MLF Experimental Report	提出日 Date of Report 01 May 2014
課題番号 Project No. 2013A0032 実験課題名 Title of experiment Partial structures of Zr-based metallic glasses 実験責任者名 Name of principal investigator Shinya Hosokawa 所属 Affiliation Kumamoto University	装置責任者 Name of responsible person Prof. T. Otomo 装置名 Name of Instrument/(BL No.) NOVA/BL-21 実施日 Date of Experiment 1-3 May 2013

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.

Sample 1: $Zr_{63}Cu_{25}Al_{12}$ bulk glass, rod

Sample 2: $Zr_{63}Ni_{25}Al_{12}$ bulk glass, rod

Sample 3: $Zr_{63}Ni_{12.5}Cu_{12.5}Al_{12}$ bulk glass, rod

Sample 4: $Zr_{50}Cu_{50}$ glass, ribbon

Sample 5: $Zr_{45}Cu_{45}Ag_{10}$ glass, ribbon

Sample 6: $Zr_{40}Cu_{40}Ag_{20}$ glass, ribbon

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.

In the last two decades, bulk metallic glasses (BMGs) with distinct glass transitions have been discovered in various multi-component metallic alloys, which show extremely excellent glass-forming abilities (GFA). Among these BMGs, some of the Zr-based alloys in this proposal have excellent critical cooling rate of some K/s, which allows forming massive BMGs with a diameter of more than 10 mm.

To understand the structural origin of such excellent GFAs in these alloys, partial structural investigations are essential. We carried out anomalous x-ray scattering (AXS) experiments on these BMGs at BM02/ESRF and BL13XU/SPring-8 close to the Zr, Ni, Cu, and Ag *K* edges, and the results were analyzed using reverse Monte Carlo (RMC) modeling [1]. To investigate them in more detail, we added neutron diffraction (ND) measurements in this project, where the scattering cross-sections for ND are different from those for x-ray diffraction (XD) and AXS.

The ND measurements were performed using the High Intensity Total Diffractometer (NOVA) installed at BL21 of MLF in J-PARC. The rod or ribbon sample was put into a thin-walled vanadium cylindrical can with a wall thickness of 0.1 mm, an inner diameter of 6 mm, and a length of about 50 mm, and set at the center of the

diffractometer. Total ND structure factors were evaluated from the scattered intensities after correcting background, container scattering, absorption, and multiple scattering, and normalizing to the scattering intensities from a reference sample of a vanadium rod. The RMC calculations were performed using the RMC++ program package [2] with the ND, XD, and AXS data.

In this report, we introduce the typical results on $Zr_{63}Ni_{25}Al_{12}$ BMG [3]. Circles in Fig. 1 show experimental structure factors of Zr and Ni AXS, total XD, and total ND, from top to bottom. As clearly seen in the figure, the Ni AXS has a spectral feature very different from others. Solid curves in Fig. 1 represent the best fits of the RMC modeling. Although the experimental results show very different scattering features from each other, the RMC modeling reproduces well all of the experimental data within the experimental errors.

Figures 2 and 3 respectively show partial pair distribution functions, $g_{ij}(r)$, and partial structure factors, $S_{ij}(Q)$, obtained from the present RMC modeling. The $g_{ij}(r)$ functions exhibit sharp first peaks. The atomic distances of Zr–related partials are in good agreement with the XAFS data [4], and the Zr–Ni distance is much smaller than the average of the Zr–Zr and Ni–Ni distances. As regards the $S_{ij}(Q)$ functions, $S_{ZrZr}(Q)$ resembles that of a typical dense–packed monatomic configuration. The first peak in $S_{ZrNi}(Q)$, however, has a large shoulder at the high Q side, indicating a non–hard–sphere Zr–Ni correlation. Of special interest is that the Ni–related partials have broad prepeaks at about 15 nm^{-1}, and the Ni–Ni partial is the most prominent, indicating the existence of weak intermediate–range correlations around the Ni atoms, in particular, in the Ni–Ni correlations. $S_{AlAl}(Q)$ shows a large increase in the small Q range. This feature resembles well the initial spectrum of random configuration of the RMC modeling. Thus, the reliability of the Al–Al correlations is still doubtful even after adding the ND data in the RMC modeling due to the very small weighting factors of A–Al in all of the experimental data.

[1] For example, S. Hosokawa et al., *Int. J. Mater. Res.* **103**, 1108 (2012).
[2] O. Gereben et al., *J. Optelectr. Adv. Mater.* **9**, 3021 (2007).
[3] S. Hosokawa et al., *J. Phys.: Conf. Ser.* **502**, 012023 (2014).
[4] S. Sato et al., *Mater. Trans.* **46**, 2893 (2005).

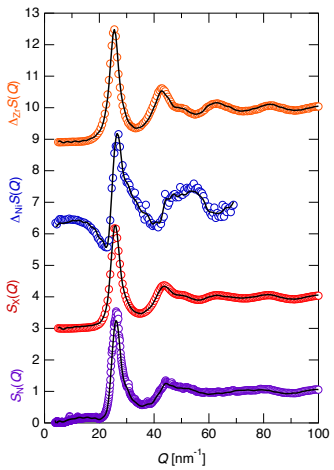

Fig. 1

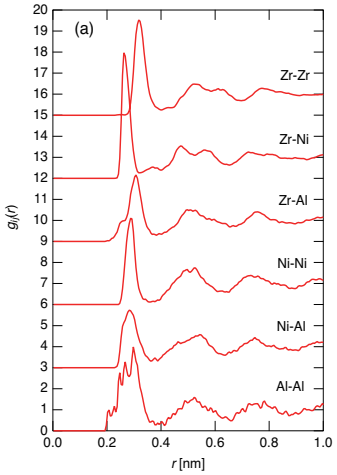

Fig. 2

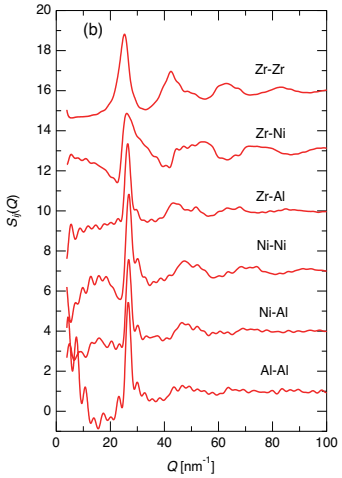

Fig. 3