ESRF	**Experiment title:** Elastic constants of a ε-Fe single crystal under pressure	**Experiment number**: HC-3402
Beamline: ID27+ID28	**Date of experiment**: from: 22/09/2017 to: 04/10/2017	**Date of report**: 20/02/2018
Shifts: 6+18	**Local contact(s)**: V. Svitlyk and A. Bosak	*Received at ESRF:*
Names and affiliations of applicants (* indicates experimentalists): **Dewaele Agnès***		

Report:

The aims of this project were: (i) to synthesize ε-Fe single crystals (on ID27); (ii) to measure their single crystal elastic constants with inelastic X-ray scattering (on ID28). For that purpose, we have compressed hydrostatically an α-Fe single crystal in a resistively-heated diamond-anvil cell.

The diamond anvil cells, loaded with iron samples embedded in neon pressure medium, were inserted in a vacuum resistive furnace which allows heating up to 850K on the samples. This device was provided by ID27. The temperature was measured by a thermocouple in contact with the back of one diamond anvil. The pressure was measured using a $SrB_4O_7:Sm^{2+}$ luminescence gauge. The phase and volume have been measured using angular-dispersive X-ray diffraction. The conditions of the experiments are summarized in **Table 1**.

Run name	Sample	Pressure medium	Pressure range (GPa)	Temperature range (K)
FeBPHT_8	Fe single crystal	Neon	6-12	300-800
FeBPHT_9	Fe single crystal	Neon	6-9	300-800
FeBPHT_10	Fe single crystal	Neon	6-20	300-800

Table 1: Conditions of the experimental runs.

The synthesis of ε-Fe single crystals can be performed by compressing the α-Fe single crystal under high temperature, and decrease the temperature in the ε-Fe stability field (see report HC-2783). Runs FeBPHT_8 and FeBPHT_9 have been terminated unsuccessfully due to a leakage in the membrane and in the capillary.

The sample synthesized in the last trial (FEBPHT_10) has been kept in the diamond anvil cell under 17 GPa at 300 K (see **Figure 1**, left) and transferred to ID28 for Inelastic X-ray scattering measurement.
There were several crystals coexisting in the sample and a crystal with size and X-ray diffracted peaks rocking curves suitable for IXS measurement has been selected on ID28. The contribution of adjacent grains was small enough to allow a quantitative analysis of IXS signal (see **Figure 1**, right).
The analysis is underway. The first data point are in correct agreement (within ±15%) with the output of DFT-GGA calculations [1], once the volume underestimate of this approximation is corrected. A more accurate calculation is currently being carried out, within dynamical mean field theory (DMFT) [2], which better describes lattice parameters and all elastic constants in ε-Fe.

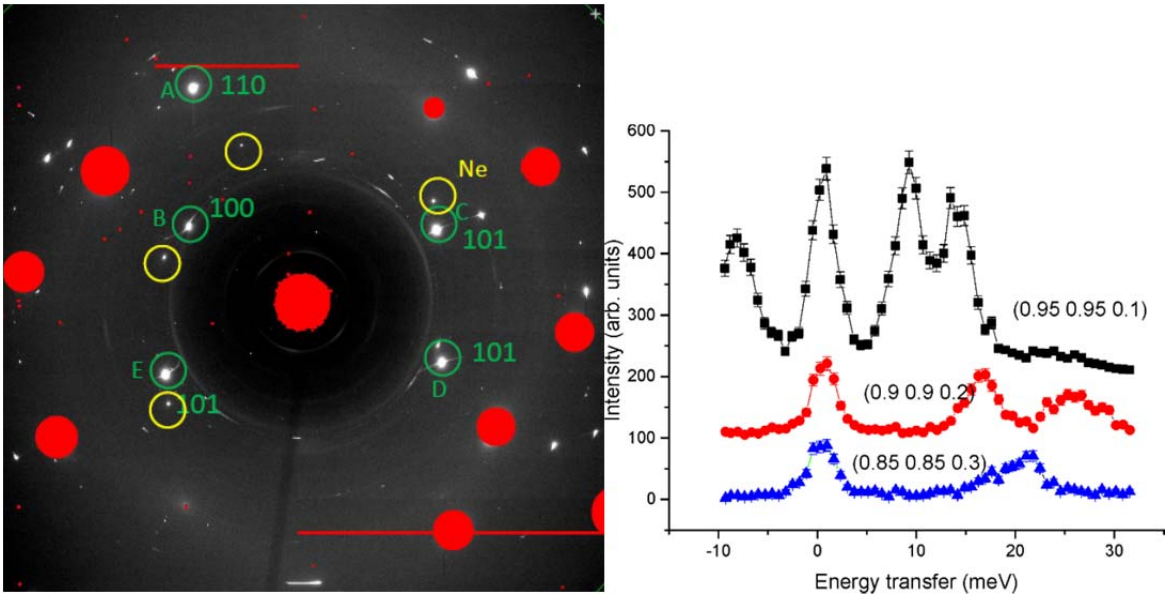

Fig. 1: Left: XRD spectrum taken in ε-Fe under 17 GPa at 300K. The red areas cover diamond anvils XRD peaks. Several XRD peaks from iron are labelled in green from A to E. **Right:** IXS spectra taken for q//112

References:

[1] X. Sha and R. Cohen, First-principles thermal equation of state and thermoelasticity of hcp Fe at high pressures, Phys. Rev. B 81, 094105, 2010

[2] L. V. Pourovskii et al., Impact of electronic correlations on the EOS and transport in ε–Fe, Phys. Rev. B 90, 155120, 2014.