	Experiment title: Can sulfur enter into the composition of the solid core of telluric planets?	**Experiment number**: ES-748
Beamline: ID28-ID15B	**Date of experiment**: from: 04.07.2018 to: 10.07.2018 (ID28)	**Date of report**: 21 February 2020
Shifts: ID-28:18 ID-15B:3	**Local contact(s)**: L. Paolasini (ID-28) M. Hanfland (ID-15B)	*Received at ESRF:*

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Report:

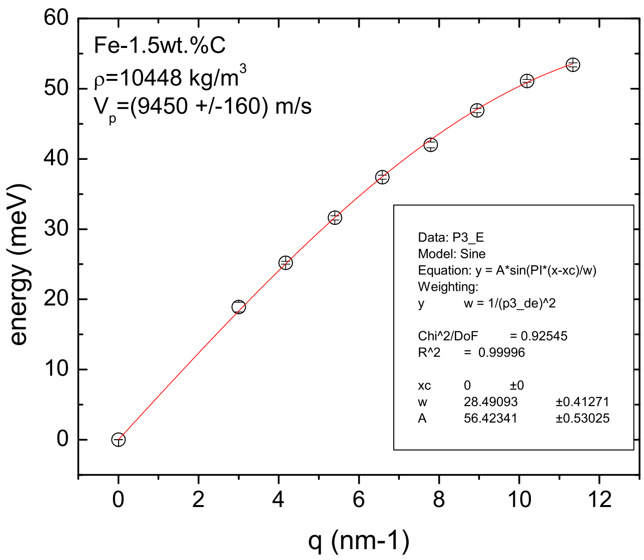
Original plan was to perform measurements on Fe-S alloys, but high-pressure synthesis resulted in chemically inhomogeneous samples and/or chemically contaminated samples, not suitable for the measurements. As such we performed inelastic x-ray scattering (IXS) and x-ray diffraction (XRD) measurements to determine sound velocity and density of polycrystalline Fe-C and Fe-C-Si alloys (high-quality, well sintered and chemically homogeneous samples, which, as Fe-S alloys, are candidates for the compositions of telluric planetary cores) in the hcp phase as a function of pressure. Specifically we carried out measurements on a binary Fe-C sample with 1.5 wt.% C and a on ternary Fe-C-Si sample with 1 wt.% C and 1.5 wt.% Si in the 30 to 140 GPa range.

Pressures were generated by membrane-driven Le Toullec type diamond anvil cells (DAC), equipped with either 100/300 μm bevelled anvils (Fe-C-Si sample) or 150/300 μm bevelled anvils (Fe-C- sample) and Re gaskets. Pressure was measured off line by collecting Raman spectra at the tip of the diamonds, and crosscheck after collection of sample diffraction by using previously established equation of state (unpublished results).

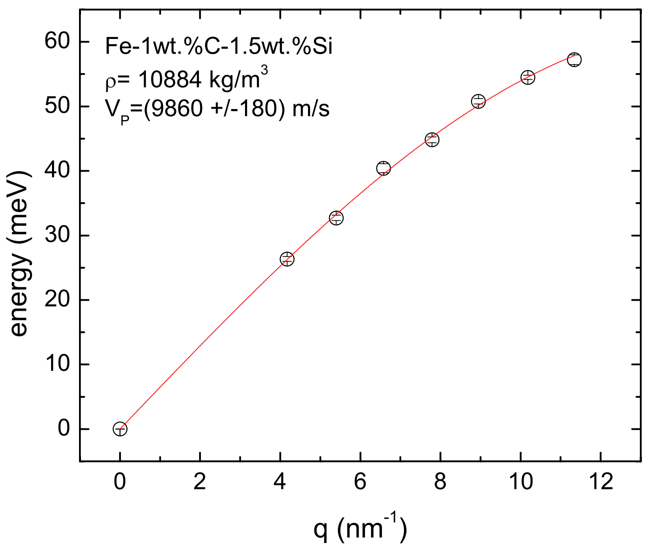
IXS measurements have been performed using the Si(9,9,9) instrument configuration. The Si(9,9,9) configuration has been proven to enhance the contrast between sample and diamonds phonons with respect to data obtained using the Si(8,8,8) configurations as typically done for powders in DAC (the widths of diamond phonons are defined by the energy resolution of the spectrometer), still providing enough flux to collect good-quality data in reasonable amount of time (~500-600 s per point). Spectra have been collected in transmission geometry, with the x-ray beam impinging on the sample through the diamonds, along the main compression axis of the cell, and hence probing exchange momenta q perpendicular to the cell-axis. The x-ray beam was focused at sample position to 40x30 μm^2 (horizontal x vertical, FWHM) by optics in Kirkpatrick-Baez configuration and slit down when necessary. Momentum resolution was set to 0.28 and 0.84 nm^{-1} in the horizontal and vertical plane. A vacuum chamber was used to minimize the quasi-elastic scattering contribution from air. At each investigated pressure point, we mapped the aggregate longitudinal acoustic phonon dispersion throughout the entire first Brillouin zone collecting 7 to 8 spectra in the 3-12.5 nm^{-1} range. The energy positions of the phonons were extracted by fitting a set of Lorentzian functions convolved with the experimental resolution function to the IXS spectra, utilizing a standard χ^2 minimization routine. We then derived the aggregate compressional sound velocity V_P from a sinus fit to the phonon dispersion, with error bars between ±1 and ±2% (see Figures 1 and 2).

At each investigated pressure point we collected 2D diffraction patterns on ID15B. Tacking advantage of the smaller beam 5x5 μm^2, we collected data over the entire sample surface, monitoring pressure gradients. Collected diffraction pattern have been analyzed to determine sample's texture as well.

IXS and XRD data have been collected for the Fe-C sample at about 50, 82 and 100 GPa and for the Fe-C-Si sample at about 41, 93 and 140 GPa. An example of the obtained acoustic phonon dispersion curve and derived velocity for Fe-C sample is illustrated in Figure 1, while Figure 2 shows an example of phonon dispersion curve and derived velocities for the Fe-C-Si sample.



<u>Figure1.</u> Example of the longitudinal acoustic phonon dispersion curve of polycrystalline hcp Fe-1.5wt.%C at high pressure. The red line is a sine fit to the experimental data.



<u>Figure2.</u> Example of the longitudinal acoustic phonon dispersion curve of polycrystalline hcp Fe-1wt.%C-1.5wt.%Si at high pressure. The red line is a sine fit to the experimental data.

Data analysis is still ongoing at the time of writing. Once finalized, we expect to be able to address the effect of C alloying on the elasticity of iron and iron-silicon alloys at high pressure.