MLF Experimental Report	提出日 Date of Report 4 July 2013
課題番号 Project No. 2012B0097 実験課題名 Title of experiment Structural analyses of Fe-based and Ni-based metal-metalloid amorphous alloys 実験責任者名 Name of principal investigator Hiroshi Arima 所属 Affiliation Tohoku University	装置責任者 Name of responsible person Toshiya Otomo 装置名 Name of Instrument/(BL No.) BL21 実施日 Date of Experiment March 21, 2013 (24 hours)

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.

The following amorphous alloy samples were produced by the single-roller melt-spinning technique with boron metal enriched by 99 % ^{11}B.

1. $Fe_{80}B_{20}$ amorphous ribbon (thickness of 0.02 mm)
2. $Ni_{60}B_{40}$ amorphous ribbon (thickness of 0.02 mm)
3. $Ni_{81}B_{19}$ amorphous ribbon (thickness of 0.02 mm)

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 neutron diffraction experiment was performed by using the time-of-flight technique and high intensity total diffractometer, NOVA at MLF, J-PARC. The amorphous ribbon samples were cut into 20 mm length and loaded into a vanadium cylinder 6 mm in diameter. The typical duration of the data collection time for each sample was about 4 hours. After the standard corrections for absorption, multiple scattering and recoil factor, the measured intensity was converted into an absolute scale with respect to the measured intensity of the vanadium standard. Pair distribution function $g(r)$ was obtained by the Fourier transformation of the structure factor $S(Q)$.

Figure 1 shows $S(Q)$ profiles of $Fe_{80}B_{20}$ calculated from the intensity profiles measured by a various detector banks, as an example. Although $S(Q)$ profiles at the high Q region is rather distorted probably due to the insufficient correction for absorption, the oscillations around unity are observed up to about 25 Å^{-1}. This result readily indicates that the present data processing works well and prompted us to study the detailed structure model by using the present experimental data. Figure 2 shows the $g(r)$s for $Fe_{80}B_{20}$, $Ni_{81}B_{19}$, and $Ni_{60}B_{40}$ calculated by the interference functions up to Q_{max} = 25 Å^{-1} .

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

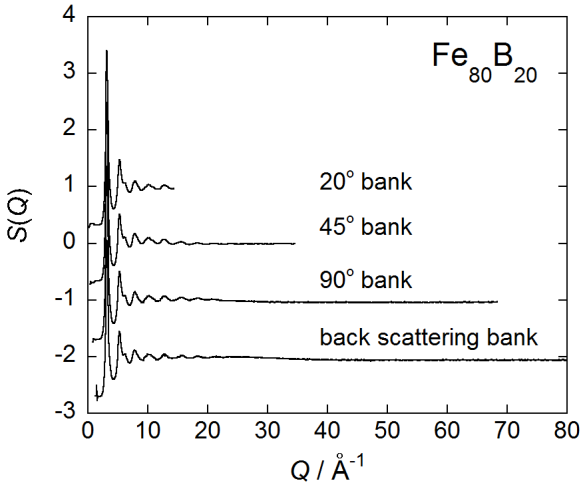

Fig. 1 The structure factor $S(Q)$ for $Fe_{80}B_{20}$ amorphous alloy.

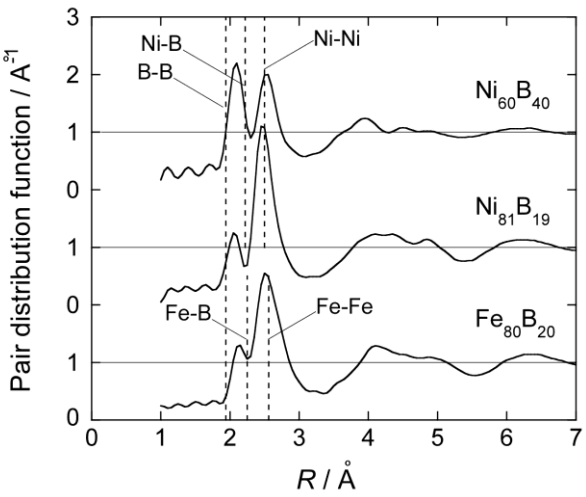

Fig. 2 The pair distribution functions for $Fe_{80}B_{20}$, $Ni_{81}B_{19}$, $Ni_{60}B_{40}$.

The dashed lines in Fig.2 indicates the interatomic distances estimated from Goldschmidt atomic radii (Fe: 1.28 Å, Ni: 1.25 Å, B: 0.97 Å). At the nearest neighbor region up to about 3 Å, the first peak could be accounted for a harmony of metal(M)–B and B–B pair correlations and the second peak is mainly contributed by the M-M pair correlation.

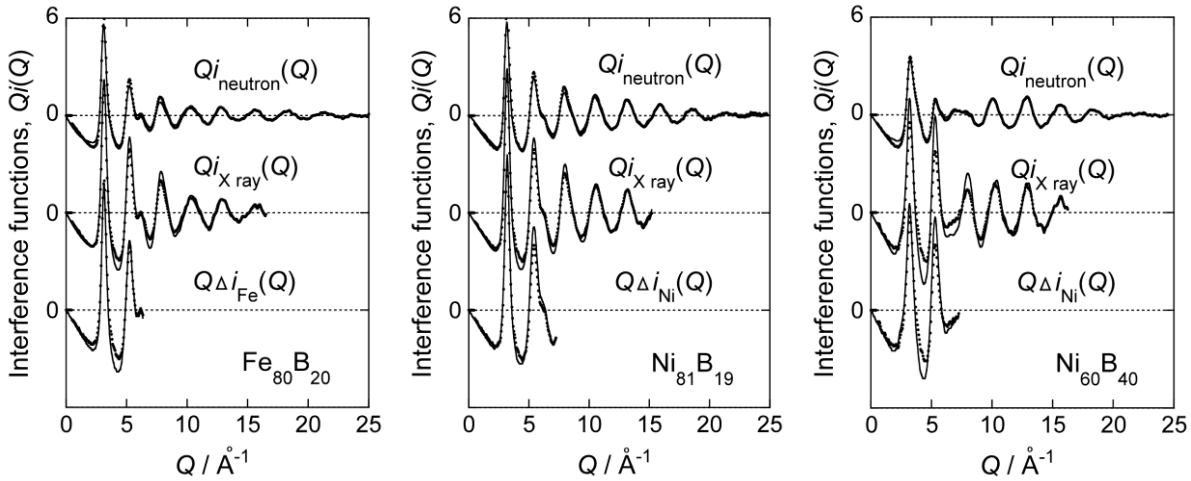

Fig. 3 The interference functions from the neutron diffraction, ordinary X-ray diffraction, and AXS measurements near Fe *K* absorption edge. Solid lines correspond to the experimental data. Dotted lines denote values calculated by the RMC method.

As for the three dimensional structural modeling of the amorphous samples, reverse Monte Carlo simulation (RMC) has been performed starting from an initial model of 2,000 atoms with the b.c.c. structure. The present simulation results are found to reproduce the three independent interference functions obtained by the neutron diffraction, ordinary X-ray diffraction, and anomalous X-ray scattering (AXS) measurements as shown in Fig. 3. We are now analyzing the obtained structural model in detail, in order to clarify local structural units around B including their arrangement.