



	Experiment title: Partial structure and glass-forming ability in glassy Pd-Ni-Cu-P alloys	Experiment number: ME1002
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Report:

In the last decade, various bulk metallic glasses with a distinct glass transition have been discovered in multicomponent alloy systems. They have an extremely excellent glass-forming ability; a far slow cooling rate such as ~ 1 K/s can avoid their crystallization. Properties of bulk glasses attract much interest both in physical and technological aspects, such as the glass transition, structural changes, phase stability, magnetic properties, elastic constant, etc. Among these glasses, $\text{Pd}_{42.5}\text{Ni}_{7.5}\text{Cu}_{30}\text{P}_{20}$ alloy is the most excellent glass-forming ability, where even the cooling rate of ~ 0.067 K/s can suppress the crystallization [1].

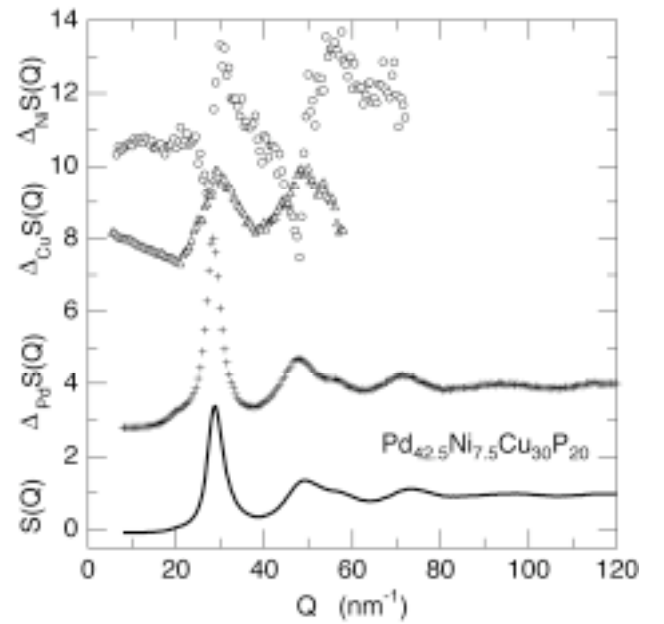
In order to clarify the excellent glass formability of $\text{Pd}_{42.5}\text{Ni}_{7.5}\text{Cu}_{30}\text{P}_{20}$ alloy in the microscopic sense, structural investigations are essential. Although many attempts of structural investigations were made for Pd-Ni-P alloys, such as XAFS and anomalous X-ray scattering (AXS), less works have been carried out on this champion glass alloy $\text{Pd}_{42.5}\text{Ni}_{7.5}\text{Cu}_{30}\text{P}_{20}$ due to its complex structural feature. Only an AXS measurement [2] provides 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 to the energies close to the Cu and Ni K edges, and the data are rather scattered due to the old generation synchrotron source of PF/KEK.

We carry out an AXS measurement on glassy $\text{Pd}_{42.5}\text{Ni}_{7.5}\text{Cu}_{30}\text{P}_{20}$ and $\text{Pd}_{40}\text{Ni}_{40}\text{P}_{20}$ alloys close to the Pd, Ni, and Cu K edges for the understanding of the local structure around these constituent elements and its relation to the excellent glass-forming properties from the

viewpoint of microscopic structure of the glasses.

Alloy ingots of $\text{Pd}_{42.5}\text{Ni}_{7.5}\text{Cu}_{30}\text{P}_{20}$ and $\text{Pd}_{40}\text{Ni}_{40}\text{P}_{20}$ bulk metallic glasses were used for the present work. The casting rate was about $\sim 100\text{-}1000$ K/s. The details of the fabrication technique were described in Ref. [1] and references therein. The AXS experiments were performed at two incident x-ray energies (-20 and -200 eV) below the K edges of Ni, Cu, or (-30 and -300 eV) below the Pd K edge, using a normal ω - 2θ diffractometer. In order to obtain differential structure factors, $\Delta_i S(Q)$, with high statistical quality, two requirements should be fulfilled: 1) A good energy resolution to discriminate the elastic signal from the fluorescence and Compton contributions, and 2) a sufficient number of scattered X-ray photons within a reasonable data collection time. We chose a graphite crystal analyzer providing a good Bragg reflection, which was placed on a 40-cm-long arm to obtain an energy resolution of 60 eV.

Figure shows results of the $\Delta_i S(Q)$ spectra of glassy $\text{Pd}_{42.5}\text{Ni}_{7.5}\text{Cu}_{30}\text{P}_{20}$ measured at energies close to the Ni (circles), Cu (triangles), and Pd (crosses) K edges. For the comparison, $S(Q)$ measured at 300 eV below the Pd K edge, is also shown by the solid curve in the figure. The phase of the oscillation of the $\Delta_{\text{Pd}} S(Q)$ spectrum looks similar to that in $S(Q)$, but systematically shifts to the smaller Q . Correspondingly, differential pair distribution functions obtained from their Fourier-transform indicate that the nearest-neighbour distance around the Pd atoms is slightly shorter than the average one. It should be noted that a small shoulder is seen at Q position below the first $S(Q)$ maximum around 20 nm^{-1} , which is not seen in the glassy $\text{Pd}_{40}\text{Ni}_{40}\text{P}_{20}$ data. Due to the contrasts between $\Delta_i S(Q)$ data and $S(Q)$, this shoulder may be composed of the Pd-Pd correlation. This result suggests that there is a small portion of a longer Pd-Pd partial coordination length than a normal dense-packed configuration in this metallic glass. Since a strong covalent correlation between the Pd and P atoms is suggested from our recent photoemission study on the same glass [3], the P atoms may selectively be located between the Pd atoms and form a strong interaction. This structural information is not visible in this AXS results due to a weak scattering intensity from the P atoms.



[1] N. Nishiyama and A. Inoue, Appl. Phys. Lett. 80, 568 (2002).

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[3] S. Hosokawa, N. Happon, H. Sato, M. Taniguchi, T. Ichitubo, M. Sakurai, E. Matsubara, and N. Nishiyama, Mater. Trans. JIM, submitted.