Experimental report

15/09/2024

Proposal: 6-05-1054 **Council:** 10/2022

Title: Unravelling the chameleon-like nature of Mg in silicate glasses

Research area: Materials

This proposal is a new proposal

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Samples: A2O·MgO·2SiO2, 1.5A2O·MgO·2.5SiO2 and 2A2O·MgO·3SiO2, A = Na or K,

Instrument	Requested days	Allocated days	From	To
D4	2	2	14/06/2023	16/06/2023

Abstract:

The coordination environment of magnesium in the silicate glasses A2O·MgO·2SiO2, 1.5A2O·MgO·2.5SiO2 and 2A2O·MgO·3SiO2, where A = Na or K, will be measured by neutron diffraction. The objective is to stabilise magnesium in a four-fold coordination environment by increasing the Na2O or K2O to MgO ratio. The results will (i) reveal the influence of the glass composition and alkali cation field strength on the Mg coordination environment; (ii) test whether four-fold coordinated magnesium plays a predominantly network-forming or network-modifying role in silicate glasses; and (iii) guide in the interpretation of 25Mg solid-state nuclear magnetic resonance experiments. Magnesium is a key component in amorphous silicates that have widespread applications ranging from commercial display glass to the models for magmatic materials in the geosciences.

Unravelling the chameleon-like nature of Mg in silicate glasses

The structure of the metasilicate composition glasses $(A_2O)_x(MgO)_{0.5-x}(SiO_2)_{0.5}$, with A = Na or K and x = 1/4 or x = 1/3, was investigated by neutron diffraction. The results were combined with those from high-energy x-ray diffraction to obtain the Mg coordination number and the distribution of Mg-O bond distances. Figure 1 shows the fitted total pair-distribution functions $D'(r)$. It is found that the alkali ions promote the formation of four-coordinated Mg^{2+} species. The results are being used to help interpret a new set of ^{25}Mg NMR experiments on these glassy materials.

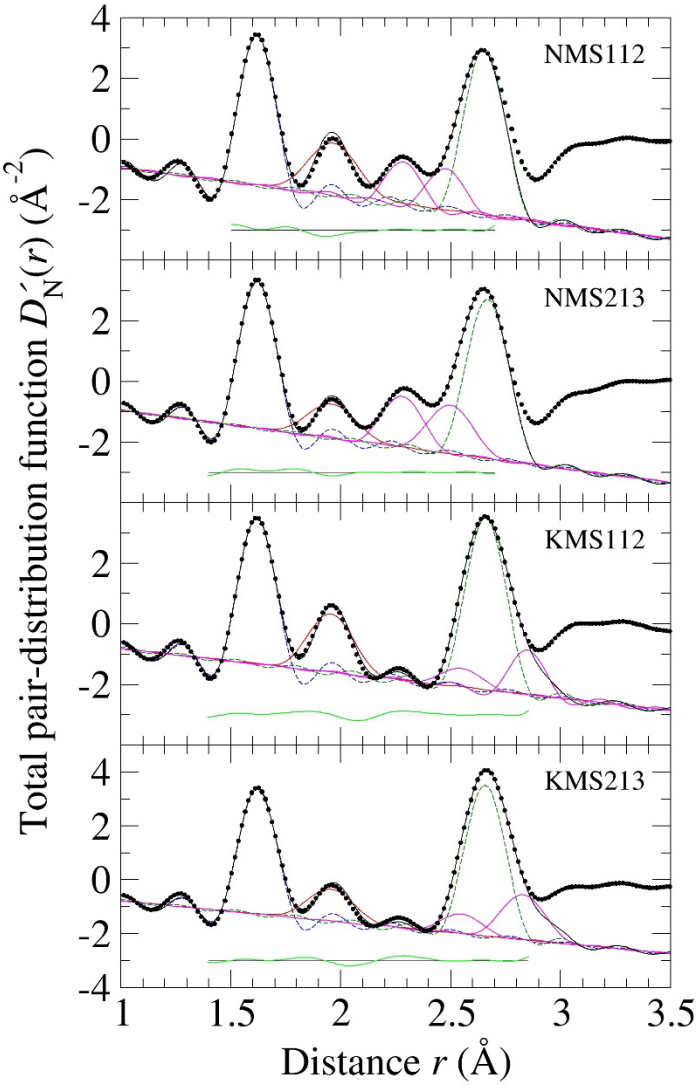

Figure 1. The fitted $D'(r)$ functions obtained from neutron diffraction where N, K, M and S denote Na_2O, K_2O, MgO and SiO_2, respectively, and the numbers refer to the ratios of these oxides.