Thermal and electrical conductivity of the Earth's core

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

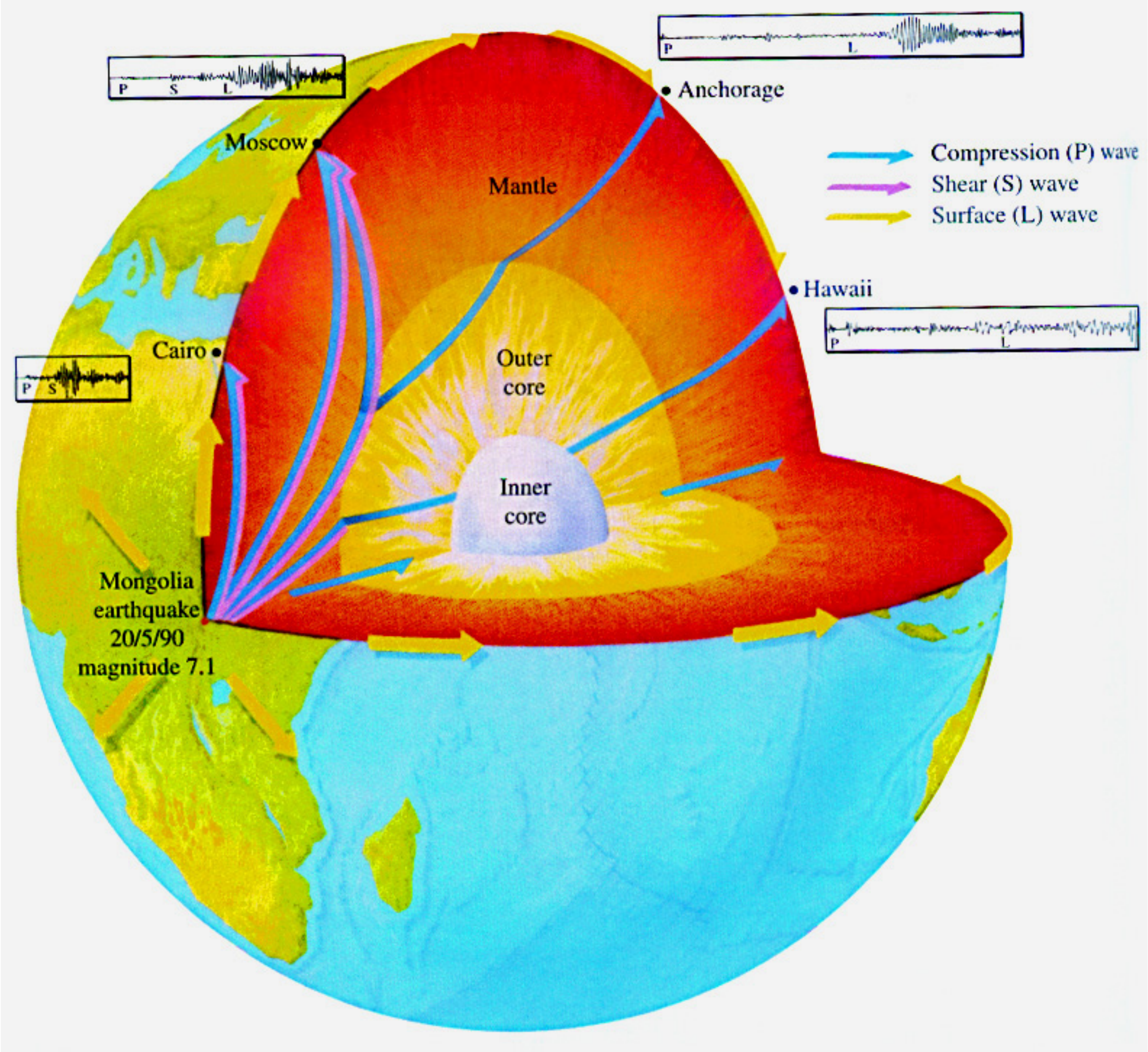
[1]*Department of Earth Sciences & Department of Physics and Astronomy, Thomas Young Centre@UCL & London Centre for Nanotechnology University College London*

[2]*School of Earth and Environment, University of Leeds*

EPSRC Engineering and Physical Sciences Research Council

THE ROYAL SOCIETY

NATURAL ENVIRONMENT RESEARCH COUNCIL



P S L
Moscow
P L
Anchorage
Compression (P) wave
Shear (S) wave
Surface (L) wave
Mantle
Hawaii
P L
Cairo
P S
Outer core
Inner core
Mongolia earthquake 20/5/90 magnitude 7.1

Electrical conductivity

- Kubo-Greenwood:

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

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

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

Thermal conductivity

- Electronic component:

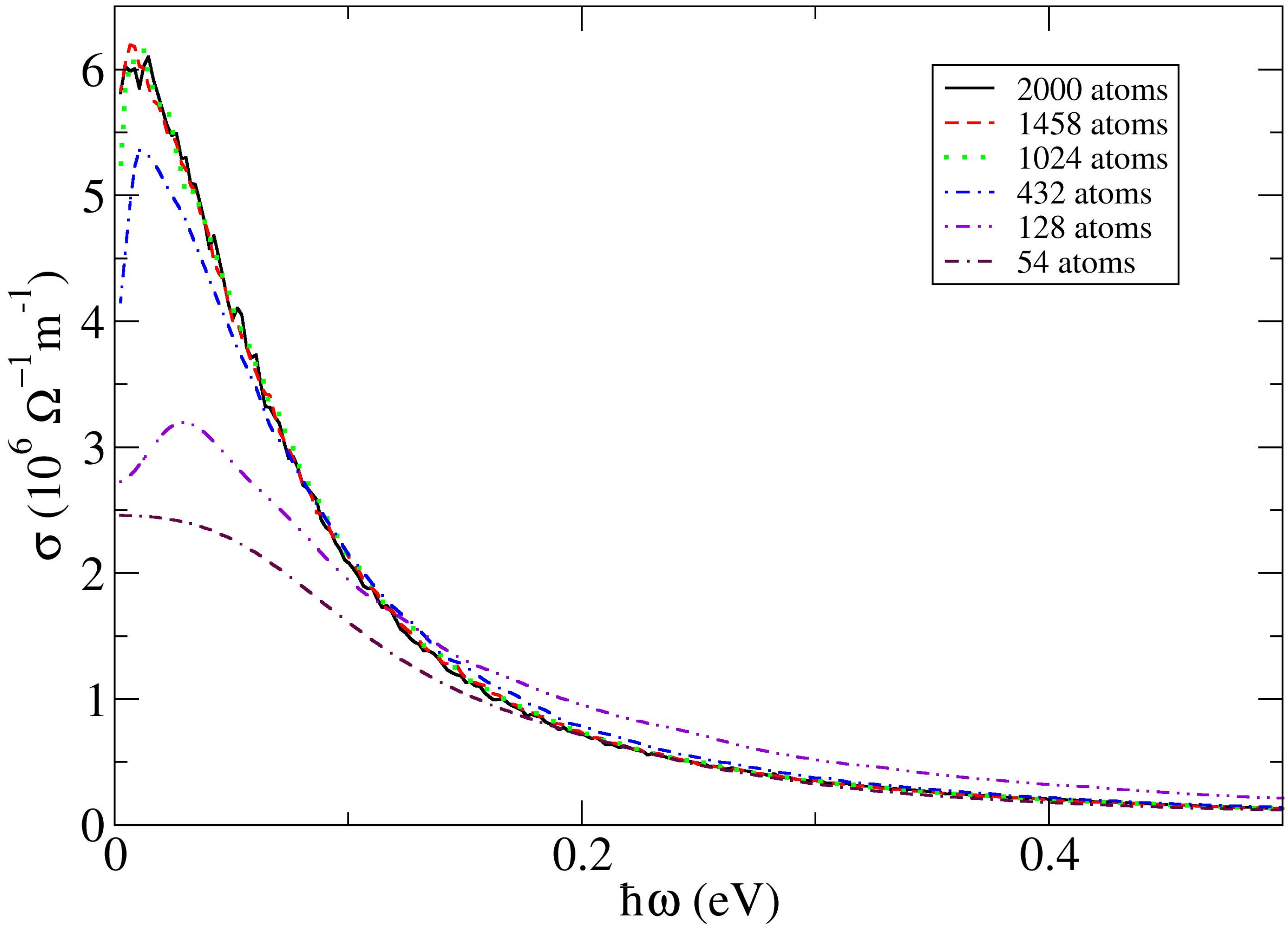
$$k = \lim_{\omega \to 0} \left\langle k(\omega, R_I) \right\rangle = \lim_{\omega \to 0} \left\langle \frac{1}{e^2 T} \left(L_{22}(\omega, R_I) - \frac{L_{12}^2(\omega, R_I)}{\sigma(\omega, R_I)} \right) \right\rangle$$

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

- Ionic component:

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

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



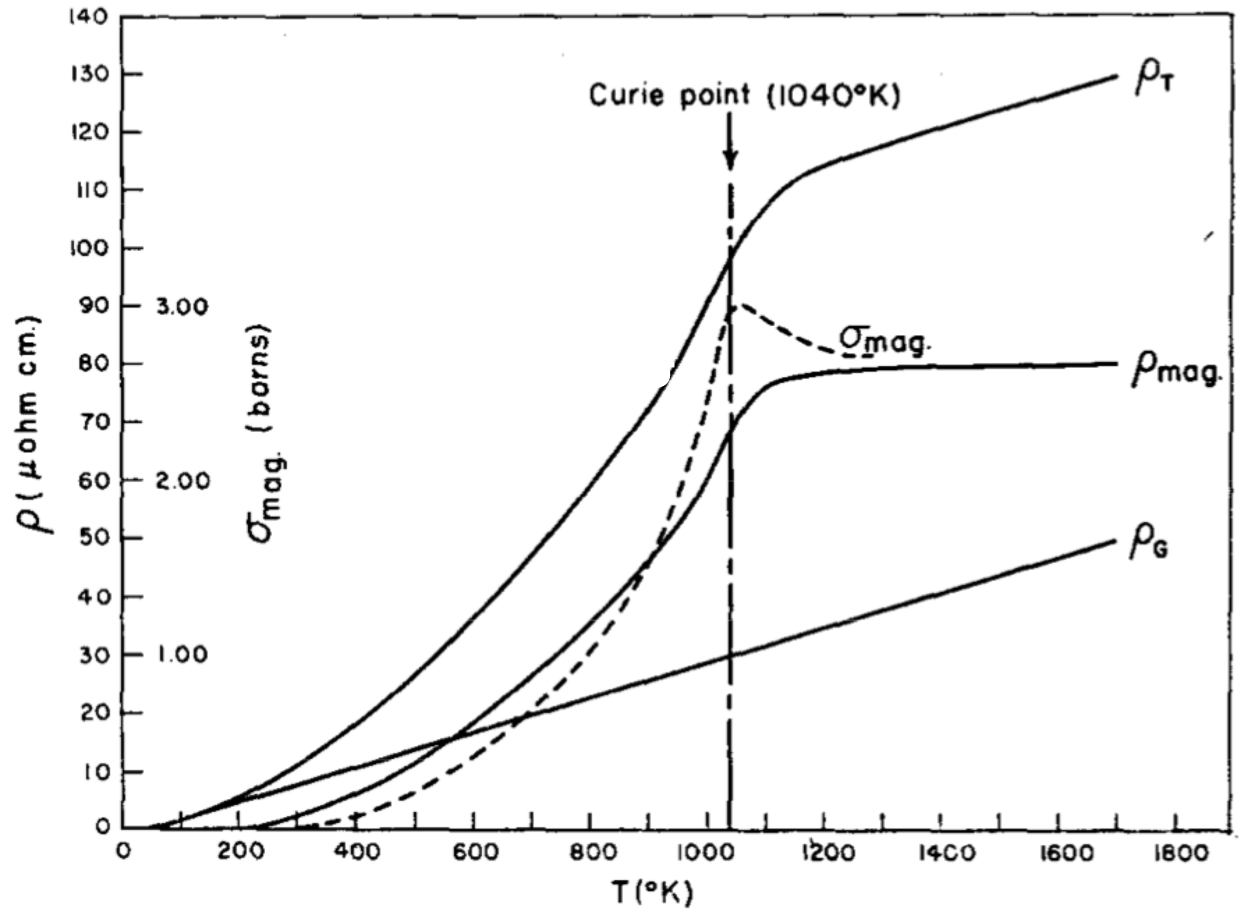
Conductivities of liquid Na at p=0 and T=400K

	σ_0 ($10^6\Omega^{-1}m^{-1}$)	κ_0 (W m^{-1} K^{-1})	L ($10^{-8}\Omega$ W K^{-2})
LDA	6.2	60	2.42
PBE	10.3	93	2.26
EXP	9.7	86	2.22

Lorenz number $L = k_0/\sigma_0 T$

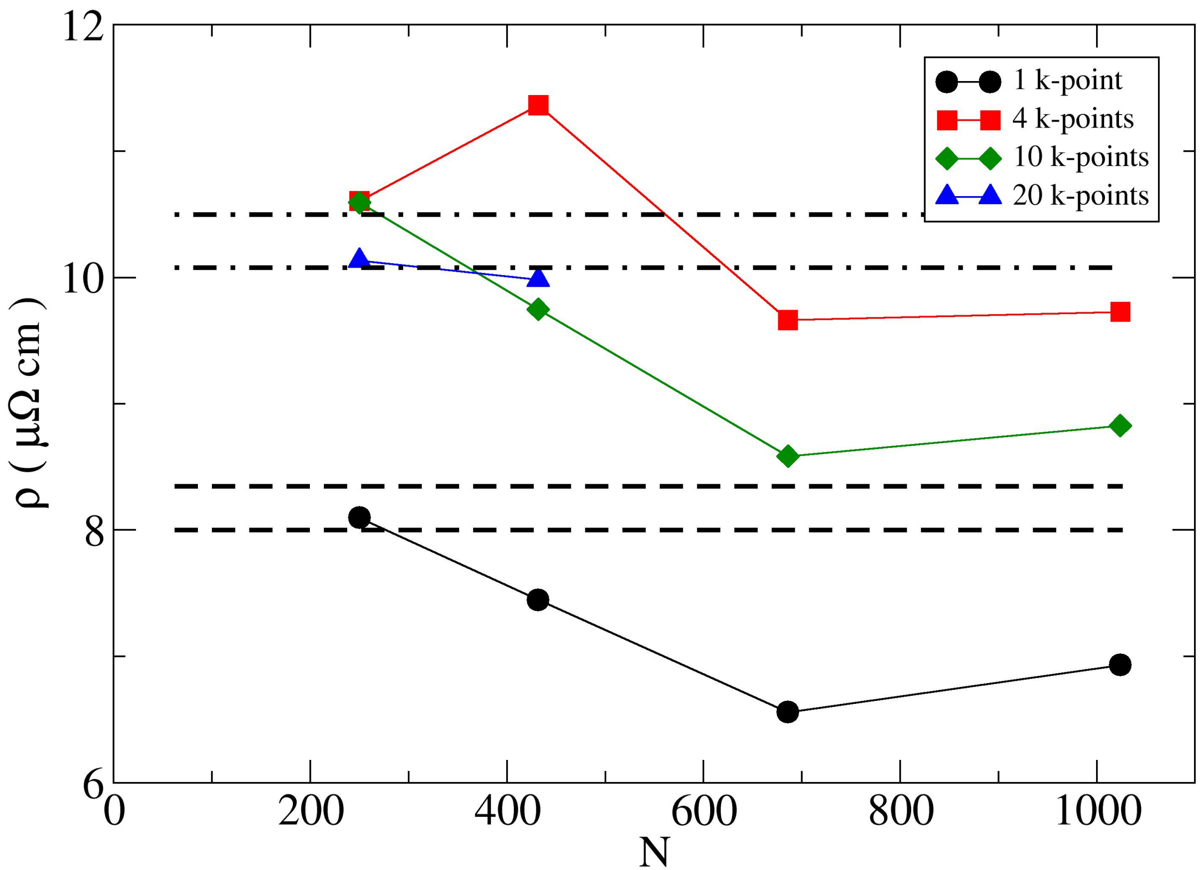
M. Pozzo, M.J. Desjarlais and D. Alfè, Physical Review B **84**, 054203 (2011).

Resistivity of iron at p=0



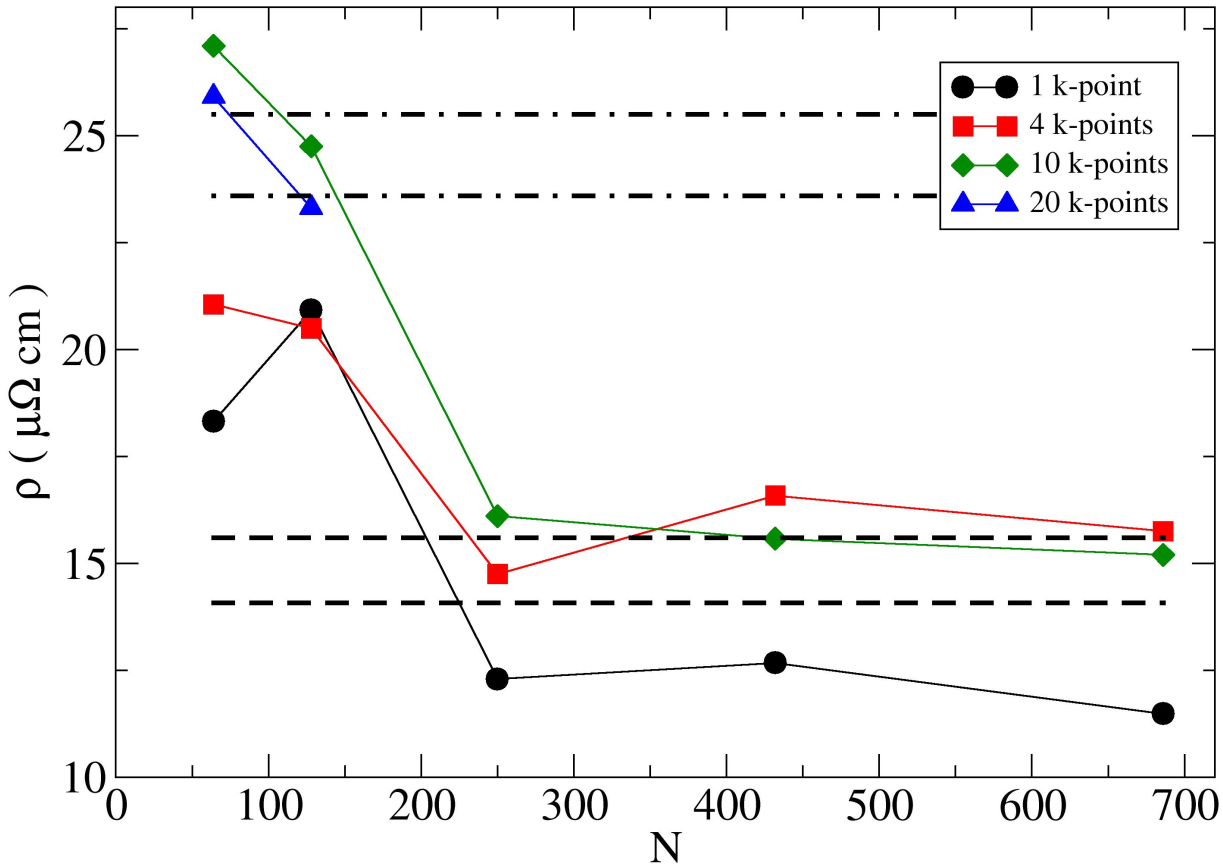
R. J. Weiss and A. S. Marotta,, J. Phys. Chem. Solids **9**, 302 (1959).

Resistivity of iron at p=0 and T= 300 K from DFT-PW91



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

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

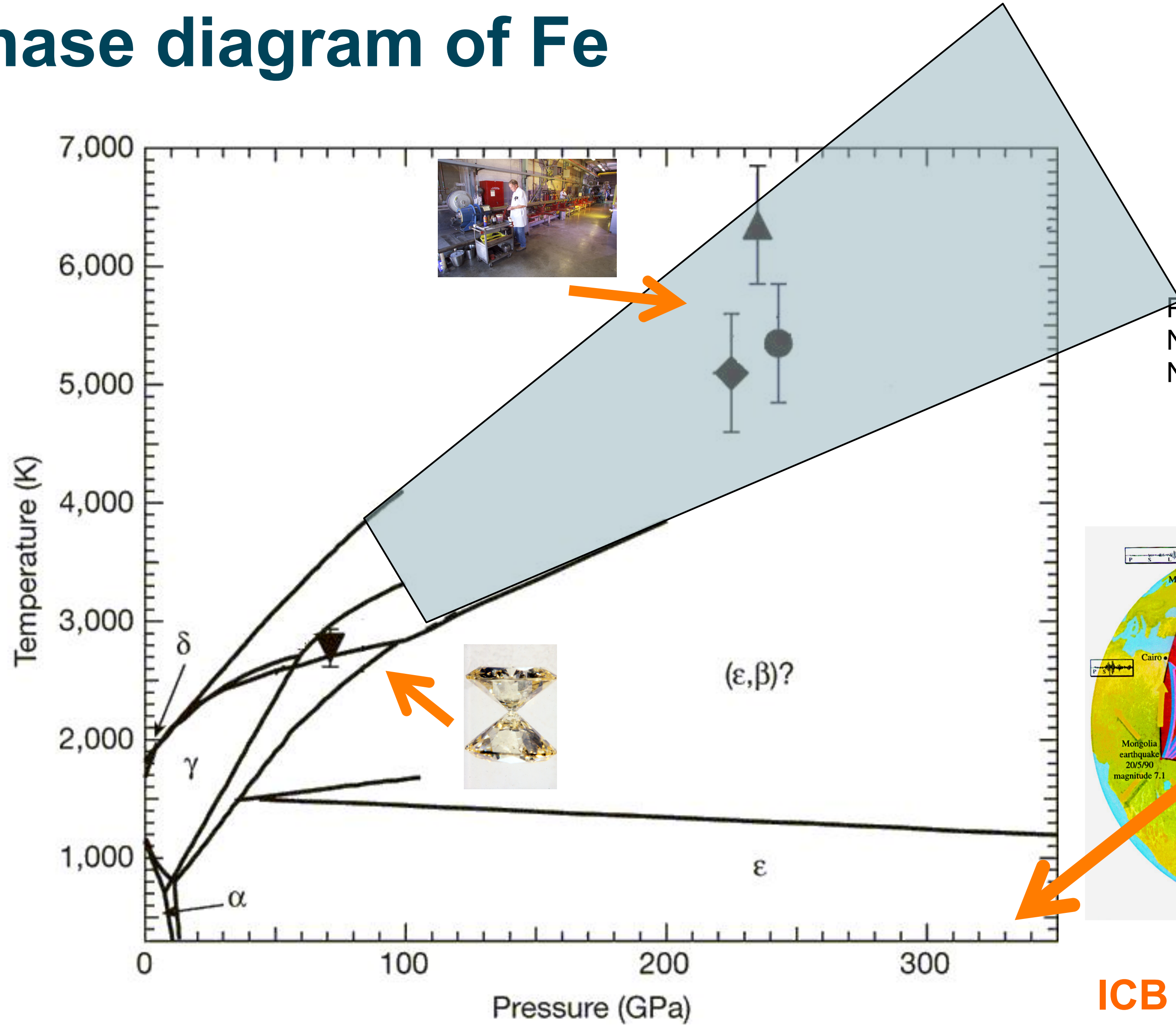


D. Alfè, M. Pozzo, and M.J. Desjarlais, Physical Review B **85**, 024102 (2012)

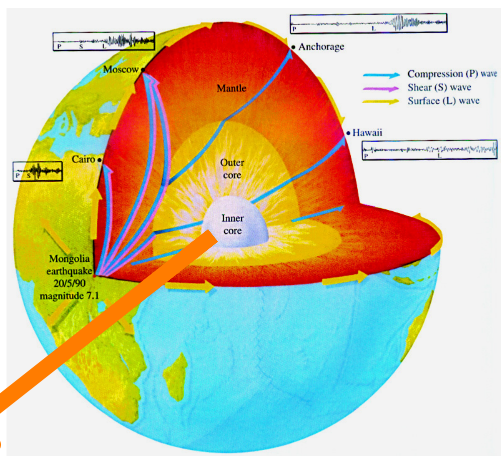
Conductivity of the Earth's core ?

- Melting curve of Fe at core pressures
- Composition of the core
  - Effect of light impurities on melting temperature
  - Effect of light impurities on conductivities

Phase diagram of Fe

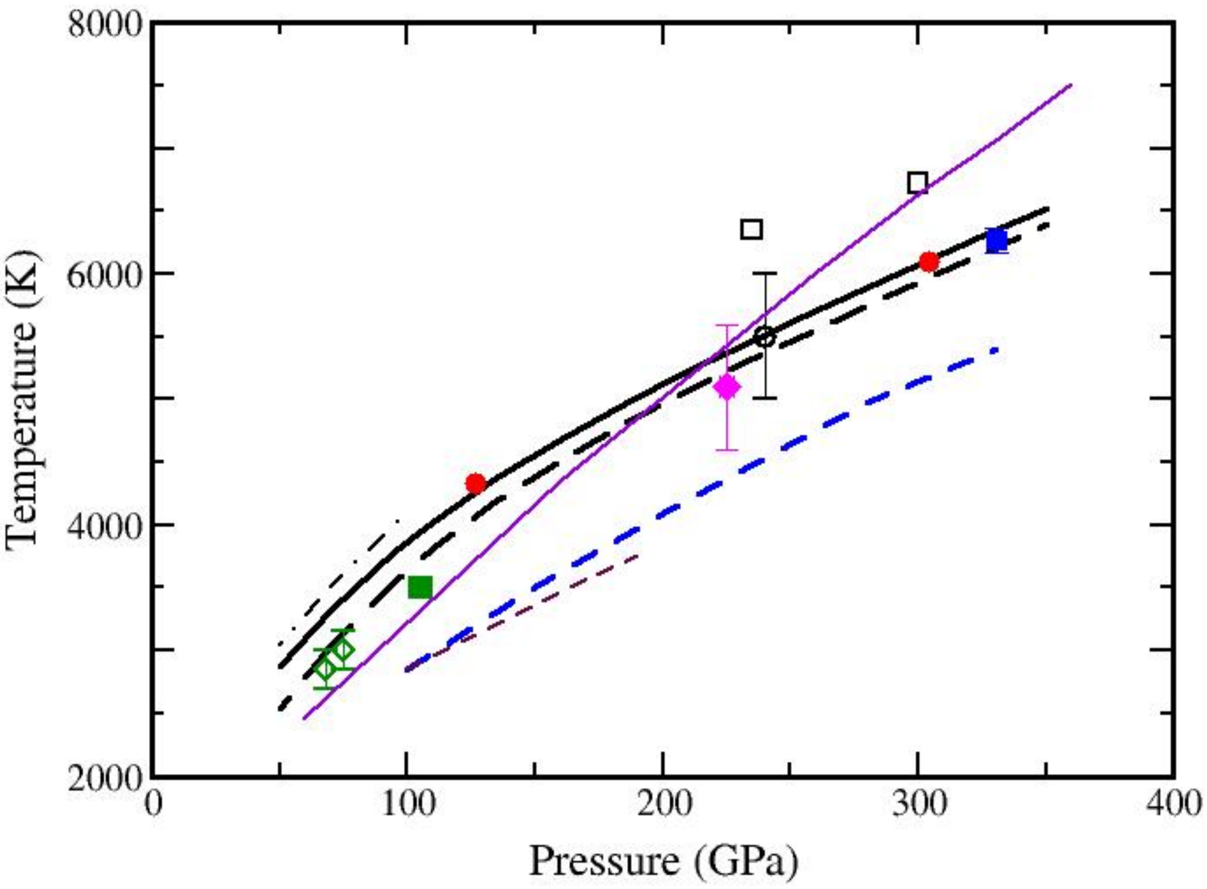


Picture adapted from:
Nguyen and Holmes,
Nature, **427**, 339 (2004)



ICB P = 330 GPa

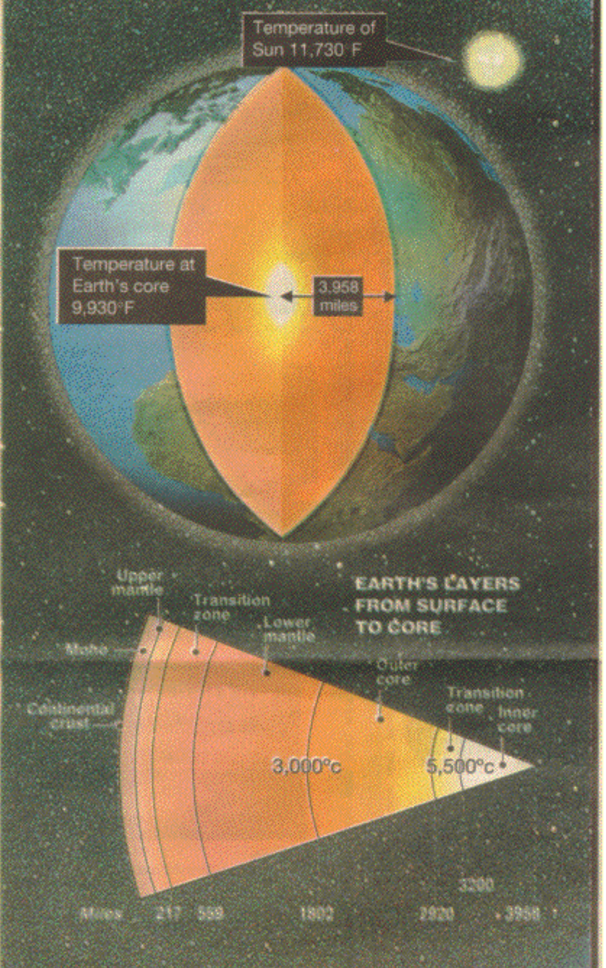
The melting curve of Fe



Alfè, Price, Gillan, Nature, **401**, 462 (1999); Phys. Rev. B, **64**, 045123 (2001); Phys. Rev. B, **65**, 165118 (2002); J. Chem. Phys., **116**, 6170 (2002)

CORE WHAT A SCORCHER

THE MIRROR, 1 October 1999



Scientists discover centre of the Earth is almost as hot as the Sun

SCIENTISTS have cracked a 100-year mystery – and found that the temperature at the centre of the Earth almost matches the heat of Sun.

The planet's core is a globe of iron which hits a blistering 9,930F. Its true temperature was a puzzle that set off more than a century of debate.

But now two powerful computers working in tandem and the mysteries of quantum physics have worked out the astonishing figure.

Professor Mike Gillan, one of the team behind the find, thinks the knowledge will improve understanding of the way the Earth works.

He said: "The Earth changes over time. Things are slowly moving and you see the effects through volcanoes and earthquakes.

"To understand this properly you need to know the temperature deep inside the Earth because that is what is driving everything. The whole dynamics of the planet depend on it."

Earth's centre is divided into an outer core of molten iron and an inner core made solid because of the pressure of rock above. Professor Gillan, of University College, London, and colleagues Dario Alfe and David Price found that the melting point of iron under such extreme pressures is 6,500C. That's 11,730F — about the temperature of the Sun.

By STEPHEN WHITE and NATHAN YATES

But because of impurities at the core, they reckon that where the molten metal turns to solid mass the temperature is 5,500C, or 9,930F.

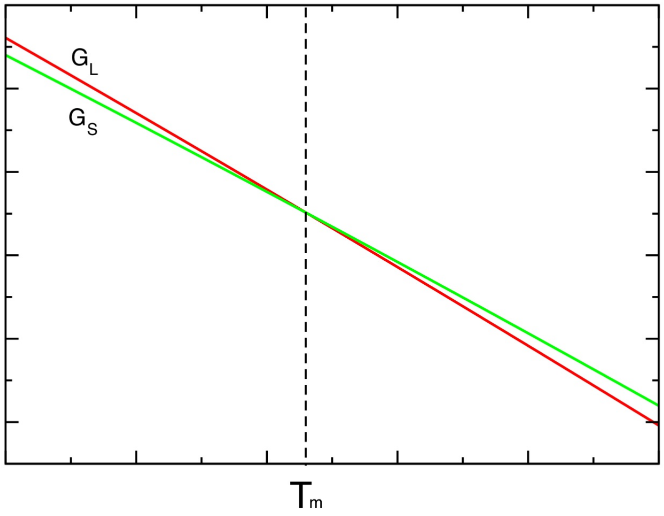
The figure is far higher than previously thought. And it could be even hotter within the inner core.

Earth's centre lies beneath a solid rock crust 9.3 miles thick, floating upon a mantle which reaches a depth of 1,800 miles and a temperature of 3,000C.

From here, the heat accelerates rapidly. The exact centre is 3,958 miles down. The study's data relates to a point 3,200 miles from the surface.

Earth's molten outer core generates the magnetic field which shelters us from the lethal solar wind. Earthquakes and volcanoes may be linked to heat variations deep down.

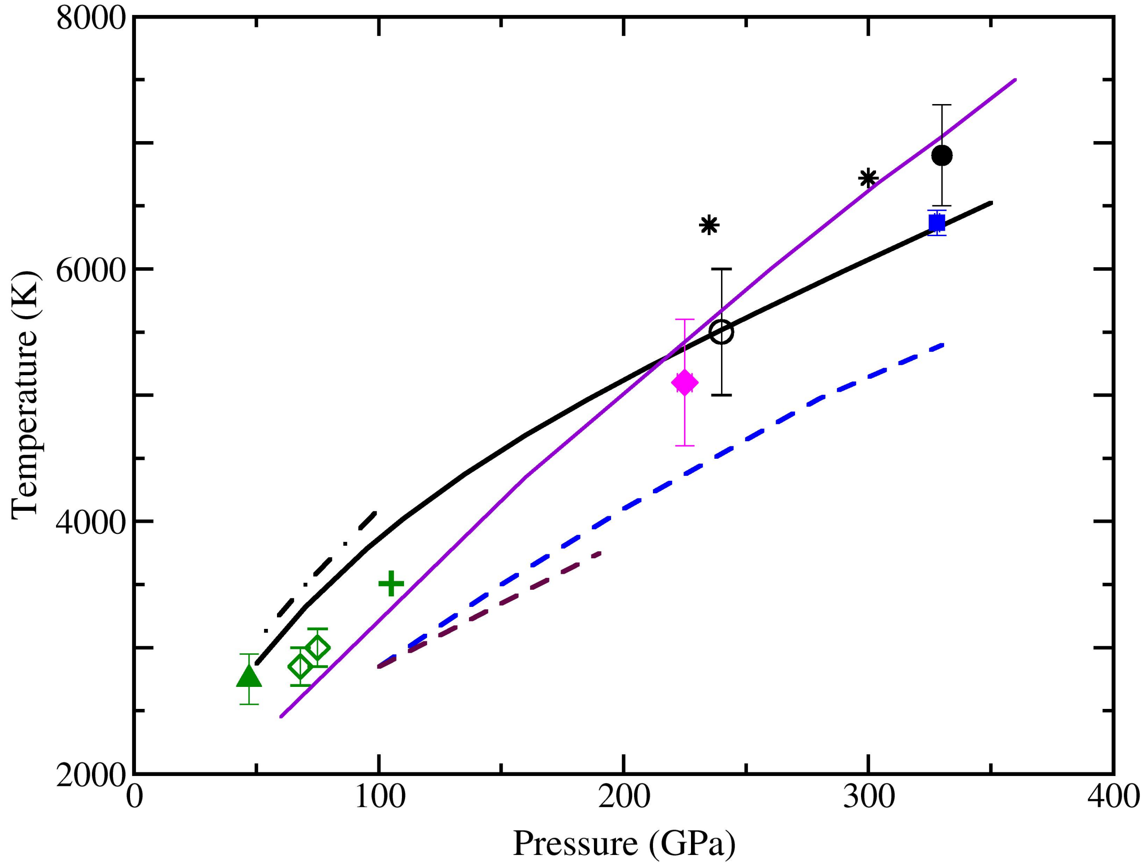
Melting of Fe from QMC:



Free energy corrections from DFT to QMC:

$$\delta T_m = \frac{\Delta G^{ls}(T_m^{ref})}{S_{ref}^{ls}}$$

Melting curve of Fe with QMC

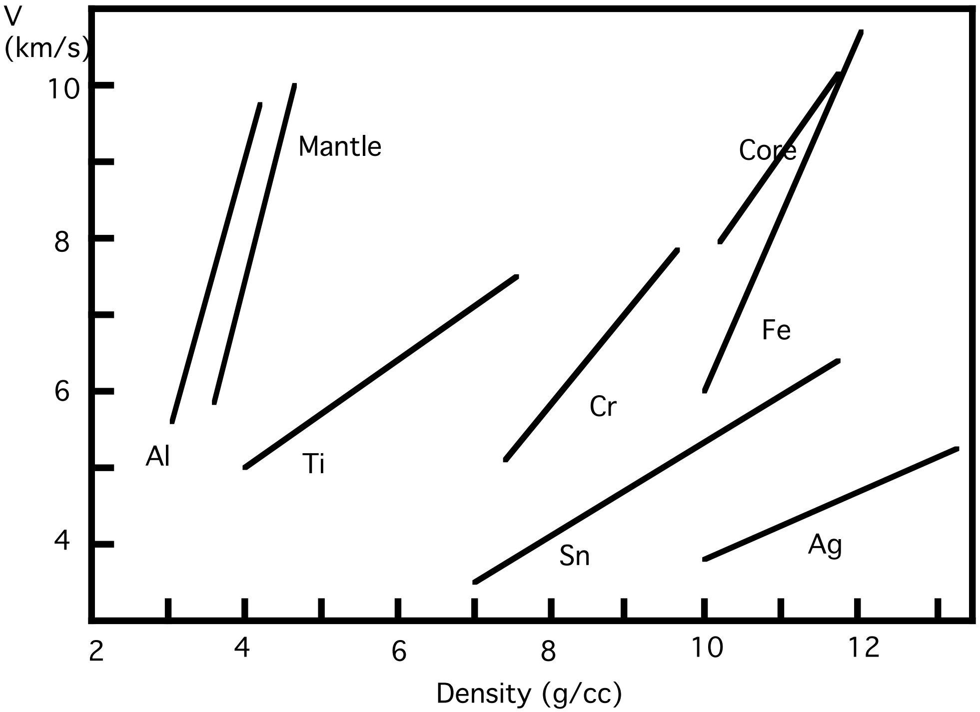


E. Sola and D. Alfè, Phys. Rev. Lett, ***103****, 078501 (2009)*

Core composition

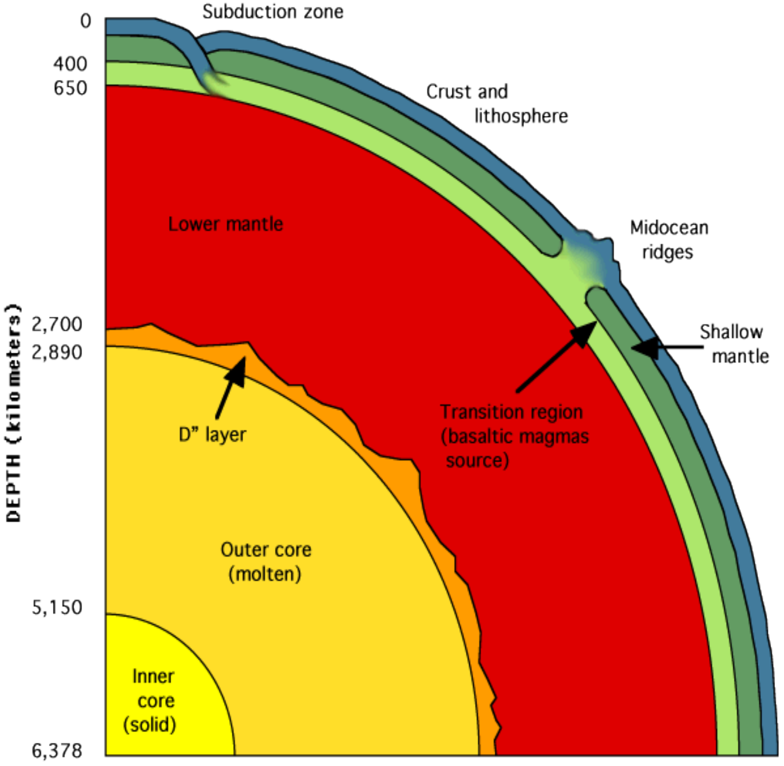
- Birch (1952) - “The Core is iron alloyed with a small fraction of lighter elements”

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



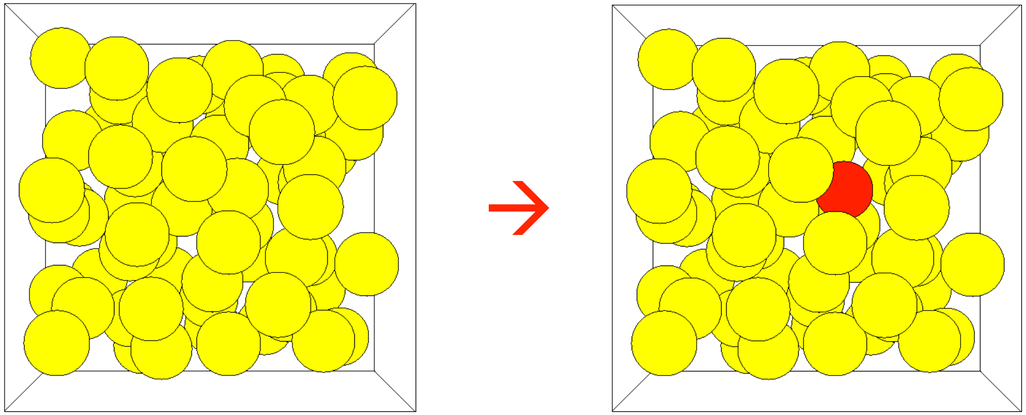
Calculating μ^{0l}_{XA} (liquid)

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

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

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

"Alchemy"

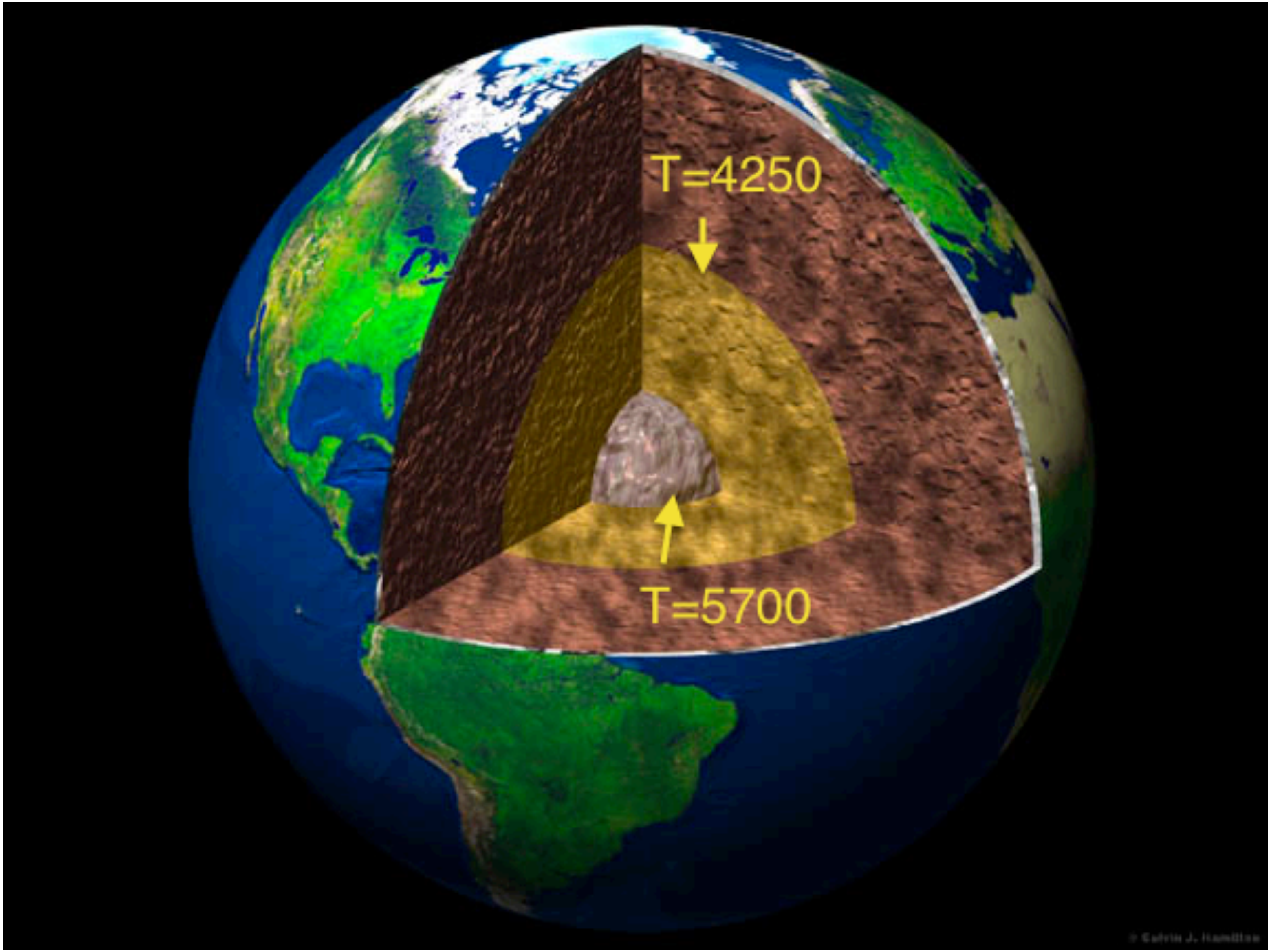


Composition of the Earth's core

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

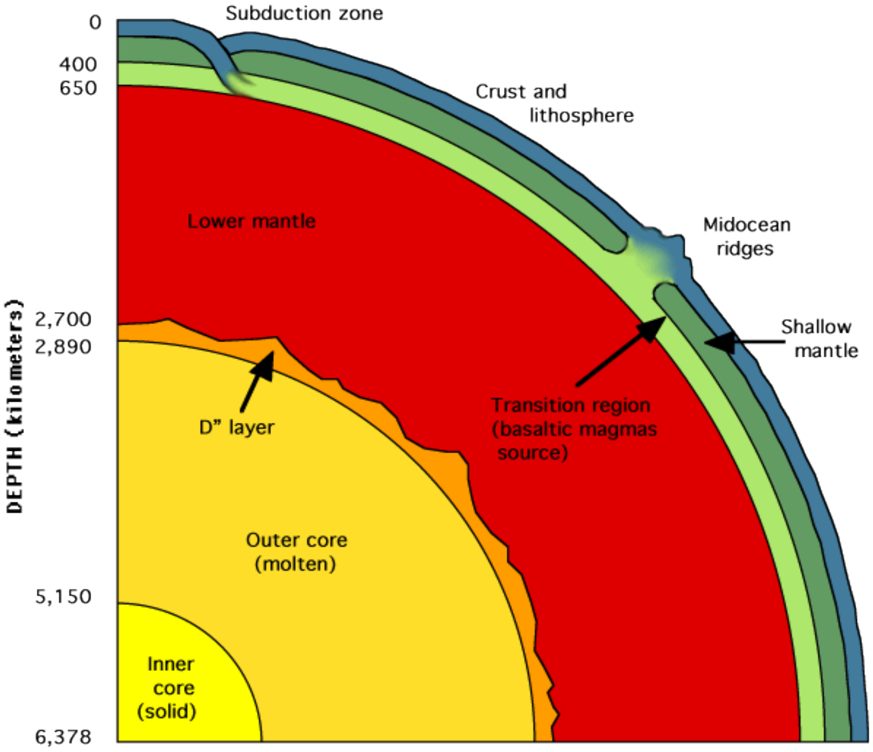
$$T - T_0 \simeq \frac{k_B T}{S_0^l - S_0^s}(c_X^s - c_X^l) \simeq -700\ \mathrm{K}$$

Alfè, Price, Gillan, Nature, **405**, 172 (2000); GRL, **27**, 2417 (2000); EPSL, **195**, 91 (2002); JCP, **116**, 7127 (2002)


T=4250
T=5700

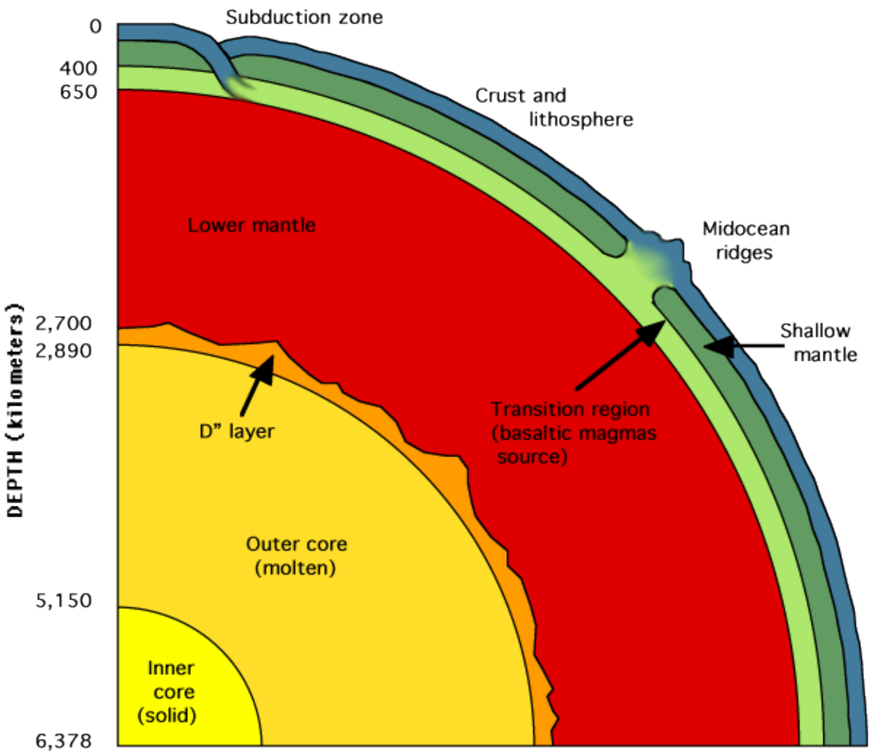
Composition of the Earth's core

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



Composition of the Earth's core

- Density change at ICB ~ 6.7 % (new seismological data, Masters and Gubbins 2003).
- Density change on melting for Fe ~ 1.7 % (from ab-initio calculations).
- ➔ Partition of light elements.

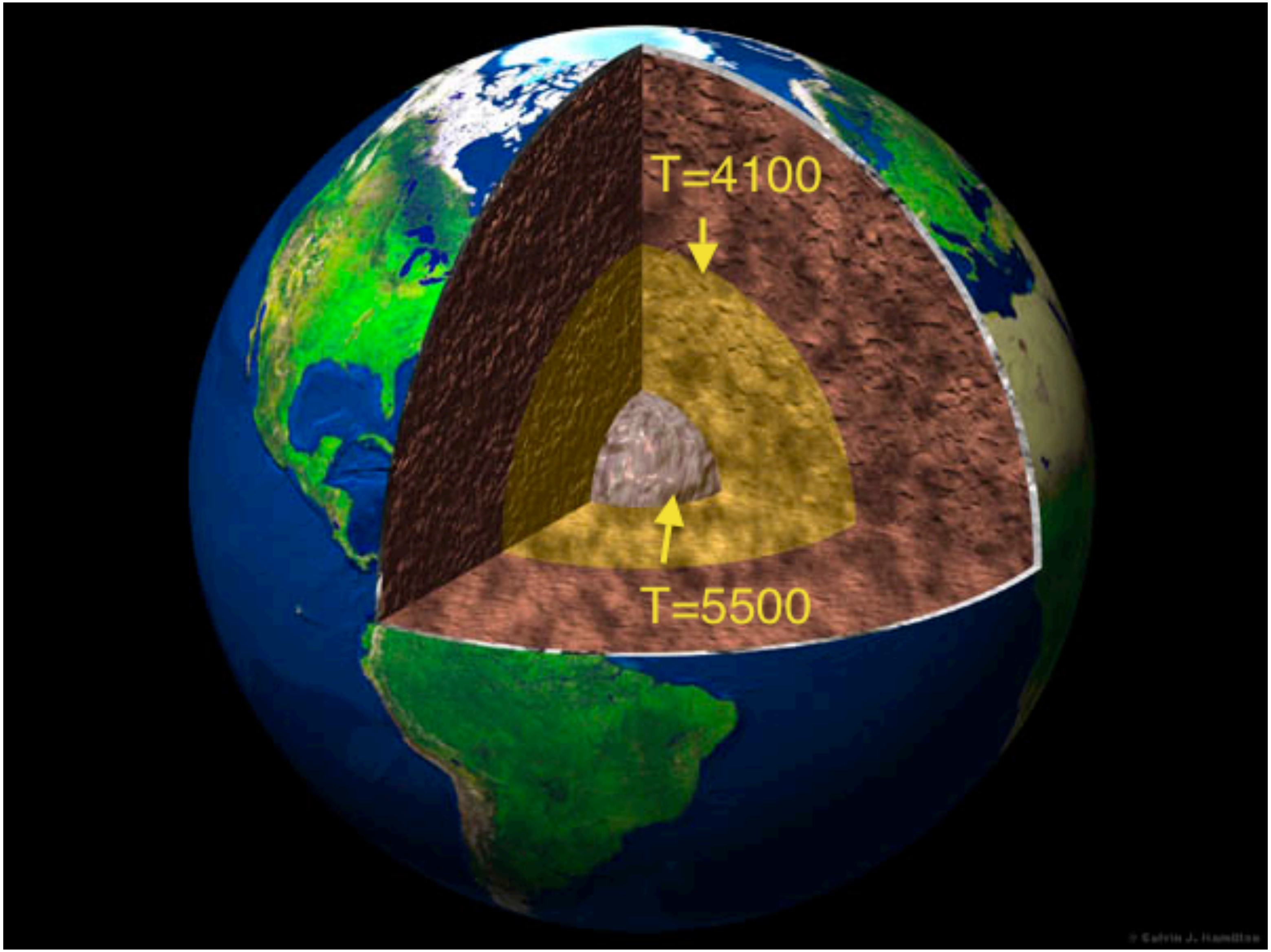


Composition of the Earth's core

	Solid	Liquid
S/Si	7.0 ± 2.5%	8 ± 2.5 %
Ox	0.2 ± 0.1 %	13 ± 2.5 %

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

Alfè, Price, Gillan, Nature, **405**, 172 (2000); GRL, **27**, 2417 (2000); EPSL, **195**, 91 (2002); JCP, **116**, 7127 (2002)


T=4100
T=5500

Electrical conductivity

- Kubo-Greenwood:

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

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

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

Thermal conductivity

- Electronic component:

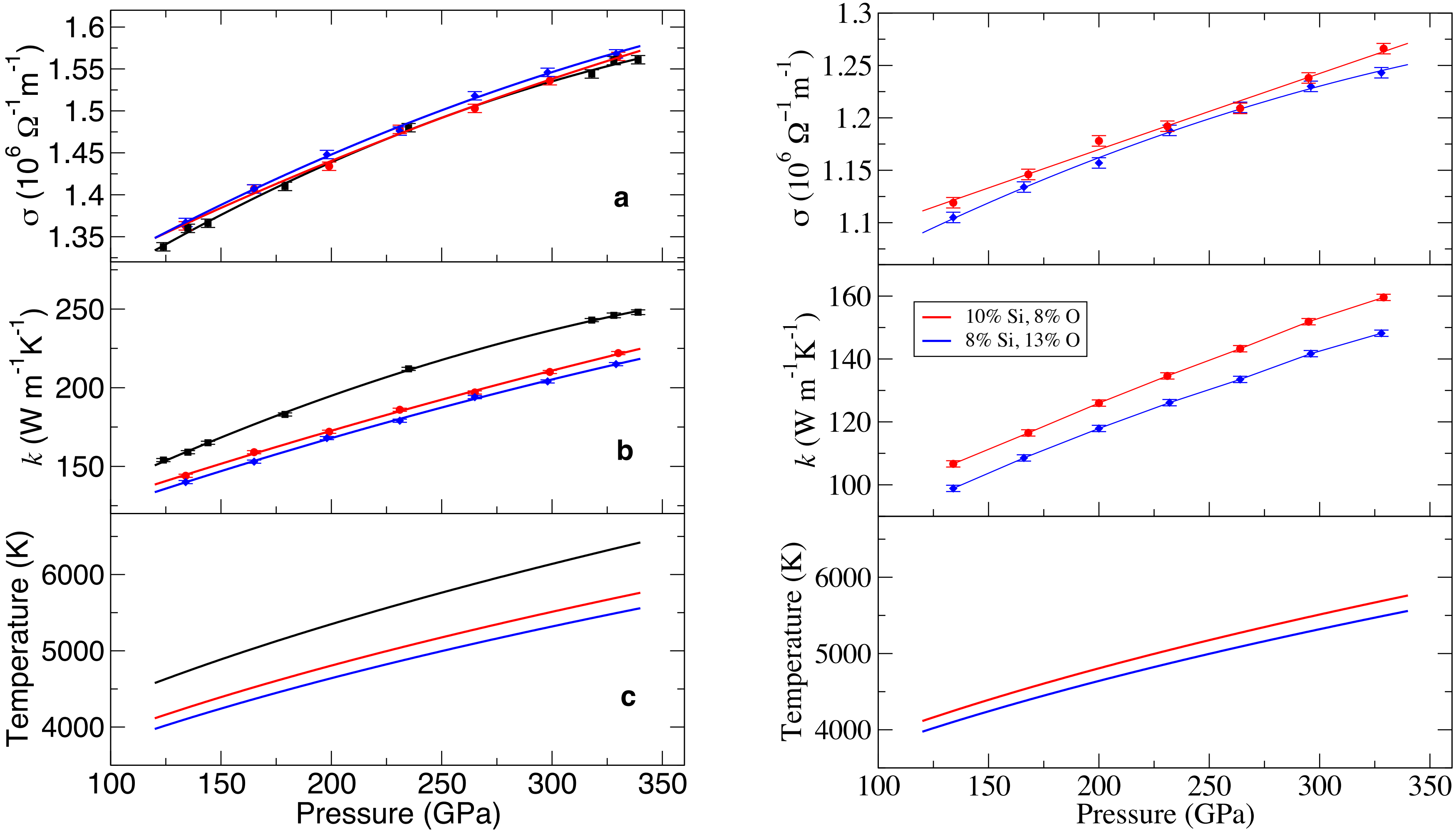
$$k = \lim_{\omega \to 0} \left\langle k(\omega, R_I) \right\rangle = \lim_{\omega \to 0} \left\langle \frac{1}{e^2 T} \left(L_{22}(\omega, R_I) - \frac{L_{12}^2(\omega, R_I)}{\sigma(\omega, R_I)} \right) \right\rangle$$

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

- Ionic component:

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

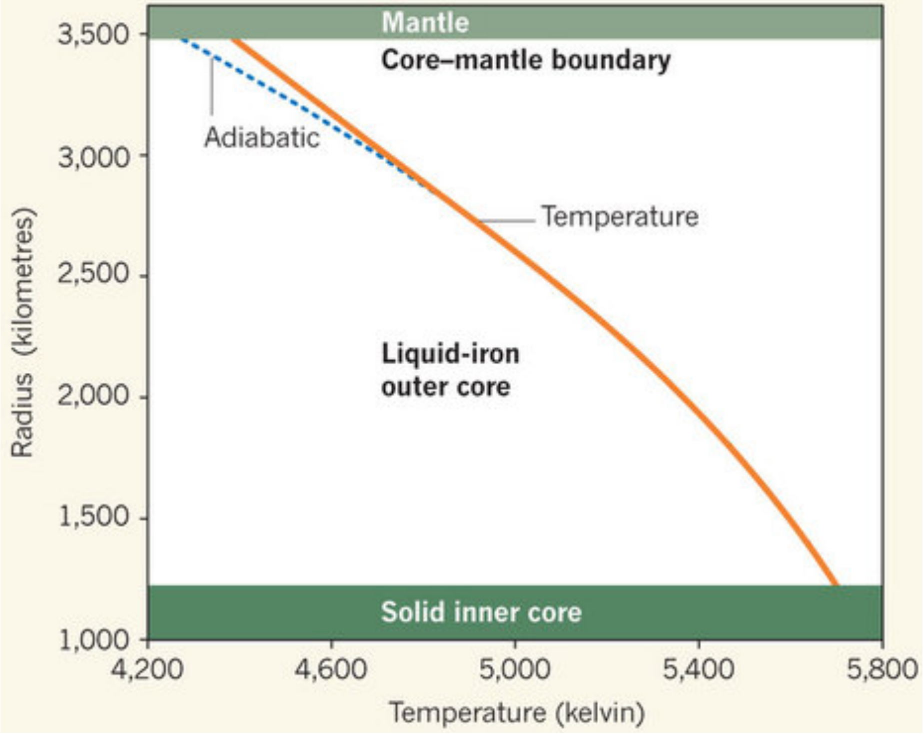
Iron at Earth's core conditions



M. Pozzo, C. Davies, D. Gubbins, & D. Alfè, Nature **485**, 355 (2012).
See also N. de Koker, G. Steinle-Neumann, G Vicek, PNAS **109**, 4070 (2012)

Conclusions

- Conductivities are 2-3 times higher than previous estimates
- Power for the geodynamo is greatly reduced
- The top of the core is probably thermally stratified



B. Buffet, News & Views, Nature **485**, 319 (2012).

- Young inner core, rapid secular cooling and/or radiogenic heating

The New York Times

Science

WORLD | U.S. | N.Y. / REGION | BUSINESS | TECHNOLOGY | SCIENCE | HEALTH | SPORTS | OPINION

ENVIRONMENT SPACE & COSMOS

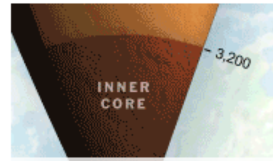
The Enigma 1,800 Miles Below Us

Sebastian Raymond/New Line Cinema

DEEP THOUGHTS Jules Verne's classic "A Journey to the Center of the Earth" has inspired several film versions, including one in 2008.

By NATALIE ANGIER
Published: May 28, 2012

Multimedia



Interactive Feature

The Structure and Movement of the Deep Earth

RSS Feed

RSS Get Science News From The New York Times »

Enlarge This Image

A diagram of the Earth's center as a giant ball of fire from the 1678 book "Subterranean World."

Enlarge This Image

20th Century Fox

A poster for the 1959 film version of the Jules Verne classic.

Geologists have long known that Earth's core, some 1,800 miles beneath our feet, is a dense, chemically doped ball of iron roughly the size of Mars and every bit as alien. It's a place where pressures bear down with the weight of 3.5 million atmospheres, like 3.5 million skies falling at once on your head, and where temperatures reach 10,000 degrees Fahrenheit — as hot as the surface of the Sun. It's a place where the term "ironclad agreement" has no meaning, since iron can't even agree with itself on what form to take. It's a fluid, it's a solid, it's twisting and spiraling like liquid confetti.

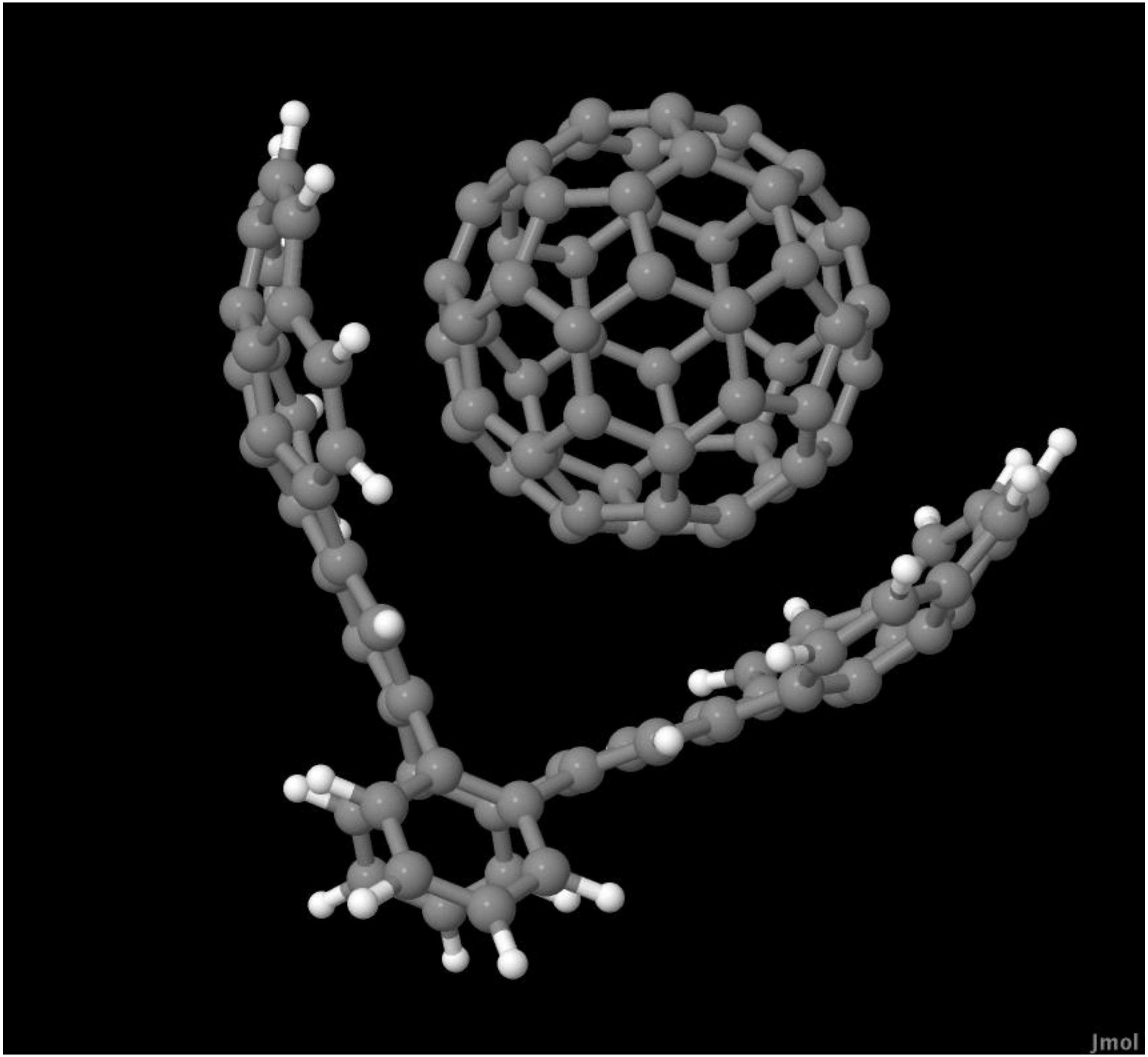
Researchers have also known that Earth's inner Martian makes its outer portions look and feel like home. The core's heat helps animate the giant jigsaw puzzle of tectonic plates floating far above it, to build up mountains and gouge out seabeds. At the same time, the jostling of core iron generates Earth' magnetic field, which blocks dangerous cosmic radiation, guides terrestrial wanderers and brightens northern skies with scarves of auroral lights.

Now it turns out that existing models of the core, for all their drama, may not be dramatic enough. Reporting recently in the journal Nature, Dario Alfè of University College London and his colleagues presented evidence that iron in the outer layers of the core is frittering away heat through the wasteful process called conduction at two to three times the rate of previous estimates.

The theoretical consequences of this discrepancy are far-reaching. The scientists say something else must be going on in Earth's depths to account for the missing thermal energy in their calculations. They and others offer these possibilities:

¶ The core holds a much bigger stash of radioactive material than anyone had suspected, and its decay is giving off heat.

¶ The iron of the innermost core is solidifying at a startlingly fast clip and releasing the latent heat of crystallization in the process.


Jmol