Inelastic X-ray scattering at extreme conditions and its geophysical applications

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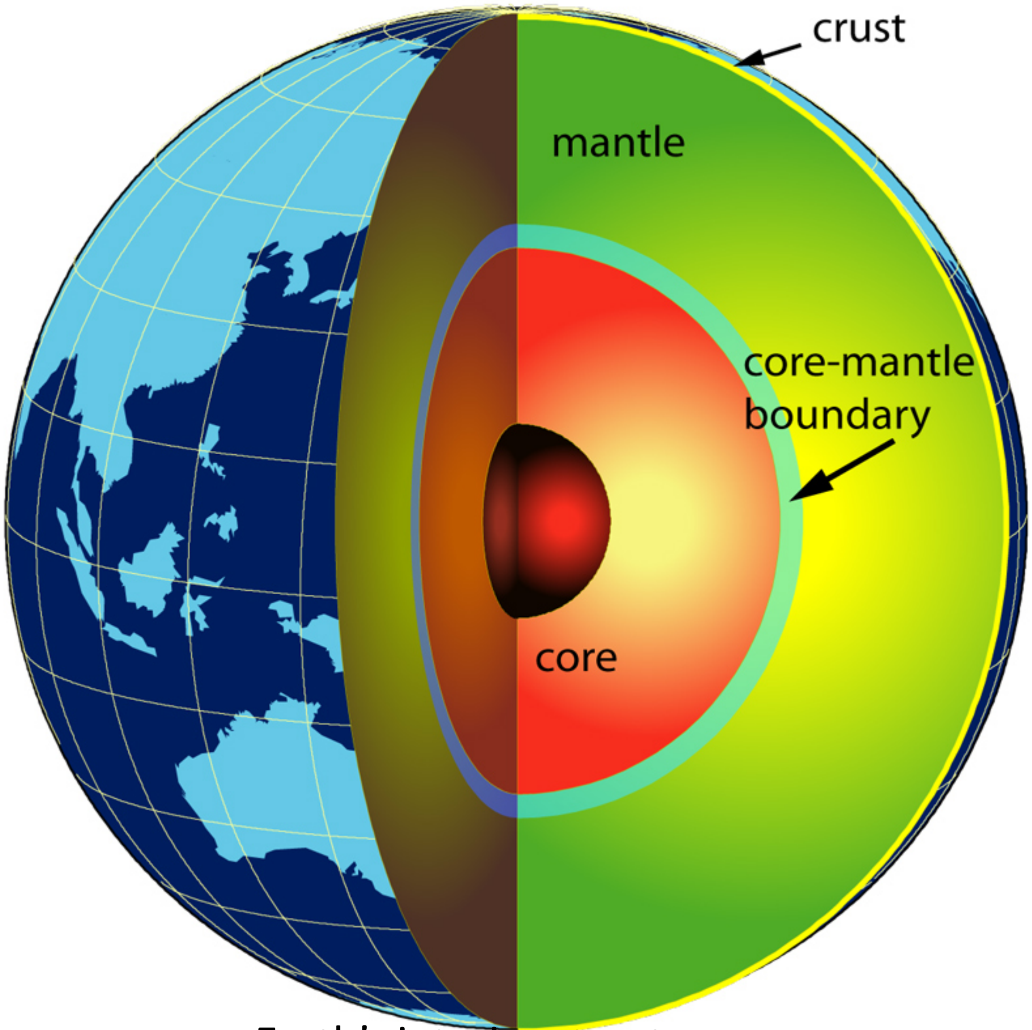
Topics

・Sound velocity of iron and its alloy compounds and the Earth’s core

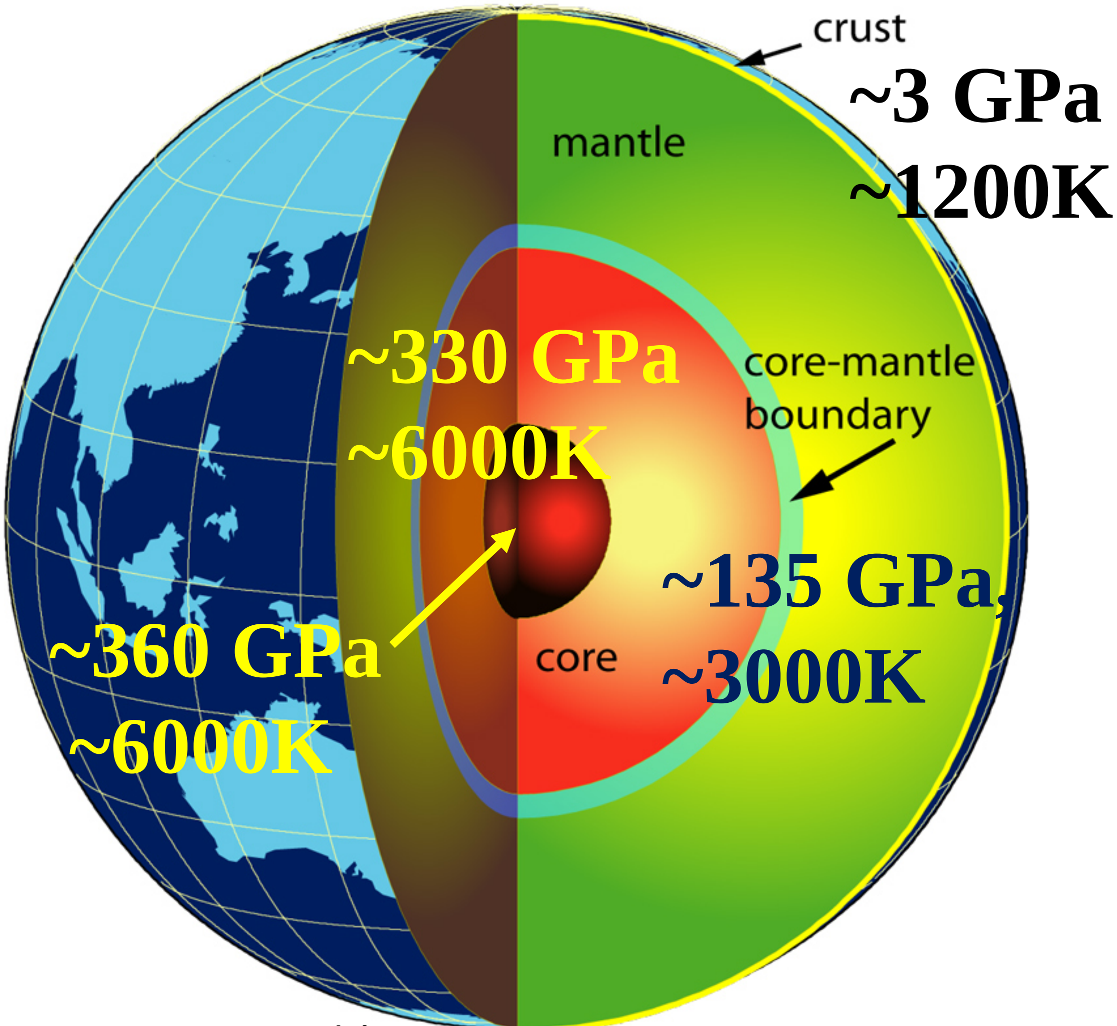
・Sound velodity measurements at multi-Megabar pressures and the primary pressure scale

Sound velocity measurements of iron-light element alloys: A challenge to the core conditions



Earth's interior structure

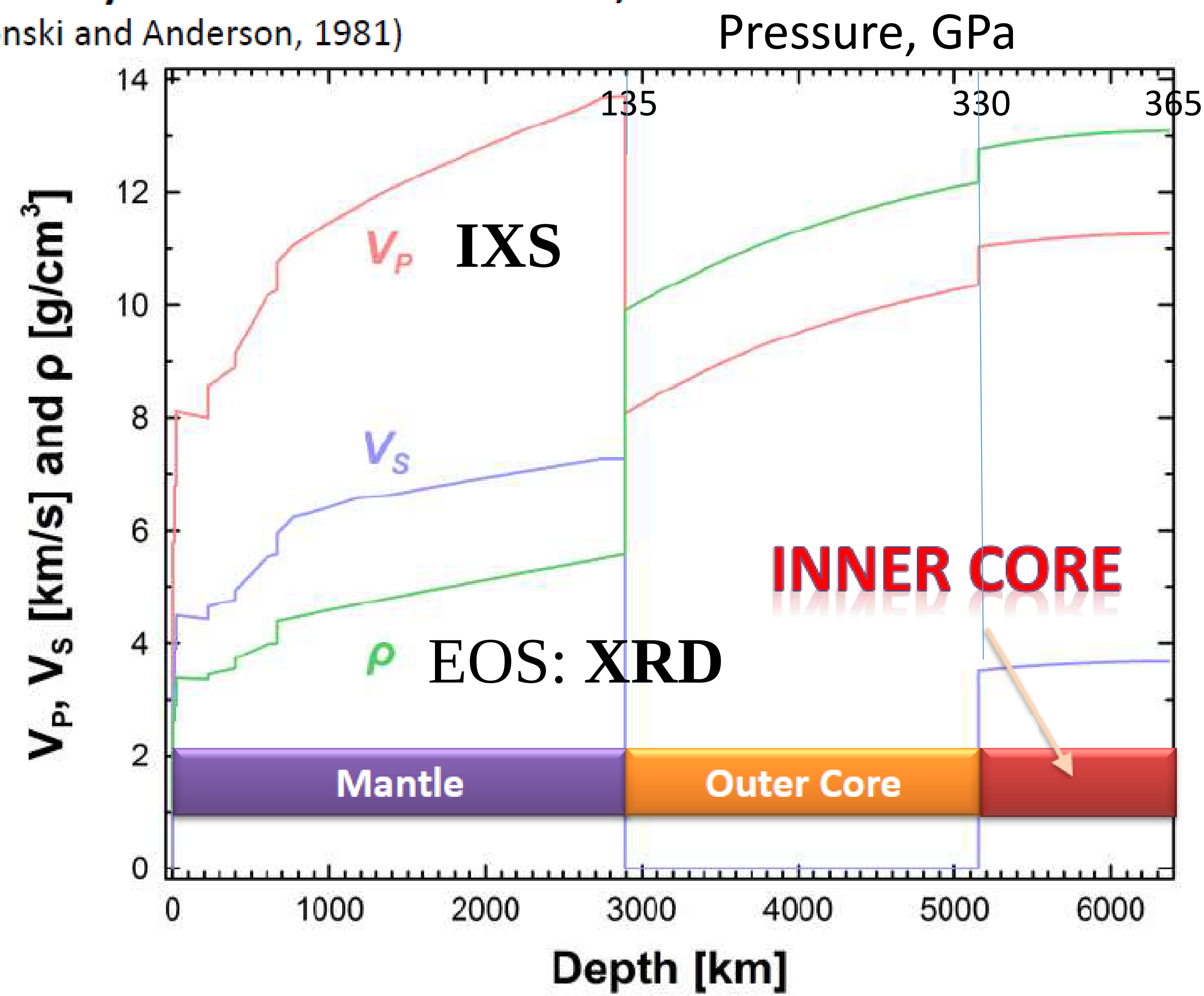
Sound velocity measurements of iron-light element alloys: A challenge to the core conditions



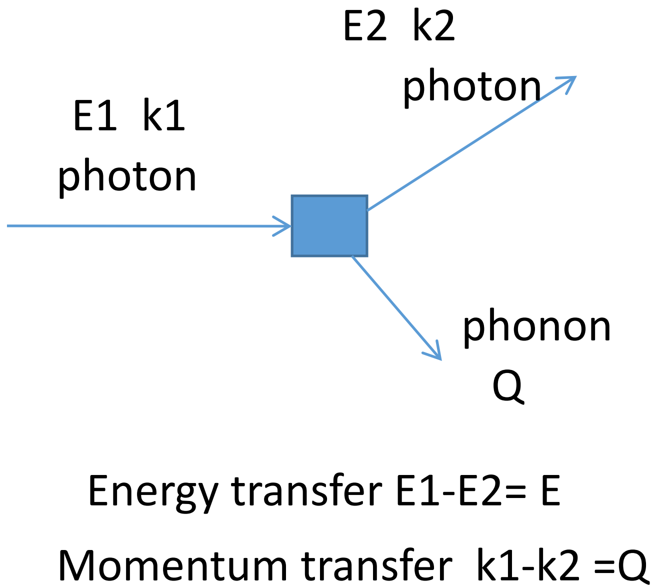
Earth's interior structure

Preliminary reference Earth model; PREM

(Dziewonski and Anderson, 1981)



Sound velocity of Fe and Iron-light element alloys



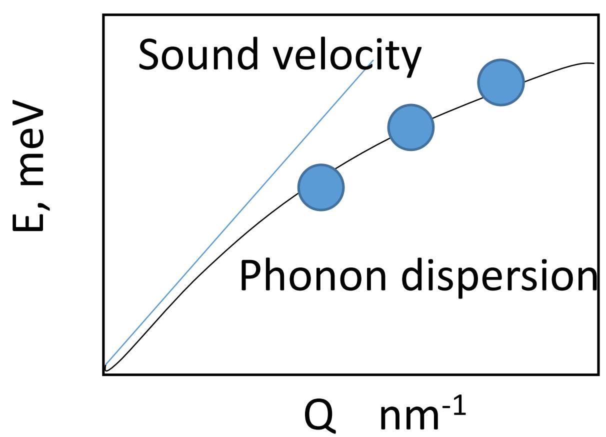
Sound velocity of Earth materials

Ultrasonic

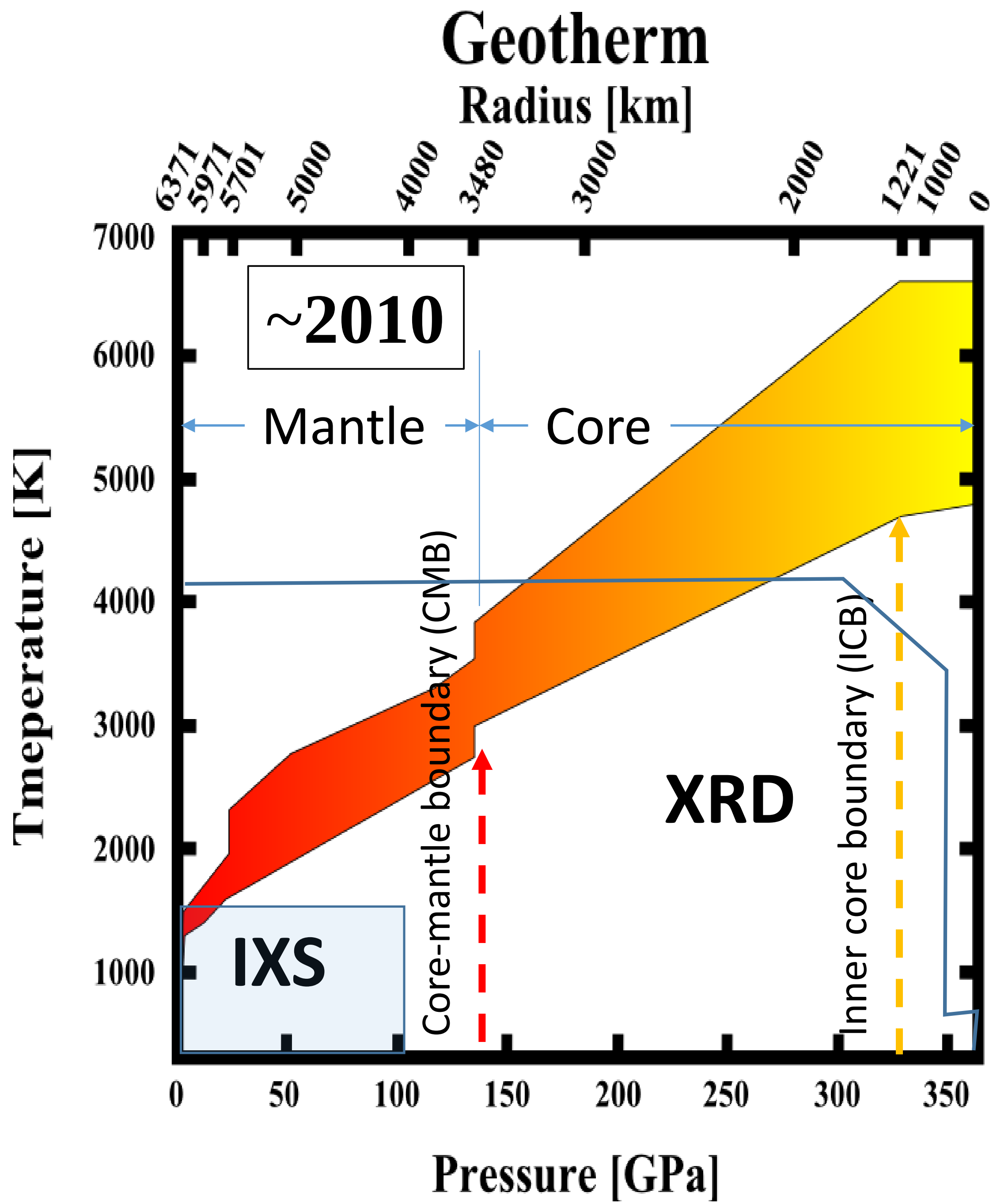
Brillouin scattering

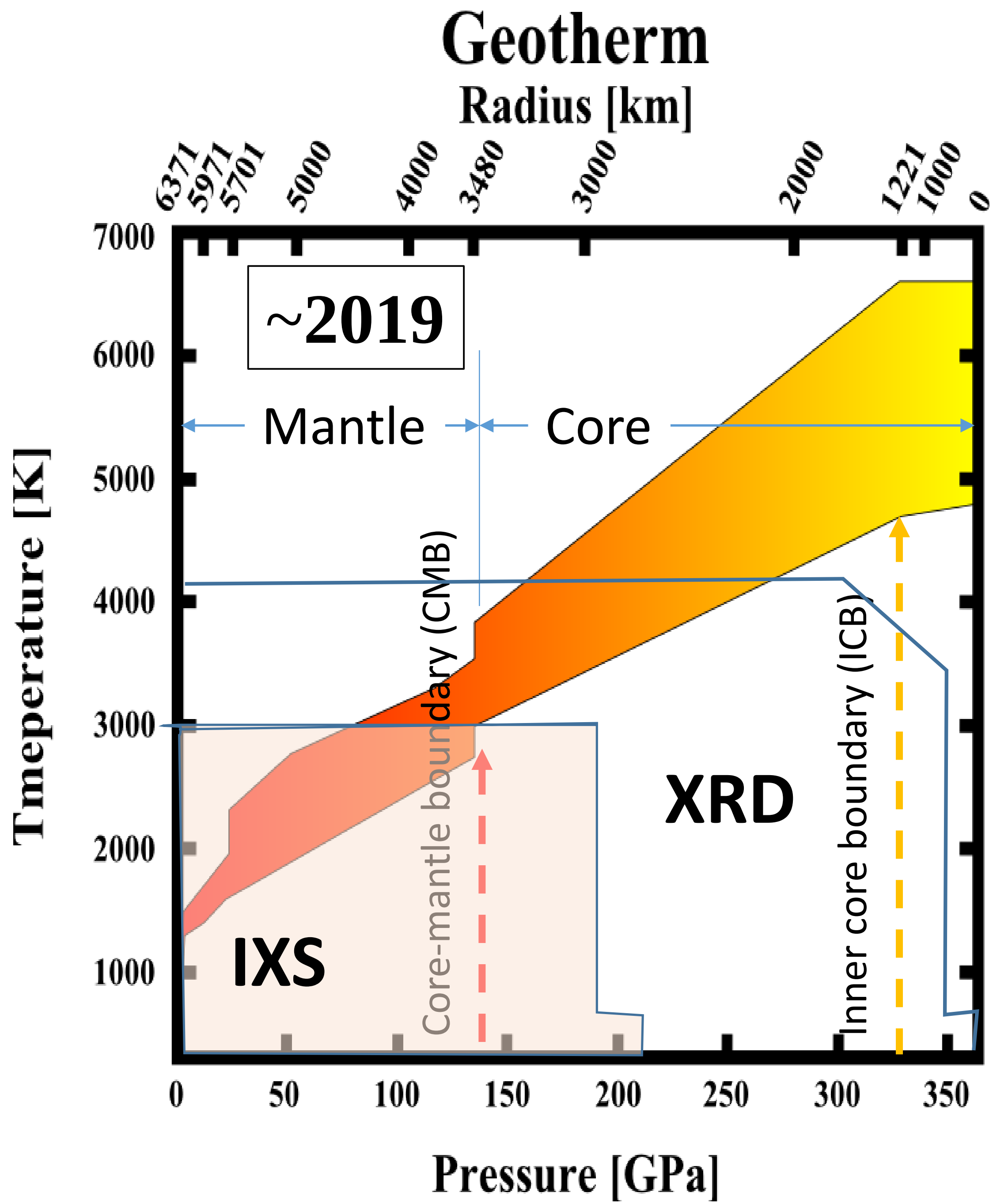
NRIXS (NIS, Nuclear Resonance Inelastic X-ray Scattering)

IXS (Inelastic X-ray scattering)



- Fiquet et al. (2001) Fe-Vp @ESRF
- Antonangeli et al. (2004) : Fe Anisotropy of Vp
- Z.Mao et al. (2012) Fe and FeSi at HP and HT @APS


Geotherm
Radius [km]
6371
5971
5701
5000
4000
3480
3000
2000
1221
1000
0
7000
6000
5000
4000
3000
2000
1000
Tmeperature [K]
~2010
Mantle
Core
Core-mantle boundary (CMB)
Inner core boundary (ICB)
XRD
IXS
0
50
100
150
200
250
300
350
Pressure [GPa]



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Pressure [GPa]

BL35XU@ SPring-8: High pressure and temperature:

IXS Optics [Baron et al., 2000]

・ Kirkpatrick-Baez mirror pair: **16 × 16 μm** beam size

XRD**:** Flat panel area detector

Heating: Portable laser heating system **COMPAT** (Fukui et al., 2013)

BL43XU@SPring-8: Higher pressure: P>200 GPa

IXS Optics [Baron et al., 2016]

・**Multilayer Kirkpatrick-Baez (KB) mirror**: **5×5 μm** beam size

・**Soller screen** [Baron, 2019]:

XRD: Flat panel area detector

BL35XU Optics

Simultaneous measurements of sound velocity and density: Flat panel detector, Image plate

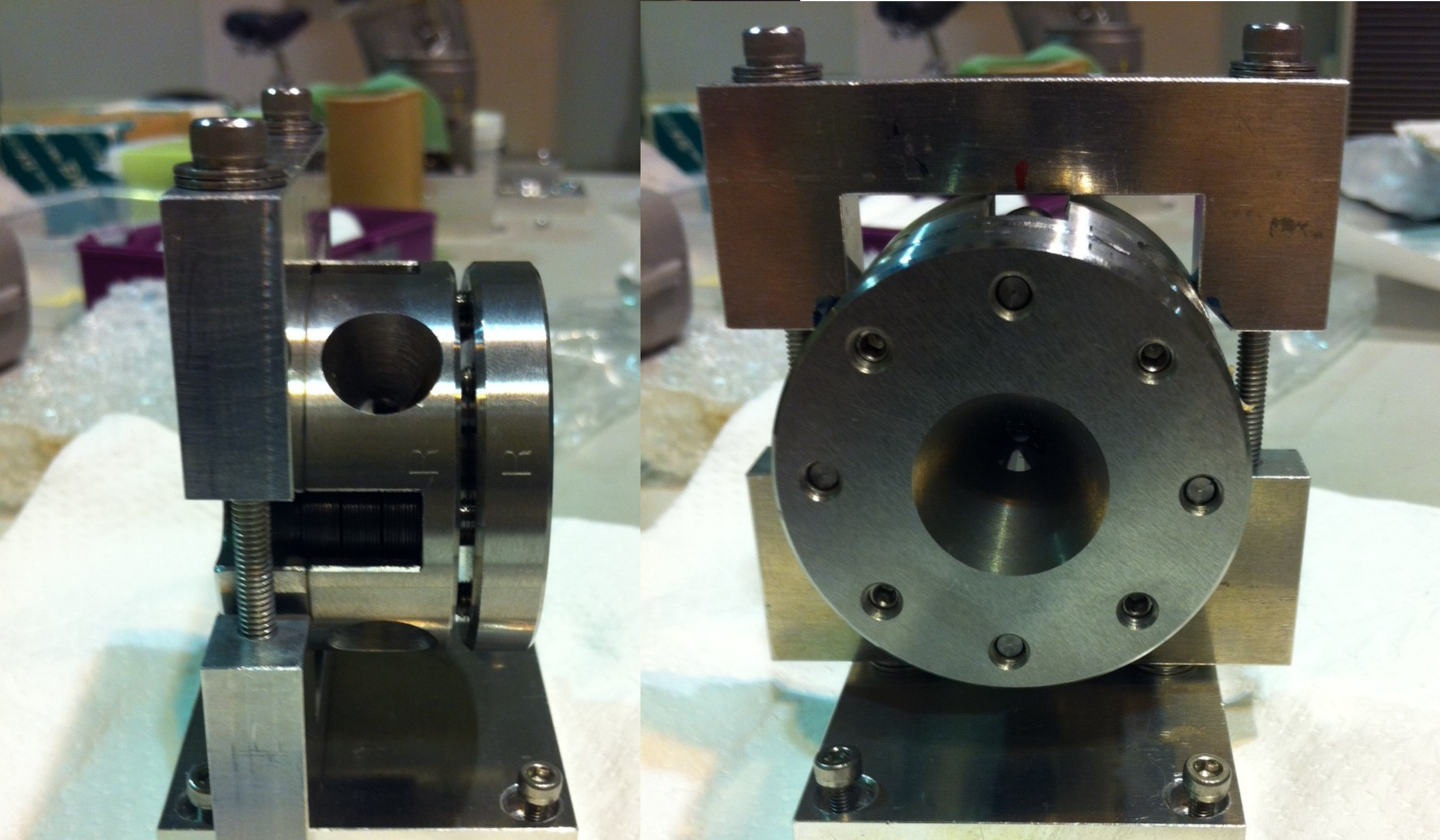
BL35XU for High pressure and temperature:

IXS Optics [Baron et al., 2000]

- Si (9 9 9) reflection: 2.8 meV resolution at 17.794 keV:
- Kirkpatrick-Baez mirror pair: **16 × 16 μm** beam size

XRD: Flat panel area detector

Heating: Portable laser heating system COMPAT (Fukui et al., 2013)

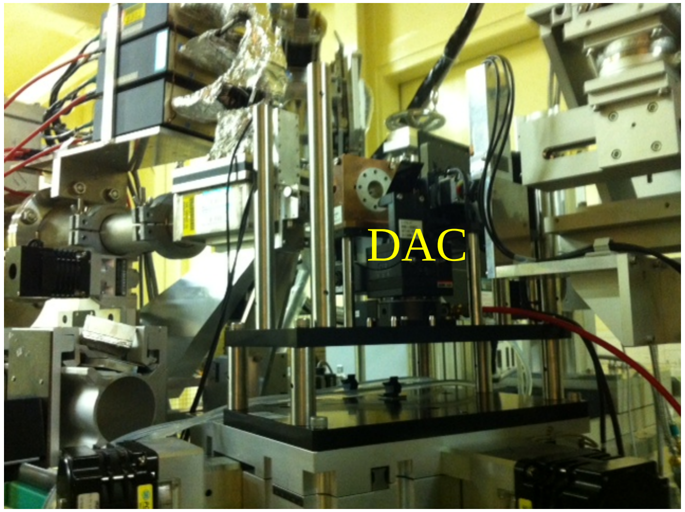


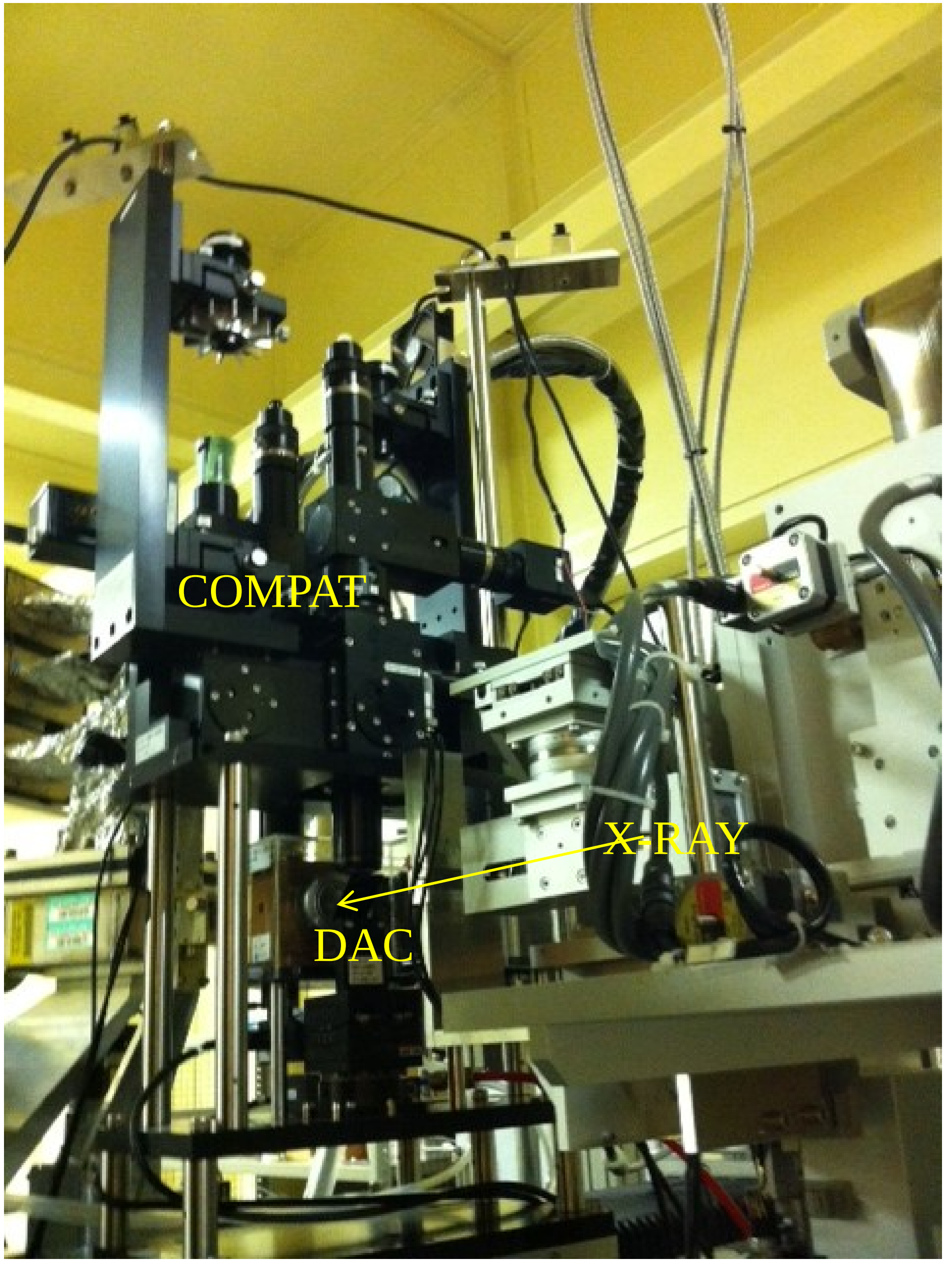
Symmetric diamond anvil cell used for IXS measurement at very high pressures: Culet size of **0.10 mm for 174 GPa and 300 K**

Portable Laser heating system for IXS:

COMPAT (COMpact system for generating extreme Pressures And Temperatures (Fukui et al., 2013)

31 hours stable heating at 2300 K and 10 hours heating at 3000 K





Sound velocity measurements:

Light elements in the inner core (BL35XU)

1. FeH: ~70 GPa at 300 K, Shibazaki et al (2012)
2. hcp-Fe : ~174 GPa, 300 K, Ohtani et al (2013)
3. Fe_3S: ~84.5 GPa, 300 K, Kamada et al. (2014)
4. hcp-Fe: ~88GPa, 1000 K, Ohtani et al (2015)
5. hcp-Fe: ~164 GPa, 3000 K. Sakamaki et al (2016)
6. Fe_3C: ~86 GPa, 2300 K, Takahashi et al. (2018)
7. $Fe_{0.89}Si_{0.11}$ alloy: 90 GPa, 1800 K Sakairi et al. (2018)
8. Fe-Ni alloy: ~160 GPa, 2500 K (in prep.)

Higher Pressure and Pressure scale to multi-Megabar (BL43XU)

1. Re: Primary scale of Rhenium ~ 210 GPa

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Higher Pressure and Pressure scale to multi-Megabar (BL43XU)

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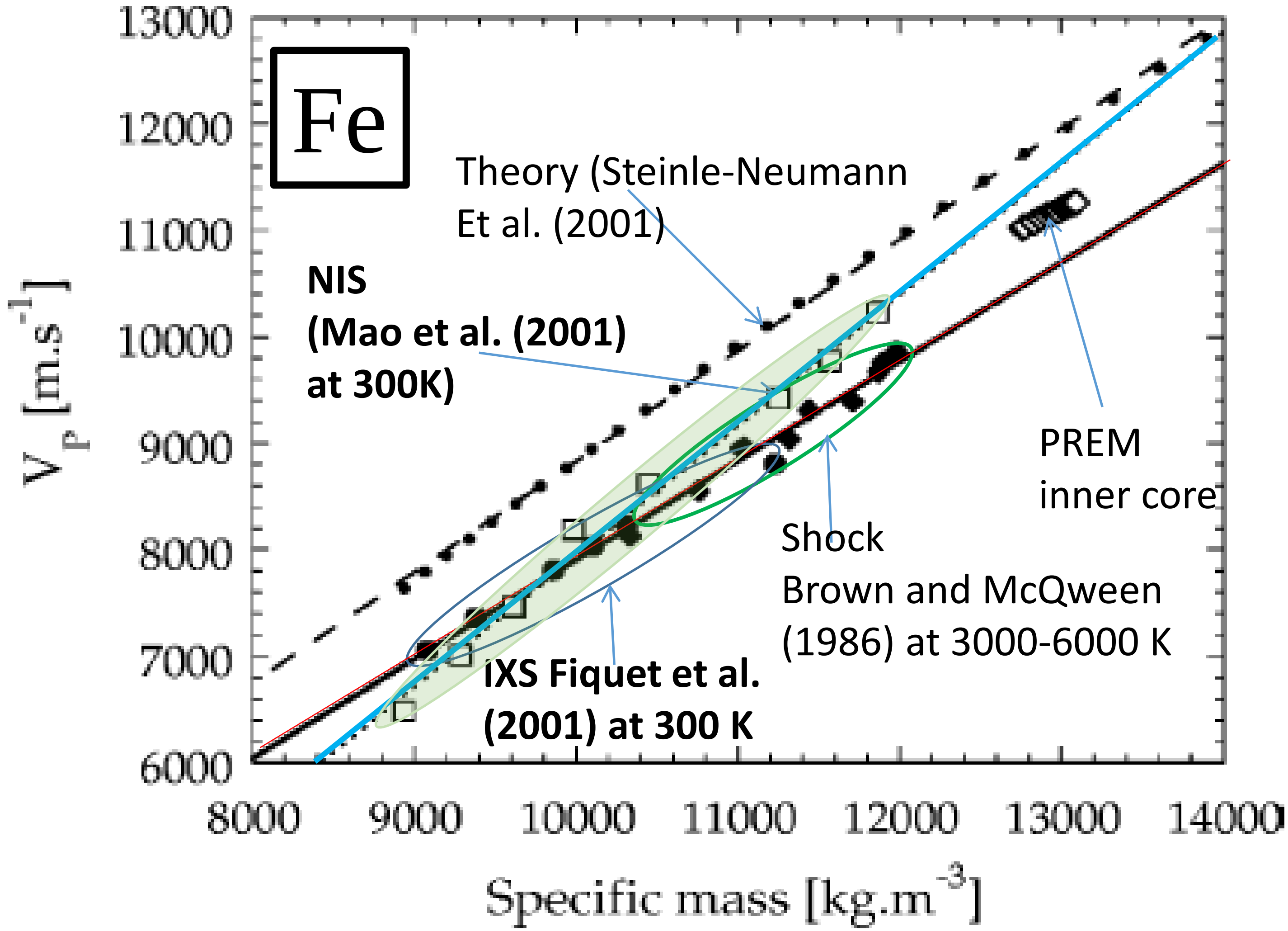
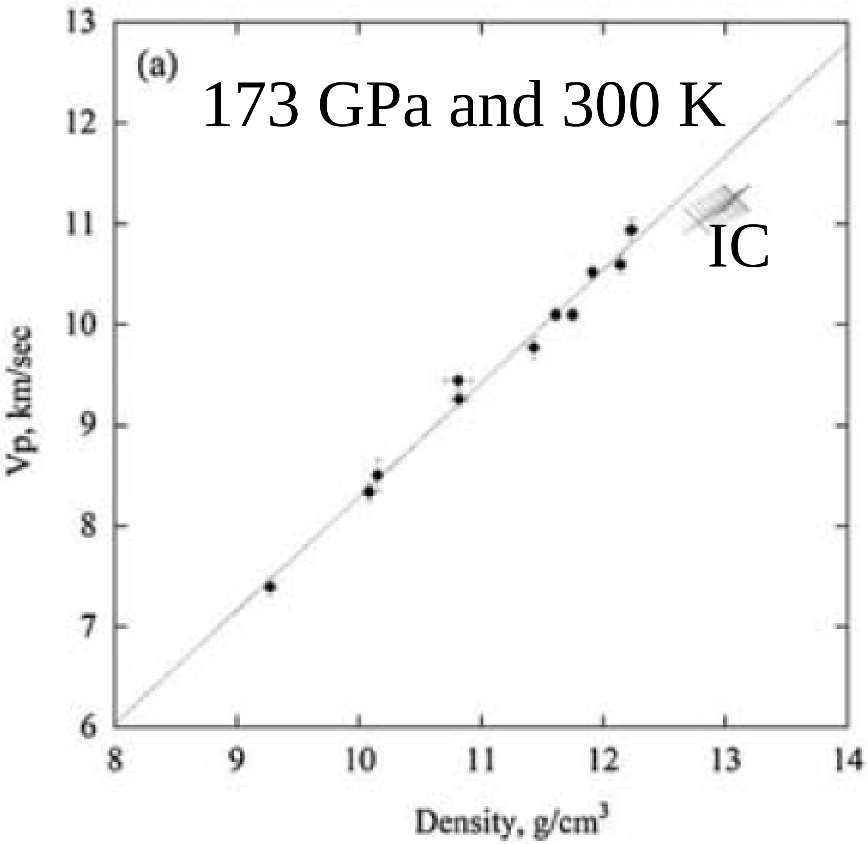
After Fiquet et al. (2004)



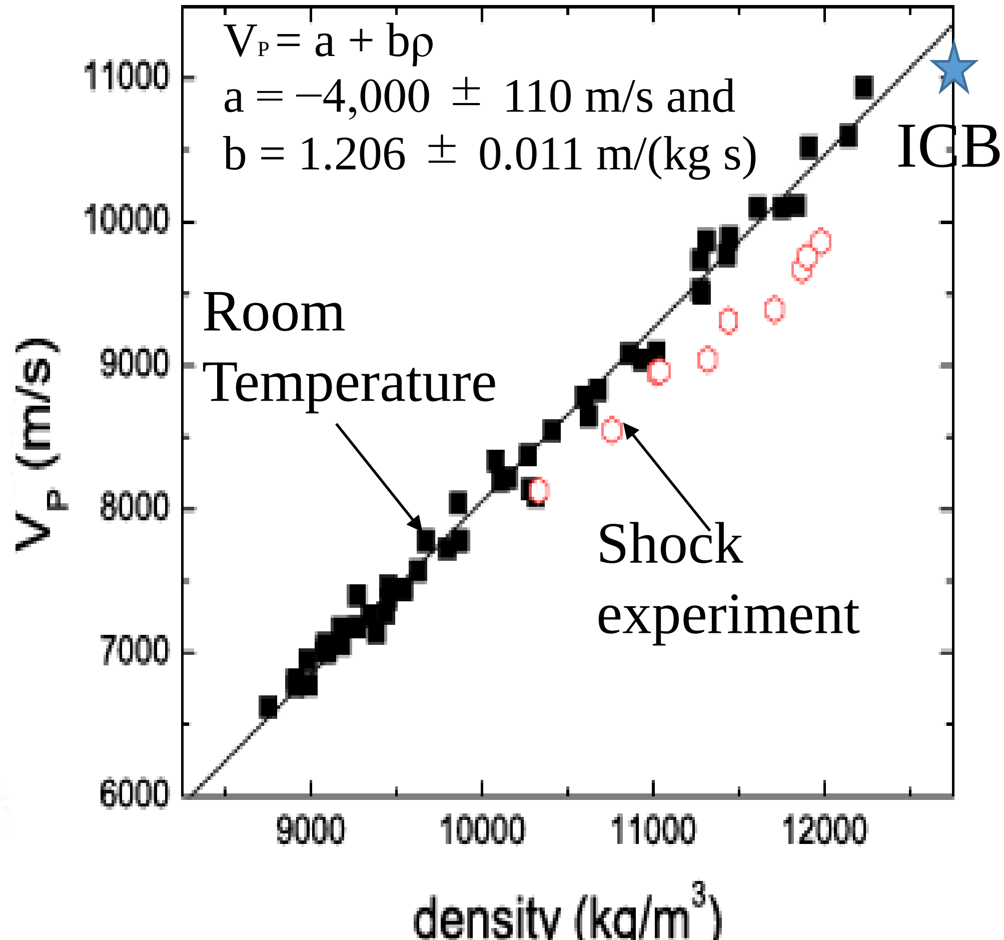
Discrepancy:
IXS and Shock vs NIS (NRIXS) ?
Temperature effect on Birch law ?

Compressional velocity of hcp-Fe at room temperature

Ohtani et al. (GRL, 2013)



Antonangeli and Ohtani (PEPS, 2015)



Data from Mao et al., 1998; Crowhurst et al., 2004; Antonangeli et al., 2004b; 2012; Ohtani et al., 2013; Decremps et al., 2014).

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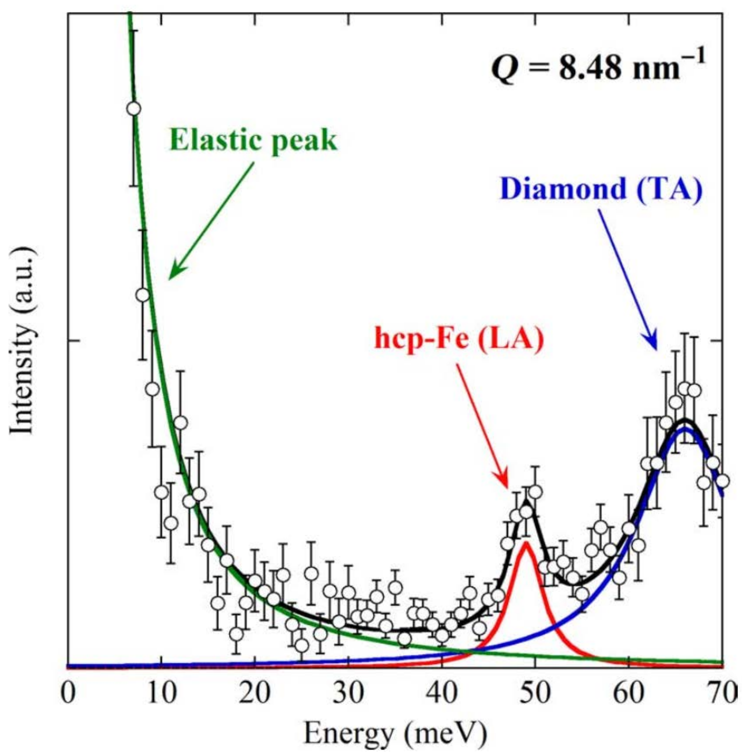
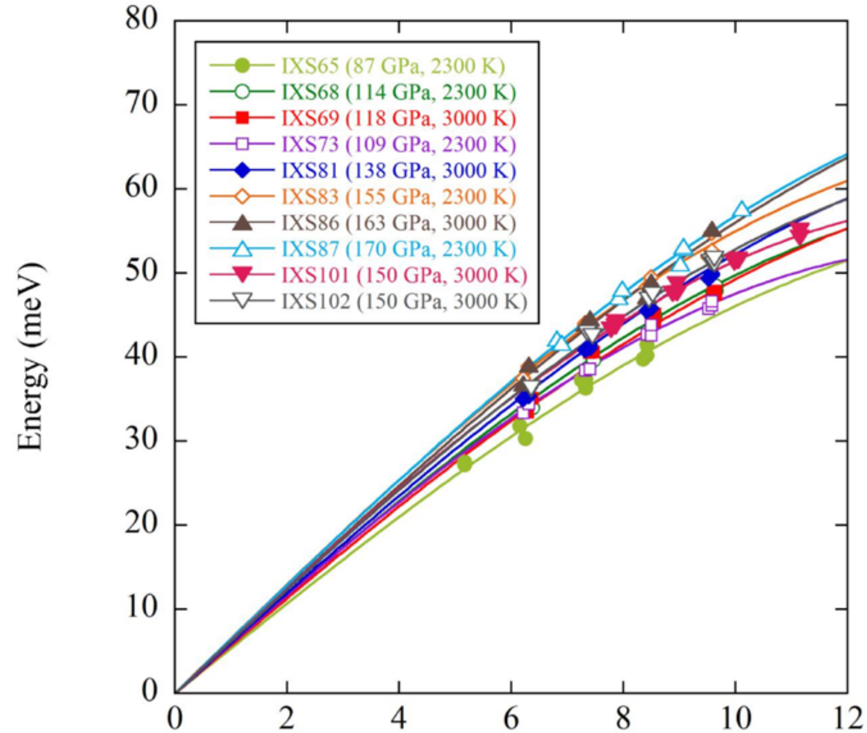
Tohoku U.

Sakamaki et al., (2016)

hcp-Fe: ~163 GPa, ~3000 K



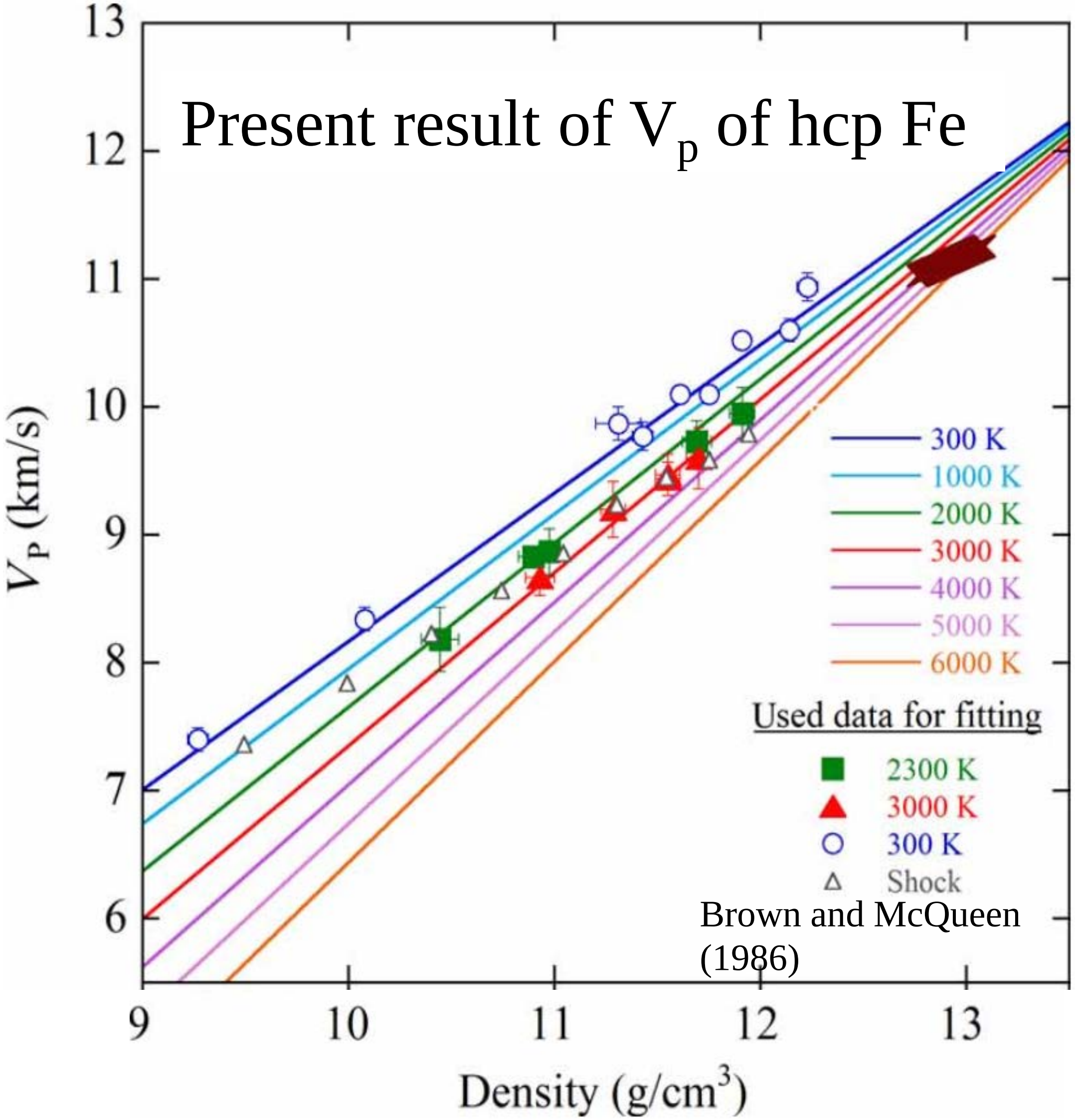


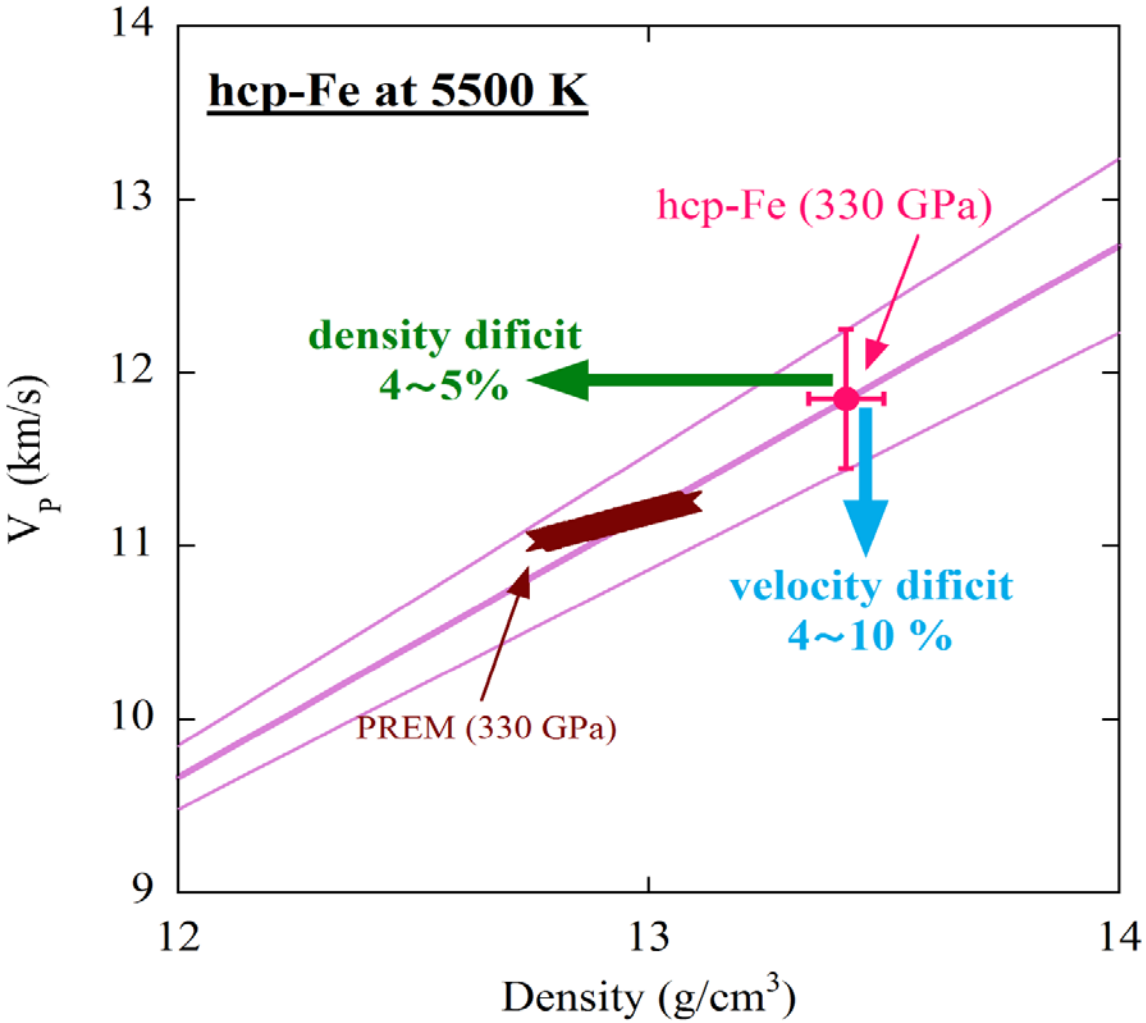
The dispersion curve was fitted by a sine function for determining Vp

$$E[\mathrm{meV}] = 4.192 \times 10^{-4}\ \mathbf{V_P[m/s]}\ Q_{MAX}[\mathrm{nm}^{-1}] \sin\left(\frac{\pi}{2}\frac{Q[\mathrm{nm}^{-1}]}{Q_{MAX}[\mathrm{nm}^{-1}]}\right)$$

Isothermal ρ-V_P fitting lines for **hcp-Fe** are expressed as

V_P (km/s)= [1.160ρ(g/cm^3) - 3.43] + [7.2 × 10^{-5} × (T(K) - 300) × (ρ (g/cm^3)– 14.2)]



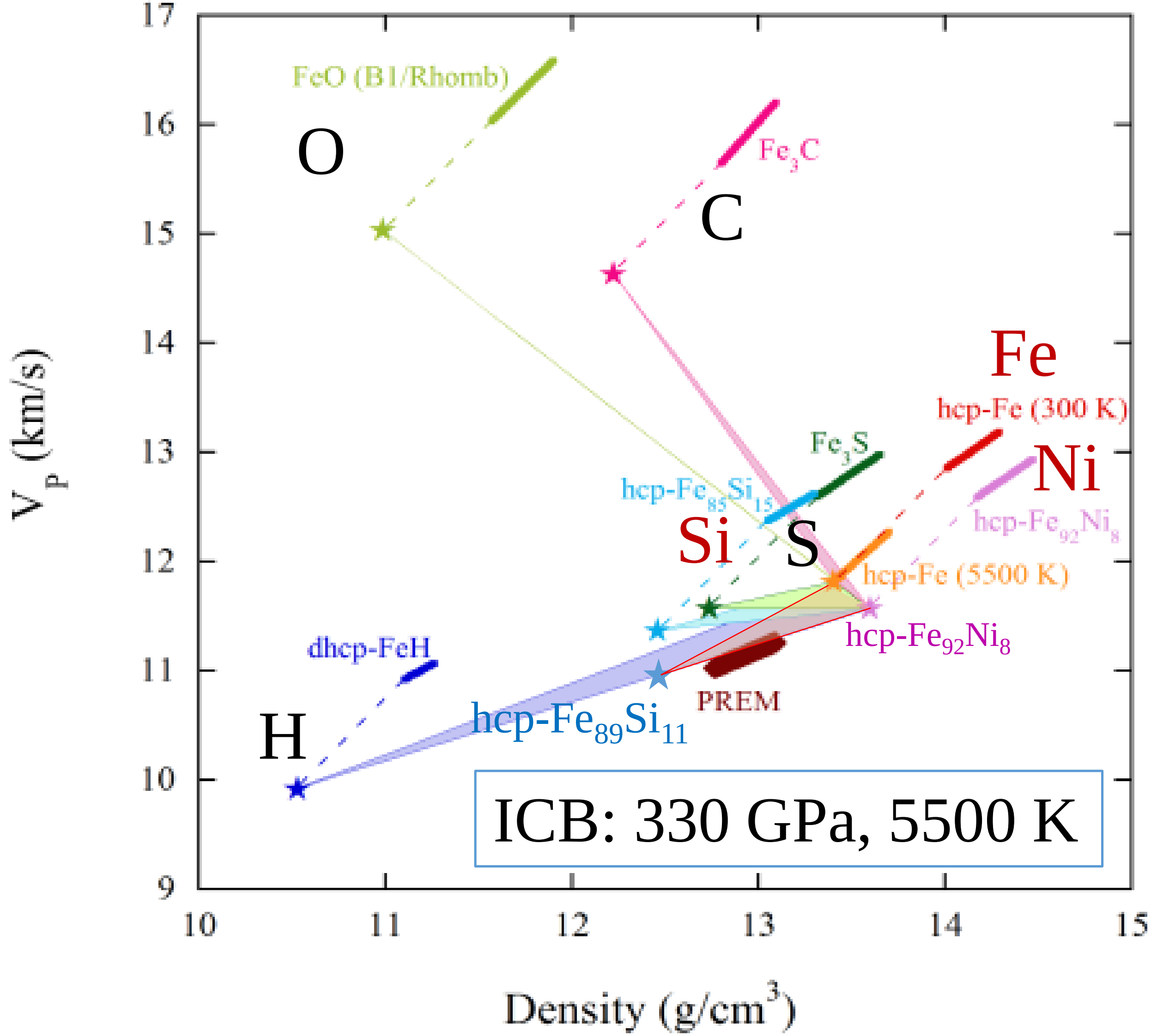


Effect of light elements:

Inner core: Vp, Vs of hcp-Fe > Vp, Vs of PREM inner core.

Outer core: V_p of liquid hcp-Fe < V_p of PREM outer core.

The effect of light elements on Birch's law of hcp-Fe



Two topics

・Sound velocity of iron and its alloy compounds and the Earth's core

・Sound velocity at multi-Megabar pressure and the primary pressure scale

BL43XU Higher pressure: P>200 GPa

IXS Optics [Baron et al., 2016]

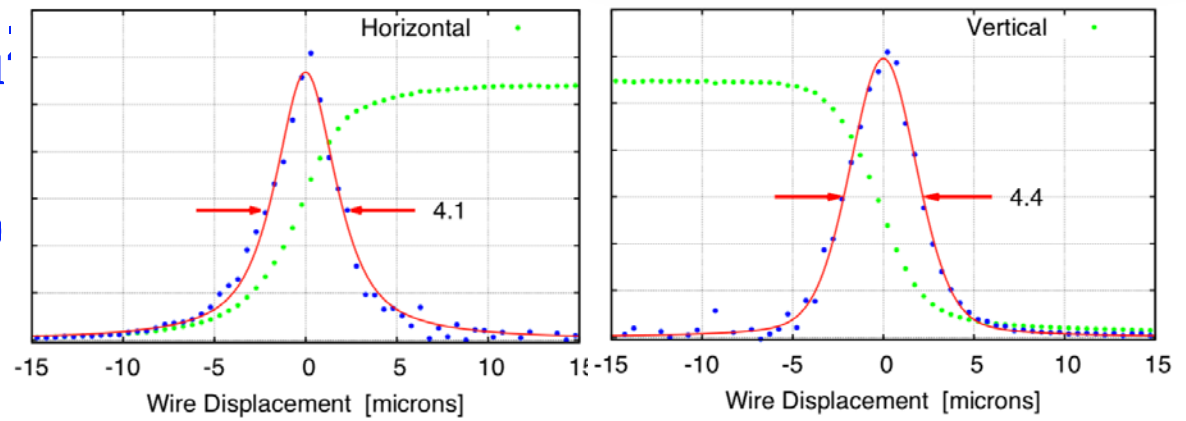
- Si (9 9 9) reflection: 2.8 meV resolution at 17.793 keV:
- Multilayer Kirkpatrick-Baez (KB) mirror pair: **5×5 μm** beam size
- **Soller screen** [Baron, 2019]: to reduce scattering backgrounds from the diamond and to improve the signal to noise ratio

XRD: Flat panel area detector

BL43XU Optics: Baron et al. (2000)

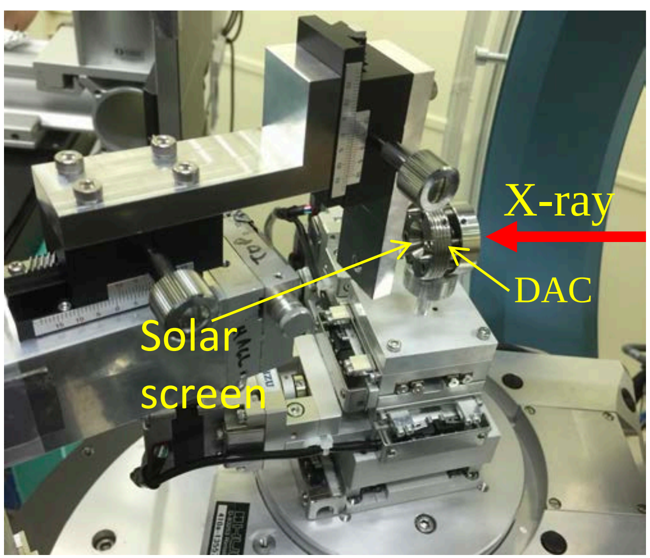
IXS with Diamond Anvil Cells (DACs) @ P> 200 GPa

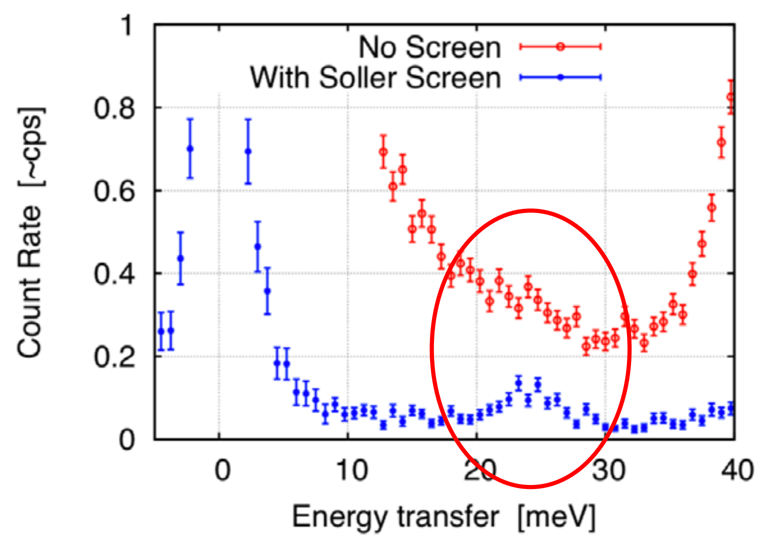
Focus Size: 5 x 5 μm
(FWHM):
Elliptical KB (Multilayer)
for 17.8 keV



Soller Screen

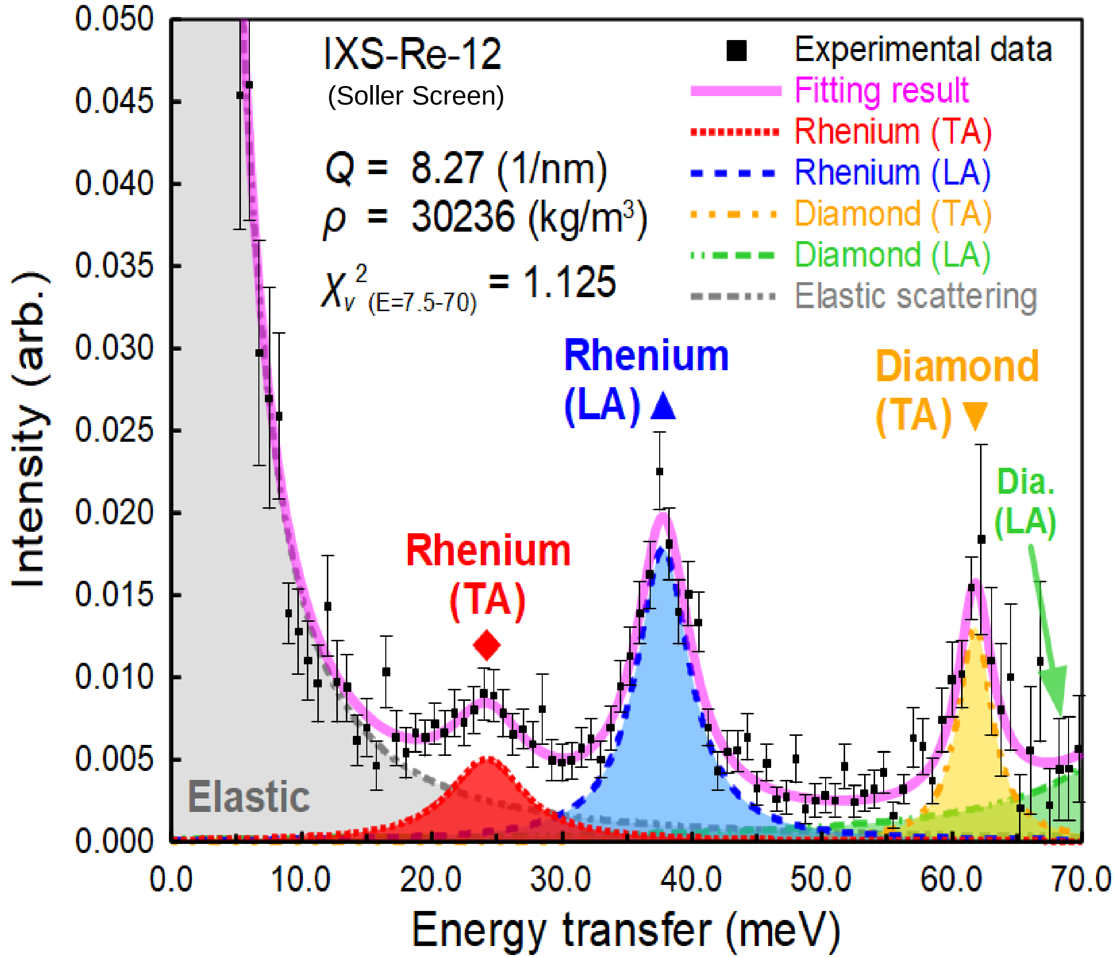
HP DAC work limited by **background from diamonds** (or Be gasket) ie: parasitic scattering from within a few mm of the sample





Shear/Transverse (TA) Modes of Rhenium

(1) Good signal to noise (Soller screen) and (2) Simple setup (**no pressure medium**) make it possible to unambiguously **identify the transverse modes of Re**



Daijo Ikuta
Tohoku U.

P~210 GPa and 300 K

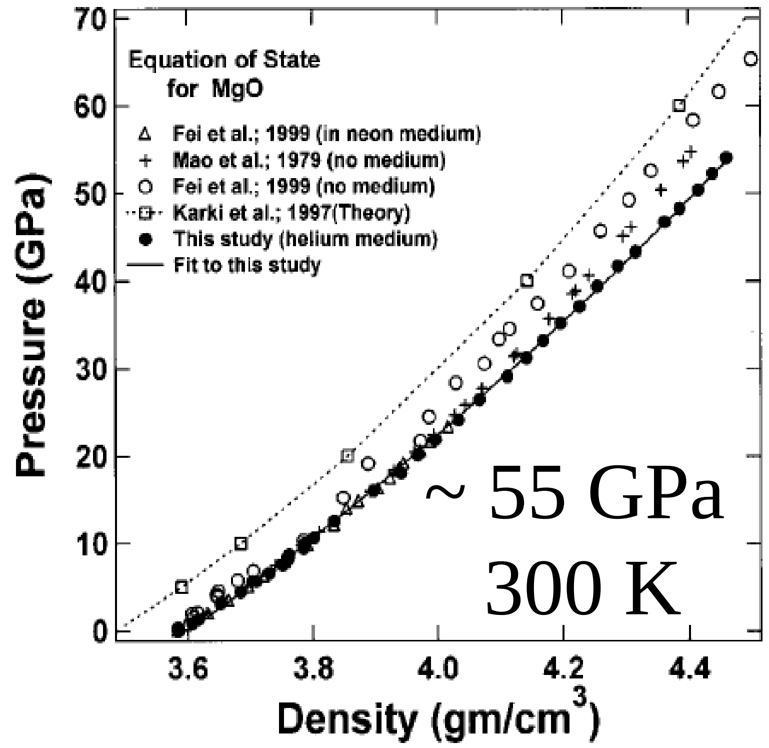
Primary Pressure Scale

Relate the density of a material (MgO, Gold, Re, etc) to P (at well-defined T)

Primary pressure scale: ρ (density), V_p and V_s

MgO Primary Scale
Brillouin Scattering with a High Pressure Cell gets both V_p and V_s at 300 K (Density from separate x-ray works)

~55 GPa at 300 K



Zha, Mao & Hemley, PNAS 2000

Primary Pressure Scale

$$v_p = \sqrt{\frac{K_S + (4/3)G}{\rho}} \qquad v_S = \sqrt{\frac{G}{\rho}}$$

$$K_{T(PT)} = \frac{K_{S(PT)}}{1 + \left[\alpha_{V(T)} \times \gamma_{(PT)} \times T\right]}$$

$$K_{T(PT)} = \rho_{(PT)} \left(\frac{\delta P}{\delta \rho}\right)_T$$

Integration of $\left(\frac{\delta P}{\delta \rho}\right)_T$ provides a primary pressure scale

Primary Pressure Scale $\quad P_{(\rho T)} = \int_{\rho_{(0T)}}^{\rho_{(PT)}} \frac{K_{T(PT)}}{\rho_{(PT)}} \delta\rho$

Summary

We determined Vp of iron, and iron-light element (Si, S, O, H…) alloys using IXS to the Earth’s core conditions

We proposed the Re primary pressure scale using Vp, Vs, and ρ of Re measured by IXS to 210 GPa.

Thank you for your attention!