ESRF	**Experiment title:** Elastic and thermal properties of (Mg,Fe)O-ferropericlase	**Experiment number**: HS-3296
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Report:

We have performed Inelastic X-ray Scattering (IXS) experiments on a single crystal of (Mg,Fe)O-ferropericlase, collecting phonon spectra along all the main crystallographic directions, missing only the longitudinal acoustic (LA) mode along the [111] direction. These preliminary measurements at ambient conditions clearly established the feasibility of experiments at high pressure (see proposal HS-3567) and open the door to the investigations of the effects of compression-induce spin-pairing transitions on the phonon dispersion of ferropericlase.

Oriented single crystals of (Mg,Fe)O have been synthesized at the Lawrence Livermore National Laboratory starting from pre-aligned crystal of MgO (normal parallel to [110] direction) by high-temperature Fe-Mg interdiffusion in a piston cylinder press. X-ray diffraction measurements on the polished sample (~100 μm thick) confirmed the alignment within few degrees, and, once compared with literature data [1], allowed to fix to ~4.5 atom% the Fe amount over the probed x-ray spot (30 μm x90 μm FWHM), in good agreement with the value estimated from electron microprobe analysis. Mosaic spreads (rocking widths) of the collected diffraction lines varied between 0.2° and 0.3°, further testifying on the good quality of the prepared crystal.

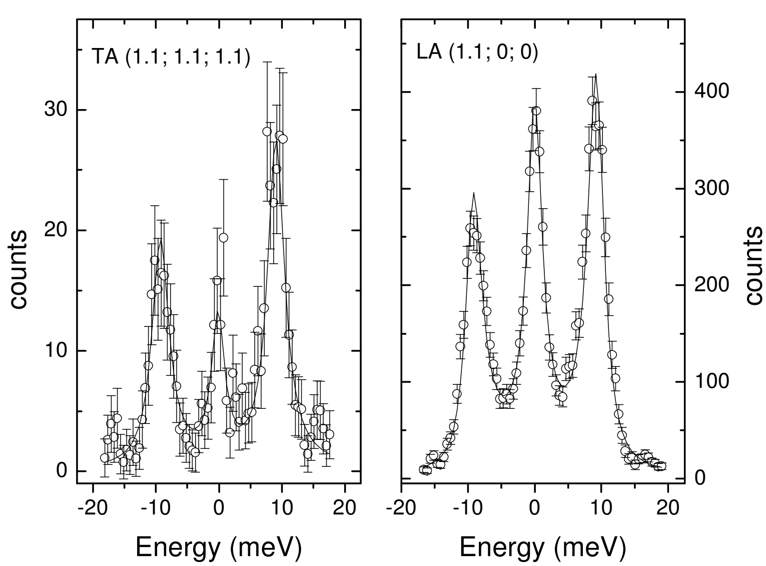

***Figure 1**: Representative IXS spectra of ($Mg_{0.955}Fe_{0.045}$)O. The experimental spectra (open circles) are shown together with their best fits.*

We collected IXS spectra along all the main crystallographic directions, missing only the LA[111] phonon mode. Typical examples of the collected data are reported in Figure 1. A detailed analysis, in particular of the zone edge phonons, is still in progress, however the good quality of the raw spectra and the first fits to the experimental data provide strong indications that, in spite of the configurational disorder and composition inhomogeneities, the quasi-elastic contribution to the inelastic spectra do not prevent the collection of high-quality data. Moreover, we did not observe any local internal vibrational modes.

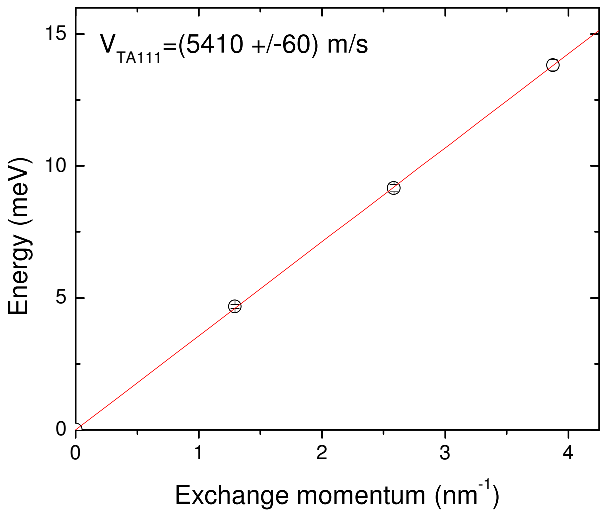

***Figure 2**: Fit to the linear part of the phonon dispersion of the TA mode along the [111] directions. The determined velocity compares well with the extrapolation of ultrasonic interferometry measurements to a similar composition: $V_{TA[111]}$ = 5540 m/s.*

From the initial slope of the acoustic phonon dispersion (see Figure 2) we determined the sound velocities which, in contrast to the nuclear resonant inelastic x-ray scattering measurements [2], compare favourably with the sound velocity obtained by ultrasonic interferometry [1] on ferropericlase of similar Fe content. In particular the analysis of the linear part of the dispersion of the LA[100], LA[110], TA [100], TA[111] and $TA[110]_{<001>}$ phonons, allowed the estimation of the full elastic tensor. The simultaneous inversion of the data provided the following values for the three independent elastic moduli: C_{11}=320 ±20 GPa, C_{44}=150 ±6 GPa, C_{12}=110 ±10 GPa. Due to the presence of compositional gradients (tens to hundred of microns domains) across the sample, the reported errors are somewhat larger than typical of the elastic moduli determined by IXS [3]. Nevertheless, the values of the various C_{ij} are in reasonably good agreement with the extrapolations of ultrasonic measurements to similar composition (C_{11}=283 GPa, C_{44}=149GPa, C_{12}=99 GPa). Furthermore, samples prepared for high-pressure experiments, with dimension compatible with diamond anvil cell geometrical constraints (~30 μm diameter disks, 10 to 15 μm thick) will be by far less affected by possible gradients, so that a higher accuracy in the determination of the elastic moduli is expected.

References:

[1] "*Structure and elasticity of single-crystal (Mg,Fe)O and a new method of generationg shear waves for gigahertz ultrasonic interpherometry"* S.D. Jacobsen *et al.*, J. Geophys. Res. Solid Earth 107, 2037 (2002).
[2] "*Sound velocities of ferropericlase in the Earth's lower mantle*", J.F. Lin *et al*, Geophys. Res. Lett. 33, L22304 (2006); Correction, Geophys. Res. Lett. 34, L0931 (2007).
[3] "*Elasticity of cobalt at high pressure studied by inelastic x-ray scattering",* D. Antonangeli, *et al.,* Phys. Rev. Lett. 93, 215505 (2004).