ESRF	**Experiment title:** In situ study of the local atomic structure of hydrous silicate melts	**Experiment number**: ES-432
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Report: The purpose of this investigation was to examine the local chemical environment of the network-modifier sodium in water bearing albite by means of x-ray Raman scattering (XRS) at high pressure and high temperature using a resistively heated diamond anvil cell (HDAC). It is well known that the solubility of water in silicate melts in form of molecular water and hydroxyl groups increases significantly when applying pressure. This incorporation of H_2O has a large effect on physical, transport and chemical properties and thus is of fundamental importance in technical processing of glass melts as well as for geological processes related to magmatism, e.g. ascent of magma in the Earth's interior and volcanic eruptions [1-3].

We studied glasses of $NaAlSi_3O_8$ (albite) and $NaAlSi_3O_8$ with 10 wt. % H_2O that were synthesized in an Internally Heated Pressure Vessel (IHPV) at the GeoForschungsZentrum Potsdam. For use with our HDAC the glasses were enclosed together with iridium gaskets in platinum capsules (with 10 wt% water for the hydrous samples) which remained for 3 days at 1200 °C and 5000 kbar in the IHPV. In this way, the melt can flow into the gasket holes significantly increases the amount of glass in the sample chamber.

During experiment ES-432 we were able to measure a complete dataset (Na, Al, O, and Si-edges) of XRS spectra of dry and hydrous albite at ambient conditions in order to evaluate the sensitivity of the edge shape on the H_2O content. Furthermore, we performed in-situ measurements of the Na and Si L-edge at approximately 500 MPa up to 400 °C with our HDAC on hydrous albite melt. The spectra of the quenched glasses at ambient conditions were measured using the Si 660 analyzer reflection at 9.7 keV with an overall energy resolution of 0.7 eV. The in-situ measurements at pressure and temperature using HDAC were

conducted using the Si 880 analyzer reflection at 12.9 keV with an overall energy resolution

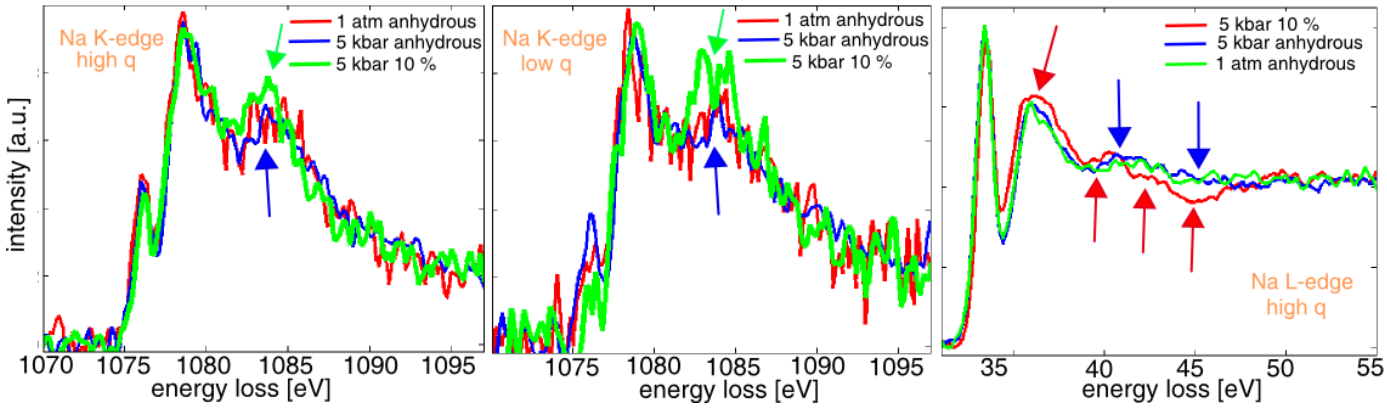

Figure 1: Measurements of the Na K-edge of $NaAlSi_3O_8$ glass, synthesized at pressure and with water content indicated at high (left) and low (center) wave vector transfer *q* at ambient conditions. XRS spectra of the Na L-edge measured at high *q* (right).

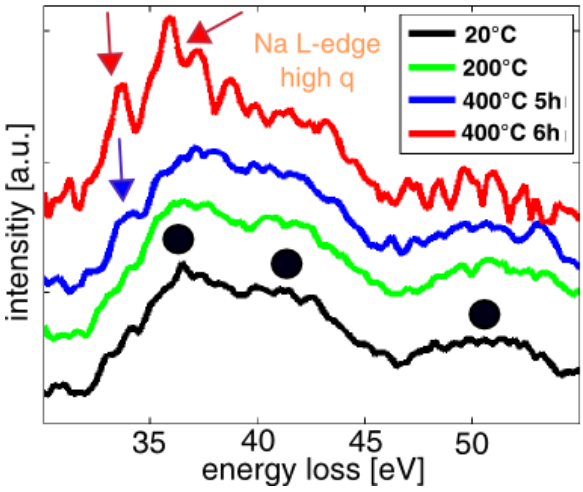

Figure 2: In-situ L-edge of hydrous $NaAlSi_3O_8$ glass and melt

of 2 eV as a compromise between flux and attenuation of the x-ray by the diamonds of the cell. The XRS spectra of the network-modifier sodium (L and K-edge) at ambient conditions are shown in figure 1. The water-incorporation predominantly affects the first post-edge maximum of the Na K-edge measured at high and low wave vector transfer *q*. For the Na L-edge strong changes in the post-edge features occur. Both observations are indicative for structural changes in the local environment of sodium due to H_2O. The in-situ measurements at the Na L-edge for hydrous albite glass are shown in figure 2. The characteristic features (labeled with a circle) as observed for the ambient XRS spectra are visible in the 25°C and 200°C measurements. Interestingly, strong spectral changes occur during the 400 °C measurement which can be attributed to melting and subsequent crystallization. The results of this experiment impressively exemplify the sensitivity of the Na L and Na K-edges to the water content in the melt.

In the next step, the experimental findings will be confronted with calculations of the XRS spectra on basis of molecular dynamics simulations of the melt which are currently under work.

[1] S.C. Kohn, Mineral. Mag. 64, 389 (2000). [2] F. Farges et al., Geochem. Cosmochim. Acta 65, 1679 (2001). [3] B. Mysen and P. Richet, Silicate Glasses and Melts: Properties and Structure, Elsevier (2005).