Geophysical applications of nuclear resonant inelastic x-ray scattering

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Workshop on Nuclear Resonant Inelastic X-ray Scattering
Advanced Photon Source, Argonne National Laboratory
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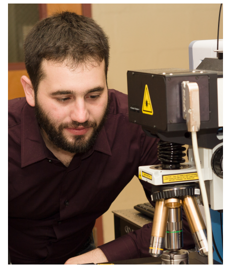
Acknowledgements



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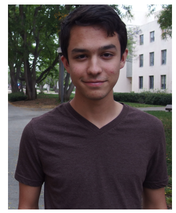

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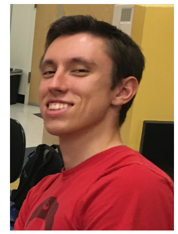

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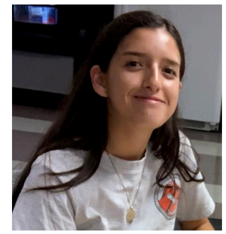

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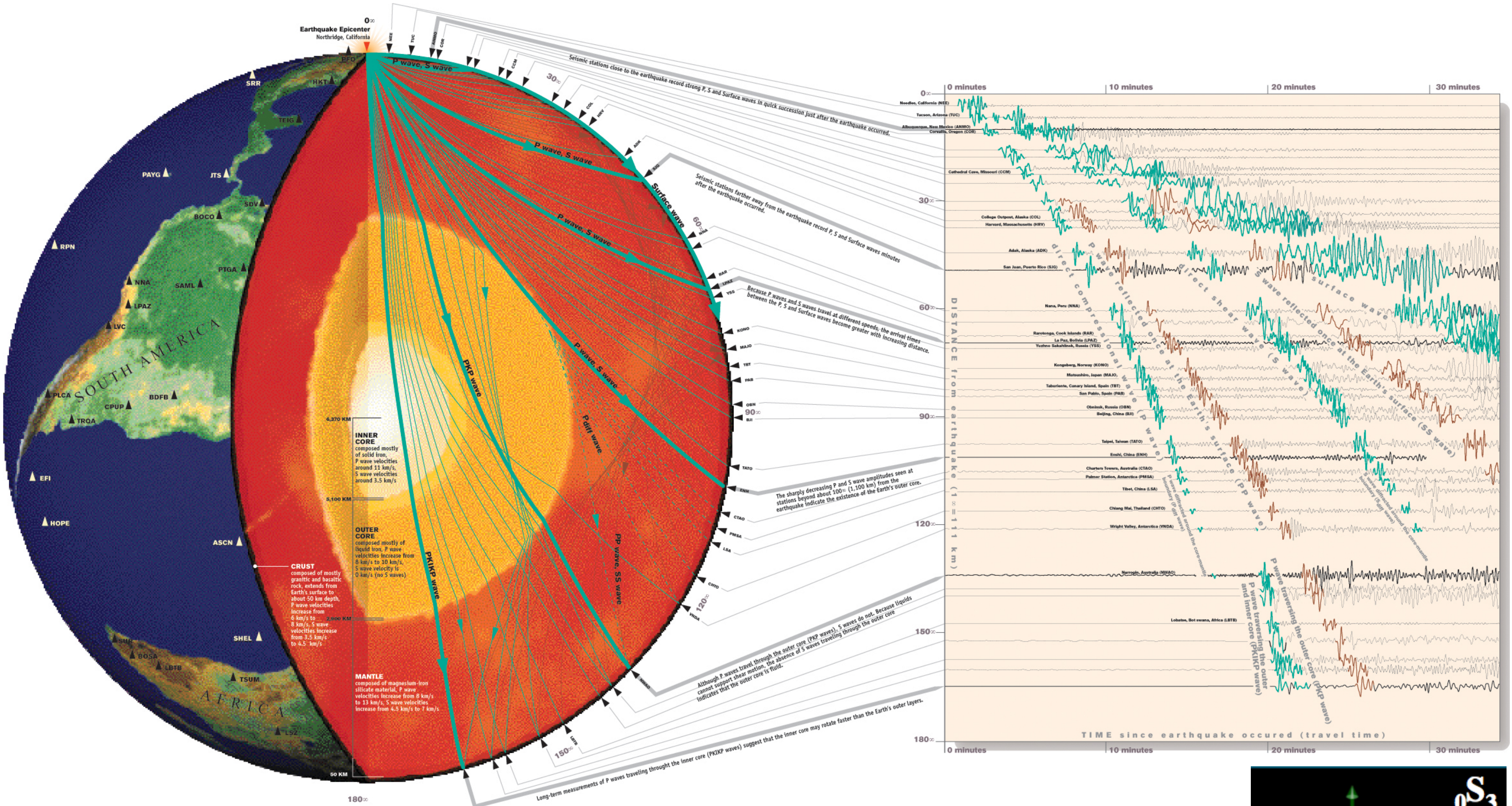
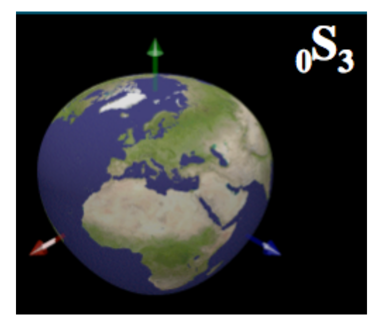
COMPRES

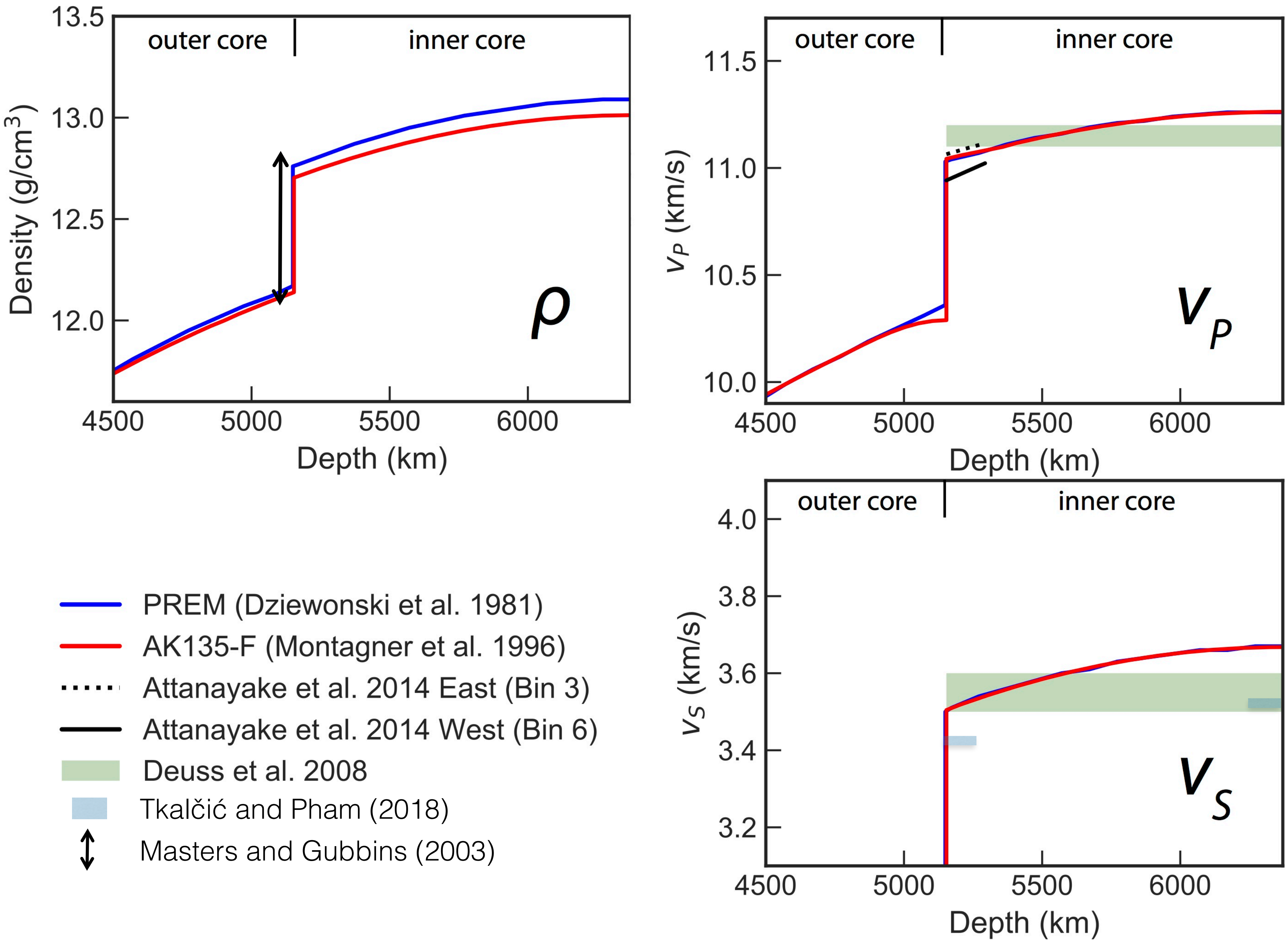




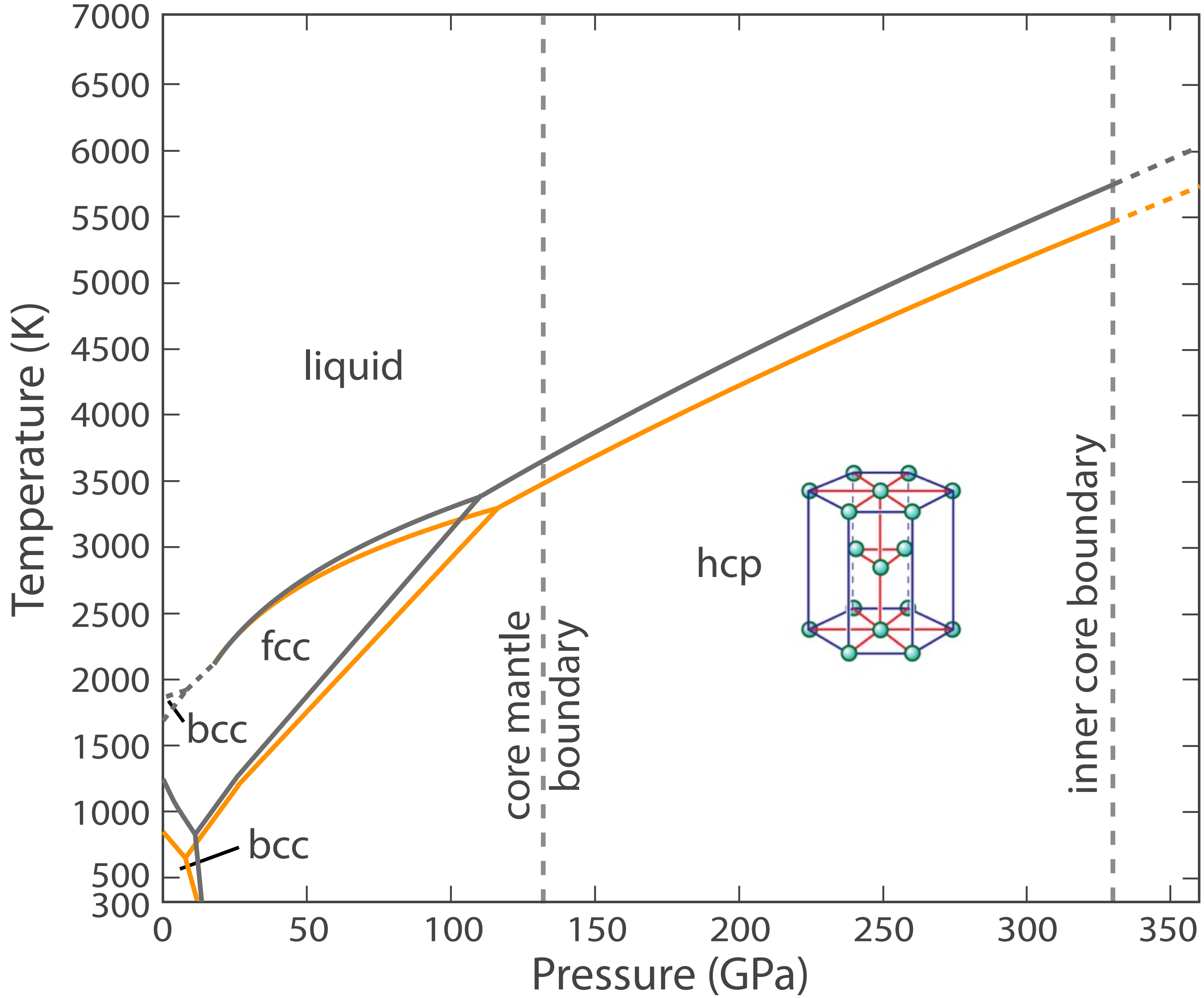
by Lucien Saviot

Seismic wave propagation through Earth's interior

Seismological Constraints



Phase diagram of Fe and $Fe_{0.91}Ni_{0.09}$



Earth's core is predominantly iron

Fe, Fe-9%Ni phase diagram: Jackson et al. (2013), Zhang et al. (2016)

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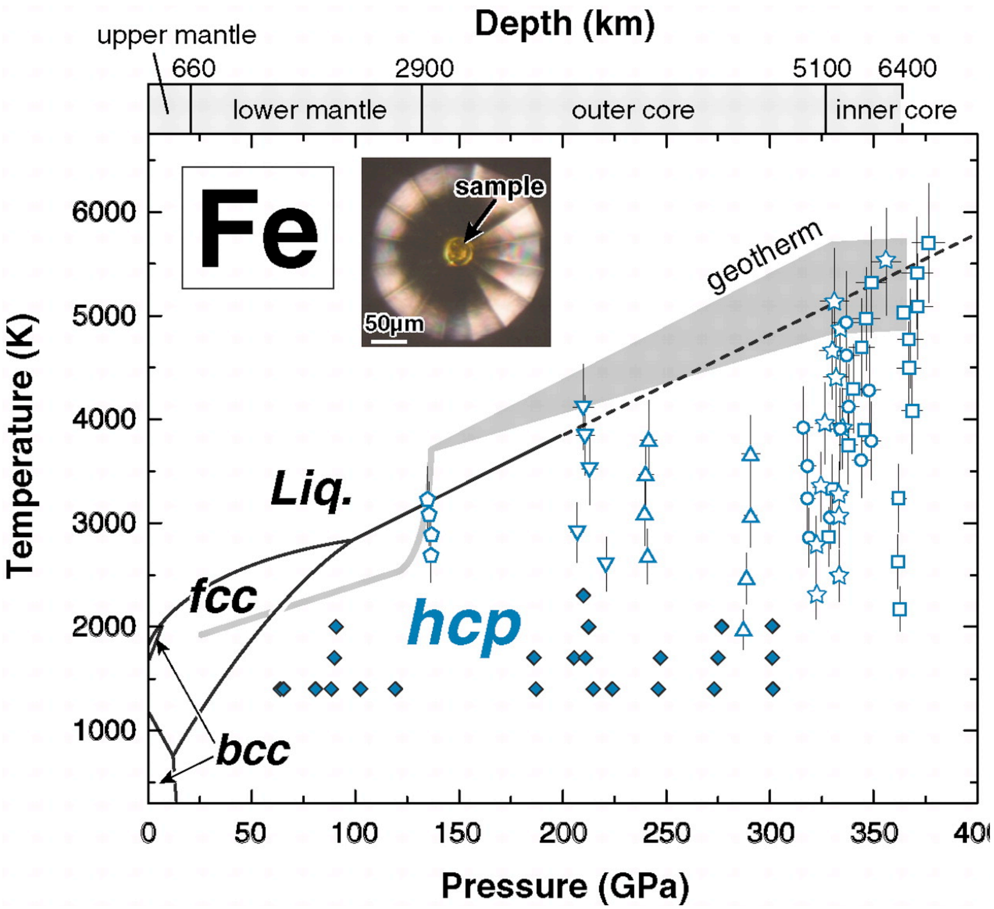
Stability of *hcp*-structured Fe-Ni-Si



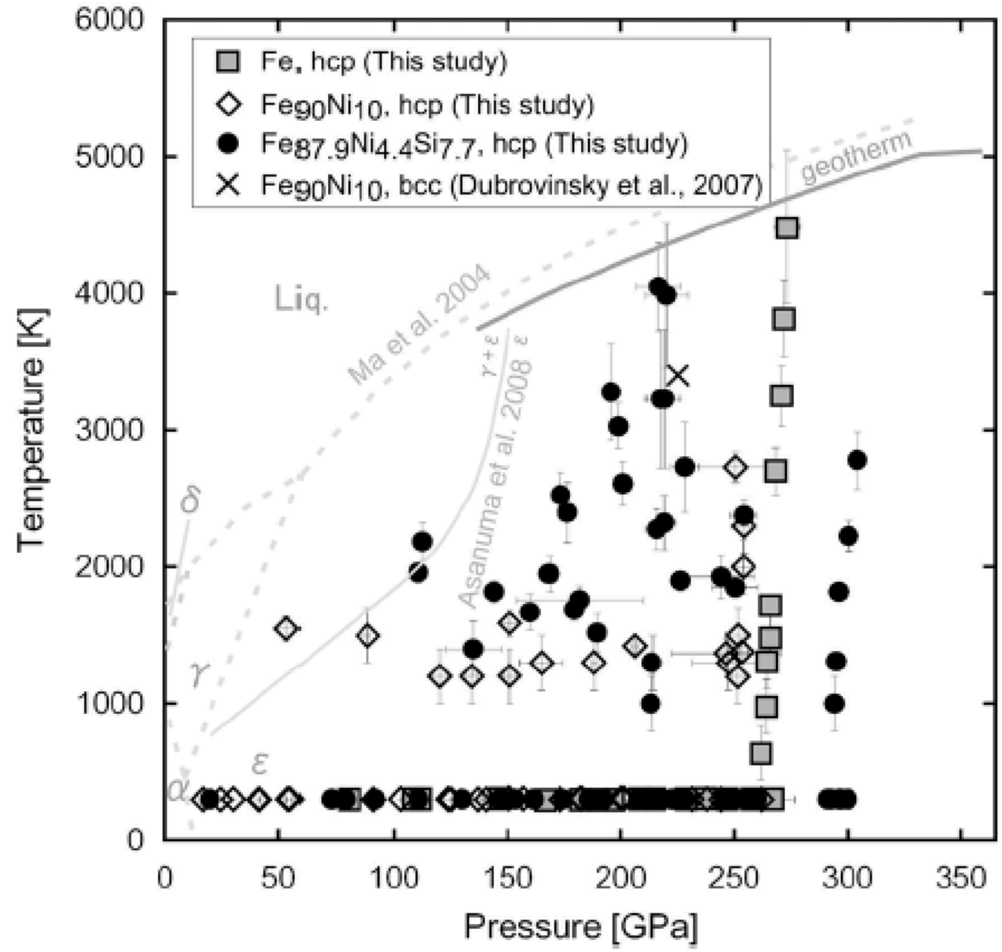


TABLE 1. LIGHT ELEMENTS SUGGESTED BEING ALLOYED WITH NICKEL–IRON IN THE FLUID CORE OF THE EARTH

C, Si, H (Birch 1952)	Si (MacDonald & Knopoff 1958; Ringwood 1958)
C, S (Urey 1960)	C, S, Si (Clark 1963)
Si, O, S (Birch 1964)	S (Mason 1966; Murthy & Hall 1970; Lewis 1973)
Mg, O (Adler 1966)	O (Bullen 1973; Ringwood 1977)

Herndon (1979), Fe Tateno et al. Science (2010); Fe-Ni-Si Sakai et al. GRL (2011); Fe-Ni: Tateno et al. GRL (2012), Sakai et al. PEPI (2014)

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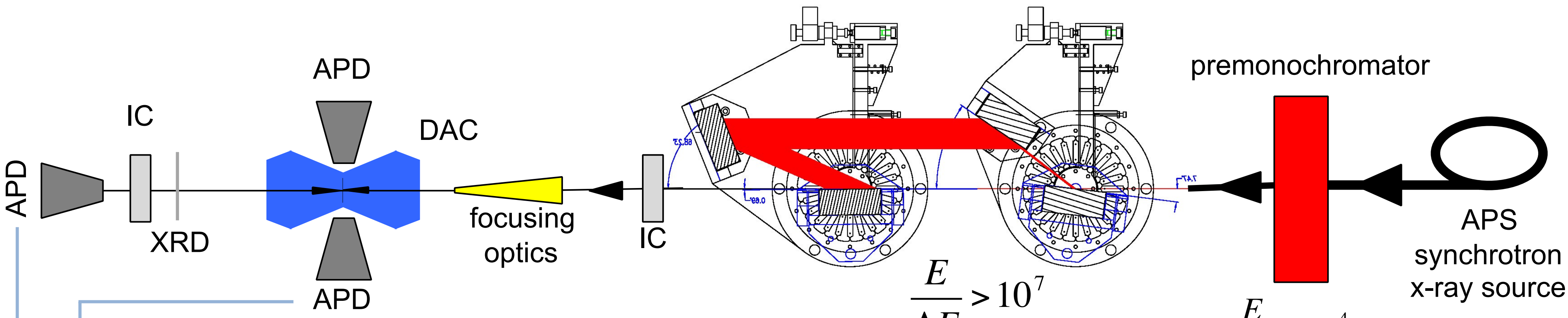
Using nuclear resonant scattering to constrain vibrational thermoelastic properties of iron-alloys: Sector 3-ID-B, Advanced Photon Source (Argonne, IL USA)



$\frac{E}{\Delta E} > 10^7$

$\Delta E = 1.0$ meV

silicon
high-resolution
monochromator

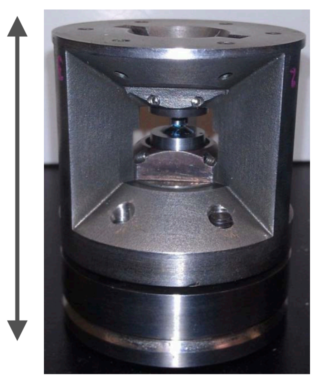
$\frac{E}{\Delta E} = 10^4$

$E = 14.4125$ keV

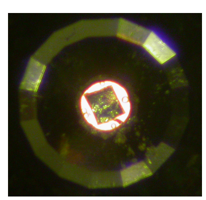
$\Delta E \approx 1$ eV

Nuclear resonant inelastic scattering
(Partial) projected phonon DOS:
thermodynamic properties (γ, P_{th} α)
sound velocities (V_D, V_P, V_S)

Nuclear resonant forward scattering



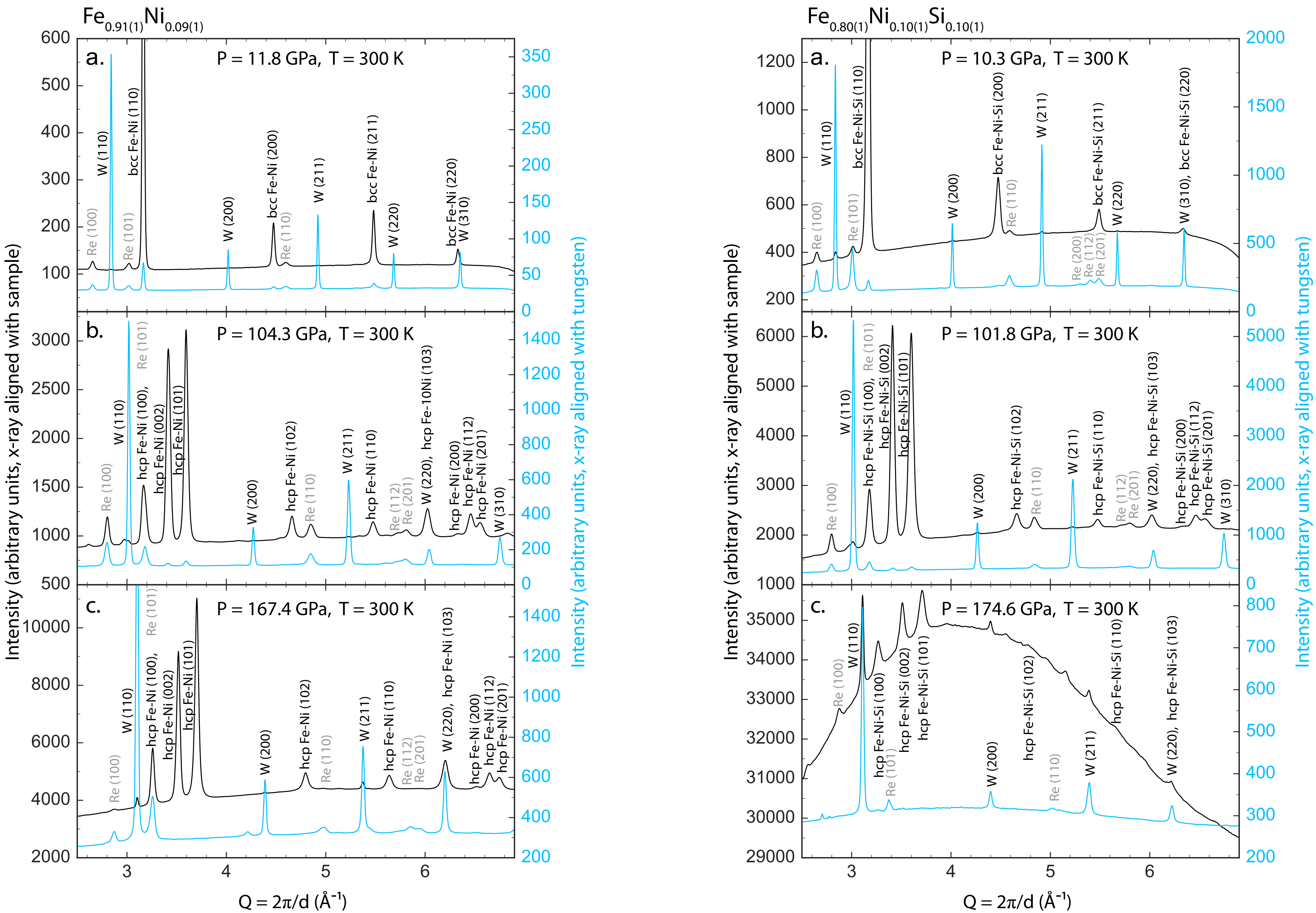
~7cm



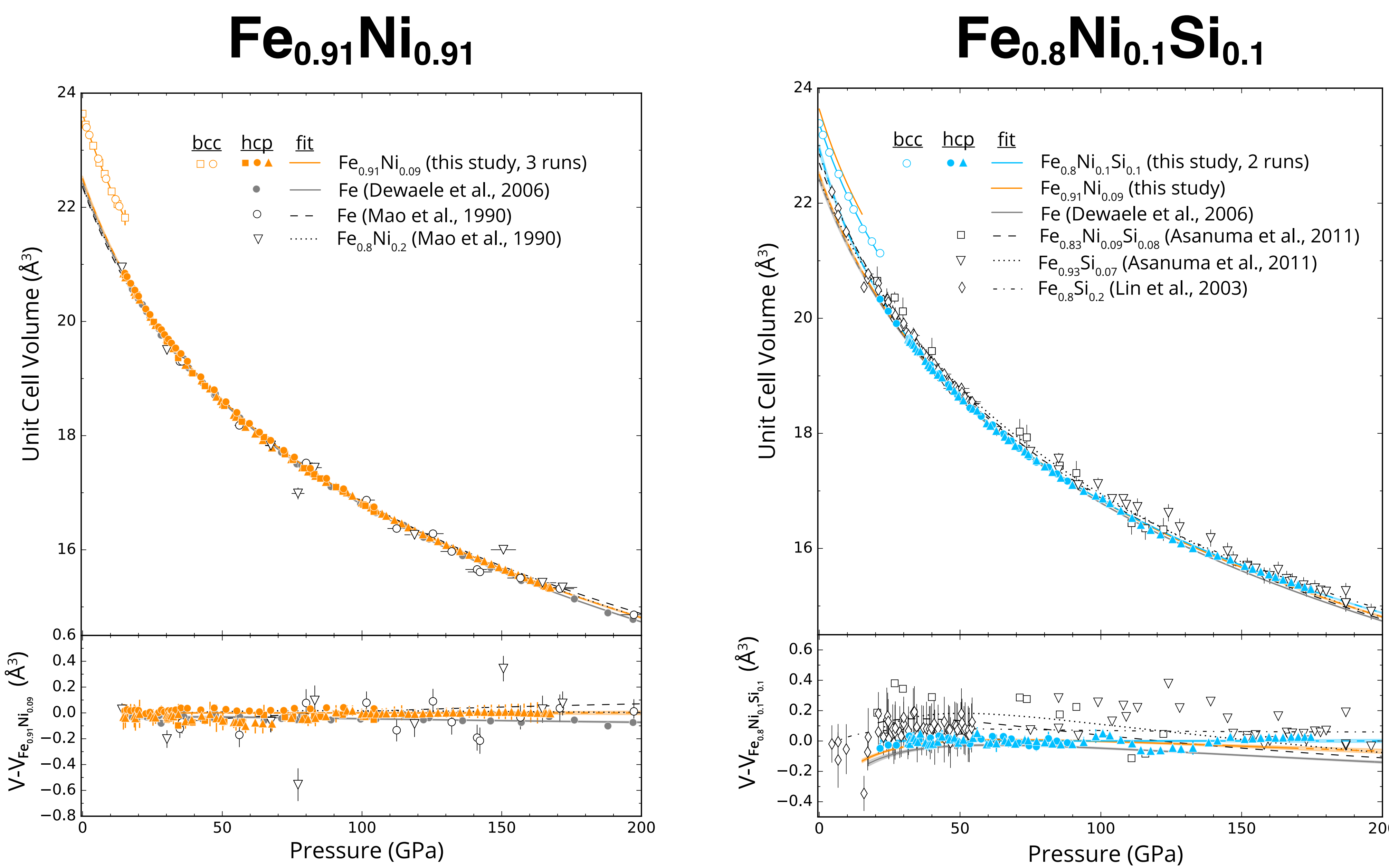
~250 um

Samples:
$^{57}Fe_{0.91}Ni_{0.09}$
$^{57}Fe_{0.8}Ni_{0.1}Si_{0.1}$

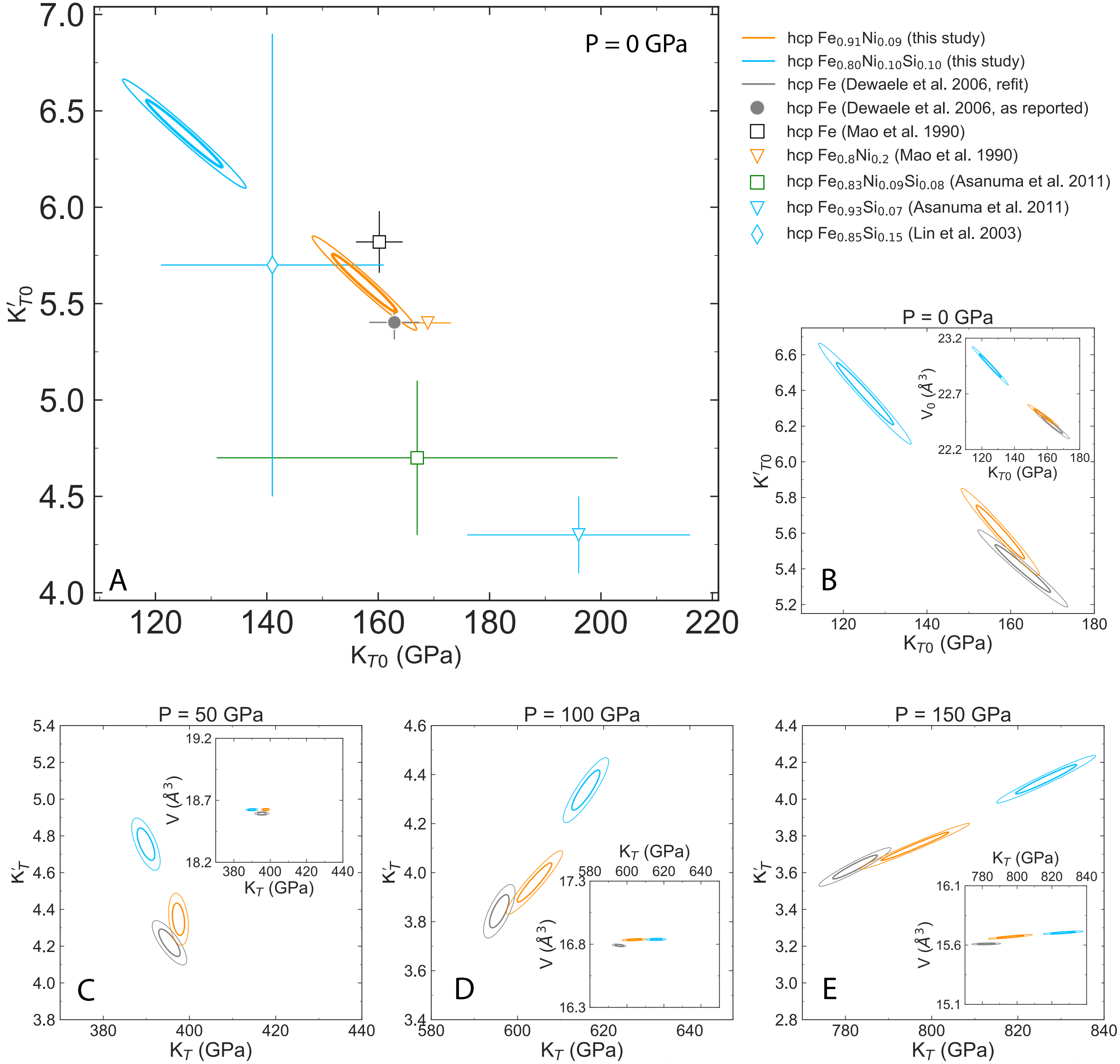
Powder XRD: He pressure medium, W pressure calibrant



Pressure-volume measurements



Parameter correlations, at a range of pressures



Morrison *et al. JGR* (2018)

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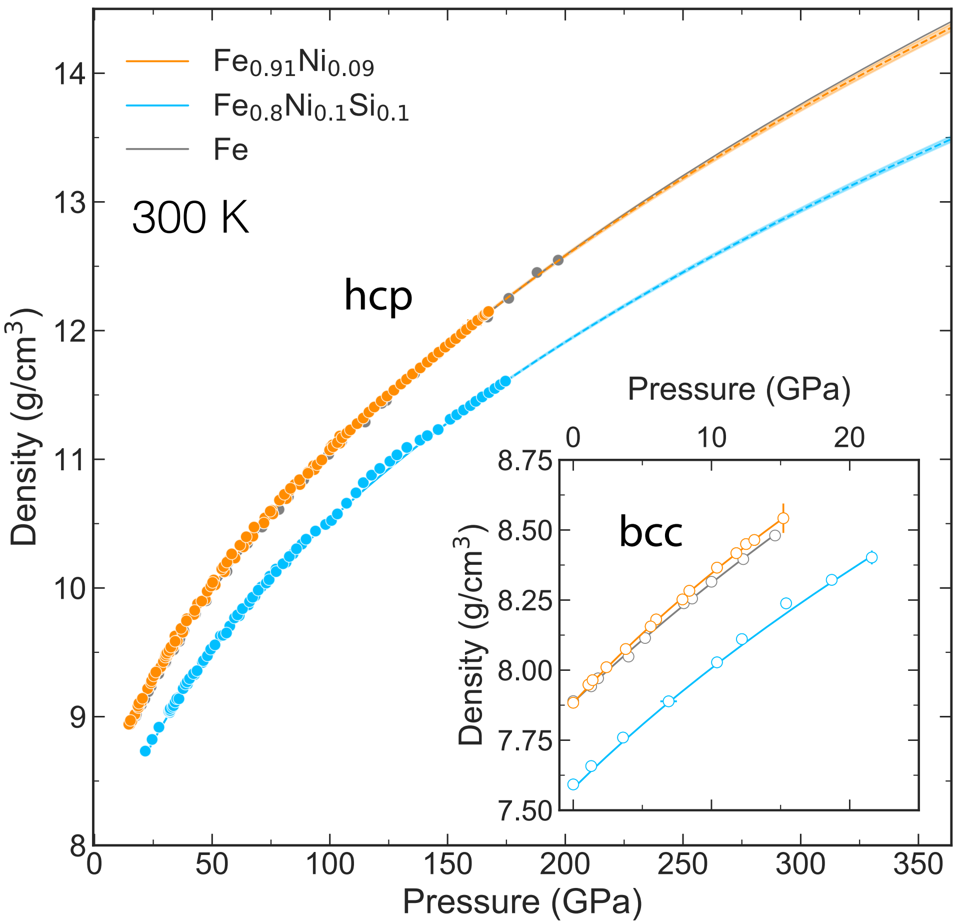
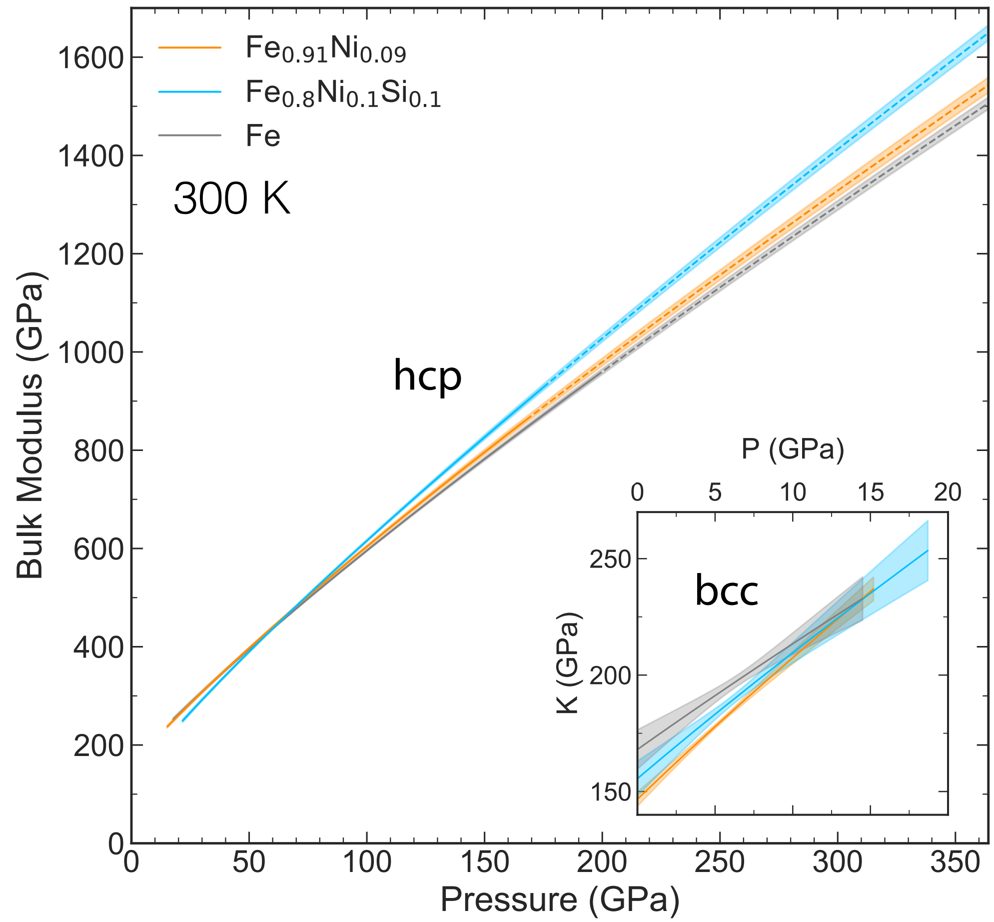
Density and bulk modulus (K_T) of these Fe-Ni-Si alloys





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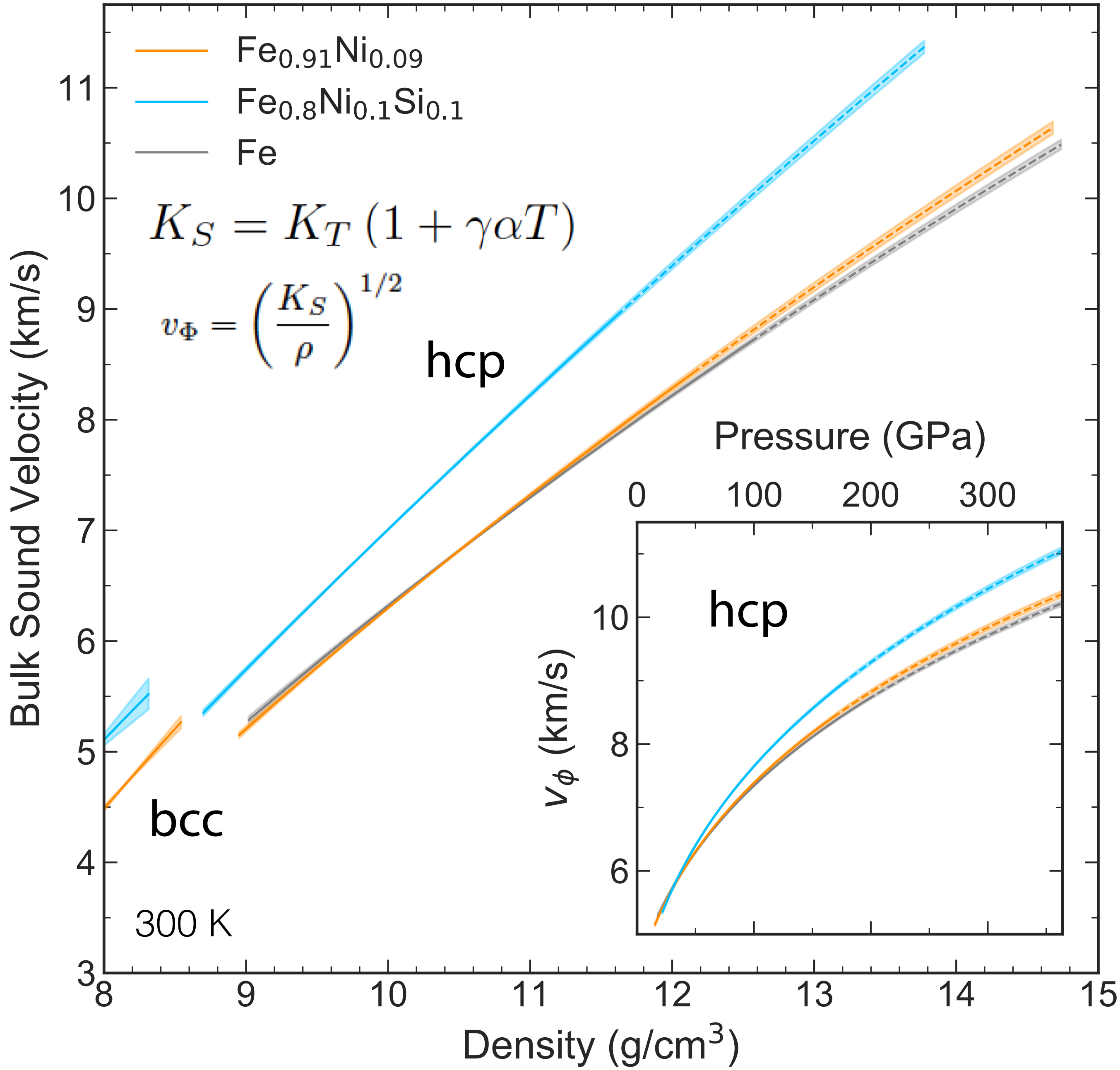
Bulk sound speed of Fe-Ni-Si alloys



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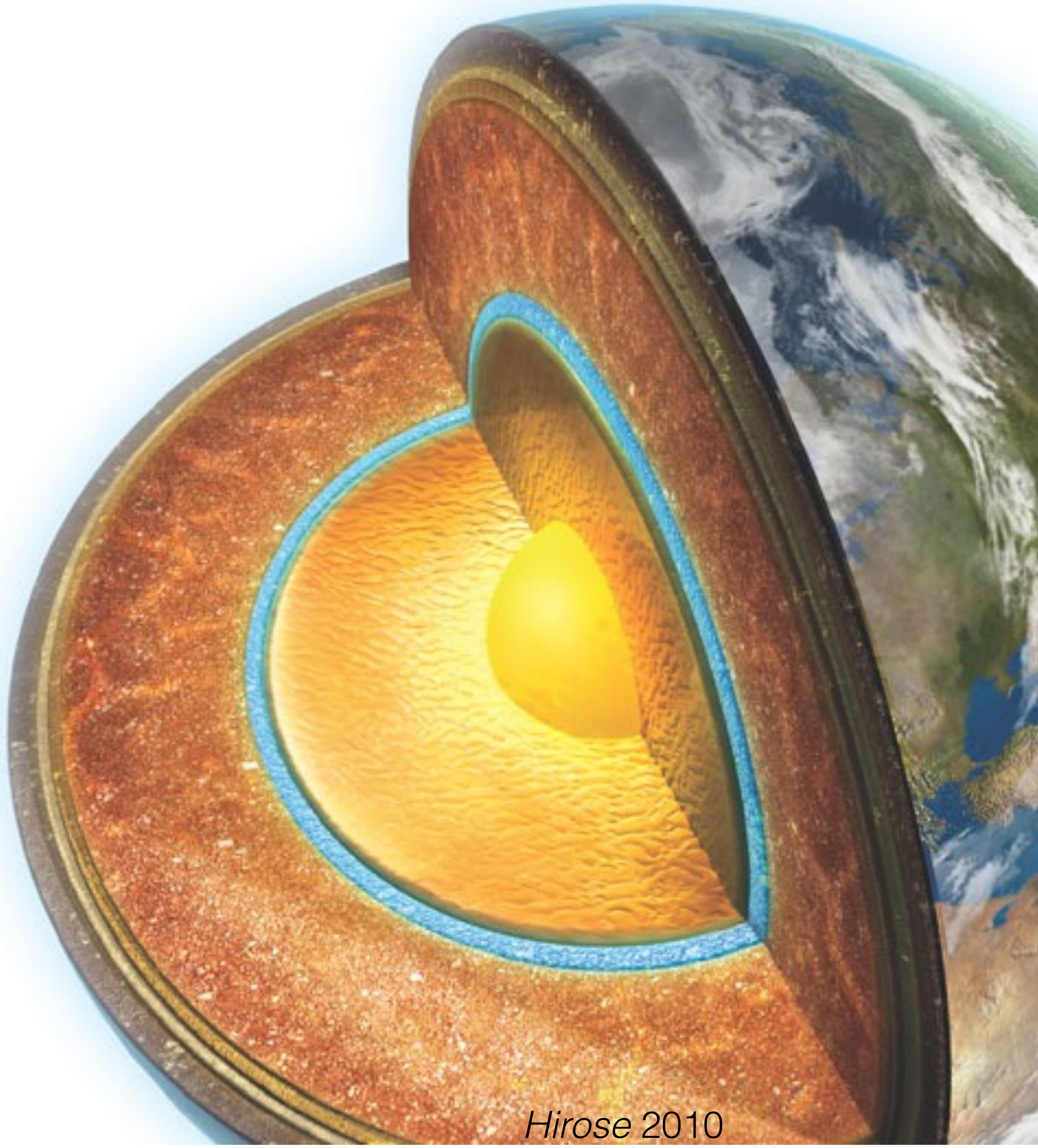
Thermal properties



Hirose 2010

Thermal equation of state

$$P(V,T) = P_{elastic}(V) + P_{th}(V,T) - P_{th}(V,T_{ref})$$

e.g., Vinet, 3rd order Birch Murnaghan

$$P_{th}(V,T) = \frac{\gamma(V)}{V}\left[9k_B T\left(\frac{T}{\Theta(V)}\right)^3 \int_0^{\Theta(V)/T} \frac{x^3 dx}{e^x - 1} + \frac{9}{8}k_B\Theta(V)\right]$$

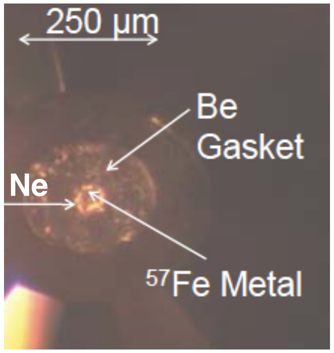
$$+ P_{\text{electronic}} + P_{\text{anharmonic}}$$

Mie-Grüneisen Debye

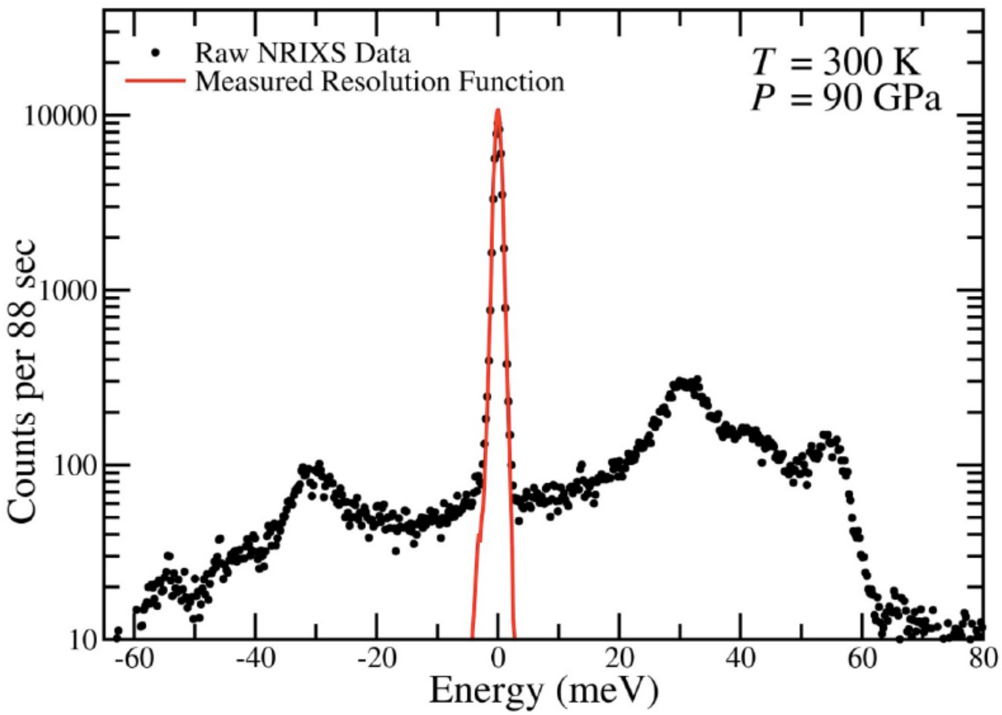
with Grüneisen parameter:

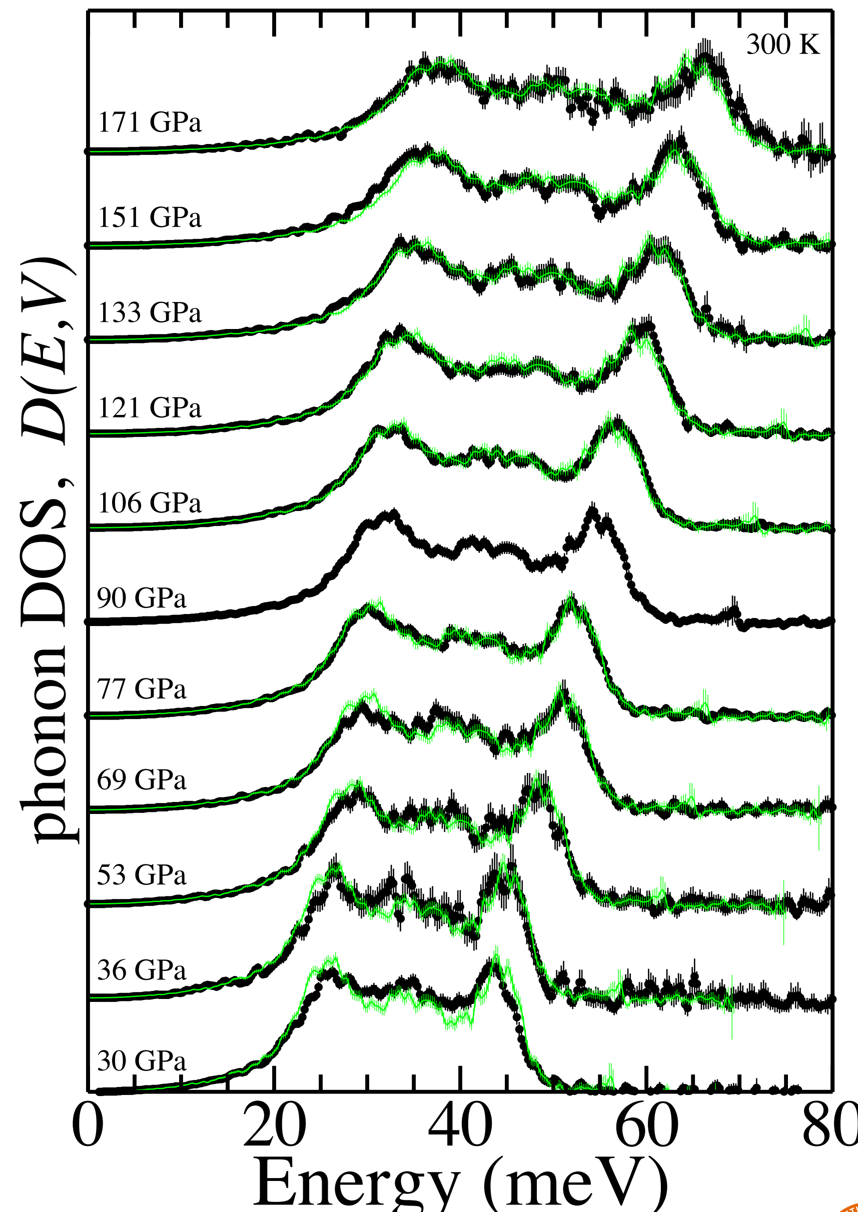
$$\gamma(V) = \gamma_0\left(\frac{V}{V_0}\right)^q$$

For example: $$P_{\text{TH}}(V,T) = \frac{9R\gamma}{V}\left(\frac{\theta}{8} + T\left(\frac{T}{\theta}\right)^3 \int_0^{\theta/T} \frac{z^3 dz}{e^z - 1}\right) + \frac{3R}{2V} m a_0 x^m T^2 + \frac{3R}{2V} g e_0 x^g T^2,$$



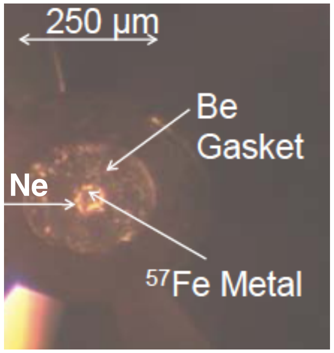
Thermal pressure terms directly determined from the volume dependence of the phonon DOS for ***hcp*-iron** to outer core pressures



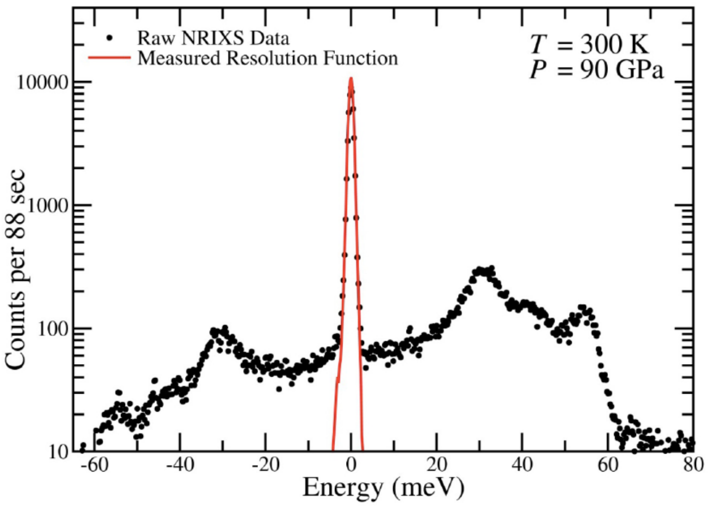


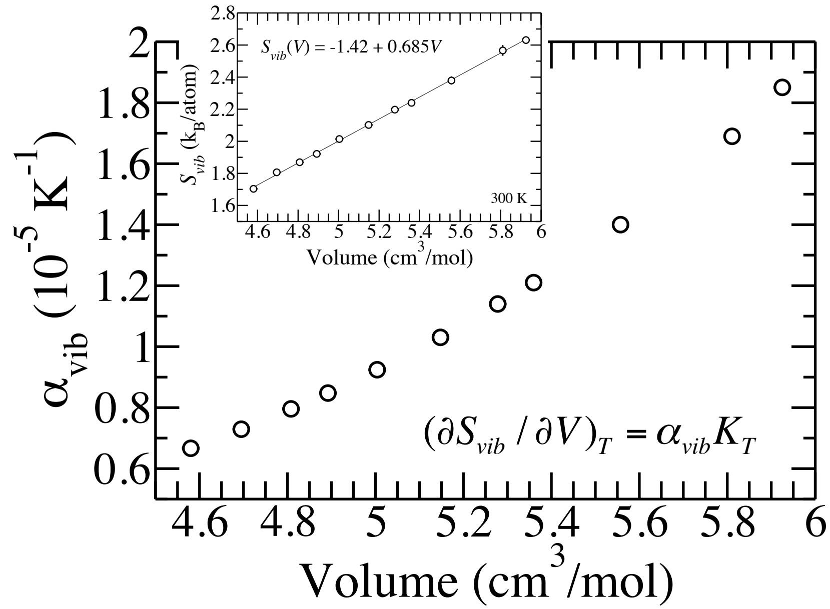
^{57}Fe sample loaded with neon
Pressure scale: Dewaele *et al. PRL* (2006)

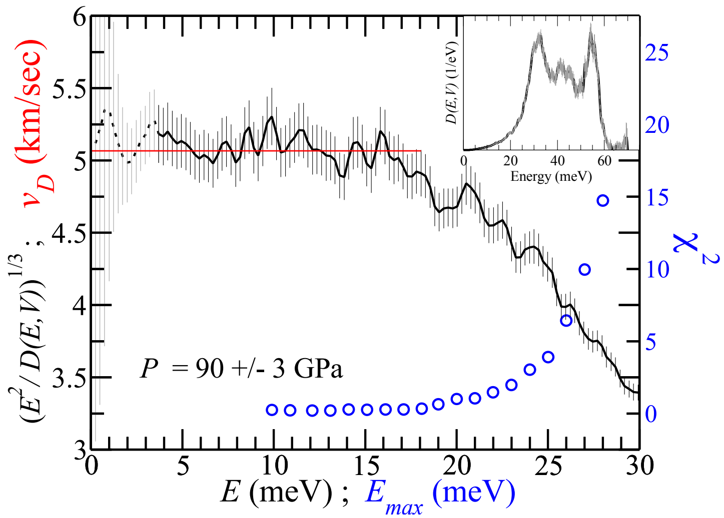
Murphy *et al. GRL* (2011), Murphy *et al. PEPI* (2011), Murphy *et al. JGR* (2013)

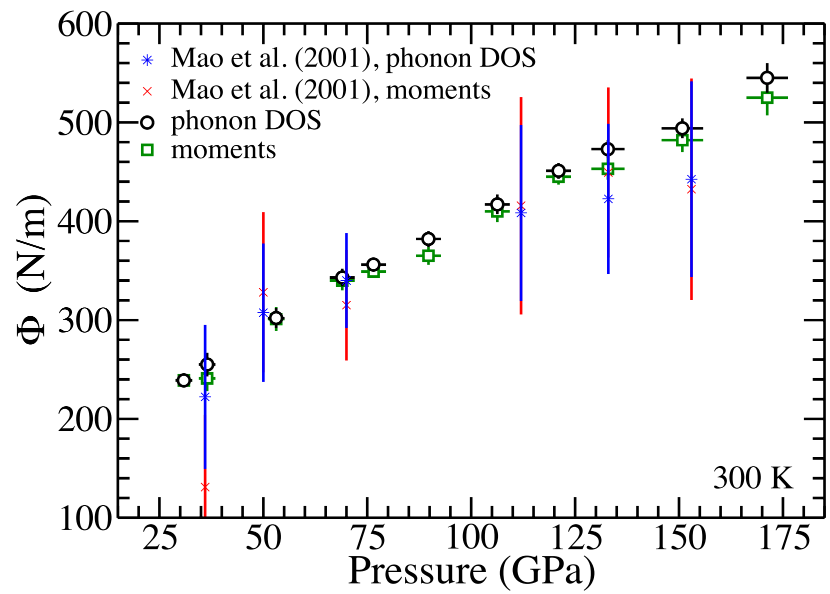


Volume dependence of the phonon DOS for ***hcp*-iron** to outer core pressures

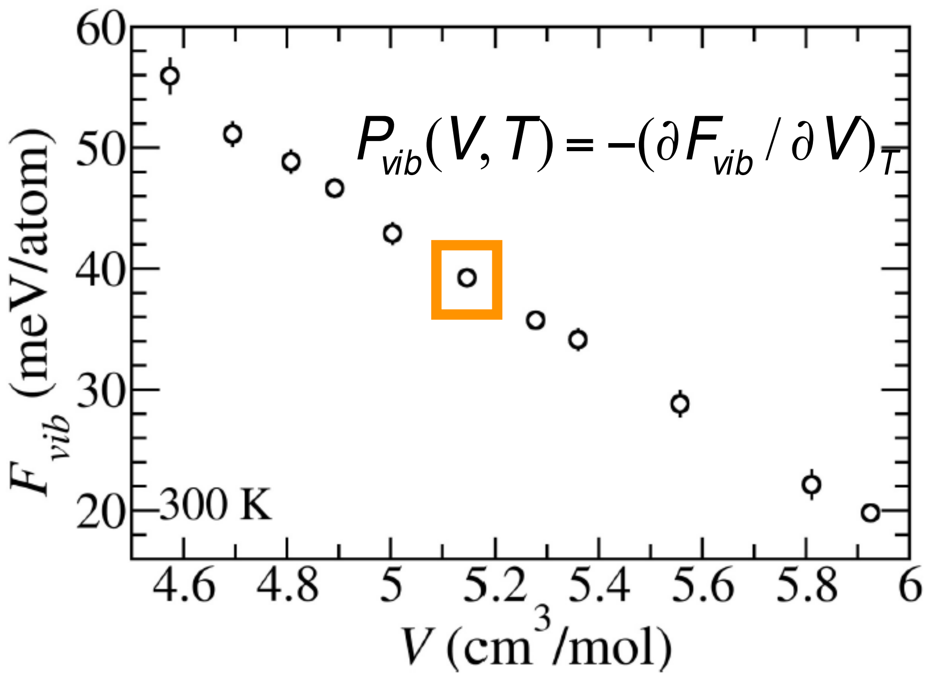


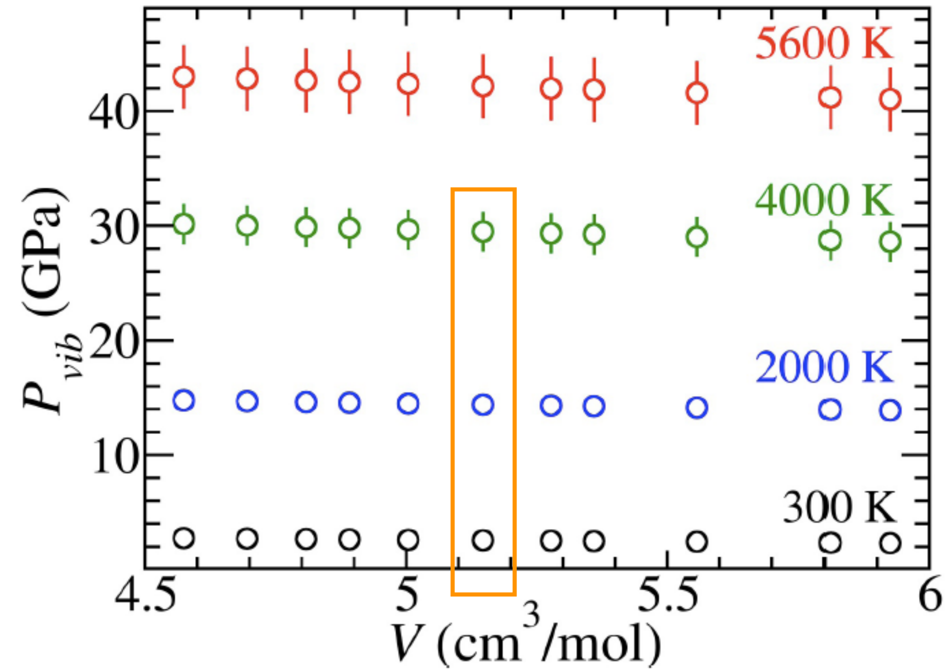


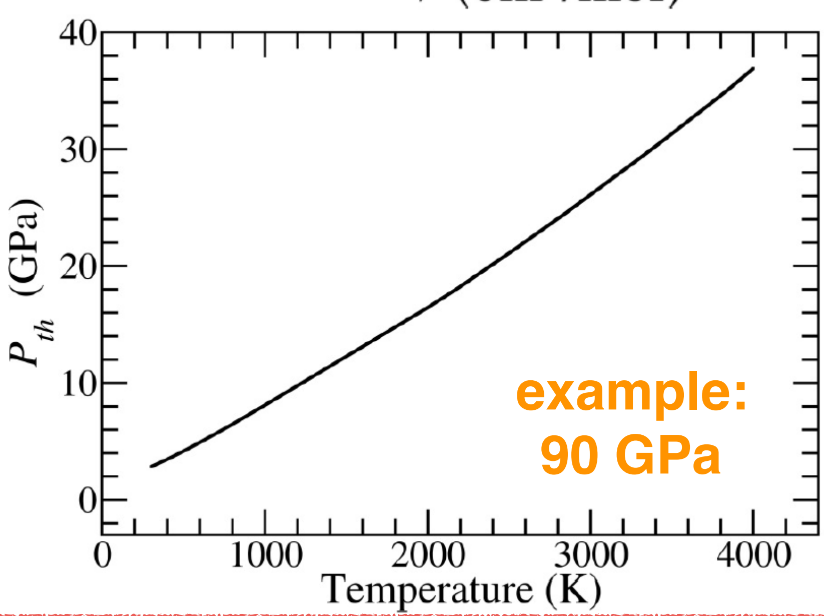




Thermal pressure from the measured volume dependence of ***hcp*-iron's** vibrational free energy







$$P_{th} = P_{vib}^{h} + P_{vib}^{anh} + P_{el}$$

Dewaele *et al. PRL* (2006)

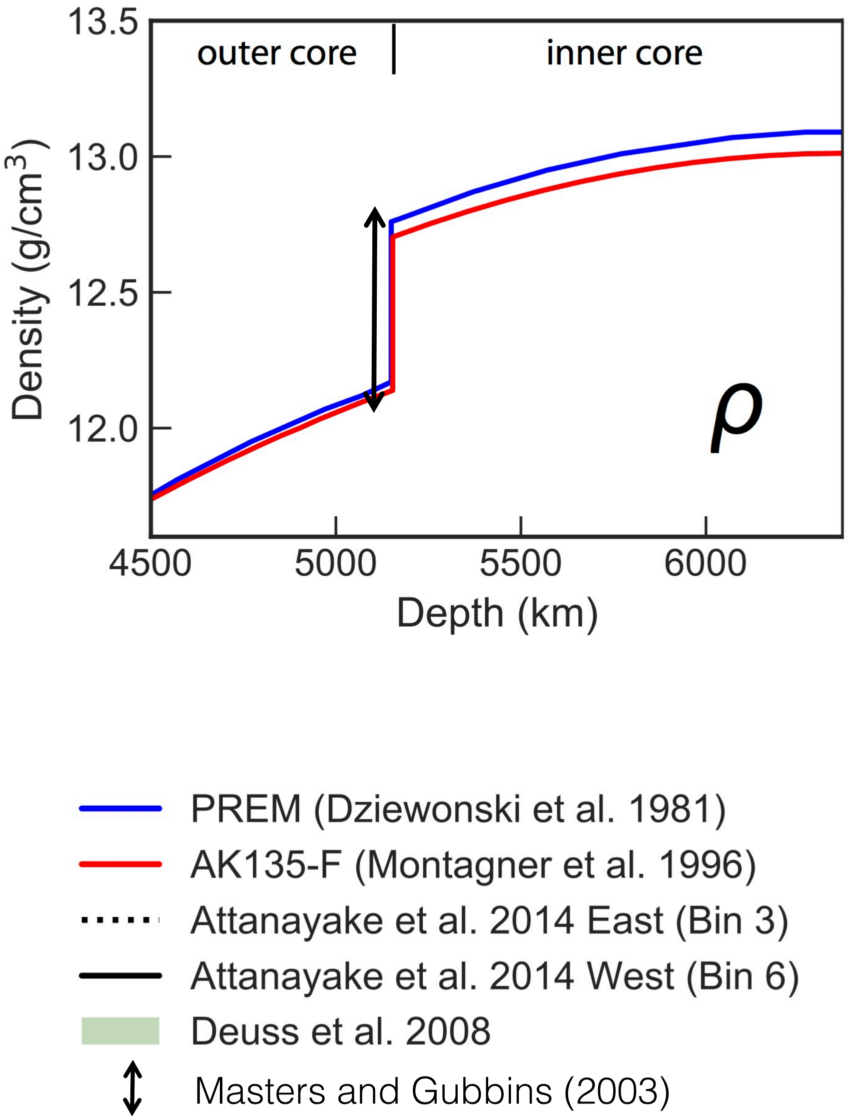
NRIXS: Murphy *et al. PEPI* (2011)

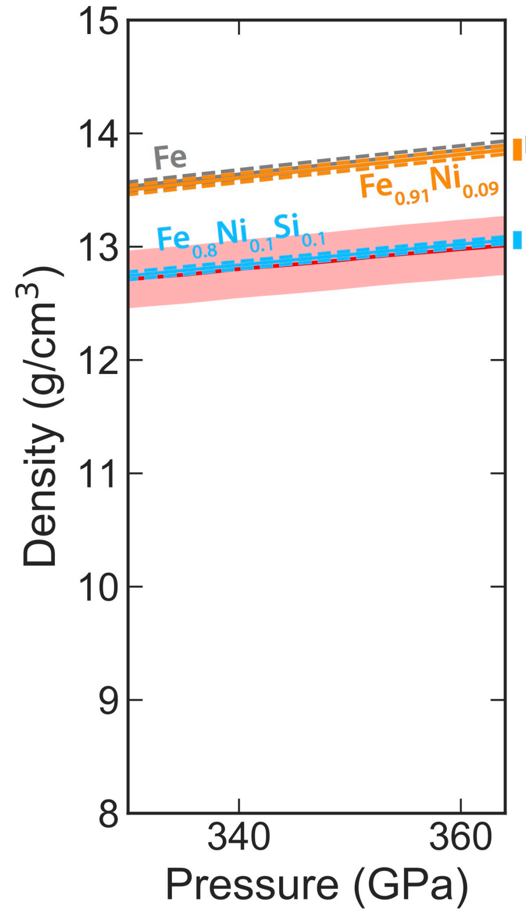
γ = 2.0±0.1

q = 1.0±0.2

PHOENIX Murphy *et al. PEPI* (2011)

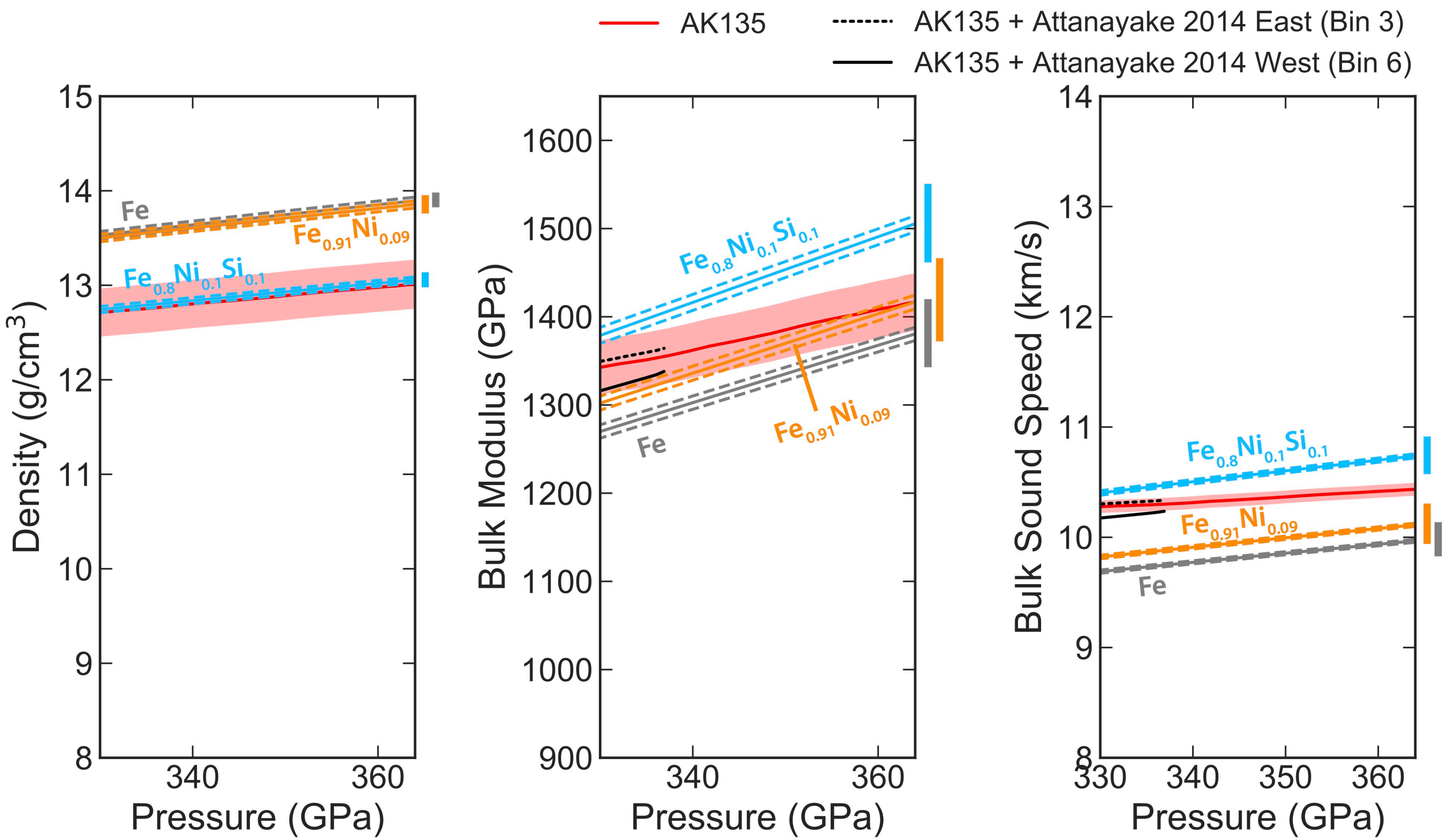
Density of Fe-Ni-Si at inner core conditions





Assume a uniform temperature:
5500 ± 500 K

Is there a composition in Fe-Ni-Si space that matches Earth's density, bulk modulus, and bulk sound velocity?



Morrison et al. JGR (2018)

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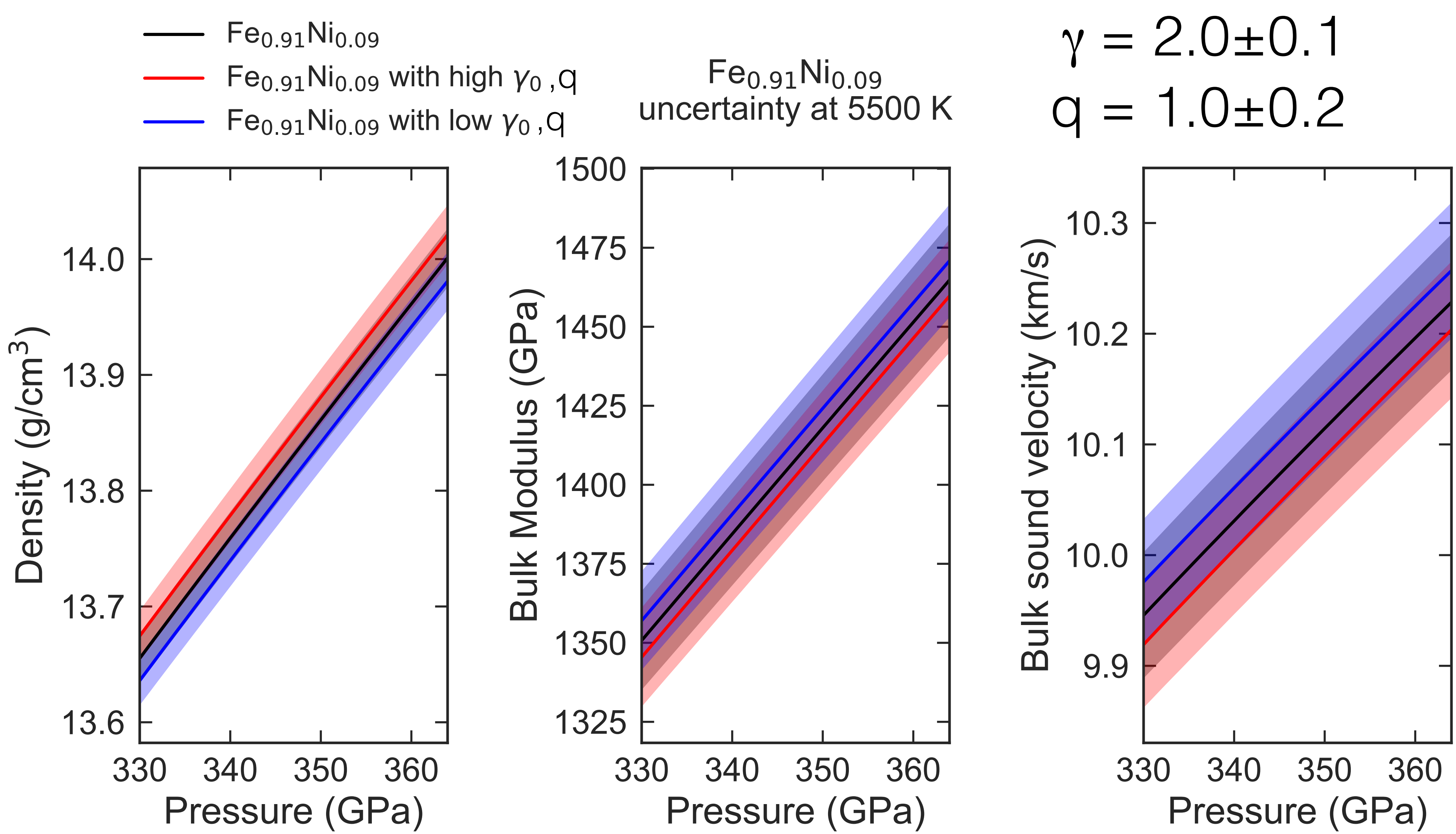
Error propagation of the quasi-harmonic thermal pressure terms to the elastic properties



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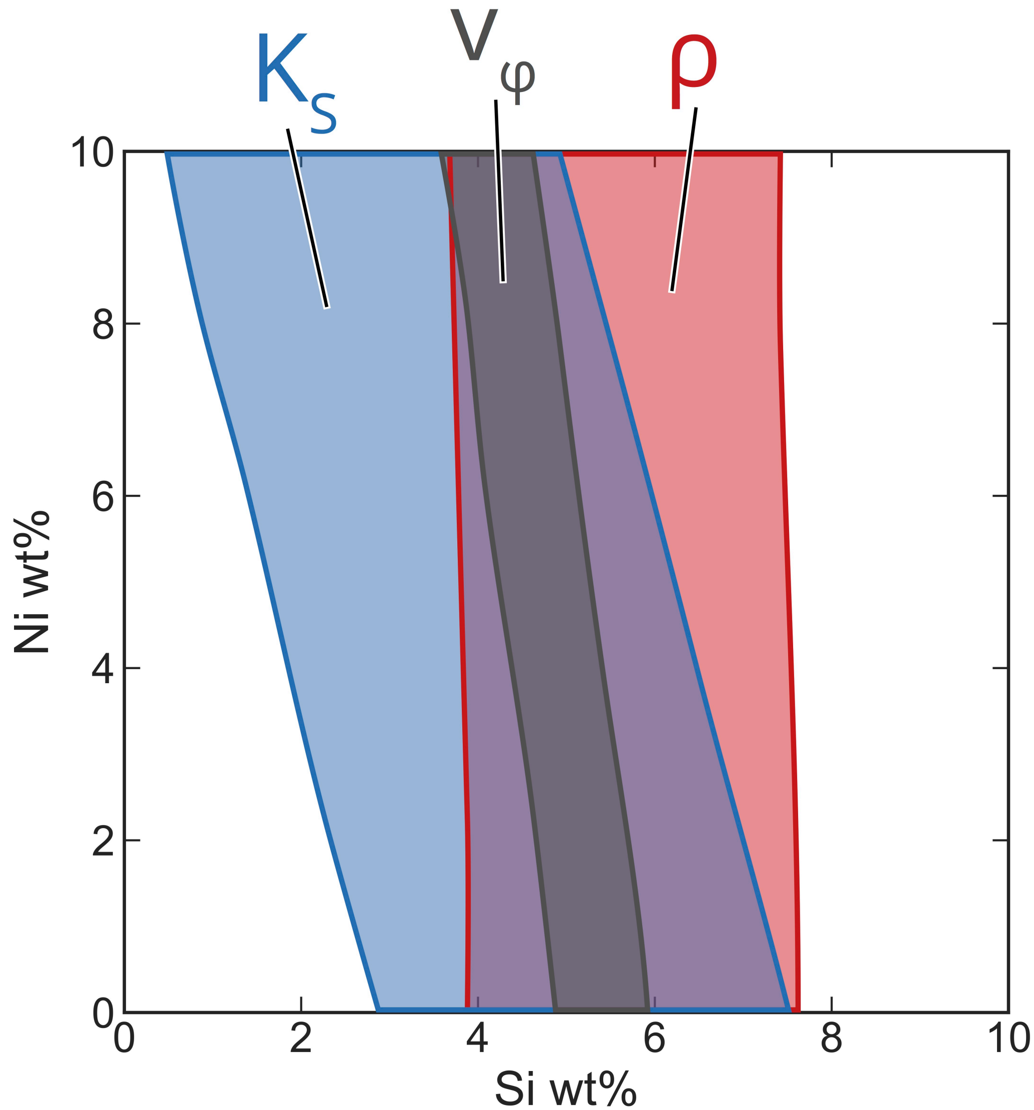
Is there a composition in Fe-Ni-Si space that matches Earth's density, bulk modulus, and bulk sound velocity?

Linear mixing model of hcp-Fe, $Fe_{0.91}Ni_{0.09}$, $Fe_{0.9}Ni_{0.1}Si_{0.1}$

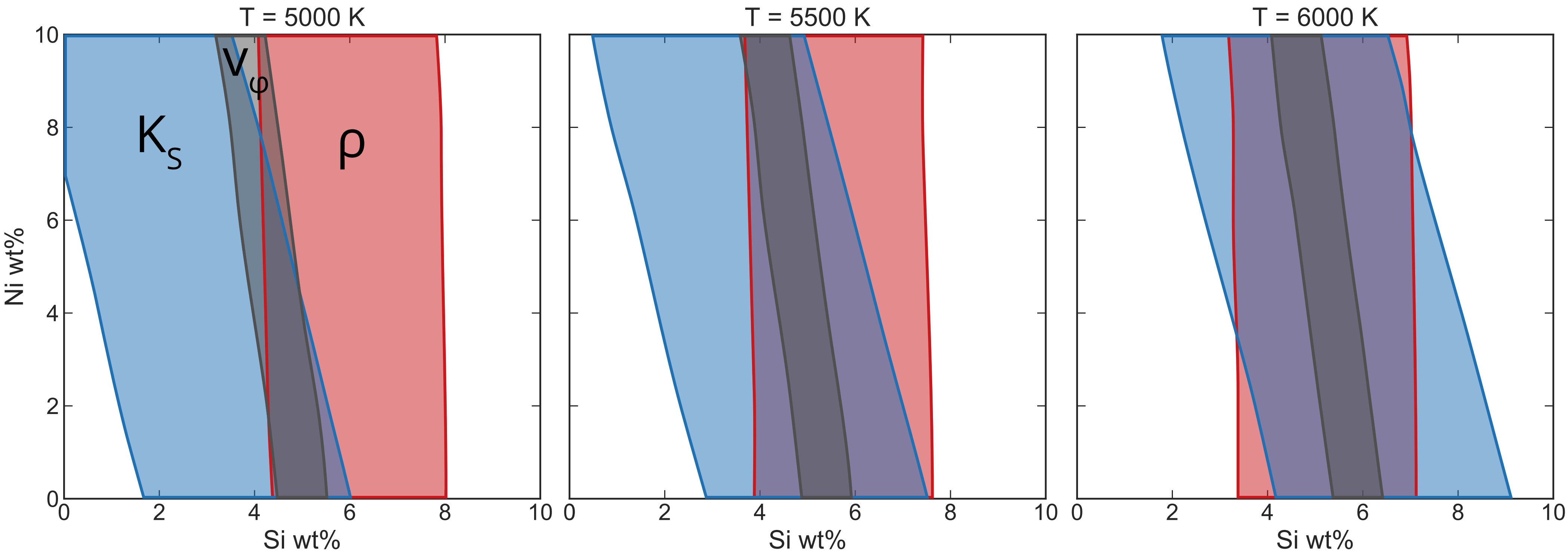
Assume core temperature of 5500 K

Pressure near ICB: 330 GPa

Result:
4.3 to 5.3 wt% silicon alone can explain the density, adiabatic bulk modulus, and bulk sound speed of the inner core



Effect of nickel, silicon, and temperature at Earth's inner-core boundary



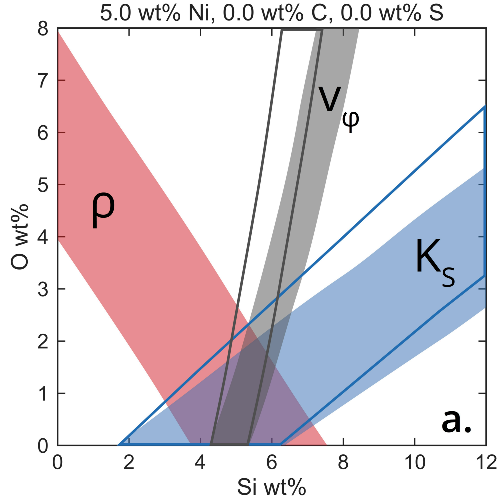
Lower temperatures: <8 wt% Ni and ~5 wt% Si required

Higher temperatures: 0 (to 10) wt% Ni, ~6 (to 5) wt% Si required

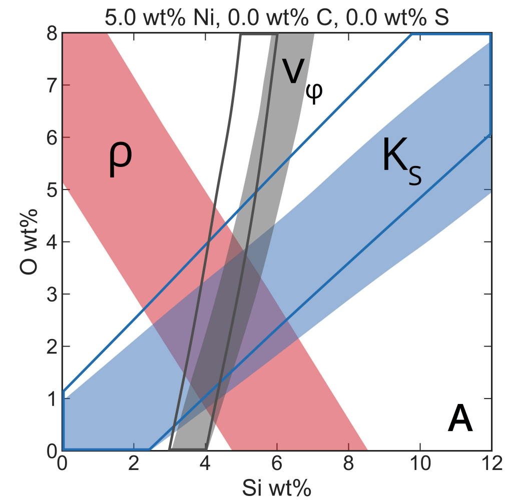
Bottom line: can match seismic quantities with an Fe-Ni-Si alloy

Compositional mixing model: Electronic and anharmonic contributions to thermal pressure

With P_{el} and P_{anh}



Without P_{el} and P_{anh}

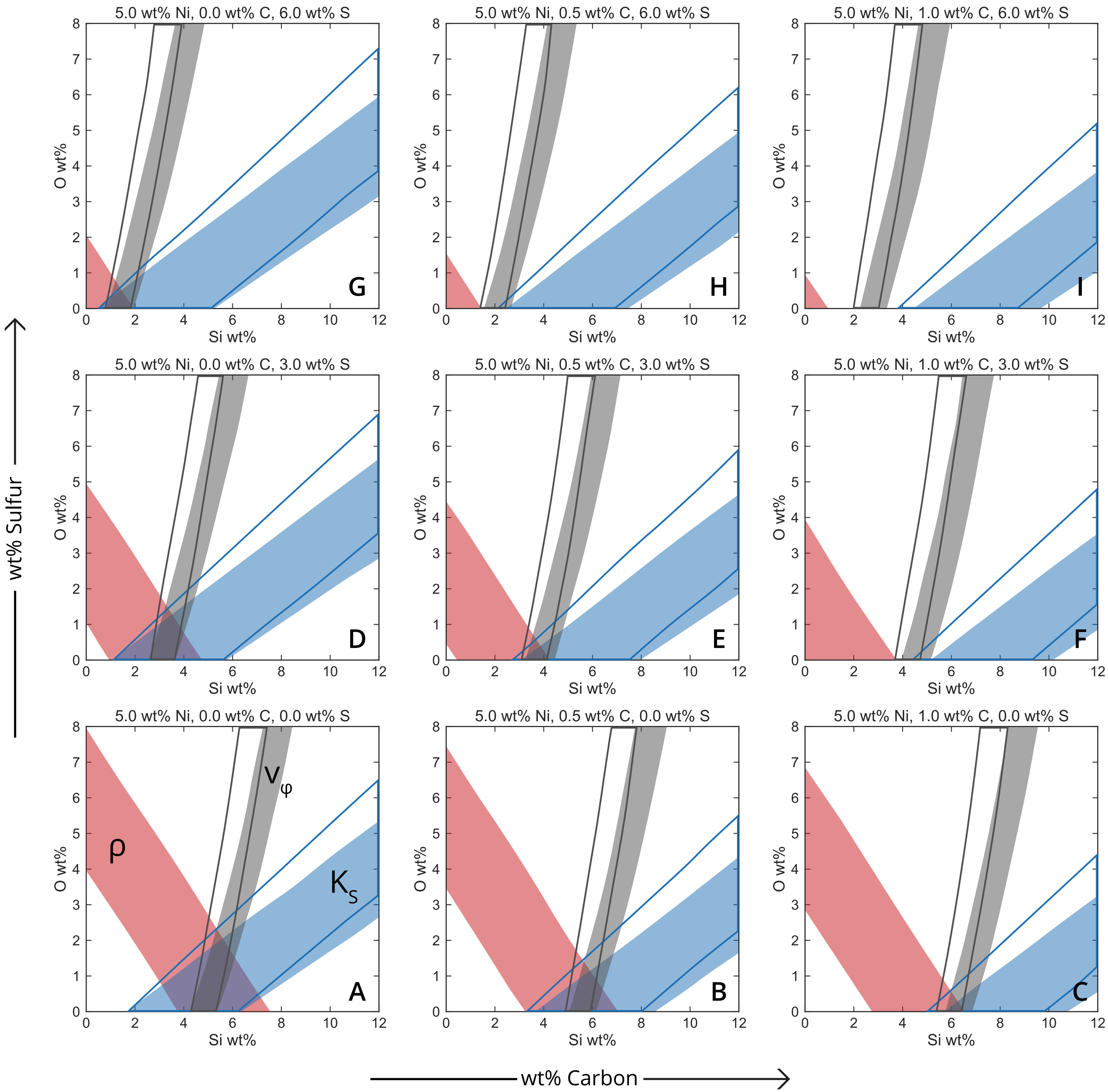


Neglecting P_{el} and P_{anh} yields results with **more** O, C, S in the inner core

<u>Upper limits (linear mixing):</u>

With P_{el} and P_{anh}	Without P_{el} and P_{anh}
6.4 wt% Si	6.2 wt% Si
2.3 wt% O	↑ 4.2 wt% O
7.5 wt% S	↑ 8.0 wt% S
1.0 wt% C	↑ 2.0 wt% C

Intersection of iron-nickel-alloy properties with AK135-F at the inner-core boundary



T = 5500 K

Morrison *et al. JGR* (2018)

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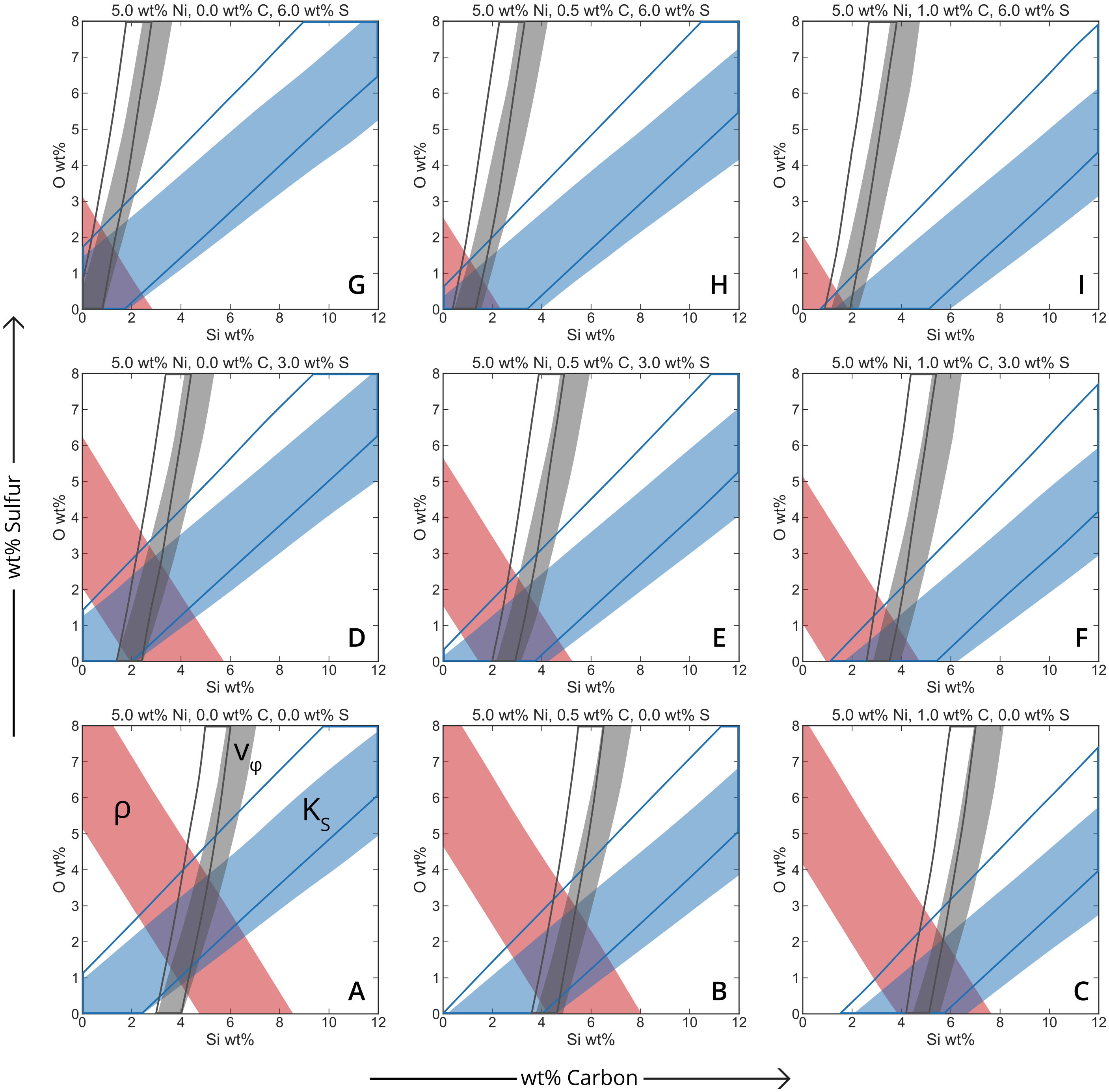
Intersection of iron-nickel-alloy properties with AK135-F at the inner-core boundary



T = 5500 K without electronic P_{el} and anharmonic P_{anh} terms

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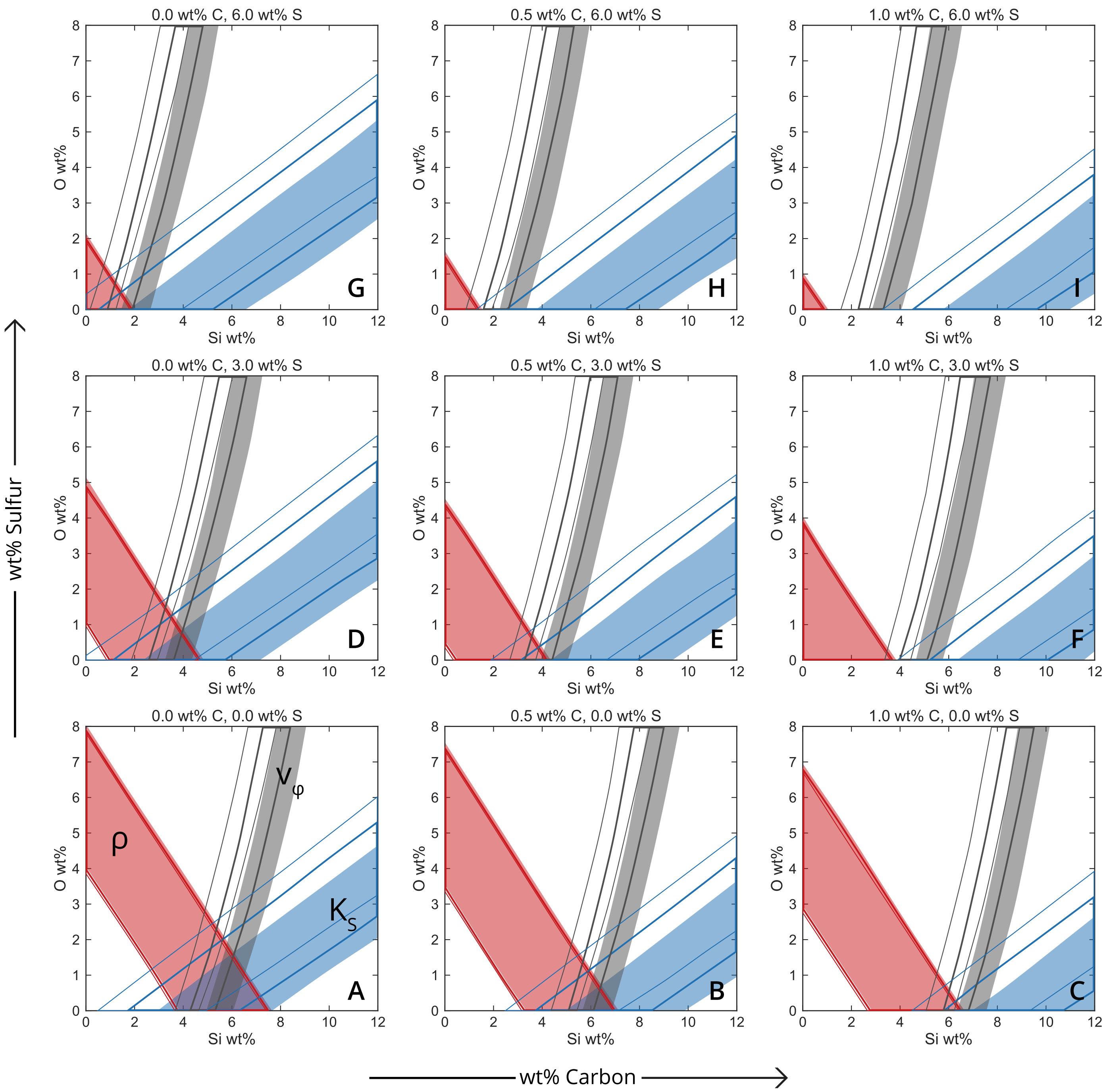
Intersection of iron-**X%**nickel-alloy properties with AK135-F at the inner-core boundary



T = 5500 K

0% Ni (shaded)
5% Ni (thick lines)
10% Ni (thin lines)

Morrison *et al. JGR* (2018)

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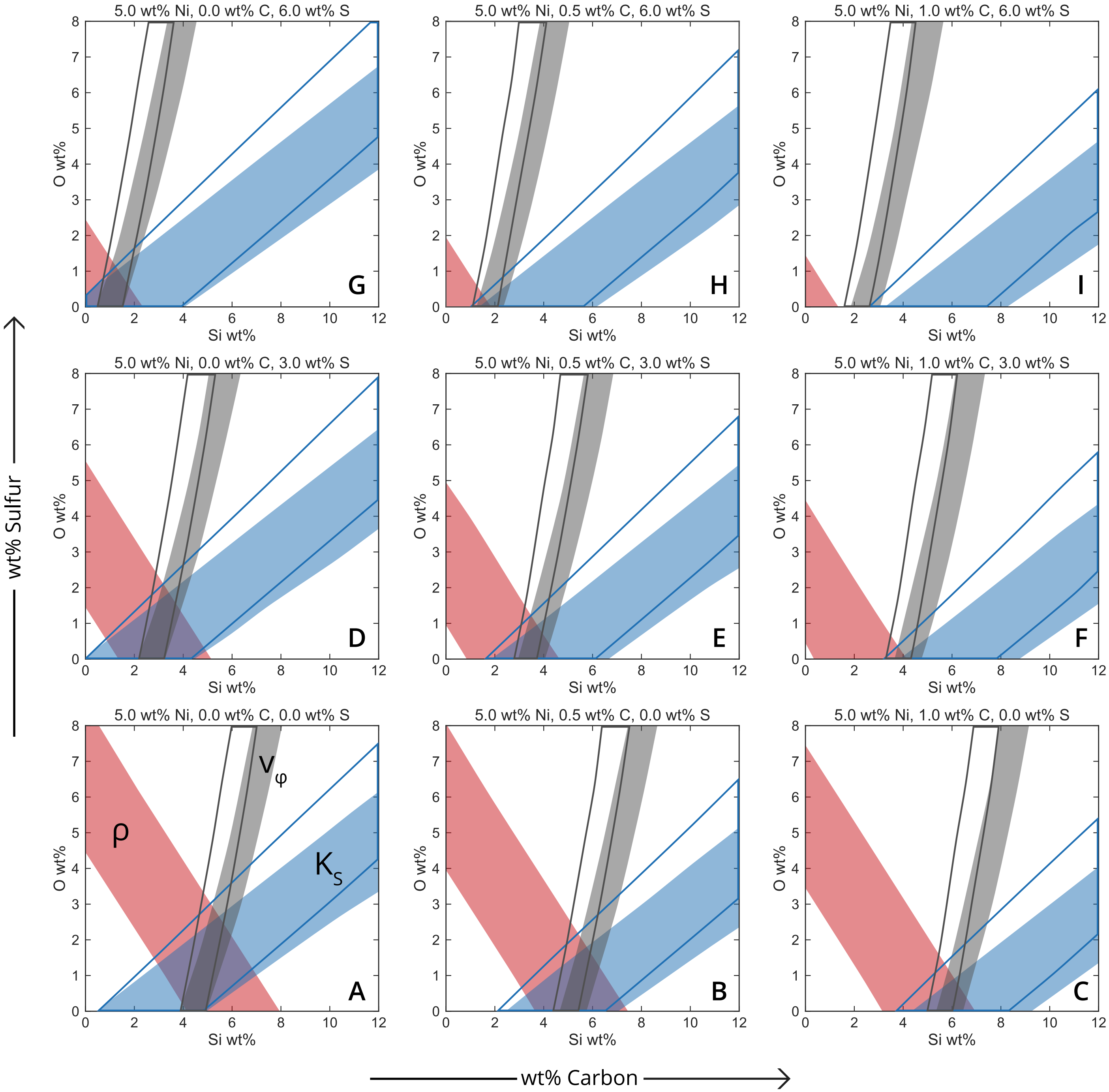
Intersection of iron-nickel-alloy properties with AK135-F at the inner-core boundary



T = 5000 K

Morrison *et al. JGR* (2018)

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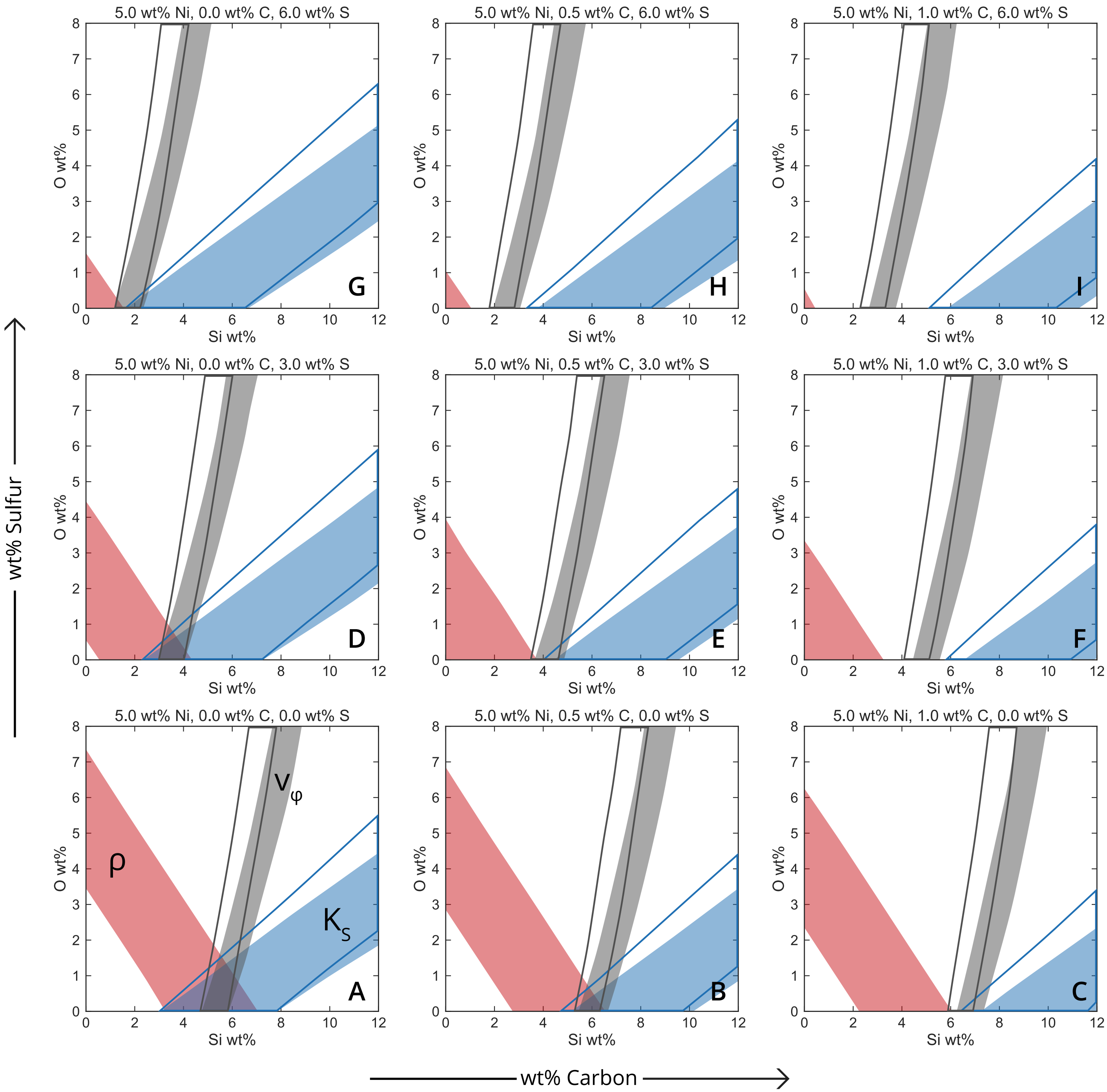
Intersection of iron-nickel-alloy properties with AK135-F at the inner-core boundary



T = 6000 K

Morrison *et al. JGR* (2018)

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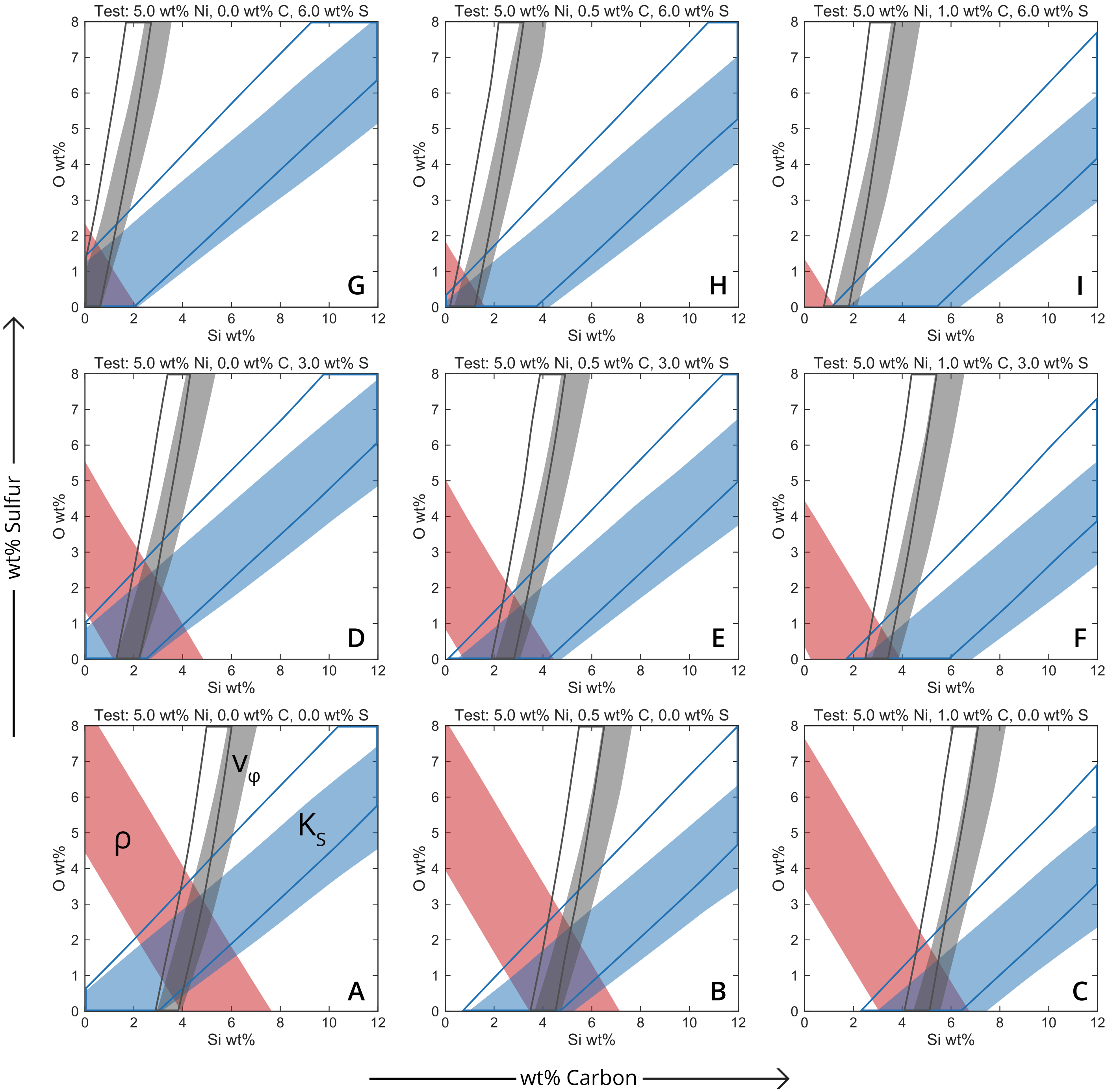
Intersection of iron-nickel-alloy properties with AK135-F



$T = 5500$ K
$P = 364$ GPa

Morrison *et al. JGR* (2018)

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Conclusions

Using nuclear resonant inelastic x-ray scattering and x-ray diffraction, we determined the sound velocities and thermal properties of Fe-Ni-Si alloys

- New method to constrain Debye velocity using probability distributions and information criteria: V_D, V_P, V_S
- thermal properties: γ, P_{vib}, α, *kinetic energy, specific heat, Lamb-Mössbauer factor*
- *Morrison et al.* (2018, under review)

Composition at Earth's inner-core boundary

Overlap of seismic observations for density, bulk modulus, and bulk sound speed, within reasonable propagated uncertainties:

- Constraints on the S,Si,C,O contents
- Incorporating electronic pressure is essential to narrow down the permissible composition of the core
- *Morrison et al. JGR* (2018)