ESRF	**Experiment title:** Local structural change in $MgSiO_3$ glass at high pressure, revealed by X-ray Raman scattering	**Experiment number**: ES291 (in run4_2015)
Beamline: ID20	**Date of experiment**: from: 1. July 2015 to: 7. July 2015	**Date of report**: 08.01.2016
Shifts: 18	**Local contact(s)**: Christoph Sahle	*Received at ESRF:*

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Report:

We were able to collect silicon L-edge, magnesium L-edge and oxygen K-edge spectra of MgSiO3 glass, compressed up to 60 GPa in plate diamond-anvil cells, at 7 pressure points. The data still require thorough analysis, and the interpretation will require modeling. However, already at the present stage, it seems, that the results of this beamtime will be a step on the way to establish X-ray Raman spectroscopy as a tool for high-pressure coordination chemistry in silicate glasses.

Our research motivation is to contribute to the understanding of the link between macroscopic properties and atomic structure of silicate melts and glasses at the Earth's mantle pressures. X-ray Raman scattering (XRS) is a powerful analytical technique for the investigation of the electronic structure of matter in-situ under extreme pressures.

In the beamtime reported here, we employed own plate-diamond-anvil cells (plateDACs) with a large opening angle, and Rhenium gaskets. With the energy of 13 keV, we used the axial geometry. This means, both incident and salient radiation went through the diamonds of the DACs (see Illustration 1). The advantage of the geometry is that we were able to measure the Si L-edge at about 100 eV, an energy region which is blocked by the Be K-edge, if Beryllium gaskets and the radial measurement geometry is used. Until today, the measurement of the Si L-edge remains very challenging.

We put emphasis on the Si L-edge, and were able to record spectra at 7 pressure steps up to 60 GPa (Illustration 2). Complementary to the Si L-edge, we measured the Mg L-edge at 6 pressure points, and the O K-edge at 5 pressure points.

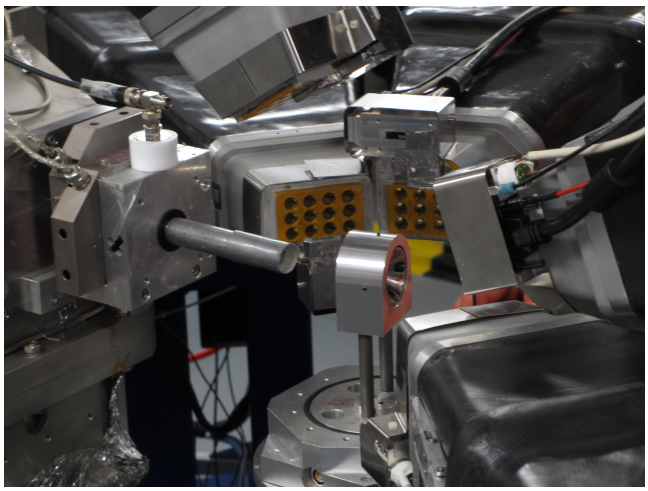

Illustration 1: The experimental axial geomtry of plate-DACs allows the use of 4 analyzer-arrays: Three in forward scattering and one in backward scattering.

The changes of the Si L-edge spectra will be interpreted in terms of changes in silicon coordination with pressure (Illustration 3) and in terms of changes in polymerization, specially at pressures below 30 GPa. The XRS data will be complemented by XRD data acquired on the same sample. Together, this allows for a more detailed description of structural changes around silicon.
The changes in the Mg L-edge spectra (lllustration 4 and 5) will be interpreted in terms of decreased Mg-O distances and increased coordination of Mg by oxygen.

We are confident to be able to publish the results of this beamtime during the year 2016.

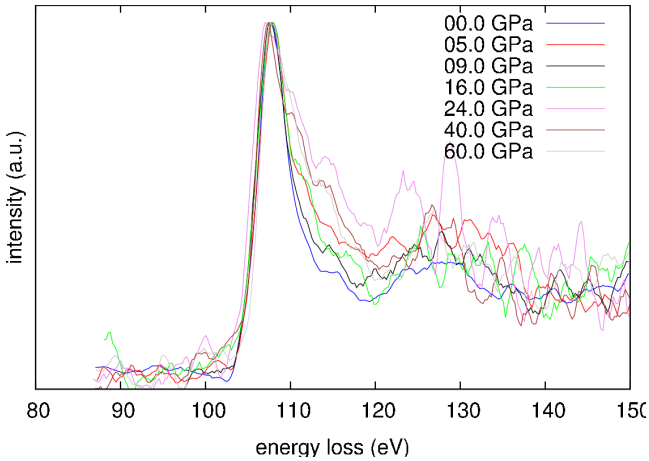

Illustration 2: The silicon L-edge reflects the structural changes under pressure, most visibly at the shoulder at 115 eV.

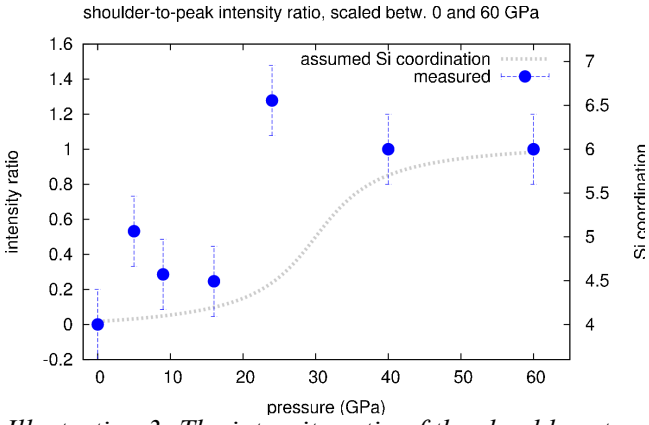

Illustration 3: The intensity ratio of the shoulder at 115 eV to the peak intensity of the Si L-edge reflects the coordination increase of Si, but the changes in the spectrum are also subject to other effect at lower pressures, such as change in polymerization.

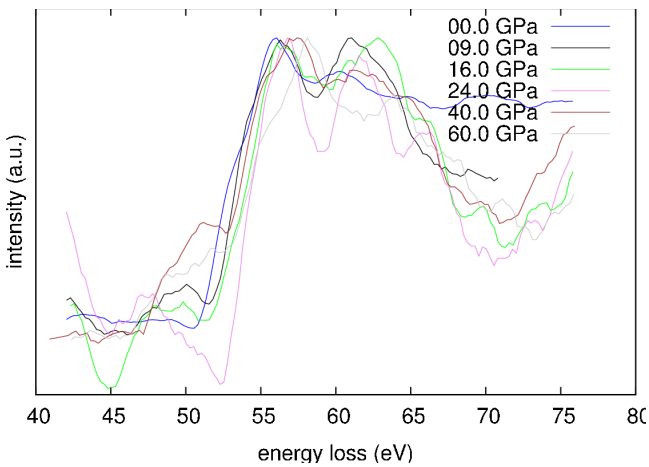

Illustration 4: The Mg L-edge is difficult to evaluate even at high q, because the signal is relatively weak compared to the inhomogeneous background from the surrounding diamond.

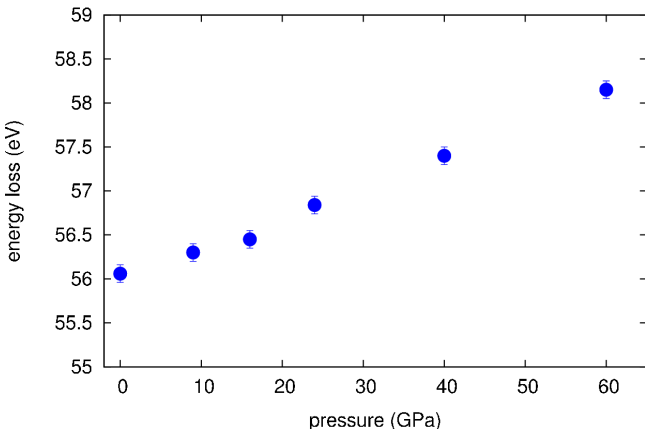

Illustration 5: The first peak position of the Mg L-edge reflects the decreasing Mg-O distances.