The Influence of Modifier Cations on the Structure of Network Glasses

A. C. Hannon\textsuperscript{1}, O. L. G. Alderman\textsuperscript{2}, E. R. Barney\textsuperscript{3}, D. Holland\textsuperscript{2}, U. Hoppe\textsuperscript{4}, S. Feller\textsuperscript{5}, A. J. Vitale\textsuperscript{5}, G. Lehr\textsuperscript{5}, L. Koudelka\textsuperscript{6}, I. Rösslerová\textsuperscript{6}, M. v. Zimmermann\textsuperscript{7}, and A. Watenphul\textsuperscript{7}

\textsuperscript{1}ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, UK
\textsuperscript{2}Physics Department, University of Warwick, Coventry, CV4 7AL, UK
\textsuperscript{3}University of Nottingham, Novel Photonic Glasses Research Group, Electrical Systems & Optics Research Division, Faculty of Engineering, Nottingham NG7 2RD, UK
\textsuperscript{4}Department of Physics, Rostock University, Universitätsplatz 3, D-18051 Rostock, Germany
\textsuperscript{5}Physics Department, Coe College, Cedar Rapids, IA 52402, USA
\textsuperscript{6}Dept of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, 532 10 Pardubice, Czech Republic
\textsuperscript{7}Deutsches Synchrotronsstrahlungslabor, HASYLAB at DESY, Notkestrasse 85, D-22603 Hamburg, Germany

A wide-ranging study of the influence of modifier cations on the structure of network glasses has been performed, using the excellent high energy X-ray diffractometer BW5.

The use of high energy synchrotron x-rays is necessary for highly absorbing materials, such as lead containing glasses. The monochromator of beamline BW5 was tuned to pass x-rays of 85 keV, allowing for a huge reduction of the absorption cross-section of the lead-containing glasses, compared to that at typical laboratory x-ray source energies, whilst also avoiding fluorescence excitation above the 88 keV Pb K-edge. The precise x-ray wavelength was calibrated using a LaB\textsubscript{6} standard. High quality data were collected for a large number of glass powders, mostly in 1.5 mm diameter thin-walled quartz glass capillaries. Data were also obtained for an empty capillary and a background. A Ge-detector was stepped over the angular range 0.5 < 2\theta < 32.0\degree, giving access to momentum transfers of magnitude up to 23.8 Å\textsuperscript{-1}. Different attenuators were used over different sections of the angular range to avoid detector saturation on account of the natural form-factor dependence of the scattering. Raw scattering data were screened for bad points, normalised to the monitor counts, scaled according to the attenuator used, and corrected for detector dead-time and the experimental geometry prior to being further corrected and reduced using the GudrunX [1] software. GudrunX was used to correct for polarisation, Compton scattering, multiple scattering and attenuation in both sample and capillary, as well as to subtract the self-scattering, background and capillary contribution to the data. No fluorescence correction was necessary due to the choice of incident x-ray energy. Normalisation by the Krogh-Moe/Norman method yields scattering data on an absolute scale. The software performs the normalisation and corrections iteratively to allow for scaling by a calibration factor accounting for unknown detector efficiencies. Suitable Fourier transforms of the extracted distinct scattering, \(i(Q)\), yielded the real-space correlation functions \(T(r)\).

The glass forming systems that were studied include the following: PbO-SiO\textsubscript{2}, PbO-GeO\textsubscript{2}, PbO-Ga\textsubscript{2}O\textsubscript{3}, PbO-MoO\textsubscript{3}-P\textsubscript{2}O\textsubscript{5}, PbO-WO\textsubscript{3}-P\textsubscript{2}O\textsubscript{5}, ZnO-WO\textsubscript{3}-P\textsubscript{2}O\textsubscript{5}, Tl\textsubscript{2}O-GeO\textsubscript{2}, CaO-GeO\textsubscript{2}, Cs\textsubscript{2}O-GeO\textsubscript{2}.

The first paper on this work has just been accepted for publication [2]. The combination of results from high energy diffraction with results from time-of-flight neutron diffraction has proved very powerful. The graphical abstract of this paper is given below.
References


Graphical abstract of reference [2]…

Lone-Pair Distribution and Plumbite Network Formation in High Lead Silicate Glass, 80PbO.20SiO₂

Oliver L. G. Alderman, Alex C. Hannon, Diane Holland, Steve Feller, Gloria Lehr, Adam Vitale, Uwe Hoppe, Martin von Zimmerman, Anke Watenphul

The structure of a lead silicate glass, 80PbO.20SiO₂, with extremely high lead content is studied by high energy x-ray and neutron diffraction, and empirical structural modelling, in order to reveal details of the plumbite based glass network and electron lone-pair distribution.