Experimental report

30/05/2022

Proposal:	**6-05-1015**	**Council:**	10/2019
Title:	Pressure-driven change to the Mg and Al coordination environments in silicate glass		
Research area:	Materials		

This proposal is a new proposal

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Samples: (MgO)0.25(Al2O3)0.25(SiO2)0.5 with 25Mg and natMg

Instrument	Requested days	Allocated days	From	To
D4	6	6	30/06/2021	07/07/2021

Abstract:

Mg and Al are two essential elements in materials that range from commercial display glass to the glasses used as models for dry basaltic melts. There is great interest in the structural response of these glasses to pressure, but little is known from in situ experiments. We will address this issue by using neutron diffraction to investigate a prototypical magnesium aluminosilicate glass at pressures up to 8 GPa. Here, the method of Mg isotope substitution will be employed to give site-specific information on both the Mg and Al coordination environments. The results will reveal, for the first time, the nature of the structural changes that take place. They will then be used to test the validity of atomic interaction models that are being developed for molecular dynamics simulations. By establishing the correct theoretical ingredients for reproducing the experimental results, these models will become transferable. This capability will enable accurate predictions for the pressure-dependent structure and properties of materials with different compositions.

Structure of lithium silicate glass by isotope substitution

The structure of the lithium silicate glasses $(Li_2O)_x(SiO_2)_{1-x}$ with $x = 0.29$, 0.33 and 0.36 was measured using neutron diffraction with ^{0}Li and ^{7}Li isotope substitution, where the zero denotes a null scattering length. For each composition, the first order difference function $\Delta D_{\mathrm{Li}}(r) = {}^0D(r) - {}^7D(r)$ was successfully obtained from the total pair-distribution functions ${}^0D(r)$ and ${}^7D(r)$ measured for the samples of $(^0Li_2O)_x(SiO_2)_{1-x}$ and $(^7Li_2O)_x(SiO_2)_{1-x}$, respectively. The $\Delta D_{\mathrm{Li}}(r)$ functions reveal the nearest-neighbour coordination environment of the mobile Li^+ ions. The results are being combined with those from high-energy x-ray diffraction and ^{29}Si magic angle spinning NMR experiments to build a complete picture of the glass network and find the effect of its rigidity on the ion mobility.

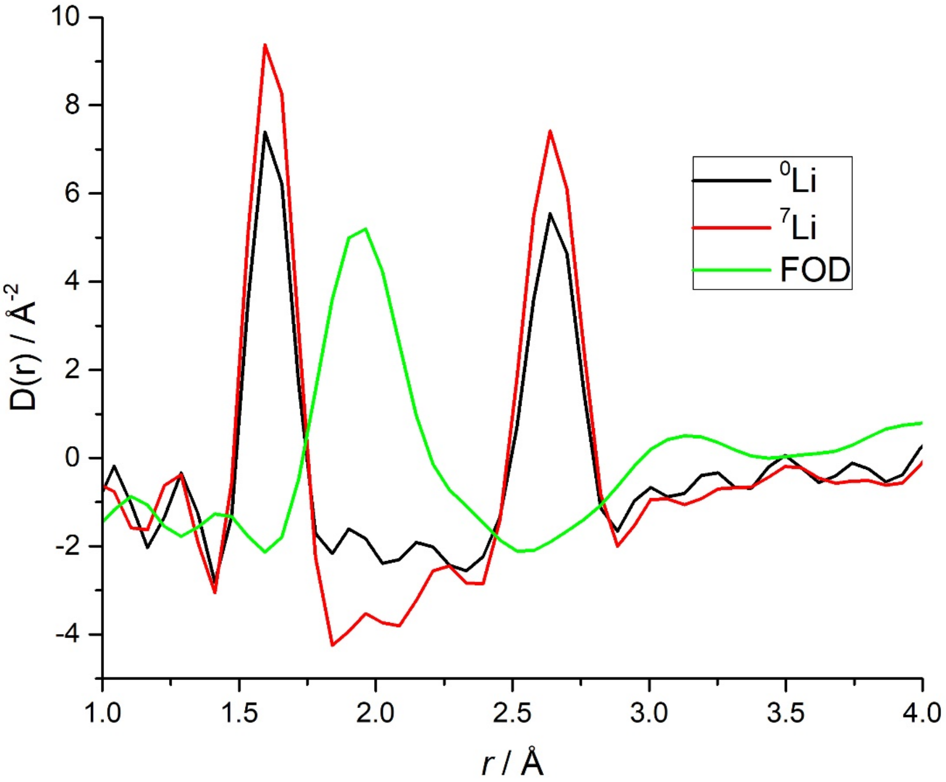

Fig. 1. The total pair-distribution functions ${}^0D(r)$ and ${}^7D(r)$ measured for samples of glassy $(^0Li_2O)_{1/3}(SiO_2)_{2/3}$ and $(^7Li_2O)_{1/3}(SiO_2)_{2/3}$, respectively, and the first order difference (FOD) function $\Delta D_{\mathrm{Li}}(r) = {}^0D(r) - {}^7D(r)$.