Composition of the Earth's inner core from sound velocity measurements on Fe and Fe-alloys

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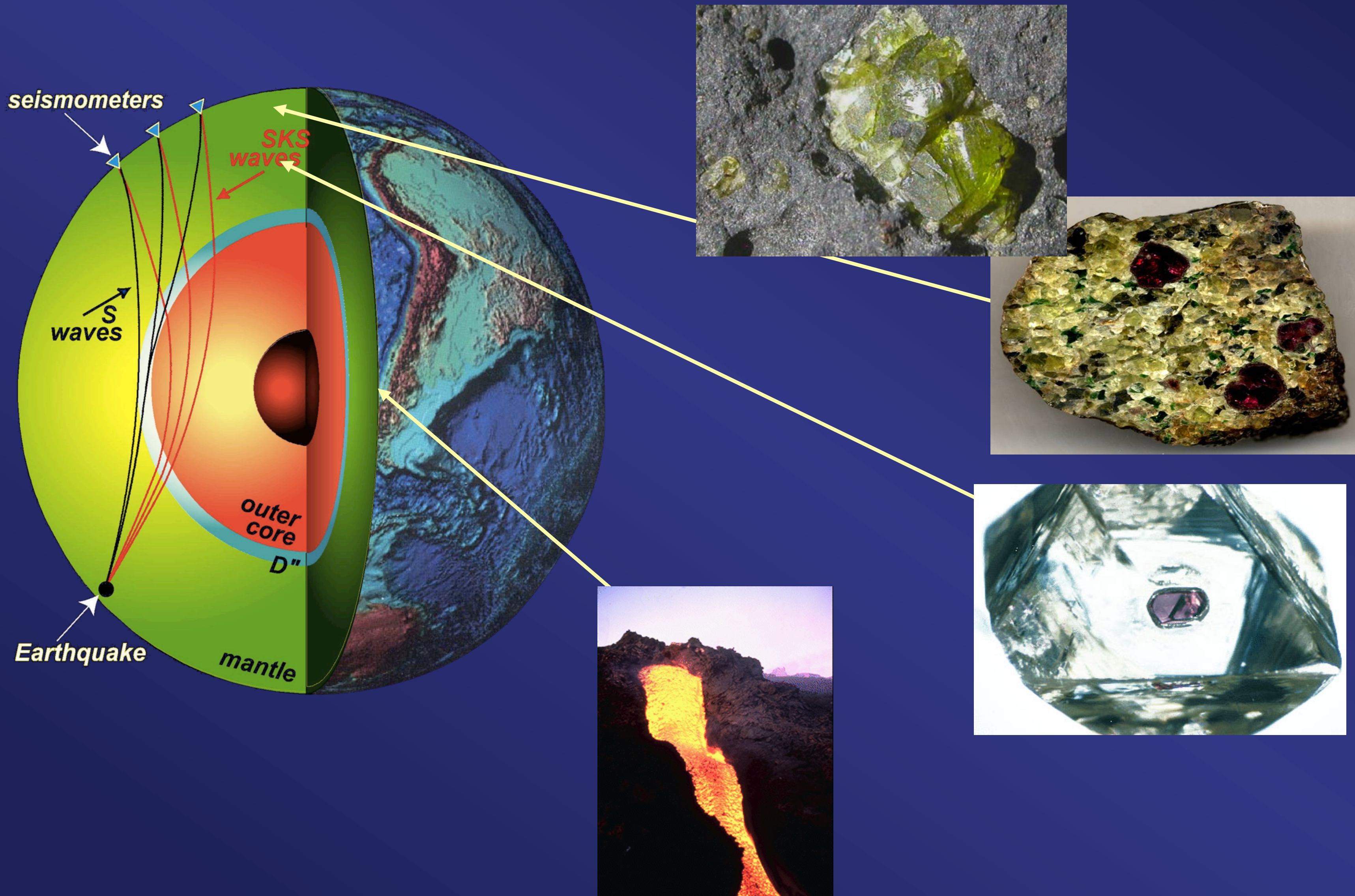
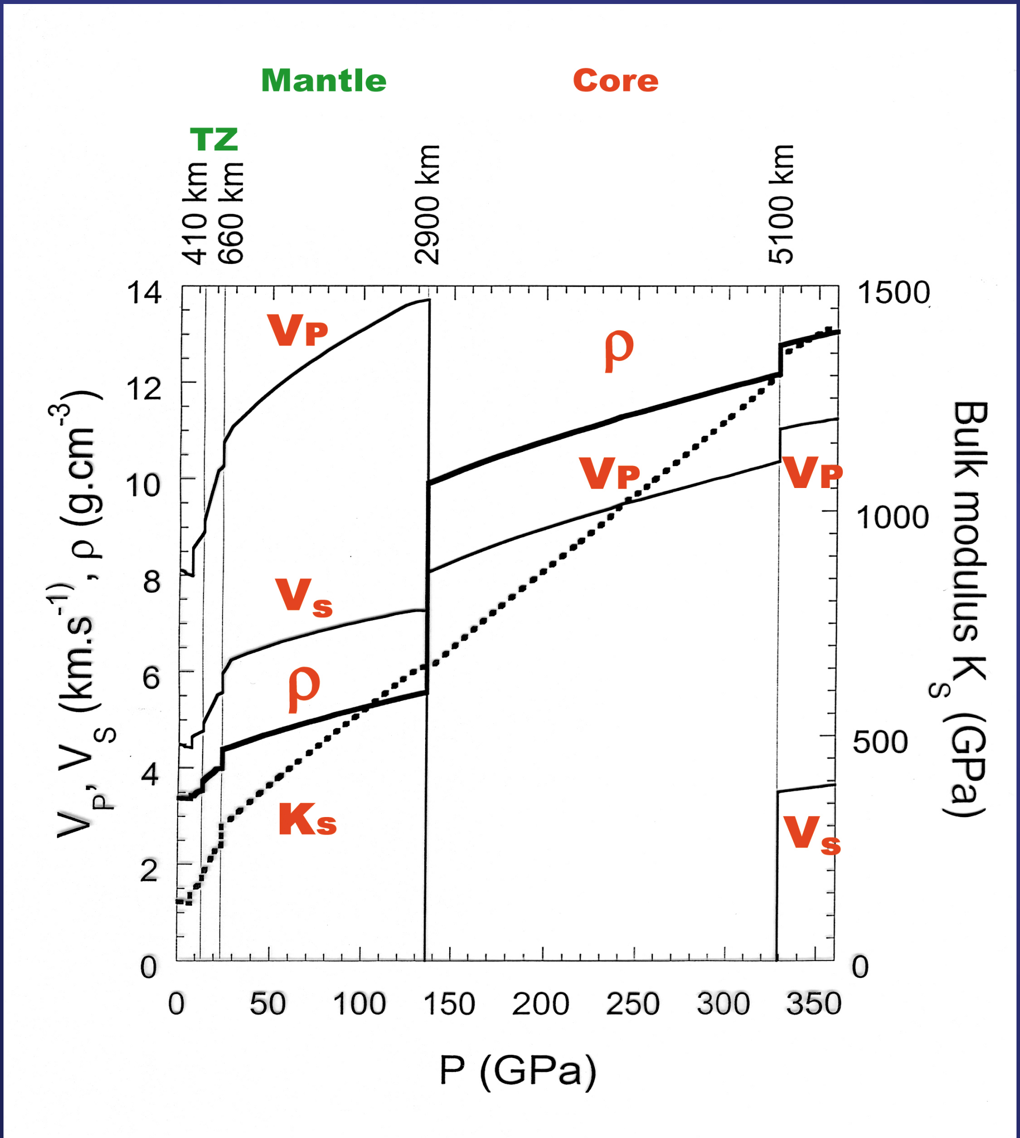
How can we probe the Earth's interior? (without having to drill to the Core…)



1-D seismic profiles ←→ Elasticity of minerals



"What materials may have the elastic properties demonstrated by the seismic waves under the conditions of the interior?"

F. Birch, 1952

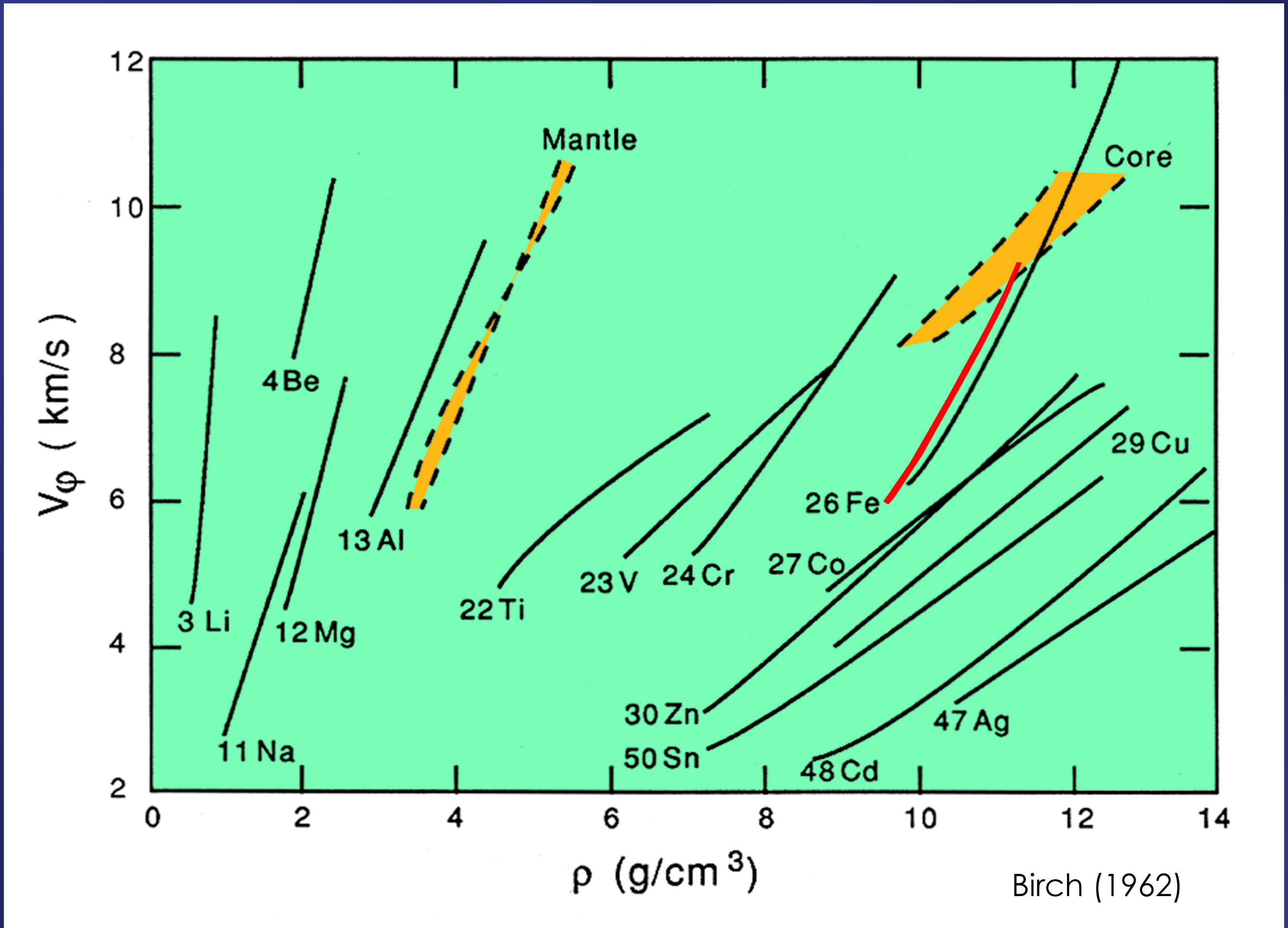
but also …

Unwary readers should take warning that ordinary language undergoes modification to a high-pressure form when applied to the interior of the Earth; few example of equivalent follow:

High-pressure form	⟷	*Ordinary meaning*
certain		*dubious*
undoubtedly		*perhaps*
positive proof		*vague suggestion*
unanswerable argument		*trivial objection*
pure iron		*uncertain mix of all the elements*

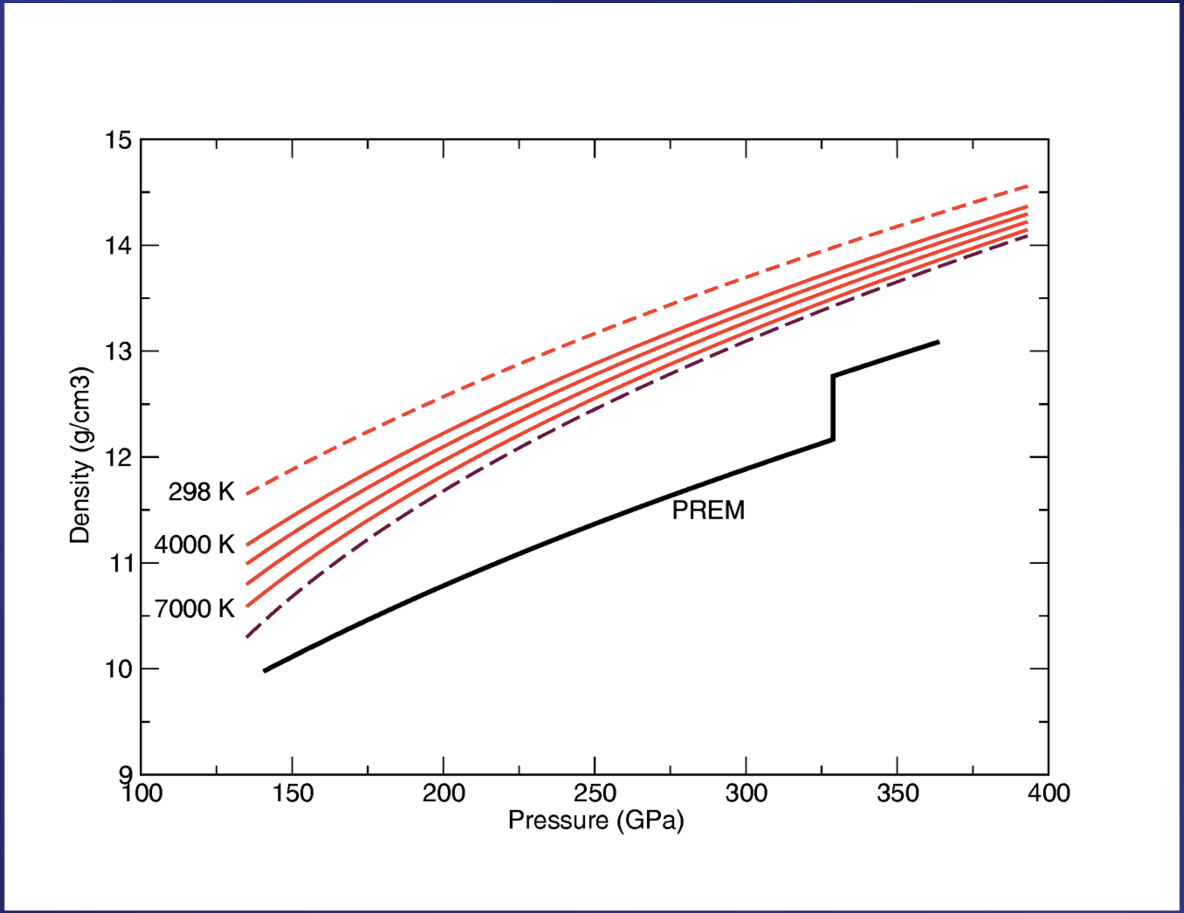
F. Birch, 1952

Velocity vs Density Systematics



Fe (+Ni) main constituent of Earth's core

EOS of hcp-Fe vs Earth's models



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

→ **Light elements in the core (Si, S, O, C …)**

Poirier, PEPI 1994

Sound velocity measurements on Fe and Fe-alloys as a function of pressure and temperature

“traditional” techniques limited

- HIGHEST ATTAINABLE PRESSURE
(large volume press, probe/sample dimensions)

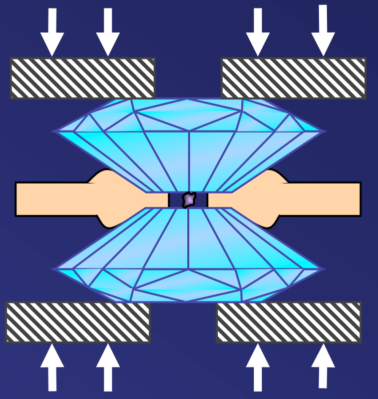
- CHOICE OF MATERIALS
(transparent samples, Mössbauer isotopes)

- INFORMATION CONTENT
(only partial, surface probe, necessary approximation, complex data inversion…)

3^{rd} generation synchrotron sources + diamond anvil cell

Sample volume < 10^{-5} mm^3

Beam size < 100 μm (<10 μm)



(Non-resonant) inelastic x-ray scattering

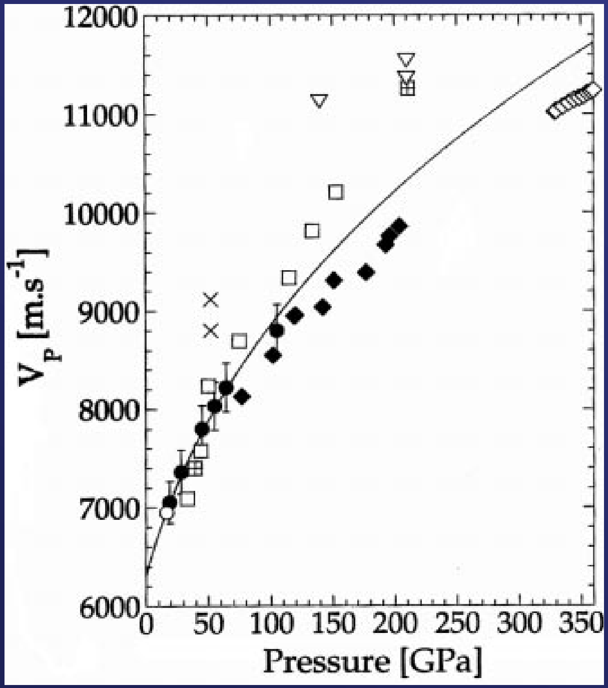
Nuclear resonant inelastic x-ray scattering

Pioneering experimental studies on Fe

Sound Velocities in Iron to 110 Gigapascals

Guillaume Fiquet,[1*] James Badro,[1] François Guyot,[1] Herwig Requardt,[2] Michael Krisch[2]

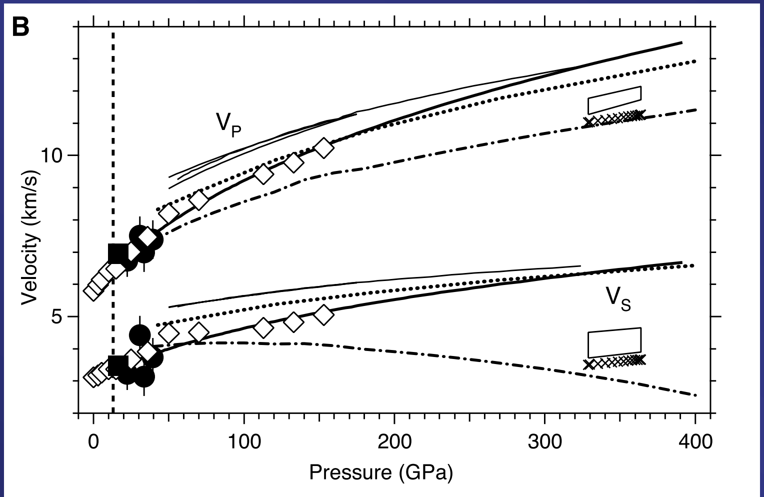
The dispersion of longitudinal acoustic phonons was measured by inelastic x-ray scattering in the hexagonal closed-packed (hcp) structure of iron from 19 to 110 gigapascals. Phonon dispersion curves were recorded on polycrystalline iron compressed in a diamond anvil cell, revealing an increase of the longitudinal wave velocity (V_P) from 7000 to 8800 meters per second. We show that hcp iron follows a Birch law for V_P, which is used to extrapolate velocities to inner core conditions. Extrapolated longitudinal acoustic wave velocities compared with seismic data suggest an inner core that is 4 to 5% lighter than hcp iron.



Phonon Density of States of Iron up to 153 Gigapascals

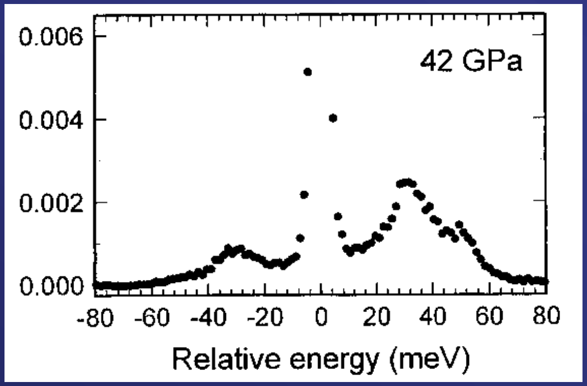
H. K. Mao,[1] J. Xu,[1] V. V. Struzhkin,[1] J. Shu,[1] R. J. Hemley,[1] W. Sturhahn,[2] M. Y. Hu,[2] E. E. Alp,[2] L. Vocadlo,[3] D. Alfè,[3] G. D. Price,[3] M. J. Gillan,[3] M. Schwoerer-Böhning,[4] D. Häusermann,[4] P. Eng,[5] G. Shen,[5] H. Giefers,[6] R. Lübbers,[6] G. Wortmann[6]

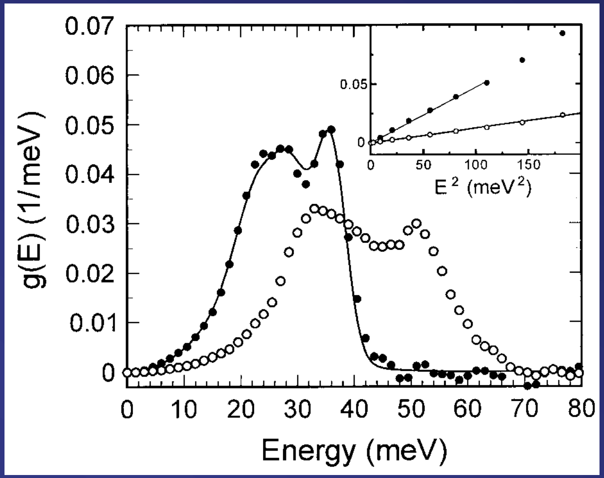
We report phonon densities of states (DOS) of iron measured by nuclear resonant inelastic x-ray scattering to 153 gigapascals and calculated from ab initio theory. Qualitatively, they are in agreement, but the theory predicts density at higher energies. From the DOS, we derive elastic and thermodynamic parameters of iron, including shear modulus, compressional and shear velocities, heat capacity, entropy, kinetic energy, zero-point energy, and Debye temperature. In comparison to the compressional and shear velocities from the preliminary reference Earth model (PREM) seismic model, our results suggest that Earth's inner core has a mean atomic number equal to or higher than pure iron, which is consistent with an iron-nickel alloy.



Basics of Nuclear Resonant Inelastic X-ray Scattering (NRIXS)

Secondary photoemission yield from Mössbauer isotopes (^{57}Fe) resonances to probe the projected partial vibrational density of states



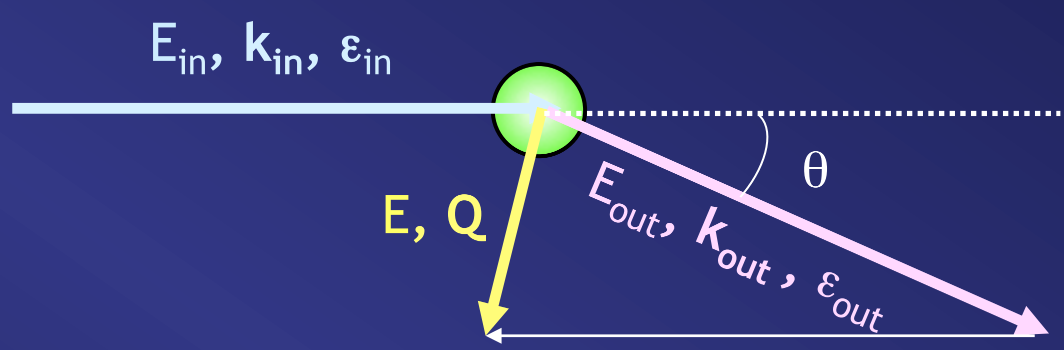


Within an harmonic approximation, for solid with Debye like low-frequency dynamics, parabolic fit to low energy range

→ Debye velocity V_D

$$3/(V_D)^3 = 1/(V_P)^3 + 2/(V_S)^3$$
$$K/\rho = (V_P)^2 - (4/3)\,(V_S)^2$$
$$G/\rho = (V_S)^2$$

Basics of Inelastic X-ray Scattering (IXS)



- Energy transfer $E = E_{out} - E_{in}$ ($E \ll E_{in}$)
- Momentum transfer $\mathbf{Q} = \mathbf{k}_{out} - \mathbf{k}_{in} = 2k \sin(\theta/2)$ ($k_{out} \approx k_{in} \equiv k$)

◆ Directional analysis of the scattered photons ⟹ Q

◆ Energy analysis of the scattered photons ⟹ E

Large variety of samples, metals as well as semiconductors or insulators

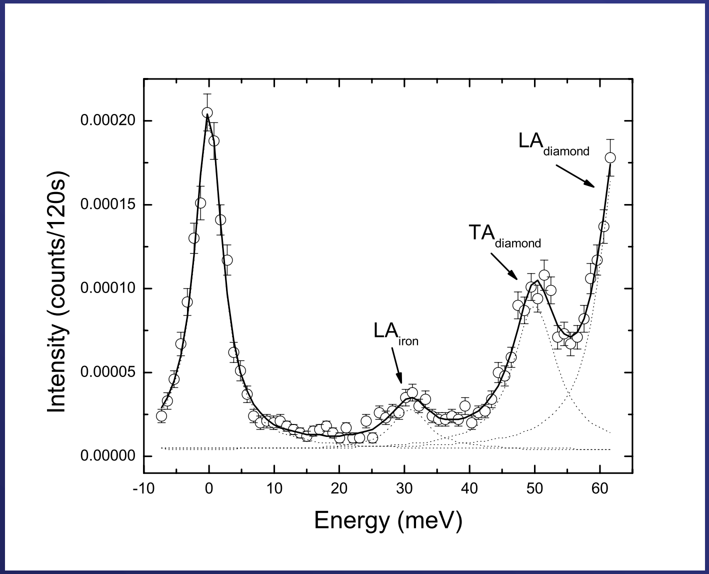
Opaque as well as transparent materials

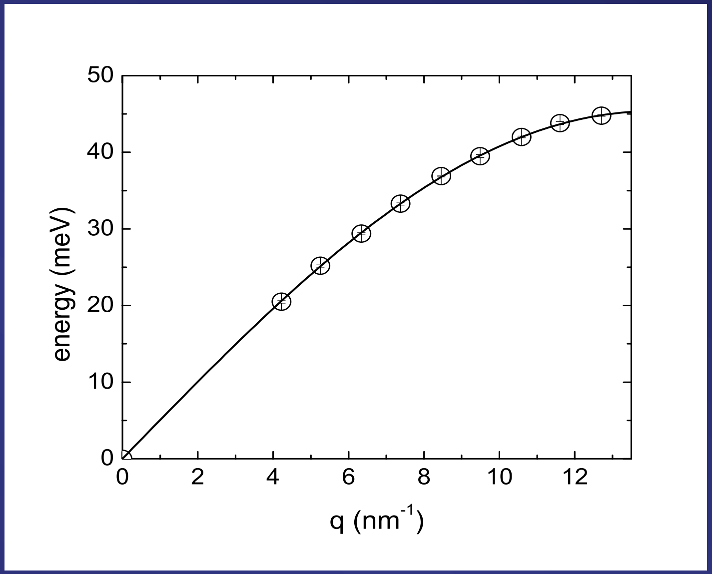
Single crystals, powders, liquid

Elasticity form IXS measurements

Single crystals: complete phonon dispersion curve → full elastic tensor (C_{ij})

Powders: averaged longitudinal dispersion

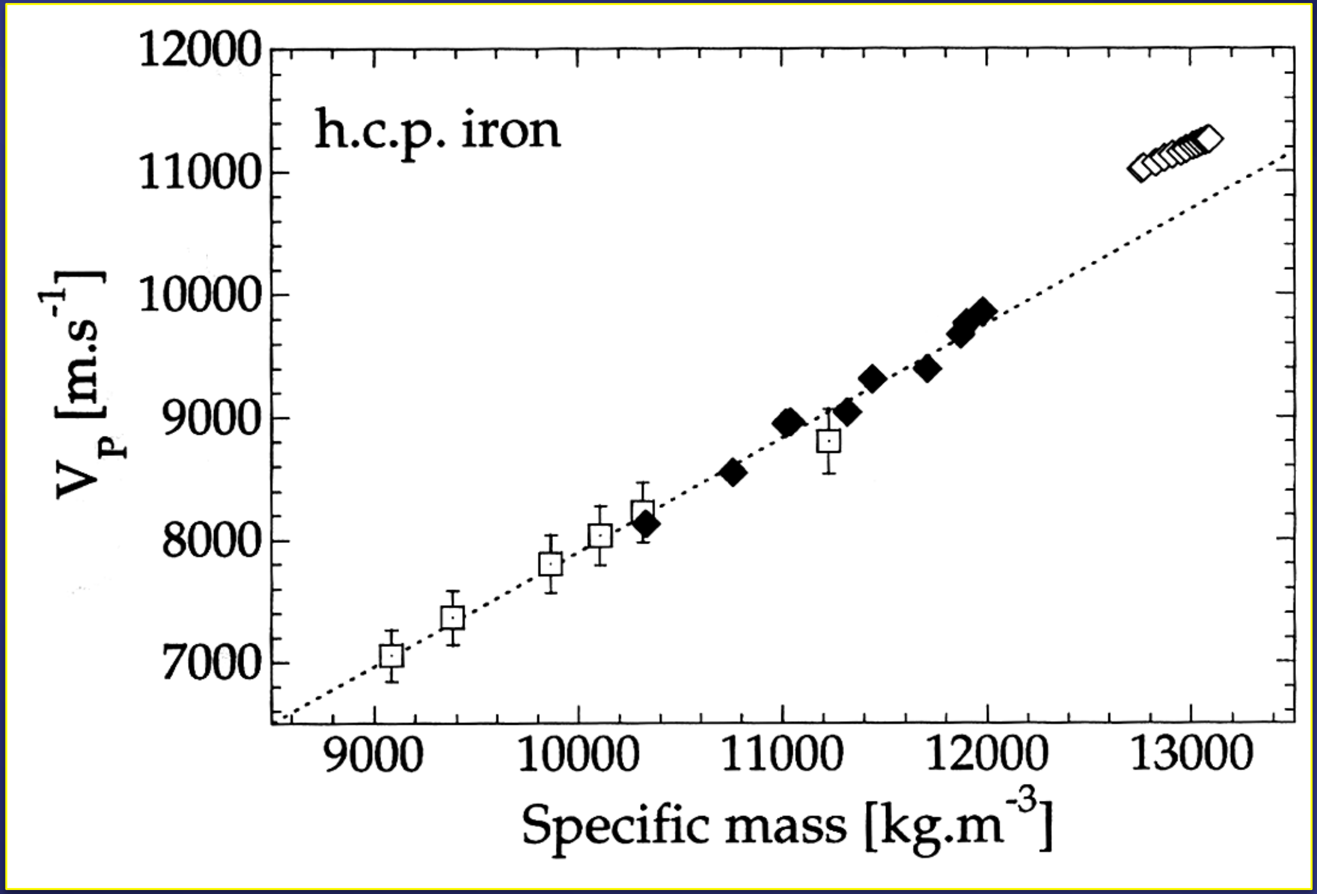




from sinus fit → aggregate compressional sound velocity V_P

(aggregate shear sound velocity V_S)

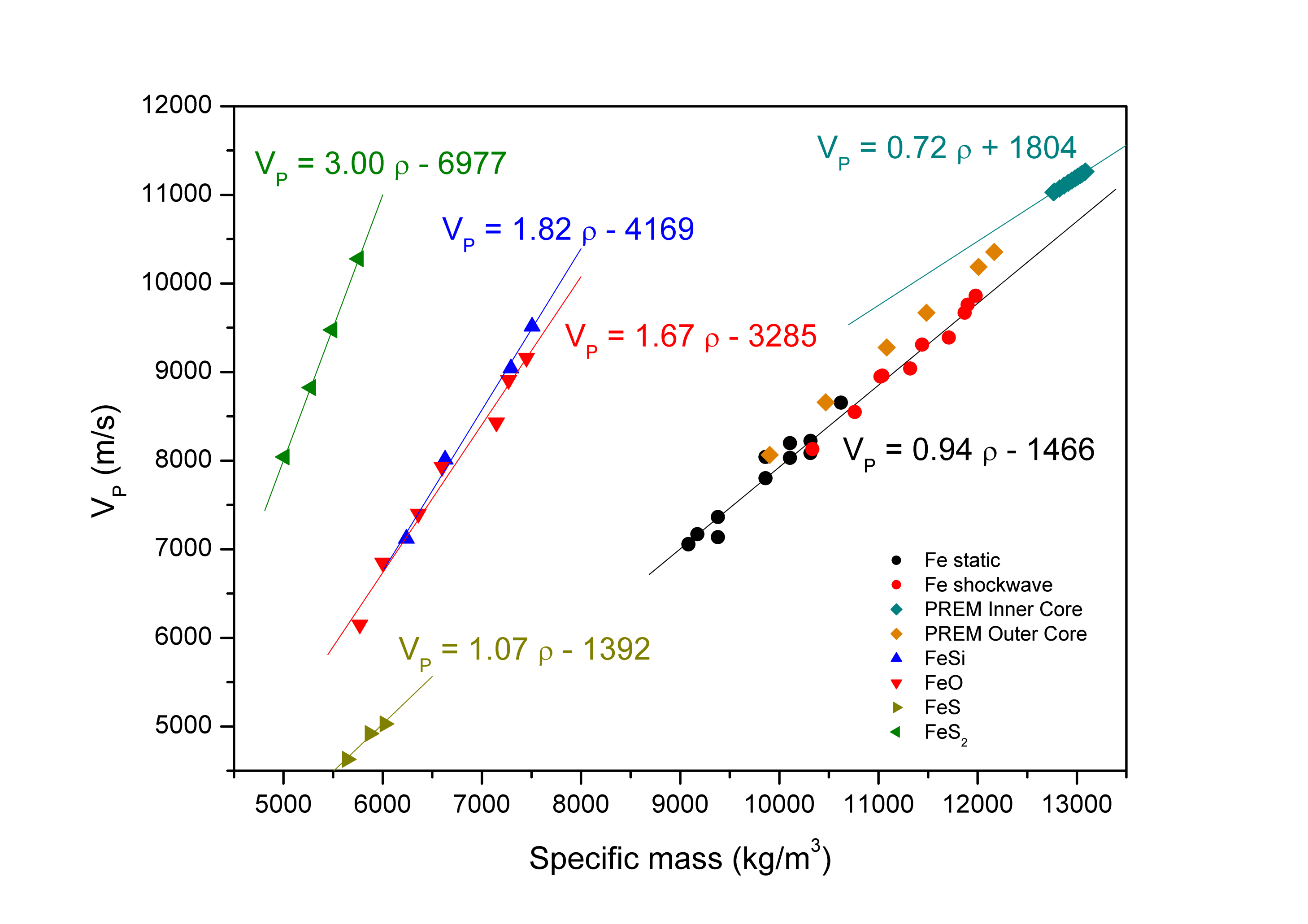
IXS on pure-Fe



Fiquet et al., Science 2001

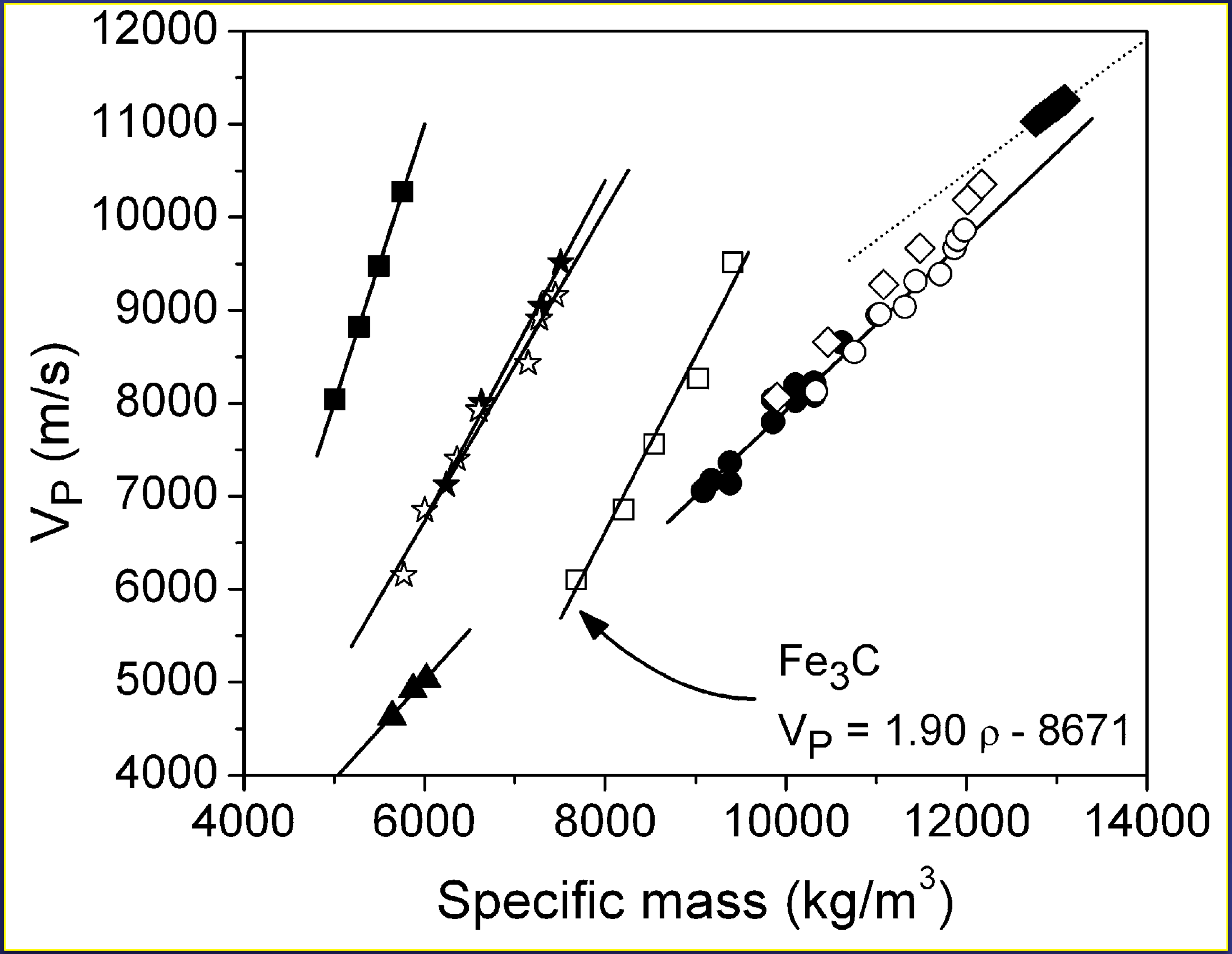
- Birch’s law
- Light elements in the inner core (Si, S, O, C …)

Sound velocities in Fe and Fe-compounds



Badro et al., EPSL 2007

Sound velocities in Fe and Fe-compounds



Fiquet et al., PEPI 2009

Composition of the core

Element	Fraction (wt%)	Compression (ρ/ρ_o)	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 2007

Main assumptions:

1) Birch's law

2) "Linear mixing" of velocities of end-members

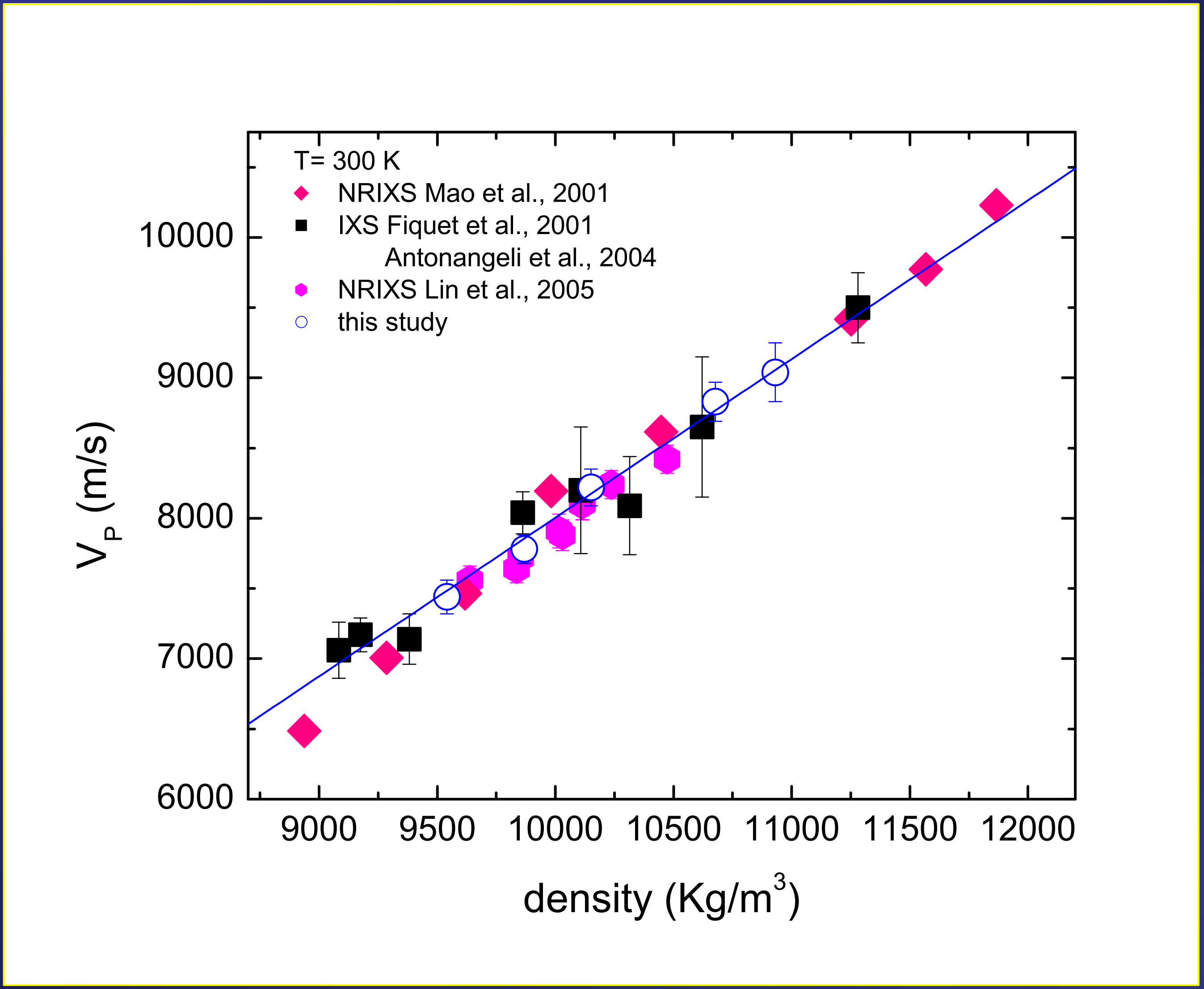
3) Inclusion of up to 15 wt% Ni is considered negligible

4) Only V_P and ρ, neglecting V_S

Sound velocities and density measurements on $Fe_{0.89}Ni_{0.04}Si_{0.07}$ to 108 GPa

+ check Fe as reference

Fe sound velocities at high P and ambient T

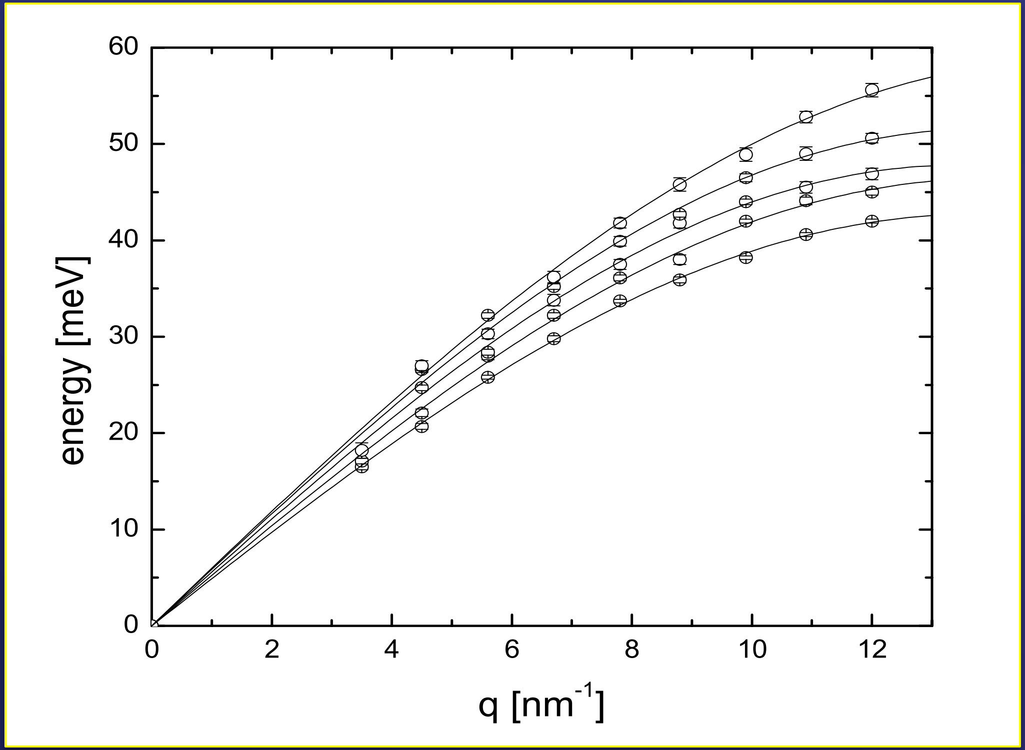


Antonangeli et al., submitted

IXS measurements to 108 GPa
(ID28-ESRF)

Polycrystalline homogeneous samples of silicon bearing iron-nickel alloy
Electron micro-probe analysis: Si → 3.7 wt%   Ni → 4.3 wt%

Compacted pellets (90 μm diameter, 20 μm thick) loaded into DAC



longitudinal acoustic phonon dispersion

↓

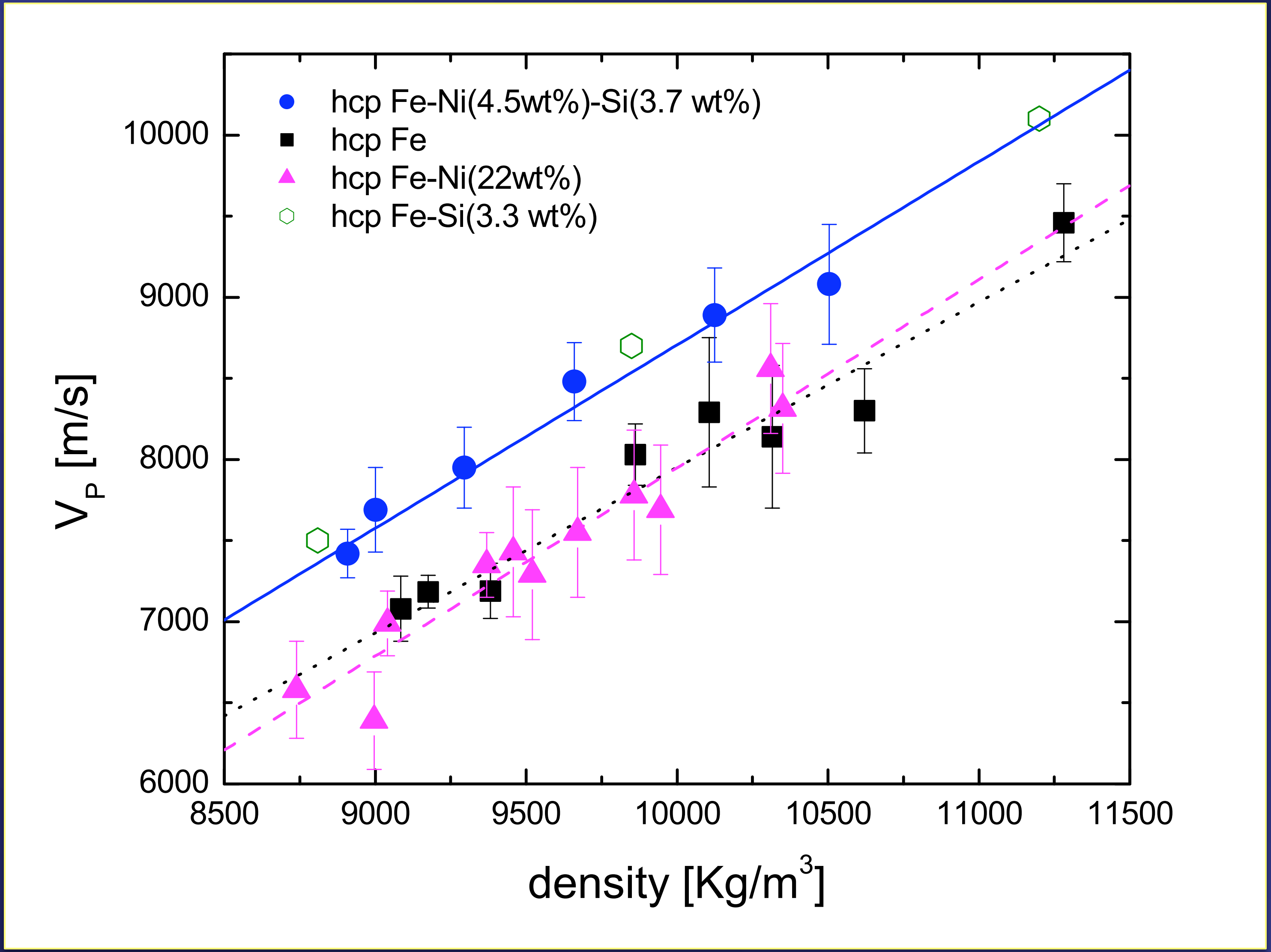
V_P and ρ

↑

diffraction

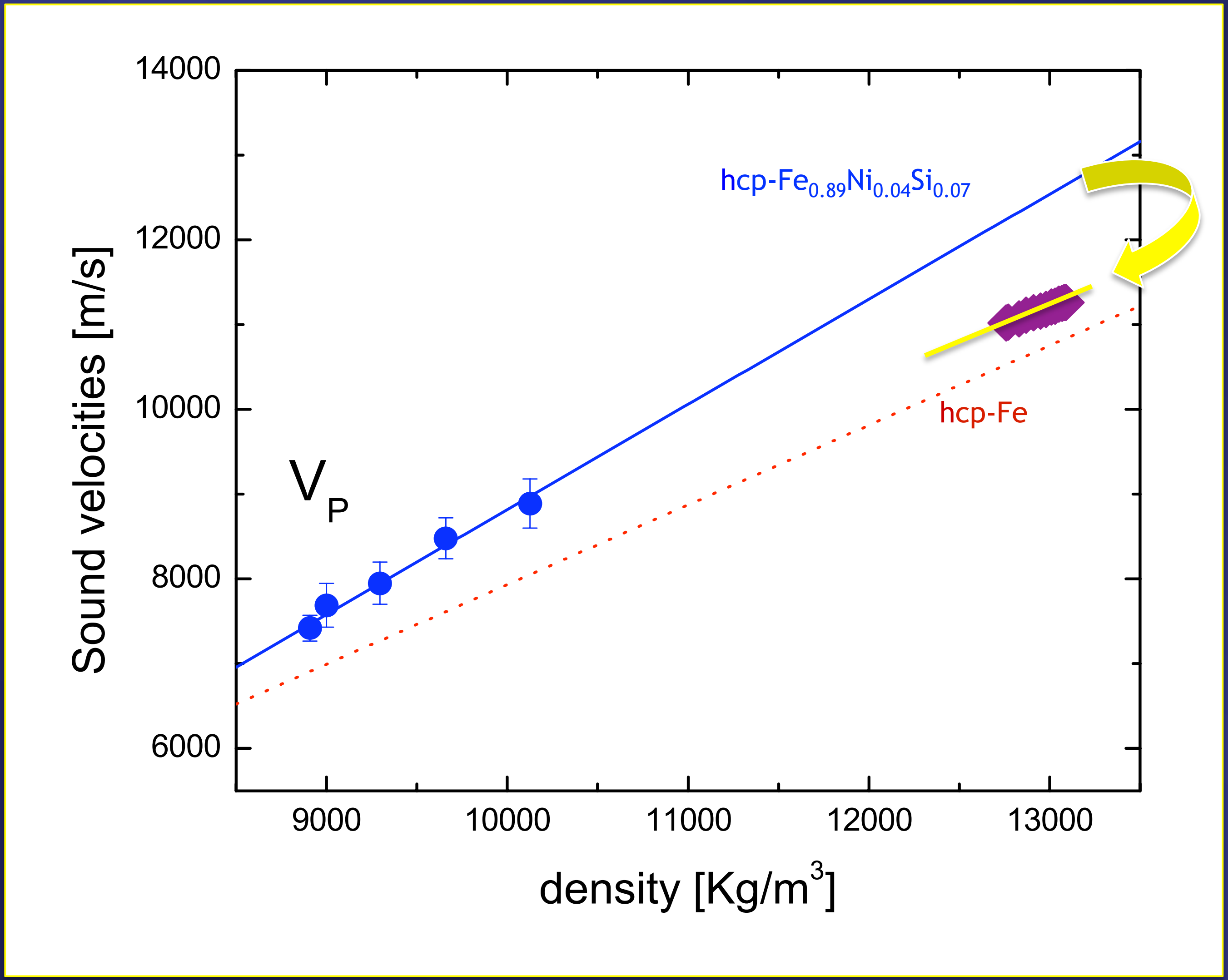
V_S combining V_P and K/ρ

Comparison with pure-Fe, Fe-Ni and Fe-Si



Antonangeli et al., EPSL 2010
Kantor et al., PEPI 2007
Tsuchiya and Fujibuchi, PEPI 2009

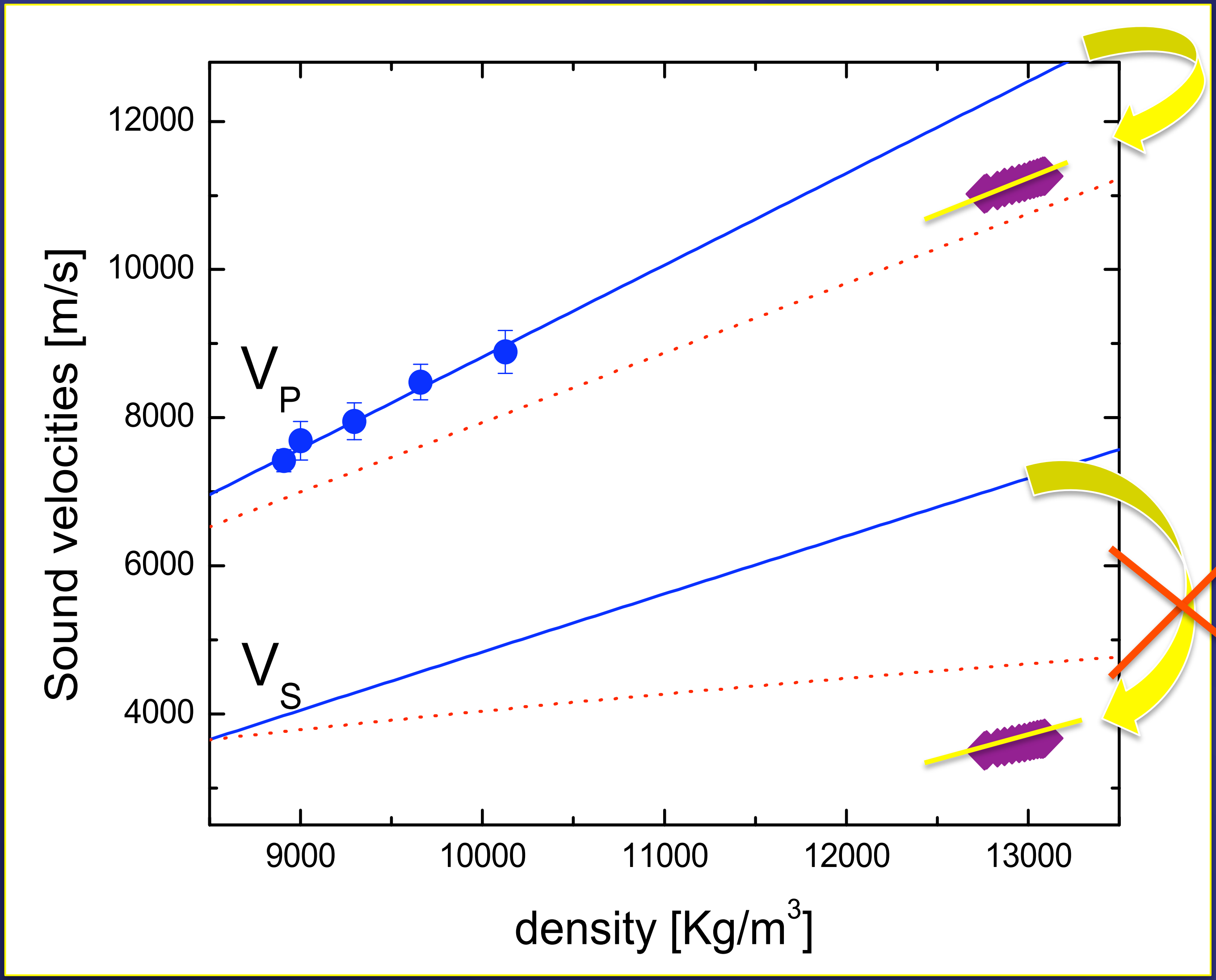
Comparison with seismic models: V_P



Down to PREM for Si ~ 1.2 wt%

Antonangeli et al., EPSL 2010

Comparison with seismic models: V_P and V_S



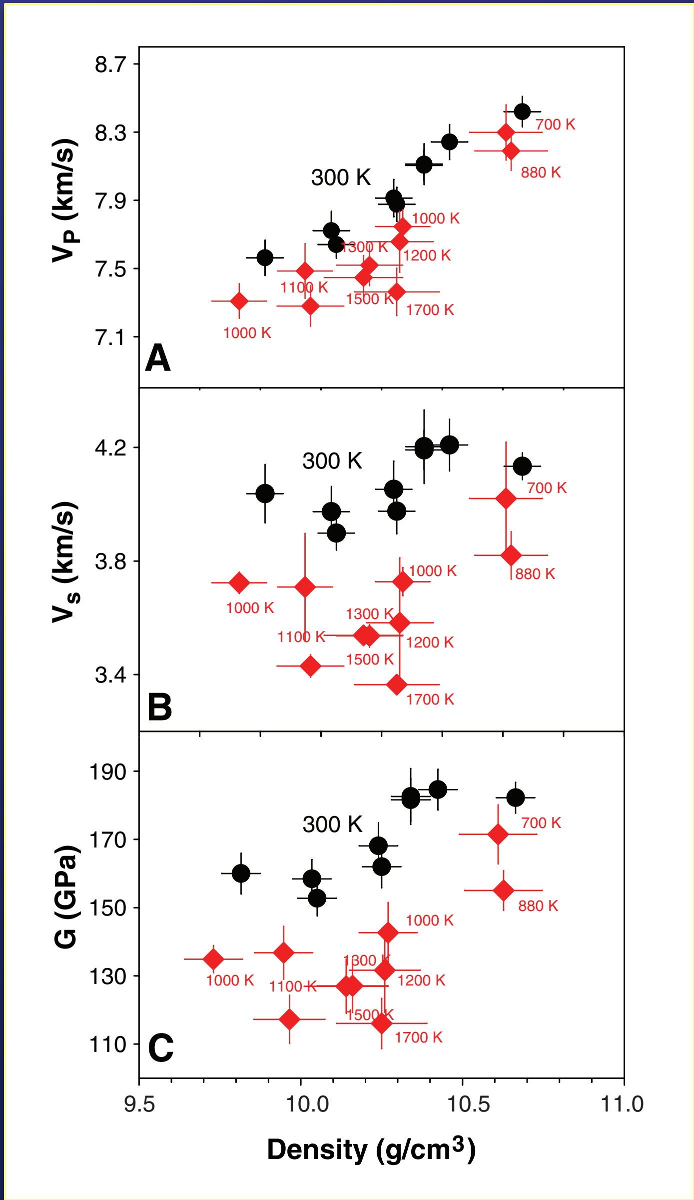
Down to PREM for Si ~ 1.2 wt%

Down to PREM ?

No for any Si concentration

Antonangeli et al., EPSL 2010

Anharmonic temperature effects?



Lin et al., Science 2005

NRIXS measurements on Fe compressed in laser-heated DAC

- Phonon density of state
- Debye velocity

- Complex data treatment
- Harmonic model
- No density determination
- Input P-V-T to solve for V_P and V_s

Is there a more direct way to probe temperature effects on sound velocity?

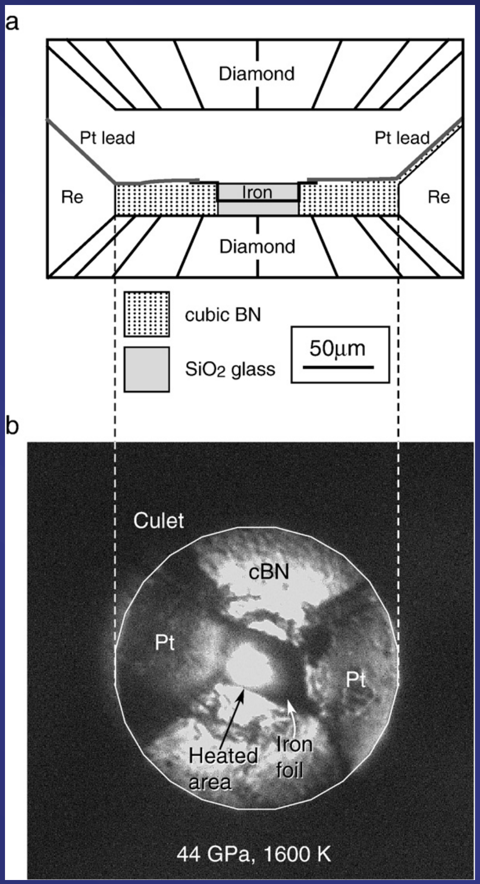
IXS measurements on Fe at high pressure and high temperature

IXS on polycrystalline sample → aggregate phonon dispersion → V_P

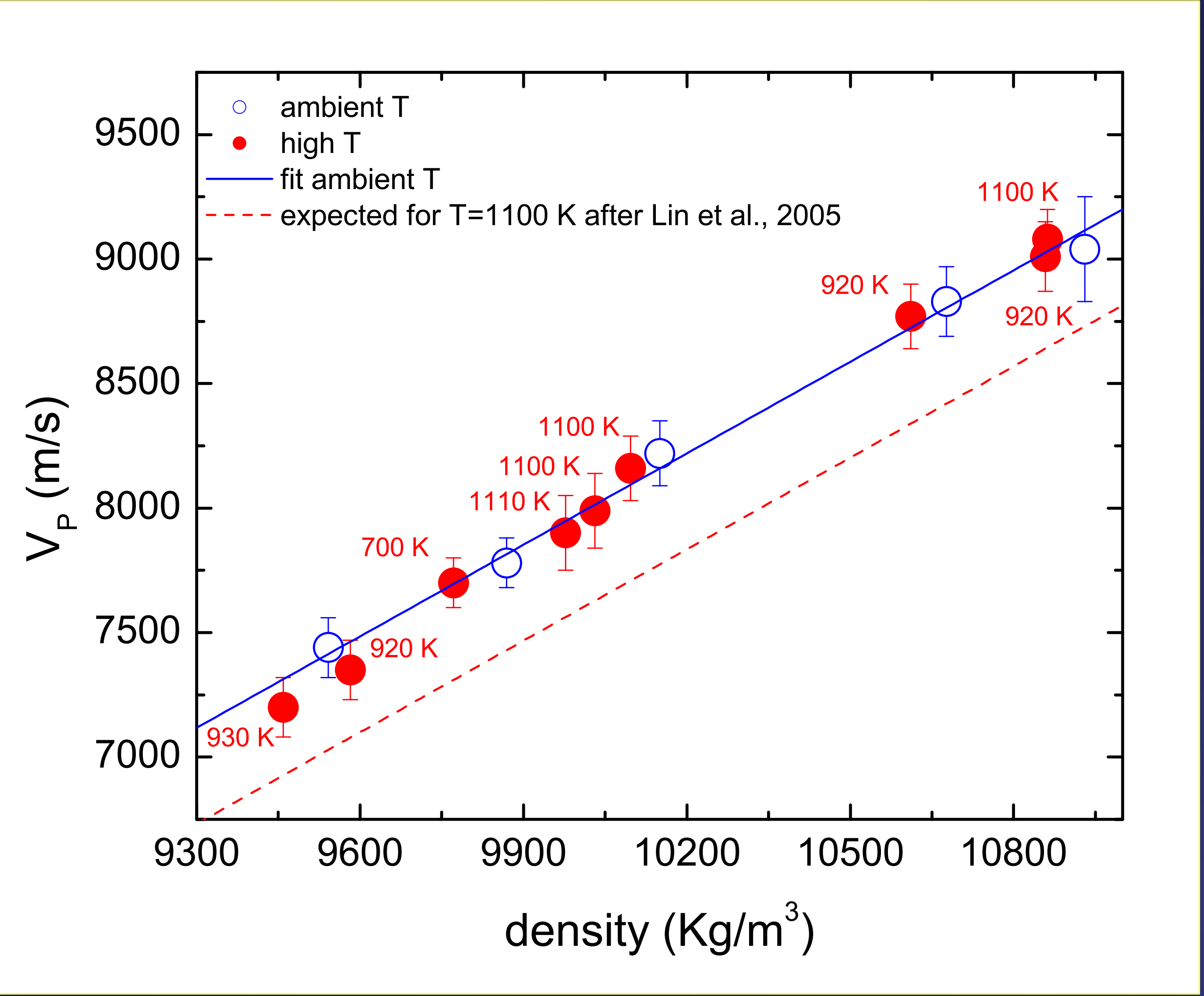
XRD → phase stability, phase purity and density

Mao type DAC
Internal and external resistive heating
In vacuum measurements

- 30 GPa < P < 93 GPa
- 300 K < T < 1100 K (for up to 12 hours)
- hcp-phase



No temperature effect up to 1100 K



Antonangeli et al., submitted

Anharmonic corrections

At core temperatures (4000-7000 K) anharmonic effects are expected

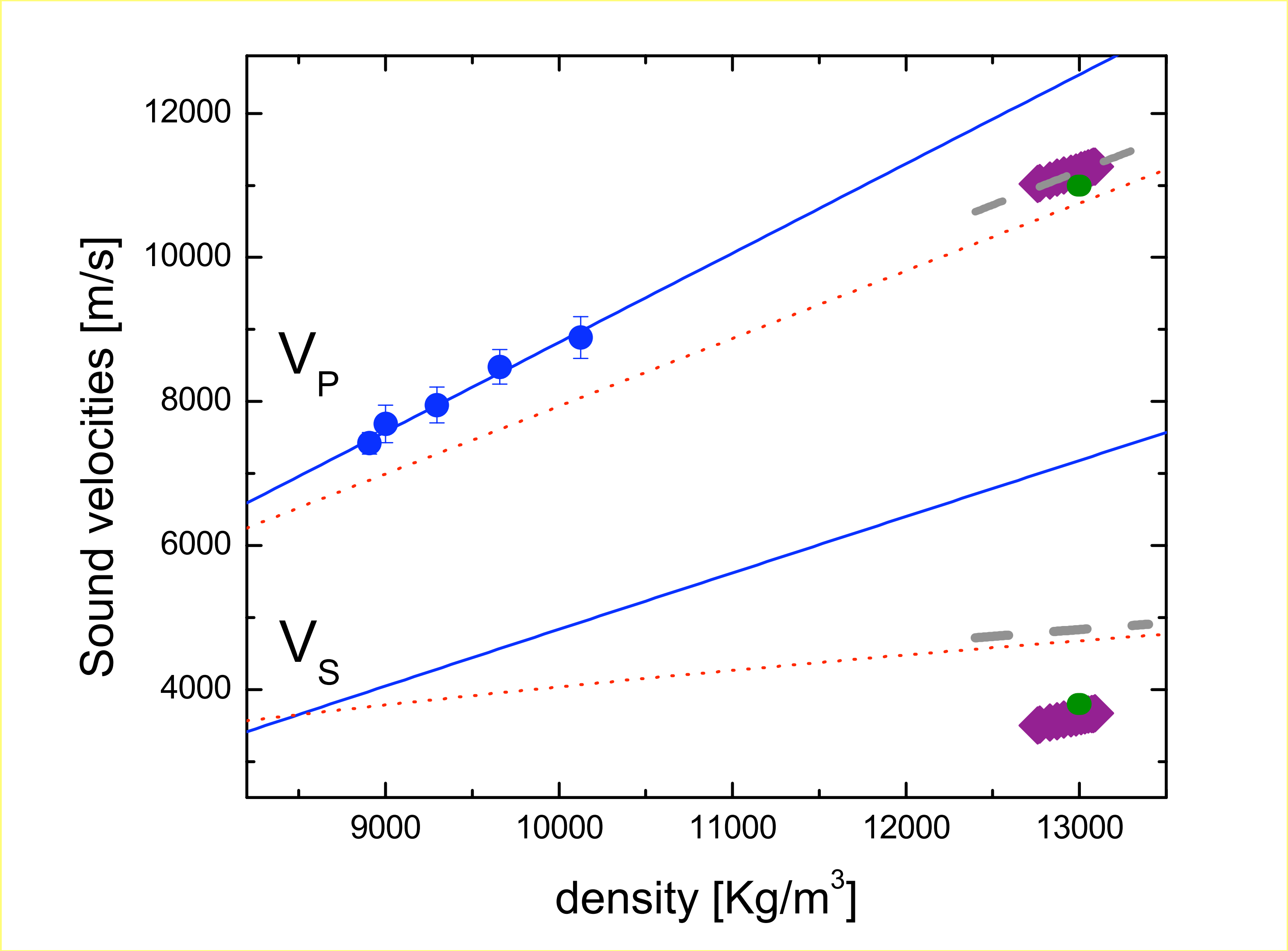
More relevant to V_S (e.g. Laio et al., 2000; Steinle-Neumann et al., 2001)

corrections at constant density (13000 Kg/m^3)

-4% on V_P and -30% on V_S at 5000 K

after calculations on pure hcp-Fe (Vočadlo et al., 2009) corrected for the 4% density variation of computational results at 300 and 5000 K

Seismic wavespeeds and density are matched for 1.5 wt% of Si at 5000 K



Antonangeli et al. EPSL 2010

Conclusions 1

- Si major light element in inner core

- Inner core containing 4-5 wt% of Ni and 1-2 wt% of Si

(exact Si amount might vary depending on temperature corrections
and if other light elements are present)

for $1.2 \leq D^{Liq/Sol} \leq 1.9$ (after Alfe et al., 2002)

- Total core composition with 1.2 wt% < Si < 4 wt%

on the lower range of core formation and core-mantle interactions models
that often call for larger Si amount in the core
e.g. 7.3 wt% (Allègre et al, 1995), 10.3 wt% (Javoy, 1995),
5-7 wt% (Wade and Wood, 2005)

Conclusions 2

- Simple model that simultaneously matches the main seismic observables: density, P-wave and S-wave velocities

Other mechanisms for lowering V_S

- Fluid inclusions (e.*g*. Singh et al., 2000; Vočadlo, 2007)

- Viscoelastic relaxation (*e.g*. Jackson et al., 2000)

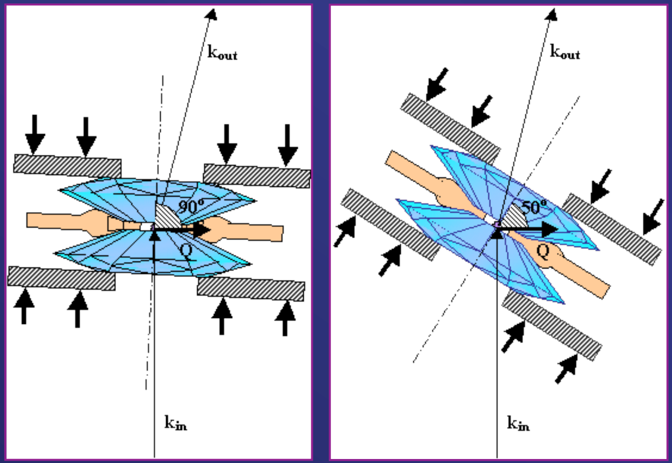
- Randomly oriented anisotropic "patches" (*e.g*. Calvet et el., 2008)

No strictly needed to explain seismic velocities

Possibly needed to account for seismic attenuation, seismic anisotropy, variation with depth, hemisphericity…

Outlooks

→ beyond radial models, single crystal properties

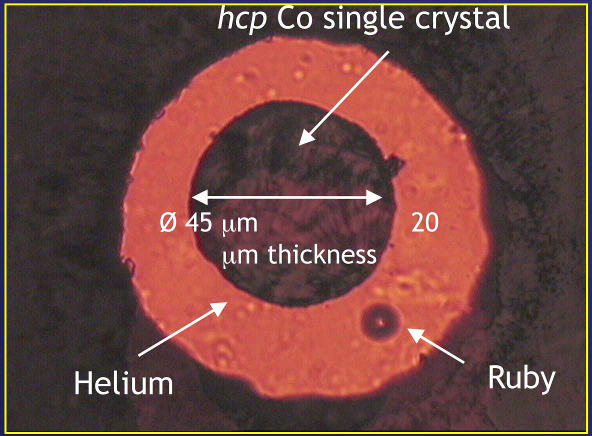


IXS from textured polycrystalline samples

$V_P\{\xi\}$ up to 110 GPa

(Antonangeli et al., EPSL 2004; Mao et al., JGR 2008)

for Fe-alloys expected limit ~150 GPa



IXS from single crystals → full phonon dispersions

C_{ij} up to 39 GPa and 1000 K

(Antonangeli et al., PRL 2004; Farber et al, PRL 2005; Antonangeli et al., PRL 2008)

so far limited by sample's availability, dimensions and quality

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