Experimental report

14/02/2020

Proposal:	**6-05-1001**	**Council:**	10/2018
Title:	Pressure-driven transformation of the Al coordination environment in oxide glass		
Research area:	Materials		

This proposal is a resubmission of 6-05-996

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Samples: (CaO)x(Al2O3)x(SiO2)(1-2x), x = 0.2, 0.3

Instrument	Requested days	Allocated days	From	To
D4	6	6	18/09/2019	25/09/2019

Abstract:

In situ high-pressure neutron diffraction will be used to investigate the pressure-induced transformation of the Al coordination environment in the prototypical aluminosilicate glass-forming system CaO-MgO-Al2O3-SiO2 (CMAS) at pressures up to 8 GPa. Aluminium is an essential component in commercial display glass, where pressures in the gigapascal regime are easily generated by sharp-contact loading, and it is an abundant element in magma-related glasses such as those from the CMAS system. The pressure-induced conversion of tetrahedral AlO4 units into higher coordinated structural motifs will change the glass structure and associated material properties. It is therefore important to measure these changes by in situ neutron diffraction in order to aid in the development of realistic models for, e.g., crack formation and propagation in display glass, and the behaviour of magma-related materials under load.

Pressure-driven transformation of the Al coordination environment in oxide glass

The structures of glassy $(CaO)_{0.2}(Al_2O_3)_{0.2}(SiO_2)_{0.6}$ and $(CaO)_{0.25}(Al_2O_3)_{0.25}(SiO_2)_{0.5}$ were measured with pressure increasing from ambient to 8.2 GPa using a Paris-Edinburgh press mounted on D4c. The structure of these materials was also measured on recovery of the glass from 8.2 GPa to ambient conditions. The measured total structure factors $F(q)$ for glassy $(CaO)_{0.2}(Al_2O_3)_{0.2}(SiO_2)_{0.6}$ are shown in Fig. 1, where q is the magnitude of the scattering vector. There is a change to the relative heights of the first-sharp diffraction peak at q ~1.70 $Å^{-1}$, which describes the intermediate range order, and the principal peak at q ~2.85 $Å^{-1}$, which originates from the formation of Al and Si polyhedral units [1]. The corresponding real-space information is being used to extract the pressure-driven changes to the Al coordination environment.

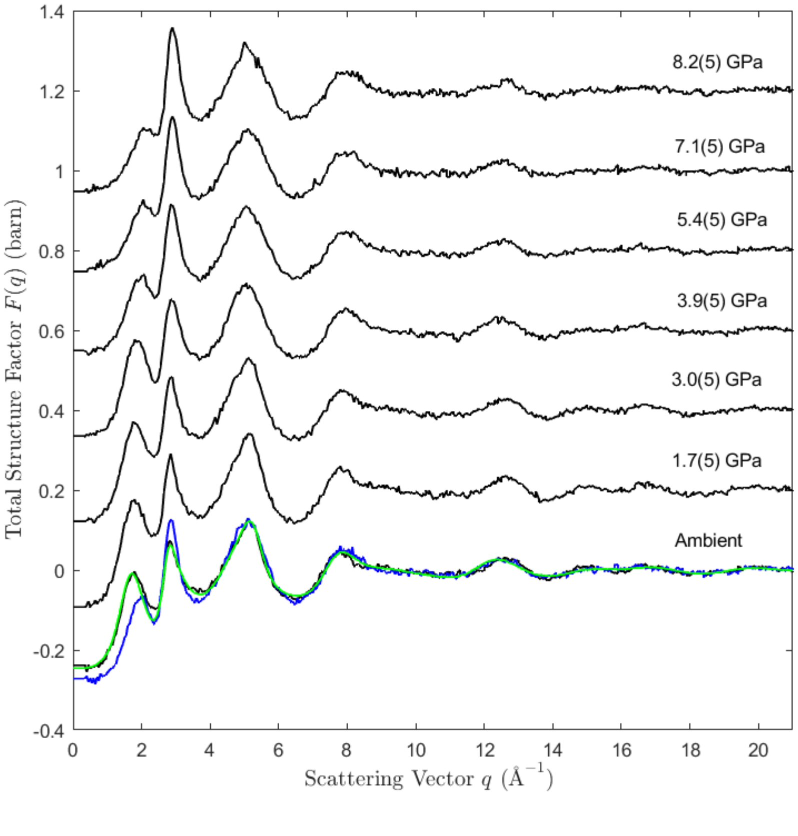

Fig. 1. The neutron total structure factors $F(q)$ for glassy $(CaO)_{0.2}(Al_2O_3)_{0.2}(SiO_2)_{0.6}$ measured using a Paris-Edinburgh press (black curves). Also shown is $F(q)$ measured at ambient for the sample recovered from 8.2 GPa (blue curve) and $F(q)$ measured at ambient for a bulk sample of the as-prepared glass in a vanadium can (green curve).

[1] Zeidler A and Salmon PS 2016 Phys Rev B **93** 214204