ESRF	**Experiment title:** Phonon spectroscopy on oriented hcp iron at pressures up to 150 GPa	**Experiment number**: HS-2083
Beamline: ID18	**Date of experiment**: from: 01.08.03 to: 07.08.03	**Date of report**: 31.08.2003
Shifts: 18	**Local contact(s)**: **Dr. Alessandro Barla**	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

H. Giefers*, U. Ponkratz*, K. Rupprecht*, G. Wortmann

Department Physik, Universität Paderborn, D-33095 Paderborn

A.I. Chumakov*

ESRF, Grenoble

Report:

The Paderborn group has specialised on phonon spectroscopy at the hexagonal (hcp) high-pressure phase of iron (ε-Fe) [1,2] and has developed a special high-pressure cell which enables the recording of phonon spectra taken in different directions with respect to the texture axis (c-axis of the pressurized ε-Fe sample) [3]. In our beamtime in July 2002 we reached 61 GPa (HS1765). In the present beamtime we measured phonon DOS spectra of ε-Fe at 5 different pressures from 43 GPa to 130 GPa, but due to the lack of beamtime the envisaged highest pressure of 150 GPa was not reached.

The nuclear inelastic scattering (NIS) experiments on ε-Fe were performed at beamline ID18 with the use of a LN_2-cooled Si(1,1,1) double-crystal premonochromator and a high-resolution (3 meV) monochromator (HRM) consisting of two pairs of ("nested") Si(3,3,3) and Si(9,7,5) crystals. Due to the focusing optics (compound refractive lenses at the beam entrance and two Kirckpatrick-Baez mirrors behind the HRM), the monochromized beam was focused on a spot of 15×8 μm (h×v). With our special high-pressure cell with a Be gasket we recorded NIS spectra through the diamonds anvils, but also at an angle of 75° with respect to the axis of the diamonds [3]. For the detection of the inelastic Fe $K_{\alpha,\beta}$ x-ray fluorescence radiation two avalanche photo diodes were used.

The Figs. 1a and 1d show the phonon density-of-states (DOS) derived from NIS spectra of ε-Fe recorded at 110 GPa and 130 GPa, the highest pressures reached in the present study. The texture effects are clearly evident and more pronounced than in our previous studies [3, HS1765]. In the present study we used no pressure- transmitting medium to increase the texture, compared to our 1st study with an alcohol-water mixture and 2nd study with mineral oil as pressure-transmitting media. A preliminary evaluation of the data yields clear evidence for a higher sound velocity in the spectra taken parallel (0°) to the texture axis (with a preferred alignment of the c-axis of hcp ε-Fe) than in the spectra taken at an angle of 75°. The observed difference in the derived elastic parameters and especially in the sound velocities, for instance $v_D(0°)$ = 5.46(4) km/s and $v_D(75°)$ = 5.25(4) km/s at 130 GPa, supports the suggestion of anisotropy in the elastic properties of ε-Fe, here of a larger sound velocity along the c-axis than perpendicular to the c-axis.

To derive the actual difference of v_D parallel and perpendicular to the c-axis (and not to the texture axis as observed here), which is of actual interest for the ongoing discussion about the reason for the anisotropy of the sound velocity in the Earth´s core [4,5], we need additional information on the amount of texture of the sample in our h.p. cell. This information can be obtained by X-ray diffraction, similar to the procedure used in [6]. Such studies are presently underway.

Another way to get this information is the method of subtracting different amounts of normalized phonon-DOS spectra of one direction (0° or 75°) from the other (75° or 0°) in order to obtain the phonon-DOS as seen parallel and perpendicular to the c-axis of ε-Fe [3]. The peaks in the difference spectra belong to modes with a high phonon-DOS. The two peaks in Fig. 1b and 1e correspond to the longitudinal and transversal optical modes, observable only along the c-axis; the lower one is the Raman active E_{2g} mode, which was studied recently to 150 GPa [7]. There is, as in our previous study, good agreement with the Raman data [7], indicating that the method of difference spectra allows for a detailed mode analysis, also for the dominant acoustic modes within the a,b-plane, derived in Figs. 1c and 1f. The final evaluation of the present data is in progress.

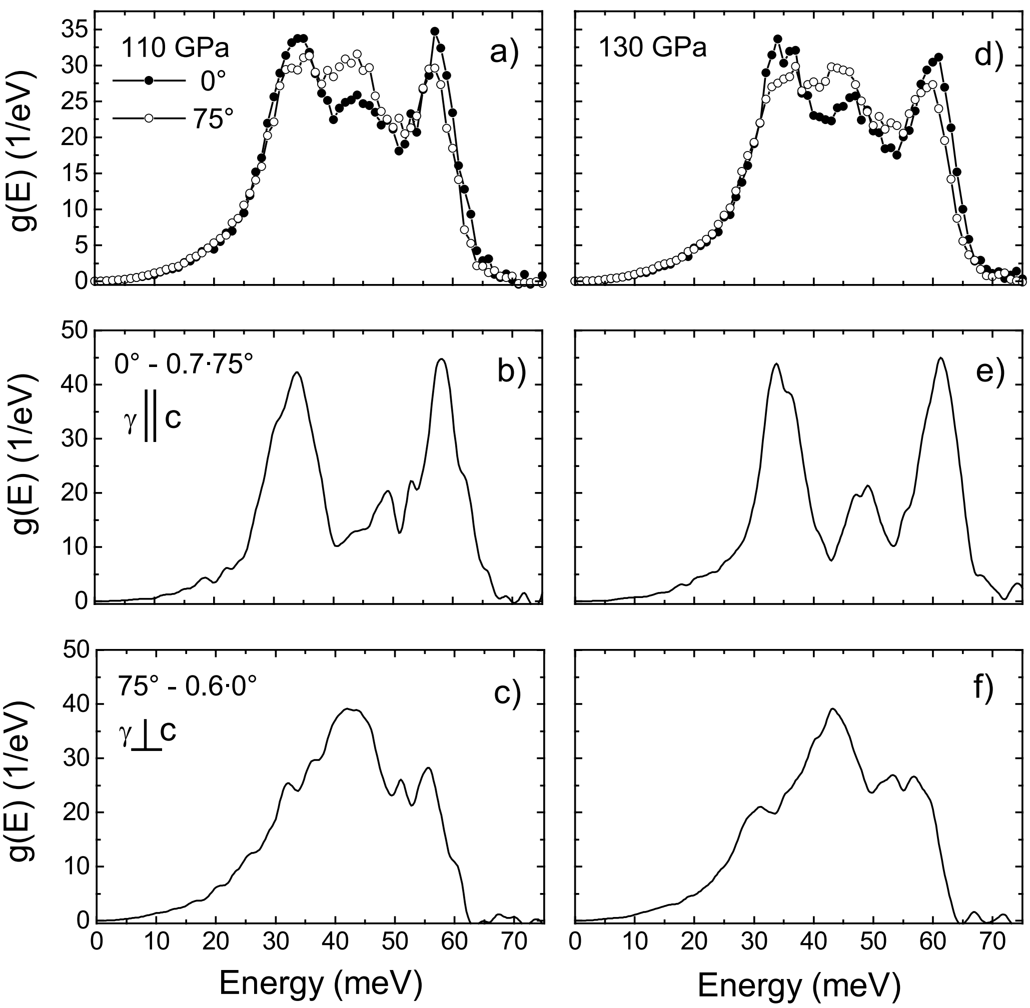

Fig. 1: *(a),(d) Phonon DOS from ε-Fe derived from NIS spectra at 110 GPa (left column) and 130 GPa (right column) measured with different directions (0° and 75°) with respect to the load axis of the HP cell. (b) and (e) Phonon DOS as obtained from the 0° DOS spectrum after subtraction of 70 % of the 75° DOS spectrum, (c) and (f) Phonon DOS as obtained from the 75° DOS spectrum after subtraction of 60 % of the 0° DOS spectrum.*

References:

[1] R. Lübbers, H.F. Grünsteudel, A.I. Chumakov, G. Wortmann, *Science* 287, 1250 (2000). [2] H.-K. Mao et al, *Science* 292, 914 (2001). [3] H. Giefers et al., *High Pressure Research* 22, 501 (2002); see also: ESRF Highlights 2000, p. 48. [4] A. Jephcoat and K. Refson, *Nature* 413, 27 (2001); G. Steinle-Neumann et al., *ibid*. p.57; B.A. Buffet and H.R. Wenk, *ibid*. 60. [5] K.C. Creager, *Nature* 356, 309 (1992) and *Science* 278, 1284 (1997). [6] H.R. Wenk et al., *Nature* 405, 1044 (2000). [7] S. Merkel et al., *Science* 288 ,1626 (2000).