MLF Experimental Report	提出日 Date of Report 11 May, 2013
課題番号 Project No. 2012B0199 実験課題名 Title of experiment Neutron diffraction studies of AgI-doped As-chalcogenide glasses 実験責任者名 Name of principal investigator Takeshi Usuki 所属 Affiliation Yamagata University	装置責任者 Name of responsible person Toshiya Otomo 装置名 Name of Instrument/（BL No.） BL-21 (NOVA) 実施日 Date of Experiment 11 -12 March, 2013 (24hr)

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。（適宜、図表添付のこと）
Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

$(AgI)_x(As_2Te_3)_{1-x}$ (x = 0, 0.2, 0.4, 0.65)
glassy samples

2. 実験方法及び結果（実験がうまくいかなかった場合、その理由を記述してください。）
Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

The time of flight measurements were made at room temperature using a standard vanadium container for $(AgI)_x(As_2Te_3)_{1-x}$ (x = 0, 0.2, 0.4, 0.65). Figure 1 shows structure factors $S(Q)$, where Q is scattering vector magnitude, obtained by the neutron diffraction experiments for both parent As_2Te_3 and 65 mol% AgI-doped glasses. Diffraction patterns at high Q region for AgI doped and undoped glasses change little, since these depend mostly on the short-range covalent bonding of host As_2Se_3 glass. On the other hand, it can be seen that there are large differences at low Q region in the $S(Q)$, especially at Q < 12 Å^{-1}. A pre-peak at 1.25 Å^{-1} in parent As_2Te_3 glass, which is considered to be an indication of intermediate-range ordering (IRO) constructed by the $As(Te_{1/2})_3$ helical chains, becomes weaker with the incorporation of AgI but remains clearly in the highly AgI-doped glasses.

Figure 2 gives pair distribution functions $g(r)$ for the present glasses. A well-defined first peak is found at 2.62 Å in the host As_2Te_3 glass. With addition of AgI, the first and second peaks shift toward higher r side.

2. 実験方法及び結果（つづき） Experimental method and results (continued)

These changes correspond to the formation of the local atomic ordering constructed by Ag and I atoms. In order to clarify such structure changes, we try to obtain quasi-partial pair distribution function of AgI-doped glass, $\Delta g(r)$, in which the As-Te pair correlation can be eliminated by the perfect cancellation of such correlation, using parent As_2Te_3 data. Figure 2 includes $\Delta g(r)$ for 65 mol% AgI-doped glasses. Indeed, positions of first and second peaks in $\Delta g(r)$ agree well with nearest neighbour Ag-I and I-I distances in crystalline AgI, suggesting that the environmental structure around mobile Ag ions in the present glasses seems to be similar to that in crystalline AgI. The present analysis for the short-range structure around As and mobile Ag atoms allows us to predict that the structure model for AgI-As_2Te_3 glasses is proposed to be a pseudo-binary mixture of the $As(Te_{1/2})_3$ network matrix and AgI-related conduction pathways. It would be responsible for the high mobility and diffusivity of mobile Ag ions in the highly doped glass systems.

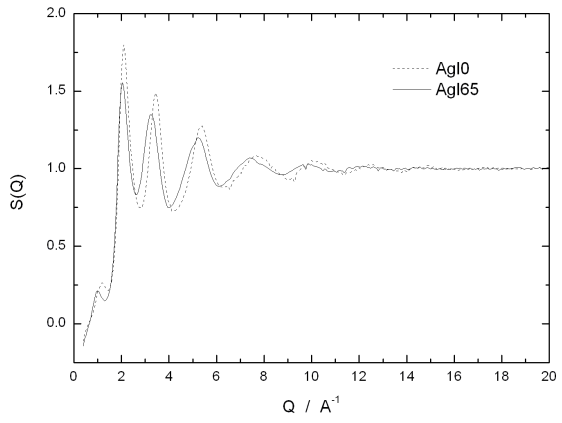

Figure 1 Total structure factor for parent and AgI-doped glasses.

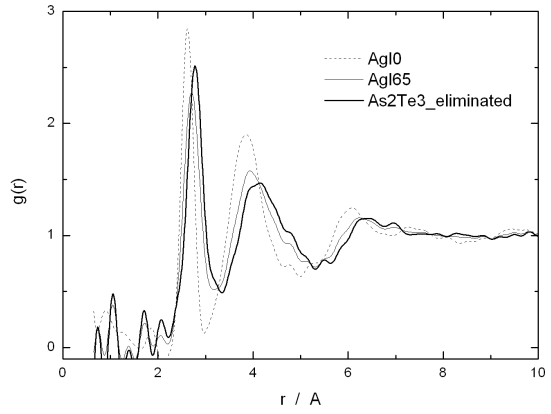

Figure 1 Total pair distribution function for parent and AgI-doped glasses.