A04-1 Theory and Computation

Member

Ab initio

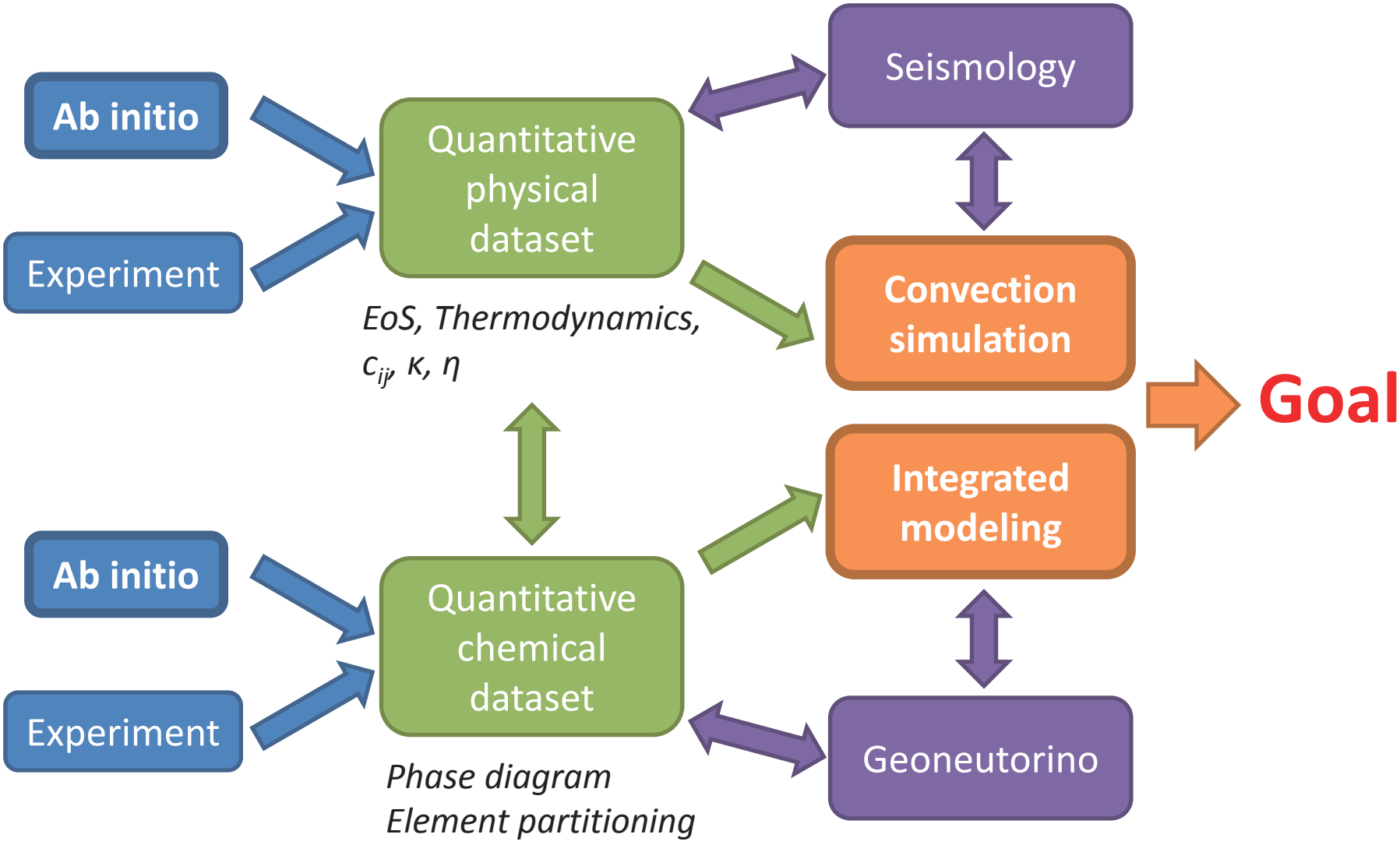
• **T. Tsuchiya (Ehime Univ, TiTech)**	Element partitioning & Diffusion
• **J. Tsuchiya (Ehime Univ, TiTech)**	Hydrous phase
• **H. Dekura (Ehime Univ)**	Thermal transport

Hydrodynamics and others

• **F. Takahashi (Kyushu Univ)**	Core dynamics
• **T. Miyagoshi (JAMSTEC)**	Mantle and Core dynamics
• **T. Nakagawa (JAMSTEC)**	Core-mantle coupling
• **J. Hernlund (TiTech)**	Integrated model

+ Kobo Researchers

Research structure



Key properties

Equilibrium

1. Structure search
2. Equation of state
3. Phase equilibrium
4. Thermodynamics
5. Elastic tensor
6. **Element partitioning**

Transport

1. **Thermal conduction**
2. **Electrical conduction**
3. **Atomic diffusion**

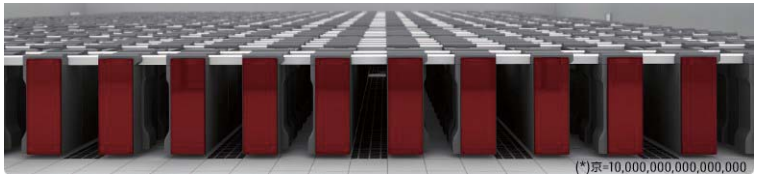
Ab initio mineral physics

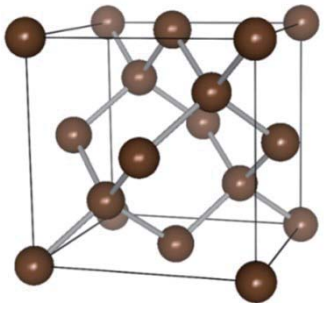
Density Functional Theory
(*Hohenberg & Kohn 64; Kohn & Sham 65*)

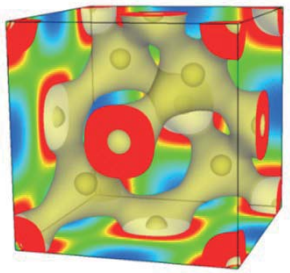
$$\left[-\frac{\hbar^2}{2m}\Delta - \sum_I \frac{Z_I}{|\mathbf{r}-\mathbf{R}_I|} + e^2\int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' + V_{XC}[n(\mathbf{r})]\right]\varphi_i(\mathbf{r}) = \epsilon_i\varphi_i(\mathbf{r})$$

$$n(\mathbf{r}) = \sum_i |\varphi_i(\mathbf{r})|^2$$

φ: 1e wavefunction
n: e density

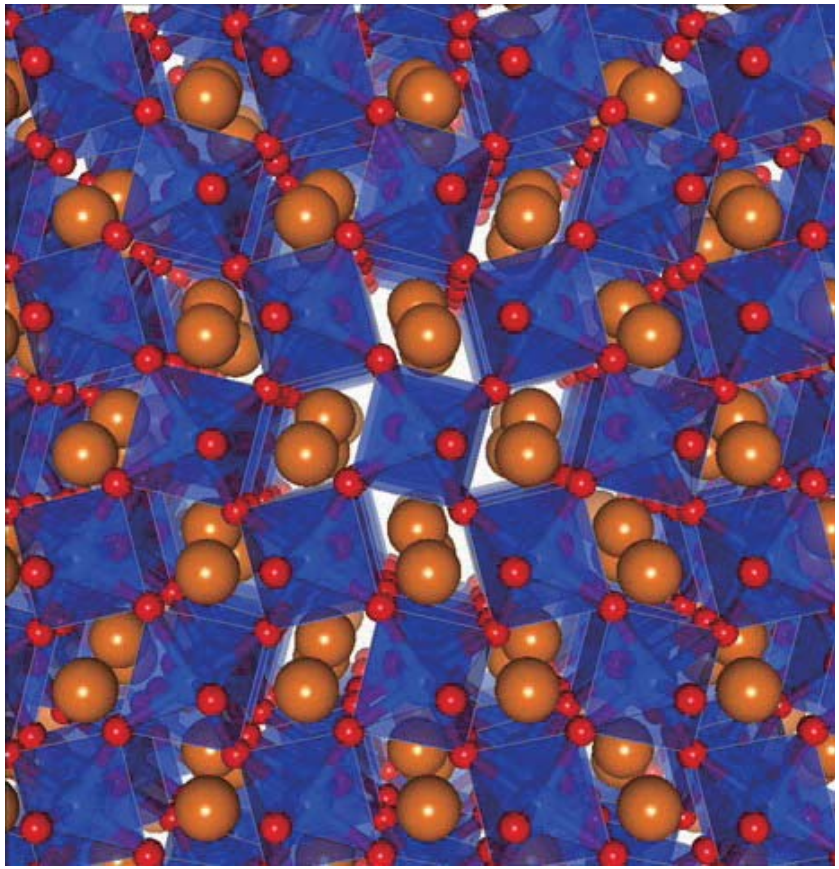




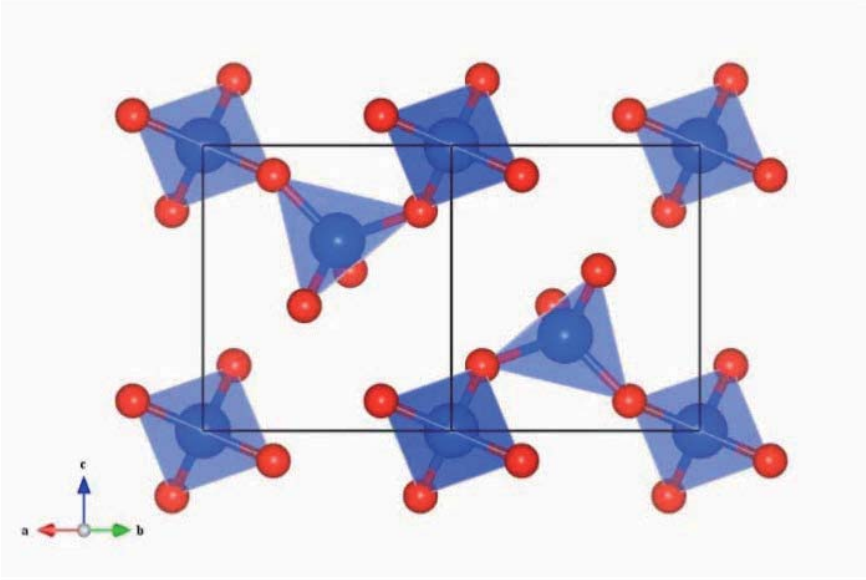


Structure search

$MgSiO_3$ Bridgmanite



SiO_2 α-Quartz



Mg

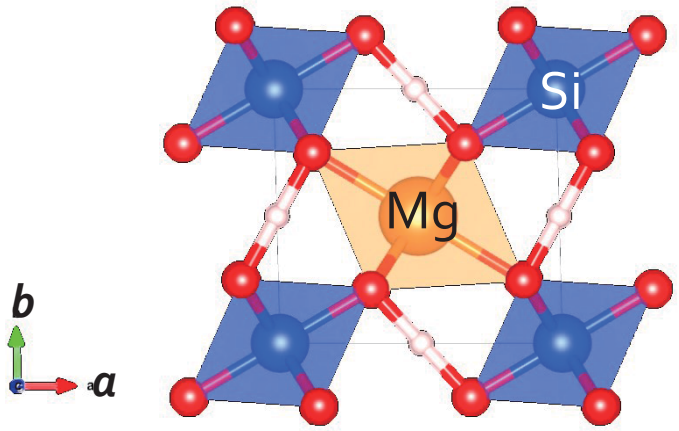
Si

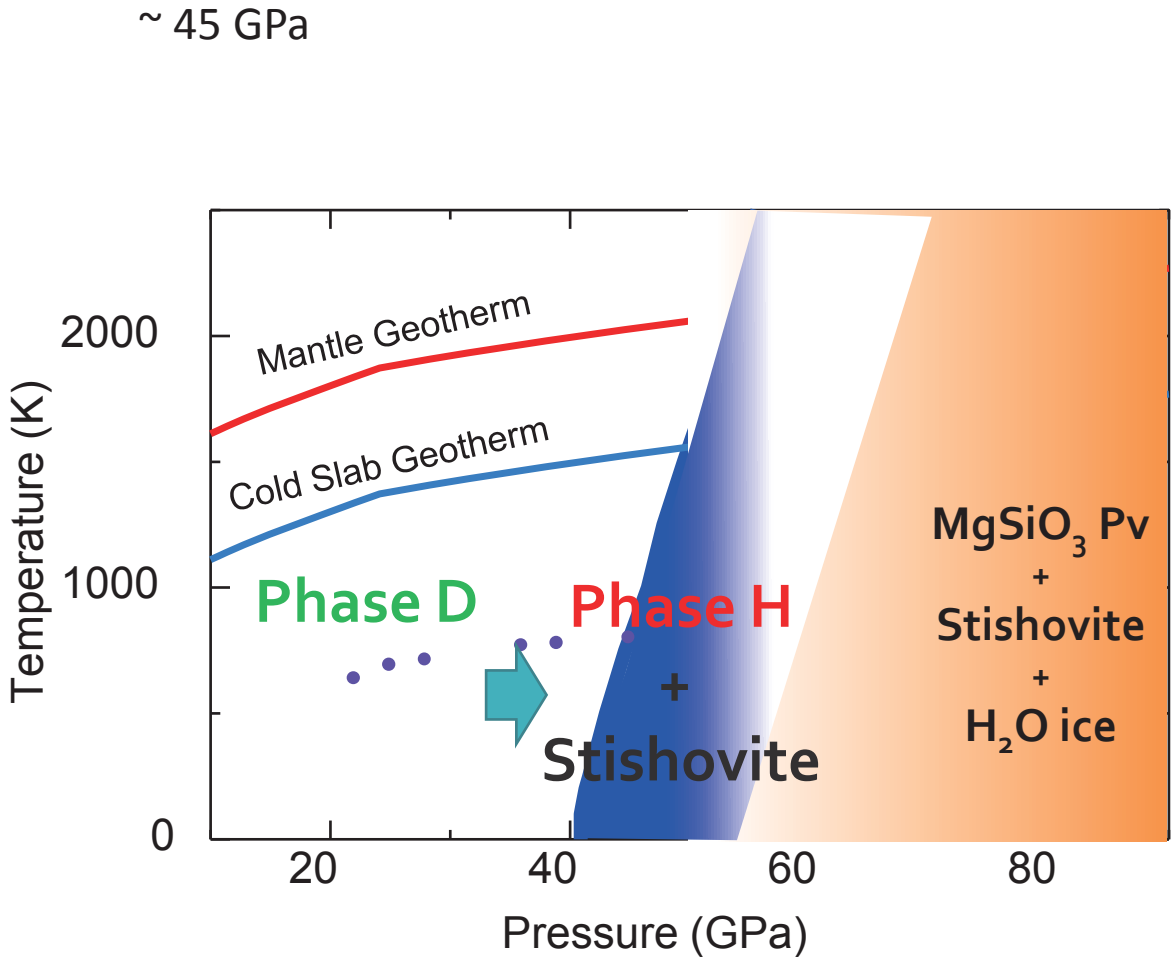
O

Tsuchiya+ (04) EPSL
Tsuchiya & Tsuchiya (11) PNAS

New high-pressure hydrous phase H

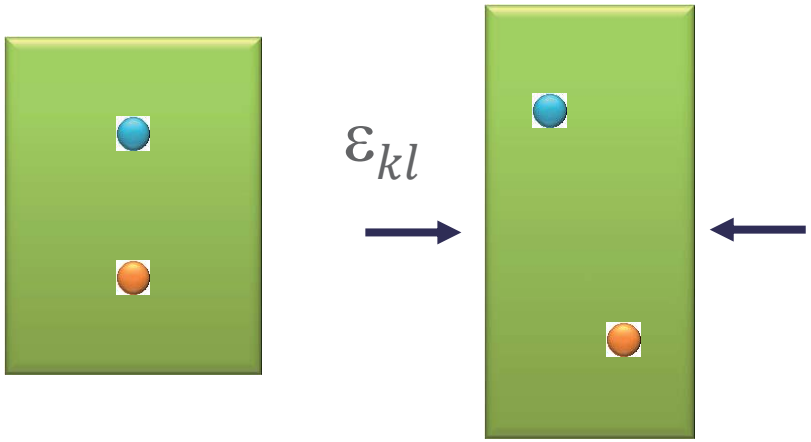
Phase D ($MgSi_2O_6H_2$) → phase H ($MgSiO_4H_2$)+SiO_2





J. Tsuchiya (13) GRL
Nishi+ (14) Nature Geosci.

High-*P,T* elasticity



Structure relaxation

Strained cell

Method-1: Stress-strain

Molecular Dynamics

$$\sigma_{ij}(P,T) = c_{ijkl}(P,T)\varepsilon_{kl}$$

Method-2: Energy-strain

Lattice dynamics + Quasiharmonic approx

$$c_{ij}^{T}(P,T) = \frac{1}{V}\left(\frac{\partial^2 G(P,T)}{\partial\varepsilon_i \partial\varepsilon_j}\right)_T$$

$c_{ij}^{S}(P,T) \rightarrow K_S$ & μ (Hill average)

$$V_P = \sqrt{\frac{K_S + 4/3\,\mu}{\rho}}, V_S = \sqrt{\frac{\mu}{\rho}}, V_\Phi = \sqrt{\frac{K_S}{\rho}}$$

Isothermal – adiabatic conversion

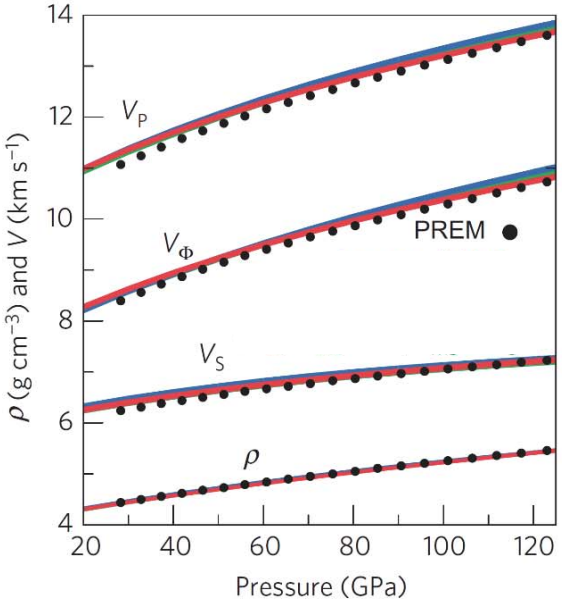
$$c_{ij}^{S}(P,T) = c_{ij}^{T}(P,T) + \frac{VT\lambda_i\lambda_j}{C_V}$$

$$\lambda_i(P,T) = \left(\frac{\partial S(P,T)}{\partial\varepsilon_i}\right)_T$$

Elastic wave velocity of aggregates

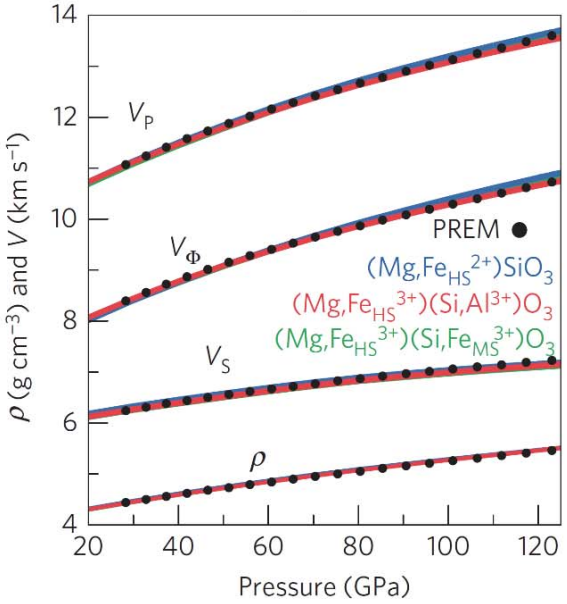
Br:Fp = 9:1

Chondrite



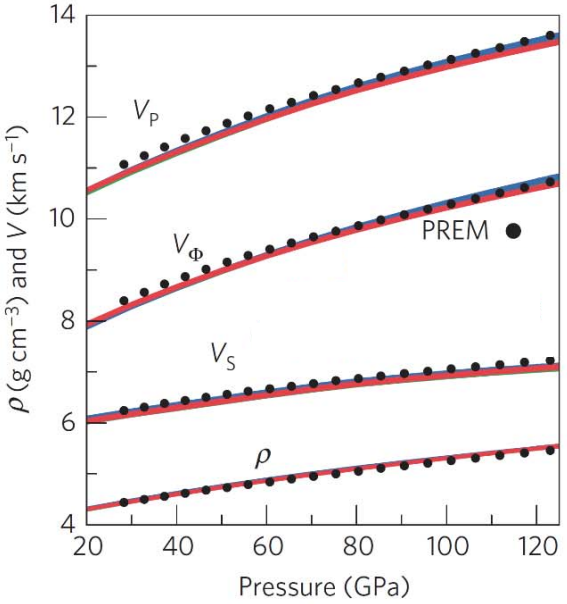
8:2

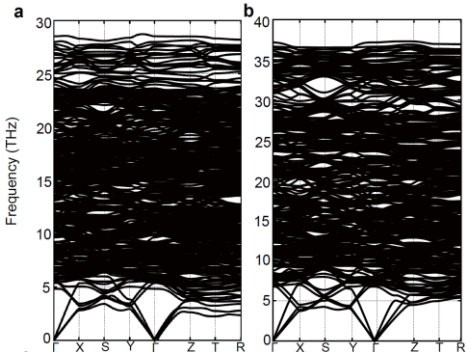
Pyrolite



7:3 in vol

Olivine





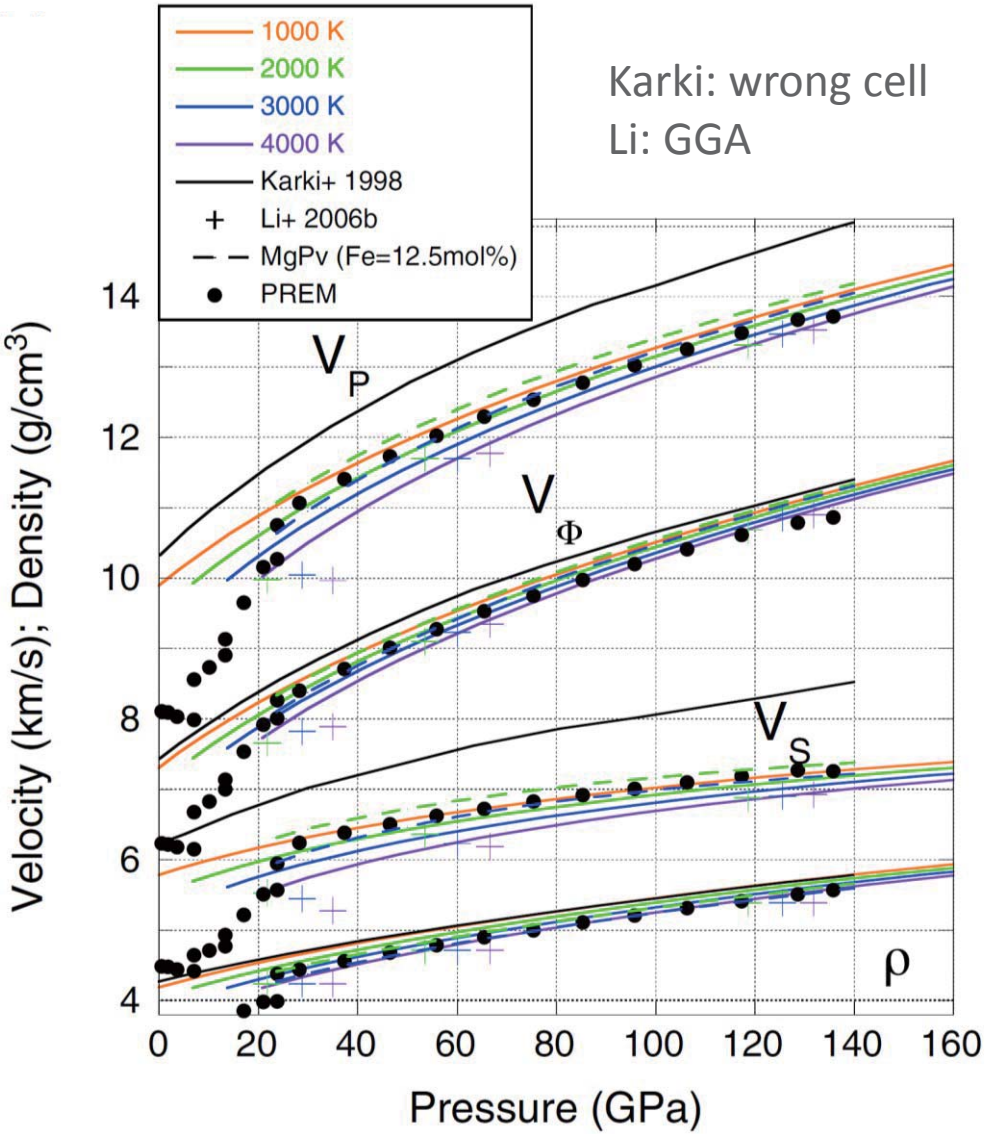
Internally consistent LSDA+U

+

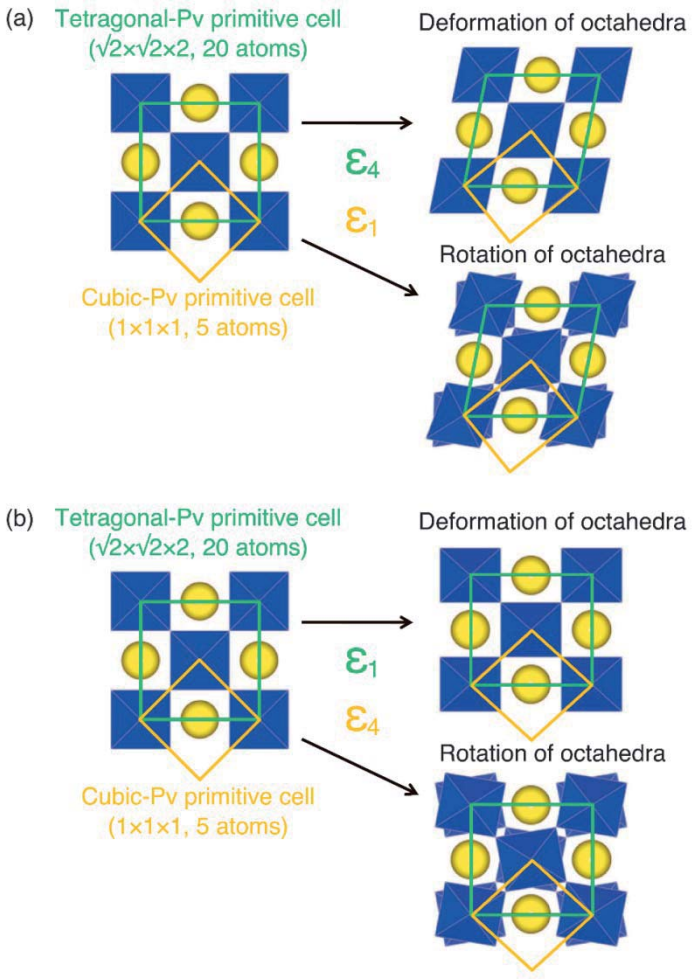
Direct LD

Wang, Tsuchiya & Hase (15) Nature Geosci.

$CaSiO_3$ Pv

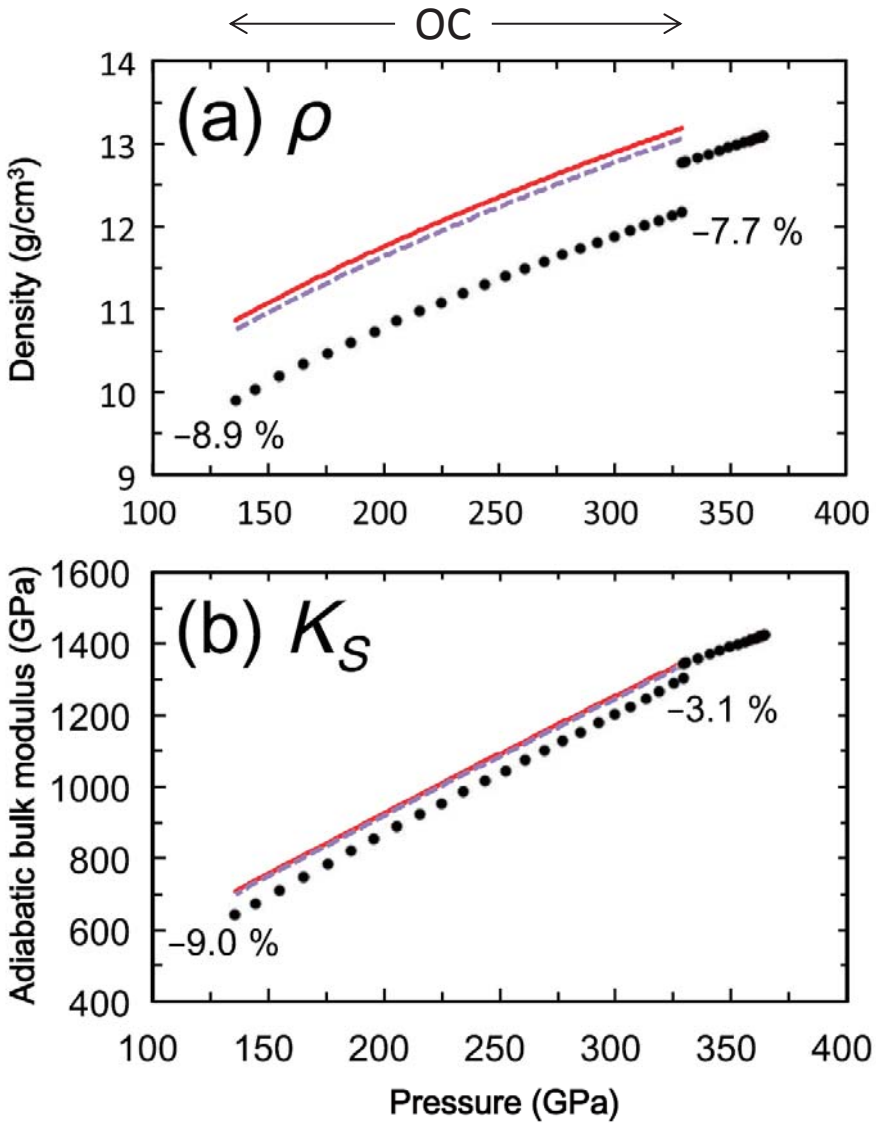


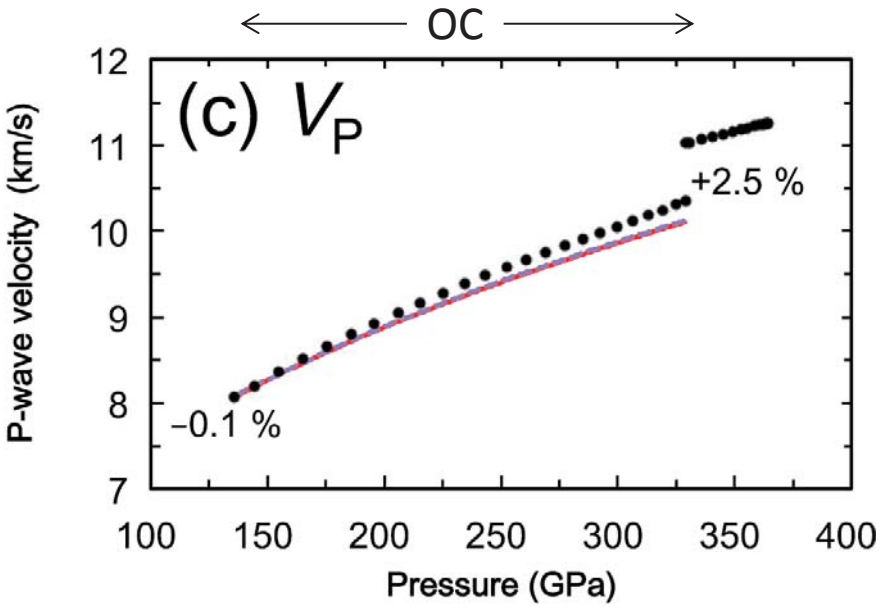
Karki: wrong cell
Li: GGA



Kawai & Tsuchiya (2014) JGR
Kawai & Tsuchiya (2015) GRL

Liquid Fe





Ichikawa, Tsuchiya, Tange (14) JGR

Liquid Fe alloy

Model:

Fe + O, S, Si, C, H, Ni

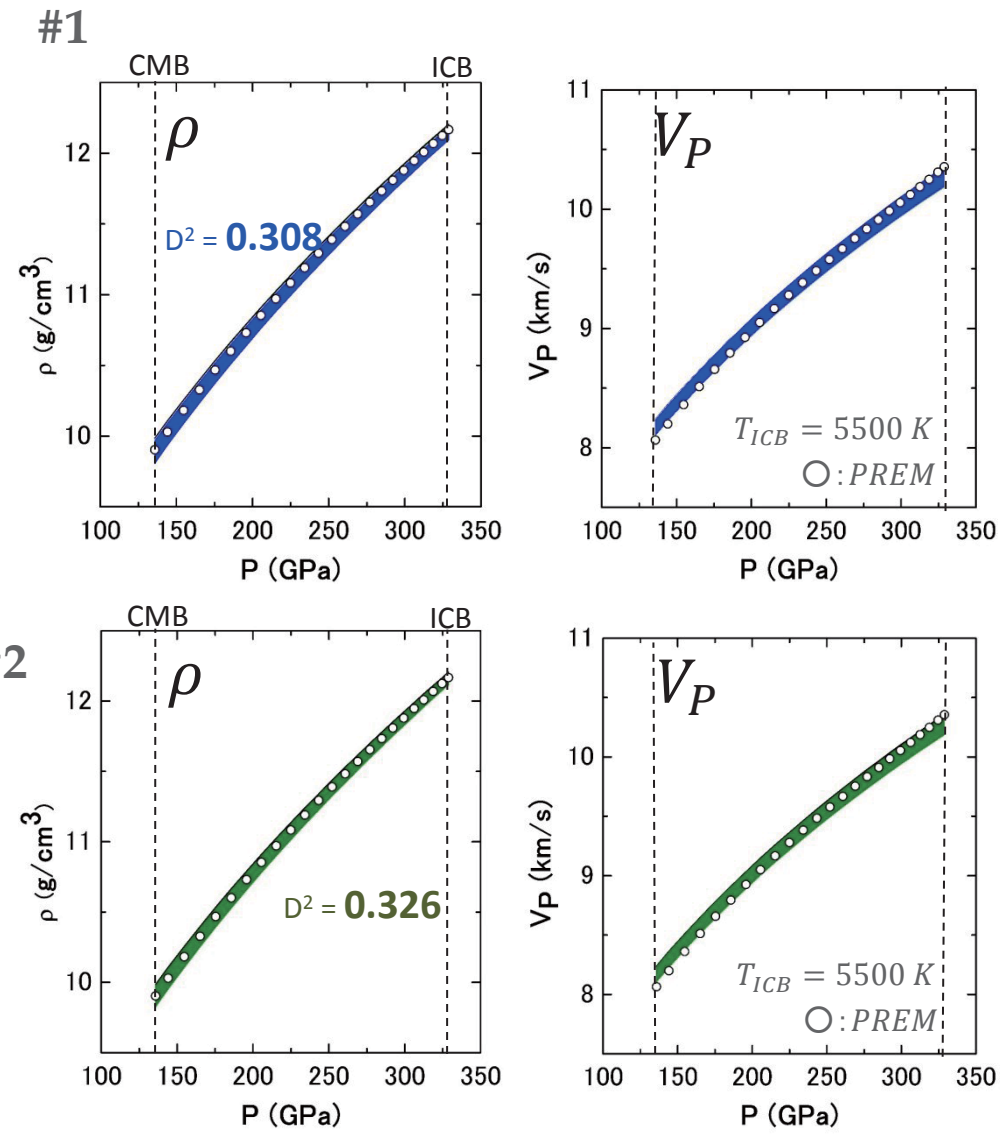
T_{ICB} = 5000, 5500, 6000

Best compositions

#1: $Fe_{0.71}Ni_{0.05}Si_{0.03}O_{0.21}$

#2: $Fe_{0.71}Ni_{0.05}S_{0.04}O_{0.20}$

Ohsumi+, in prep.



Lattice thermal conductivity

$$\kappa_{\mathrm{lat}} = \frac{1}{3}\sum_{s}^{3n}\int \mathbf{v}_{\mathbf{q},s}^{2} c_{\mathbf{q},s}\tau_{\mathbf{q},s} d\mathbf{q}$$

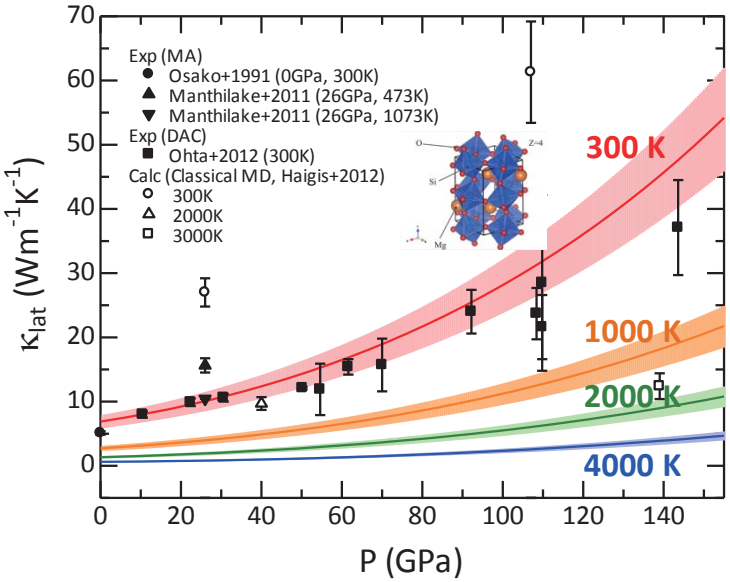
$$\tau_{\mathbf{q},s} = \frac{1}{2\Gamma(\omega_{\mathbf{q},s})}$$

Third-order dynamical tensor

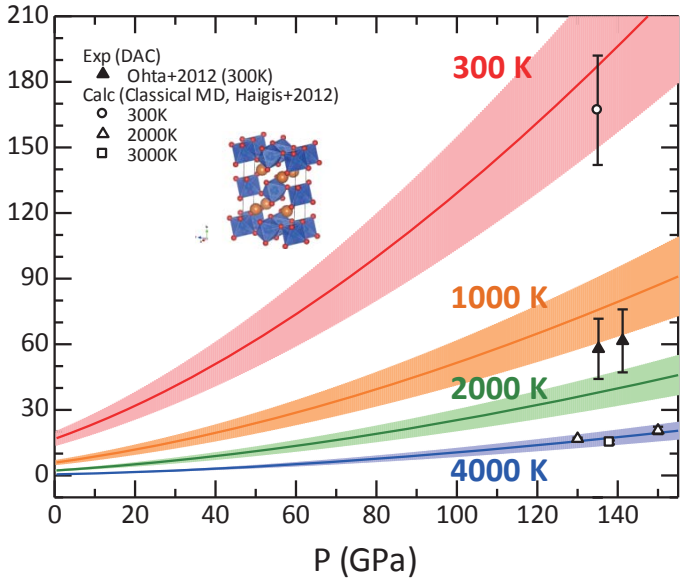
$$\Gamma_{\mathbf{q},s}(\omega) = \frac{\pi}{2N_{\mathbf{q}'}}\sum_{\mathbf{q}',s',s''} |V_3(\mathbf{q}s, \mathbf{q}'s', \mathbf{q}''s'')|^2 \times [\{1 + n_{\mathbf{q}',s'} + n_{\mathbf{q}'',s''}\}\delta(\omega_{\mathbf{q}',s'} + \omega_{\mathbf{q}'',s''} - \omega) + 2\{n_{\mathbf{q}'',s''} - n_{\mathbf{q}',s'}\}\delta(\omega_{\mathbf{q}',s'} - \omega_{\mathbf{q}'',s''} - \omega)]$$

$$\mathbf{q}'' = -\mathbf{q} - \mathbf{q}' + \mathbf{G}$$

MgPv



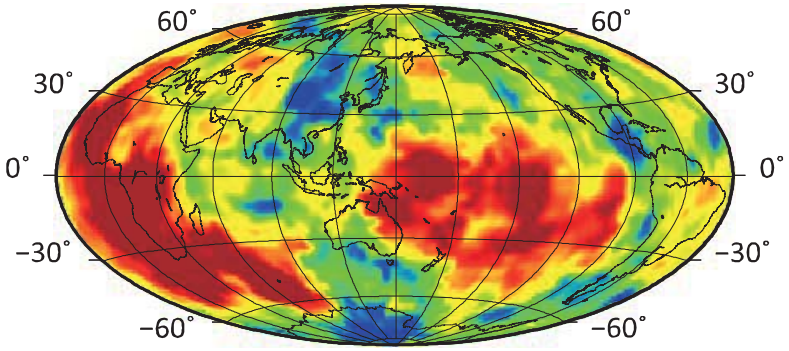
MgPPv

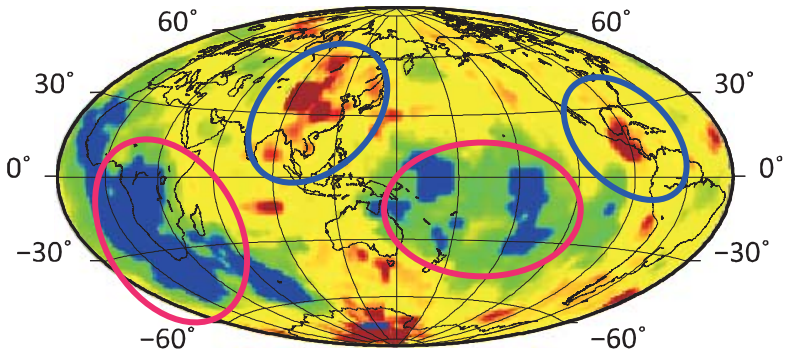


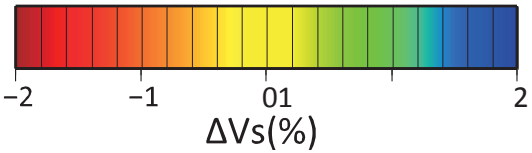
Dekura, Tsuchiya, Tsuchiya (13) PRL

Local CMB heat flux interpreted from V_S tomography

$d\ln V_S$ → $d\ln T$ → $d\ln q_{CMB}$

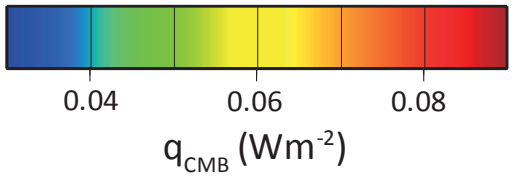






Grand (2000) z=2770km

$$q_{\mathrm{CMB}} = \frac{\Delta T_{\mathrm{TBL}}}{\int_0^{\delta_{\mathrm{TBL}}} \frac{dz}{\kappa_{\mathrm{LM}}}}$$



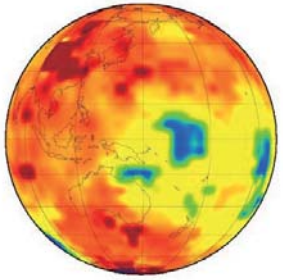
Hot regions = Low heat flux (~0.03 W/m²)

Cold regions = High heat flux (~0.09 W/m²)

Total CMB heat flow estimated using *κ* of pure phases

$$J_{\mathrm{CMB}} = \int dS\, q_{\mathrm{CMB}}$$

$$\sim 9 \text{ TW}$$



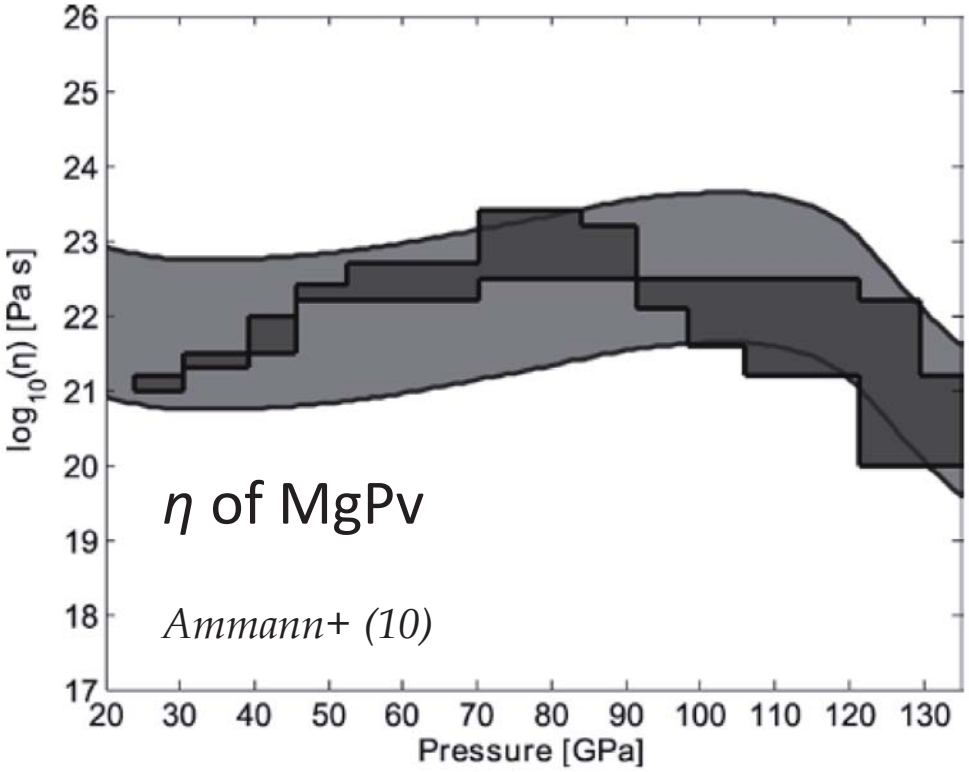
Viscosity (diffusion creep)

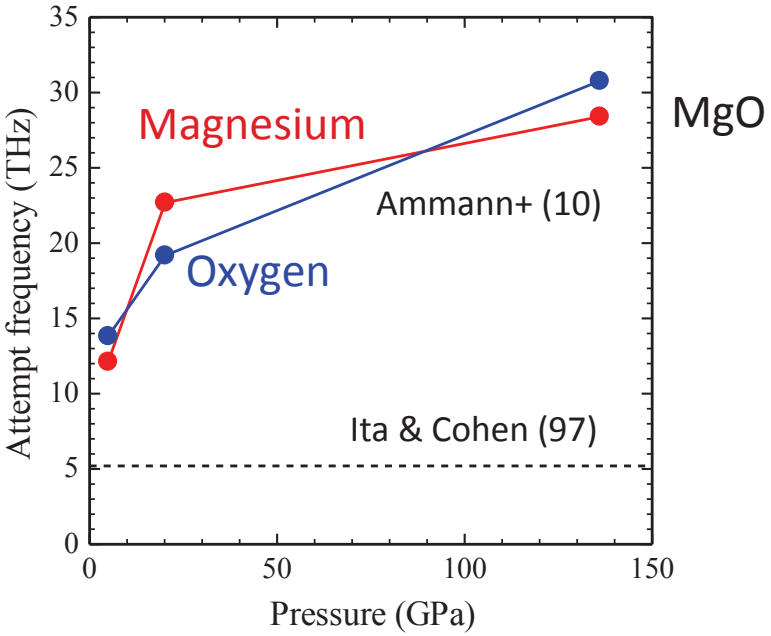
Nabarro-Herring viscosity

$$\eta \propto \frac{d^2 k_B T}{D_{eff}\Omega}$$

$$D = N_V \frac{Z_m}{6} l^2 \nu \exp\left(-\frac{\Delta H_m}{k_B T}\right)$$

Trial frequency





Application to element partitioning

Partitioning condition

$$\mu^{\text{phase } A}_{\text{component } i} - \mu^{\text{phase } A}_{\text{component } j} = \mu^{\text{phase } B}_{\text{component } i} - \mu^{\text{phase } B}_{\text{component } j}$$

Chemical potential

$$\mu_i = \left(\frac{\partial G}{\partial n_i}\right)_{P,T,N}$$

Free energy

$$G(P,V,\{n_i\}) = H(P,V,\{n_i\}) - TS(P,V,\{n_i\})$$

Entropy:
Hard to estimate

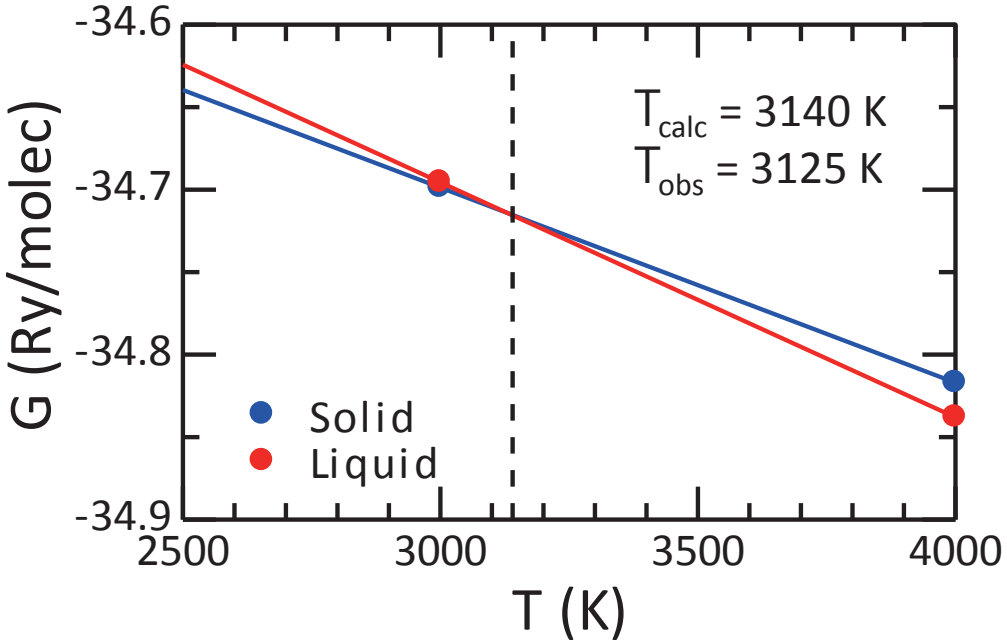
Thermodynamic integration

$$F_1 = F_2 + \int_0^1 \left\langle \frac{\partial U}{\partial \lambda} \right\rangle d\lambda$$

Potential energy of a combined system $U(\lambda) = \lambda U_1 + (1 - \lambda) U_2$

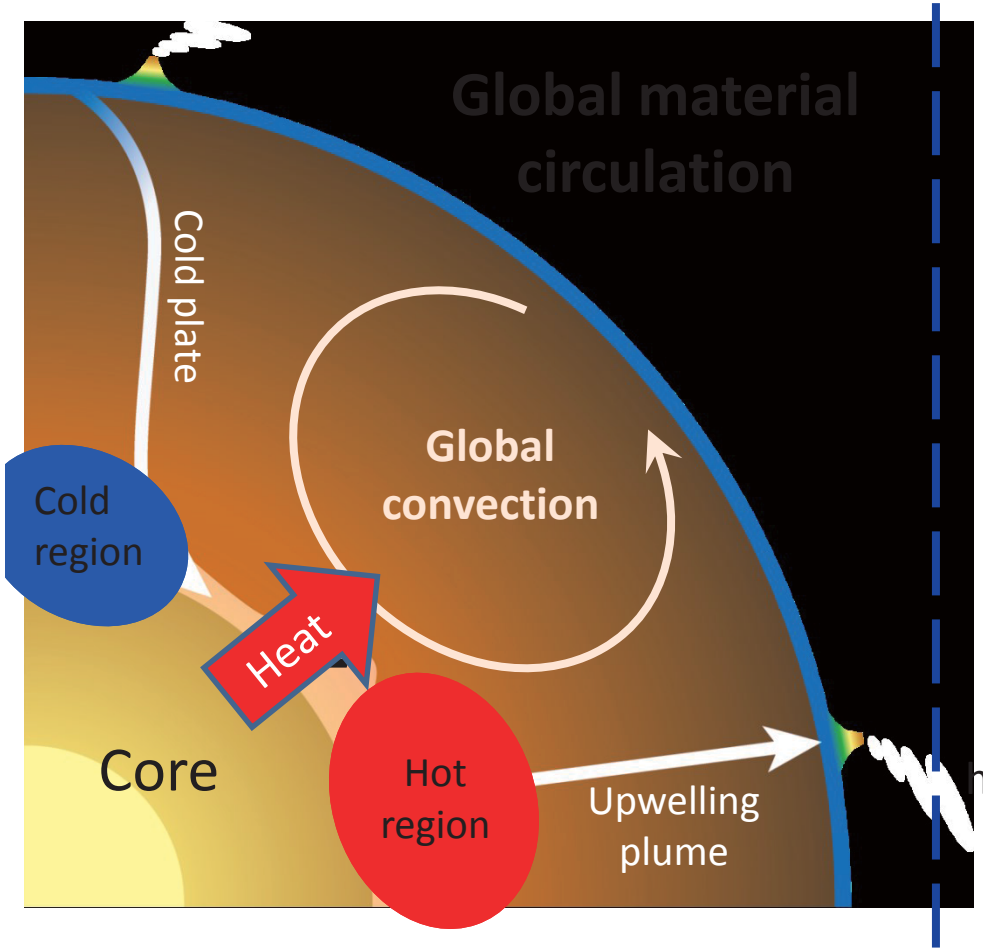
We have developed one-step (ideal → ab initio) TI-MD code (Taniuchi in prep).

Melting point of MgO at 0 GPa

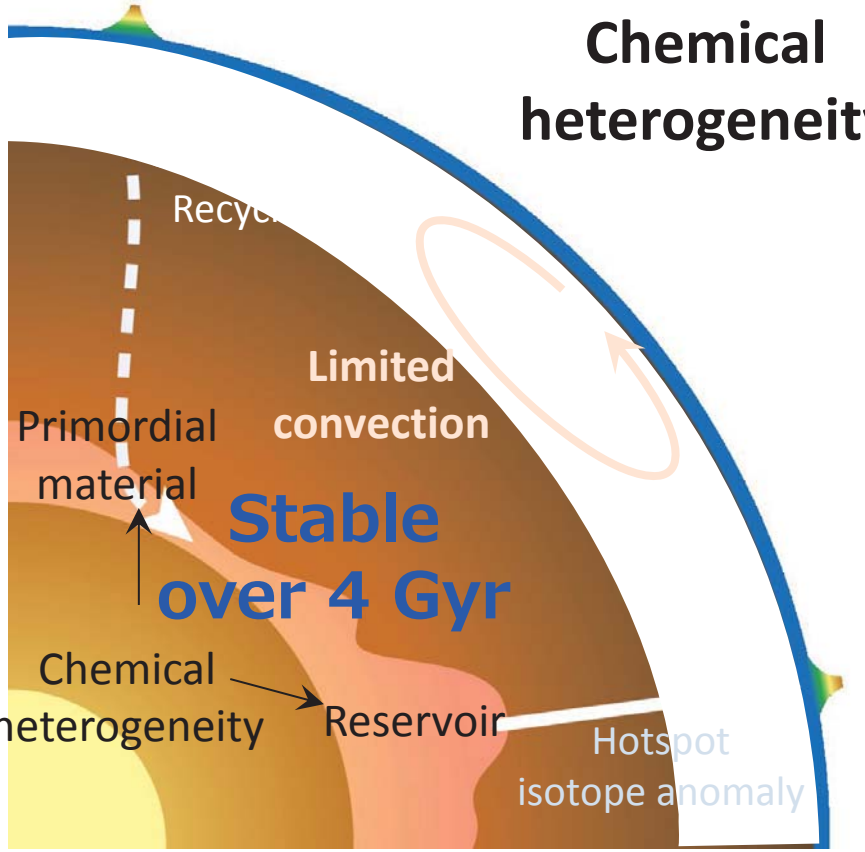


Chemical heterogeneity/Heat source distribution

Geophysical picture

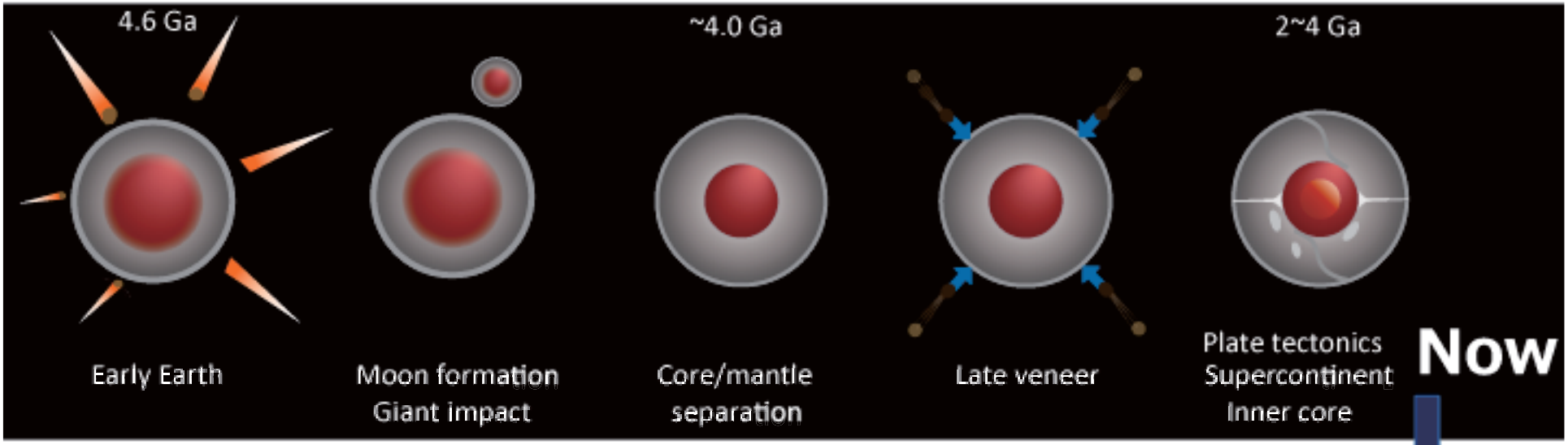


Geochemical picture



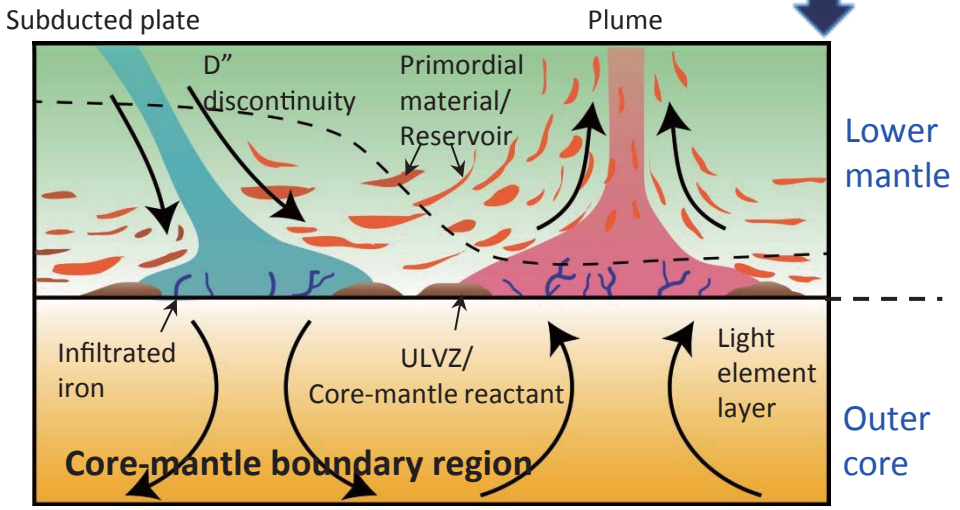
Details/ Origin/ Evolution

Formation processes of chemical heterogeneity



Time & Scale?

Quantitative data of high-*P,T* element partitioning and thermal property



Many factors of chemical heterogeneity