EUROPEAN SYNCHROTRON RADIATION FACILITY

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 via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can 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:** **Microscopic manifestation of magneto-lattice interplay in FeGe**	**Experiment number**: HC3846
Beamline: ID28	**Date of experiment**: from: 03.09.2018 to: 04.09.2018	**Date of report**: 03.03.2020
Shifts: 3	**Local contact(s)**: Pavel Sedmak	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

FeGe shows a spiral magnetic ordering below ≈ 278 K. While at the temperatures of ~ 211 – 245 K the magnetic spirals alter the propagation direction from [100] to [111]. The crystal structure of FeGe despite being cubic is of rather low symmetry – it belongs to an unusual B20 type (space group $P2_13$, Z = 4), in which each species has sevenfold coordination. The atomic positions in FeGe are slightly removed from the ideal structure, in which the iron and germanium both occupy 4*a* (U, U, U) sites with U = ±0.15451. Recent studies have shown the presence of a magnetic contribution to the specific heat [1].

In order to study the structural variation of FeGe, which is expected to accompany the changes of the magnetic structure in the range of ~ 100 - 300 K, powder sample of FeGe was

placed into 0.3 mm diameter capillary for x-ray diffraction experiment. The wavelength of x-ray radiation was as small as 0.18934 A according to the calibration with the help of Si standard (NIST 640C).

The fitting of x-ray diffraction patterns performed by Fullprof Suit Software package resulted in a good agreement of the experimental and theoretical diffractograms as exemplified in Fig.1 (conventional Rielveld R-factors: $R_p \approx 4\%$, $R_{wp} \approx 4\%$).

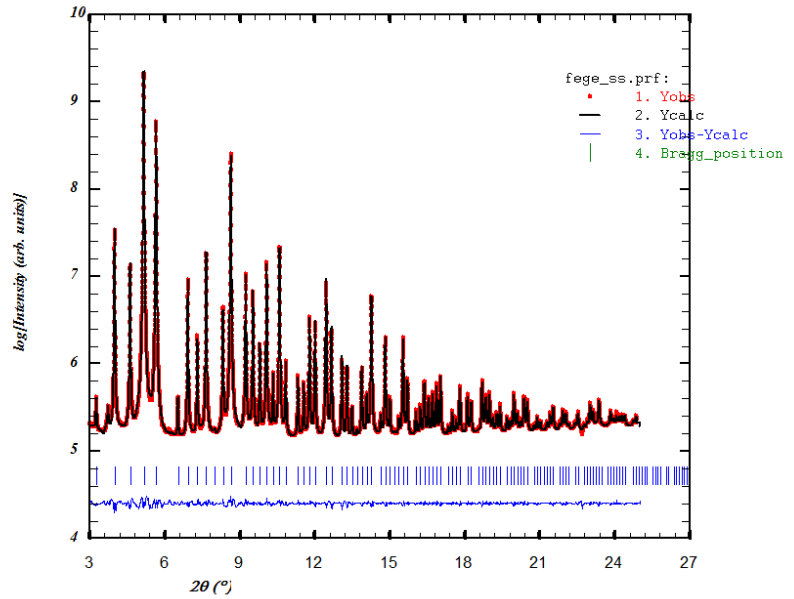
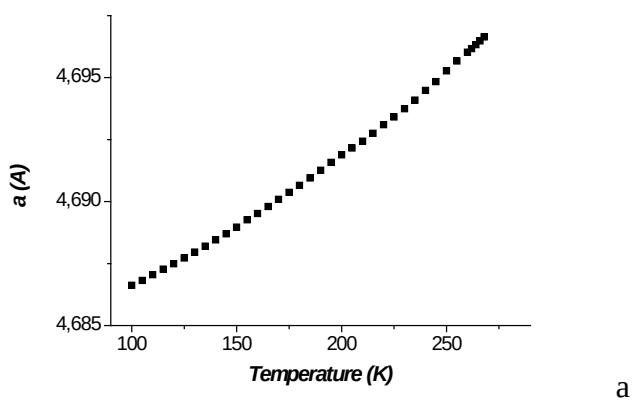
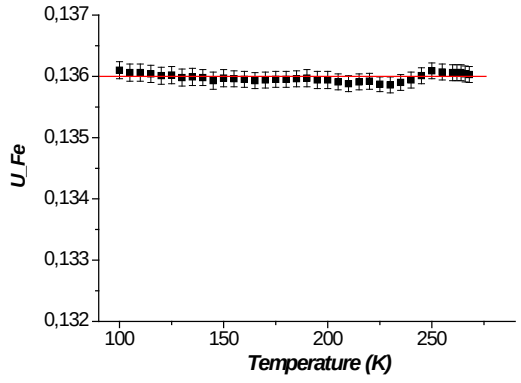


Fig. 1. An example of x-ray diffraction fitting for FeGe powder (T= 268 K, semi-logarithmic scale).



a



b

Fig. 2. The temperature dependences of the: a) lattice parameter, b) atomic position parameter of Fe-atoms

The fitting of the set of diffractograms at a number of temperatures provided the temperature dependence of the lattice parameter presented in Fig. 2a. It does not show any significant peculiarities. The approximation of this dependence to the room temperature give the lattice parameter of ~ 4.698 Å, that is close to the previously obtained values (4.6995(2) Å [1], 4.700 Å [2], 4.70585(4) Å our measurements at BM25).

The atomic position parameter of Fe-atoms (U_Fe) as a function of temperature is shown in Fig. 2b. There are no drastic changes of this parameter in the studied temperature range, rather it remains constant within the experimental error. It means that at least in the temperature range corresponding to the change of the magnetic spiral propagation direction (211 – 245 K) the crystal structure does not rearrange particularly. The data obtained at higher temperatures is characterized by a larger experimental error and does not allow to evaluate the temperature dependence of U_Fe. The further work is in progress.

[1] H. Wilhelm, A.O. Leonov, U.K. Rossler et al., Phys. Rev. B. 94, 144424 (2016).
[2] Richardson, Acta Chem Scand. 21, 753 (1967)