Local- and intermediate-range structures of room-temperature superionic Ag-GeSe3 glasses

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Abstract

Recently, much attention has been paid for investigating superionic conductors, which can be used as solid electrolytes for solid-state batteries. Superionic glasses with a high ionic conductivity of 10-6-10-2 S/cm are promising materials for such applications. It is well-known that superionic behavior in Ag containing chalcogenide glasses is observed at room temperature, such as for Ag-GeSe3 alloys, in contrast to high temperatures needed in crystalline superionic conductors.
To investigate the ion conduction mechanism in Ag ion conducting glasses Agx(GeSe3)1-x with x = 0.15 [1], 0.28, 0.33 and 0.50 [2] from the local structural point of view, we carried out anomalous x-ray scattering (AXS) experiments near the x-ray energies close to the Ge, Se, and Ag K absorption edges. Details of the experiment and analysis are given elsewhere [3]. This method can provide insight into the structural properties enabling the effect of superionic conductivity for compositions with $x >$ 0.30 in the amorphous phase. The experimental results were analyzed with reverse Monte Carlo (RMC) modeling, providing the partial structure factors and the corresponding partial pair-distribution functions. Evidence is found for a high level of intermediate range order for low silver concentrations, whereas the superionic conducting phase formed at high silver concentrations is characterized by cluster-like configurations of Ag atoms on a nanometer scale.

In the presentation, we will show full sets of partial structural information obtained in combination with Ge, Se, and Ag K edge AXS data and RMC modeling, and explain the structural information on the ion conduction mechanism in Agx(GeSe3)1-x glasses by also citing the previous works [1-3].

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