



	Experiment title: Structural changes in CaSiO ₃ glass at high pressure by means of X-ray Raman Scattering (XRS)	Experiment number: HC-3775
Beamline: ID20	Date of experiment: from: 20/06/2018 to: 26/06/2018	Date of report: 29/02/2020
Shifts: 18	Local contact(s): Sahle Christoph	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Petitgirard Sylvain*, Bayerisches Geoinstitut, Bayreuth, Germany Spiekermann Georg*, Universitaet Potsdam, Potsdam, Germany Albers Christian*, Technische Universitaet Dortmund, Dortmund, Germany Sakrowski Robin*, Technische Universitaet Dortmund, Dortmund, Germany Sternemann Christian*, Technische Universitaet Dortmund, Dortmund, Germany Wilke Max*, Universitaet Potsdam, Potsdam, Germany		

Report:

Scientific Background

Knowledge of the density and structure of silicate melts is of great importance to model fate of a magma ocean that could form in the early Earth mantle. To understand the crystallization sequence and product of fractional crystallisation and their fate it is important to measure the behaviour and properties of multi-component melts in the deep Earth. In particular, it is relevant to look at the different end-members to characterise the effect of individual elements in such processes.

Among the compositions of interest for the Earth's interior, CaSiO₃ is of particular importance. Indeed, the CaSiO₃ solid (or Ca-Perovskite) is the third most abundant mineral in the Earth's lower mantle after bridgmanite (MgFeSiO₃) and magnesowustite (Mg,Fe)O. From experimental data on melting relationship, Ca-perovskite is the first one to crystalize from a magma ocean. Thus the CaSiO₃ component of magma is of great importance to understand magma crystallization and crystal settlements in such contest. However, so far, CaSiO₃ glass under high pressure has been investigated with XRS only at the Ca K-edge and only up to 20 GPa []. This is insufficient for a comprehensive investigation of important structural changes in silicate glasses under compression.

Experimental procedure

The CaSiO₃ glass was synthetized using an aerodynamic levitation set-up coupled with a CO₂ laser at the CEMThi lab in Orleans. The glass was grinded and loaded in BX90 cells equipped with miniature diamonds. We collected the absorption spectra for the three different edges of the sample: Si L-edge, Ca L-edge and O K-edge up to 60 GPa.

Preliminary results

Here, we present the preliminary results for the Ca L-edge up to 60 GPa (Figure-1). For the first time we collected data on three different edges at the same time and beyond 20 GPa for Ca L-edge with an energy resolution of 0.7 eV. From the analysis of the Ca L-edge we observe a smooth decrease with pressure up to 60 GPa and a sudden change just beyond 60 GPa. We need to measure more data point at higher pressure to characterise and confirm this change most probably related to a coordination evolution in the glass.

To understand the compaction mechanism of the amorphous phase relative to the crystalline phase, we will also measure the reference crystal that show the main form of coordination at ambient conditions but also under pressure to follow their absorption edge features and compare with the amorphous phase.

Our XRS data collected so far will be compared with calculations utilizing the OCEAN code on basis of MD simulations and will shade a new light on the structural changes that occur in amorphous silicate networks at high pressure.

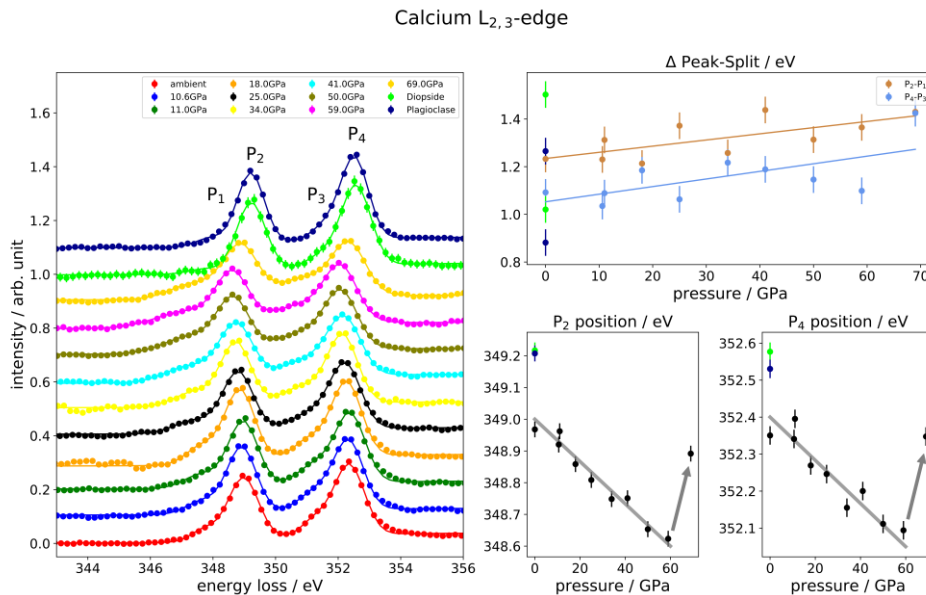


Figure 1. Results for the Ca L_{2,3} edge. On the left side, collected spectra of the amorphous phase under pressure and few reference crystals. Right side, data evaluation with on top the splitting between the two main peak and bottom the evolution of the peak position as a function of pressure.