Local Structure of xAs_2S_3-$(1-x)Ag_2S$ Glasses (x = 0,0.4,0.6)

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Glasses of the As_2S_3-AgS_2 family have a unique combination of properties that make them useful as fast ion conductors. The conductivity has been found to change nonlinearly with Ag content, and a hypothesis has been put forward that the nonlinearity reflects the change in the distribution of Ag in the As_2S_3 glassy matrix with increasing x. However, no experimental evidence has been advanced so far. This prompted us to investigate the atomic ordering in three glasses with composition xAs_2S_3-$(1-x)Ag_2S$ glasses (x=0,0.4,0.6). The experiments were carried out at the SRI-CAT 1-ID beamline with the use of x-rays of energy 80.6 keV. The experimental structure factors, S(Q), are shown in Fig. 1 and the corresponding atomic pair distribution functions (PDF), g(r), in Fig. 2. As can be seen, the experimental structure factors extend up to 30 $Å^{-1}$, making it possible to resolve the contributions of As-S, Ag-S and Ag-Ag atomic pairs to the experimental atomic PDFs, as shown in Fig. 2. The individual peaks in the experimental PDFs have been fit with Gaussians, and the corresponding coordination numbers and distances determined. It has been found that both As and Ag maintain a rather uniform coordination sphere of approximately 3 and 2.5 sulfur atoms, respectively, for all values of x. The Ag-Ag coordination number, however, increases with increasing x from 1.5 for x=0.4 to 2.2 for x=0.6. This shows that the distribution of Ag atoms in the As_2S_3 matrix is far from random: it changes from a single-chain to a cross-linked-chain/sheet-like with increasing x. Further analyses are under away; the results will be reported elsewhere.

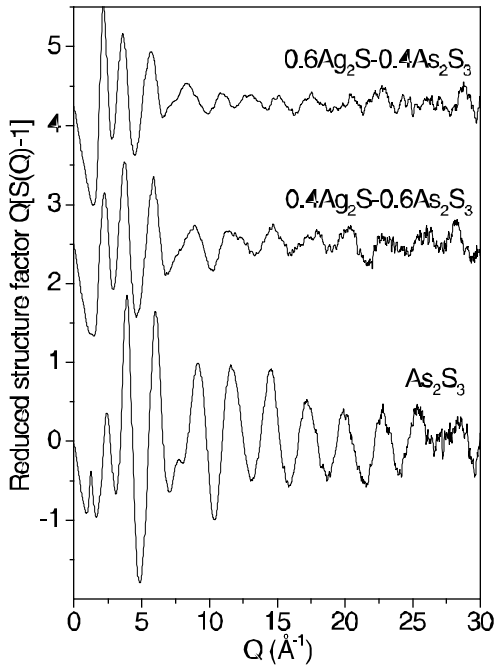

FIG. 1. Experimental structure factors for As-S-Ag glasses.

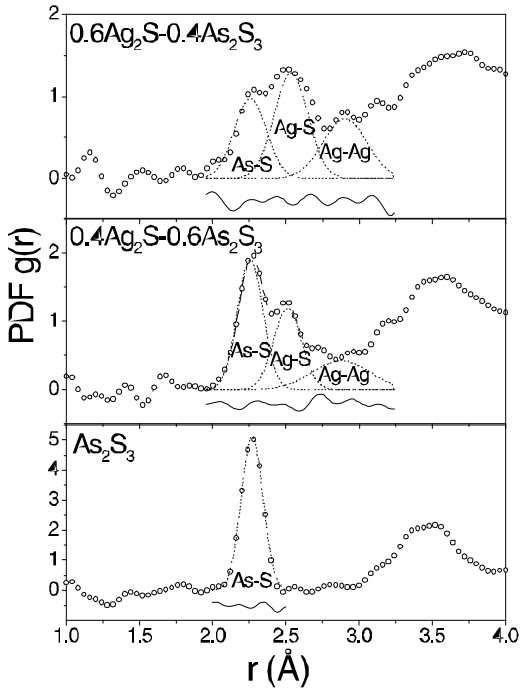

FIG. 2. Gaussian fit to the first peaks in the PDFs, $g(r) = \rho(r)/\rho_o$, for As-S-Ag glasses. Experimental data: symbols; individual Gaussians: broken lines; residual difference: full lines (bottom of each panel). Peaks are labeled with the corresponding atomic pairs.

Acknowledgments

Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Basic Energy Sciences, Office of Science, under Contract No. W-31-109-ENG-38. The work was supported by NSF Grant No. CHE-9903706.