**E**UROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

# 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:**<br>Measurement of Pressure-Temperature phase diagram on a SmFeAsO single crystal | **Experiment number**:<br>HS-4467 |
| **Beamline**: | **Date of experiment**:<br>from: 30 Nov 2011 to: 04 Dec 2011 | **Date of report**:<br>21-06-12 |
| **Shifts:** | **Local contact(s)**:<br>Wilson A. Crichton<br>Michael Hanfland | *Received at ESRF:* |


**Names and affiliations of applicants** (* indicates experimentalists):

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## Report:

X ray diffraction measurements on single crystals of SmFeAsO were performed under high pressure and low temperature conditions. The major purpose of this beamtime was the investigation of the tetragonal-to-orthorhombic phase transition of the compound with the increase of external pressure. For that reason we focused our interest on determining the structural phase transition temperature at various pressures, acquiring datasets with small temperature steps of 2K at each pressure value; given the big number of datasets required for such a detailed investigation and the time constraints imposed by the heating and cooling of the pressure cell, the highest pressure we could reach was limited to 85kbars.

The mentioned structural phase transition is clearly mirrored in the temperature evolution of the tetragonal 220 Bragg reflection which splits into a doublet (040 and 400) in the orthorhombic phase (Fig.1); therefore an estimation of the structural transition temperature could be given by the temperature evolution of the $(220)_T$ reflection's width. Based on a first stage analysis of our data, we detect the $(200)_T$ peak splitting for every studied pressure, a result which indicates the retention of the structural transition upon external pressure at least up to the highest reached value of 85kbars (Fig.2); as expected, pressure suppresses the transition temperature towards lower values (Fig.2 inset). Although the structural transition is present in the whole studied pressure range, it evidently broadens with pressure (Fig.2) suggesting that with further increase of pressure the transition would be totally suppressed; additional XRD data at higher pressure values would be necessary to verify this and to accurately determine the pressure where the structural transition disappears.

However, correlating these results with our preliminary transport measurements under high pressure, it becomes clear that, at least up to 85kbars, superconductivity appears at the orthorhombic phase of the compound.

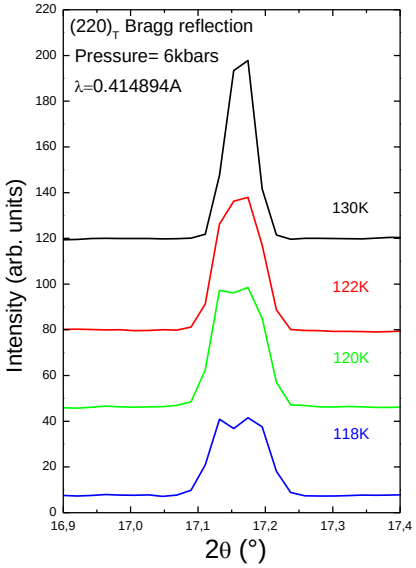


Fig. 1: Selected region of the XRD profiles of SmFeAsO showing the temperature evolution of the $(220)_T$ Bragg reflection at P= 6kbars.

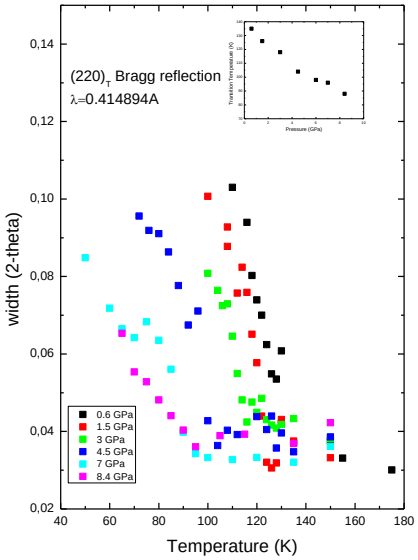


Fig.2: Temperature evolution of the FWHM for the $(220)_T$ Bragg reflection at various pressures. Inset: Pressure evolution of the structural transition temperature as estimated by the $(220)_T$ peak width .