ESRF	**Experiment title:** Elasticity of (Mg,Fe)O across the spin-pairing transition: spin-phonon coupling?	**Experiment number**: HS-4110
Beamline: ID28	**Date of experiment**: from: 07.04.2010 to: 13.04.2010	**Date of report**: 25 February 2011
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Report:

We carried out inelastic x-ray scattering (IXS) measurements on $Mg_{0.83}Fe_{0.17}O$-ferropericlase single crystals compressed in diamond anvil cells (DAC) at 9, 34 and 70 GPa. These data complement previous measurements (see Experimental Report HS-3864).

We performed IXS measurements on beamline ID28, operating the instrument in the Si(9,9,9) configuration, which provides 3 meV total energy resolution full-width-half-maximum (FWHM). The direction and size of the momentum transfer were selected by an appropriate choice of the scattering angle and the sample orientation in the horizontal scattering plane. The momentum resolution was set to 0.28 nm^{-1} and 0.84 nm^{-1} in the horizontal and vertical planes, respectively. The focused x-ray beam of 30 x 90 μm^2 FWHM was further reduced in the vertical by slits to match sample dimensions. Measurements have been performed in transmission geometry, with the incoming x-ray impinging along the cell axis, across the diamonds.

At each investigated pressure point we collected 2-3 spectra in the linear part of the dispersion of four to five independent acoustic phonons, LA (100), TA (100), LA(110), $TA(110)_{<001>}$ and $TA(110)_{<-110>}$, deriving the sound velocity from the initial slope of the dispersion. Bragg angles of the [111], [200] and [220] reflection were also recorded, to provide the crystal orientation and a direct determination of the density for each pressure point. We then obtained the three independent element of the elastic tensor (C_{11}, C_{12} and C_{44}) solving the Christoffel equation.

The obtained results are reported in Figure 1, together with results from previous run (HS-3864) and literature values. Up to ~ 40 GPa, all the elastic moduli exhibit a monotonic increase with pressure, as is expected with compression. In the 40 to 60 GPa pressure range, where the spin transition occurs, we observe a distinct softening of C_{44}, and a small variation in C_{12}, while C_{11} retains a continuous trend. Above 60 GPa, the usual monotonic increase with pressure is observed for all the moduli, although with a larger pressure derivative. The back extrapolations of our results to ambient pressure are within few percent of the ultrasonic determinations for the same composition [1]. However, if we compare our high-pressure measurements with ISLS [2] and Brillouin [3,4] data obtained on samples with lower iron content, we observe qualitative agreement for C_{44} and $C'=1/2(C_{11}-C_{12})$, which display softening in the pressure range of the spin transition for all methods (quantitative differences are at least partially due to differences in iron concentration), but disagreement for C_{12} and, notably, for C_{11}. Indeed, whereas both optical studies [2, 4] report a large softening of C_{11} in the 40-60 GPa range, the direct determination of C_{11} by IXS does not show any anomaly.

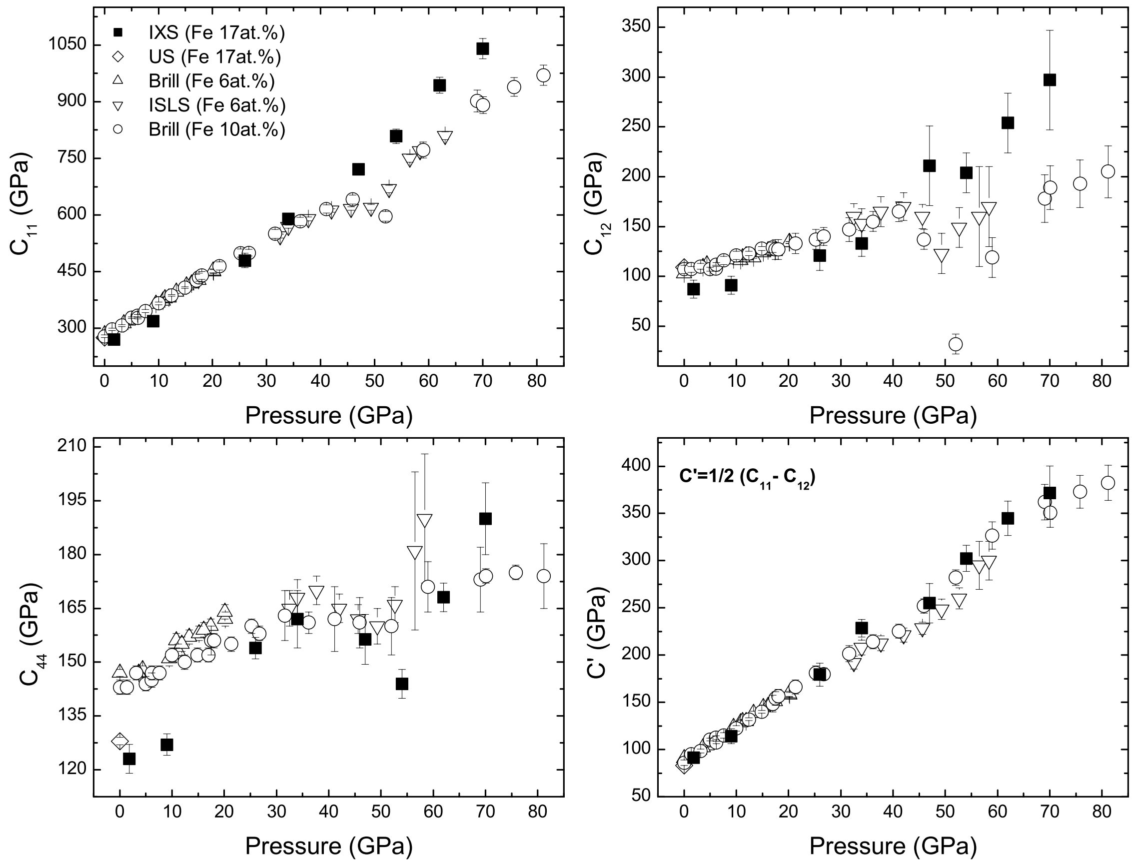

Figure 1: Pressure evolution of the single-crystal elastic moduli of $(Mg_{1-x},Fe_x)O$-ferropericlase. Solid square, IXS data for x=0.17, open diamonds, ambient pressure ultrasonic determination for x=0.17 [1]; open triangles, Brillouin measurements for x=0.6 [3]; open inverted triangles, ISLS results for x=0.06 [2]; open circles, Brillouin determination for x=0.10 [4].

Further discussion on the obtained results and geophysical implications can be found in Antonangeli et al., Science 331, 64 (2011).

References

[1] S.D. Jacobsen *et al.*, J. Geophys. Res. 107, 2037 (2002).
[2] J.C. Crowhurst *et al.,* Science 319, 451 (2008).
[3] J.M. Jackson *et al.*, J. Geophys. Res. 111, B09203 (2006).
[4] H. Marquardt *et al.,* Earth Planet. Sci. Lett. 287, 345 (2009).