ESRF	**Experiment title:** Acoustic phonon dispersion of $SrTiO_3$ perovskite and sound velocities of $MgSiO_3$ to core-mantle boundary pressures	**Experiment number**: HS1338
Beamline: ID28	**Date of experiment**: From: 12/11/2000 to: 20/11/2000	**Date of report**: 18/07/2001
Shifts: 24	**Local contact(s)**: Matteo d'Astuto	*Received at ESRF:*

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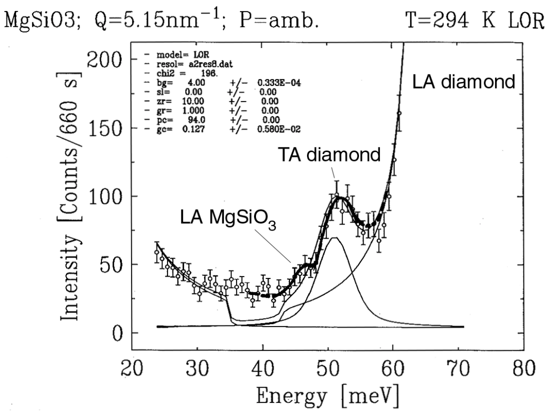
Report:

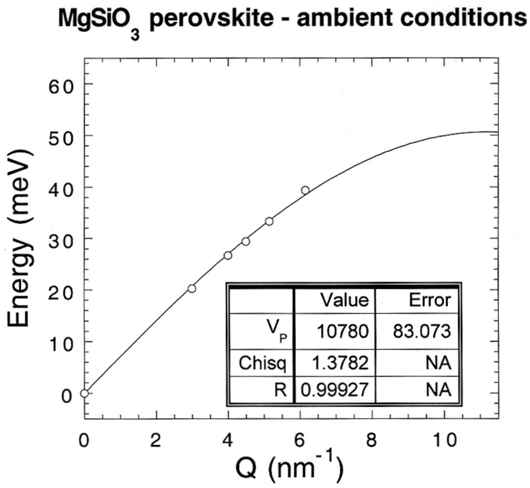
Physical properties of $MgSiO_3$ with perovskite structure is of first interest to better understand both the composition and current state of the Earth's mantle (670 to 2900 km in depth). The knowledge of the elastic constants of this compound, which makes up to 80-100 wt% of the lower mantle, is for instance essential for comparison with Earth's global models, which are based on seismic waves velocity profiles. To date, ambient conditions elastic moduli have been determined by a single experiment of Brillouin spectroscopy [1] and pressure and temperature derivatives have been inferred from an ultrasonic experiment [2].

The proposal was aimed to investigate the elastic properties of $MgSiO_3$ perovskite under very high-pressure. An $MgSiO_3$ perovskite sample was synthesized in a multi-anvil press [3] and subsequently loaded in helium in a diamond anvil-cell. A typical IXS spectrum is presented below, at pressure conditions close to ambient.



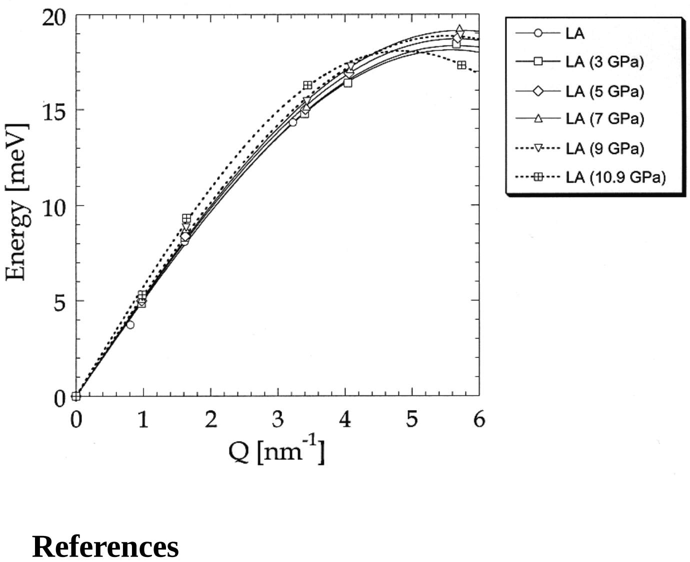
As shown in this figure, the acoustic longitudinal excitation from the sample is almost at the same energy as the signal related to the transverse acoustic phonon of the diamond anvil. The diamond window is indeed characterized by very high acoustic velocities, which makes any analysis impossible at high-pressure in the geometry we had during the experiment.

On the other hand, we could record for the first time a full dispersion curve of the longitudinal acoustic branch of silicate perovskite at ambient pressure. The analysis shown below yields an independent direct determination of the sound velocity for this material.



Assuming a sine function for the dispersion of this longitudinal acoustic mode, we obtain a mean longitudinal acoustic velocity V_P of 10780 ± 83 ms^{-1}, which is in good agreement with the value of 10940 ms^{-1} determined by Brillouin spectroscopy [1].

Perovskite structure exhibits a wide variety of behaviour, with a multitude of possible phase transition [4]. The vibrational dynamics of these transitions is very important since they are likely to proceed via soft-mode mechanisms [5]. In this respect, the second part of the proposal was dedicated to the study of the acoustic phonon dispersion relations of an analogue perovskite ($SrTiO_3$), to characterize one of the key phase transition described above. High quality single crystals are available for that compound, that seems to undergo with increasing pressure a transition from a cubic (Pm3m) to a tetragonal structure (I4/mcm) for which transition pressure is still controversial (*i.e.* between 6 and 12 GPa). A single crystal perovskite of $SrTiO_3$ perovskite was embedded in helium in a diamond-anvil cell and IXS pattern were recorded with increasing pressure.



In addition to sound velocities determination as a function of pressure, the preliminary results presented below might indicate that such a transition indeed proceeds via a softening of the longitudinal branch along ζ00, which starts at 9 GPa and is clear at 10.9 GPa close to the edge of the first Brillouin zone. However, complementary experiments on other crystal orientations are needed to strengthen such conclusions.

References

[1] Yeganeh-Haeri A., Weidner D.J. and Ito E. Elasticity of MgSiO3 in the perovskite structure. *Science* 243, 787-789 (1989).

[2] Sinelnikov Y.D., Chen G., Neuville D.R., Vaughan M.T. and Liebermann R.C. Ultrasonic shear wave velocities of $MgSiO_3$ perovskite at 8 GPa and 800 K and lower mantle composition. *Science* 281, 677-679 (1998).

[3] The high-pressure synthesis was conducted by J. Zhang with the joint support of SUNY at Stony Brook and the Technology Center for High Pressure Research.

[4] Lines M.E. and Glass A.M. Principles and applications of ferroelectrics and related materials. Clarendon Press, Oxford (1977).

[5] Hemley R.J. and Cohen R.E. *Ann. Rev. Earth Planet. Sci*., 20, 553-560 (1992).