Structure and conductivity of Na-P-S superionic conducting glasses studied by neutron and X-ray diffraction

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All-solid-state sodium batteries with excellent safety have attracted much attention as one of candidates of post-lithium ion batteries because of great abundance and low cost of sodium. Recently, it was found that Na_3PS_4 glass-ceramic solid electrolyte synthesized by annealing of $(Na_2S)_{75}(P_2S_5)_{25}$ glass has a conductivity in the order of 10^{-4} Scm^{-1} at room temperature [1].

In this paper, we report results of structural analysis based on neutron and X-ray diffraction for $(Na_2S)_x(P_2S_5)_{100-x}$ superionic conducting glasses (x = 50, 60, 67, 70). Neutron and synchrotron X-ray diffraction experiments were carried out with the high intensity total diffractometer (NOVA) at the BL21 beam line of MLF in J-PARC and with a horizontal two-axis diffractometer at the BL04B2 beam line in SPring-8, respectively. Furthermore, reverse Monte Carlo (RMC) modeling based on neutron and X-ray structural factors, $S(Q)$, was performed to derive three-dimensional atomic configurations of $(Na_2S)_x(P_2S_5)_{100-x}$ glasses. Figure 1 shows experimental $S(Q)$s and calculated $S(Q)$s by the RMC modeling for $(Na_2S)_{50}(P_2S_5)_{50}$ glass.

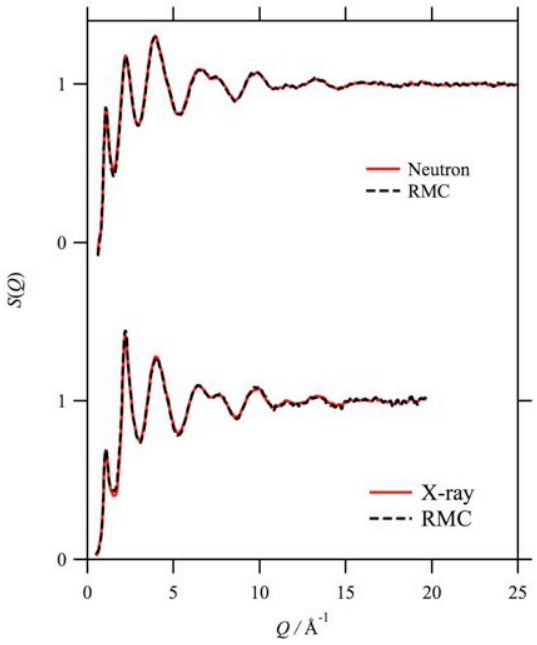

Fig. 1 Neutron and X-ray structure factors, $S(Q)$, of $(Na_2S)_{50}(P_2S_5)_{50}$ glass. Red lines were experimental $S(Q)$s and black broken lines were calculated $S(Q)$s by the RMC.

In the presentation, we will show results of an analysis focused on "void distribution" in the atomic configurations and discuss about conduction pathways of Na^+ ions for the Na-P-S system.

[1] A. Hayashi, K. Noi, A. Sakuda, M. Tatsumisago, Nat. commun., **3**, 856:1-5 (2012).