MR43C-0105: Physical Properties of Fe-S and Fe-C-S Alloys Under Planetary Core Conditions

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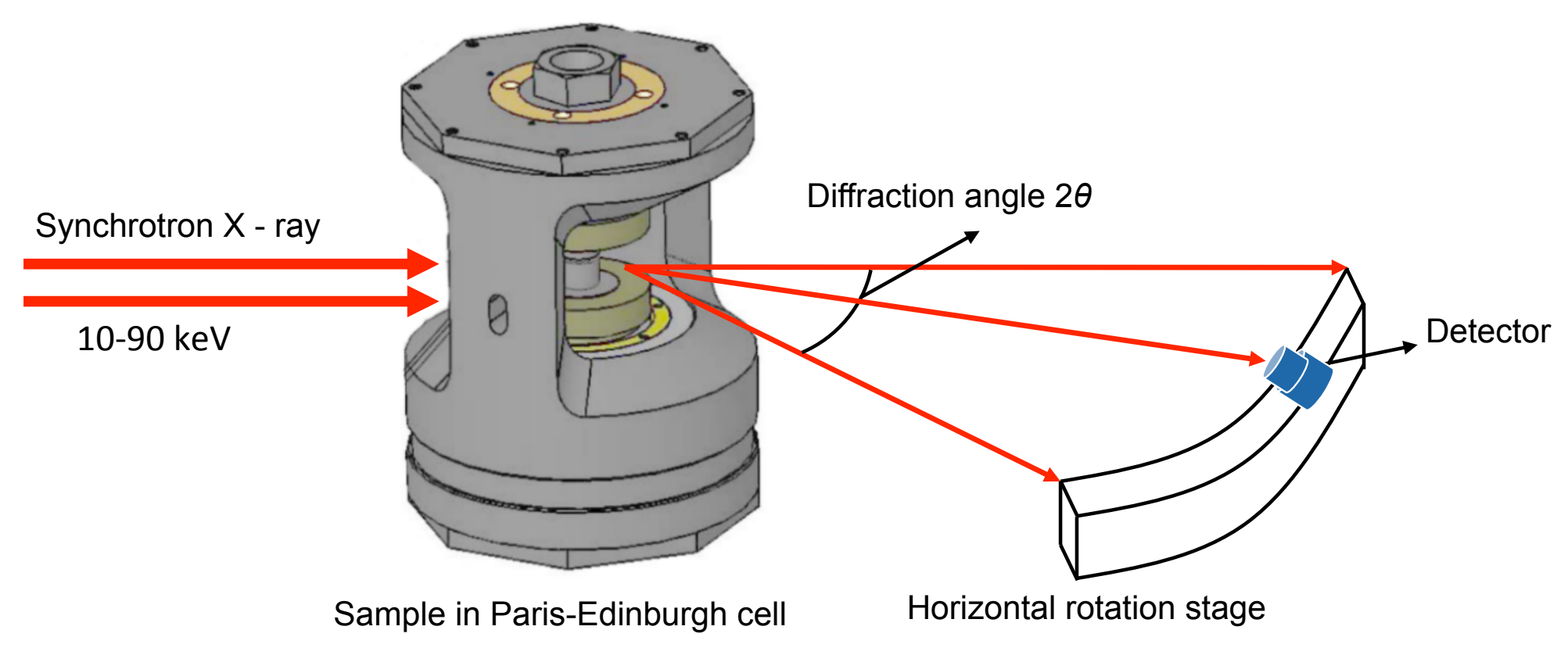
Context: The Fe-FeS binary is largely seen as the archetypal system to model the properties of the core of small to medium-sized telluric bodies. Noteworthy, while at the low pressures characteristic of the Moon the Fe-FeS is a simple binary eutectic, at the conditions relevant for planets such as such as Mercury, or satellite such as Ganymede, Io, and Europa, the Fe-S phase diagram is quite complex, with intermediate compounds of narrow stability field that incongruently melt.
Carbon is another light element as sulfur commonly found in meteorites and potentially present at a few wt% in the core of terrestrial planets, it is thus important to understand its effects on the properties of Fe-S alloys

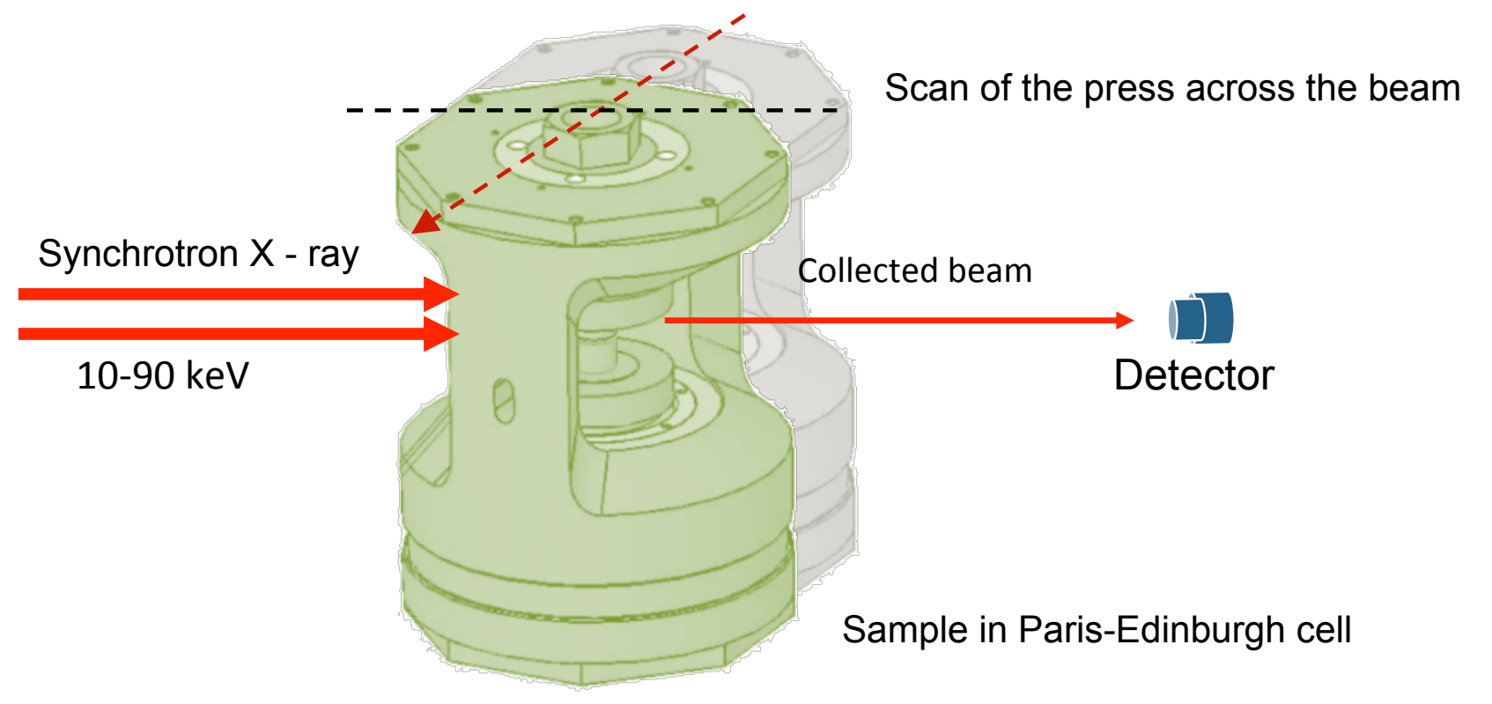
Combined in situ X-ray diffraction and absorption experiments on liquids at high pressure and high temperature

Diffraction mode: CAESAR



Amorpheus
(Boccato et al. DOI: 10.1080/08957959.2022.2032032 https://github.com/CelluleProjet/Amorpheus)

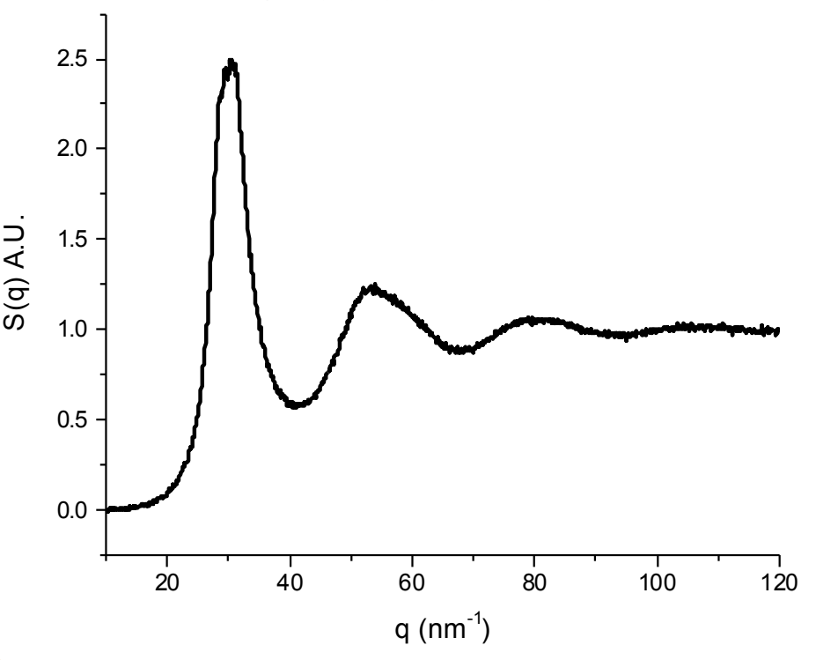
Absorption mode: Beer-Lambert + tomography



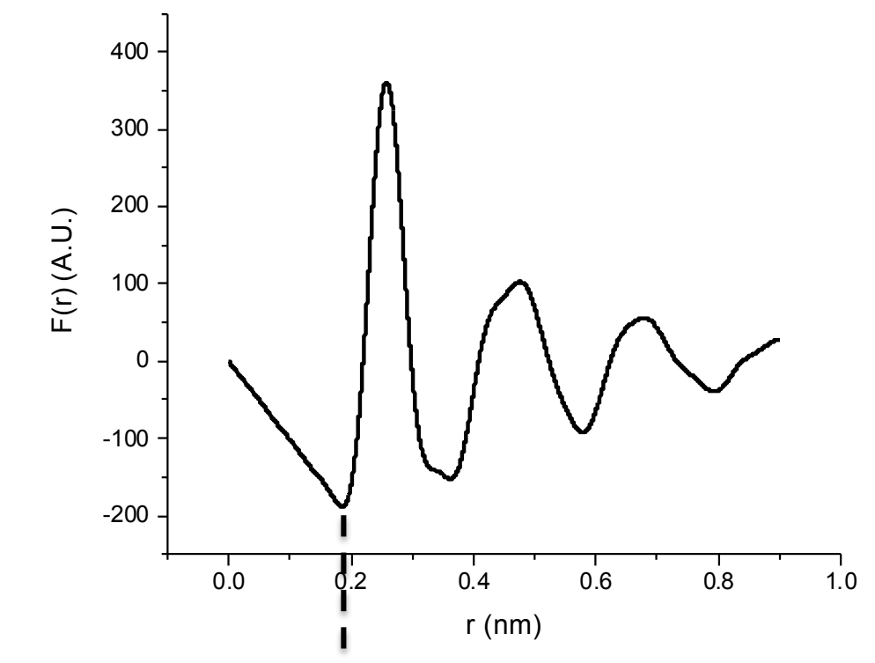
$I=I_0e^{-\mu\rho t}$

Local structure and density

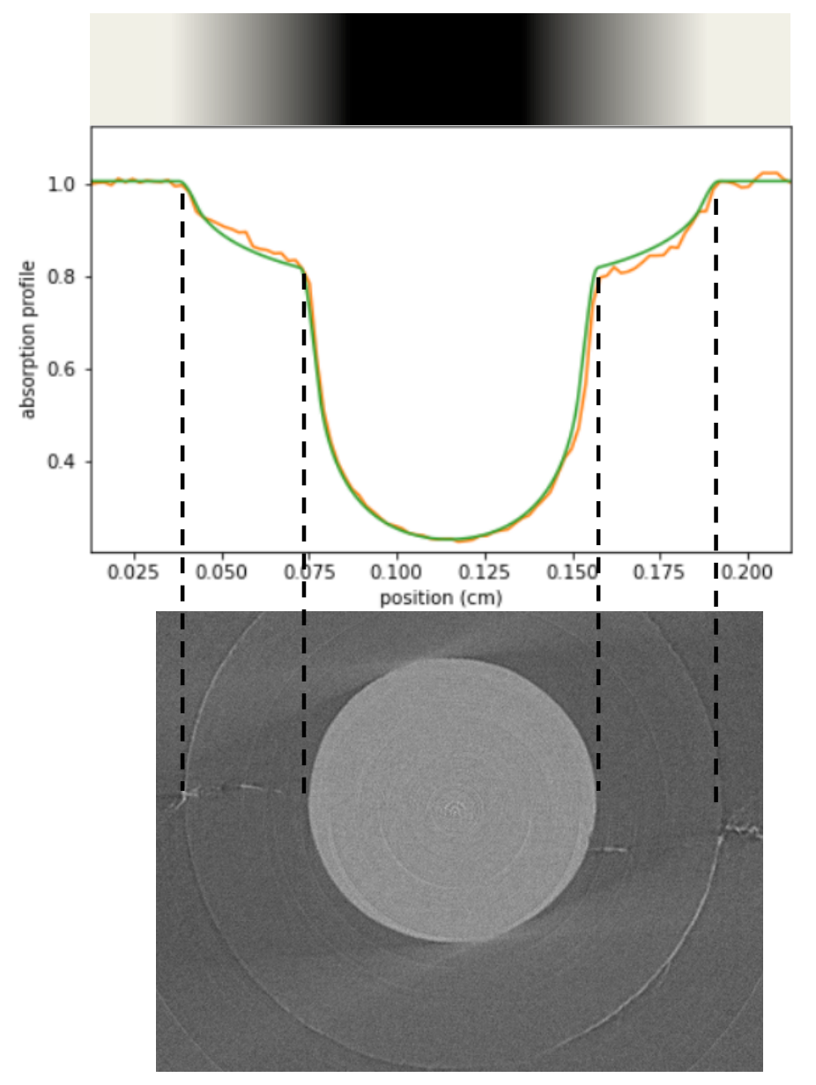
Structure factor



Distribution function



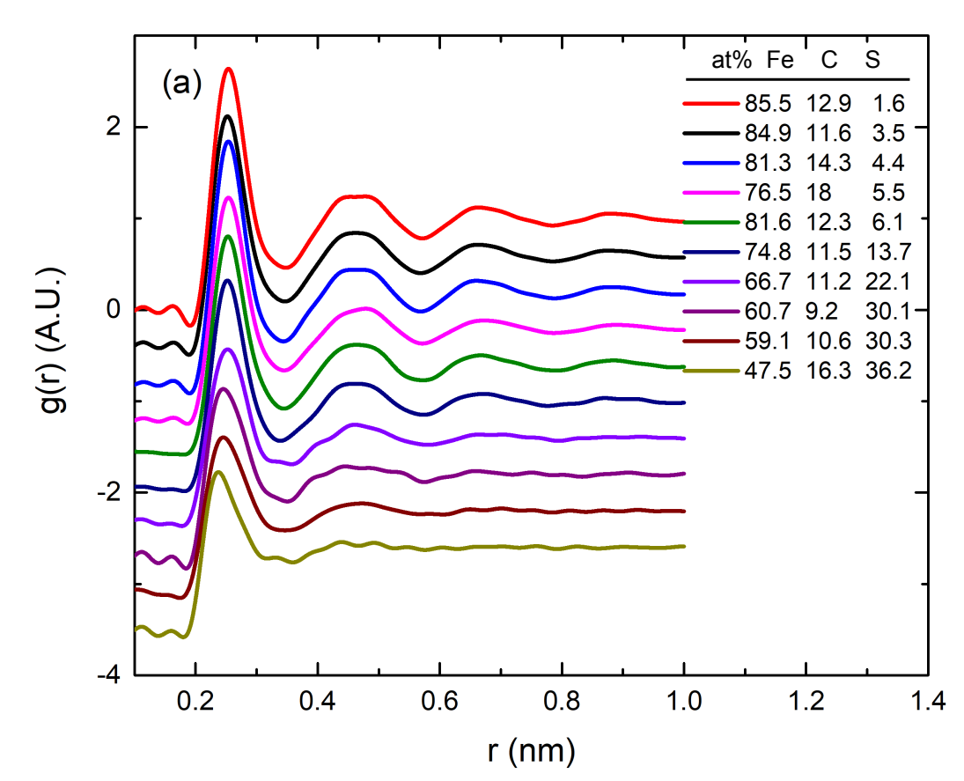
$F(r) = -4\pi\rho_0 \ (r < r_{min})$



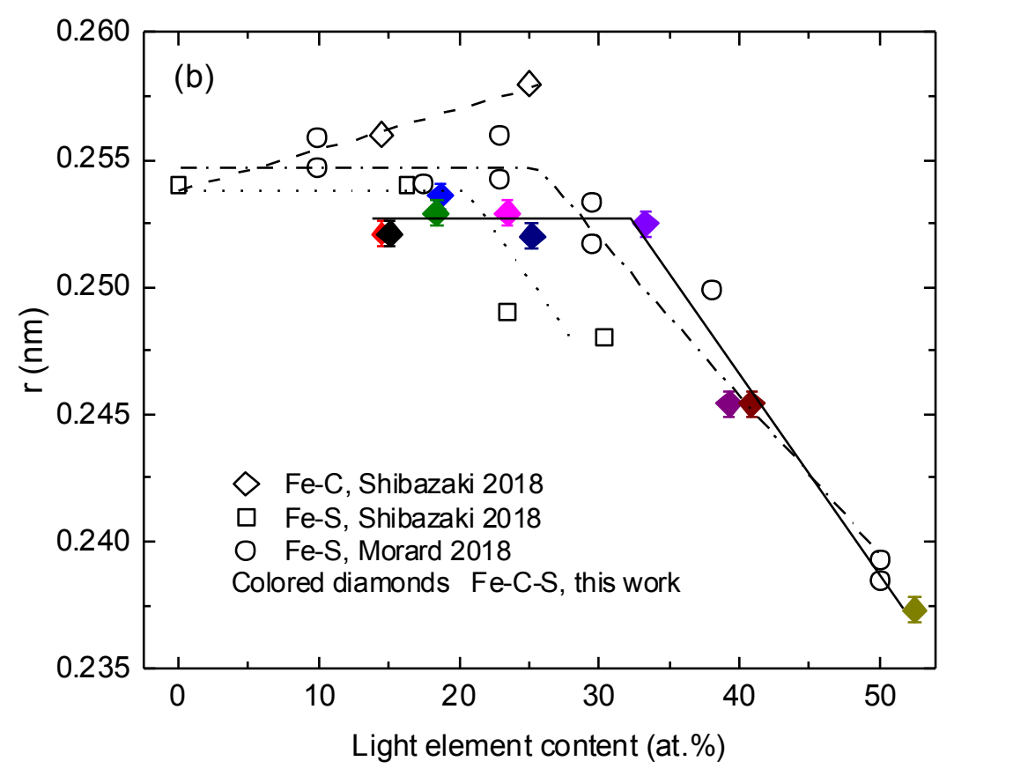
Density and 3D imaging

Local structure and density of liquid Fe-C-S alloys at high pressure and high temperature

Effect of S and C on local order

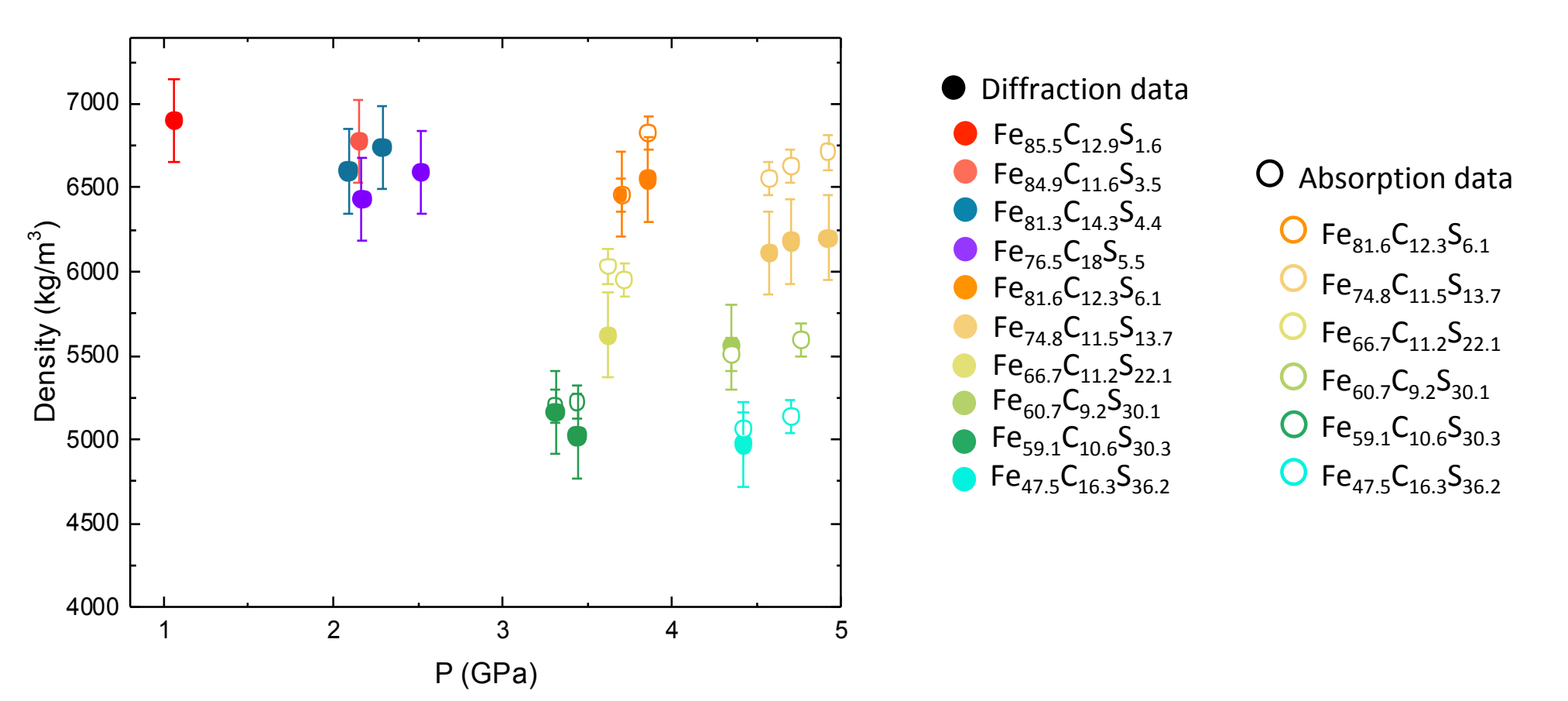


Fist peak position vs. light element content



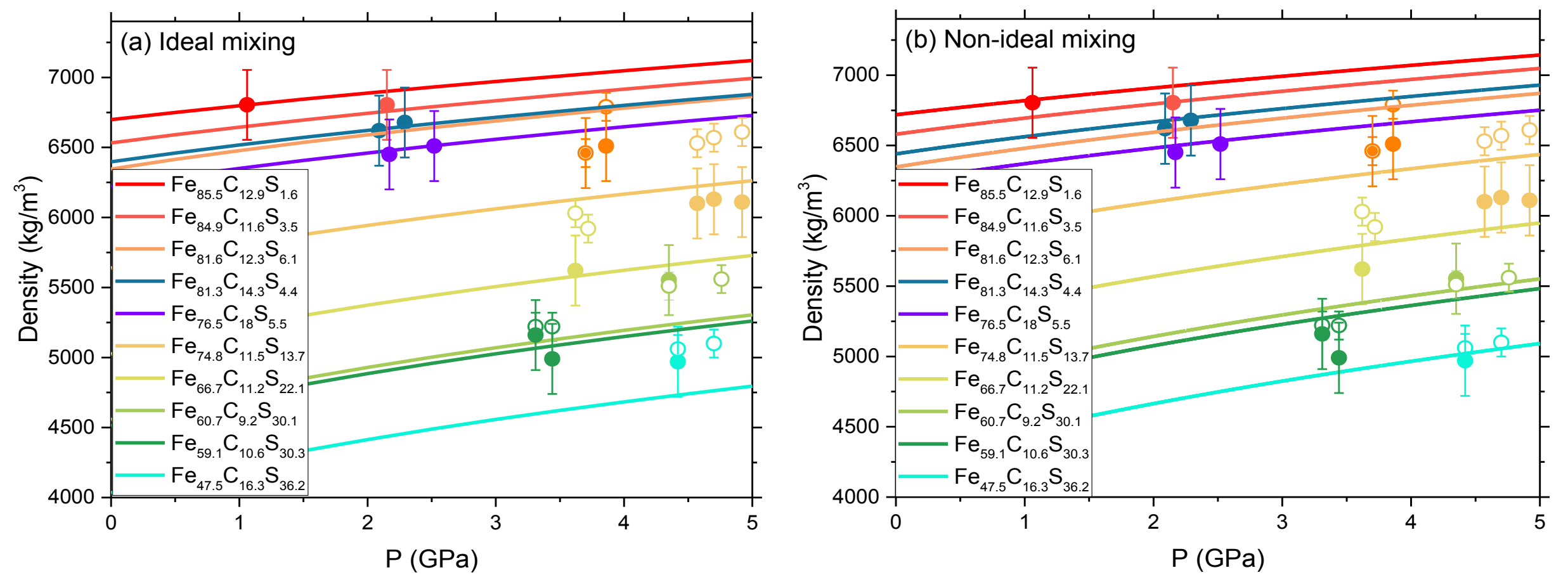
Structure modification visible for S> 22.1 at% → perturbation of the Fe-Fe network
C interstitially incorporated in liquid iron, without affecting much the Fe-Fe bonds

Density as a function of pressure (1-5 GPa) at high temperature (1600-1900 K)



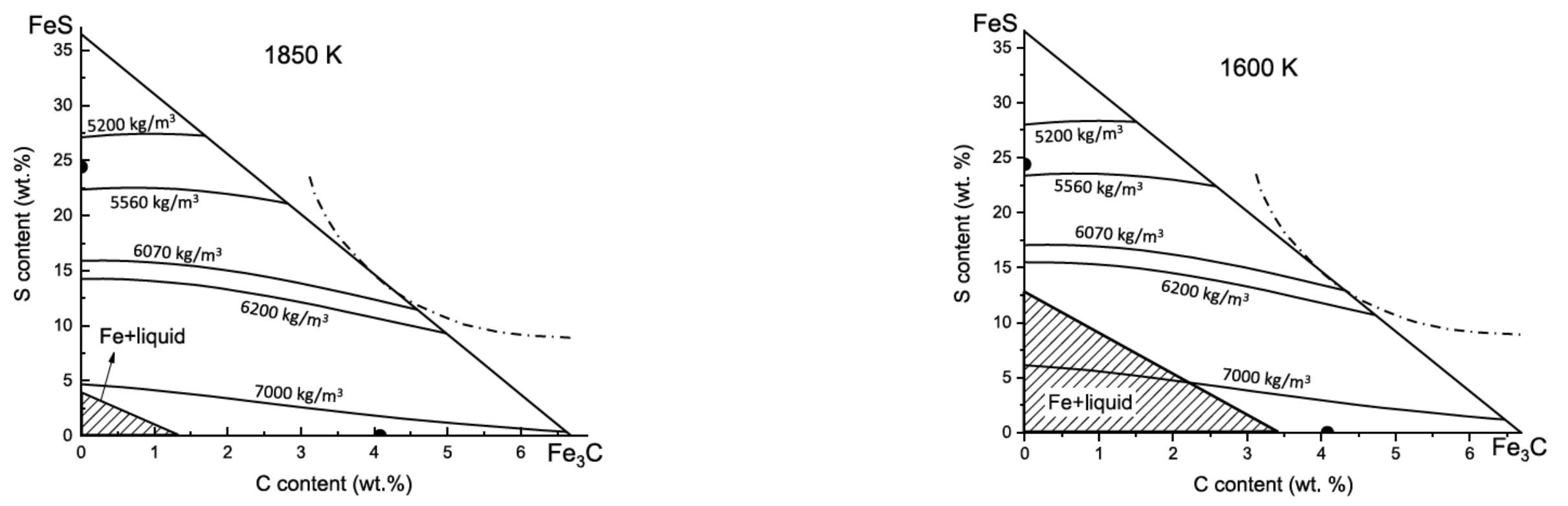
Reliable density determination, independently confirmed by two methods

Thermodynamic model



Thermodynamic solution model of the Fe-C-S liquid built on the thermal EOSs of Fe, FeS, and Fe_3C with their interactions modeled by an asymmetric Margules formulation

Implications for the Moon's core composition

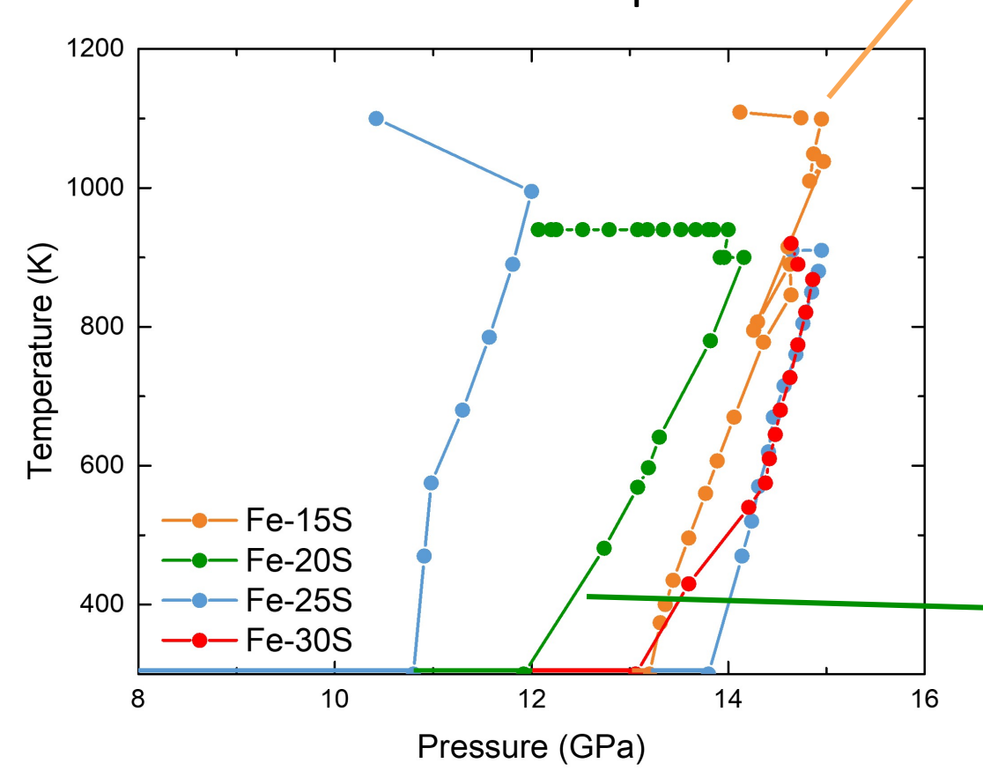


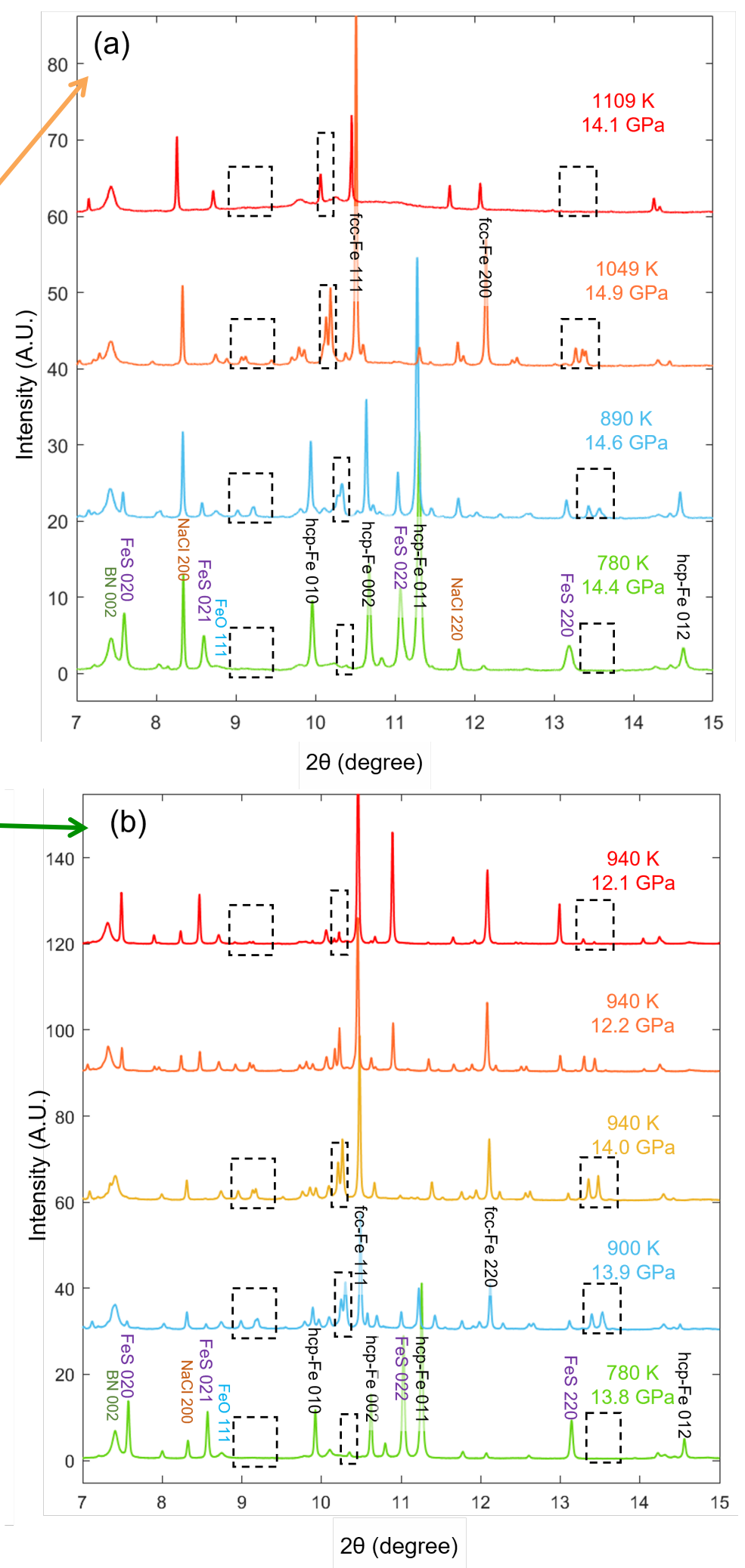
Recently proposed density for the Moon's (outer) core:
G19 (no inner core): 4200-5200 kg/m^3 → S: 27-36 wt%; C: 2-0 wt%
V19 (no inner core): 5560-6070 kg/m^3 → S: 12-23 wt%; C: 4.6-0 wt%
K21 (inner core): 6200-700 kg/m^3 → no solutions for T = 1850 K;
S: 5-13 wt%; C: 2.3-0 wt% for T=1600 K
B23 (no inner core): 6010-9510 kg/m^3 → S: 0-12 wt%; C: 7-0 wt%
B23 (inner core): 4420-5630 kg/m^3 → no solutions for any considered T

Study of the subsolidus phase diagram of the Fe-FeS binary in the 11-15 GPa range

- In situ angle dispersive XRD on sample in Paris-Edinburgh press at the ID27 beamline of ESRF
- Electron microscopy analysis of recovered samples

Experimental P-T paths for five Fe-S samples

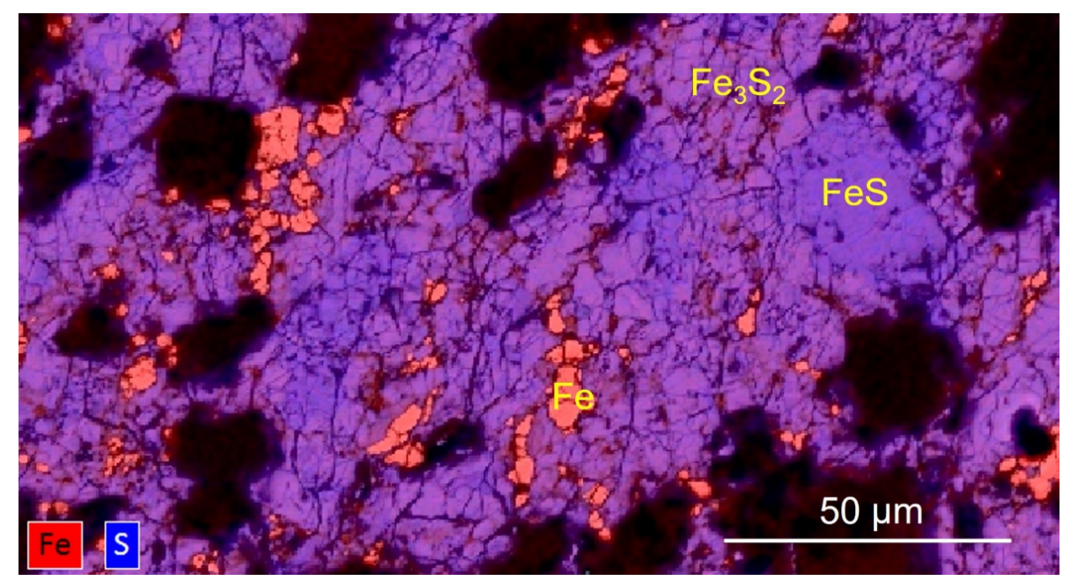




Maximum P, T and products of each run

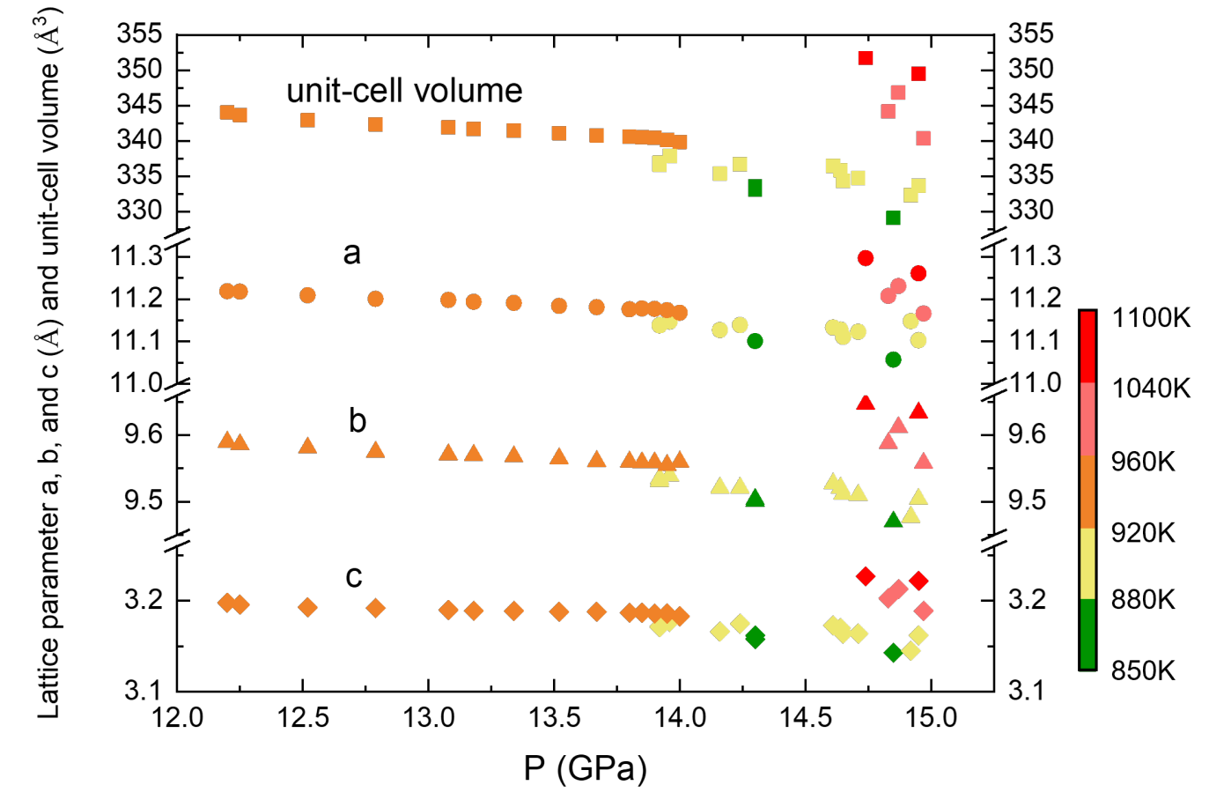
Run	P_{max} (GPa)	T_{max} (K)	Products
Fe-15S	15.0	1110[a]	Fe+Fe_3S_2+ trace FeO[b]
Fe-20S	14.2	940	Fe+Fe_3S_2+ trace FeO
	(Decompressed to 12.1)	(Kept at 940)	(Fe+FeS + trace FeO)
Fe-25S (low-P)	12.0	1100[a]	Fe+FeS + trace FeO[b]
Fe-25S (high-P)	15.0	910	FeS+Fe_3S_2+ trace FeO
Fe-30S	14.9	920	FeS+Fe_3S_2+ trace FeO

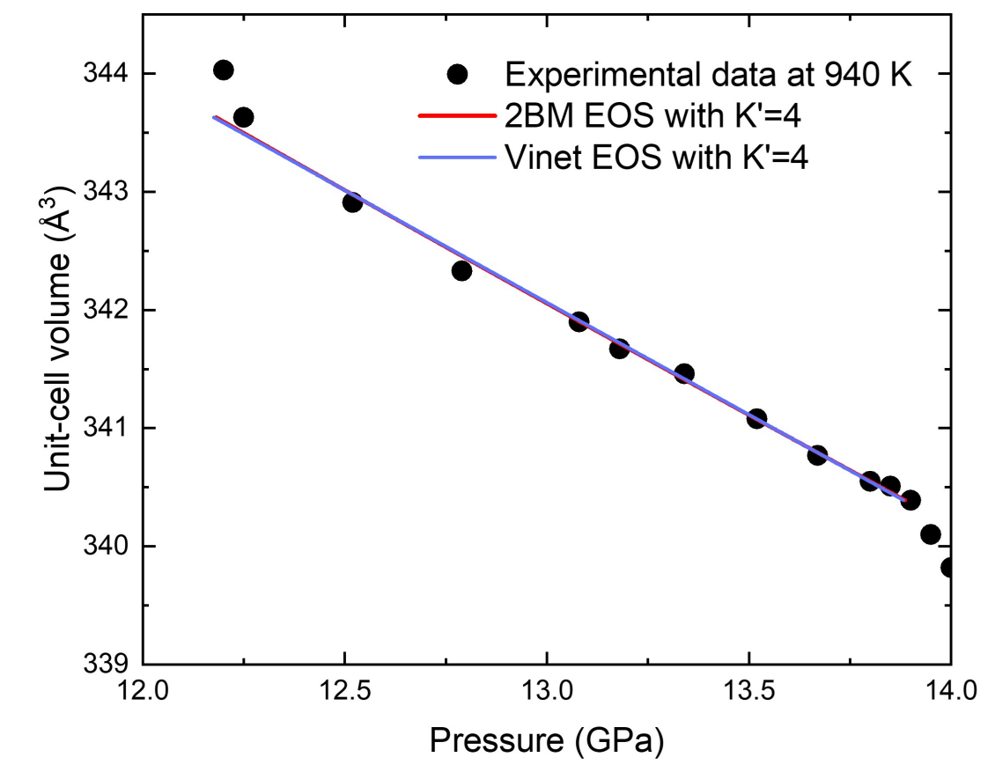
[a] Partial melting.
[b] Observed already before melting



EDS mapping of Fe-25S run product

EoS of Fe_3S_2





T_0 (K)	940 K	
Formalism	2nd-order Birch-Murnaghan	Vinet
$V_{0(T_0)}$ (Å^3)	372.2 (0.8)	367.3 (0.6)
$K_{0(T_0)}$ (GPa)	130(4)	185 (4)
K'_{T_0}	4[a]	4[a]
α (×10^{-5} K^{-1})	26.5[b]	

Implications for the S-rich cores in the 12-20 GPa range

- Fe_3S_2 stable below melting in the 12-20 GPa range → possible crystallizing phase in the core of telluric planets
- Fe_3S_2 end-member phase for thermodynamic modeling in the range 12-20 GPa, together with Fe or FeS depending on whether the S content is below or above 27 wt%
- Change in the slope of the pressure evolution of the eutectic temperature from negative to positive at 12 GPa, in concomitance to the stabilization of Fe_3S_2 ?
- Central pressure of Europa, Io, and Ganymede < 11 GPa → crystallizing phase Fe or FeS
- Mercury and Mars big enough to possibly have Fe_3S_2, but:
  Mars is currently expected fully molten (if solid core, very small and at P> 20 GPa)
  Mercury is most likely is not rich enough in S (even at a late stage of inner-core growth)

Main references: Zhao et al., J. Geophys. Res.: Planets 128, e2022JE007577 (2023); Zhao et al., Earth Planet. Sci. Lett. (under review)
Other references: Anderson & Ahrens, J. Geophys. Res. 99(B3), 4273 (1994); Briaud et al., Nature 617, 743 (2023); Garcia et al., Space Science Reviews 215, 1 (2019); Knibbe et al., J. Geophys. Res.: Planets 126, e2020JE006651 (2021); Komabayashi, J. Geophys. Res.: Solid Earth 119, 4164 (2014); Kuskov et al., Geochem. International 59, 1018 (2021); Viswanathan et al., Geophys. Res. Lett. 46, 7295 (2019).