	Experiment title: Study of the bcc-Fe to hcp-Fe phase transition under high pressure	**Experiment number**: hs4468
Beamline: id27	**Date of experiment**: from: 29-oct-2011 to: 01-nov-2011	**Date of report**: 15-mar-2012
Shifts: 9	**Local contact(s)**: Sylvain Petitgirard	*Received at ESRF:*

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Report:

In this experiment, we wanted to study the effects of the bcc to hcp phase transition in iron. Upon compression, this transition is known to occur around 15 GPa, depending on the pressure medium. Upon decompression, transition pressure is lower (around 10 GPa). X-ray diffraction was used to follow the accommodation of stress and texture induced by the transition.

Two samples, consisting of a sheet of pure, rolled, polycrystalline Fe, about 40x40 μm^2, were loaded in diamond anvil cells equipped with 300 μm culet diameter anvils and a rhenium gasket. Methanol-ethanol and helium were used as pressure medium for the first and the second sample, respectively. In both cases, we collected x-ray diffraction data at regular load intervals while increasing and decreasing pressure repetitively between 6 and 20 GPa. This procedure was performed in order to study the effect of sample history and microstructure on the transition as well as the microstructures induced by the transition itself.

2D diffraction data, collected in angular dispersive geometry using a monochromatic beam can now be processed using the 2D Rietveld analysis software MAUD in order to extract the cell parameters, phase proportions, grain sizes and sample textures during this experiment. Fig. 1, for instance, shows the proportion of α-Fe as a function of pressure during the 3 subsequent cycles of pressure increase and decrease performed for sample 1. In helium, the transition from α-Fe to ε-Fe is sharp, at about 15 GPa, and independent of the cycle number. Similarly, the transition for ε-Fe to α-Fe is sharp, at about 10 GPa, and independent of the cycle number.

In parallel, 2D x-ray diffraction images are used in order to extract information about grain orientation statistics within the polycrystals at all points during the experiment. Figure 2a, for instance, presents pole figures for the 110, 200, and 211 directions for α-Fe in sample 2, before the first transition to ε-Fe. The strong texture of the original rolled Fe sheet used as starting material can be observed. Figure 2b presents the texture obtained in ε-Fe, after the transition from α-Fe. A strong texture can be observed as well.

We are now in the process of interpreting this dataset and relate our observations to possible transition mechanisms between those two phases. In the future, the results will be used to improve our understanding of the bcc-hcp phase transition in Fe. We will also use our model in order to predict the effects on texture of a hypothetical hcp to bcc transition in Fe in the Earth core.

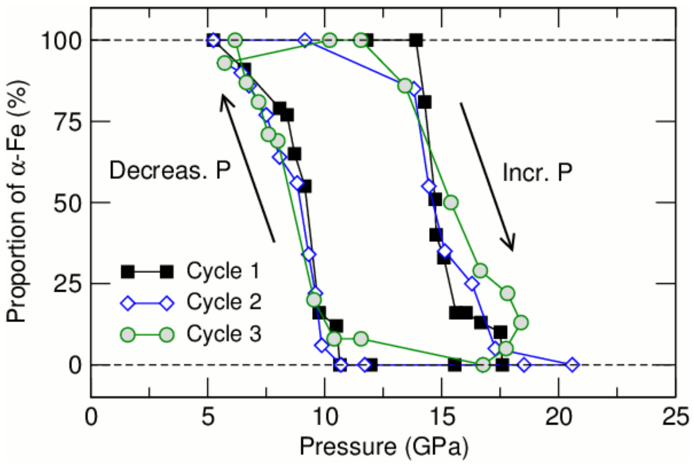

Figure 1: *proportion of α-Fe as a function of pressure for the 3 subsequent cycles of pressure increase and decrease performed on sample 2, loaded in helium.*

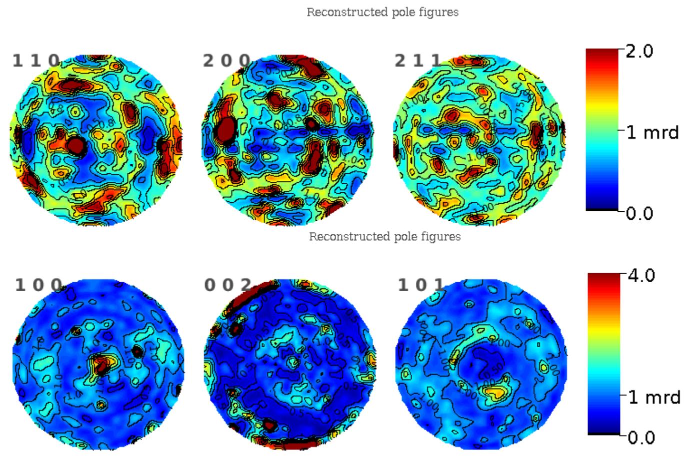

Figure 2: *(a) 110, 200, and 211 pole figures representing grain orientation statistics in α-Fe in sample 2, before the first transition to ε-Fe. (b) 100, 002, and 101 pole figures representing grain orientation statistics in ε-Fe in sample 2, after the first transition from α-Fe. Area projection, linear scale in multiples of a random distribution. Axial compression direction is at the center of the pole figure.*