Structural Study of $Fe_{80}B_{20}$ Amorphous Alloy by Anomalous X-ray Scattering Coupled with Neutron Diffraction

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The Fe-based metal-metalloid amorphous alloy system is applied for the soft magnetic glassy alloys and counted as one of the prominent categories in the field of amorphous alloy technology. Although several advanced techniques have been applied for elucidating the detailed structural model for these interesting alloys (e.g. [1]), the arrangement by local structural units of typical icosahedra and/or trigonal prisms is still unclear. In order to discuss the detailed structure of Fe-based metal-metalloid amorphous alloys, the information of partial structural factors for any pairs of the constituents is strongly required. In this study, we determined the partial structural functions for a $Fe_{80}B_{20}$ amorphous alloy by the combinational use of anomalous X-ray scattering (AXS) and neutron time of flight diffraction (ND), which is one of the most advanced methods in order to obtain the reliable structural model for amorphous samples.

The AXS measurement at Fe *K* absorption edge was carried out at BL-7C of Photon Factory, KEK, Tsukuba. The ND experiment was performed by using high intensity total diffractometer, NOVA at MLF, J-PARC.

As for the three dimensional structural modeling of the $Fe_{80}B_{20}$ amorphous sample, reverse Monte Carlo simulation (RMC) has been performed starting from an initial model of 2,000 atoms with a random packing structure. The present RMC simulation well reproduces the three independent interference functions obtained by Fe-AXS, the ordinary X-ray diffraction, and ND as shown in Fig. 1. The obtained structural model allows us to discuss the fundamental local structural units together with their arrangements.

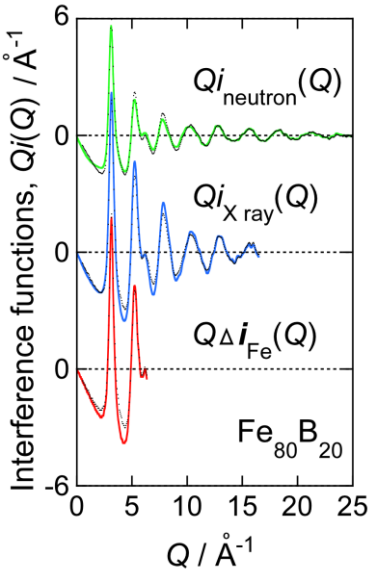

Fig. 1 The three interference functions obtained by Fe-AXS, the ordinary X-ray diffraction, and ND. Solid and dotted lines indicate the experimental data and the results of RMC, respectively.

[1]A. Hirata, Y. Hirotsu, T. Ohkubo, T. Hanada, and V..Z.Bengus, Phys. Rev. B **74**, 214206 (2006).