| ESRF | **Experiment title:**<br>Elastic properties of (Mg,Fe)SiO3 perovskite and post-perovskite at high P,T | **Experiment number**:<br>HE-2901 |
|---|---|---|
| **Beamline**:<br>ID18 | **Date of experiment**:<br>from: 12.11.2008 to: 28.11.2008<br>(concurrent with HE-2893; setup 12.-17.11.08) | **Date of report**:<br>01.03.2009<br><br>*Received at ESRF:* |
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## Report:

Seismology and its associated parameters (density, compressional and shear wave velocities) is our primary method for directly probing the Earth's interior; therefore techniques such as nuclear inelastic scattering (NIS) which provide information on the sound velocities of relevant minerals are an important tool to determining the nature of the Earth's interior. The aim of experiment HE-2901 was to carry out NIS measurements, combined with nuclear forward scattering (NFS), on lower mantle minerals at high pressure and temperature.

In our previous experiments on ID18 at ESRF (HE2157, HE2577 and HE2750), we used a diamond anvil cell (DAC) equipped with an external heater to achieve higher temperatures. This approach allowed us to collect NFS data to 1000 K at high pressures (HE2157 and HE2750), but diamond failure prevented high temperature data collection for NIS (HE2577). We therefore used a different approach for the current experiment, and installed a prototype portable laser-heating system on ID18.

Experiment HE2901 was carried out at the same time as HE2893 since both experiments used exactly the same setup, only different samples, and took place during operation in 7/8+1 mode (setup), hybrid mode (19.-25.11.08) and 16-bunch mode (27.-28.11.08). For all measurements the beam was focussed to ca. 4 µm × 20 µm using a K-B mirror, and a MAR CCD camera was installed on the beam line to enable collection of XRD data at the same P,T conditions as the NIS and NFS spectra. For NIS data collection the DAC was oriented with the gasket horizontal to the beam (i.e., both the beam and the incoherent signal passed through the gasket), while NFS data was collected in either horizontal or vertical geometry (or both). We discovered two problems associated with NIS data collection in horizontal geometry: (1) the beam excites resonance in iron contained in the Be gasket; and (2) the beam excites resonance in parts of the sample that were not heated. The first effect can be corrected for by subtraction of a "Fe in Be" signal from the NIS data, while the second effect simply results in an averaging of signals from the sample at different temperatures; in both cases data are still usable. However we are currently redesigning the laser heating system so that NIS data can be collected in vertical geometry, hence removing these two problems in future experiments.

We collected 12 NIS spectra for $Fe_{0.12}Mg_{0.88}SiO_3$ perovskite, the most abundant lower mantle phase, at pressures to 100 GPa and temperatures to 1000 K, as well as 2 NIS spectra of other perovskite compositions at ambient conditions for comparison. Since we were not able to synthesise post-perovskite due to kinetic problems, we collected instead 14 NIS spectra for $Fe_{0.12}Mg_{0.88}O$ ferropericlase, the second most abundant lower mantle phase, at pressures to 95 GPa and temperatures to 2000 K. Both perovskite and ferropericlase are known to undergo spin transitions within the P,T range of our experiments (McCammon et al., 2008; Lin et al., 2007).

From the NIS data we determined the phonon density of states (PDOS), which we then used to extract the mean velocity of sound using the Debye model.For both perovskite and ferropericlase, the main peak in the PDOS shifts to higher energies with increasing pressure at room temperature (Figs. 1 and 2, left), consistent with general expected behaviour. The mean sound velocities derived from the room temperature $Fe_{0.12}Mg_{0.88}SiO_3$ perovskite data show the same behaviour as the data from $Fe_{0.18}Mg_{0.82}O_3$ perovskite (see Report HE-2750), namely that vibrations of the iron sub-lattice are different from those of the bulk structure at low frequencies, in contrast to the behaviour of most all other silicate and oxide minerals. Ongoing collaboration with computational groups are expected to provide insight into this anomalous behaviour.

The PDOS spectra in some of our data show a shift of the main peak to higher energies with increasing temperature at constant pressure (Figs. 1 and 2, middle and right), contrary to the general expectation that higher temperatures cause softening of the lattice, and hence a shift of the peak to lower energies (e.g., Chumakov et al., 1996). This behaviour might result from the effect of changing spin populations, and analysis of the NFS spectra is continuing in order to constrain this parameter.

**References:**

Chumakov, A.I. *et al.*, *Phys. Rev. B* **54**, R9596-R9599 (1996).
Lin, J.-F. *et al.*, *Science* **317**, 1740-1743 (2007).
McCammon, C. *et al.*, *Nature Geoscience* **1**, 684-687 (2008).


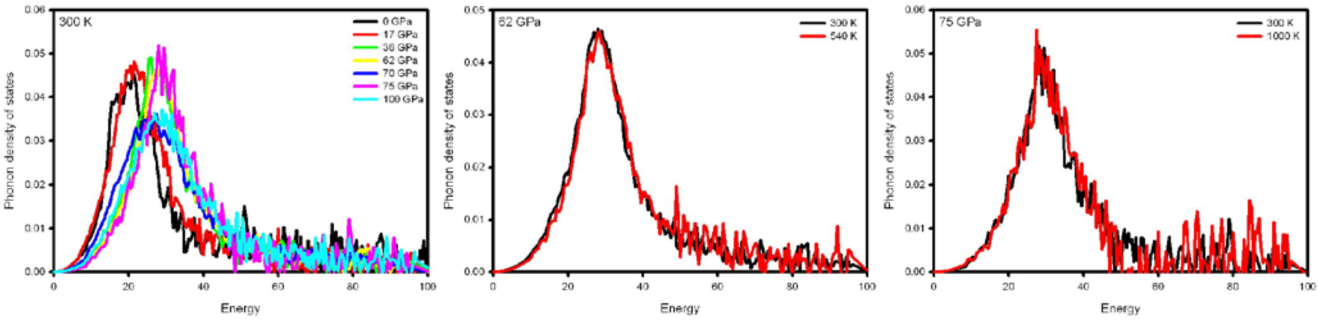


Fig. 1. Phonon density of states derived from NIS data of $Fe_{0.12}Mg_{0.88}SiO_3$ perovskite as a function of pressure at room temperature (left), and high temperature at constant pressure (centre and right)

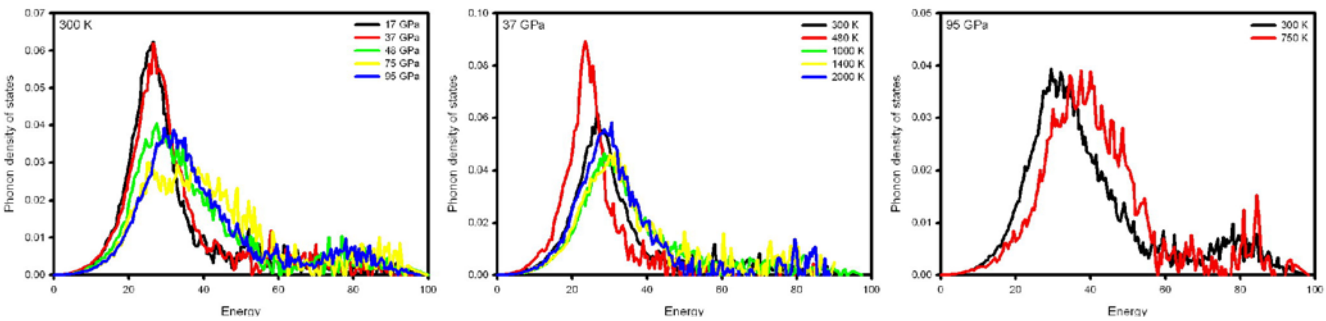


Fig. 2. Phonon density of states derived from NIS data of $Fe_{0.12}Mg_{0.88}O$ ferropericlase as a function of pressure at room temperature (left), and high temperature at constant pressure (centre and right)