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Report:

The issue of the anisotropy of sound wave propagation in hcp-iron at very high pressures [1] has been addressed by inelastic x-ray scattering (IXS). Iron develops, when compressed under non-hydrostatic conditions, texture above 30 GPa with a preferential alignment of the c-axis along the compression axis of the diamond-anvil cell. The effect of texture on the sound wave propagation can be probed with IXS by varying the measurement of longitudinal acoustic phonon propagation with respect to the compression axis. To this purpose, a special large angular opening diamond anvil cell (DAC) was developed.

Polycrystalline 99.99% iron from Sigma Aldrich was loaded in a 90 μm diameter hole drilled in a rhenium gasket, pre-indented to 28 μm (initially 200 μm), and pressurized in a DAC equipped with beveled diamonds (150 μm flat beveled from 300 μm culets at an angle of 8^o). No pressure-transmitting medium was used. The dispersion of longitudinal acoustic phonons was determined at 22, 69 and 112 GPa. Two different geometries were employed (see Figure 1), corresponding to a longitudinal sound propagation of 50^o and 90^o with respect to the loading axis. The pressure was determined *in situ* by conventional ruby fluorescence technique and crosschecked by x-ray diffraction, making use of the known equation of state of iron [2]. The experiment was performed with an overall energy resolution of 5.5 meV and a momentum resolution of 0.25 nm^{-1}. Data were collected at 5 different momentum transfers q at the lowest pressure, at 8-9 q values at higher pressure.

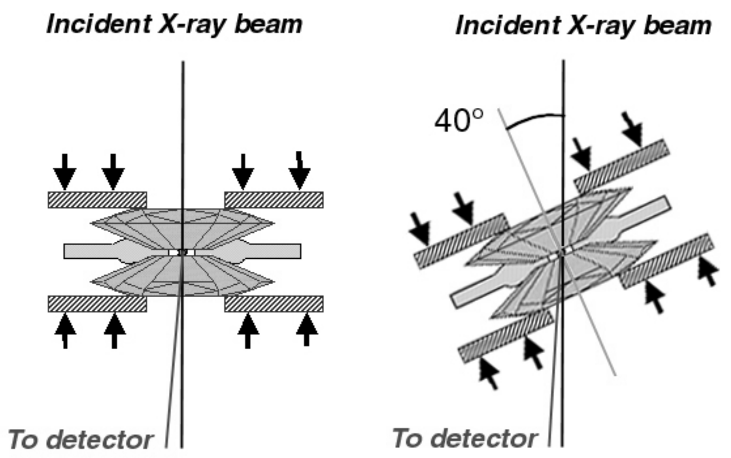

***Figure 1**: Schematic representation of the diamond-anvil cell and the two different scattering geometries. The probed propagation direction of the sound waves is either at 90^o or 50^o from loading axis of the DAC.*

Figure 2 shows the dispersion curves for the two orientations of the DAC, recorded at 22 GPa (left panel) and 112 GPa (right panel). The low *q* region, especially for 0^{o} incidence, is not accessible due to the presence of the longitudinal acoustic phonon of diamond whose intensity is much higher than the one of iron. The sound velocity V_p is obtained by a sine function fit to the dispersion curve:

$$E\ [\mathrm{meV}] = 4.192\times10^{-4}\ V_p[\mathrm{m/s}] \times q_{Max}[\mathrm{nm}^{-1}]\ \sin\{\pi/2\times(q[\mathrm{nm}^{-1}]/q_{Max}[\mathrm{nm}^{-1}])\}$$

where q_{Max} is the value of *q* corresponding to the Brillouin zone boundary where the slope of the dispersion is zero. For P=22 GPa, q_{Max} was either fixed to the value derived from x-ray diffraction assuming a perfect orientational average of the grains or kept free. Utilising these two procedures, the resulting sound velocities for the two orientations are identical within error bars.

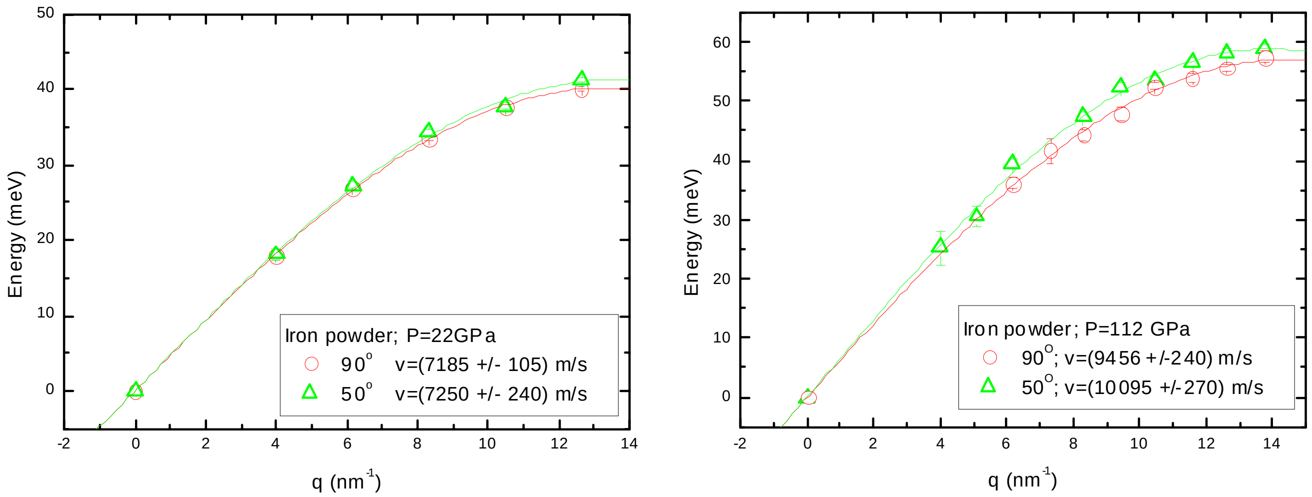

***Figure 2**: Phonon dispersion curves at 22 GPa (left) and 112 GPa (right) for propagation directions of 90^{o} and 50^{o} with respect to the loading axis of the DAC. The lines are the sinus fits to the experimental data with* q_{Max} free. *The derived values for the sound velocity are reported as well.*

For P=112 GPa differences in the dispersion curve can be appreciated. More specifically, the phonon energies for the "50^{o} –curve" are systematically higher. The derivation of the respective sound velocities, keeping the value of q_{Max} free in the fit, yield q_{Max} [50^{o}] < q_{Max} [90^{o}]. This is in qualitative agreement with the known preferred orientation of the c-axis along the loading axis, leading to a smaller value of q_{Max}. A complete analysis, quantifying the value of q_{Max} for the two orientations utilising results from radial diffraction measurements, is currently underway.

The deduced sound velocity for the "50^{o}-orientation" is 5-6% higher than the one for the "0^{o}—orientation". This anisotropy measured on a textured polycrystalline sample at 112GPa is comparable with the one observed for the Earth (3-4%, with the fast direction oriented parallel to the Earth's rotation axis), relaxing the requirement of a nearly perfect alignment claimed by first principle calculation [3] to justify this feature.

Moreover keeping account of such anisotropy it is possible to explain the discrepancies between the sound velocity measured by IXS [4] and NRIXS [5]. Actually the former probed essentially perpendicularly to the compression axis (lower velocity) while the latter along this axis (higher velocity).

References

[1] Wenk *et al.*, *Nature* **405**, 1044 (2000)
[2] Mao *et al.*, *Geophys. Res.* **95**, 21737 (1990)
[3] Sixtrude and Cohen, *Science* **267**, 1972 (1995)
[4] Fiquet *et al.*, *Science* **291**, 468 (2001)
[5] Mao *et al.*, *Science* **292**, 914 (2001)