ESRF	**Experiment title:** Acoustic-phonon dispersion in iron and $MgSiO_3$ perovskite under high pressure	**Experiment number:** HS1067
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Report:

The dispersion of longitudinal acoustic phonons has been measured by inelastic x-ray scattering in the hexagonal closed-packed structure of iron (h.c.p.Fe) from 19 to 110 gigapascals. Phonon dispersion curves have been recorded in the momentum transfer region $Q = 4$ to 12 nm^{-1} on polycrystalline iron compressed in a diamond-anvil cell. The present IXS experiment was carried out at the inelastic scattering beamline ID28 at the European Synchrotron Radiation Facility (ESRF, Grenoble, France). The undulator X-ray beam was monochromatized by a cryogenically cooled silicon (111) crystal and by a very-high-energy resolution monochromator, operating in backscattering geometry and utilizing the silicon (888) reflection order. This beam, with an energy of 15.618 keV and an energy resolution of 3.9 meV, was focused with a gold-coated mirror down to a beam size of 270 µm X 80 µm (horizontal X vertical; full-width-half-maximum) at sample location. These incident beam dimensions were further reduced by slits to avoid scattering from the high-pressure cell gasket. The scattered photons were collected by 5 spherical silicon crystal analysers operating in backscattering and Rowland circle geometry at the same reflection order as the high-resolution monochromator. The momentum transfer Q ($Q=2k_0\sin(\theta_S/2)$ where k_0 and θ_S are the wave vector of the incident phonon and the scattering angle, respectively) was selected by rotating the 7m-long spectrometer arm in the horizontal plane. Spectra were collected at five different momentum transfers simultaneously, spanning Q-values between 4 and 12 nm^{-1}. A powdered sample (99.999% purity) was loaded into the 120-µm hole of a rhenium gasket compressed between diamond anvils. Pressures were determined with the ruby fluorescence technique (*1*) and cross-checked by X-ray diffraction (*2*).

The experiment was performed on a polycrystalline sample of iron since it is impossible to preserve a single crystal while crossing the phase boundary from the low pressure body-centered cubic structure (b.c.c. or α phase) to the h.c.p. structure between 12 and 15 GPa (*3*). The observed increase of the phonon frequencies corresponds to an increase of the longitudinal wave velocity (V_P) from 7000 to 8800 $m.s^{-1}$ (see Figs. 1 and 2). Extrapolated longitudinal acoustic wave velocities compared with seismic data suggest an inner core slightly lighter than pure iron (*8*).

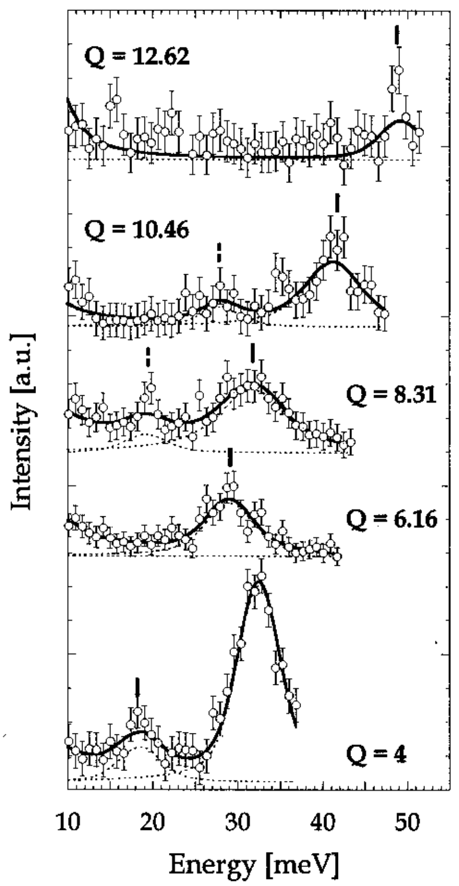

Fig. 1. Dispersion of iron longitudinal acoustic (LA) phonon with increasing Q values (in nm^{-1}). (LA) phonons of iron are indicated by ticks. A transverse acoustic (TA) mode detected at Q= 8.31 and Q= 10.46 nm^{-1} is indicated by broken ticks. Data are normalized to the intensity of the iron (LA) phonon peak. Integration time for each point was of the order of 700s, obtained by summation of 4 to 6 scans in the range 0-50 meV.

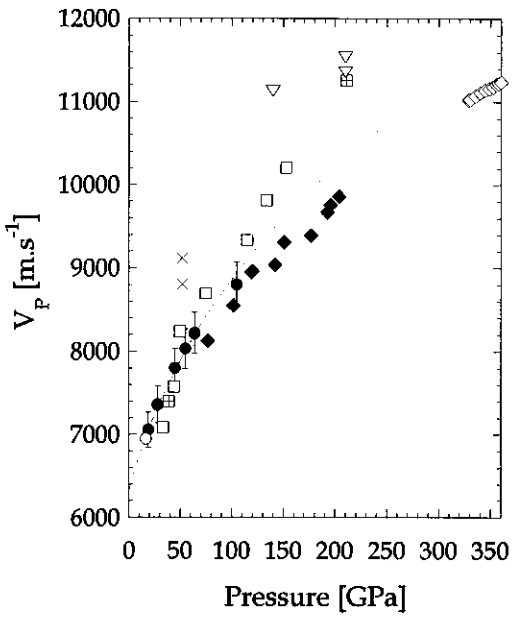

Fig. 2. Longitudinal acoustic wave velocities (V_P) of iron as a function of pressure: (●) the present work, extrapolated at higher pressure after a Birch fit to our data (solid line) and plotted along with (○) ultrasonic and (⊞) XRD measurements (*5*), (×) XRD measurements (*2*), (□) NRIXS data (*7*), (◆) shock-wave measurements, (◇) observations for the inner core, (▽) *ab initio* calculations.

The present IXS measurements represent the first direct measurements of V_P at very high pressure, and hence an alternative method to XRD measurements (*4, 5*). In contrast to NRIXS (*6, 7*) measurements which are limited to elements which possess Mössbauer isotopes, sound velocity measurements by IXS experiments under pressure can be used on a variety of materials of geophysical interest, including periclase or $MgSiO_3$ perovskite. Such a technique should be suited to map optical phonons dispersion curves as well.

References

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