Transport and structural properties of silver bromide doped chalcogenide glasses

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Abstract

Silver-halide doped glasses which show high Ag+ **ionic conductivity** at room temperature are suitable materials for the sensors' development. They are also suitable model materials to investigate the structural origin of conductivity changes in fast ionic conducting glasses. To this end, the quasi-binary AgBr-As2S3 glass system has been synthesized and characterized. X-ray diffraction (XRD) shows that the glass-forming range for the (AgBr)x(As2S3)1–x compositions varies between $0.0 \leq x \leq 0.5$. The glass transition and crystallization temperatures (Tg and Tx), density (d), and the total conductivity (σ) have been measured for all the samples ($0.0 \leq x \leq 0.6$). The ionic conductivity increases by 13 orders of magnitude with increasing the Ag atomic concentration ([Ag]max = 18.75 at.%) and two distinctly ion transport regimes, above the percolation threshold at xc, are distinguished. Glass-phase separation occurs over a wide range of Ag content, i.e. $7.3 \leq$ [Ag] $\leq$ 18.75 at.% and is confirmed by both thermal and SEM studies. Raman spectroscopy, high-energy X-ray diffraction and neutron diffraction experiments have been carried out to elucidate the structural aspects at both short- and intermediate-range order. The results suggest that the dominant structural entities in **AgBr-poor** glasses ($x \leq$ 0.1-0.2) are isolated edge-sharing **ES-Ag2Br2S4/2 dimers** distributed more or less randomly in the corner-sharing **CS-AsS3/2** host network. Meanwhile, for the **AgBr-rich** glasses ($0.2 < x \leq 0.4$), the silver structural entities are formed by **tetrahedral** chains (AgBr2/2S2/2)n. Further increase of the AgBr content, thus for the **high-AgBr rich** glasses (x 0.4), new **AgBr3/3S1/2** mixed tetrahedra appear giving rise either to 2D layers or 3D sub-network.

Keywords: Chalcohalide glasses, Electrical properties, Raman spectroscopy, High energy Xray diffraction, Neutron diffarction

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