

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://www.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.



	Experiment title: Direct measure of the phonon dispersion in single-crystal MnGe	Experiment number: HC2515
Beamline: ID28	Date of experiment: from: 08.04.2016 to: 12.04.2016	Date of report: 07.10.2016
Shifts: 12	Local contact(s): Alexei Bosak	<i>Received at ESRF:</i>
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Report:

An anomalous phonon behavior has been discussed in recent papers on transition metal monogermanides (MnGe) and monosilicides (FeSi) with the cubic B20 structure [1-4]. In order to study the phonon peculiarities in FeSi, which accompany the insulator-metal transition at 150 – 180 K [2-4], single-crystal of FeSi was selected and prepared for inelastic x-ray scattering experiment. The actual crystal size was 100 – 105 mkm being unessentially higher than the optimal value at the photon energy of 17794 eV (i.e. 65 mkm).

The single-crystal was mounted in such a way that the phonon dispersion was studied in the (hk0) plane. The measurements were carried out in a constant-Q mode (9 different Q-points were detected simultaneously with 9 analysers) by keeping the analyser temperature

fixed, and scanning the temperature of the monochromator. Herewith, relative change of the monochromator temperature results in a relative energy variation. The corresponding energy resolution was ~ 3 meV.

All the allocated beamtime was fruitfully utilized. The first part of the experiment was aimed at studying the phonon dispersion at room temperature and selecting reasonable points for the temperature-dependent investigations. The following phonon dispersion at 300 K can be extracted from the data obtained: $(0, 3+\xi, 0)$, $(\xi, 4, 0)$, $(2+\xi, 2+\xi, 0)$, $(2+\xi, 2-\xi, 0)$. During the second part of the experiment we measured temperature-dependent constant wave-vector scans at the Γ point of $(3, 0.5, 0)$, M point of $(2.5, 2.5, 0)$ and two symmetric (from the crystallography viewpoint) X points of $(0.5, 4, 0)$ and $(4, 0.5, 0)$. The latter measurements were performed at 100, 150, 200 and 300 K.

The obtained spectra were further analyzed with the help of locally developed software based on Matlab in order to derive the energy positions and phonon linewidths (Fig 1 a). Our preliminary results have revealed a moderate phonon softening with temperature, e.g. maximum at ~ 19 meV shifted at $\sim 3-4$ % upon heating from 100 to 300 K (Fig 1 b). More rigorous approximation of the spectra is to be done. A complete analysis of the data collected is in progress.

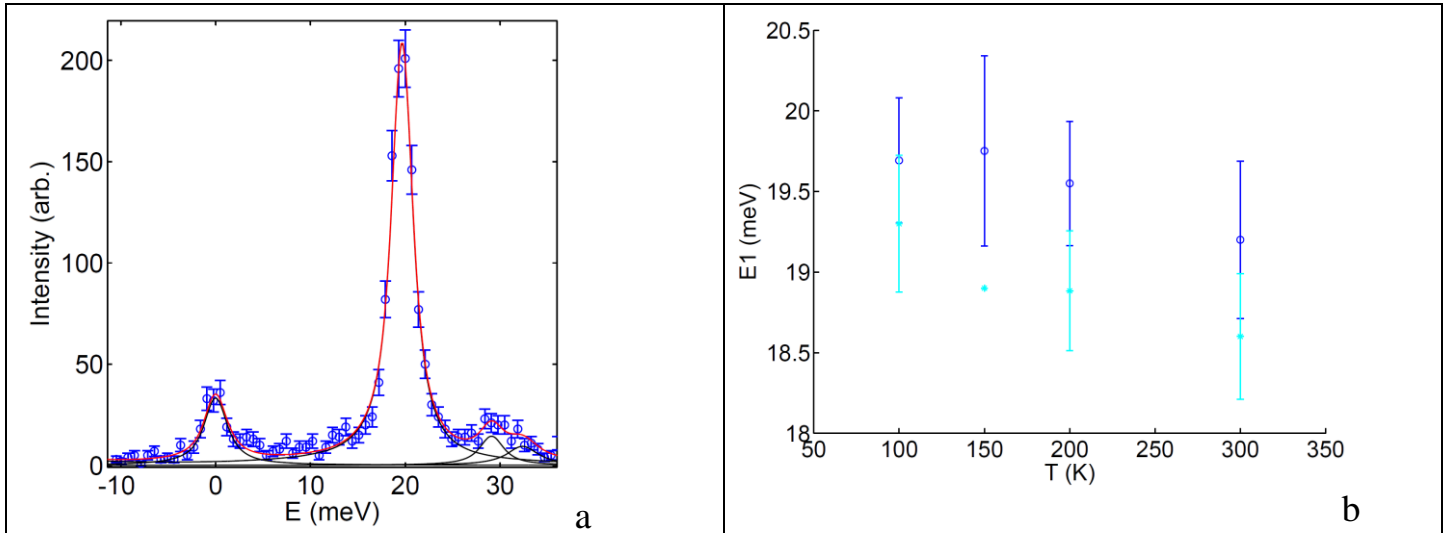


Fig. 1. (a) An example of approximated phonon spectrum, at X point $(0.5, 4, 0)$, $T=100$ K and (b) temperature dependence of the maxima position, the peaks at ~ 19 meV were taken from X points of $(0.5, 4, 0)$ and $(4, 0.5, 0)$ – blue and green symbols, respectively.

- [1] G.A. Valkovskiy, et. al., J. Phys. Cond. Matter, 28, 375401 (2016).
- [2] S. Krannich, et. al., Nature Communications. 6, 8961 (2015).
- [3] P.P. Parshin, et. al., Phys. Rev. B, 93, 081102(R) (2016).
- [4] O. Delaire, et. al., Proceed. Nat. Acad. Sci. U.S.A., 108, 4725 (2011).

