Experimental report

14/02/2020

Proposal: 6-05-982 **Council:** 10/2016

Title: Structure of Permanently DensifiedGeO2 Glass

Research area: Materials

This proposal is a new proposal

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Samples: Four GeO2 samples with 70Ge isotopes
Four GeO2 samples with 73Ge isotopes

Instrument	Requested days	Allocated days	From	To
D4	5	5	09/09/2019	14/09/2019

Abstract:

GeO2 is a prototypical network-forming glass that can be processed under high pressure and temperature conditions to give a permanently densified material, with a density that can be more than 20% greater than the density of the pristine glass prepared at ambient pressure. This low- to high-density amorphous transition has a profound effect on the material properties, but little is known about the accompanying structural changes and the associated mechanisms of network collapse. We will address this problem by using neutron diffraction with Ge isotope substitution to measure the structures of carefully chosen permanently densified GeO2 glasses. The results will be combined with those obtained from high-energy x-ray diffraction to build realistic structural models by refining molecular dynamics configurations via the reverse Monte Carlo method. Hence, we will elucidate the mechanisms of topological change.

Structure of permanently densified GeO_2 glass

The structures of as-prepared and densified GeO_2 glass were measured by neutron diffraction. The densified samples were prepared by compression at a temperature around 650 K and pressure of 4 or 8 GPa. The maximum densification was ~17%, and the sample size was small at ~50 mg. The measured total structure factors $F(q)$ 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 ~1.5 Å^{-1} and the principal peak at q ~2.66 Å^{-1}. These peaks originate from length scales that are commensurate with the organisation of tetrahedral GeO_4 motifs on an intermediate length scale and with the size of these GeO_4 motifs, respectively [1]. The diffraction results therefore indicate structural changes on both length scales. The corresponding total pair-distribution functions $G(r)$ are shown in Fig. 2, where r is a real-space distance [1]. Here, there is a change to the relative heights of the peaks at r ~2.83 Å and r ~3.16 Å that originate from intra-tetrahedral O-O distances and inter-tetrahedral Ge-Ge distances, respectively [2].

Complementary x-ray diffraction patterns have also been measured at SPring-8. The combined neutron and x-ray diffraction data sets are being used to construct realistic structural models to elucidate the mechanisms of pressure-induced deformation.

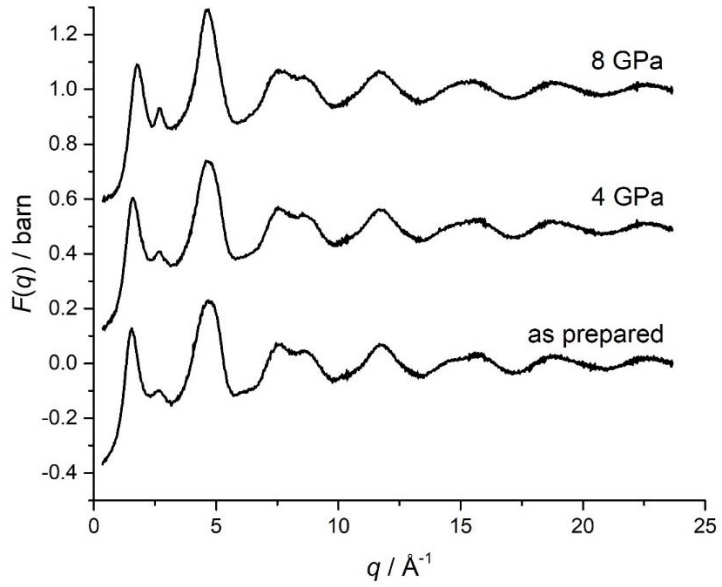

Fig. 1. The measured neutron total structure factors $F(q)$ for as-prepared and densified GeO_2 glass.

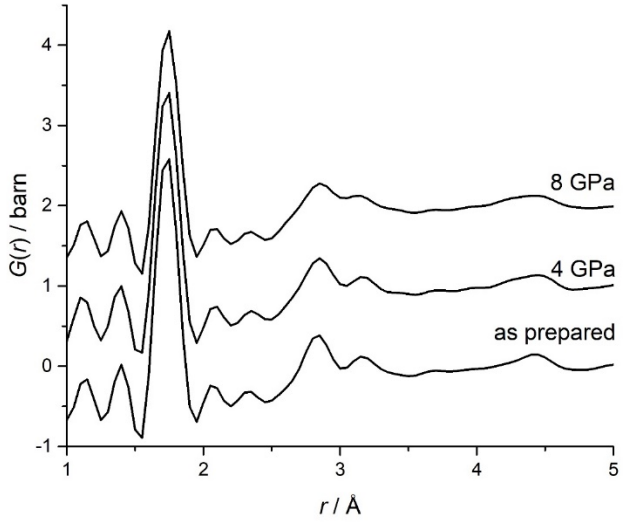

Fig. 2. The neutron total pair-distribution functions $G(r)$ for as-prepared and densified GeO_2 glass, obtained by Fourier transforming the $F(q)$ functions shown in Fig. 1.

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

[2] Salmon PS et al. 2007 J Phys: Condens Matter **19** 415110