EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

http://193.49.43.2:8080/smis/servlet/UserUtils?start

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** Electron states and magnetic ordering in Fe_3BO_6 studied by "forbidden" Bragg reflections	**Experiment number**: 28-01/745
Beamline: BM28	**Date of experiment**: from: 05.07.2006 to: 11.07.2006	**Date of report**: 31.08.2006
Shifts: 18	**Local contact(s):** Laurence Bouchenoire	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

Iron orthobrarate (Fe_3BO_6) is a complex magnetic material from spacegroup *Pnma* with two distinct iron sites. Preliminary measurements on XMaS beamline as well as computer simulations predicted interesting multipole effects in the x-ray resonant scattering at the Fe K-edge. Due to the lower symetry of the resonant atomic scattering tensor compared to the crystal symmetry, diffraction occur at forbidden Bragg reflections. The quadrupole-dipole and quadrupole-quadrupole terms of the resonant scattering yield diffraction in the pre-edge region with azimuthal dependence different from the main resonance lines.

In this experiment, we measured several forbidden Bragg reflections from a Fe_3BO_6 single crystal at room temperature. Measurements were carried out with XMaS diffractometre in vertical 4-circle configuration. Motorized slits in front of the sample were used to restrict the beam to the size of the sample (a plate of surface ~ 2 mm x 3 mm with crystal a-axis normal to the surface). Data were collected with a Vortex Si Drift Diode providing energy resolution, thus allowing separation of elastic scattering from fluorescence.

We studied the 300, 500, 700, 710 and 7-10 reflections, which are all forbidden Bragg reflections of the *Pnma* spacegroup and present various interference effects between both Iron sites. Rocking curves revealed a quite high mozaicity of the crystal. Therefore we systematically measured rocking curves at several energies and on full azimuthal range, in order to correct the data with reliable integrated intensities. The azimuthal dependence of intensities integrated over the rocking curves is shown on Figure 1. Full bidimentional energy/azimuth maps were measured (Fig. 2). 710 and 7-10 reflections could be measured on partial azimuthal range only, because of the limitation on theta rotation. The data are of very high quality, with good statistics and low noise. However, multiple scattering effects are responsible for numerous parasitic peaks. Data analysis should carefully identify them in order to provide a reliable data set for simulation.

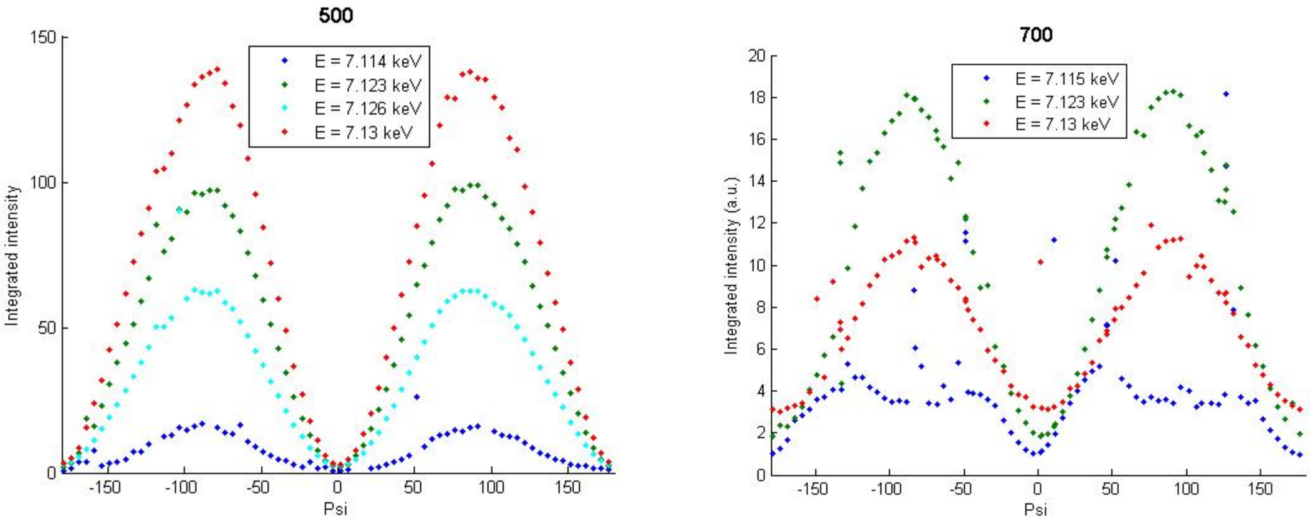

Figure 1: Azimuthal scans of 500 and 700 reflections at several energies, measured by integration of rocking curves

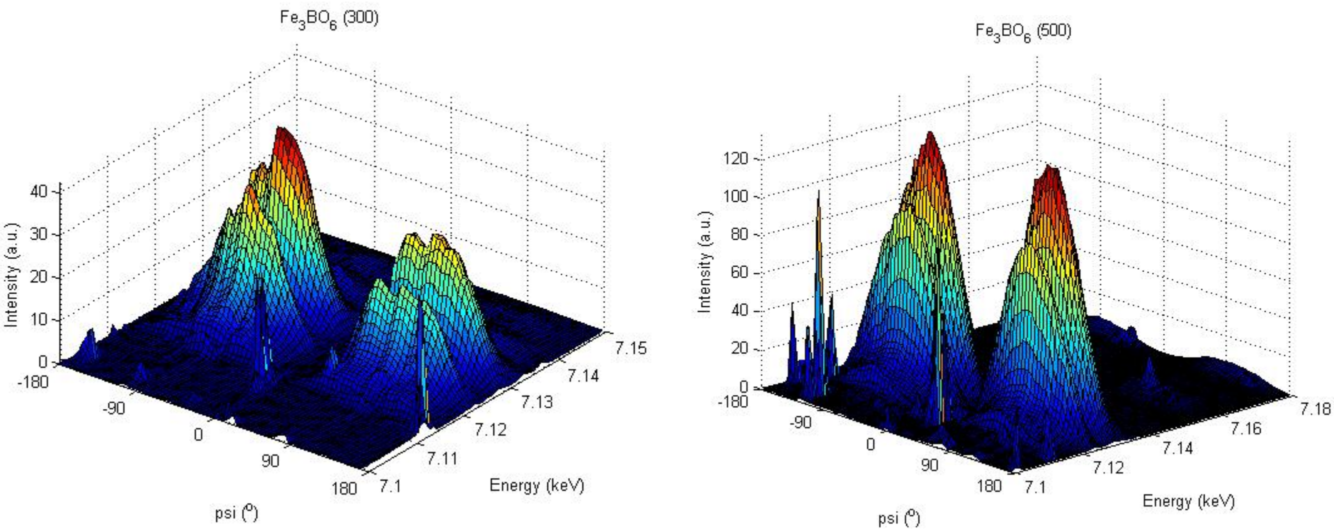

Figure 2: Energy/azimuth map of the 300 & 500 reflections, after data reduction.

These measurements will be compared with simulations performed with the code FDMNES, developed by Yves Joly (Lab. Cristallographie, Grenoble).