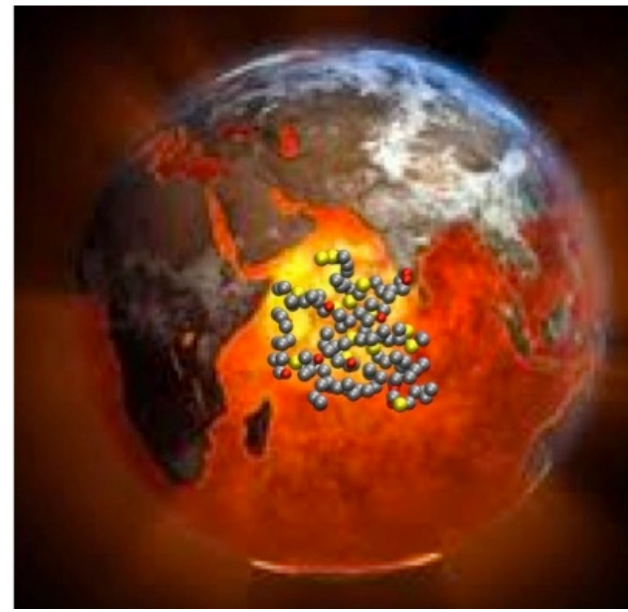
Transport properties of iron mixtures at planetary conditions



Dario ALFÈ[1]
Monica Pozzo[1], Chris Davies[2], David Gubbins[2]

[1]*Department of Earth Sciences & Department of Physics and Astronomy,*
Thomas Young Centre@UCL & London Centre for Nanotechnology
University College London
[2]*University of Leeds and University of California San Diego*

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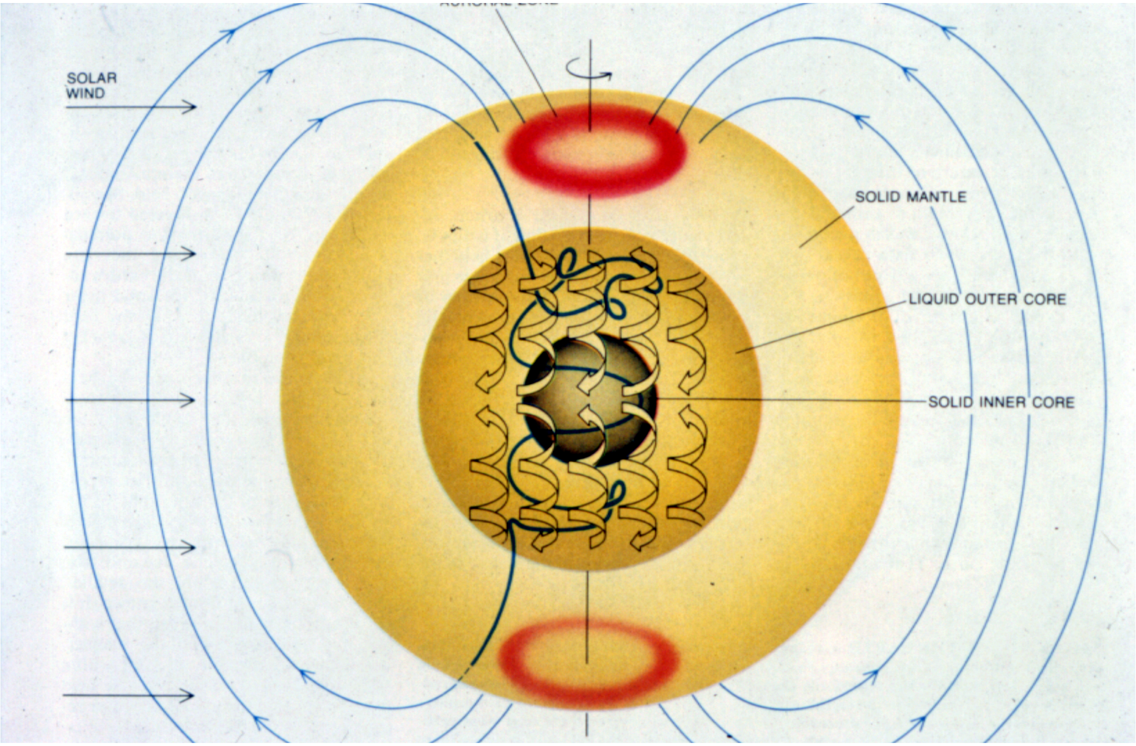
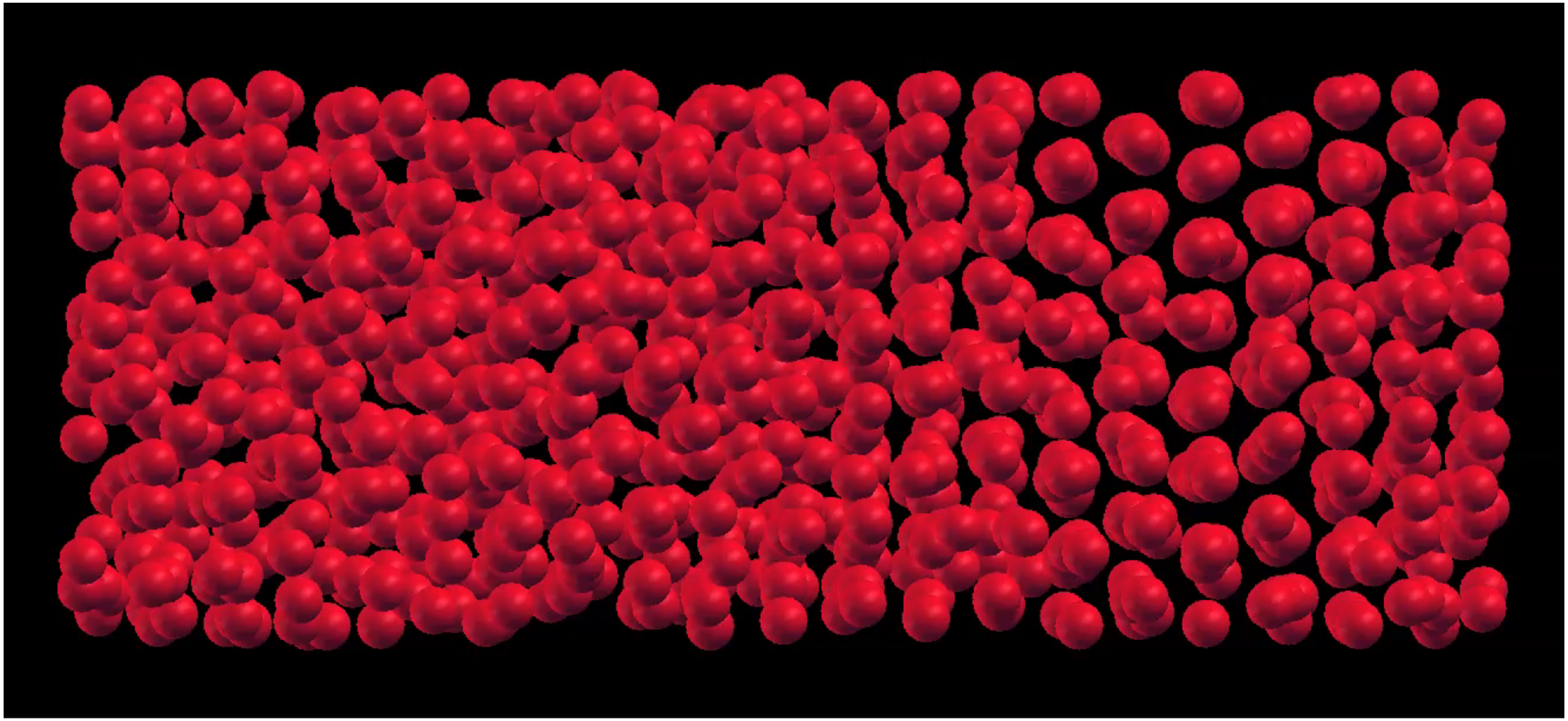
Transport in the Earth's core



- Thermal conductivity (heath transport)
- Electrical conductivity (Ohmic dissipation)

Computer modelling



How do the atoms interact with each other ?

Density Functional theory

Hohenberg & Kohn 1964
Kohn & Sham 1965

$$H\psi = E\psi$$

$$\psi(r_1,\ldots r_N)$$

$$\Downarrow$$

$$n(r)$$

$$H_{KS}\psi_i = E_i\psi_i \quad i = 1, N$$

$$H_{KS} = T + V + V_H + V_{XC}$$

Electrical conductivity

- Density functional theory
- Kubo-Greenwood:

$$\sigma_{\mathbf{k}}(\omega, R_I) = \frac{2\pi e^2 \hbar^2}{3m^2 V_{\text{cell}}} \frac{1}{\omega} \sum_{\alpha=1}^{3} \sum_{i,j=1}^{N} \left(f_{i,\mathbf{k}} - f_{j,\mathbf{k}} \right) \left| \left\langle \psi_{i,\mathbf{k}} \middle| \nabla_\alpha \middle| \psi_{j,\mathbf{k}} \right\rangle \right|^2 \delta\left(\varepsilon_{i,\mathbf{k}} - \varepsilon_{j,\mathbf{k}} - \hbar\omega \right)$$

$$\sigma(\omega) = \left\langle \sigma(\omega, R_I) \right\rangle$$

$$\sigma = \lim_{\omega \to 0} \sigma(\omega)$$

Implementation in VASP: **Desjarlais 2002**

Thermal conductivity

- Electronic component:

$$k = \lim_{\omega \to 0} \left\langle k(\omega, R_I) \right\rangle = \lim_{\omega \to 0} \left\langle \frac{1}{e^2 T} \left(L_{22}(\omega, R_I) - \frac{L_{12}^2(\omega, R_I)}{\sigma(\omega, R_I)} \right) \right\rangle$$

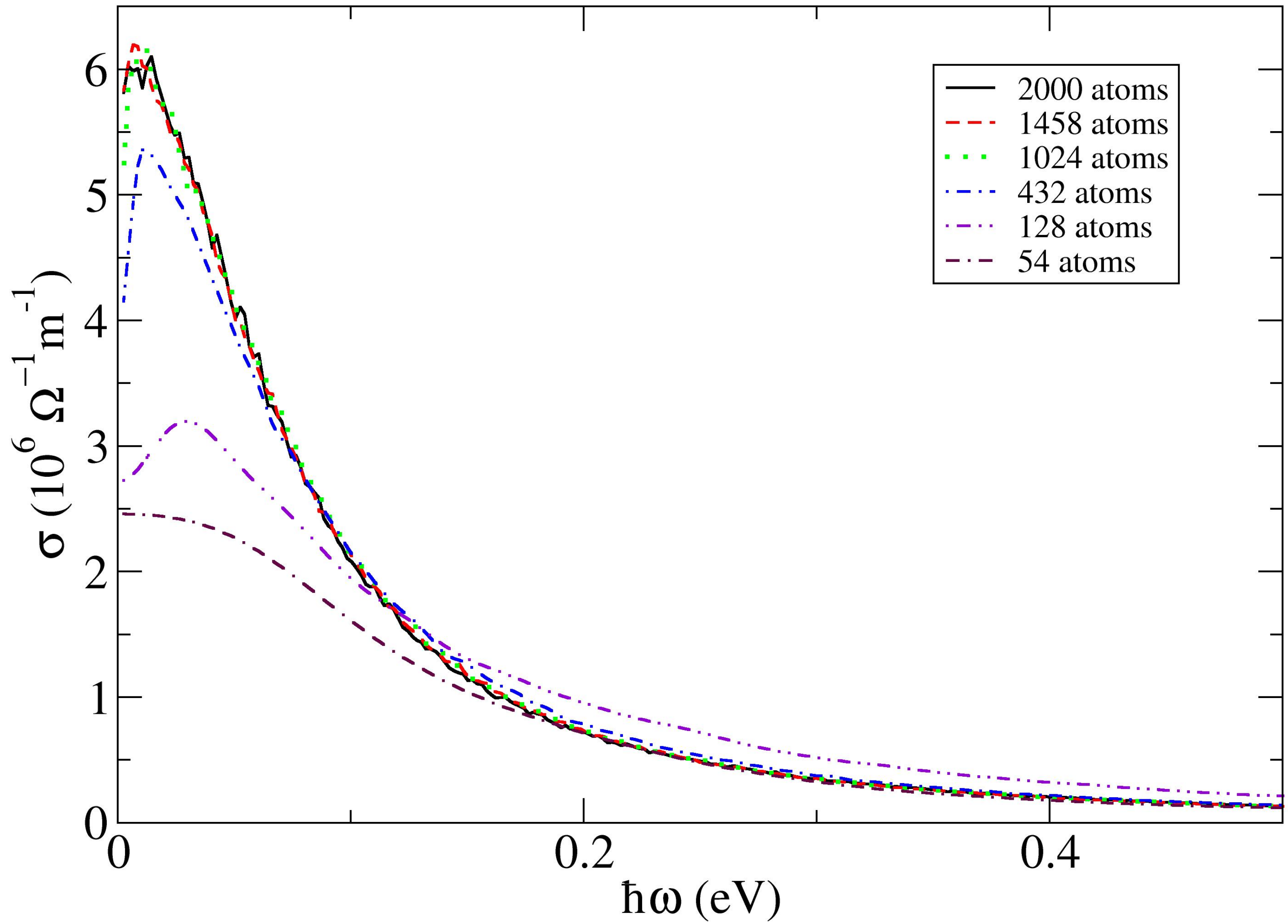
$$L_{l,m}(\omega, R_I) = (-1)^{l+m} \frac{2\pi e^2 \hbar^2}{3m^2 V_{\mathrm{cell}}} \frac{1}{\omega} \sum_{\alpha=1}^{3} \sum_{i,j=1}^{N} \left(f_{i,\mathbf{k}} - f_{j,\mathbf{k}} \right) \left| \left\langle \psi_{i,\mathbf{k}} \middle| \nabla_\alpha \middle| \psi_{j,\mathbf{k}} \right\rangle \right|^2 \delta\left(\varepsilon_{i,\mathbf{k}} - \varepsilon_{j,\mathbf{k}} - \hbar\omega \right) \left(\varepsilon_{i,\mathbf{k}} - \mu \right)^{l-1} \left(\varepsilon_{j,\mathbf{k}} - \mu \right)^{m-1}$$

- Ionic component (Green-Kubo):

$$\kappa = \frac{1}{3V_{cell} k_B T^2} \int_0^\infty \left\langle \mathbf{j}(0)\mathbf{j}(t) \right\rangle dt$$

Implementation in VASP: **Desjarlais 2002**

Example: liquid Na at p=0 and T=400 K



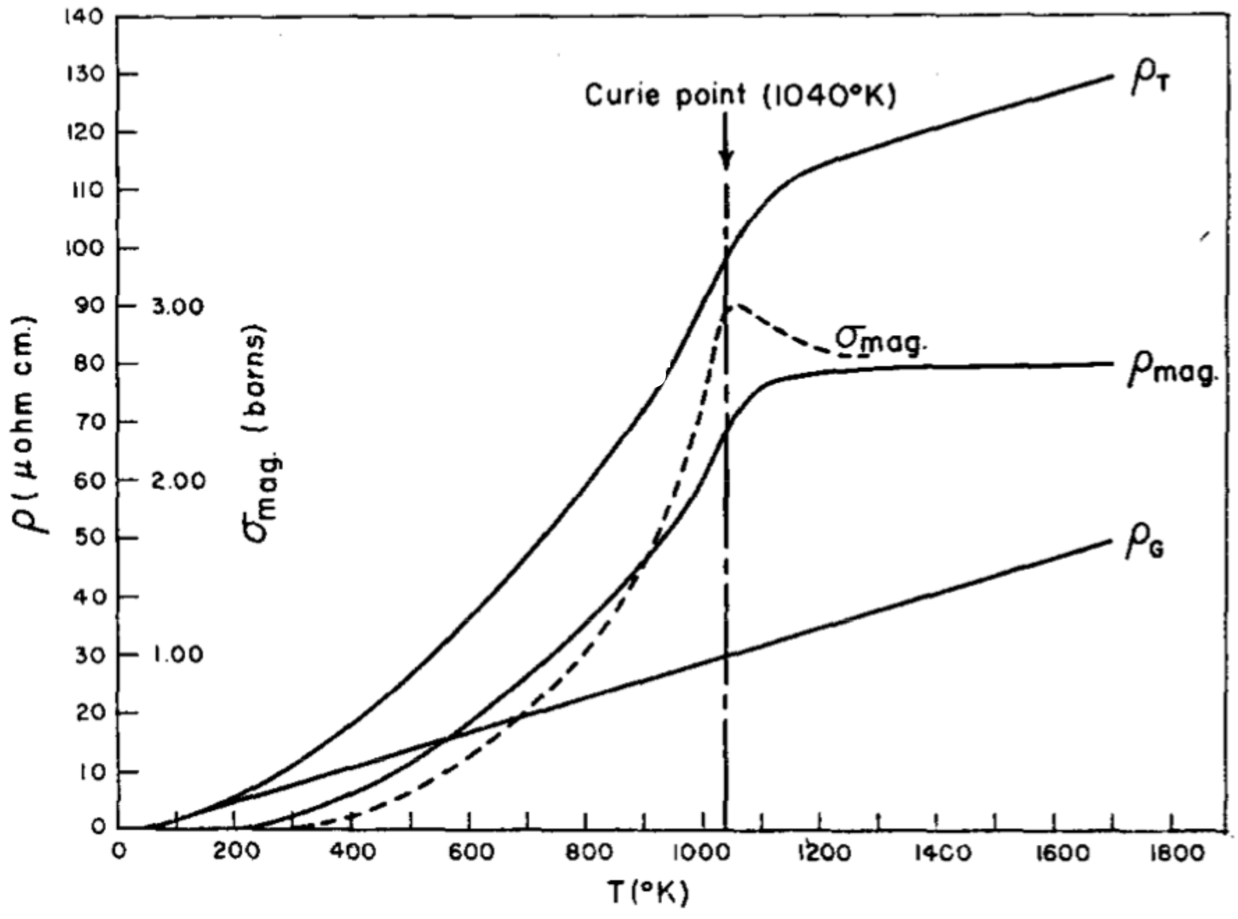
Conductivities of liquid Na at p=0 and T=400K

	σ_0 ($10^6\Omega^{-1}m^{-1}$)	κ_0 (W m^{-1} K^{-1})	L ($10^{-8}\Omega$ W K^{-2})
PBE	10.3	93	2.26
EXP	9.7	86	2.22

Lorenz number $L = k_0/\sigma_0 T$

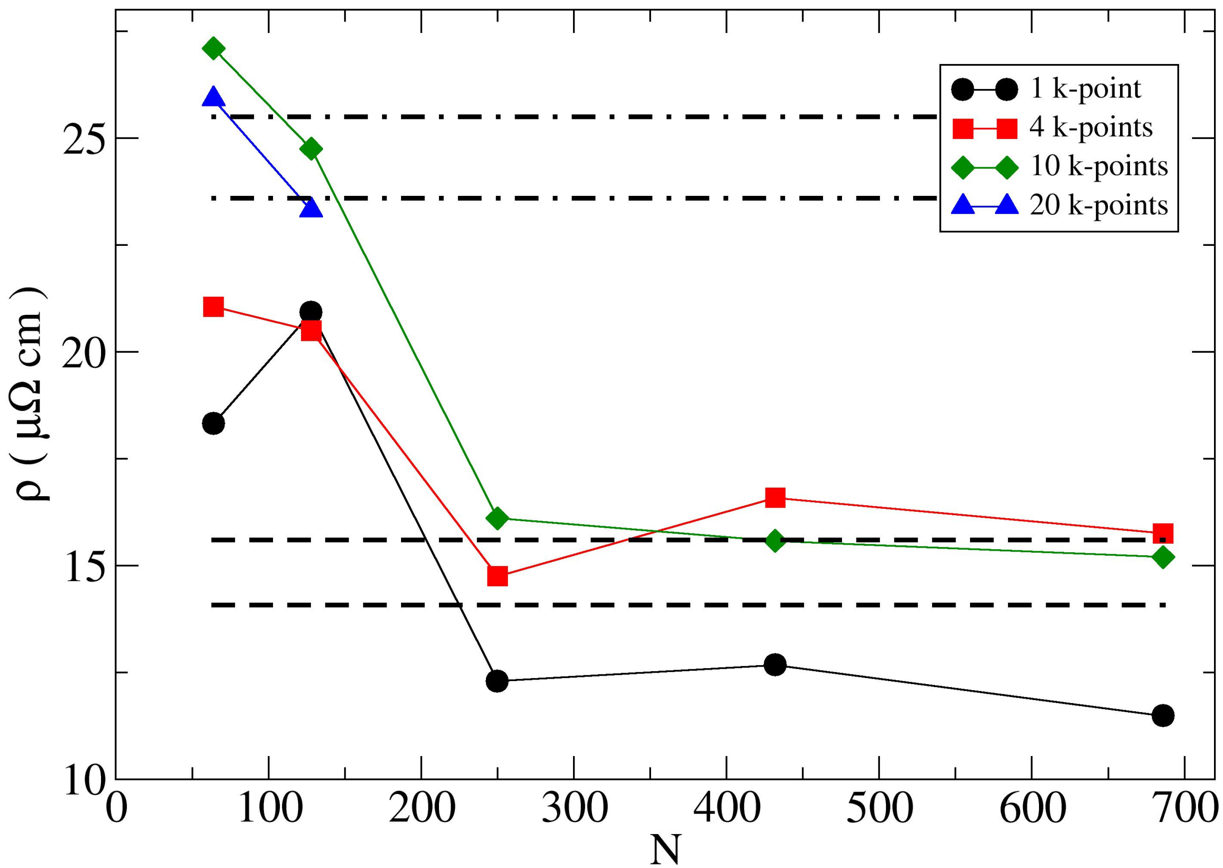
M. Pozzo, M.J. Desjarlais and D. Alfè, Physical Review B **84**, 054203 (2011).

Resistivity of iron at p=0



R. J. Weiss and A. S. Marotta, J. Phys. Chem. Solids **9**, 302 (1959).

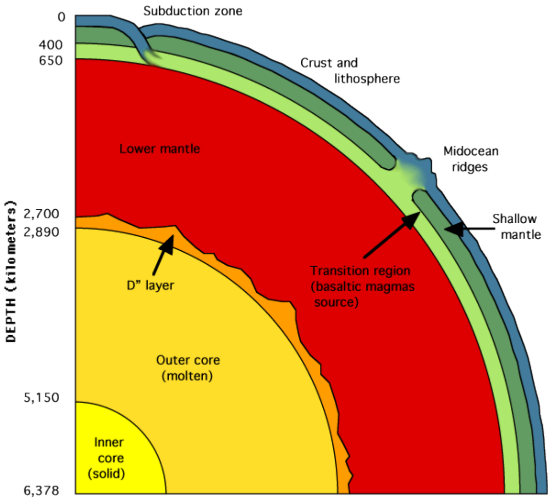
Resistivity of iron at p=0 and T= 500 K from DFT-PW91



D. Alfè, M. Pozzo, and M.J. Desjarlais, Physical Review B **85**, 024102 (2012)

Conductivity of the Earth's core

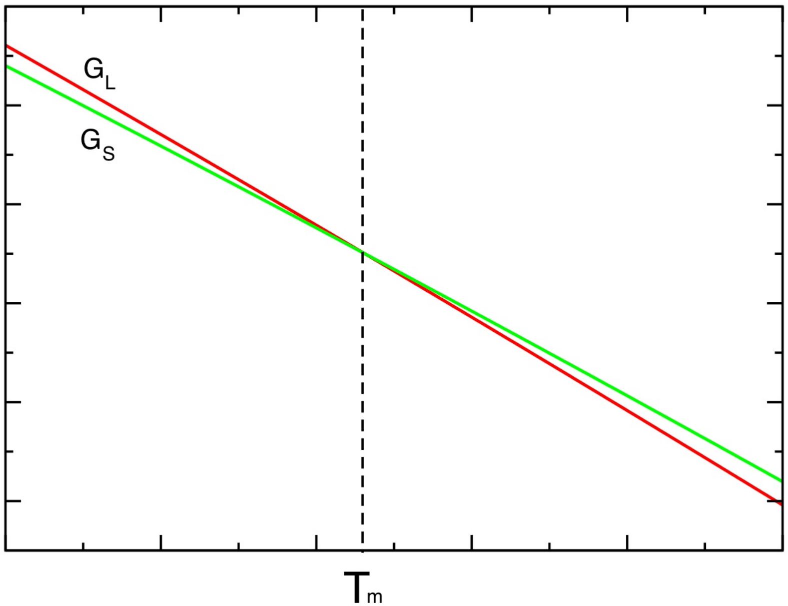
- Melting temperature of Fe at ICB pressure.
- Isentropic temperature profile in the outer core.
- Composition of the core
  - Effect of light impurities on melting temperature
  - Effect of light impurities on conductivities



Melting:

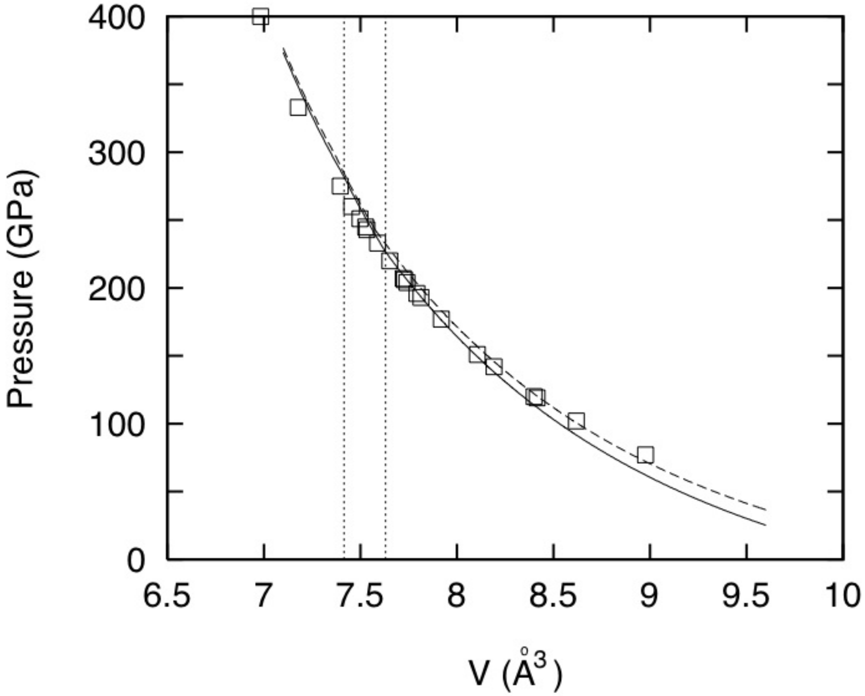
- Free Energy:
  - Helmholtz free energy: $F(V,T) = E(V,T) - TS(V,T)$
  - Gibbs free energy: $G(p,T) = F(V,T) + pV$

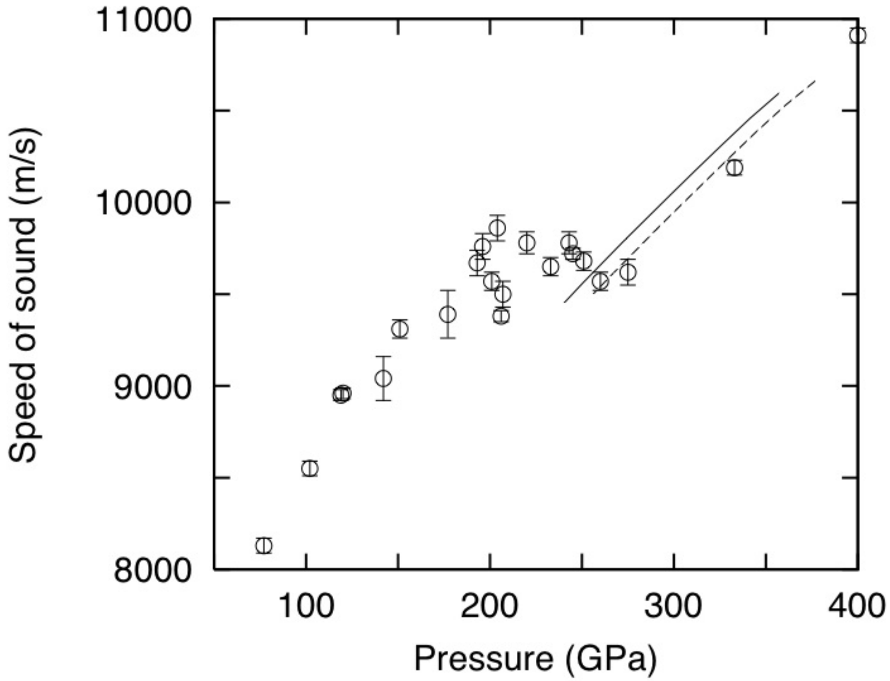
$$p = -dF/dV$$



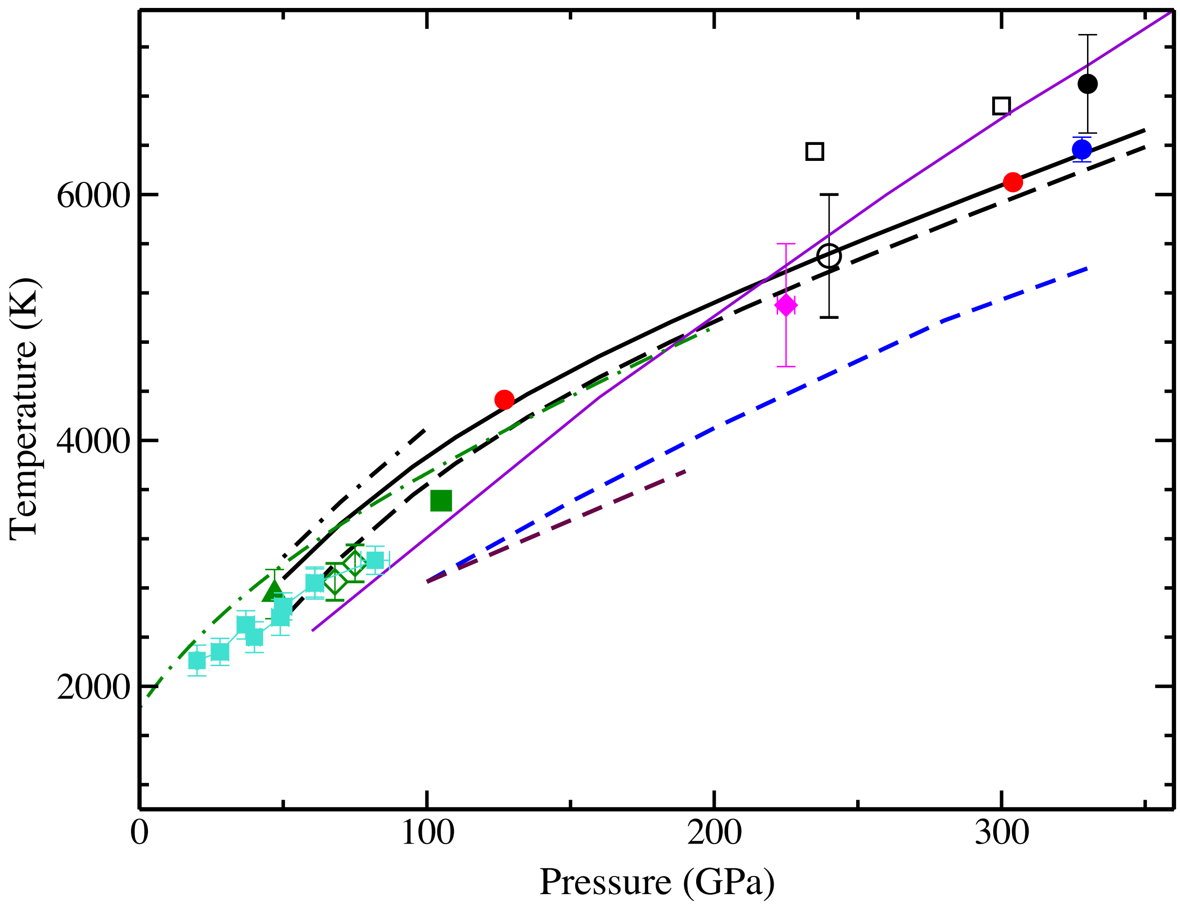
Hugoniot of Fe

$$\frac{1}{2}p_H(V_0 - V_H) = E_H - E_0$$





The melting curve of Fe

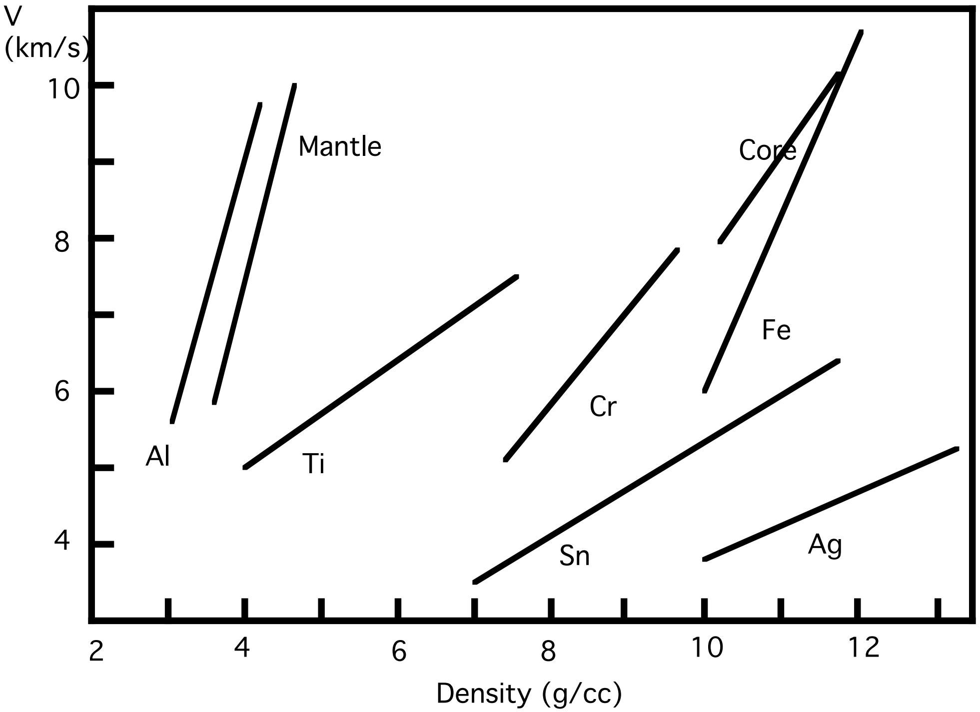


Alfè et al 1999, 2001, 2002, 2009; Belonoshko et al 2000; Laio et al 2000; Boehler 1993; Jephcoat 1996; Williams et al. 1986; Ma et al 2004; Shen et al. 1998; Brown & McQueen 1986; Yoo et al 1993; Nguyen&Holmes 2004; Jackson et al. 2013; Anzellini et al 2013; Bouchet et al. 2013.

Core composition

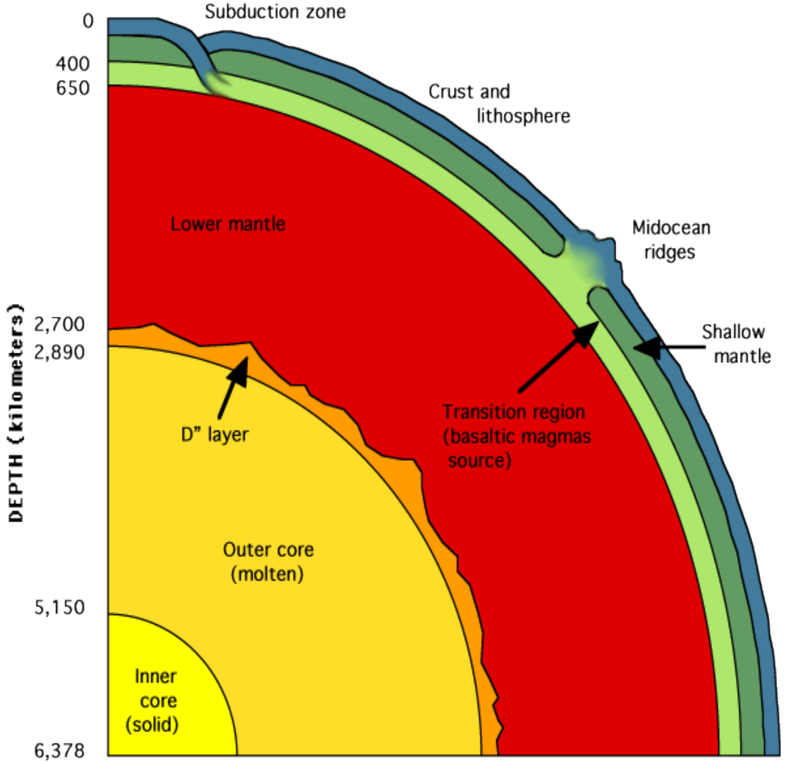
- Birch (1952) - "The Core is iron alloyed with a small fraction of lighter elements"

- Nature of light element inferred from:
  - •Cosmochemistry
  - •Meteoritics
  - •Equations of state

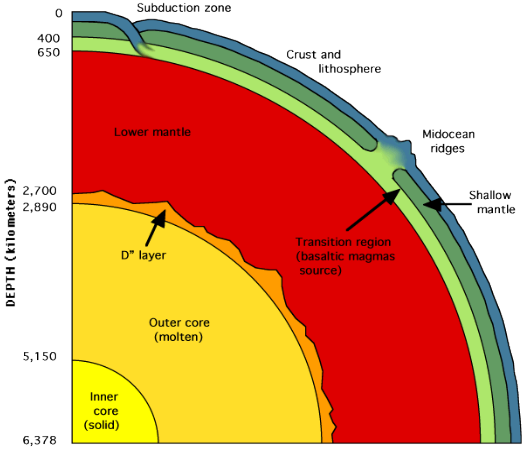


Strategy to constrain the composition of the Earth's core

- Density change at ICB ~ 5-6.5 % (seismological data).
- Density change on melting for Fe ~ 1.7 % (from ab-initio calculations).
- ➔ Partition of light elements.



Solid-liquid equilibrium



- Binary mixture, solvent A, solute X
- Equality of chemical potentials

$$\mu_X^l(p,T_m,c_X^l) = \mu_X^s(p,T_m,c_X^s) \qquad (1)$$

$$\mu_X(p,T_m,c_X) = k_B T \ln c_X + \tilde{\mu}_X(p,T_m,c_X)$$

$$c_X^s / c_X^l = \exp\left[(\tilde{\mu}_X^l - \tilde{\mu}_X^s)/k_B T_m\right]$$

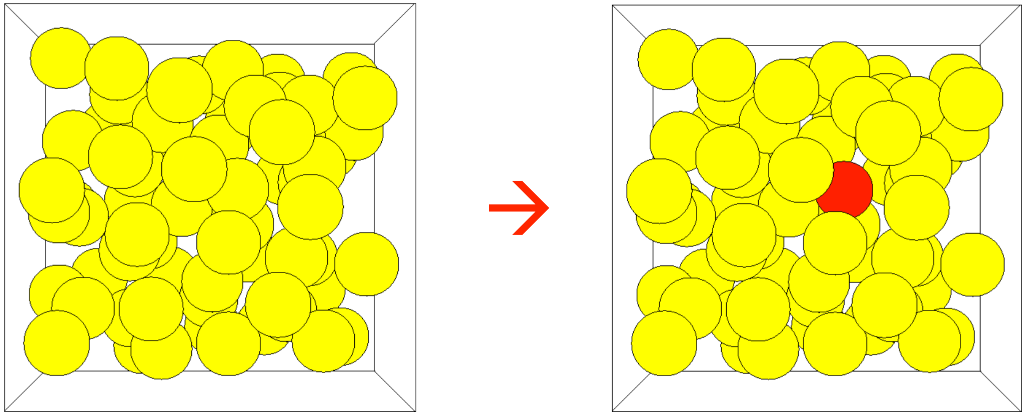
Calculating $\mu^{0l}{}_{XA}$ (liquid)

$$F_{A/X} - F_A = \int_0^1 d\lambda \, \langle U_{A/X} - U_A \rangle_\lambda$$

$$U_\lambda = (1-\lambda)U_A + \lambda U_{A/X}$$

$$\mathbf{f}_\lambda = -\frac{\partial U_\lambda}{\partial \mathbf{R}} = (1-\lambda)\mathbf{f}_A + \lambda \mathbf{f}_{A/X}$$

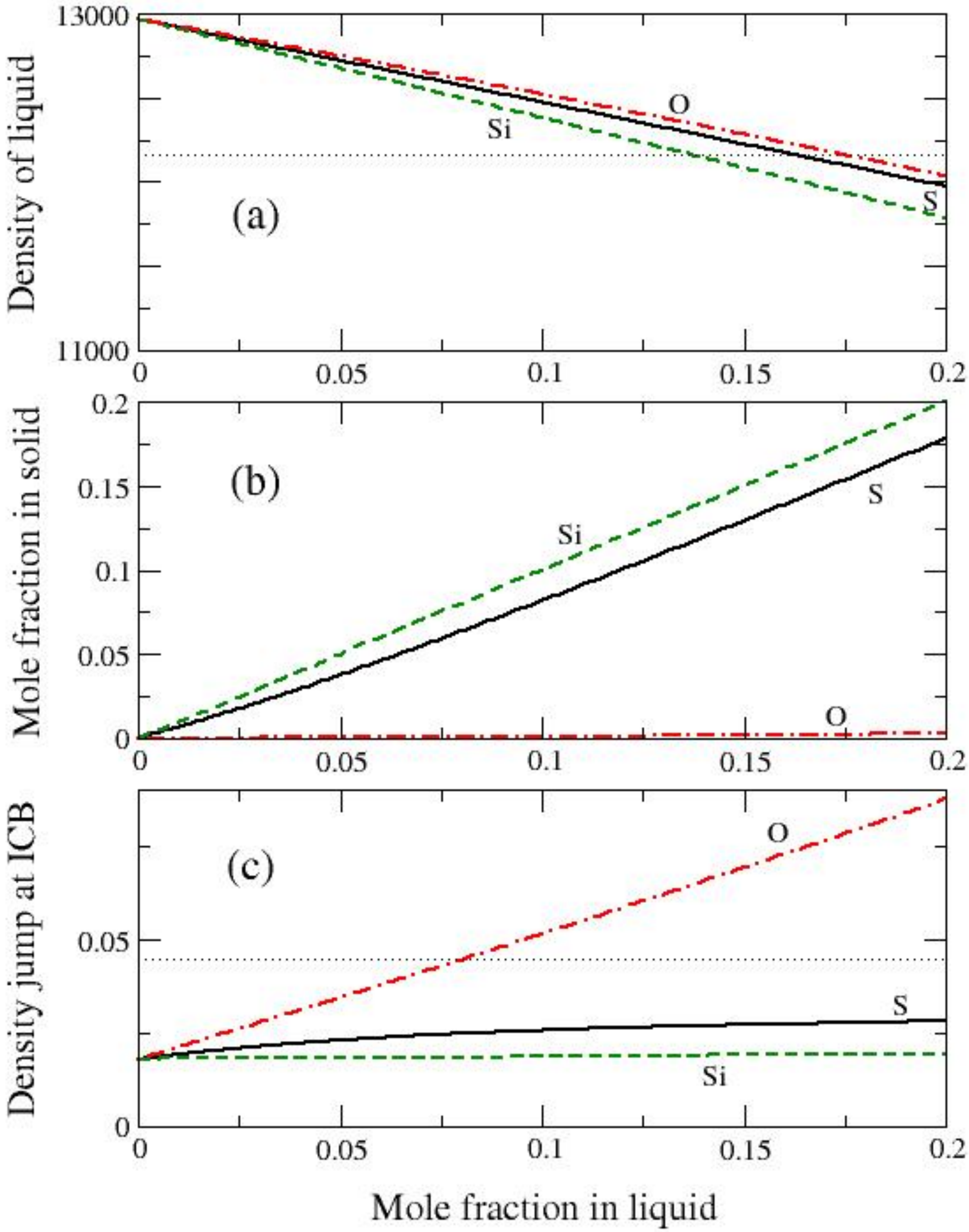
“Alchemy”



Results

$$c_X^s / c_X^l =$$

$$= \exp\left[(\tilde{\mu}_X^l - \tilde{\mu}_X^s) / k_B T \right]$$



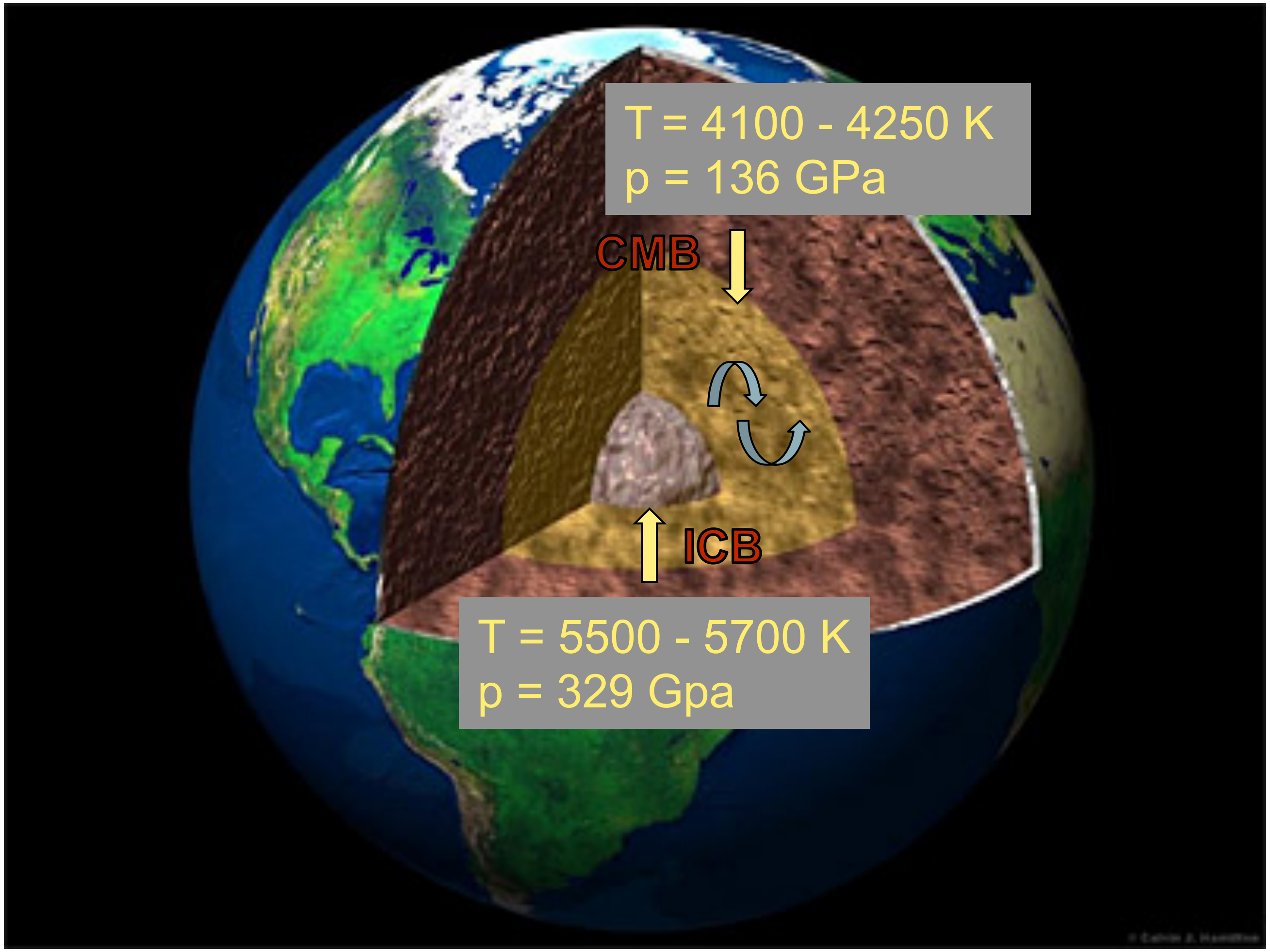
Composition of the Earth's core

	Solid	Liquid
S/Si	8.5 ± 2.5%	10 ± 2.5 %
O	0.2 ± 0.1 %	8-13 ± 2.5 %

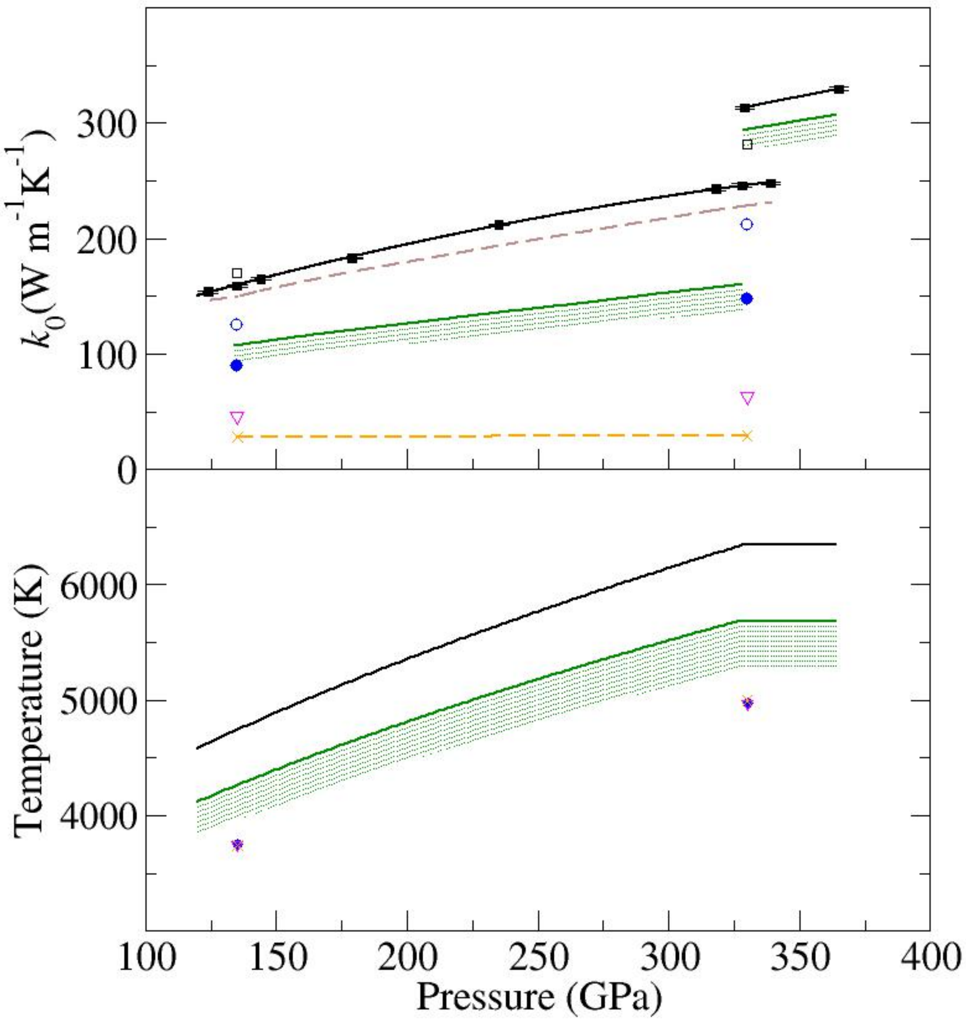
$$T - T_0 \simeq \frac{k_B T}{S_0^l - S_0^s}(c_X^s - c_X^l) \simeq -700, -900 \text{ K}$$

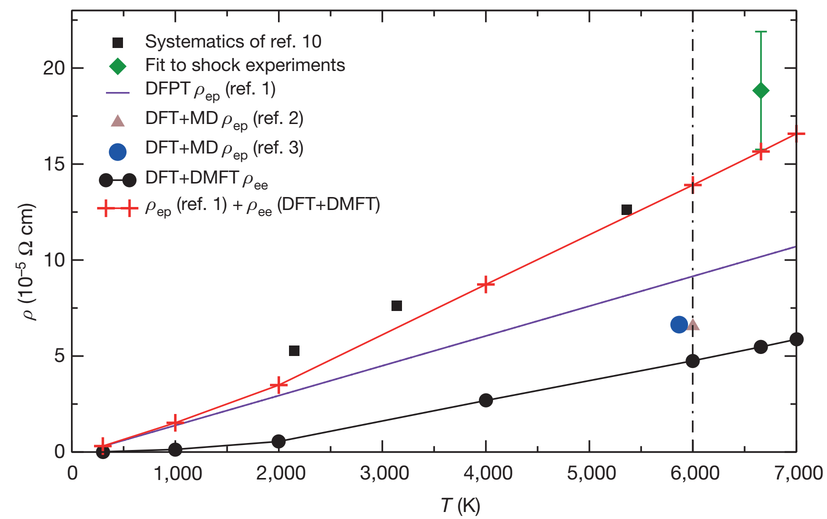
Alfè, Price, Gillan, Nature, **405**, 172 (2000); GRL, **27**, 2417 (2000);
EPSL, **195**, 91 (2002); JCP, **116**, 7127 (2002);
See also Badro et al, PNAS, **111**, 7542 (2014)

Earth’s outer core temperatures



Iron and iron alloys at Earth's core conditions



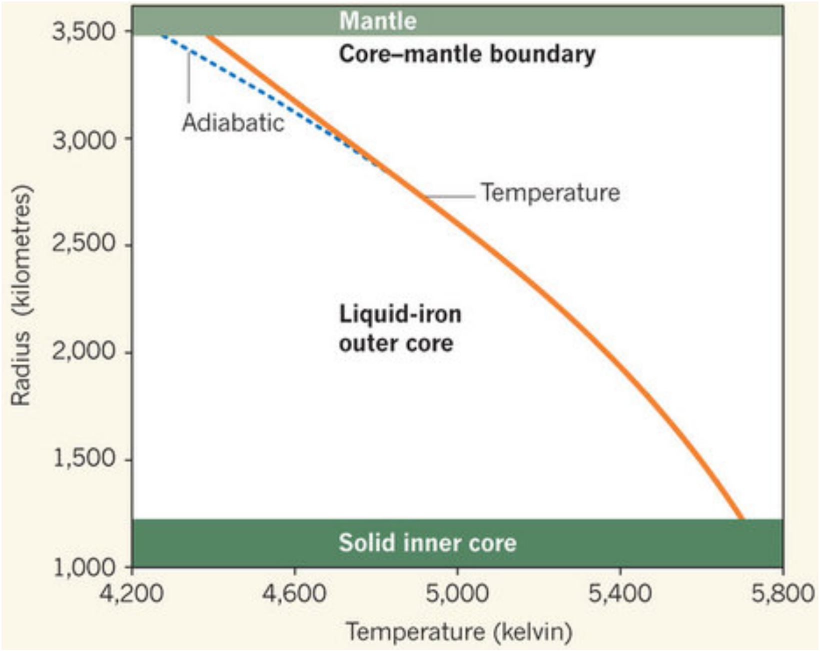


Zhang et al, Nature 2015

M. Pozzo, C. Davies, D. Gubbins, & D. Alfè, Nature **485**, 355 (2012); PRB **87**, 014110 (2013); EPSL **393**, 169 (2014).
News & Views by B. Buffet, Nature **485**, 319 (2012).
See also N. de Koker et al, PNAS **109**, 4070 (2012); Gomi et al, PEPI **224**, 88 (2013). Ohta et al, AGU abstract (2014).

Conclusions

- Conductivities of the Earth's core are 2-3 times higher than previous estimates.
- Power for the geodynamo is greatly reduced (but longer magnetic decay time, which stabilises the magnetic field).
- Young inner core, rapid secular cooling and/or radiogenic heating.
- The top of the core may be thermally stratified



B. Buffet, Nature **485**, 319 (2012).