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# Structural analysis of $Pd_{40}Cu_{40}P_{20}$ and $Pd_{45.5}Cu_{35.5}P_{19}$ metallic glasses

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## Introduction

Pd-Cu-P alloy system is a constituent of Pd-Cu-Ni-P glass system, showing an extremely small critical cooling rate for vitrification and high resistance to crystallization [1]. Another component, Pd-Ni-P ally system has been examined well about the structure. However, the structural analysis of Pd-Cu-P glass system has not been presented. Although Hi et al. reported [1] that a bulk Pd-Cu-P glass is capable to produce over a large compositional range, a typical $Pd_{40}Cu_{40}P_{20}$ glass has not been reported to be obtained in a bulk shape. We have carefully searched an adequate composition for bulk glass formation and succeeded to produce a bulk glass with the $Pd_{45.5}Cu_{35.5}P_{19}$ composition by water-quenching. This suggests that the glass forming ability (GFA) was remarkably improved by a small adjustment of alloy composition. The objective in the present report is to check the difference of amorphous structure between $Pd_{40}Cu_{40}P_{20}$ and $Pd_{45.5}Cu_{35.5}P_{19}$ glasses.

## Experimental Results

A bulk $Pd_{45.5}Cu_{35.5}P_{19}$ glass with a rod shape of 6 mm in diameter and 20 mm in length was prepared by water-quenching. A ribbon $Pd_{40}Cu_{40}P_{20}$ glass was prepared by melt-spinning with a cupper roll. The structural analysis for these glasses was performed by normal scattering with Mo-Kα radiation (17.5 keV) and anomalous X-ray scattering (AXS) experiments near the Cu-K absorption edge (8.980 keV) with a far-edge energy of 8.680 keV and a near-edge energy of 8.955 keV at BL7C station. AXS enables us to examine the species-specified local structure of the glass, i.e. Cu-P, Cu-Cu and Cu-Pd correlations

Figure 1 presents the radial distribution functions (RDFs) for AXS-experiments, where the number densities, 75.3 and 74.1 $nm^{-3}$, were used for $Pd_{40}Cu_{40}P_{20}$ and $Pd_{45.5}Cu_{35.5}P_{19}$ glasses. The $1^{st}$ peaks of RDFs were fitted well by a linear combination of three Gaussian functions, corresponding to the nearest Cu-P, Cu-Cu and Cu-Pd atomic correlations. The nearest neighbour distance $r_{ij}$ and coordination number $N_{ij}$ were estimated and the result is summarized in Table I. The $r_{ij}$ is physically acceptable, when compared to the atomic radius $r_{Pd}$=0.141, $r_{Cu}$=0.127 and $r_P$=0.100 in ref. [3]. Nearest neighbour metallic atoms $Z$ around the centred P atom, assuming the statistical distribution of the metallic atoms, is predicted to be $Z$=1.7x(0.4/0.2)x2≈6.8 for the $Pd_{40}Cu_{40}P_{20}$ glass, and this result is compatible with various metal-metalloid binary glasses [4]. The coordination number of Cu and Pd atoms around the centred Cu atom, $N_{CuCu}$ and $N_{CuPd}$, are compatible with each other for $Pd_{40}Cu_{40}P_{20}$ glass, while $N_{CuCu}$ is rather larger for $Pd_{45.5}Cu_{35.5}P_{19}$ glass than $Pd_{40}Cu_{40}P_{20}$ glass. Also, $N_{PCu}$≈3.5x(0.355/0.19)=6.5 is obtained, and this value is approximately two times larger than $N_{PCu}$ =1.7x(0.4/0.2)=3.4 of $Pd_{40}Cu_{40}P_{20}$ glass. When the tri-capped triangular prism constitutes a predominant part of the local structural unit of a glass with the composition of $TM_{80}M_{20}$ (TM: transition metal, M: metalloid) [4], $N_{MTM}$ should range over 6 – 9. Therefore, under the assumption that the local amorphous structure for $Pd_{45.5}Cu_{35.5}P_{19}$ glass is similar to that for $Pd_{40}Cu_{40}P_{20}$ glass, the present results suggest that micro-phase separative tendency might increase in $Pd_{45.5}Cu_{35.5}P_{19}$ glass.

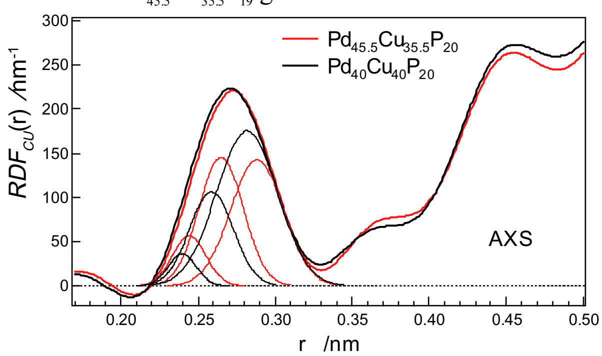


Fig. 1 AXS radial distribution functions. Fine lines show the de-convolution of $1^{st}$ peaks due to Gaussian functions.

| | Cu-P | | Cu-Cu | | Cu-Pd | |
|---|---|---|---|---|---|---|
| | $r_{ij}$ | $N_{ij}$ | $r_{ij}$ | $N_{ij}$ | $r_{ij}$ | $N_{ij}$ |
| Pd40 | 0.240 | 1.7 | 0.259 | 4.8 | 0.282 | 5.9 |
| Pd45.5 | 0.244 | 3.5 | 0.265 | 7.8 | 0.288 | 3.8 |

Table I.Comparison of $r_{ij}$ and $N_{ij}$ for $Pd_{40}$ and $Pd_{45.5}$ glasses.

## References

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