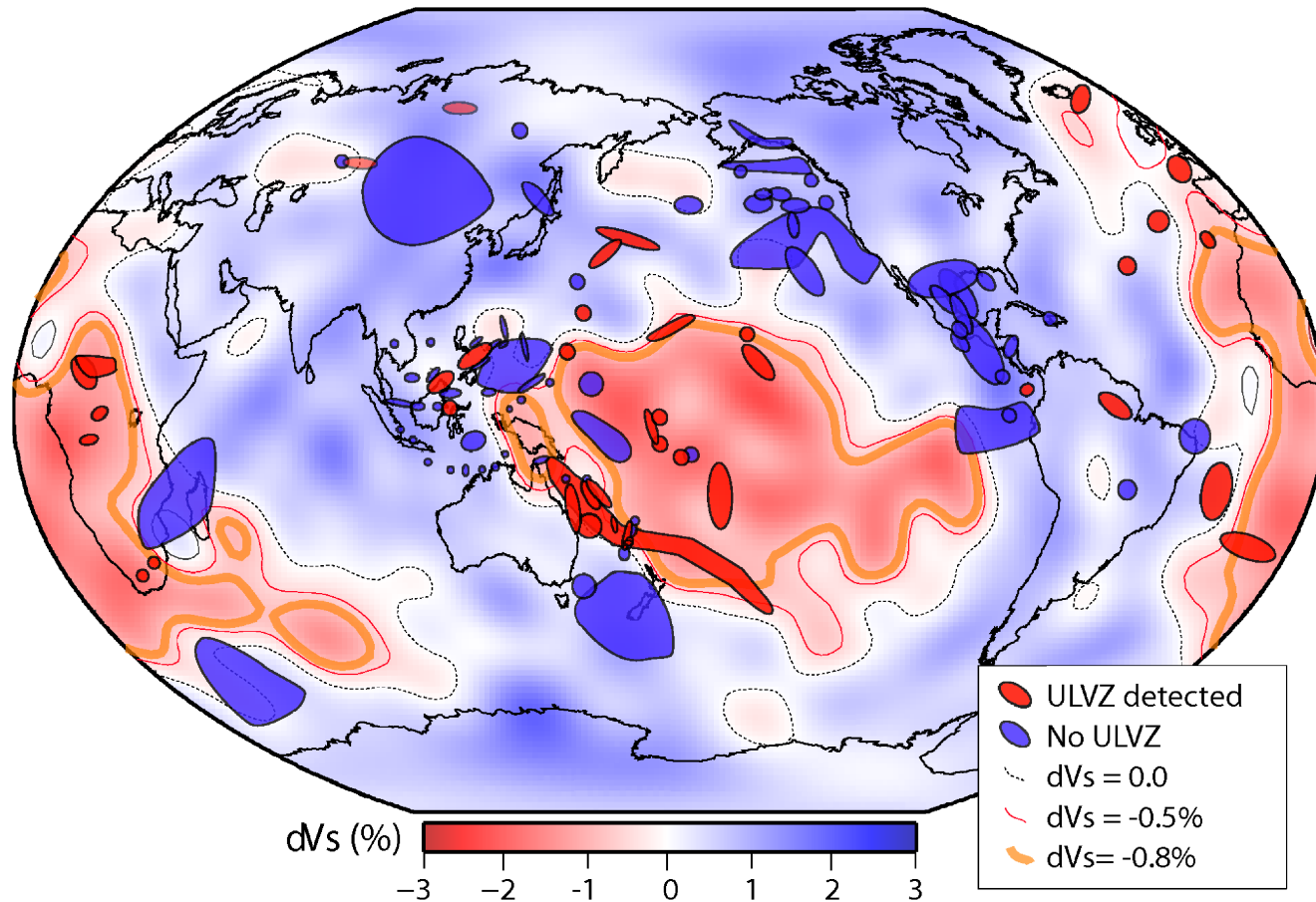


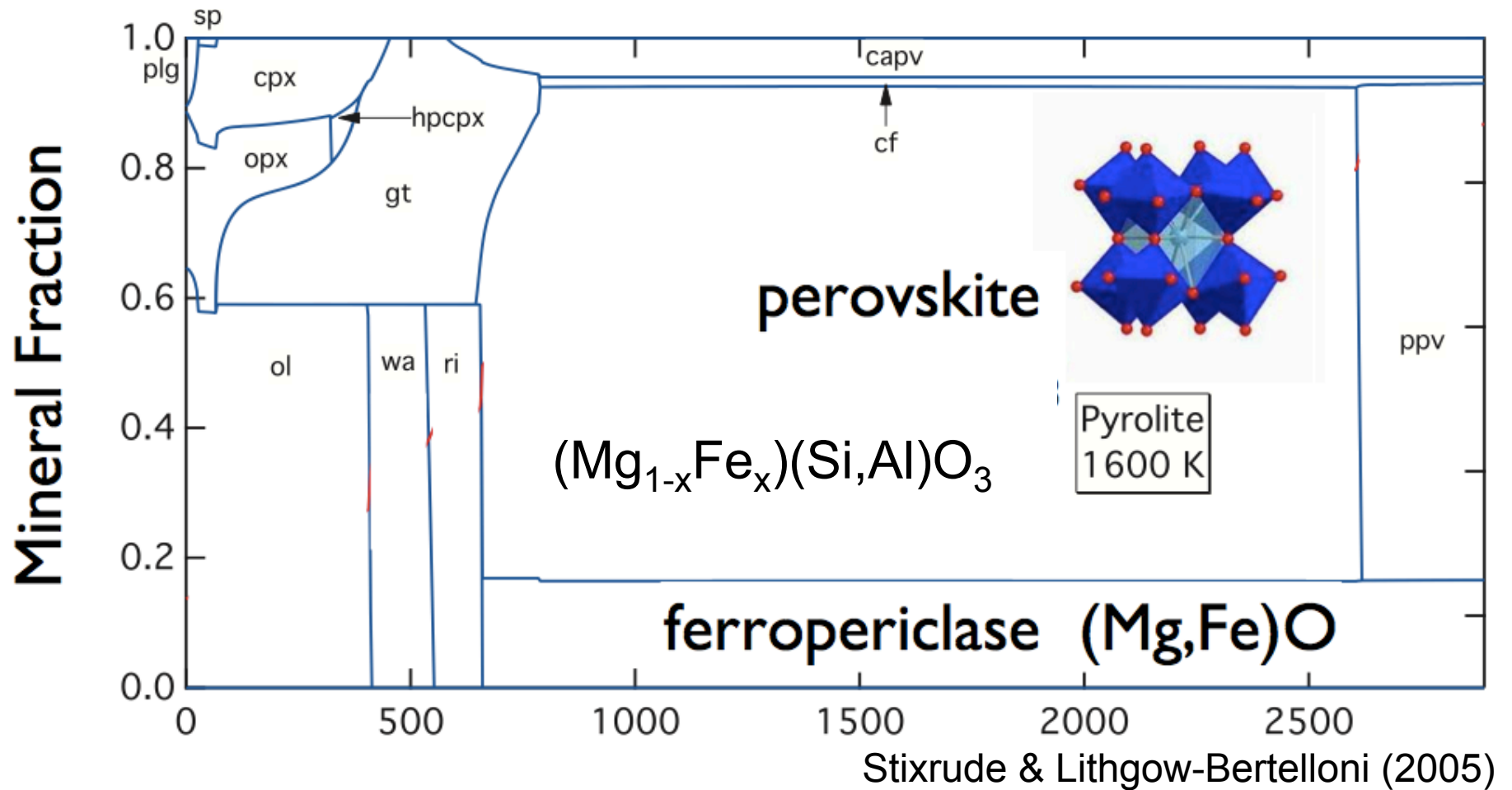
# Distributions of ultra-low velocity zones (ULVZs)



McNamara *et al.* *EPSL* 2010

- Slow
  - ~10 to 30% drop in  $V_s$
  - ~5 to 20% drop in  $V_p$
- Variable
  - $V_p/V_s$  range ~1 to 5
  - Not well-constrained
- Density
  - Constrained?

# Major minerals in Earth's mantle



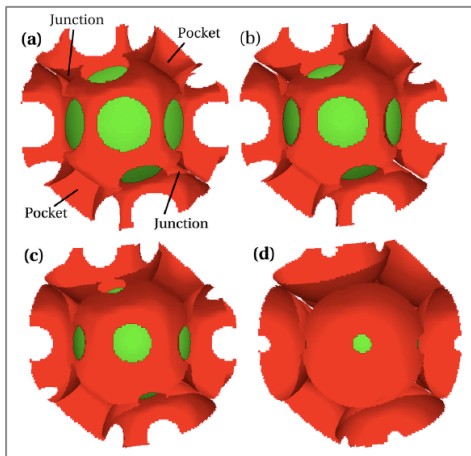
$$0.05 \leq x \leq 0.35$$

Fe<sup>2+,3+</sup>  
spin state

# Explanations of low velocities in ULVZs

## Partially Molten ULVZ

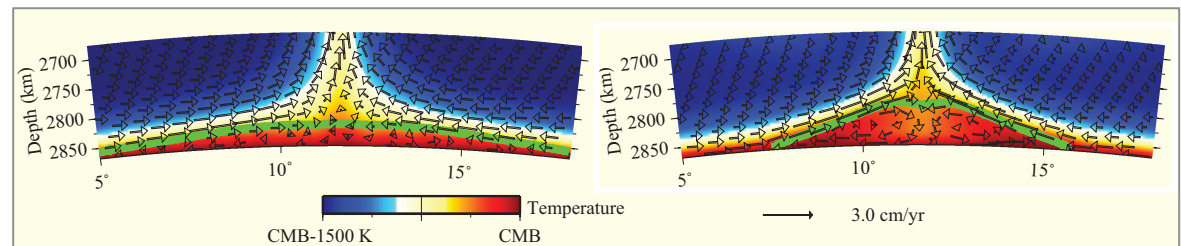
- Increased melt fraction  
→ lower velocities
- How to make dense enough melts?
  - Shock melting on Mg-Fe silicates indicate melts are not dense enough to stick around (Thomas *et al.* 2012)
- How to maintain enough melt 10s of km high?



Wimert and Hier-Majumder, 2012

## Solid ULVZ

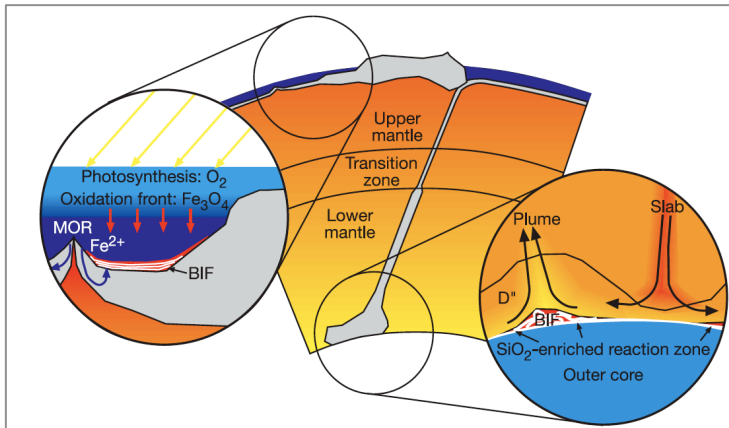
- Increased iron content  
→ lower velocities
- Relationship between sound velocity and density?
  - Iron-rich post-perovskite (Mao *et al.*, 2004)
- How to decrease velocities without making it too dense?
  - Iron-rich (Mg,Fe)O (this study)



Bower *et al.* EPSL 2011

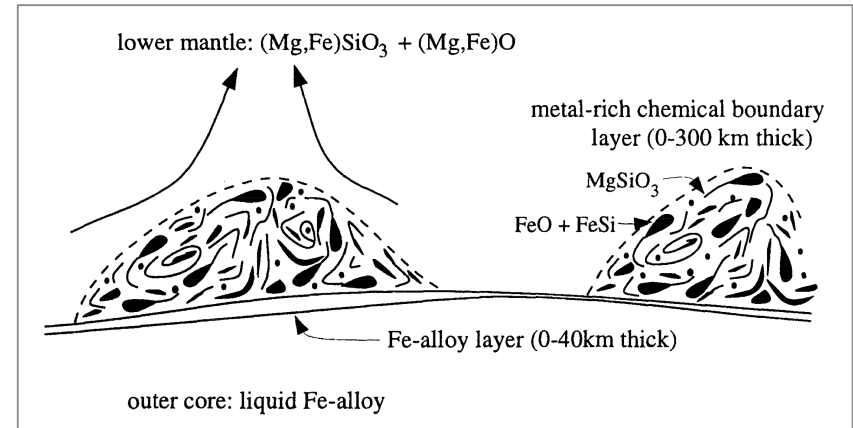
# Formation mechanisms suggested for ULVZs

## Dense, subducted material



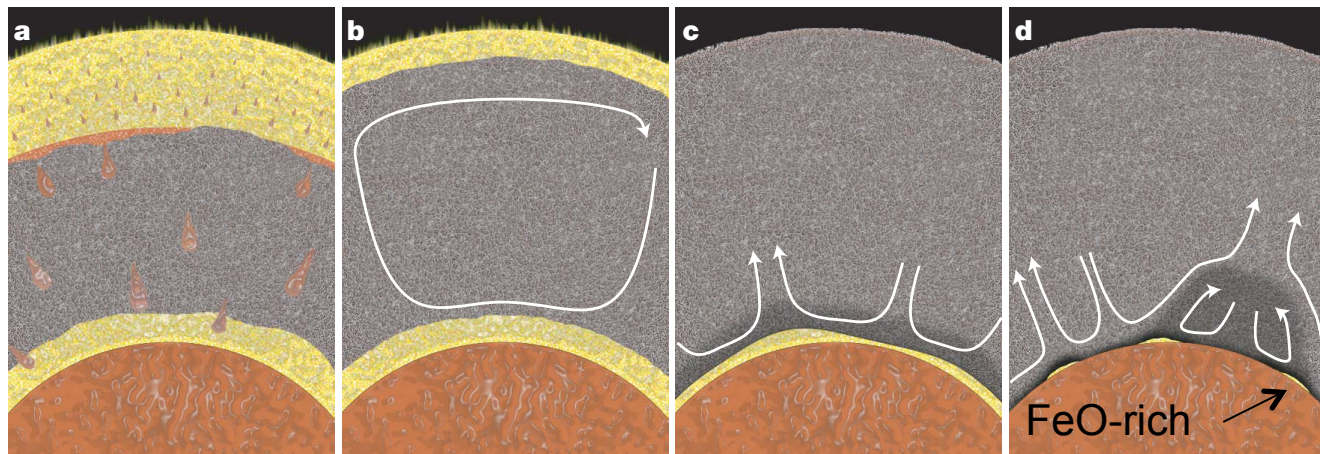
*Dobson and Brodholt (2005)*

## Interaction with the core



*Manga and Jeanloz (1996)*  
*Otsuka & Karato (2012)*

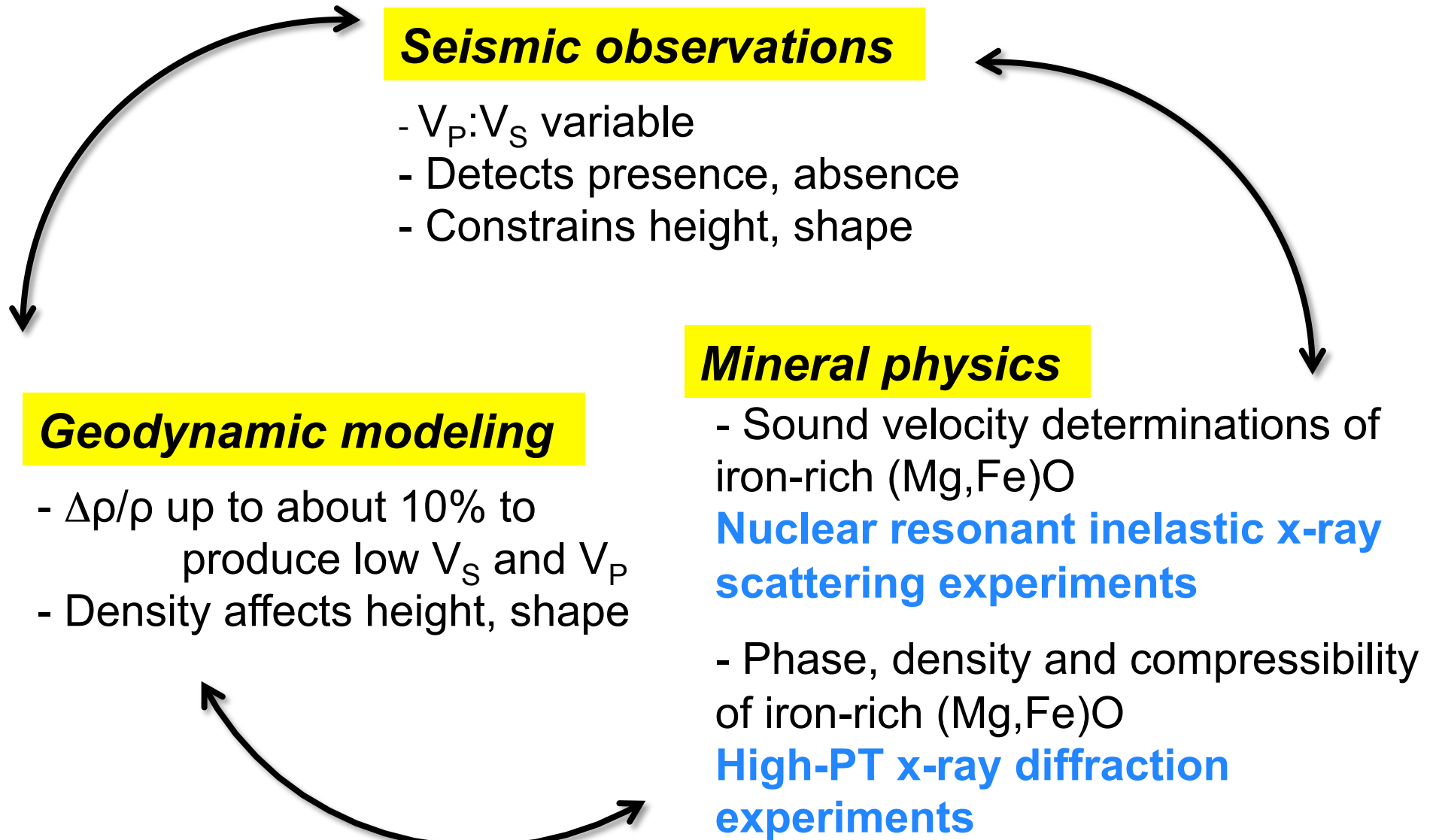
## Residues of a crystallizing magma ocean



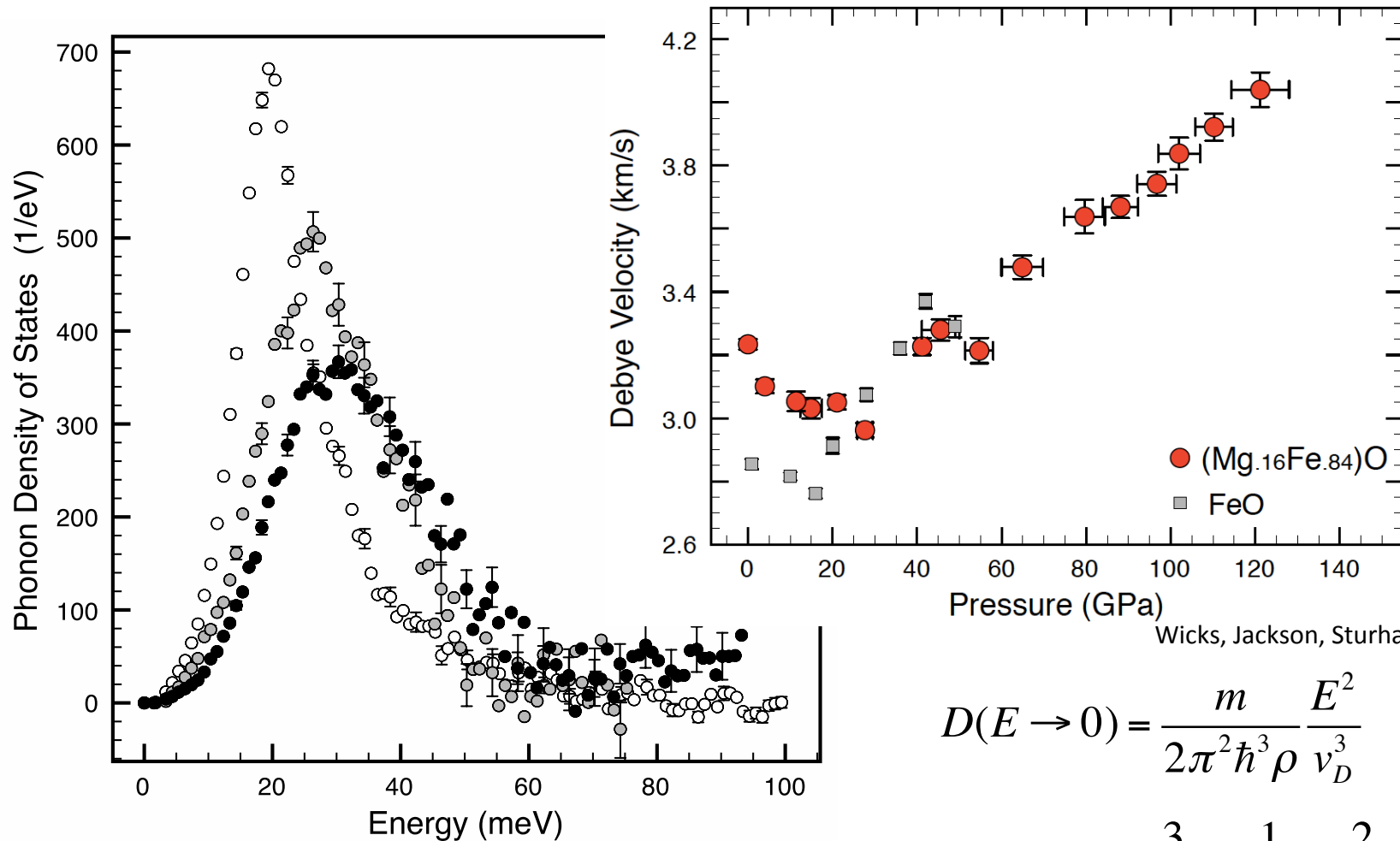
*Labrosse et al. (2007)*



# Approach to investigate ULVZs



# Partial phonon density of states of $(\text{Mg}_{0.16}\text{Fe}_{0.84})\text{O}$ , “iron-rich”



Wicks, Jackson, Sturhahn. (*GRL* 2010)

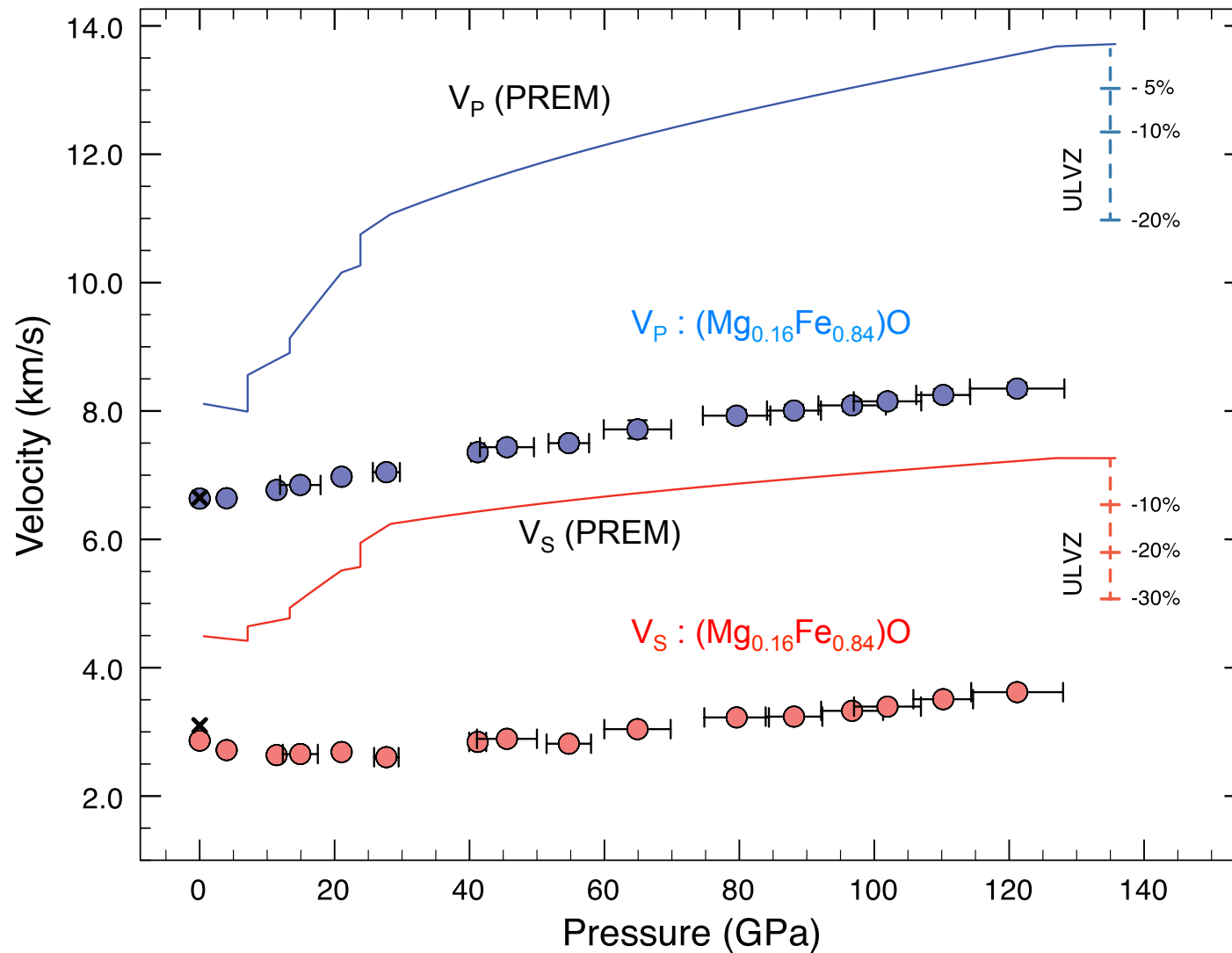
$$D(E \rightarrow 0) = \frac{m}{2\pi^2 \hbar^3 \rho} \frac{E^2}{v_D^3}$$

$$\frac{3}{V_D^3} = \frac{1}{V_P^3} + \frac{2}{V_S^3}$$

$$\frac{K_S}{\rho} = V_P^2 - \frac{4}{3} V_S^2$$

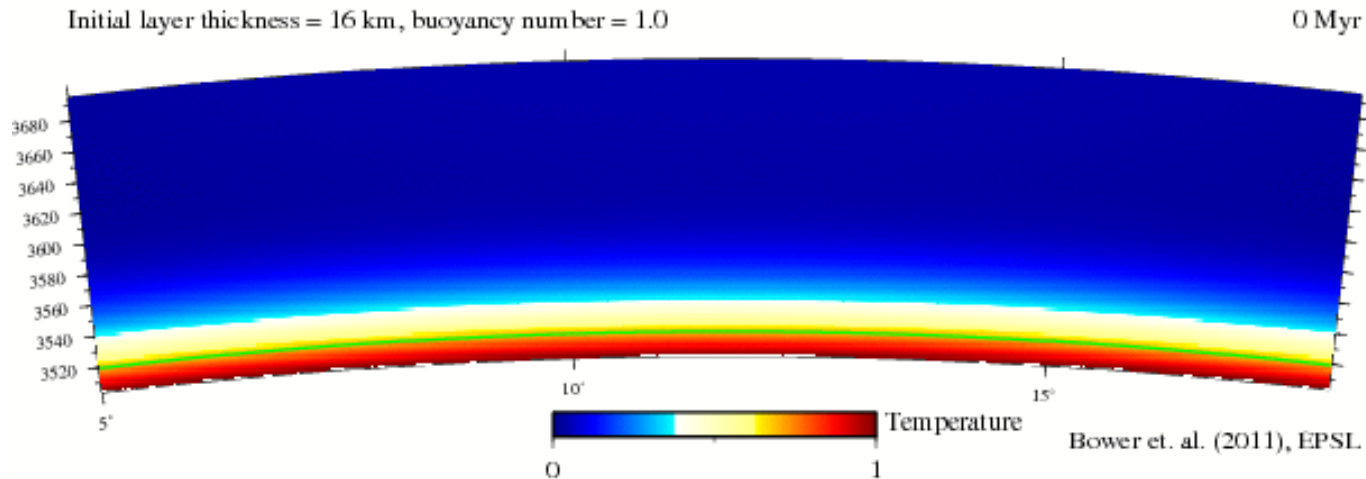
Software: **PHONIX**  
[www.nrinx.com](http://www.nrinx.com), Sturhahn,  
 Hyp. Int. 2000

# Iron-rich (Mg,Fe)O: Very low sound velocities at pressures approaching Earth's CMB

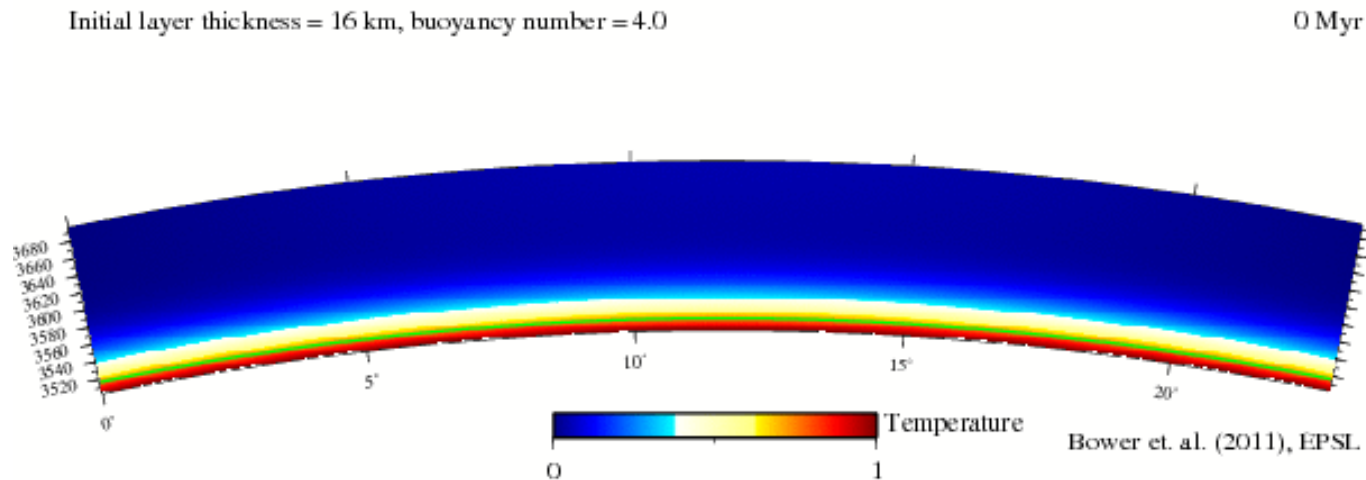


Revised from Wicks *et al.* GRL 2010

Density of iron-rich (Mg,Fe)O-bearing chemical layer:  
Constrains buoyancy and shape of structures near Earth's core-mantle  
boundary

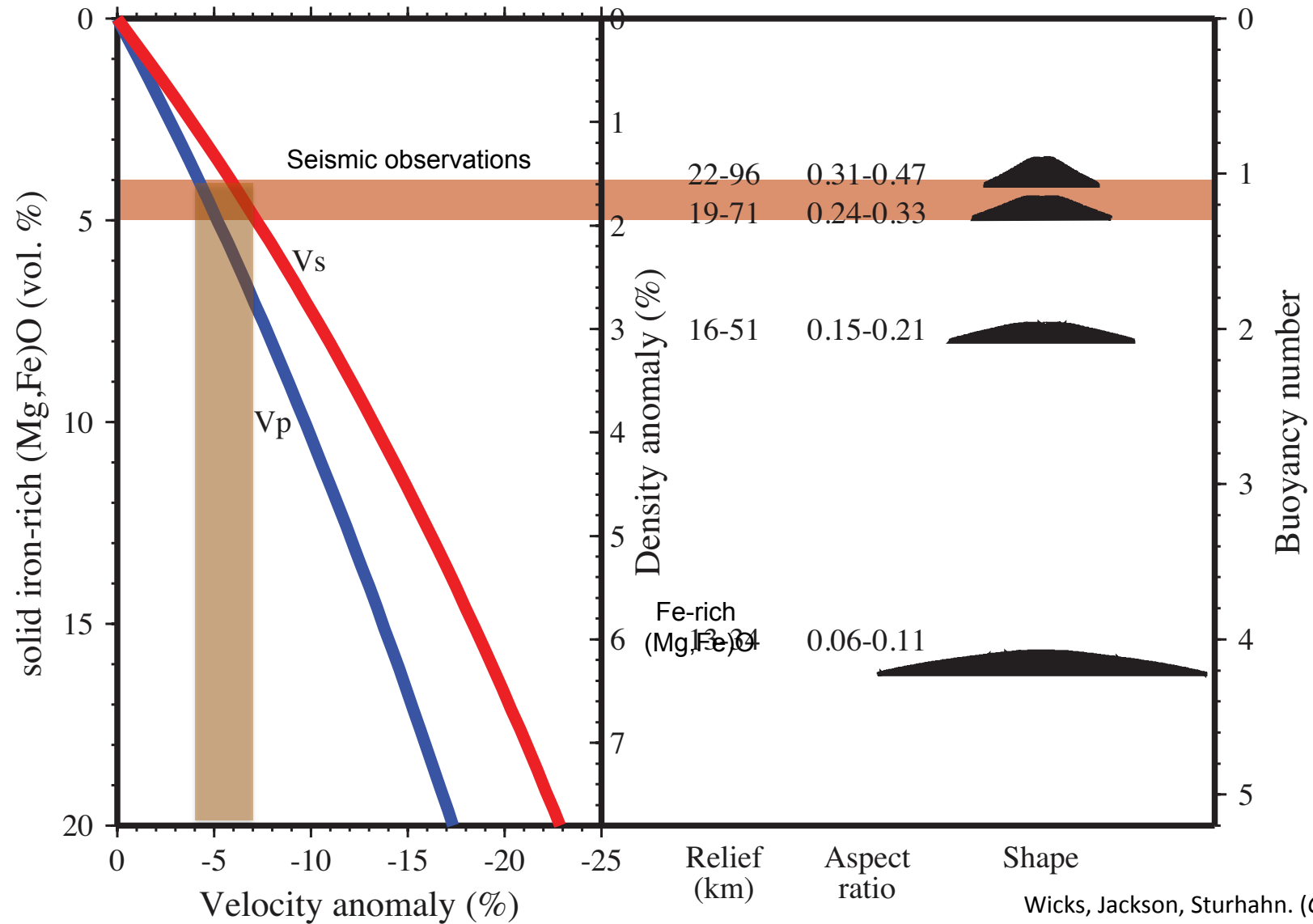


A few percent  
of iron-rich  
(Mg,Fe)O



About 10% of  
iron-rich  
(Mg,Fe)O

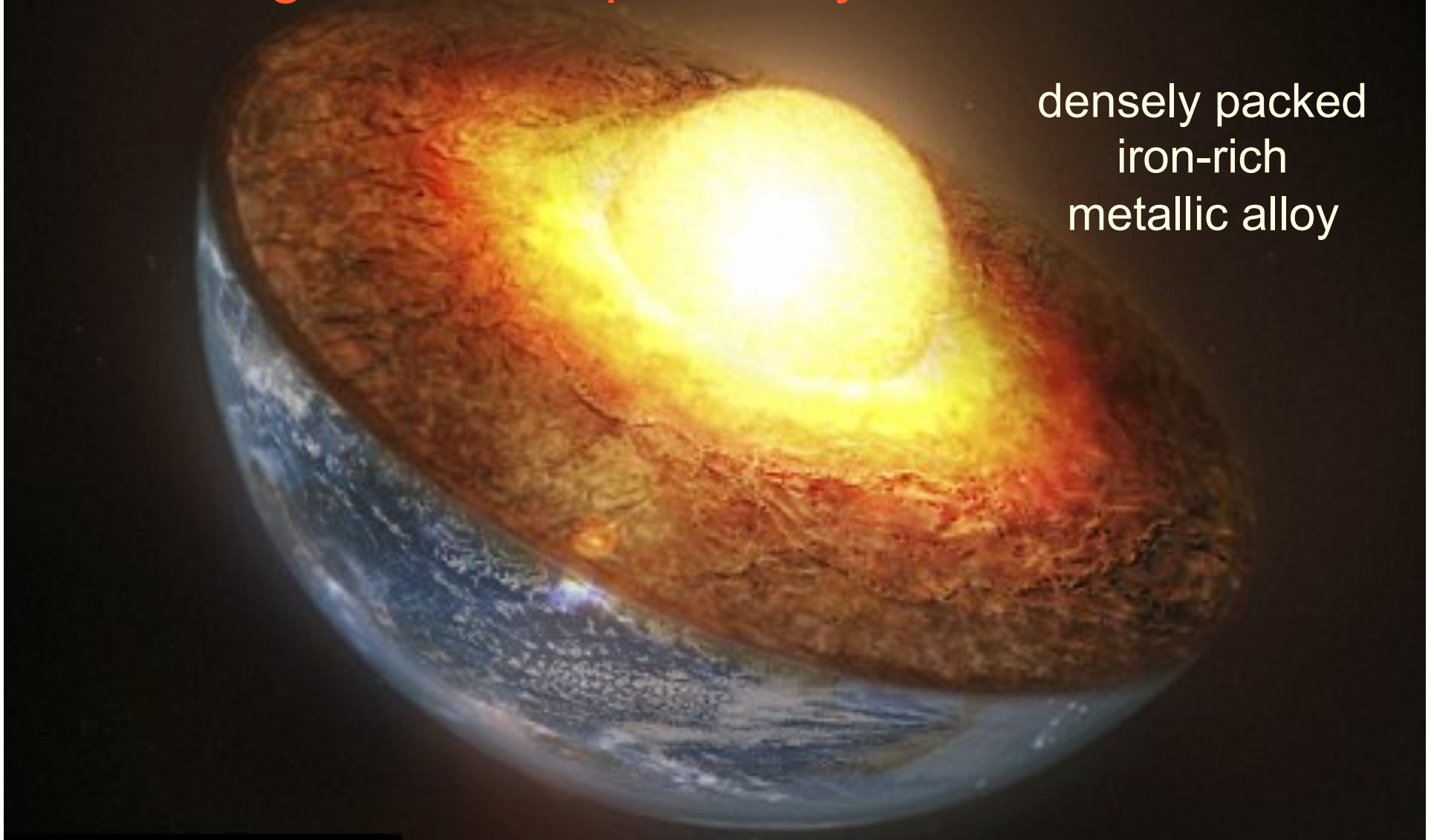
# Wave velocities and relief (shape) of iron-rich (Mg,Fe)O-bearing layer near Earth's core-mantle boundary



Wicks, Jackson, Sturhahn. (*GRL* 2010)  
 Bower, Wicks, Gurnis, Jackson. (*EPSL* 2011)  
 Sun, Helmberger, Jackson, Clayton, Bower. (*EPSL* 2013)

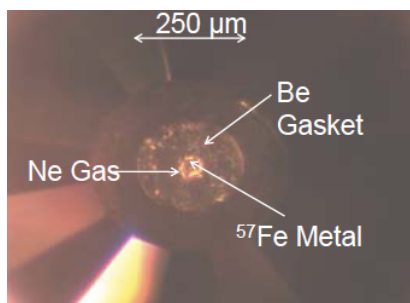


# Accessing terrestrial planetary cores

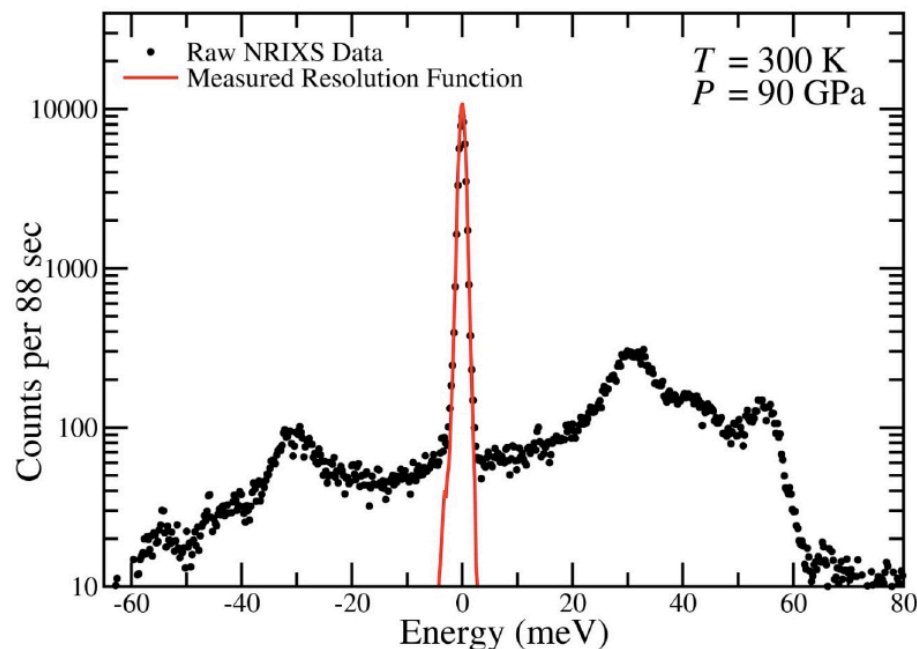


densely packed  
iron-rich  
metallic alloy

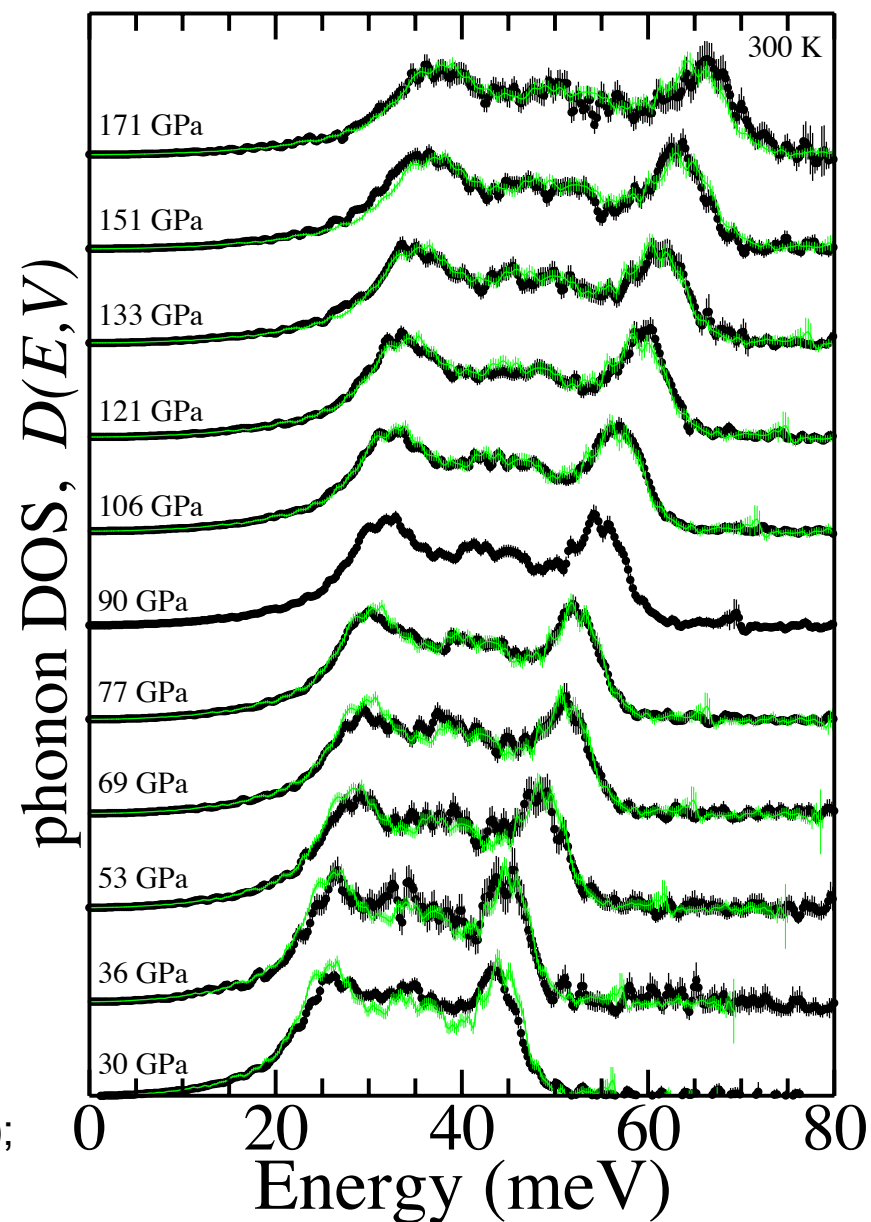
*Image credit: Discovery Channel*



# Volume dependence of the phonon DOS for *hcp*-iron to outer core pressures

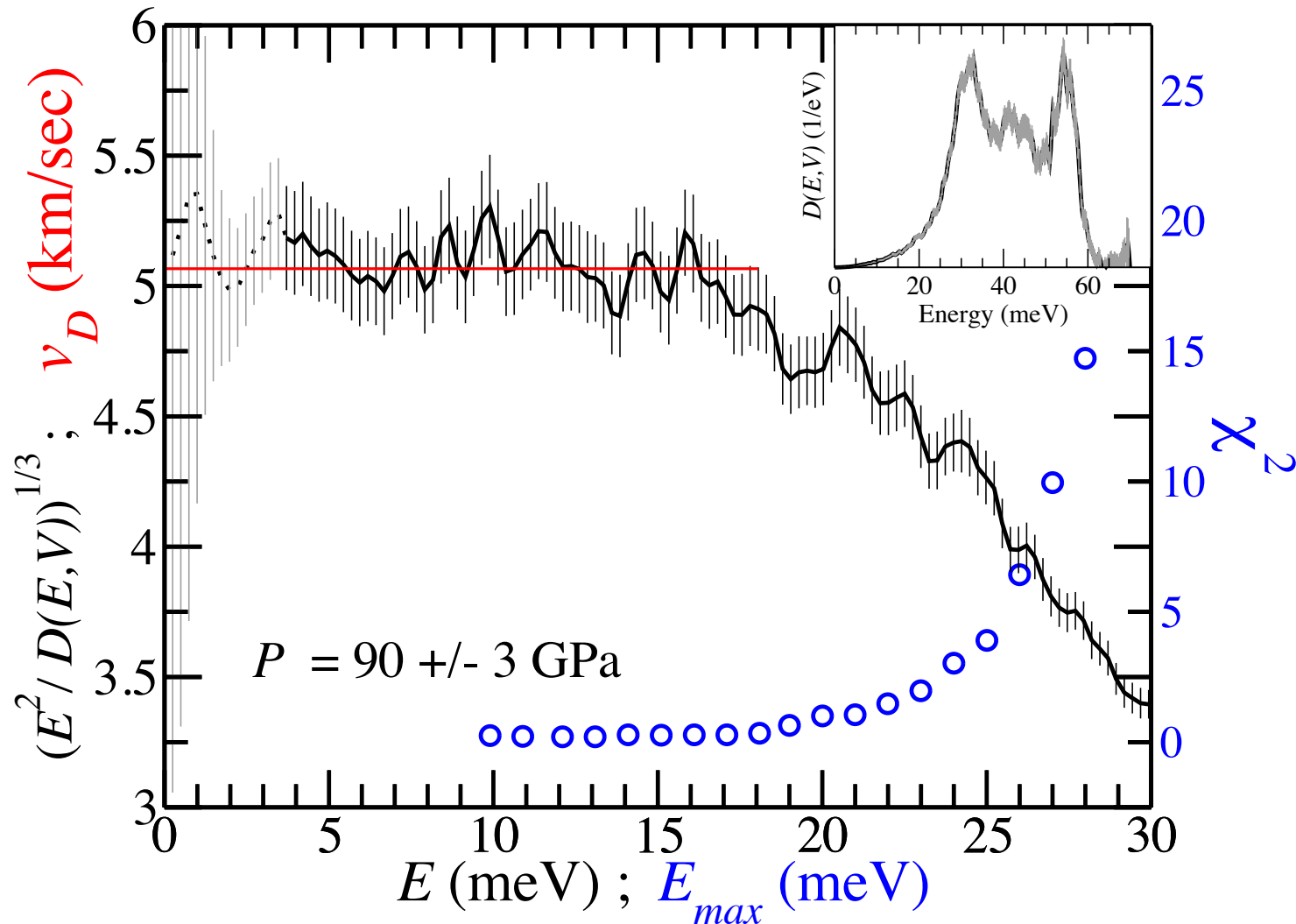


Fe sample loaded with neon  
Pressure scale: *Dewaele et al. PRL* (2006)

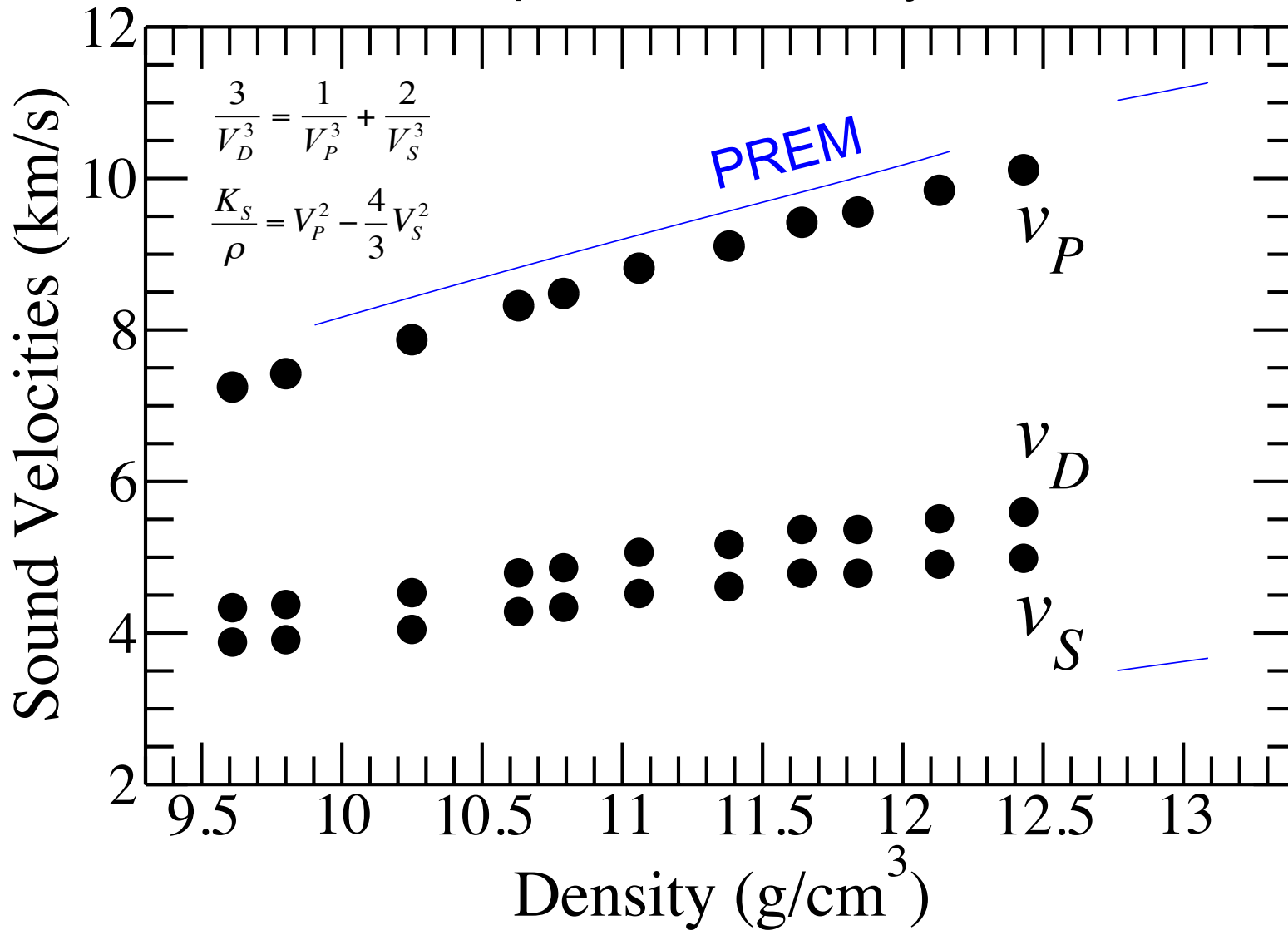


Murphy *et al. GRL* (2011); Murphy *et al. PEPI* (2011);  
Murphy *et al. JGR* (2013)

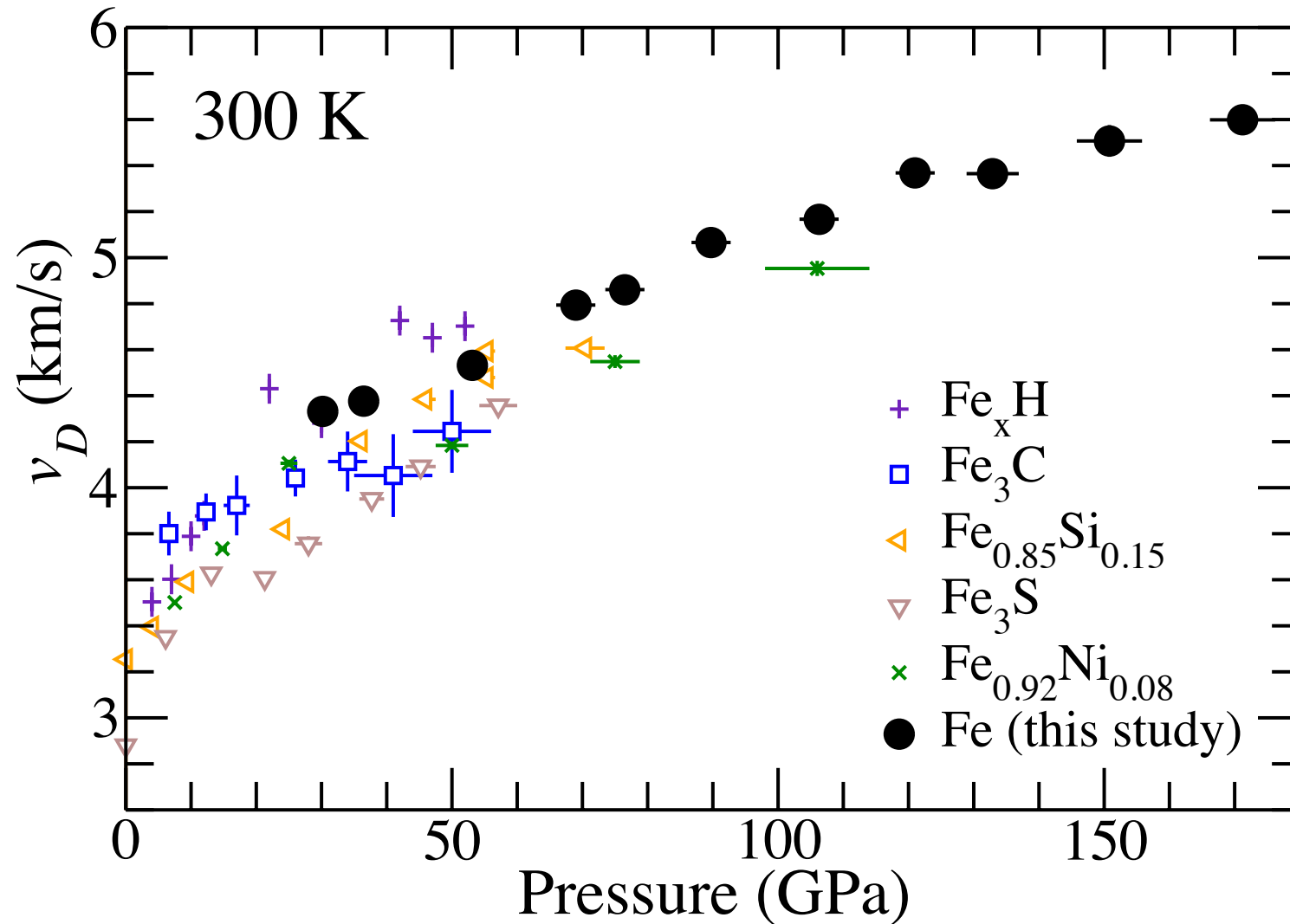
# Determination of the Debye sound velocity of *hcp*-iron from the measured phonon density of states



# Sound velocities of *hcp*-iron from the measured phonon density of states

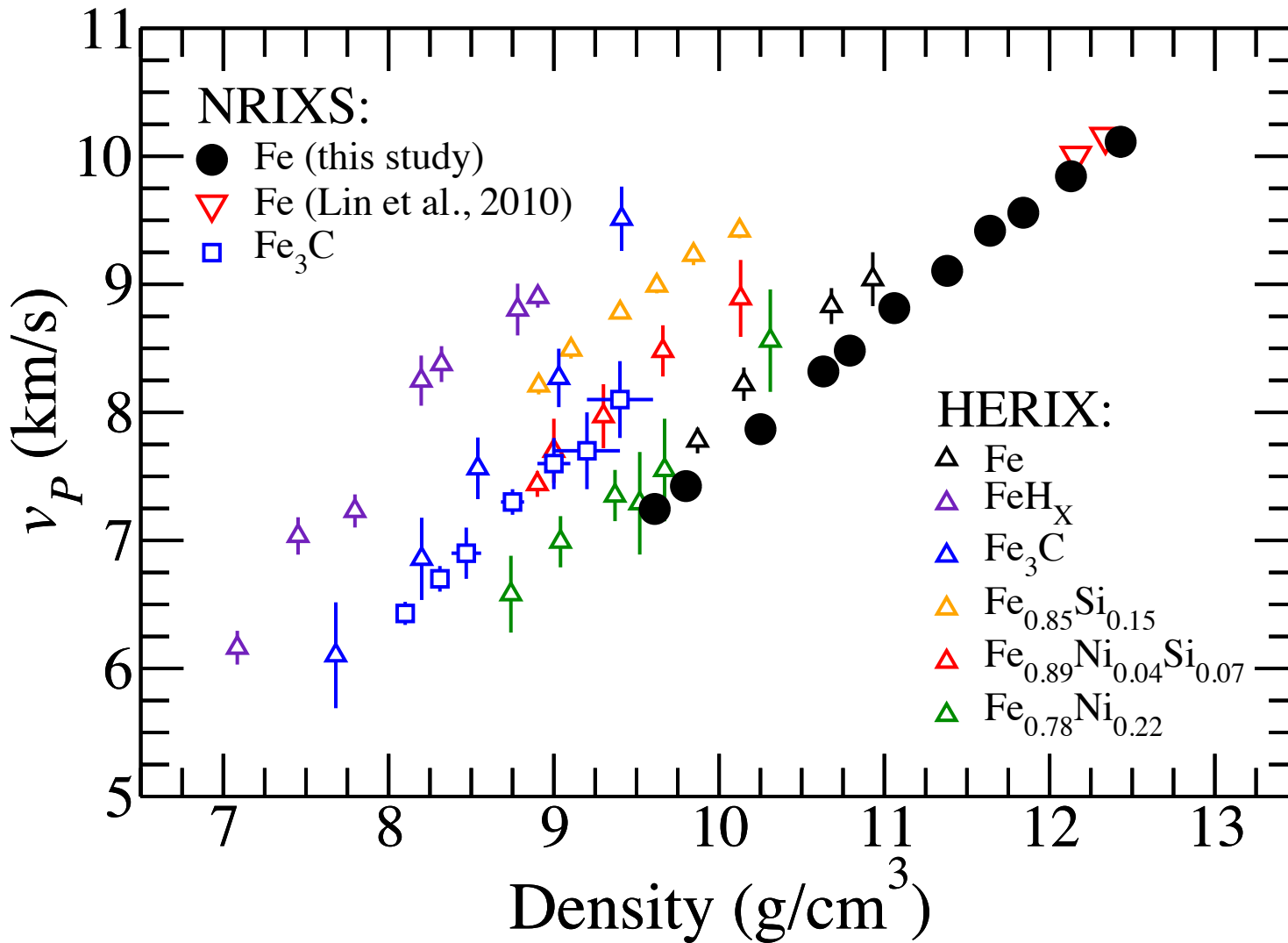


# Debye sound velocities of *hcp*-iron and iron-alloys from nuclear resonant inelastic x-ray scattering measurements

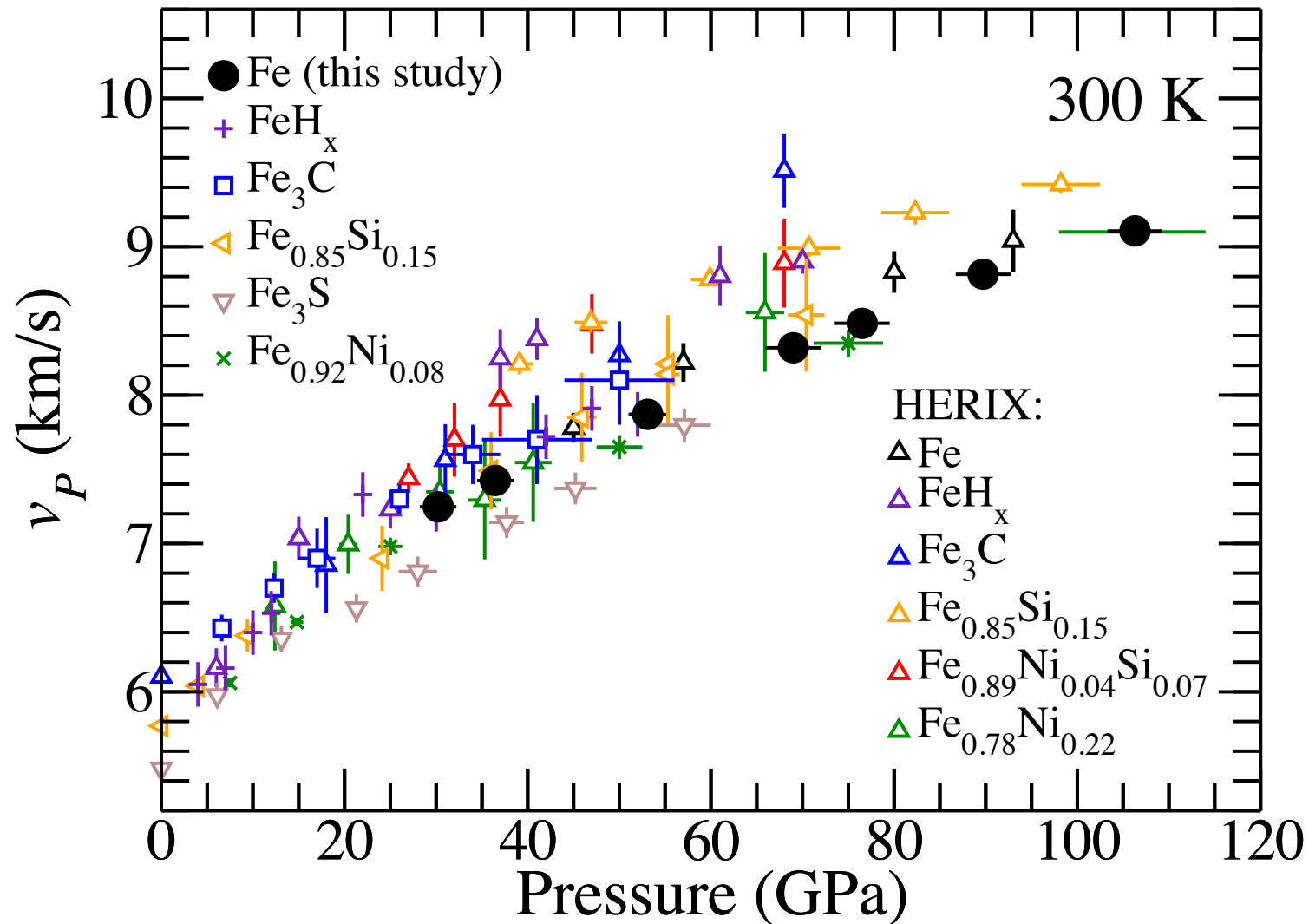




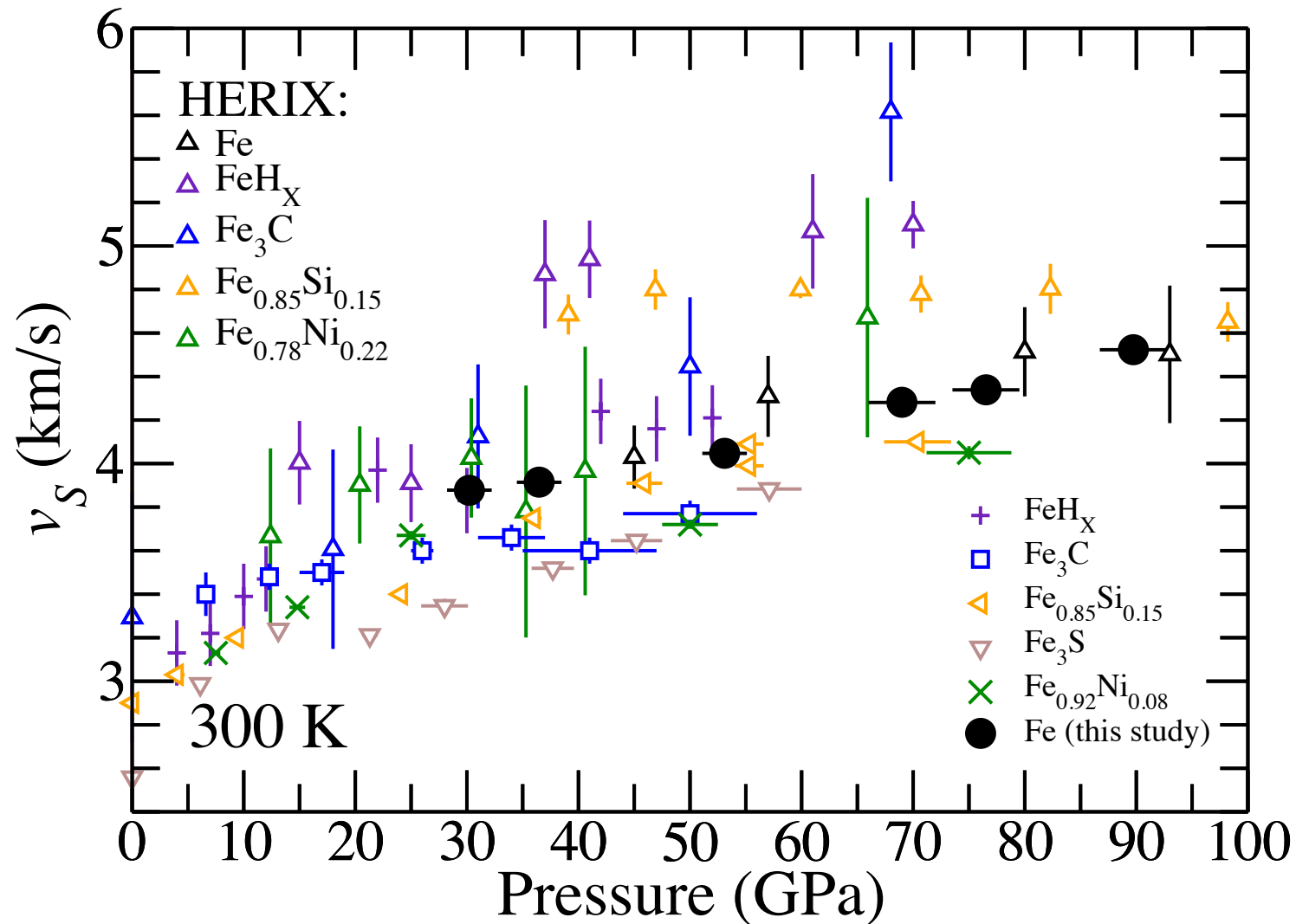
# Compressional wave velocities of *hcp*-iron and iron-alloys from inelastic x-ray scattering measurements



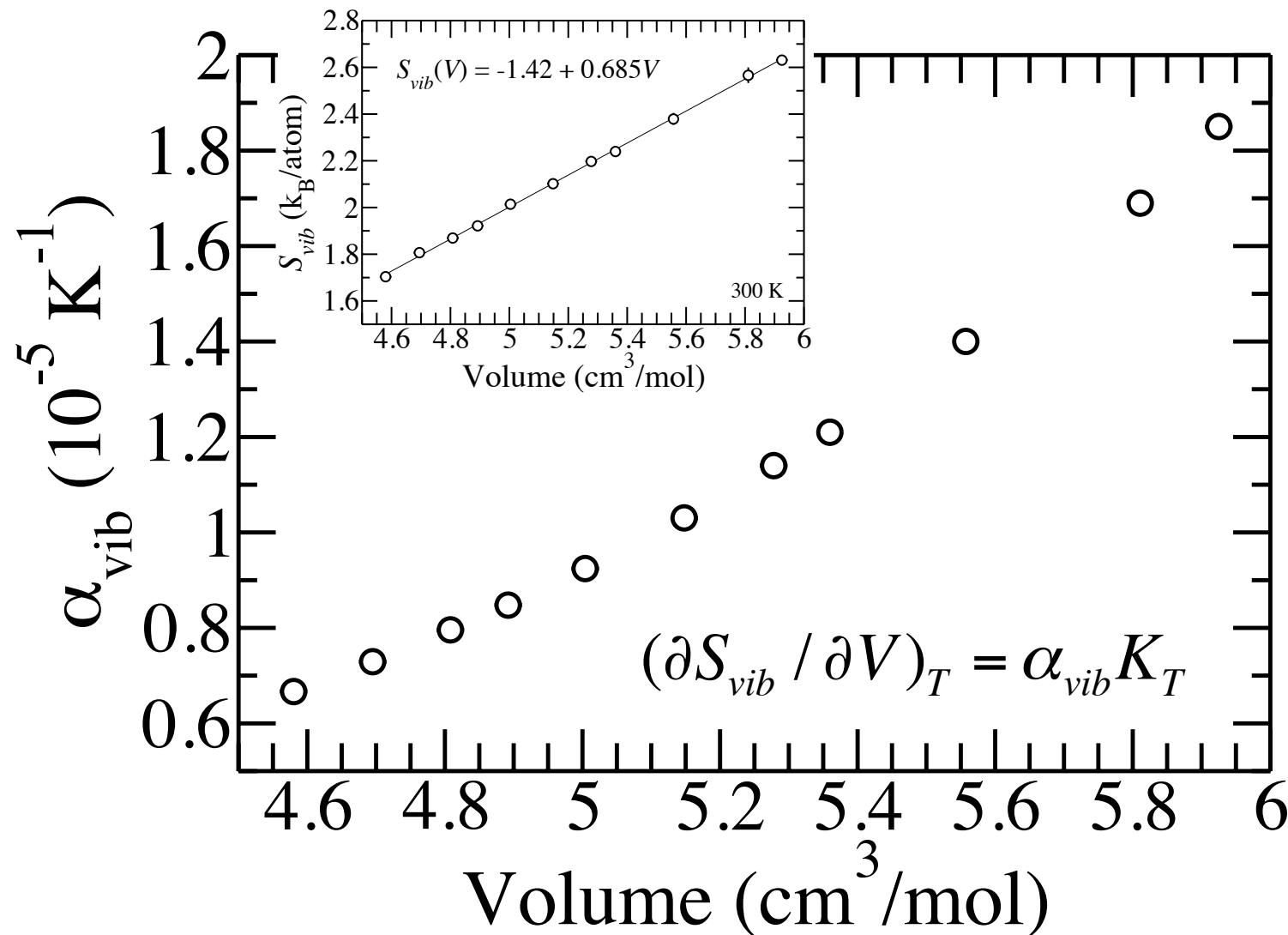
# Compressional wave velocities of *hcp*-iron and iron-alloys from inelastic x-ray scattering measurements



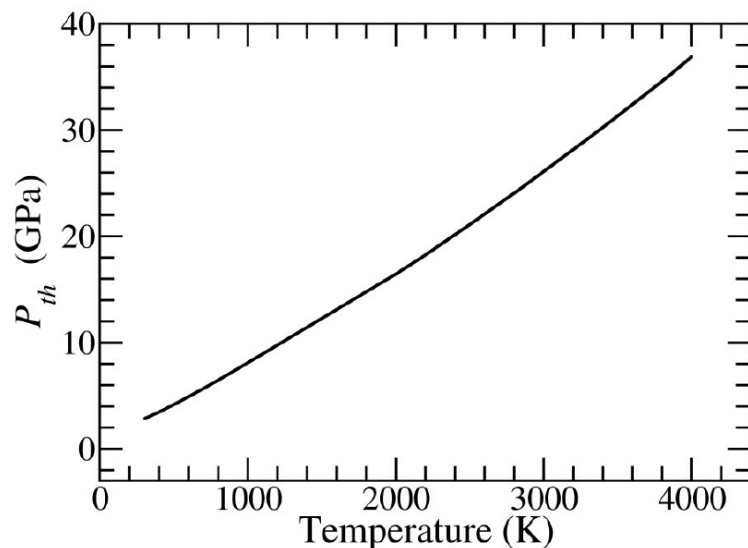
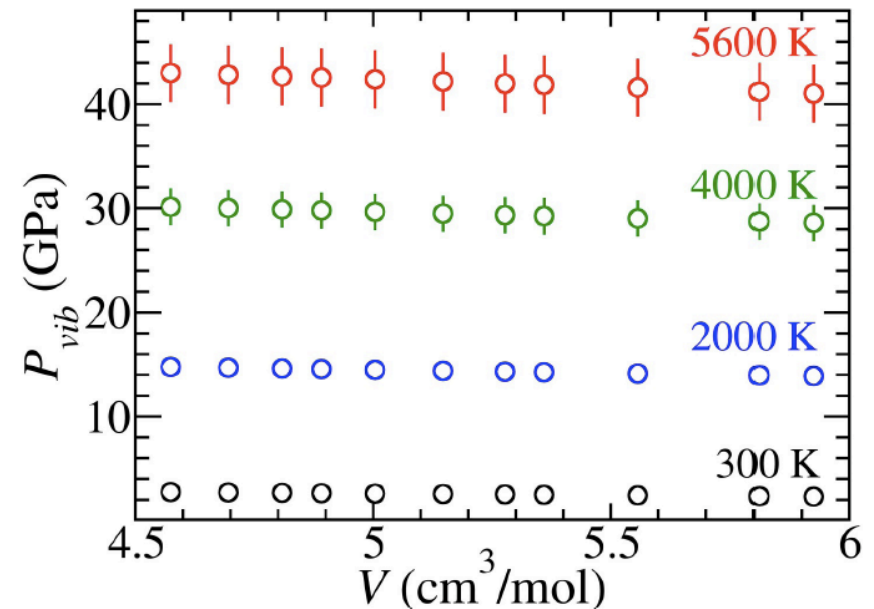
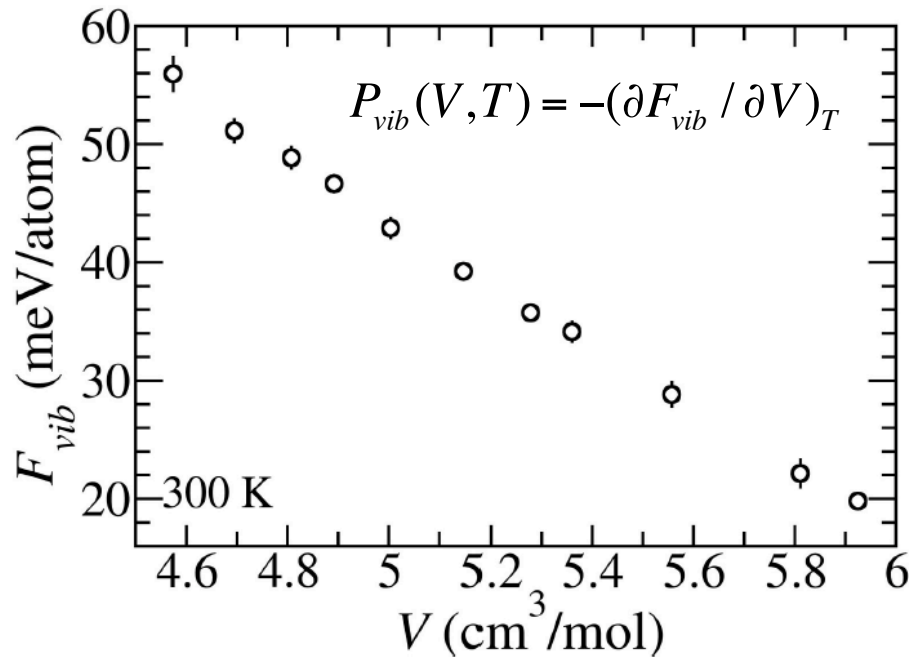
# Shear wave velocities of *hcp*-iron and iron-alloys from inelastic x-ray scattering measurements



# Thermal expansion of *hcp*-iron from the measured volume-dependence of vibrational entropy



# Thermal pressure from the measured volume dependence of *hcp*-iron's vibrational free energy



$$P_{th} = P_{vib}^h + \underbrace{P_{vib}^{anh}}_{\text{Dewaele et al. PRL (2006)}} + P_{el}$$

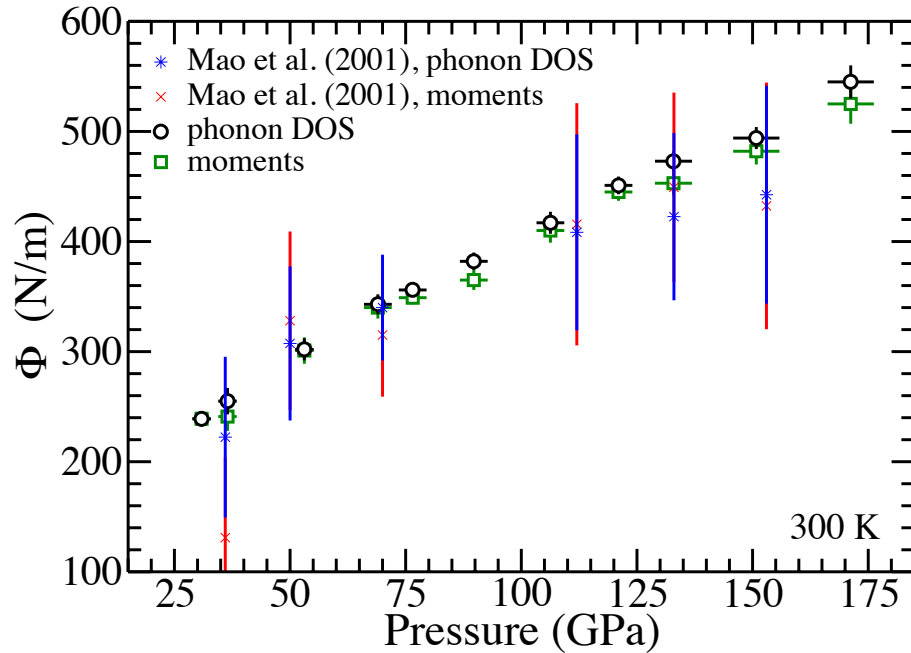
Murphy et al. PEPI (2011)

$$\rho_{ICB}^{hcp-Fe} = 13.50 \pm 0.03 \text{ g / cm}^3$$

$$\Rightarrow 5.5 \pm 0.2\%$$

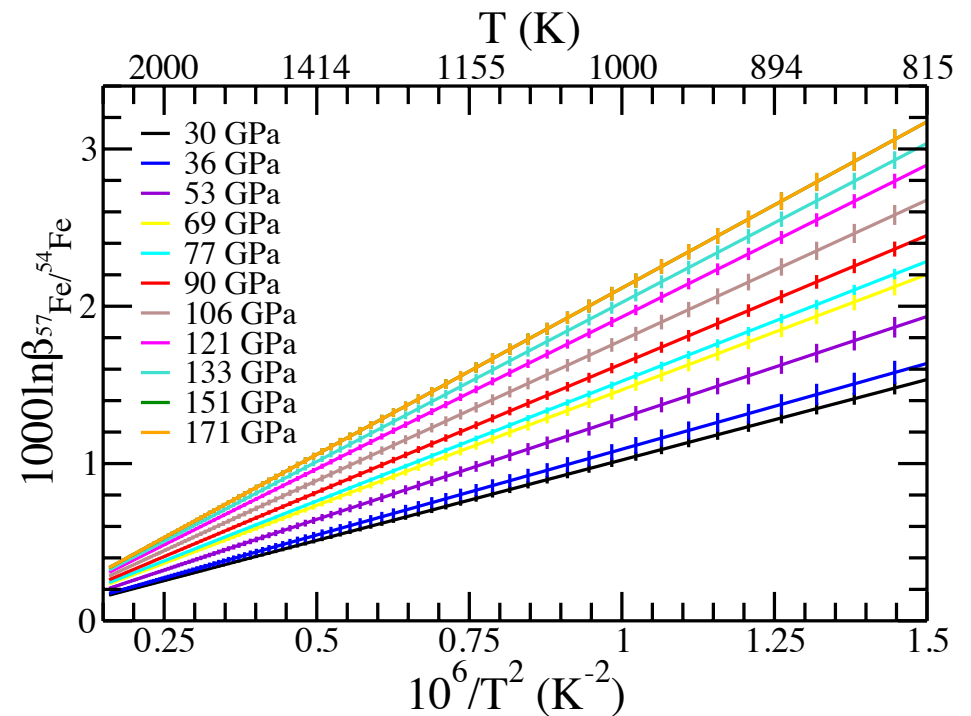


# Isotope fractionation factors of *hcp*-iron from the measured force constants

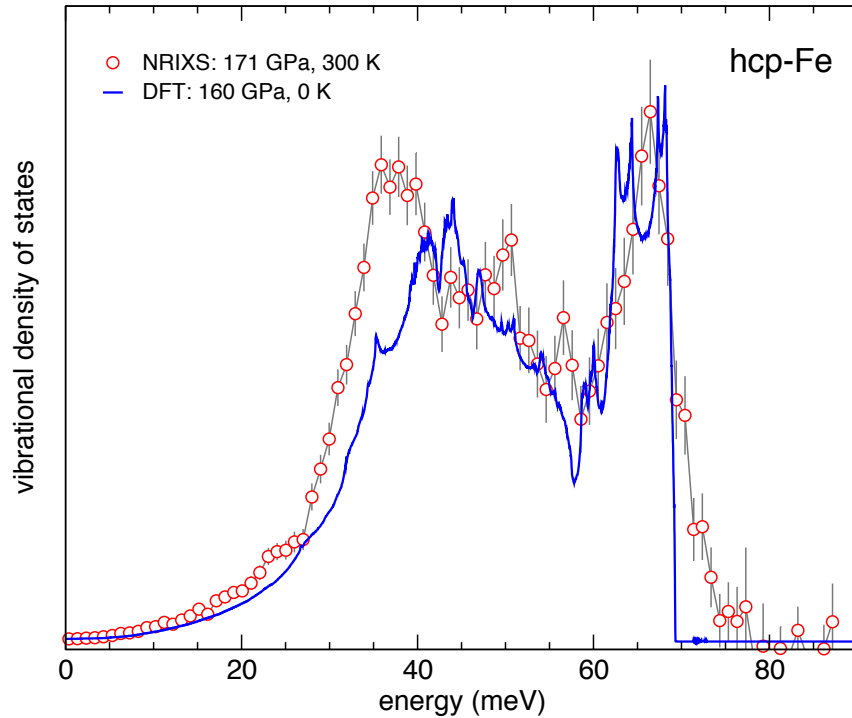


$$\Phi = \frac{k^2}{2E_R^2} \int (E - E_R)^3 S(E) dE$$

$$\ln \beta(V, T) = - \frac{\Delta m \hbar^2 \Phi(V, T)}{mm^* 8(k_B T)^2}$$



# Combining density functional theory with measured data:



Collaboration with R. Caracas (ENS Lyon)

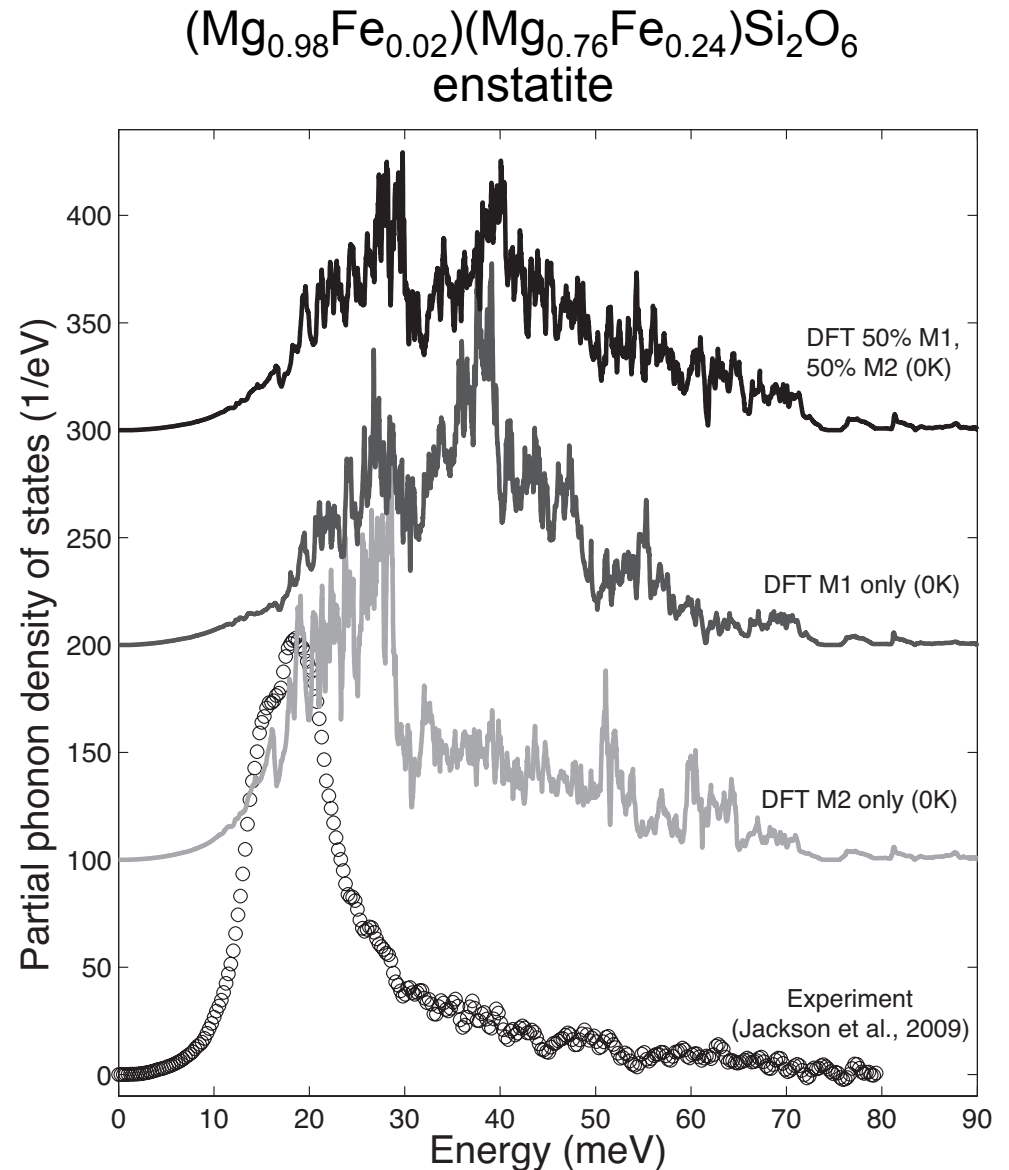
## Candidate core alloys

✧ Thermal equations of state

Independent of theory:

✧  $V_P$  and  $V_S$

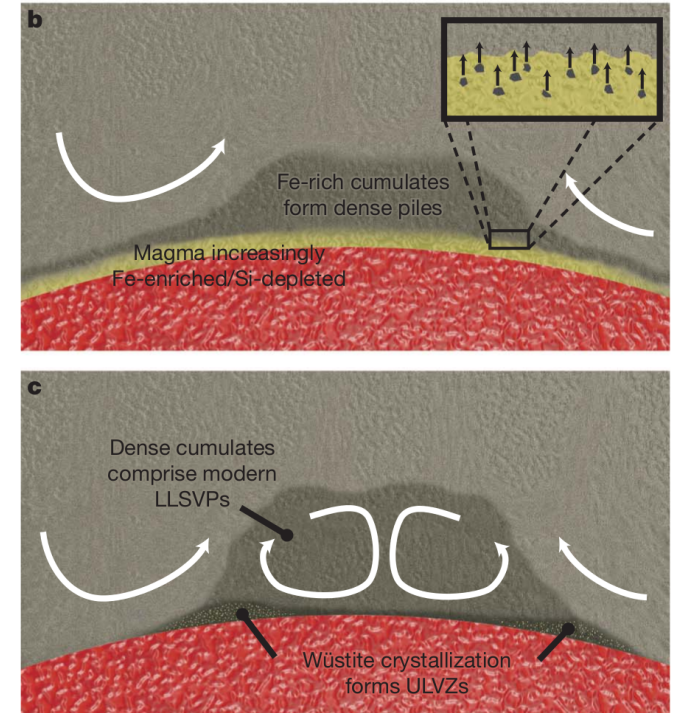
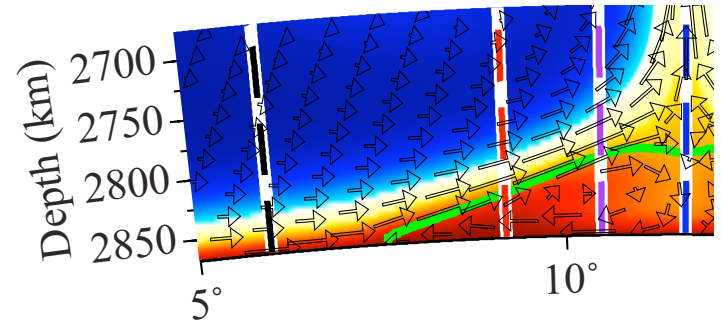
✧ Iron isotope  $\beta$ -factors



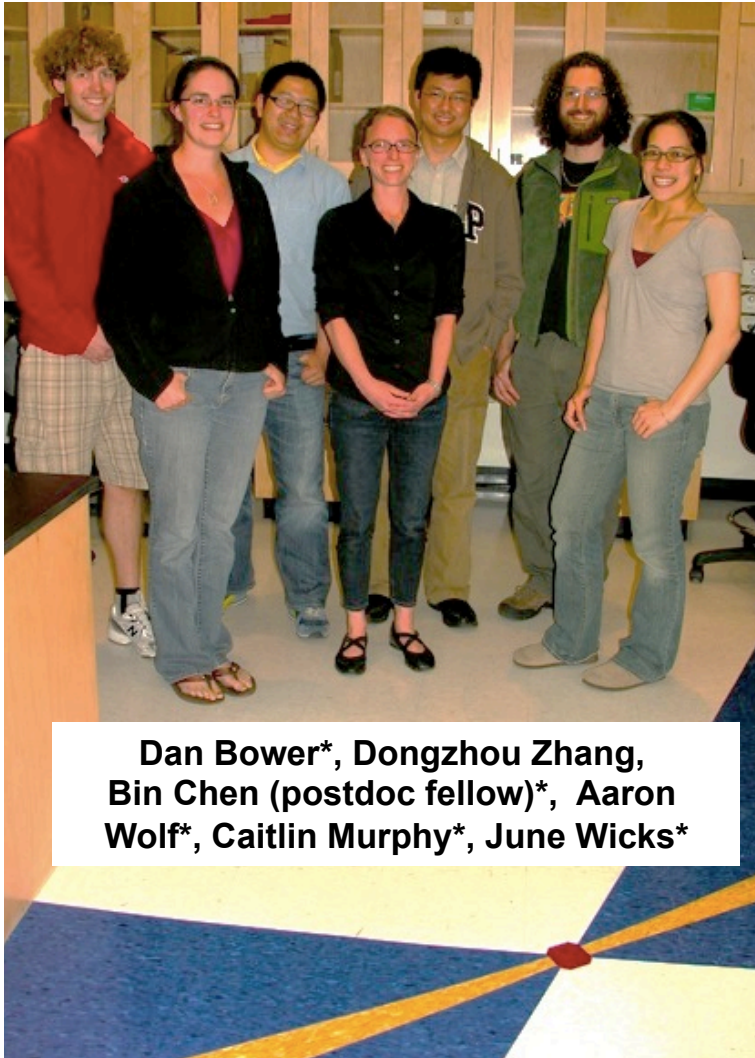
(Zhang, Jackson, Caracas, et al. 2013)

# Conclusions

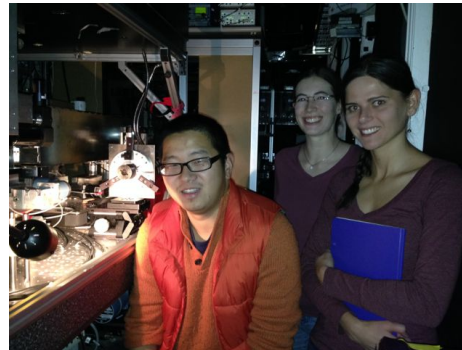
- ✧ Enstatite, an upper mantle mineral, exhibits shear softening near a pressure-induced phase transition
- ✧ Sound velocities and density of iron-rich (Mg,Fe)O provides a plausible explanation of heterogeneous patches at Earth's core-mantle boundary
  - ✧ Distinct, matches seismic observations
  - ✧ Could be a residue of a deep magma ocean
- ✧ Sound velocities of thermoelasticity of iron-alloys, together with seismic observations, will help constrain the composition of Earth's core



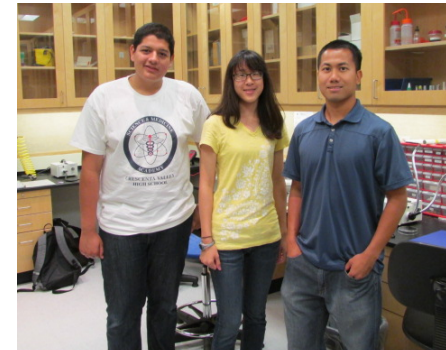
# Acknowledgements



Dan Bower\*, Dongzhou Zhang,  
Bin Chen (postdoc fellow)\*, Aaron  
Wolf\*, Caitlin Murphy\*, June Wicks\*



Rachel Miller Natalia  
Solomatova



High school students & teacher  
Ed Margaret Chuong  
Guzman Yu Vu

## Advanced Photon Source: Inelastic X-ray and Nuclear Resonant Scattering Group (Sector 3)

Wolfgang Sturhahn (*now at Caltech*),  
Jiyong Zhao, Tom Toellner, E. Ercan Alp, Michael Hu

**GSE-CARS (Sector 13):** V. Prakapenka and P. Dera

**Dan Bower:** *now a Postdoctoral Fellow at ETH, Zurich*

**Dongzhou Zhang:** *PhD student, Caltech*

**Bin Chen:** *now Asst. Prof. at Univ. of Hawaii*

**Aaron Wolf:** *now a Turner Postdoc Fellow at Univ. of Michigan*

**Caitlin Murphy:** *now a Carnegie Postdoc Fellow at the Geophysical Laboratory*

**June Wicks:** *now a Hess Postdoc Fellow at Princeton*

**YoungHee Kim,** *now Asst. Prof. at Seoul National Univ.*

**Zhongwen Zhan,** *now Asst. Prof. at UT Austin*



*Thank You!*