ESRF	**Experiment title:** Antiphase Bragg Ptychography	**Experiment number**: HS-4761
Beamline: ID10A	**Date of experiment**: from: 24/11/2012 to: 30/11/2012	**Date of report**:
Shifts: 18	**Local contact(s)**: Y. Chushkin and F. Zontone	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

A. Madsen, European XFEL, Hamburg*
J. Hallmann, European XFEL, Hamburg*
T. Roth, European XFEL, Hamburg*
V. Chamard, Institut Fresnel, Marseille*

Report:

The aim of the experiment was to image the density of a small Fe_3Al crystallite using Bragg ptychography. Like in regular ptychography overlapping exposures was be taken and at every position the crystal is rocked through the (001) reflection and the intensity pattern (speckle) measured at every position. Due to the coherent illumination in this manner it is possible to retrieve the density of the object, in this case in 3 dimensions due to rocking through the Bragg reflection, see figure 1.

For Fe_3Al it is expected that the density is a complex function (i.e. it has both amplitude and phase) due to the presence of domain walls in the crystal structure. Along the (001) direction the phase shift over an antiphase boundary is +/- π in Fe_3Al's B2 structure and this should be detectable in the reconstructed density as sudden phase jumps. The ptychography approach (overlapping exposures) allows getting an extra handle on the iterative phase retrieval procedure and hence the difficult problem of correctly retrieving both amplitude and phase in 3D should be possible.

The beamline was prepared for the experiment and a small crystallite was identified in the sample and speckle patterns taken at 16 overlapping regions.

In order for the phase retrieval to work oversampling of the speckle pattern is required. In this case the sample is larger than the beam so it is the beam size that determines the speckle size.

The oversampling criterion (Nyquist-Shannon theorem) states that the detector resolution has to be two times finer than the speckle size, at least. In general, the finer detector resolution the better as it allows releasing other constraints of the phase retrieval algorithm. Also, one can better deal with low signal-to-noise ratios.

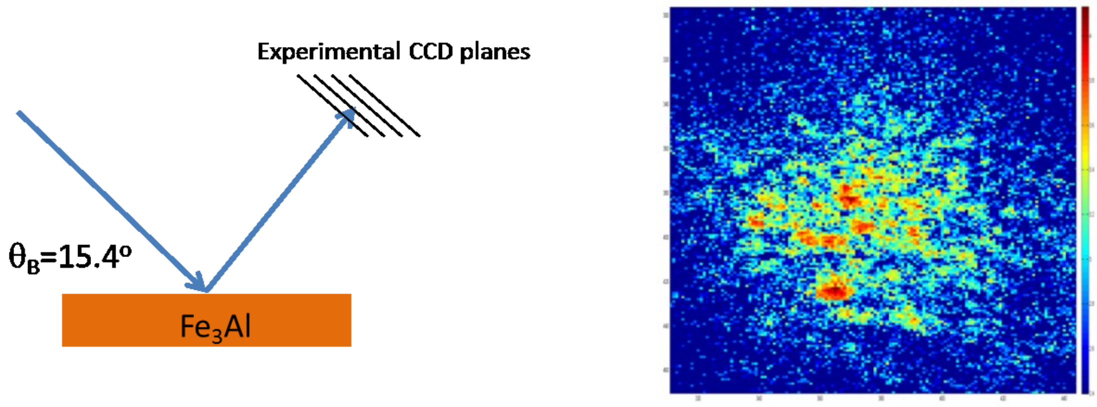

Figure 1: *(left) sketch of the experimental setup. When the sample is rocked through the (001) reflection the experimental CCD planes sweep through the crystallite that is probed. (right) example of a speckle pattern from the (001) reflection.*

As of today (August 2014) unfortunately we have not managed to perform a reliable 3D reconstruction of the data set. One of the problems is the beam size that was too large and hence the speckle size smaller than expected. By back propagation of the measured direct beam profile we estimate the FWHM of the beam on the sample to be ~5 micron (~10 micron between first minima on either side, see figure 2). Even if the oversampling criterion is still fulfilled this is more than twice as big as the 2 micron we estimated were necessary for a successful experiment.

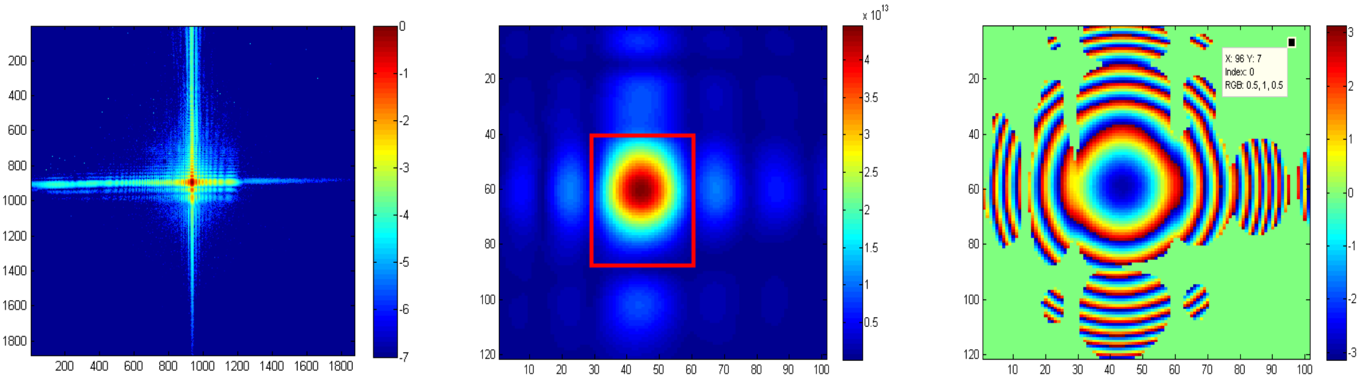

Figure 2: *(left) measured intensity in the far field, (middle) back propagated beam amplitude at the sample position, (right) back propagated beam phase at the sample position. The beam size marked by the red square in the middle panel is about 10 x 12 micron.*

It also means that the size of overlapping regions is way too big as the beam was only displaced 0.8 micron between successive exposures and then the redundancy in the ptychographic reconstruction is too large. Unfortunately, online monitoring of the beam size was not available and the aforementioned back propagation result (figure 2) was only achieved after the experiment.