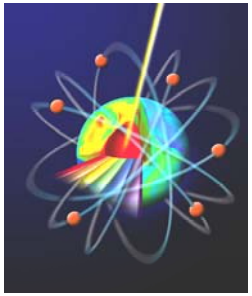

Synchrotrons: a core business ?

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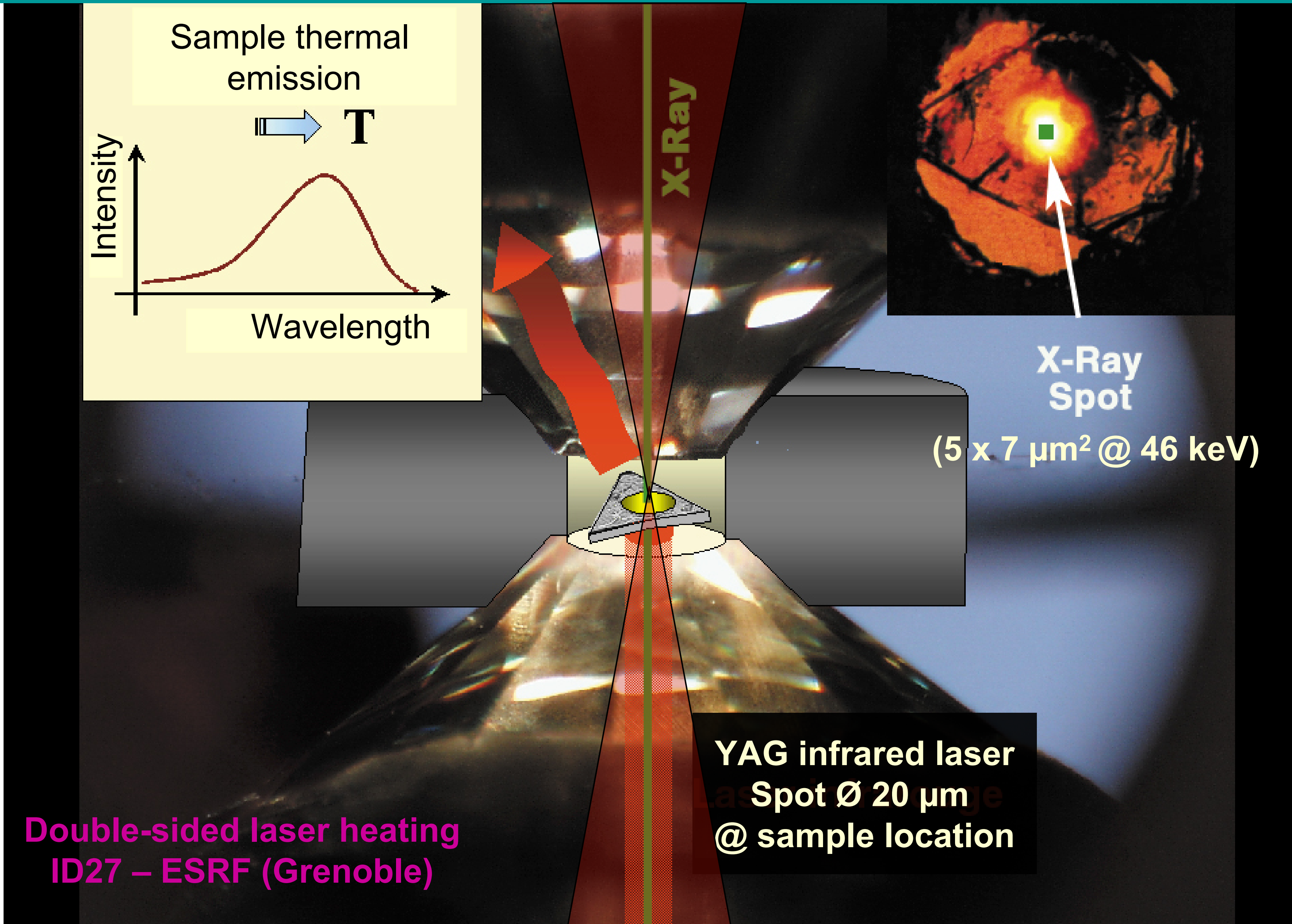
75015 Paris

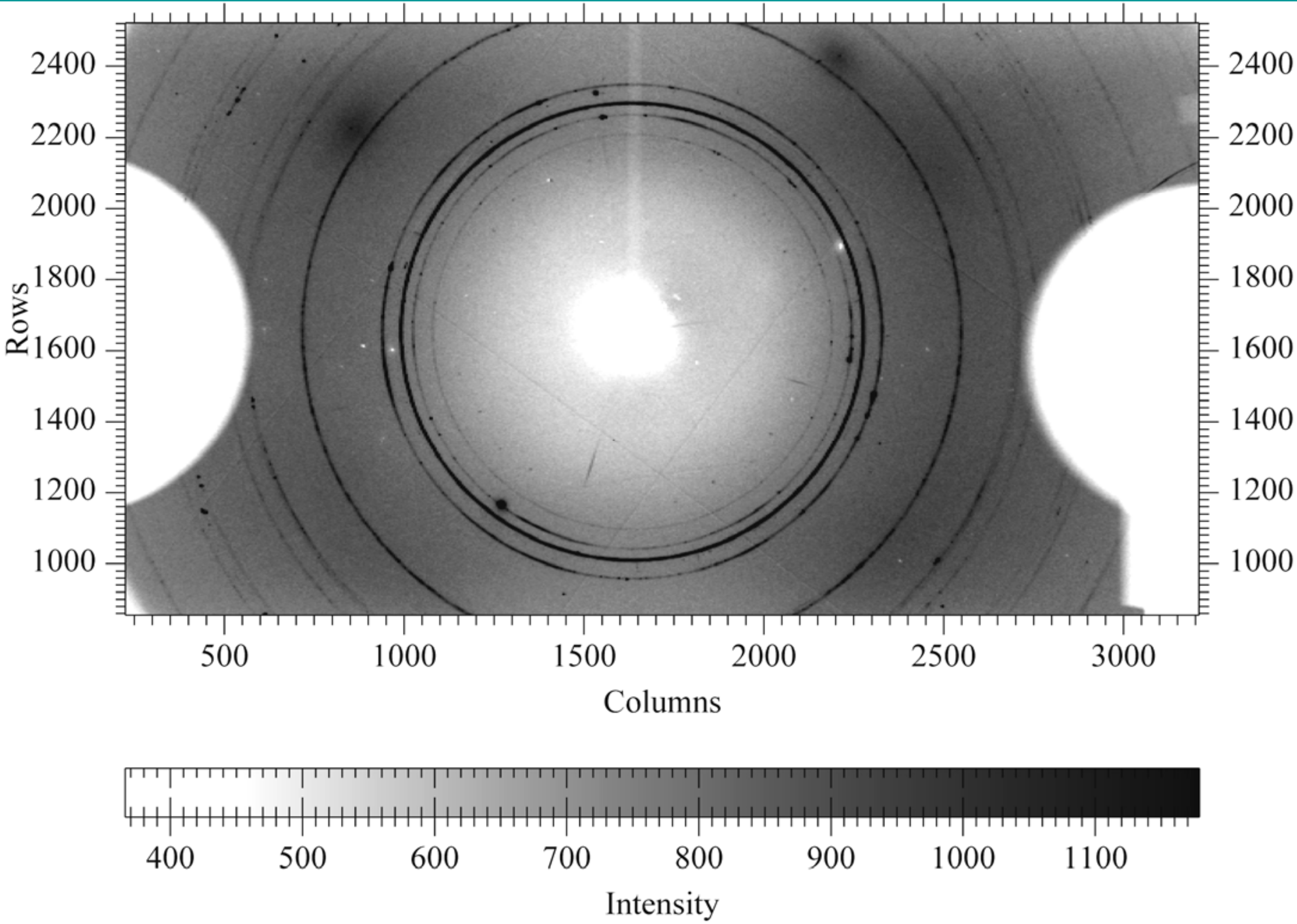
OUTLINE

- Phase diagram (iron structure)
- c/a ratio @ HP / HT (elastic anisotropy)
- Thermal equation of state
- Fe_3C high-pressure acoustic properties and inner core carbon content

In situ X-ray diffraction ID27 @ ESRF



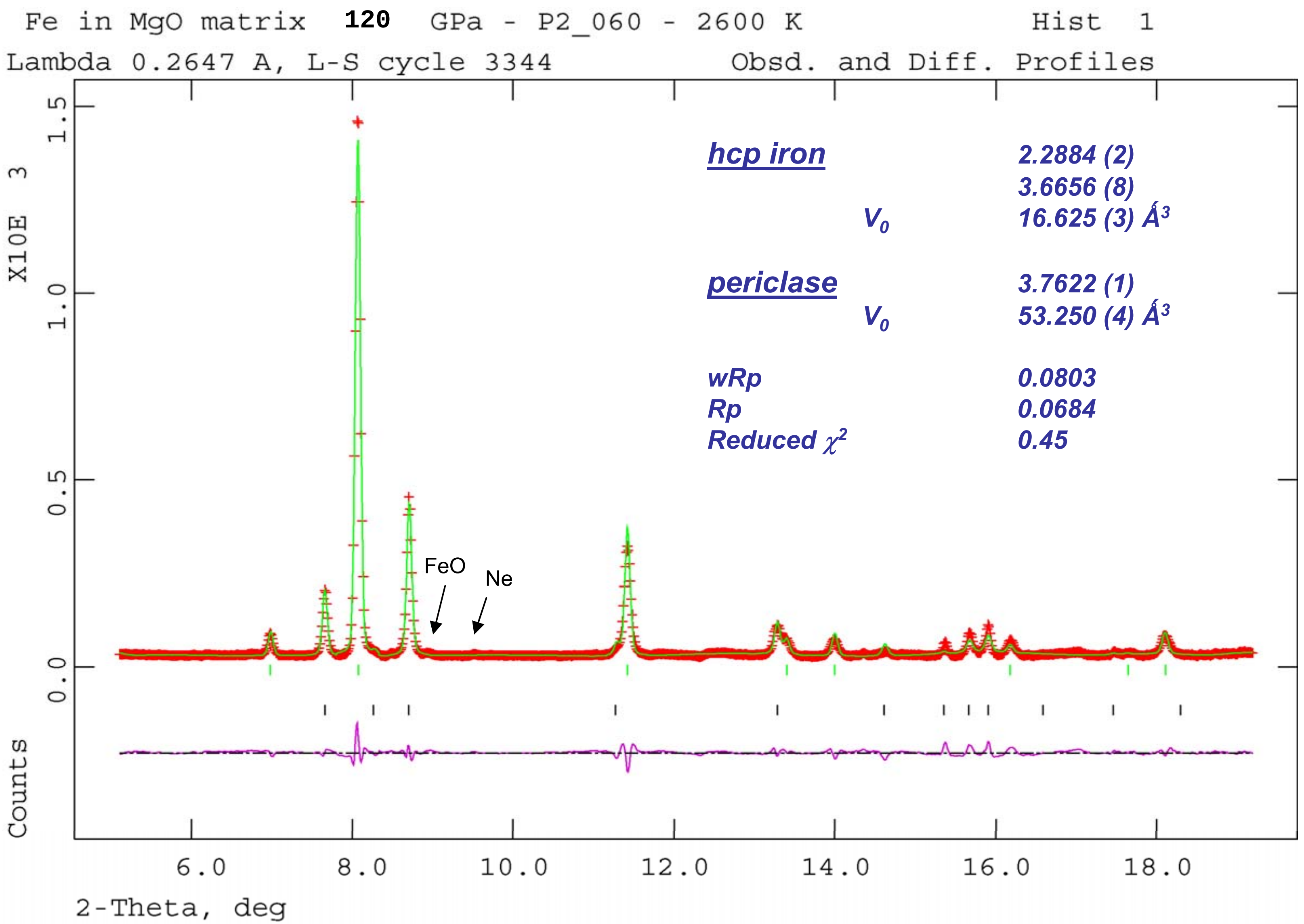
In situ X-ray diffraction



-Hot pressed sample MgO + iron
(800° C / 24 h / 15 kbar in MgO capsule / graphite furnace)
- Neon pressure transmitting medium
- 120 GPa – 3300 K

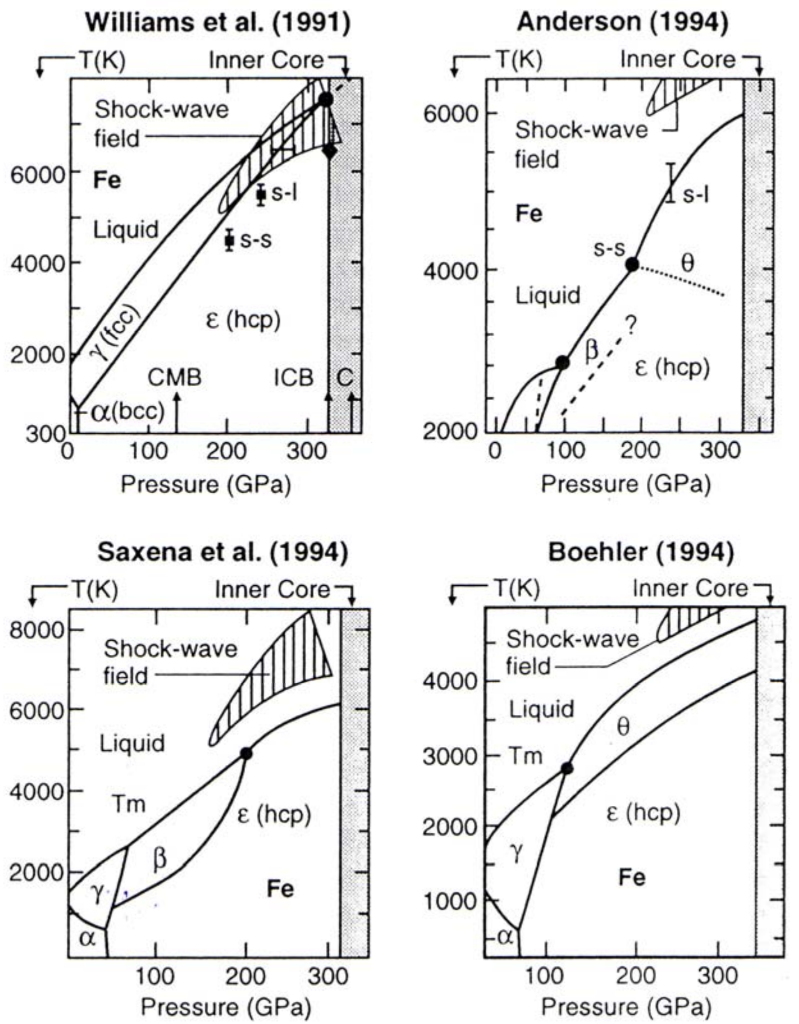
ID27 @ ESRF

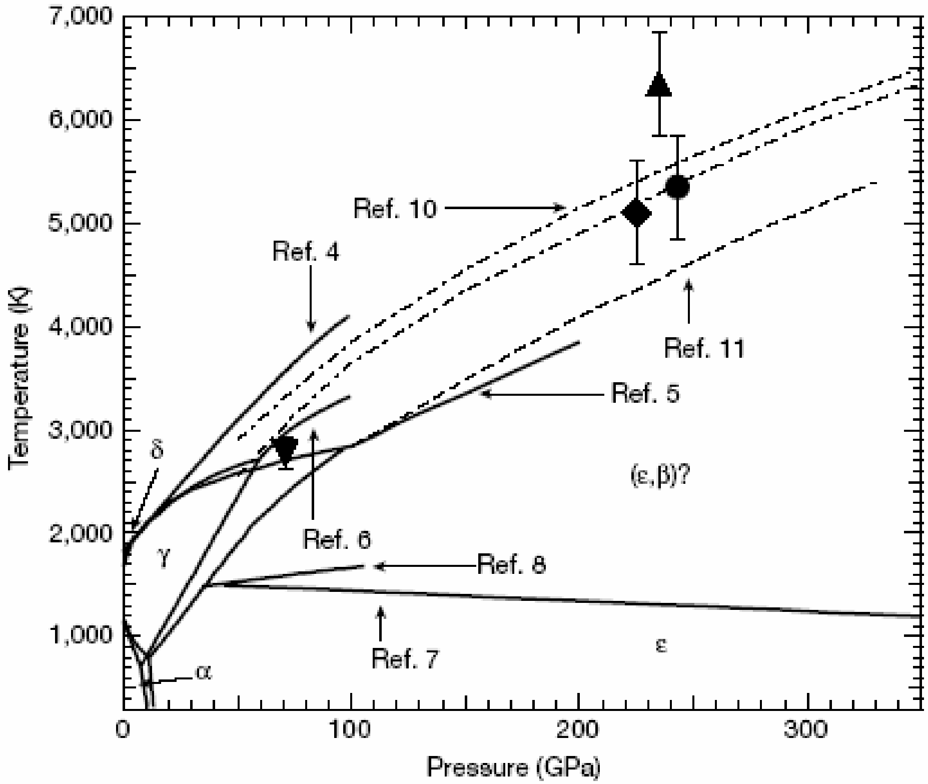
In situ X-ray diffraction



→ hcp iron …

Phase diagram

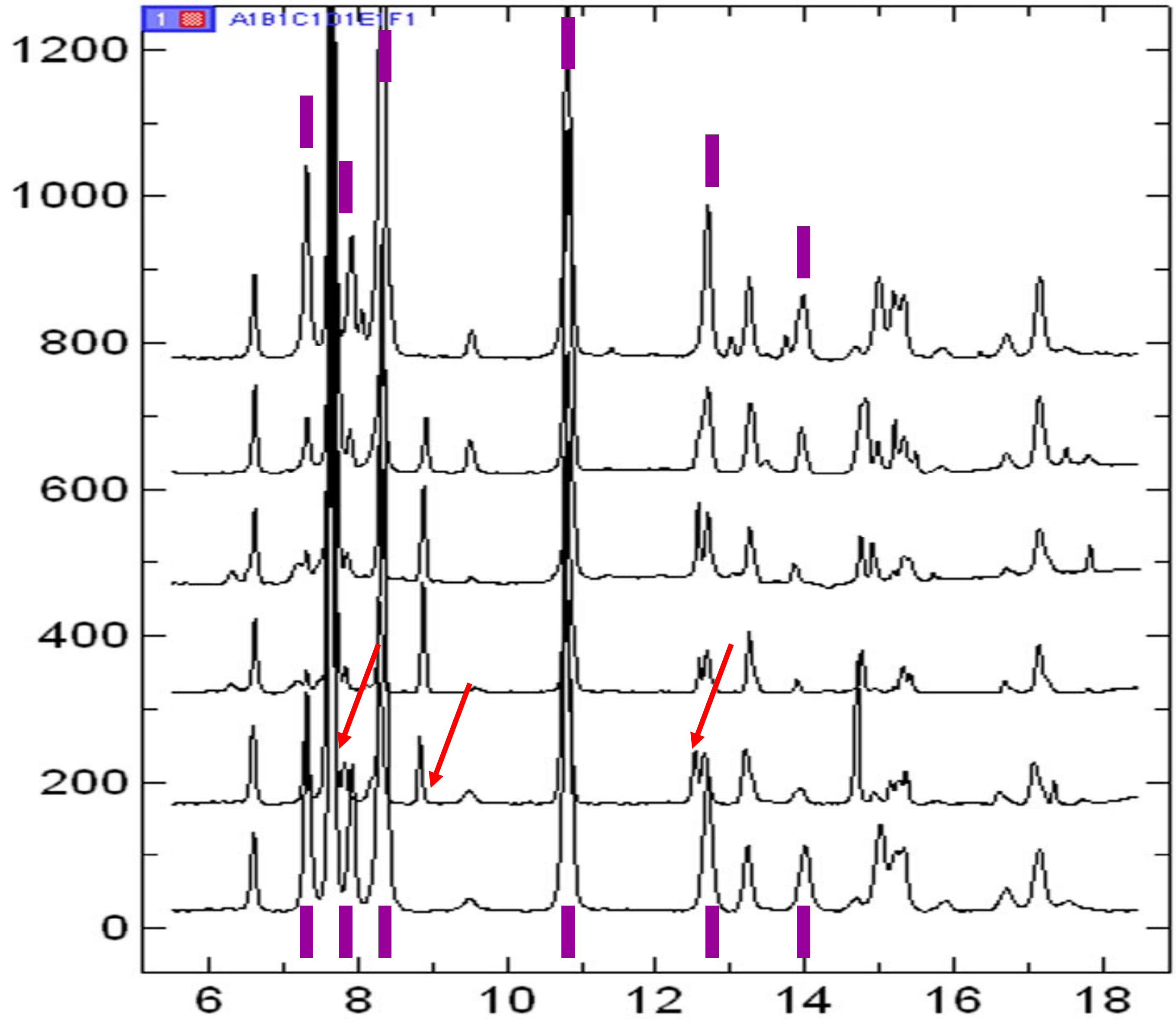




Nguyen J.H. and Holmes N.C., *Nature*, 427, 339, 2004.

Anderson O.L., *Reviews of Geophysics*, Suppl., U.S. National Report to International Union of Geodesy and Geophysics, 429, 1995.

In situ X-ray diffraction



(ε) hcp – (γ) fcc phase transition

P= 40.1 GPa - RT

P= 50 GPa – 1710 K

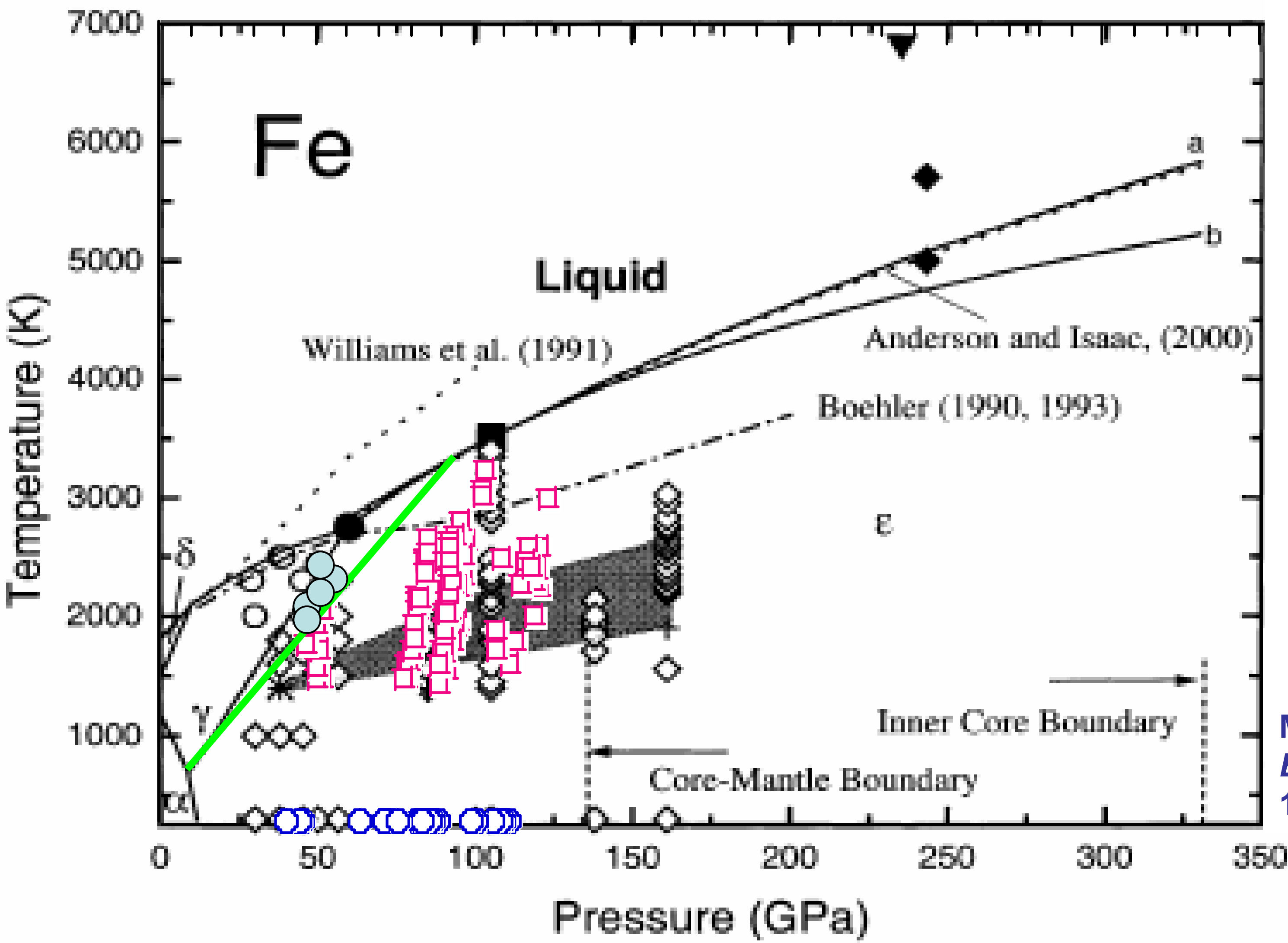
P= 52.5 GPa – 2170 K

P= 50.2 GPa – 1950 K

P= 46.7 GPa – 1790 K

P= 40.4 GPa - RT

Phase diagram



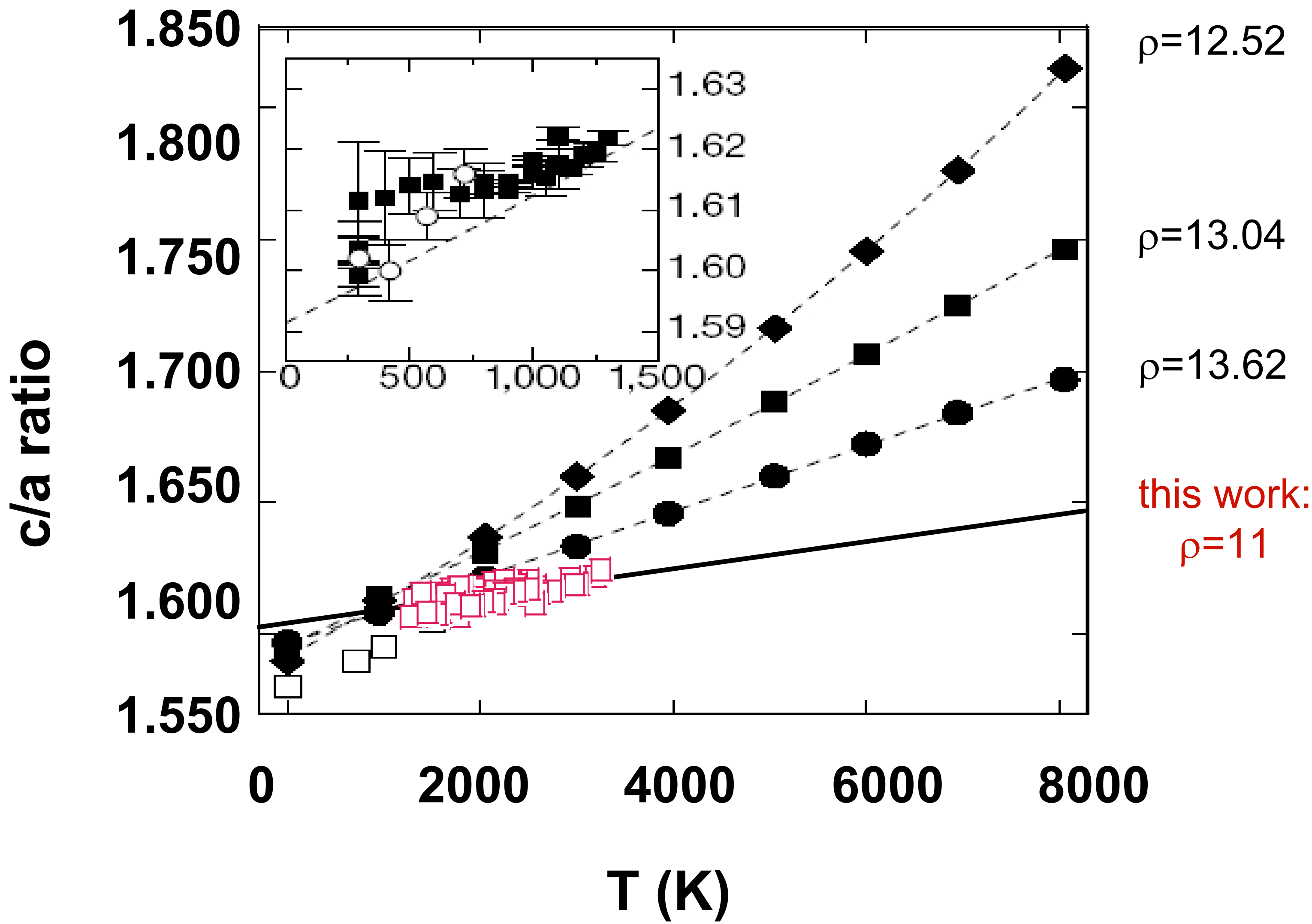
Ma Y. et al., *Phys. Earth Planet. Int.*, 143-144, 455, 2004.

→ triple point hcp-fcc-liquid iron @ 95 GPa, 3300 K

→ no β-phase (Pbcm, dhcp…)

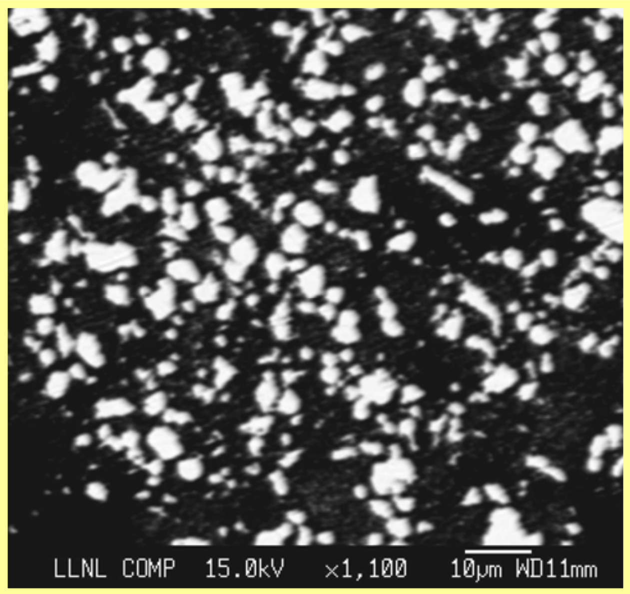
→ melting line above 3350 K @ 100 GPa

c/a ratio



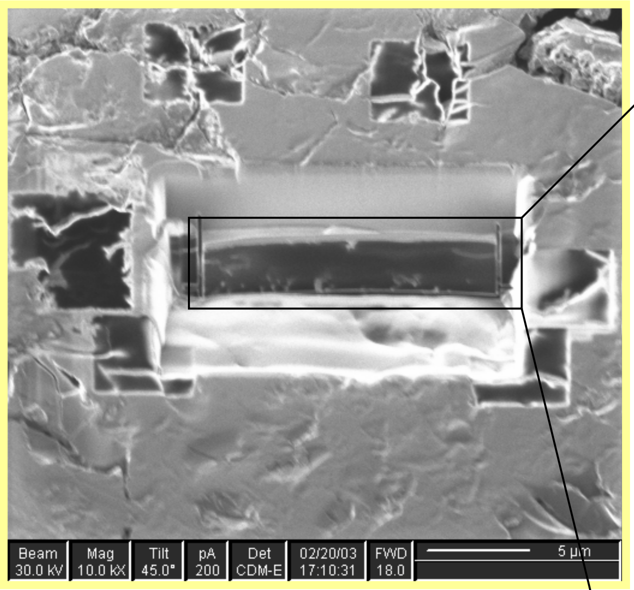
Steinle Neumann et al., *Nature*, 413, 57, 2001.

Recovered sample – FIB preparation

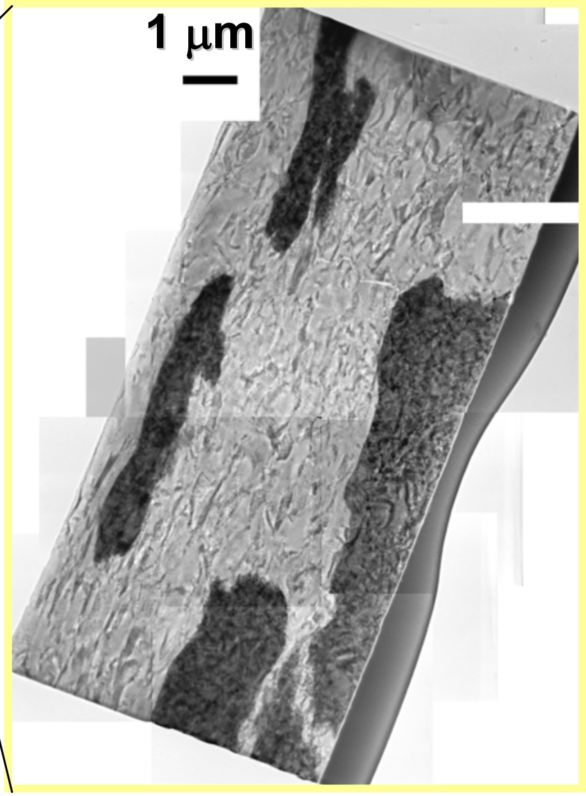


Hot pressed sample:
MgO + iron – low fO_2

High-pressure high-temperature experiments



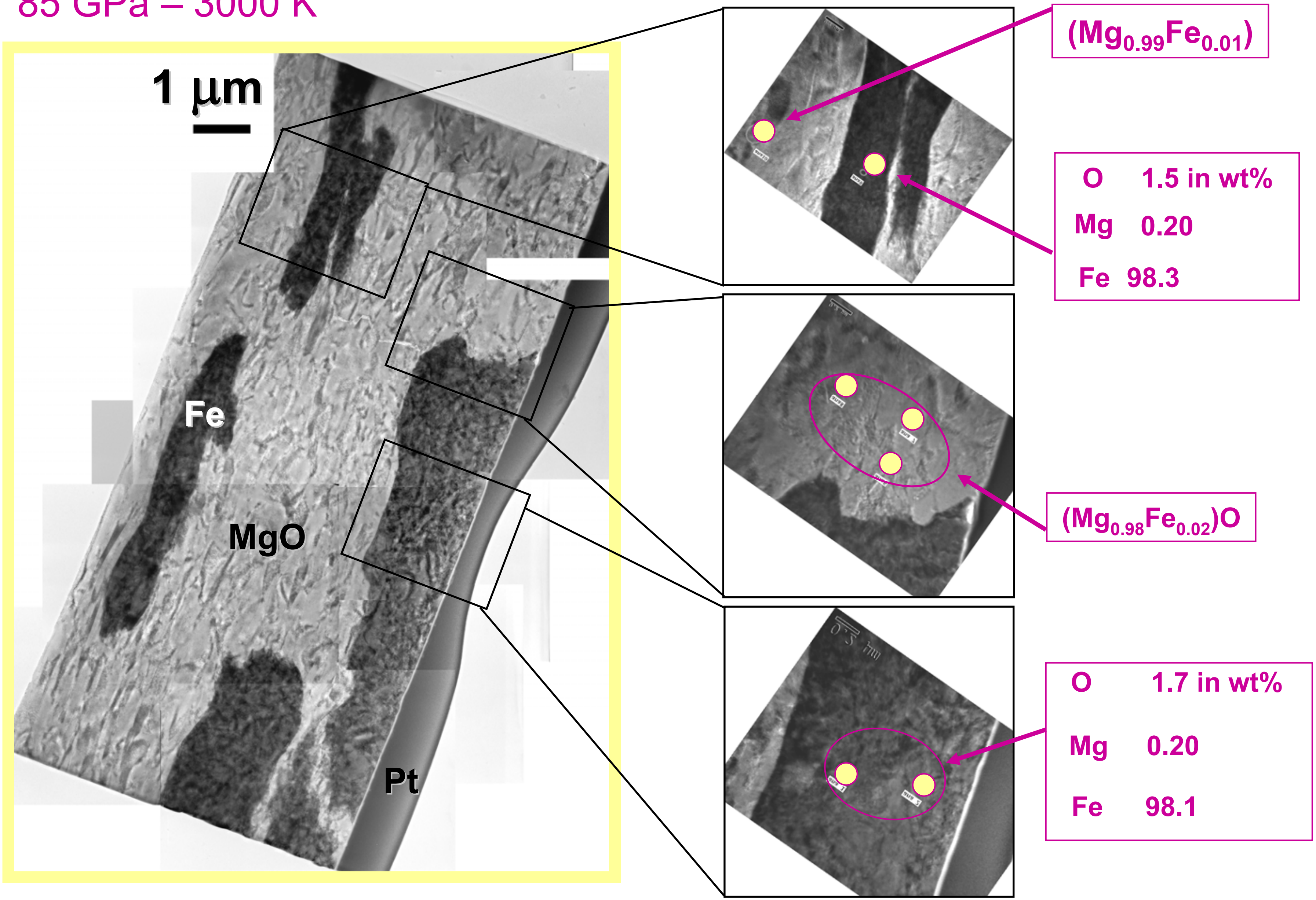
FIB preparation



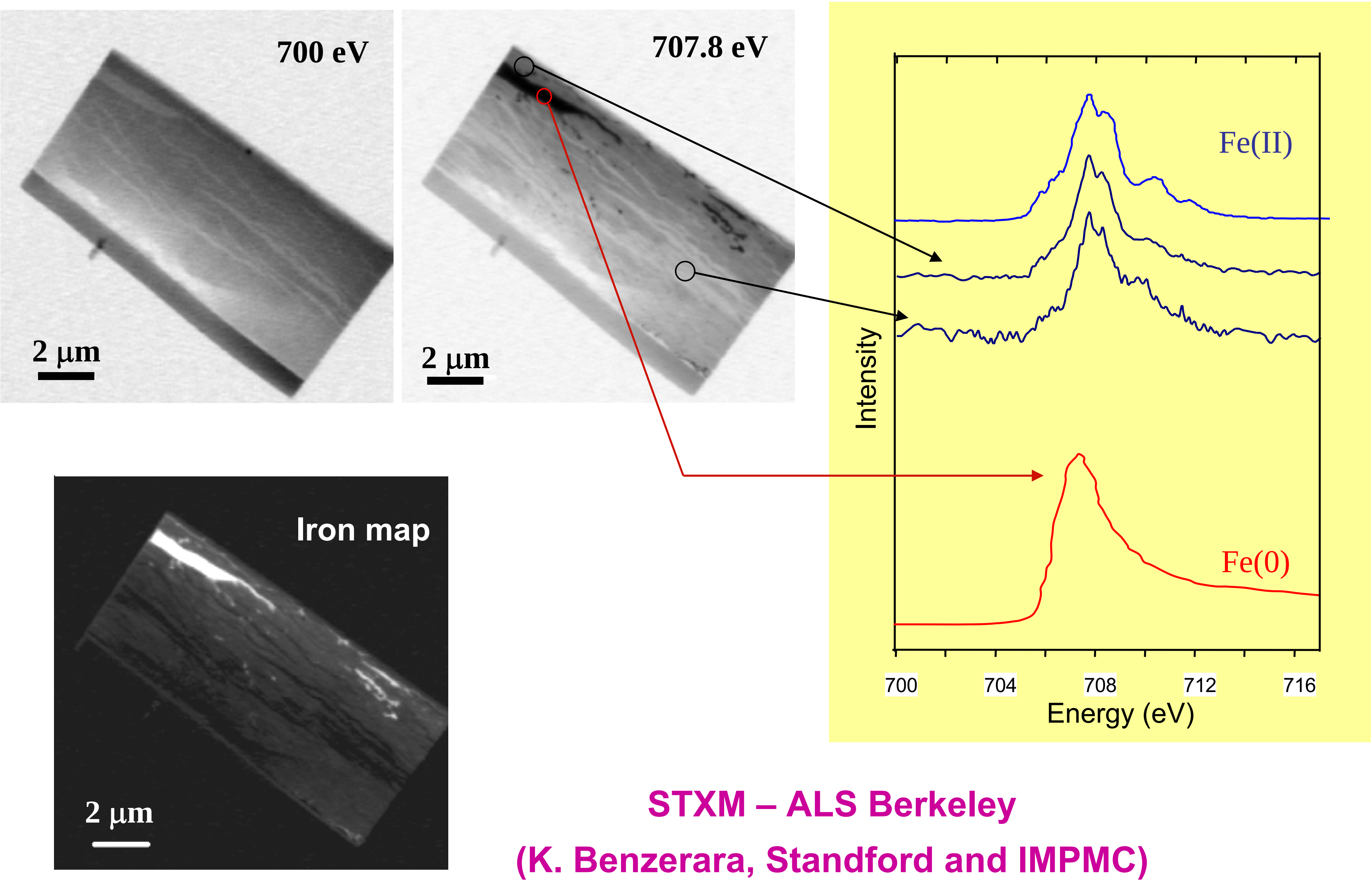
TEM – STXM ready

Recovered sample – FIB preparation – ATEM analysis

85 GPa – 3000 K



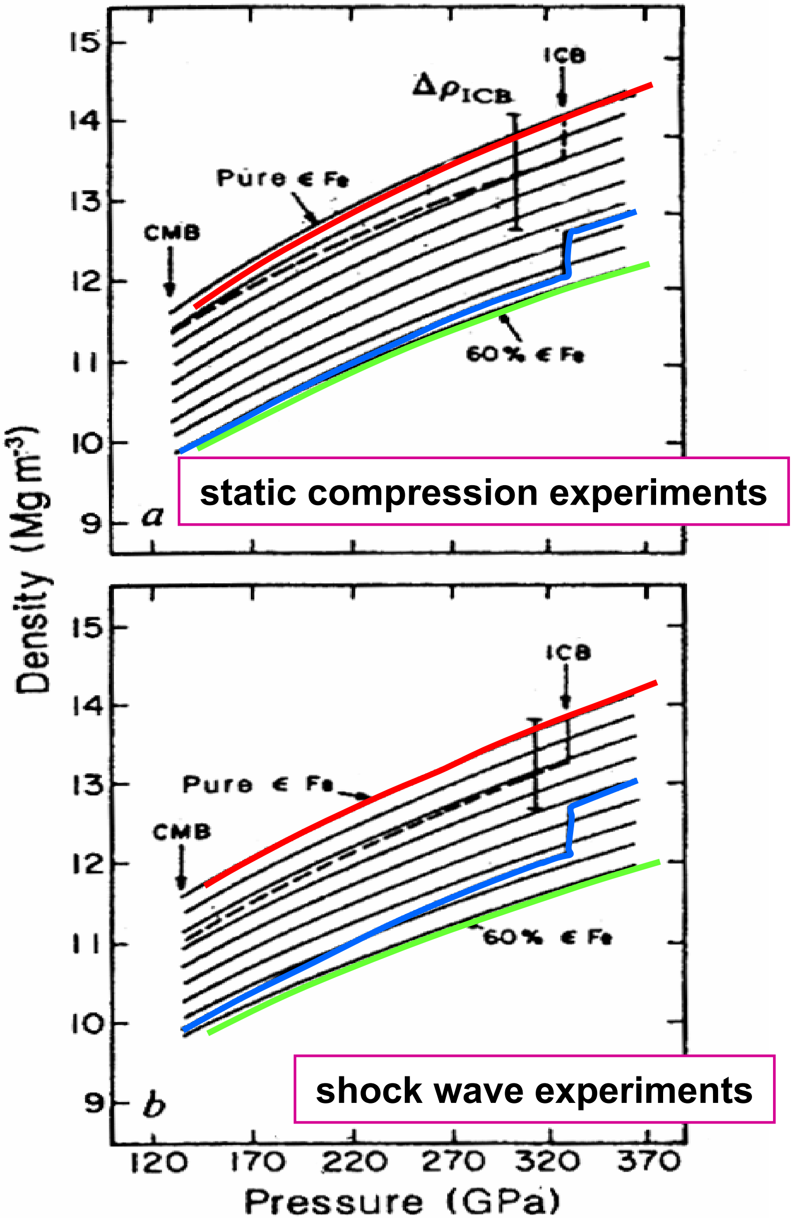
Recovered sample – FIB preparation – STXM study

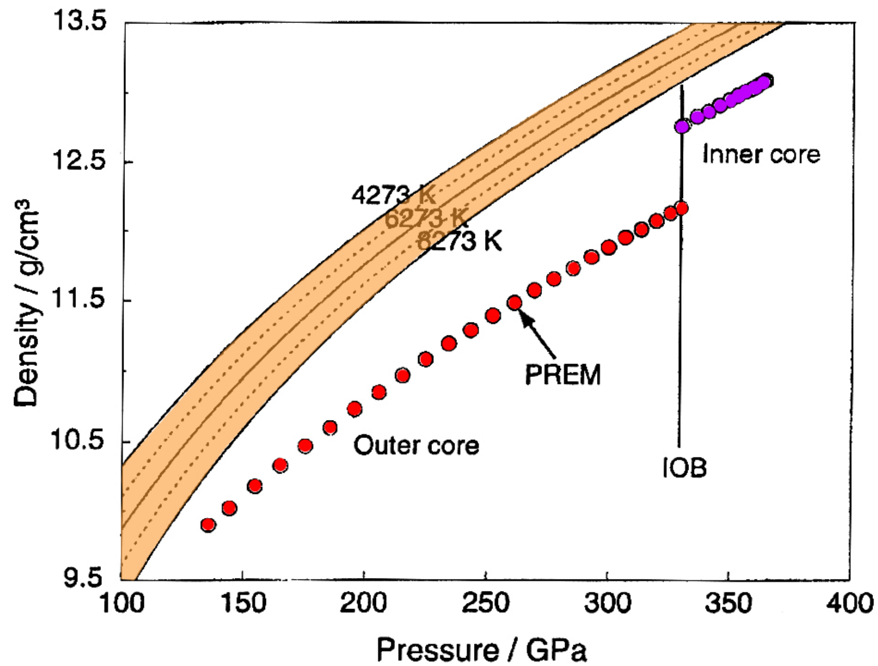


STXM – ALS Berkeley

(K. Benzerara, Standford and IMPMC)

Equation of state





Uchida et al., *J. Geophys. Res.*, 106 21799, 2001.

After Jephcoat and Olson, *Nature*, 325 332, 1987.

Equation of state

- 15 data points room-temperature in helium
  Pressure range: 14 – 30 GPa (this work)

- 37 data points room-temperature in helium
  Pressure range: 18 -198 GPa **Dewaele et al. Phys. Rev. Lett., 2006**

- 87 data points HP-HT laser heating in neon
  Pressure range: 47 -120 GPa
  Temperature range: 1500 - 3300 K (this work)

- Temperature : black body thermal emission
  Pressure scale: MgO **Speziale et al. J. Geophys. Res., 2001**

Equation of state

- Third order Birch-Murnaghan equation of state (static EoS)

$$\frac{P}{K_T(P_0,T_0)} = \frac{3}{2}x^{5/3}\left[x^{2/3}-1\right]\times\left\{1-\frac{3}{4}(4-K_0')\left[x^{2/3}-1\right]\right\}$$

- Mie-Grüneisen thermal Eos

$$P_{th}(V,T) = \frac{3n\gamma RT}{V}D(x) \quad \text{with} \quad D(x) = \frac{3}{x^3}\int_0^x \frac{\xi^3}{e^\xi - 1}d\xi$$

- Quasi-harmonic approximation (Debye temperature and Grüneisen parameter function of volume only)

$$\Theta_D(V) = \Theta_{D_0}(V_0)\exp\left(\frac{\gamma_0-\gamma}{q_0}\right), \quad \gamma(V) = \gamma_0(V_0)\left(\frac{V}{V_0}\right)^{q_0}$$

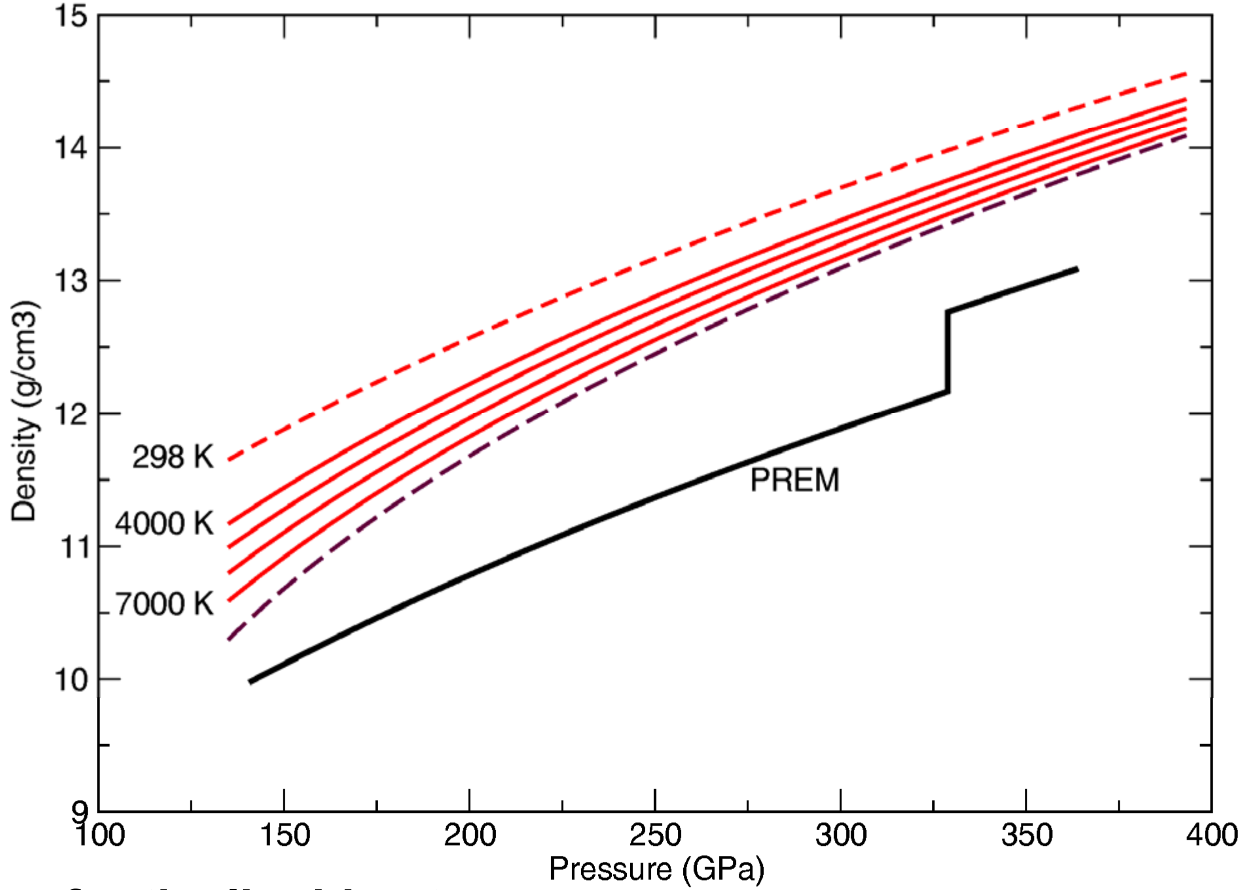
- Anharmonic and electronic contribution to thermal pressure

$$P_{\mathrm{TH}}(V,T) = \frac{9R\gamma}{V}\left(\frac{\theta}{8}+T\left(\frac{T}{\theta}\right)^3\int_0^{\theta/T}\frac{z^3dz}{e^z-1}\right) + \frac{3R}{2V}ma_0x^mT^2 + \frac{3R}{2V}ge_0x^gT^2$$

Dewaele et al., *Phys. Rev. Lett.*, 97, 215504, 2006

Equation of state

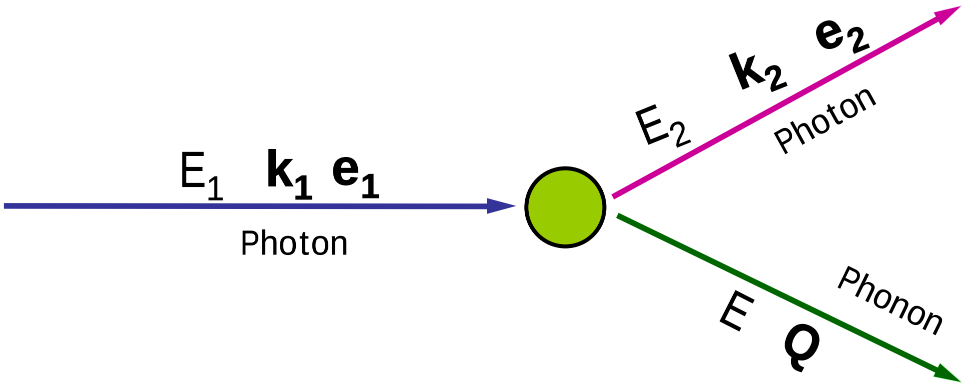
V_0	22.420	0.053
K_0	166.8	5.5
K'_0	4.98	0.14
Θ_D	1023	375
γ	2.50	0.36
q	2.28	0.45



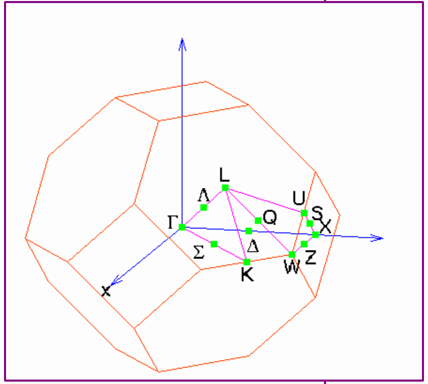
- 11% density difference for the liquid outer core
- 6 % for the solid inner core

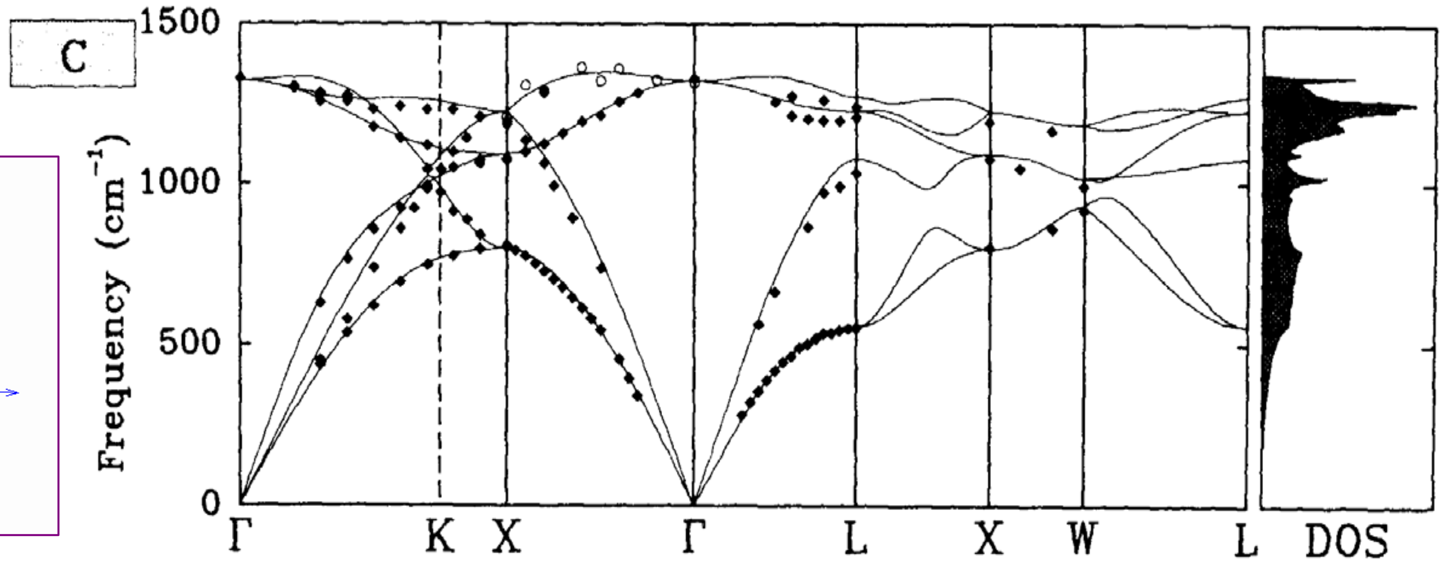
→ light elements in the inner core …

High-resolution inelastic X-ray scattering ID28 @ ESRF

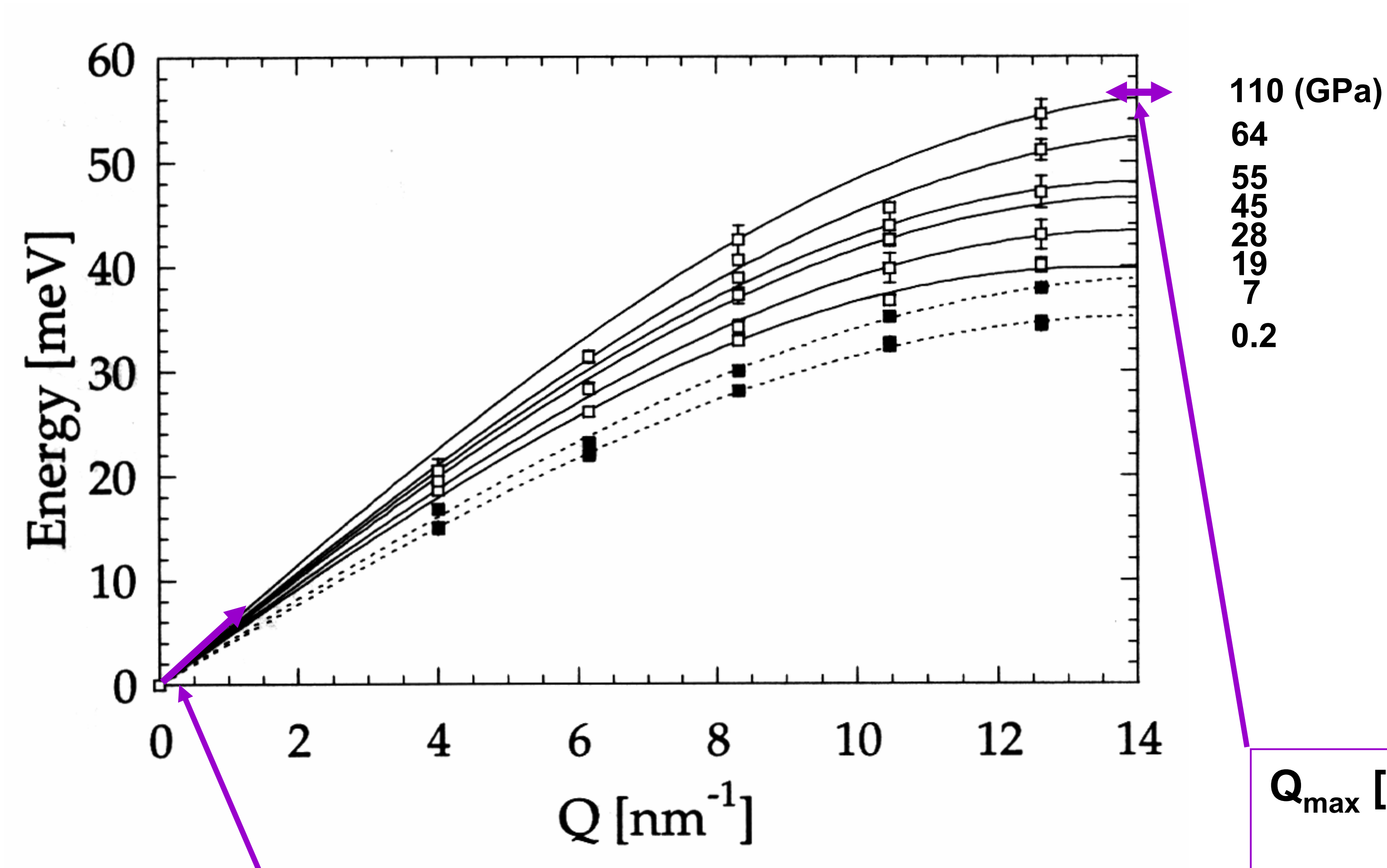


• Energy transfer:	$E_1 - E_2 = E$	(1 – 200 meV)
• Momentum transfer:	$k_1 - k_2 = Q$	(1 – 100 nm^{-1})





Polycrystalline sample: average dispersion curve

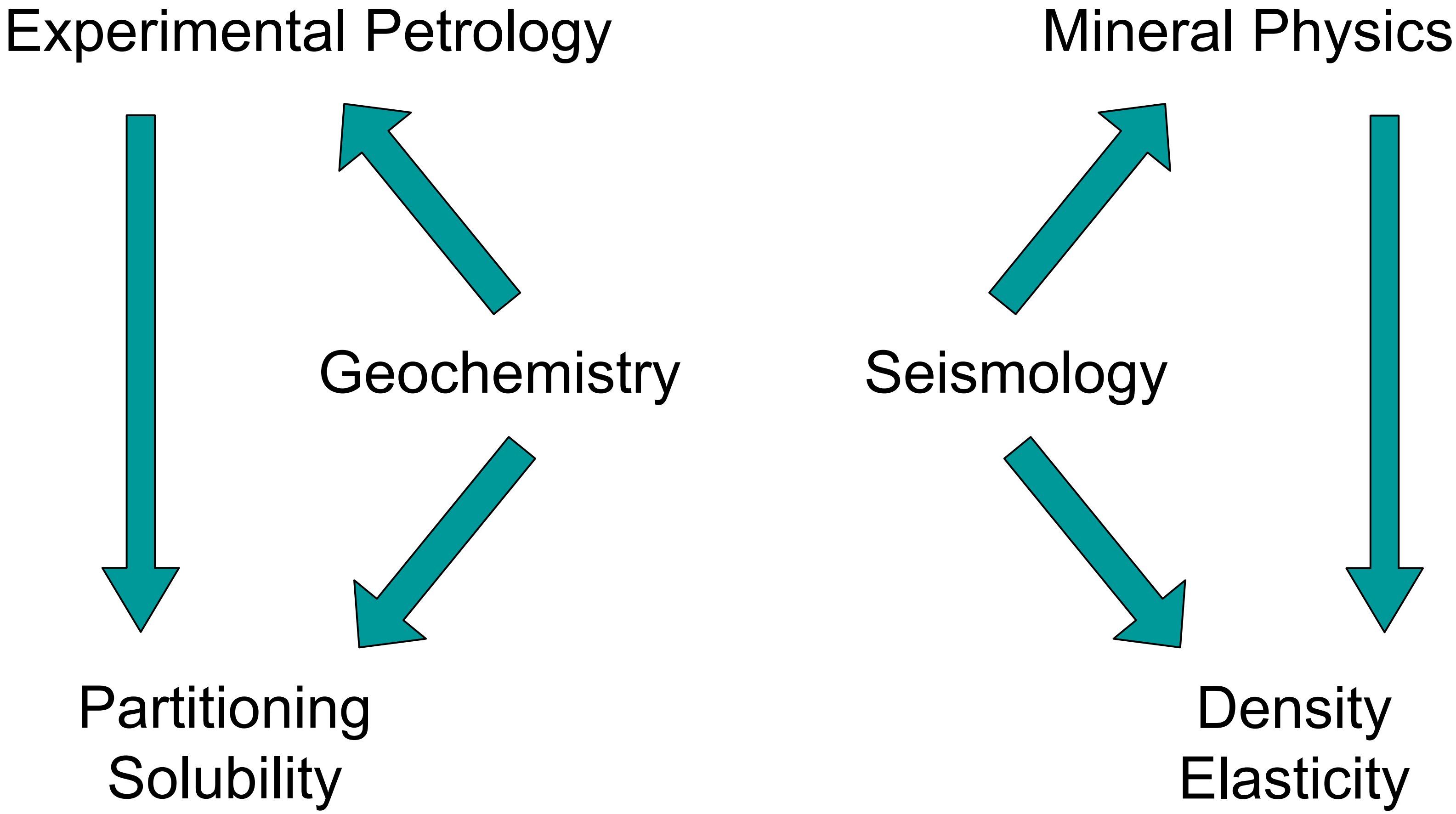


Q_{max} [nm^{-1}]

V_P=0
E max

V_P [ms^{-1}] – slope at Q=0

What light elements ?



What light elements ?

Major element: Fe

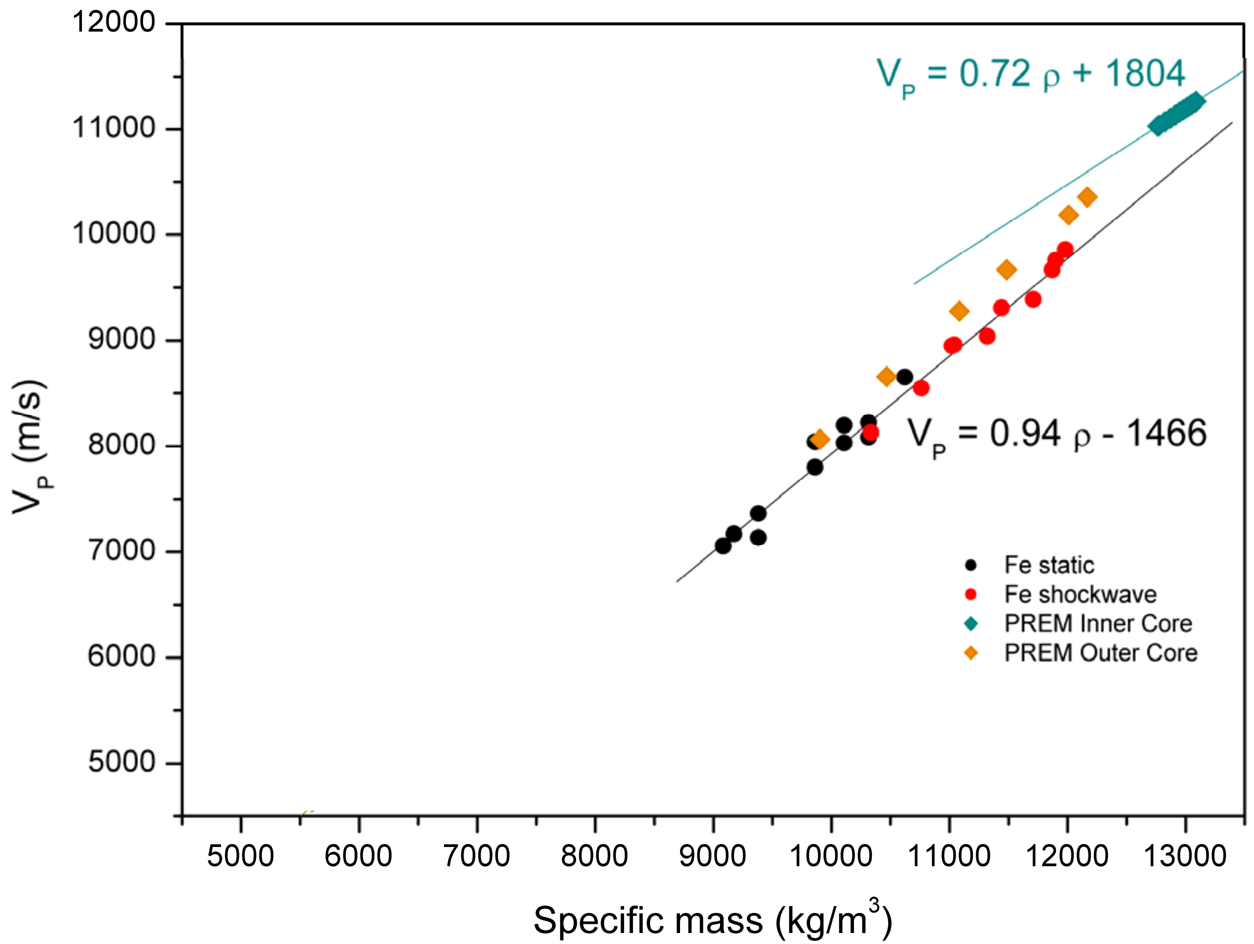
Minor elements: **FeO, $FeSi$, FeS, FeS_2, Fe_3C**

Diamond anvil cell up to 112 GPa

High-resolution inelastic x-ray scattering

IXS beamline ID28 at the ESRF

Sound velocities in the core



Badro et al., *EPSL*, 254, 1-2, 233, 2007

Composite model

$$\rho = (1 - x)\rho_{Fe} + x\rho_{le} = \rho_{seismic}$$

$$V = \frac{V_{Fe} \cdot V_{le}}{(1 - x)V_{le} + xV_{Fe}} = V_{seismic}$$

$$V_{Fe} = a_{Fe}\rho_{Fe} + b_{Fe}$$

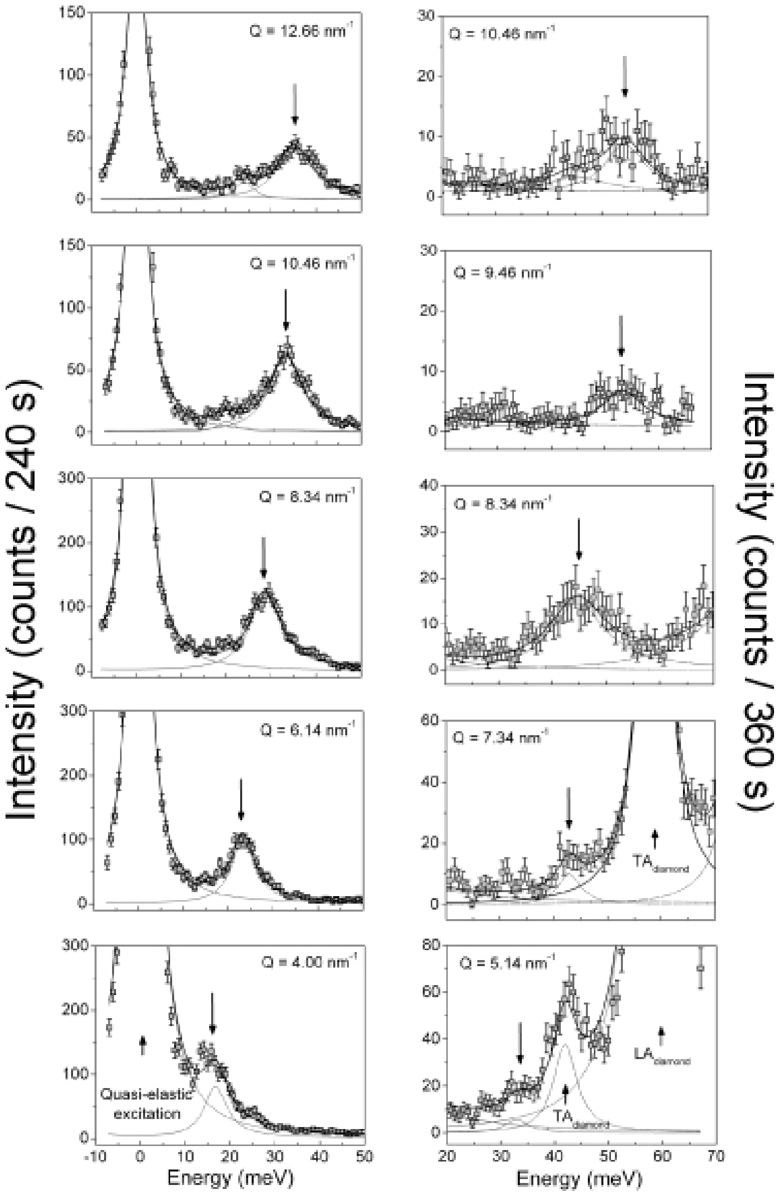
$$V_{le} = a_{le}\rho_{le} + b_{le}$$

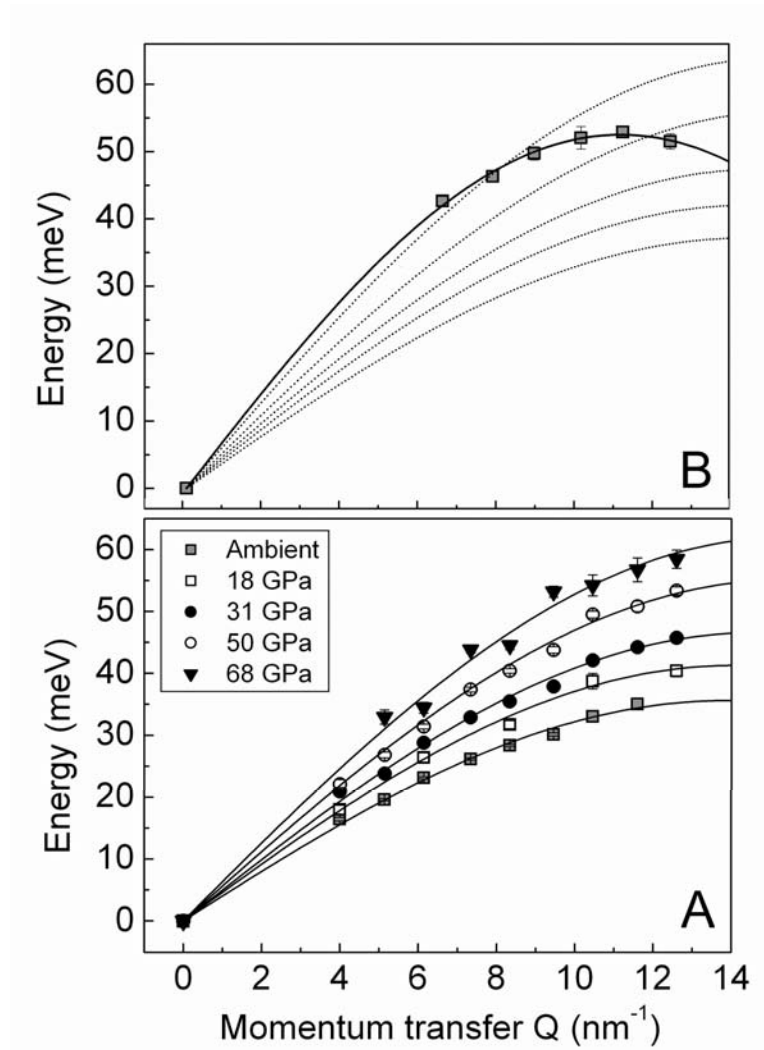
Composition of the core

Element	Fraction (wt%)	Compression (ρ/ρ_0)	Model Inner Core (wt%)	Model Outer Core (wt%)
Si	2.3	1.28	2.3	2.8
O	1.6	1.33	minor	5.3
S^{2-}	9.7	2.51	minor	minor
S^{-}	3.6	1.05	minor	minor

Badro et al., *EPSL*, 254, 1-2, 233, 2007

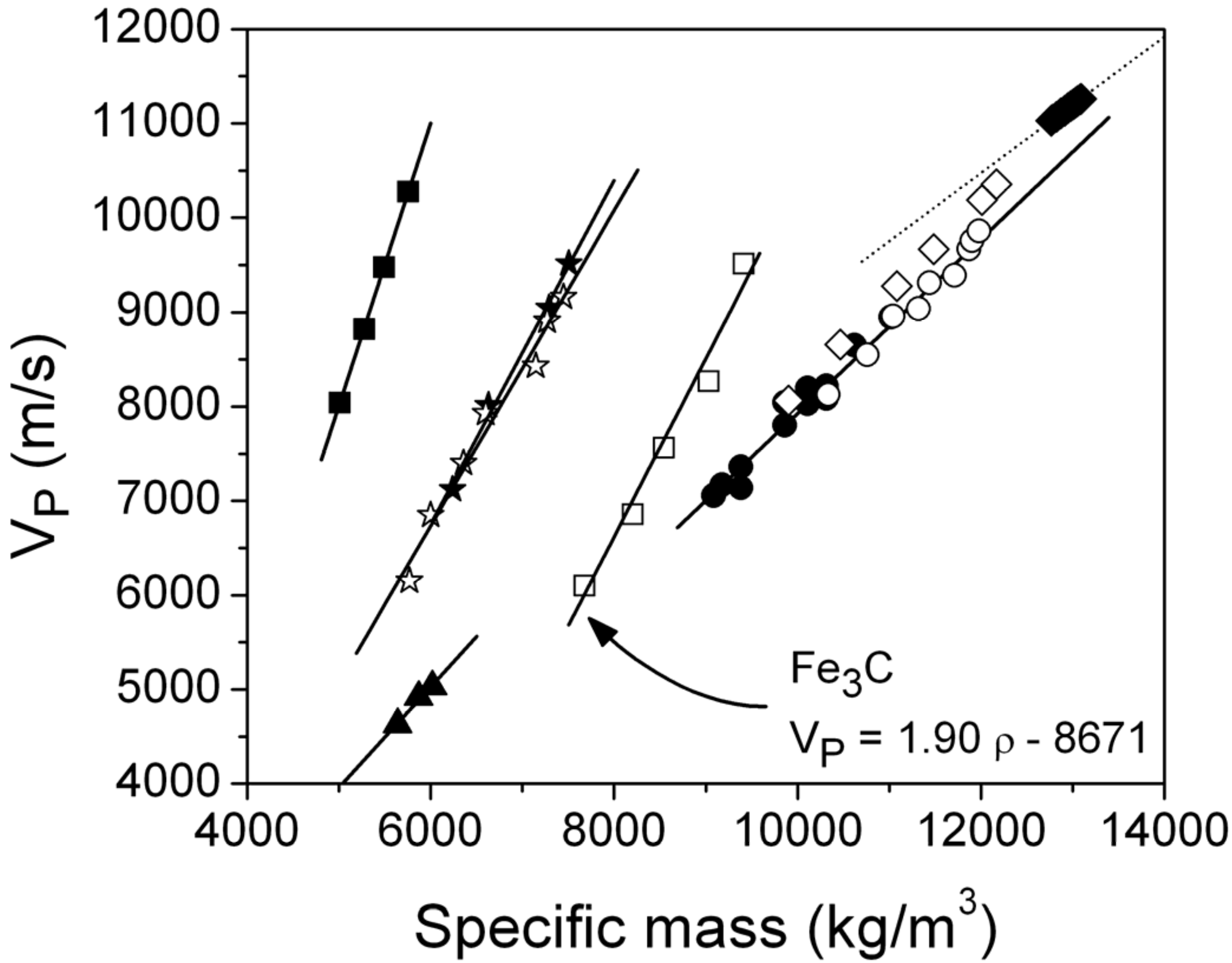
Sound velocity in Fe_3C





Fiquet et al., *Phys. Earth Planet. Int.*, submitted

Sound velocity in Fe_3C



Fiquet et al., *Phys. Earth Planet. Int.*, submitted

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O	1.6	1.33	minor	5.3
S^{2-}	9.7	2.51	minor	minor
S^{-}	3.6	1.05	minor	minor
C	1.0	1.40	1.0	—

4.9 % nickel – 7.3 % silicon – 4.1% oxygen – 2.3 % sulfur (Allègre et al., 1995)

5.6 % nickel – 9.6 % silicon – 1.9 % oxygen – 2.2 % sulfur (Javoy, 1999)

W.F. McDonough, S.S. Sun, Chem. Geol. 120, 223–253, 1995.

G. Dreibus, H. Palme, Geochim. Cosmochim. Acta 60, 1125–1130, 1996.

< 2 wt% S

SUMMARY

- *Phase diagram (iron structure)*

- fcc – hcp – liquid triple point @ 95 GPa / 3300 K
- hcp iron at high pressure and temperature – no β phase (orthorhombic or d-hcp)
- Melting temperature above 3300 K @ 100 GPa

- *c/a ratio @ HP / HT (elastic anisotropy)*

- Reversal of anisotropy of longitudinal waves @ high P high T questionable

- *Equation of state (core composition)*

- On the way to a well constrained thermal equation of state for iron

- *Light elements in the solid inner core*

- Silicon is our best choice
- Carbon at 1 wt% level provided electronic / magnetic state stays similar as that at low pressure (1wt % much lower carbon content than that of Fe_3C)
- Provided Fe is hcp in the inner core (cf *bcc* report from Dubrovinsky et al., 2007 for a 10% nickel alloy)
- This need to be checked !

Acknowledgments

- James Badro, Anne Line Auzende, Karim Benzerara *(IMPMC / IPGP)*
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- Nicolas Guignot, Michael Krisch *(ESRF)*