ESRF	**Experiment title:** Local compaction mechanisms in Earth's mantle related glasses,revealed by X-ray Raman scattering: The case of MgSiO3	**Experiment number:** HC-3182 (in run3_17)
Beamline: ID20	**Date of experiment:** from: 28. June 2017 to: 4. July 2017	**Date of report:** 12.09.2017
Shifts: 18	**Local contact(s):** Christoph Sahle	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Georg Spiekermann,(*) University of Potsdam, 14469 Potsdam, Germany, geospiek@uni-potsdam.de

Report:

We have collected X-ray Raman scattering (XRS) spectra of MgSiO3 glass at the silicon L-edge, magnesium L-edge and oxygen K-edge spectra of MgSiO3 glass, compressed up to 60 GPa in diamond-anvil cells (DAC), equipped with recently developed miniature diamonds of 1 mm diameter and 0.5 thickness. Some measurements were carried out with Beryllium gaskets in a radial geometry.

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.

The spectral quality that we collected is much superior to the one achieved in a prior beamtime, ES-291. This is due to the miniature diamonds that we tested for the first time in beamtime ES-431. Figure 1 shows the Mg L-edge up to 57 GPa at high momentum transfer in hitherto unrivaled spectral quality. Figure 2 shows the Si L-edge.

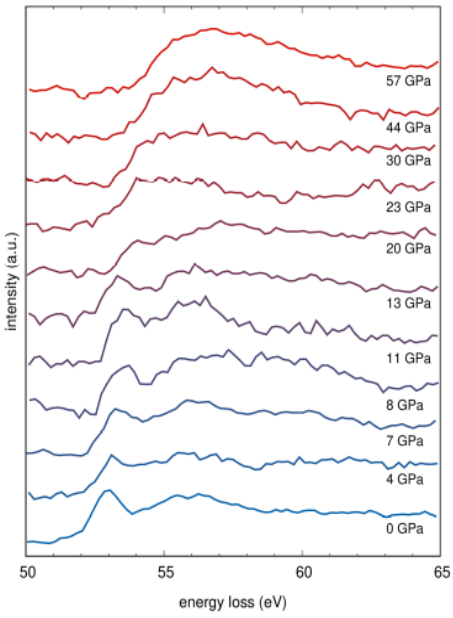

Figure 1: XRS spectra of the Mg L-edge up to 57 GPa, with a pronounced shift of the edge onset.

The evaluation of the observed spectral changes in terms of coordination changes of silicon and magnesium is challenging and requires modelling of

spectra. We will compute spectra at the Bethe-Salpeter equation (BSE) level with the OCEAN code. Figure 3 shows the excellent agreement of the Mg L-edge as observed by XAS and the calculated XRS spectrum at high momentum transfer.

The coordination increase of silicon in compressed silicate glasses has been investigated before, but no consensus has been reached, as the diverging results from several studies show. On the coordination increase of magnesium, not much has been established.

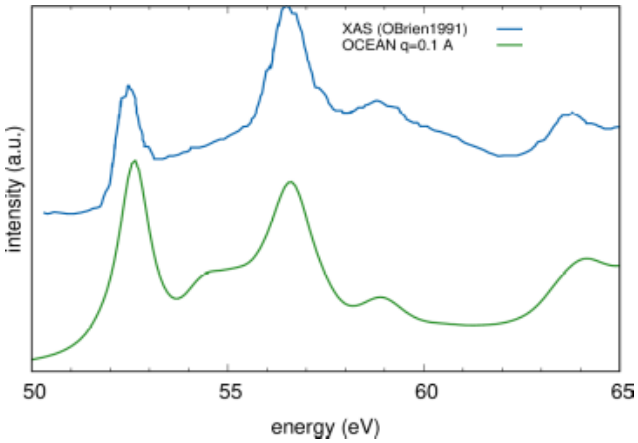

Figure 3: Comparison of the measured Mg L-edge of MgO (XAS, O'Brien1991), compared to the computed spectrum with the OCEAN code.

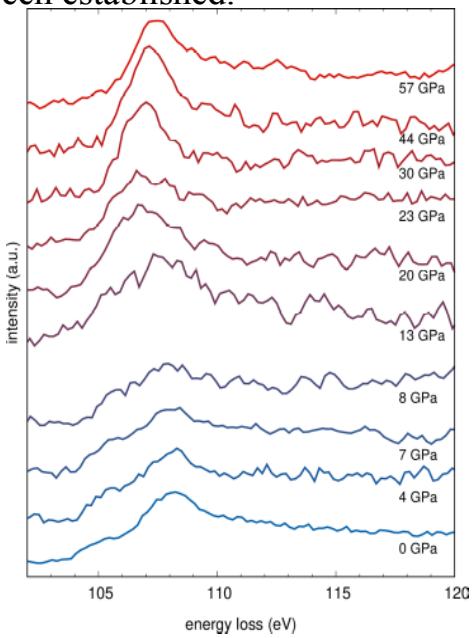

Figure 2: Si L-edge at high momentum transfer up to 57 GPa