



**Experiment title:**  
Partial structure and glass-forming ability of Zr-Ni-Cu-Al bulk metallic glasses

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**Report:**

In the last two decades, bulk metallic glasses with a distinct glass transition have been discovered in various multicomponent alloy systems. They have an extremely excellent glass-forming ability (GFA); a far slow cooling rate such as  $\sim 1$  K/s can avoid their crystallization. Properties of bulk glasses have attracted much interest in both physical and technological aspects, such as the glass transition, structural changes, phase stability, magnetic properties, elastic constant, etc. Among these glasses, the sample in this proposal,  $Zr_{63}(Ni,Cu)_{25}Al_{12}$  alloys, have excellent GFAs, where even the cooling rate of some K/s can suppress the crystallization [1]. In particular, the GFA of the  $Zr_{63}Ni_{12.5}Cu_{12.5}Al_{12}$  metallic glass is better than those of the end-members of  $Zr_{63}Ni_{25}Al_{12}$  and  $Zr_{63}Cu_{25}Al_{12}$  alloys.

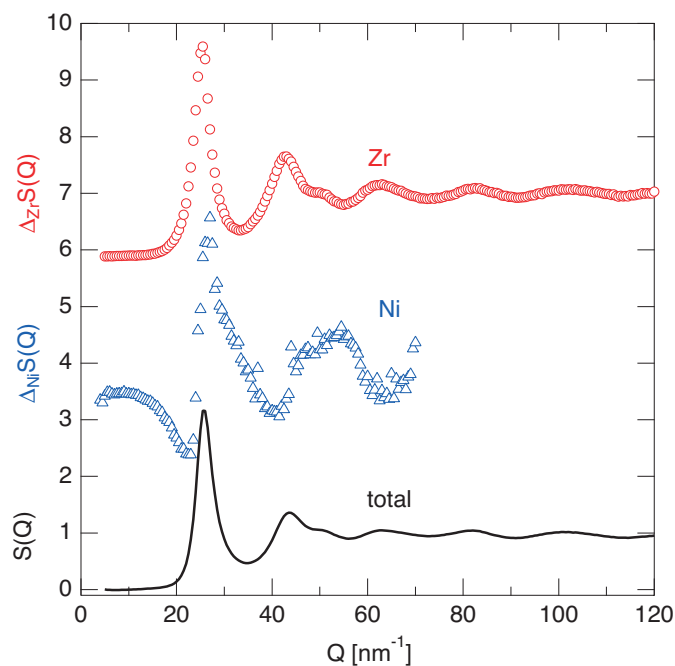
In order to clarify the excellent GFA of  $Zr_{63}Ni_{12.5}Cu_{12.5}Al_{12}$  alloy in the microscopic sense, structural investigations are essential. Although many attempts of structural investigations were made, such as x-ray absorption fine structure (XAFS) [2] and X-ray diffraction (XD) [2,3], less works have been carried out on even three component alloys due to its complex structural feature. We carried out an anomalous x-ray scattering (AXS) measurements on  $Zr_{63}Ni_{12.5}Cu_{12.5}Al_{12}$ ,  $Zr_{63}Ni_{25}Al_{12}$ , and  $Zr_{63}Cu_{25}Al_{12}$  bulk metallic glasses close to the Zr K (17.998 keV), Ni K (8.333 keV), and Cu K (8.979 keV) edges to understand the local- and intermediate-range structures around these constituent elements and its relation to the excellent GFA from the view point of microscopic atomic structure.

The glass alloys were used for the present work, which were manufactured by arc-melting the elemental metals with the purities of better than 99.999 %, and then

rapid-quenching into a Cu mold under pure Ar atmosphere. The AXS experiments were performed at two incident x-ray energies,  $-30$  and  $-300$  eV below the Zr K edge and  $-20$  and  $-200$  eV below the Ni and Cu K edges, using a normal  $\omega - 2\theta$  diffractometer. The experimental details are given elsewhere [4].

Figure shows the differential structure factors,  $\Delta_i S(Q)$ , of glassy  $\text{Zr}_{63}\text{Ni}_{25}\text{Al}_{12}$  alloy measured close to the Zr (circles) and Ni (triangles) K edges, together with the total structure factor,  $S(Q)$  (solid curve). As seen in the figure, the  $\Delta_{\text{Zr}} S(Q)$  spectrum looks similar to  $S(Q)$  except the amplitude of the oscillations. On the other hand,  $\Delta_{\text{Ni}} S(Q)$  has a feature very different from  $\Delta_{\text{Zr}} S(Q)$  and  $S(Q)$ . In particular, out-phases in the oscillations are seen beyond  $30 \text{ nm}^{-1}$ . The  $\Delta_i S(Q)$  data were obtained in other two glassy alloys similarly.

These AXS data with good qualities will be analyzed using RMC modelling to evaluate a complete set of partial structure factors,  $S_{ij}(Q)$ , and to draw three-dimensional atomic configurations of these metallic glasses. We also plan to perform neutron diffraction experiments for these glasses in the near future, from which we can reliably determine the positions of Al atoms.



- [1] A. Inoue et al., Mater. Trans. JIM **34**, 1234 (1993).
- [2] S. Sato et al., Mater. Trans. **46**, 2893 (2005).
- [3] E. Matsubara et al., J. Alloys Compd. **434-435**, 119 (2006).
- [4] S. Hosokawa and J.-F. Bérar, AIP Conf. Proc. **879**, 1743 (2007).