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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:** **Temperature dependence of the lattice dynamics of ordered and disordered $Fe_{72}Pt_{28}$ studied by NIS**	**Experiment number**: HE-1687
Beamline: ID18	**Date of experiment**: from: 12.07.04 to: 18.07.04	**Date of report**: 31.08.04
Shifts: 18	**Local contact(s)**: **Dr. Alexandr Chumakov**	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report: This beamtime was actually devoted to "Phonon spectroscopy on oriented hcp iron at high pressures and temperatures". It turned out, however, that the envisaged pressure experiments in the Mbar range with 0.5 meV energy resolution (instead of 3 meV as in our proposal HS-2083) were extremely time consuming (with estimated two NFS spectra in the whole 18 shifts). In addition, we had, no access to the XRD facilities of the high-pressure beamline ID30 (due to the closing of this beamline and rebuilt at ID 27). XRD analysis was essential to analyse the degree of texture in the hcp iron samples. So we changed, in agreement with the beamline scientists, to our proposal "Lattice dynamics in $Fe_{72}Pt_{28}$ Invar alloys as function of temperature and pressure", which got a high ranking from the HS committee.

This proposal was based on previous successful investigations of the lattice dynamics in the classical Invar system $Fe_{65}Ni_{35}$ as function of pressure and temperature by ^{57}Fe-nuclear inelastic scattering (NIS) of SR [1, 2, reports on HS-1614, HS-1765]. An exploratory NIS study of ordered $Fe_{72}Pt_{28}$ Invar as a function of temperature (see proposal HE-1807) provided the phonon densities-of-states (DOS) at the Fe sites. Due to the spectral resolution of 3 meV, we could not resolve the structures of the phonon-DOS in the energy range below 10 meV, where the TA_1[110] phonon mode is located, which is strongly correlated with the Invar properties, e.g. the anomalous small thermal expansion, even negative for ordered and disordered $Fe_{72}Pt_{28}$ [3].

We measured at beamline ID18 the phonon spectra of ordered and disordered $Fe_{72}Pt_{28}$ Invar alloys in the temperature range from 20 K up to 550 K with the best possible energy resolution of actually 0.45 meV. For the low and high temperature measurements the samples were placed in a He flow cryostat and in a vacuum oven, respectively. The magnetic properties of the samples (enriched with 30% of ^{57}Fe) as function of temperature and pressure were previously studied with conventional ^{57}Fe-Mössbauer spectroscopy [4]. First of all, we observe characteristic differences between the ordered (near to Cu_3Au structure) and disordered (random fcc structure). As expected the phonon-modes are better resolved in ordered $Fe_{72}Pt_{28}$, e.g. peaked structures of the optical modes around 16 - 32 meV, and exhibit a stronger variation of the properties in the low-energy range below 10 meV. Secondly, we observe for both systems a very unusual and contrary temperature variation of the DOS, an increase of the low-energy modes and a decrease of the high-energy modes with rising the temperature (see Fig. 1).

We analysed the DOS spectra in the same way as done for $Fe_{65}Ni_{35}$ [1, 2]. From integrating over the whole DOS, the so-called high-temperature Debye temperatures $\Theta_{D,HT}$ were derived.

From the initial slope of the phonon DOS the mean sound velocities v_D were obtained, which are proportional to the low-temperature Debye temperature $\Theta_{D,LT}$. The temperature dependence of $\Theta_{D,HT}$ and $\Theta_{D,LT}$ is shown in Fig. 2 (top). While $\Theta_{D,HT}$ remains almost constant over the temperature range investigated (which can be attributed the negligible thermal expansion), $\Theta_{D,LT}$ increases strongly with temperature up to the respective magnetic ordering temperatures, T_c = 380 K for disordered and T_c = 510 K for ordered $Fe_{72}Pt_{28}$. One should also note that $\Theta_{D,LT}$ is always smaller than $\Theta_{D,HT}$ even above the magnetic ordering temperature, a behavior opposite to that of normal d-metals, but characteristic for Invar systems as observed by us for $Fe_{65}Ni_{35}$ [1,2]. We expect, similar to the case of $Fe_{65}Ni_{35}$, that $\Theta_{D,LT}$ will surpass $\Theta_{D,HT}$ by the application of pressure, when the magnetic properties change from high-spin to low-spin behaviour [1,2] .

The mean sound velocity v_D, which represents in the Debye model by $1/v_D^3 = 1/v_l^3 + 2/v_t^3$ an average of the longitudinal and transversal sound velocities, is also shown in Fig. 2 (bottom). The temperature dependence of v_D and of $\Theta_{D,LT}$ nicely reflects the anomalous behavior of the TA_1[110] mode as well as the transversal sound velocity in [110] direction [3].

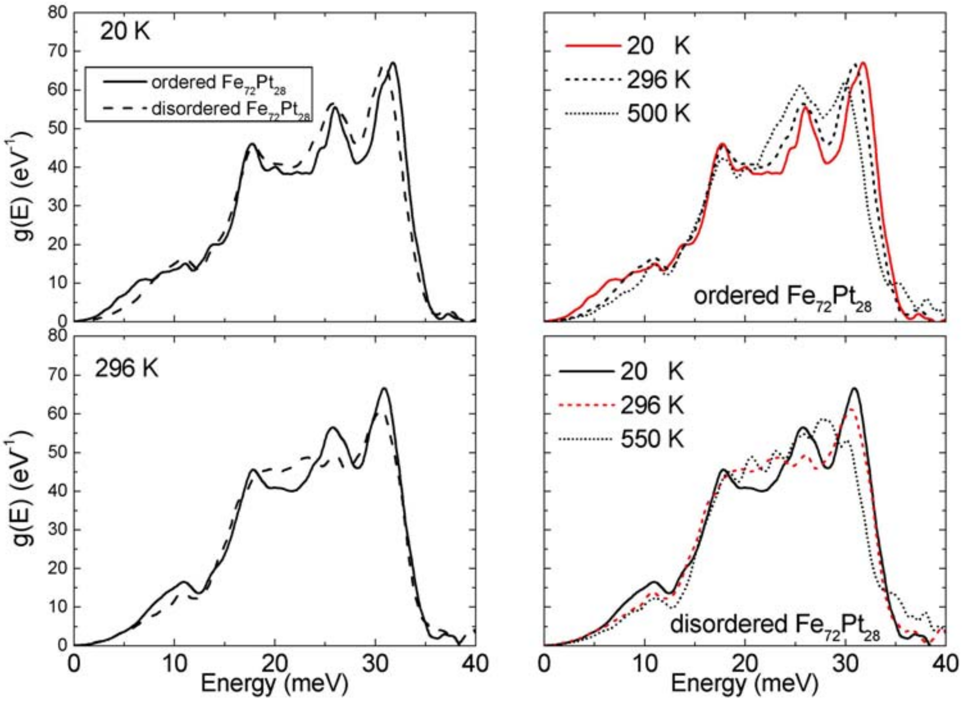

Fig 1. Partial phonon density of states for ordered and disordered $Fe_{72}Pt_{28}$ Invar at different temperatures.

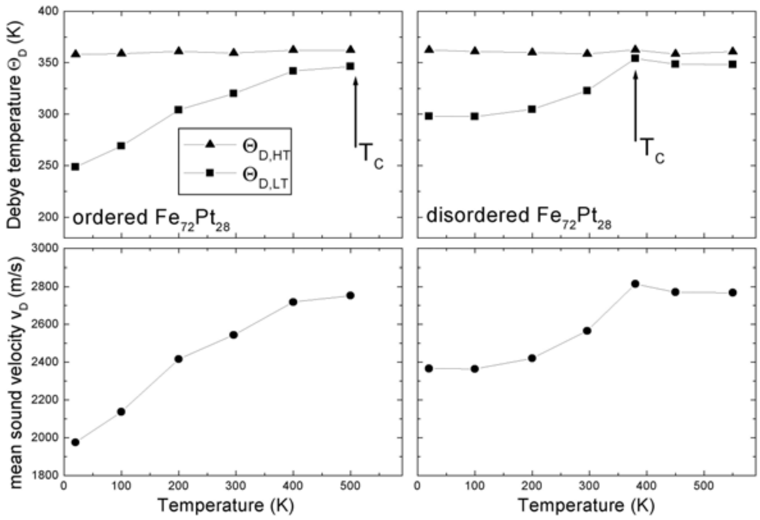

Fig 2. High temperature and low temperature Debye temperature and mean sound velocity of ordered and disordered $Fe_{72}Pt_{28}$ Invar as function of temperature.

References: [1] H. Giefers, PhD thesis, Paderborn University, 2004. [2] H. Giefers, K. Rupprecht, U. Ponkratz, O. Leupold, G. Wortmann, submitted. [3] E. Wassermann, J. Magn. Magn. Mat. 100, 346 (1991). [4] M.M. Abd-Elmeguid, H. Micklitz, Phys. Rev. B 40, 7395 (1985).