ESRF	**Experiment title:** Partial structure and glass-forming ability in glassy Pd-Ni-Cu-P and Pd-Pt-Cu-P alloys	**Experiment number:** HD162
Beamline: BM02	**Date of experiment:** from: 20 Feb. 2008 to: 26 Feb. 2008	**Date of report:** 22 Dec. 2014
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Report:

In the last two decades, bulk metallic glasses (BMG) with distinct glass transitions have been discovered in various multi-component alloys. They show extremely excellent glass-forming abilities (GFA), where even a very slow cooling rate such as ∼1 K/s can avoid crystallization. Among these BMGs, the $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ alloy has at present the most excellent GFA, where even the cooling rate of ∼ 0.067 K/s can suppress the crystallization, and can form a massive bulk glass with a diameter of more than 40 mm [1].

To clarify the excellent GFA of this alloy in the microscopic sense, structural investigations are essential. An anomalous x-ray scattering (AXS) measurement was already performed by Park et al. [2] to provide useful information on the local structure in this glass, suggesting that a peculiar atomic association related to Cu atoms may play an important role. However, the experiment was limited in the low Q range due to the low energies close to the Ni and Cu K edges, and the data are rather scattered due to the use of an old generation synchrotron source of PF-KEK.

In this study, we have performed AXS on the $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ BMG close to the Pd [3], Ni, and Cu K absorption edges.The obtained differential structure factors $\Delta_k S(Q)$ were analyzed together with a complementary neutron diffraction result $S_{\rm N}(Q)$ using reverse Monte Carlo (RMC) modeling to evaluate the partial structure factors $S_{ij}(Q)$ and the corresponding partial pair distribution functions $g_{ij}(r)$.

The $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ rod with a diameter of 3 mm was prepared by arc-melting mixtures of pure Pd, Ni, Cu, and the prealloyed Pd-P in an pure Ar atmosphere. To eliminate heterogenous nucleation due to the oxide contamination, a B_2O_3 flux treatment was carried out more than ten times in a highly purified Ar atmosphere. The melts was kept at about 1,000°C for more than six days and then quenched into iced water.

The AXS experiments were carried out near the Pd (24.350 keV), Ni (8.333 keV) and Cu (8.979 keV) K edges at BM02. For obtaining $\Delta_k S(Q)$s, scattering experiments were performed at two different incident x-ray energies of 30 and 200 eV below the the Pd K edges, and 20 and 200 eV below the Ni and Cu K edge, using a standard $\omega - 2\theta$ diffractometer installed at the beamline. The RMC simulations were carried out using three $\Delta_k S(Q)$s, the x-ray total structure factor $S_{\mathrm{X}}(Q)$, and $S_{\mathrm{N}}(Q)$.

The left panel of the figure shows $\Delta_k S(Q)$s close to the Pd, Ni, and Cu K edges, $S_{\mathrm{X}}(Q)$, and $S_{\mathrm{N}}(Q)$ measured at ILL from top to bottom. The circles indicate the experimental data and the solid curves denote the best fits of the RMC modeling. As clearly seen in the figure, the coincidences between the experiments and the RMC fits are excellent.

The middle panel of the figure shows $S_{ij}(Q)$s obtained from the RMC fits. $S_{\mathrm{PdPd}}(Q)$ and $S_{\mathrm{PdNi}}(Q)$ show large shoulders at the smaller Q side of the first peaks, indicating the existence of Pd-Pd and Pd-Ni intermediate-range correlations. On the other hand, enhancements are observed at the low Q region in $S_{\mathrm{PdCu}}(Q)$ and $S_{\mathrm{NiCu}}(Q)$, indicating phase separation tendencies around the Cu atoms.

The right panel of the figure shows $g_{ij}(r)$s obtained from the RMC fits. From those, the partial interatomic distances were obtained, and are in good agreement with the previously obtained AXS results [3]. For the further discussion, Voronoi analyses using the obtained atomic configurations are now in progress.

[1] N. Nishiyama and A. Inoue, Appl. Phys. Lett. **80**, 568 (2002).
[2] C. Park et al., Mater. Trans. JIM **40**, 491 (1999).
[3] S. Hosokawa et al., Phys. Rev. B **80**, 174204 (2009).