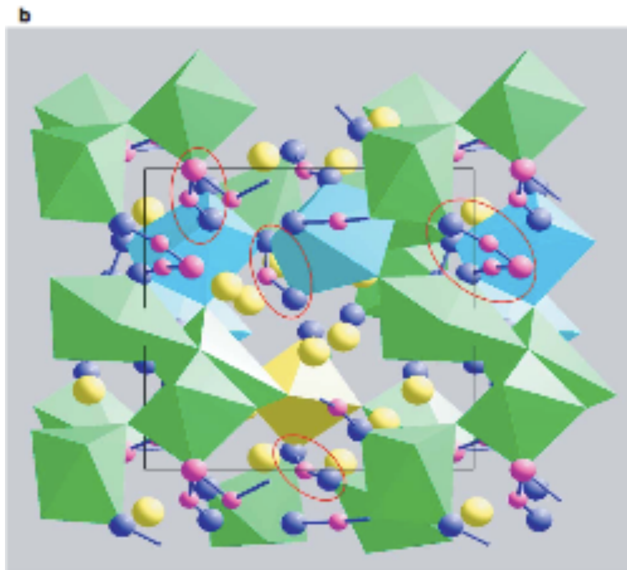
Mookherjee et al. (2008) Nature

$MgSiO_3$-H_2O (10 wt. %)

~0 GPa



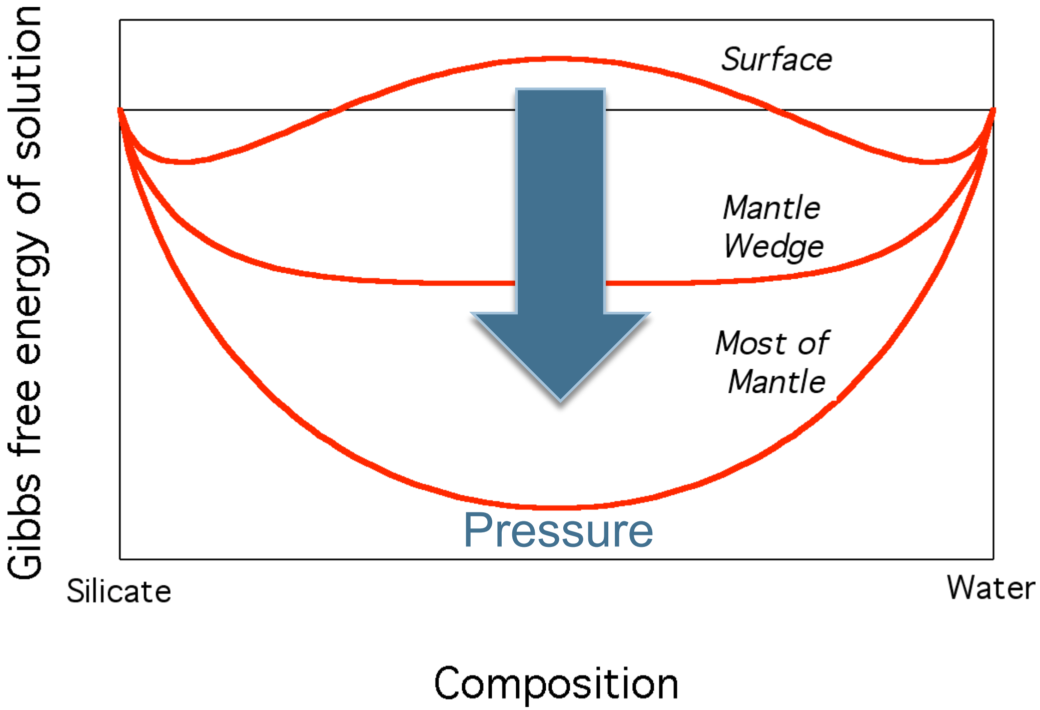
~100 GPa



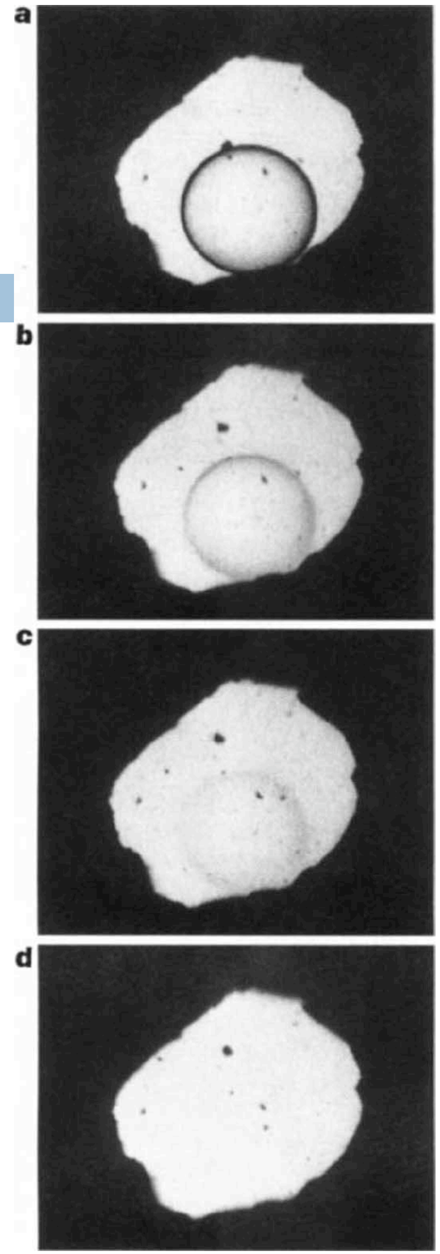
$MgSiO_3$-H_2O

- Complete miscibility of silicate liquids and water over nearly entire mantle

$$\left(\frac{\partial G_{sol}}{dP}\right)_T = V_{sol} \leq 0$$



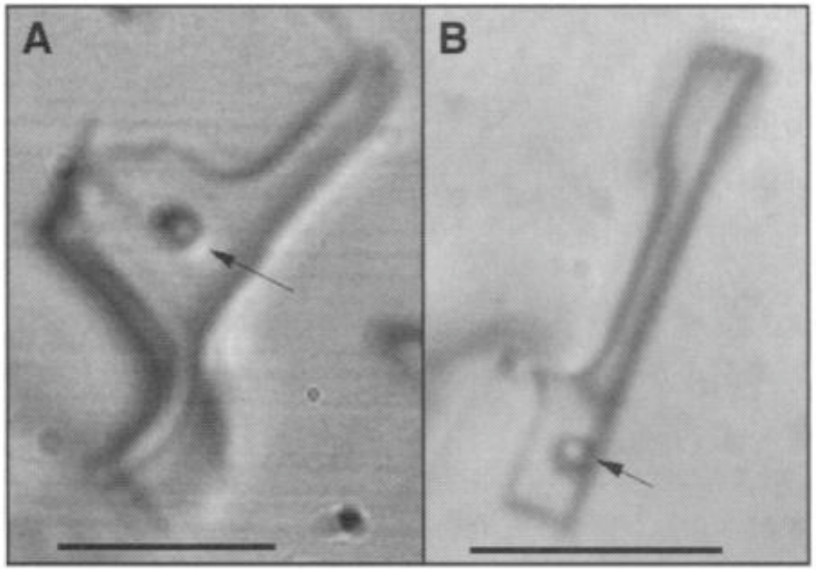
Mookherjee et al. (2008) Nature



Shen & Keppler (1997) Nature
P ~ 1.5 GPa

Initial Water Content of Earth

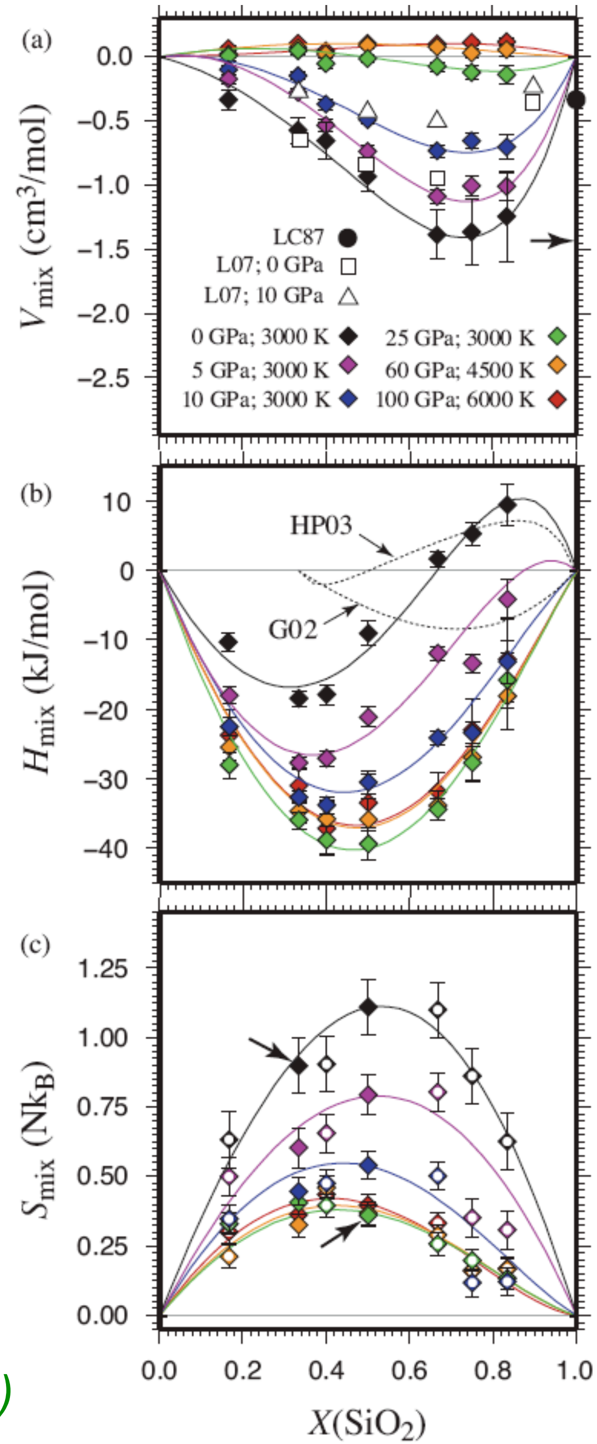
- Unlimited solubility of water in deep magma ocean has implications for
  - Deep mantle solidus
  - Origin of atmosphere
  - Present water content of interior
- Why is the magmatically probed mantle much drier than CI chondrites?
  - Most water never accreted
  - Accreted and then removed
  - Currently stored at depth?



Fluid inclusions in a chondritic meteorite
Zolensky et al. (1999) Science

First Principles Petrology of the Deep Earth

- Predict solution properties with first principles molecular dynamics
- MgO-SiO_2 join
- Large, negative volume of mixing approaches zero on compression
- Enthalpy of solution is large and positive at low pressure and silica-rich end
- Everywhere negative at high pressure
- No immiscibility at depth



MgO-SiO_2

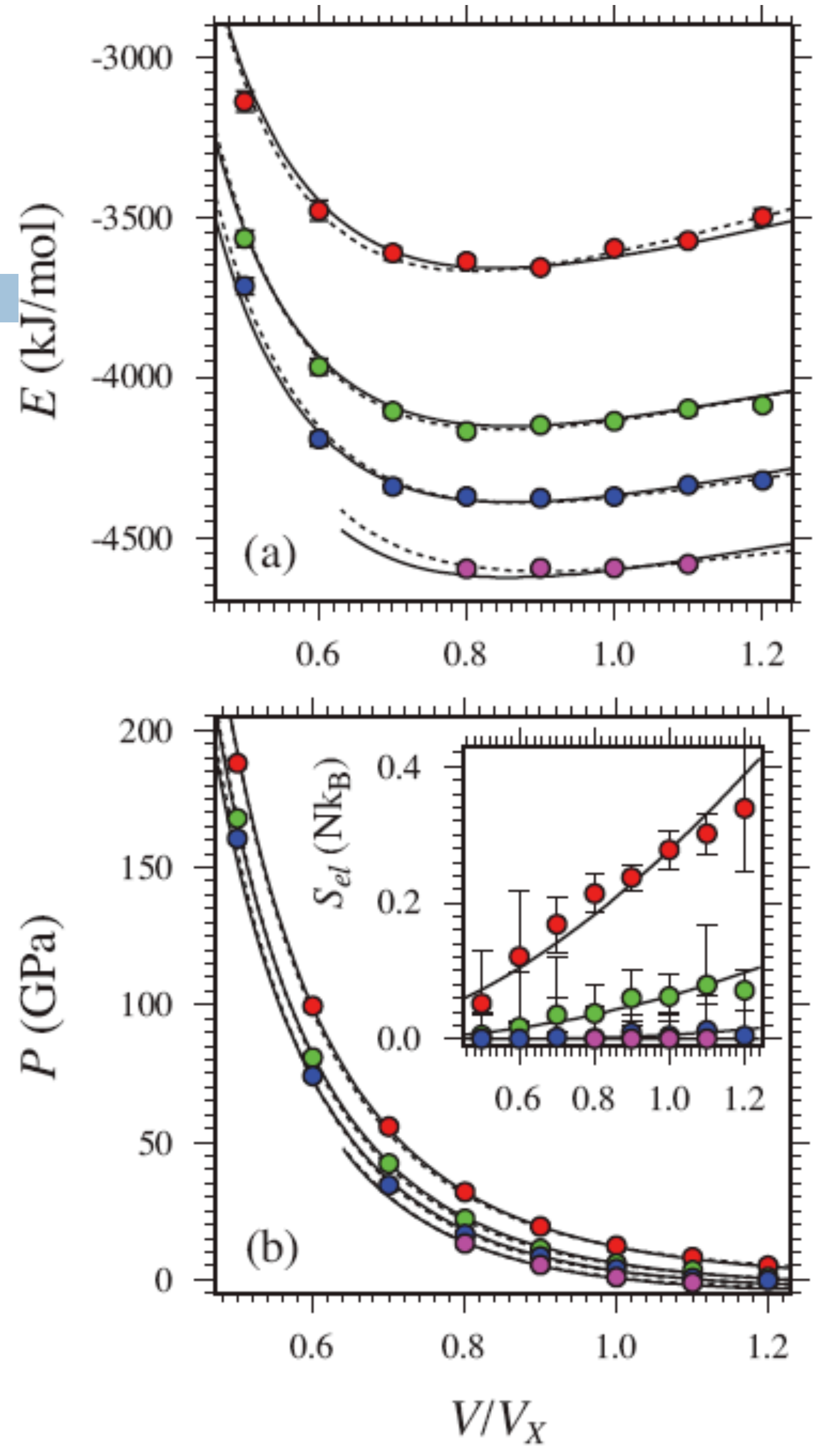
De Koker et al. (to be published)

Liquid Fundamental Thermodynamic Relation

- New analytical formulation *F*(*V*,*T*)
- Accounts self-consistently for all thermodynamic properties
- Based on our FPMD results
- Birch-Murnaghan finite strain theory
- Generalized Rosenfeld-Tarazona thermal contributions
- Electronic contributions are important

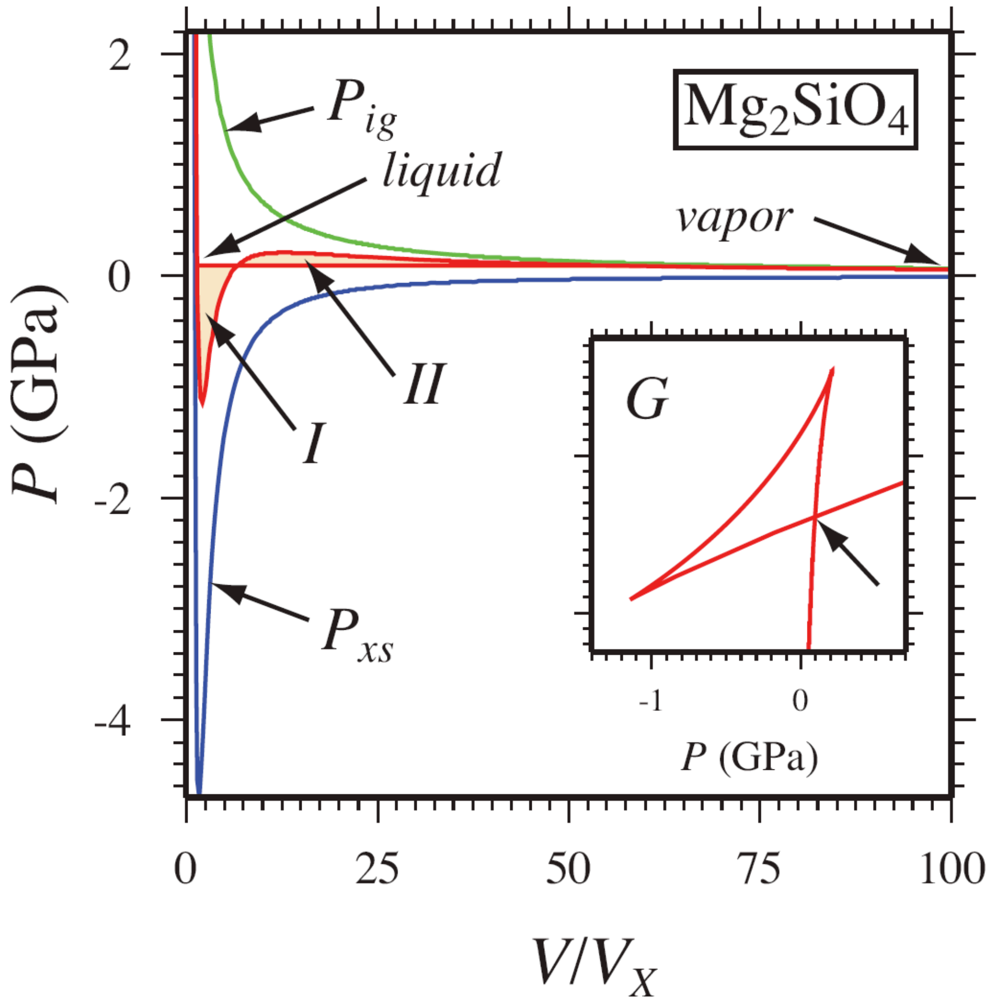
Mg_2SiO_4

de Koker & Stixrude (2009) GJI



Liquid Fundamental Thermodynamic Relation

- New formulation correctly captures liquid-gas transition
- Important for early Earth heat transfer
- Prediction for Mg_2SiO_4 at 6000 K
  - Vapor pressure = 0.09 GPa (900 bars)
  - Heat of vaporization = 1130 kJ/mol



de Koker & Stixrude (2009) GJI

Mg_2SiO_4

Conclusions

- First principles molecular dynamics simulations a powerful means of studying silicate liquids
- Predict gradual four-fold to six-fold Si-O coordination change over mantle pressure range
- Predict large Grüneisen parameter of silicate liquids
- ULVZ may be partially molten
- Early Earth may have been completely molten
- Began crystallizing from the mid-mantle
- Unlimited solubility of water in magma ocean
- Deep mantle may be a reservoir of primordial water