The Influence of Modifier Cations on the Structure of Network Glasses

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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_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 $0.5 < 2\theta < 32.0^o$, giving access to momentum transfers of magnitude up to 23.8 $Å^{-1}$. 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: $PbO-SiO_2$, $PbO-GeO_2$, $PbO-Ga_2O_3$, $PbO-MoO_3-P_2O_5$, PbO-WO3-P_2O_5, ZnO-WO3-P_2O_5, Tl_2O-GeO_2, $CaO-GeO_2$, Cs_2O-GeO_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

1. *A.K. Soper, E.R. Barney, Extracting the pair distribution function from white-beam X-ray total scattering data, J. Appl. Cryst. 44(2011)714.*
2. *O.L.G. Alderman, A.C. Hannon, D. Holland, S. Feller, G. Lehr, A. Vitale, U. Hoppe, M. v. Zimmerman, A. Watenphul, Lone-pair distribution and plumbite network formation in high lead silicate glass, 80PbO.20SiO$_2$, Phys. Chem. Chem. Phys. (2013) in press.*

Graphical abstract of reference [2]…

Lone-Pair Distribution and Plumbite Network Formation in High Lead Silicate Glass, 80PbO.20SiO$_2$

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The structure of a lead silicate glass, 80PbO.20SiO$_2$, 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.