ESRF	**Local structure around network modifiers and formers in quenched silicate melts at high pressure**	**Experiment number**: ES 449
Beamline: BM23	**Date of experiment**: from: 19.10.16 to: 25.10.16	**Date of report**: 3.8.17
Shifts: 18	**Local contact(s)**: Angelika Rosa	*Received at ESRF:*

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Report:

This study aims at understanding the structural properties of silicate melts and glasses at extreme pressure conditions. We study the structural effects of compression by using the local structure around Ge, Sr, and Y as a function of pressure. In the studied systems, Ge and Sr partially replace the major elements Si, Na, and Ca. While Ge will monitor changes of network-forming cations, Sr will do so for network modifiers, whereas Y represents the geochemically important rare earth elements.

EXAFS spectra of Ge and Sr were acquired on glasses with the nominal composition $Na_{0.5}Sr_{0.5}Al_{1.5}Si_2Ge_{0.5}O_8$ and $Na_{0.45}Ca_{0.1}Mg_{0.05}Sr_{0.5}Al_{1.35}Si_{1.95}Ge_{0.5}O_{7.8}$, both doped with 5000 ppm Y. For Y only XANES spectra for selected pressures could be acquired due to the low XRF signal. Spectra were recorded using the KB-mirror micro-focus station at beamline BM23 with a beamsize of 7 x 20 μm^2 and a Si(111) fixed-exit monochromator. Sr and Ge were measured in transition mode whereas Y was measured in fluorescence mode using a con-focal XRF setup to minimize background from elastic and inelastic scattering (Wilke et al. 2010). For this, a long working-distance polycapillary half-lens was located between the diamond anvil cell and the Si drift-chamber EDS detector. The diamond anvil cells were equipped with nano-polycrystalline diamonds to avoid glitches in the spectra by Bragg diffraction from the diamond anvils.

Fourier transforms of the EXAFS for Ge and Sr are shown in figure 1 and 2 as a function of pressure. Preliminary analysis of the spectra reveal increases in the Ge-O distance by ca. 3% and the coordination number from 4 to 6 between 5 and 30 GPa. At higher pressure, the distance decreases slightly. The change of these parameters is quite similar for the two investigated glass compositions. In comparison, the conversion from 4 to 6-fold coordination and associated increase of the Ge-O distance in GeO_2 glass takes place between 4 and 20 GPa (e.g. Hong et al. 2014). In case of Sr, there are only small changes in the Sr-O distance, however the number oxygen neighbors increases from 6 at ambient pressure to 8 at 30 GPa.

The XANES spectra of Ytrrium are shown in figure 2. There is a distinct change in the fine structure of the white line at 17050 to 17070 eV between ambient pressure and the two higher pressures but virtually no difference at the first EXAFS maximum. This might indicate that the Y-O distance does not change significantly and only the site symmetry is affected.

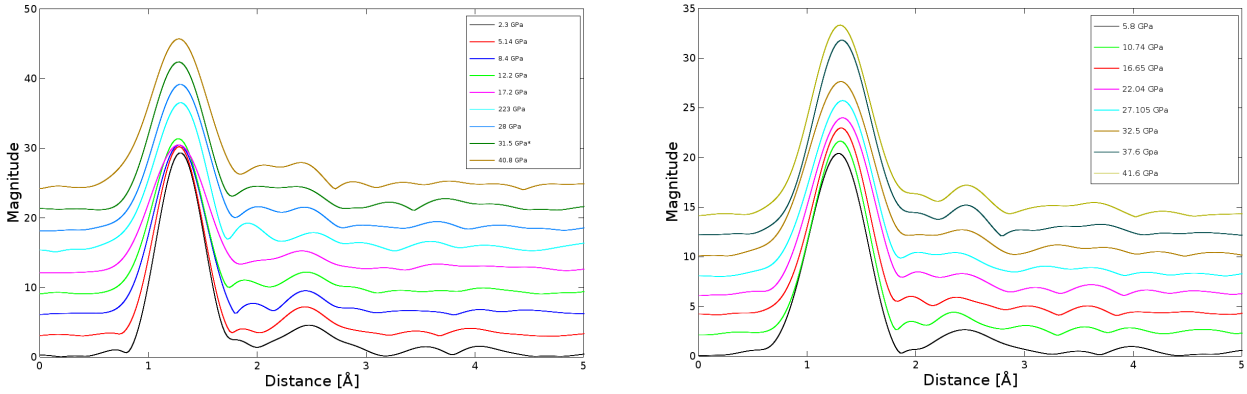

Figure 1: Fourier transform of EXAFS measured at the Ge K-edge at pressures indicated. (left) Ab-Glass; (right) Ab-Di Glass.

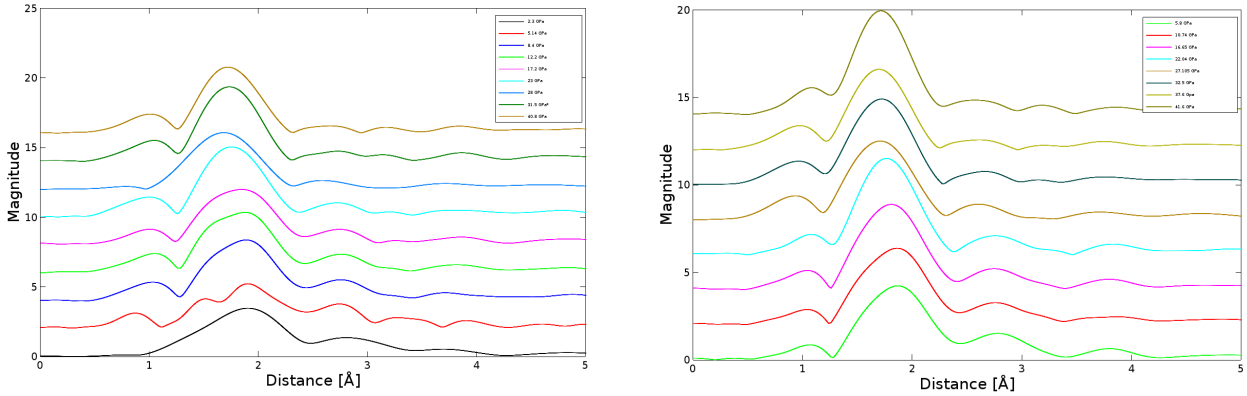

Figure 2: Fourier transform of EXAFS measured at the Sr K-edge at pressures indicated. (left) Ab-Glass; (right) Ab-Di Glass.

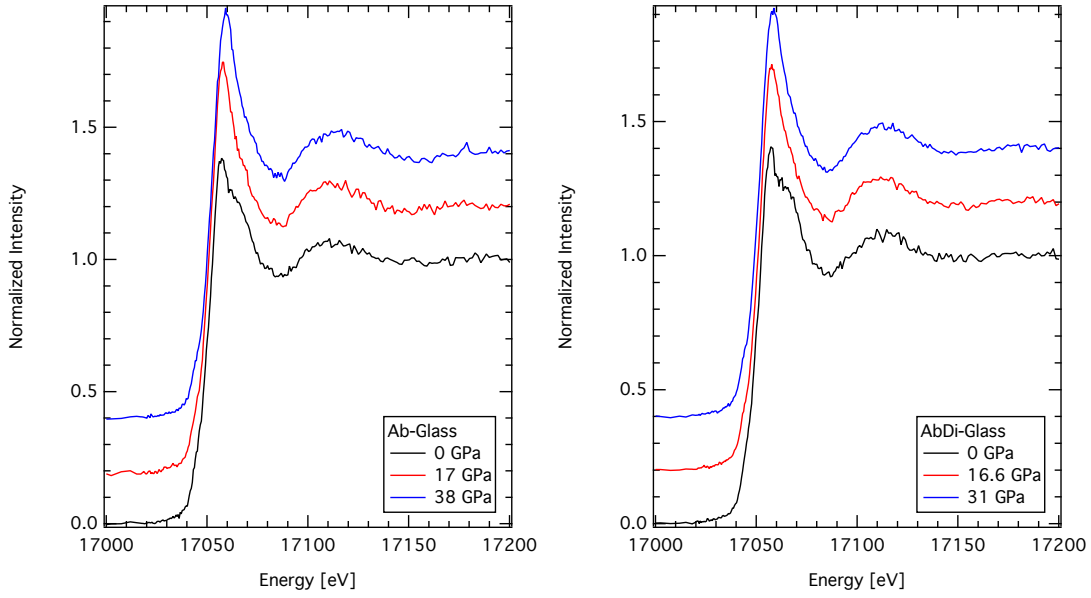

Figure 3: XANES spectra measured at the Y K-edge at the pressures indicated. (left) Ab-Glass; (right) Ab-Di Glass.

References:

Wilke et al. (2010) J Synchrotron Rad, 17, 669-675.
Hong et al. (2014) J. Phys.: Condens. Matter, 26, 035104.

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