

Local structures and electrochemical properties of $\text{Li}_2\text{S}\text{--}\text{GeS}_2$ superionic glasses

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It is well known that $\text{Li}_2\text{S}\text{--}\text{GeS}_2$ glasses, which can be synthesized by rapid quenching and mechanical alloying (MA), show a high ionic conductivity in the order of 10^{-4} S/cm at room temperature (RT) [1, 2]. In order to understand the conduction mechanism for lithium ions in solids, the detailed information on the atomic structures requires. In this work, we performed reverse Monte Carlo (RMC) modeling with neutron data to get the three-dimensional atom locations of each element for the $\text{Li}_2\text{S}\text{--}\text{GeS}_2$ glasses.

$(^7\text{Li}_2\text{S})_x(\text{GeS}_2)_{100-x}$ glasses ($x = 40, 50, 60,$ and 67) were synthesized by MA of $^7\text{Li}_2\text{S}$ and GeS_2 powders in the appropriate molar proportions. The samples were characterized using X-ray diffraction (XRD) with $\text{Cu-K}\alpha$ radiation and differential scanning calorimetry (DSC) at the temperatures between RT to 520°C . The electrical conductivities σ were measured by the ac impedance method. We performed time-of-flight (TOF) neutron diffraction experiments with the total scattering spectrometer NOVA at the BL21 beam line of the Materials and Life Science Experimental Facility (MLF), Japan Proton Accelerator Research Complex (J-PARC).

In the conduction measurements σ increased with increasing the Li content, particularly σ for $(^7\text{Li}_2\text{S})_{60}(\text{GeS}_2)_{40}$ glass showed $\sim 10^{-4}$ S/cm at RT. Figure 1 shows the structure factor, $S(Q)$, for $(^7\text{Li}_2\text{S})_{40}(\text{GeS}_2)_{60}$ glass at RT. In the presentation, we will show the three-dimensional structures of $(^7\text{Li}_2\text{S})_x(\text{GeS}_2)_{100-x}$ glasses ($x = 40, 50, 60,$ and 67) obtained from RMC modeling, together with their XRD, DSC, and electrical conductivity data.

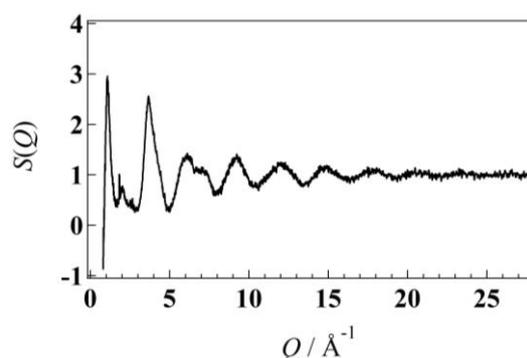


Fig. 1. Structure factor, $S(Q)$, for $(^7\text{Li}_2\text{S})_{40}(\text{GeS}_2)_{60}$ glass obtained from the time-of-flight (TOF) neutron diffraction experiment.

References

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