

alignment of the c-axis of the iron crystallites along the Earth's rotation axis, in an otherwise randomly oriented medium, can alone qualitatively explain compressional travel time anomalies observed in Earth's inner core.

References

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Principal publications and authors

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High-pressure Phonon Spectroscopy of Oriented hcp Iron

The hexagonal (hcp) high-pressure phase of iron (ϵ -Fe) is the most relevant constituent of the Earth's inner core. The thermodynamic and elastic properties of this phase are therefore of actual geophysical interest.

Using Nuclear Inelastic Scattering (NIS) with the 14.413 keV transition of Fe-57, the phonon density-of-states (DOS) in hcp iron was measured for the first time up to 42 GPa at ID22N of ESRF [1] and later up to 153 GPa at the APS [2]. Using the texture of the pressurised sample, we developed a new method to study the orientation dependence of the phonon density-of-states in ϵ -Fe up to 40 GPa [3]. The use of texture enables a search for a possible anisotropy in the sound velocity. Here we report on such a high-resolution NIS study of oriented ϵ -Fe up to 130 GPa.

Synchrotron radiation of 14.413 keV with a bandwidth of 3 meV was focused onto the sample of about 50 μm in diameter, contained in a Be gasket between the diamonds in the high-pressure cell [3]. NIS spectra were measured in two different directions, 0° and 75° , with respect to the axis of the diamonds, which is also the preferred c-axis orientation of the ϵ -Fe sample. NIS spectra of ϵ -Fe were recorded from 28 GPa up to 130 GPa. The phonon-DOS spectra, derived from the NIS spectra [1,3], are shown in Figure 1. They exhibit clear pressure-induced shifts of their characteristic peaks to higher energy as well as characteristic differences for the two orientations.

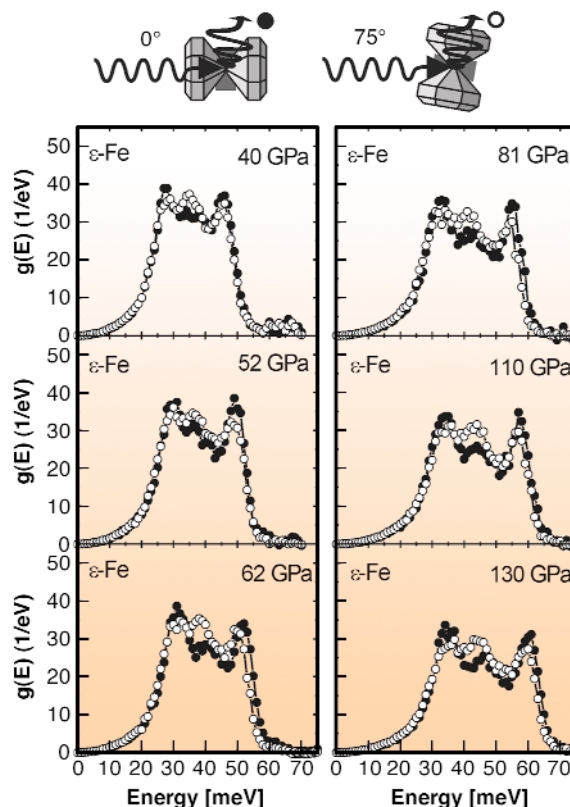


Fig. 1: (above) Transmission of the SR beam through the Fe sample at 0° and 75° with respect to the diamond anvil axis in the high-pressure cell. (below) Phonon-DOS $g(E)$ of ϵ -Fe derived from NIS spectra at various pressures. Full dots correspond to the 0° direction and open dots to the 75° direction.

To explain the orientation dependence of the observed phonon DOS, theoretical calculations of the phonon dispersion relations and phonon-DOS were performed for ϵ -Fe at 40 GPa [3]. In addition, we demonstrated that the observed texture effects can be enforced by difference spectra, producing projected phonon-DOS as seen by NIS parallel and perpendicular to the hexagonal c-axis [3].

From the thermodynamic and elastic parameters derived from the phonon-DOS spectra of Figure 1 we concentrate here on the mean sound velocity v_m , connected in the Debye model with the longitudinal and transversal sound velocity, v_p and v_s , by $3/(v_m)^3 = 1/(v_p)^3 + 2/(v_s)^3$. The sound velocities v_m of ϵ -Fe, derived from the low-energy range (0 - 15 meV) of the DOS are shown in Figure 2. They exhibit a systematic difference between the two directions, increasing with pressure and amounting to about 4% at 130 GPa. One can use the known bulk modulus K and shear modulus G of ϵ -Fe to derive the corresponding v_p and v_s values from the measured v_m values [2]. The results for v_p are shown in Figure 2 and exhibit a smaller, but well-resolved difference. The 75° data agree nicely with v_p data obtained by IXS, a complementary technique (see D. Antonangeli *et al.*, preceding article). All other elastic parameters derived from the full phonon-DOS exhibit

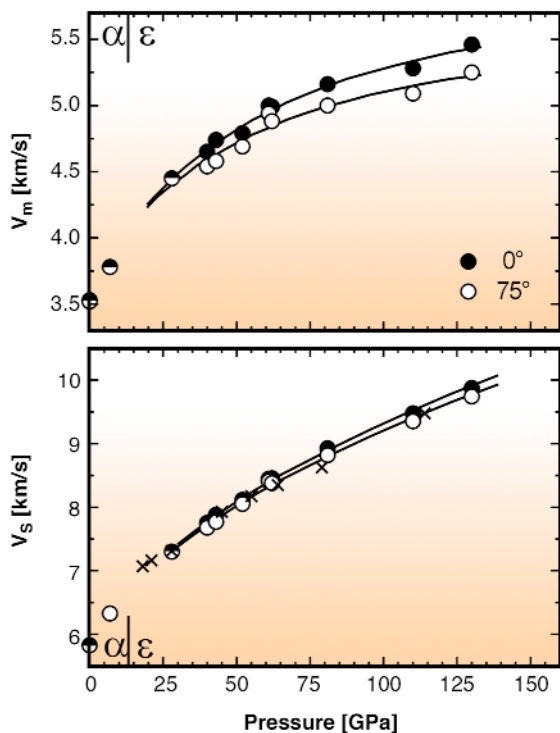


Fig. 2: (above) Mean sound velocity v_m in ϵ -Fe derived from the phonon-DOS spectra shown in Figure 1. (below) Longitudinal sound velocity v_p derived from v_m as explained in the text. Full and open dots have the same meaning as in Figure 1. The v_m and v_p data for α -Fe are also shown [3]. The crosses mark v_p values measured by IXS preferentially perpendicular to the c -axis.

similar differences indicating that the lattice is stiffer parallel to rather than perpendicular to the hexagonal c -axis. One reason for this behaviour might be the observed decrease of the c/a ratio with pressure.

Bearing in mind that the present data of v_m and v_p were obtained from a textured sample (and not from a single crystal) and that the NIS probability varies with $\cos^2 \vartheta$, where ϑ is the angle between the k -vector of the incident synchrotron radiation and the polarisation vector of the excited or annihilated phonons, the experimentally observed v_m values at 0° and 75° provide only lower limits of the actual difference in v_m and the derived v_p and v_s values as seen parallel and perpendicular to the c -axis. When we derive v_m and, accordingly, v_p and v_s from the projected DOS, we obtain considerably larger differences, up to 10% for v_m and v_p at 130 GPa [4]. An exact determination of the difference depends on the degree of texture in the ϵ -Fe samples, which will be determined independently in future studies. The present data demonstrate the high-resolution power of NIS for precise determination of the sound velocities and other elastic parameters well above 100 GPa.

References

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Fe K pre-edges Revealed by Resonant X-ray Emission

The pre-edge structures at the K absorption edge of transition metals obtained from X-ray absorption spectroscopy (XAS) are known to be extremely sensitive to the chemical and structural local environment, and can be used as a fingerprint of the transition metal properties [1]. Compared to L edge measurements, this method is advantageously bulk-sensitive, because it is performed in the hard X-ray energy range, and can be applied to a vast variety of materials such as bio-complexes and Earth science related materials, under various sample environments.

In XAS, however, the pertinence of data analysis hinges on the broadening effect related to the $1s$ core-hole lifetime. This limitation can be overcome to a certain degree by using a second order process instead, namely resonant X-ray emission spectroscopy (RXES). This method consists of measuring a specific decay channel on resonance as the incident energy is tuned to an absorption edge. As a benchmark of this technique, we have applied RXES in a series of Fe-bearing minerals. We focused on the K_α emission line ($2p \rightarrow 1s$ transition) in the vicinity of the Fe-K edge ($1s2p$ -RXES). In these model systems, Fe can be either of valence $2+$ or $3+$ and sits in a supposedly pure octahedral (O_h) or tetrahedral site (T_d). All the spectra were obtained on the **ID26** beamline using a Rowland circle spectrometer and a spherically-bent Si analyser.

Figure 1 shows the absorption edges obtained by RXES in the partial fluorescence yield mode (PFY). Here, the emitted energy E_2 is kept fixed at the maximum of the K_α line while the incident energy E_1 is varied through the Fe-K absorption edge. The presence of a shallower core-hole in the RXES final state, when compared to XAS, yields to a remarkable sharpening effect. Notably, the pre-edge exhibits a clear dependence on both Fe site-