Electronic structure of $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ excellent bulk metallic glass former: Comparison to the reference $Pd_{40}Ni_{40}P_{20}$ glass

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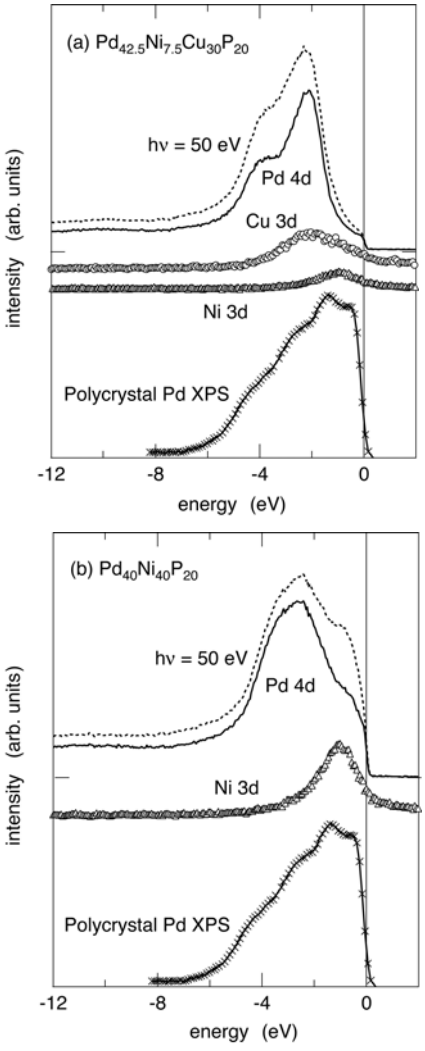
Bulk metallic glasses of Pd-Ni-Cu-P alloys, discovered by Nishiyama and Inoue [1], have intensively been studied due to their good glass-forming ability (GFA). They have optimized the concentration dependence of the critical-cooling-rate (CCR), and found that $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ has at present the slowest CCR of 0.067 K/s and can form a massive bulk glass with a diameter of more than 40 mm by simple water-quenching [2].

In order to clarify the origin of the excellent GFA from the viewpoint of electronic structure, photoemission spectrum (PES) [3], and soft X-ray emission (SXES), and core absorption spectra were measured at BL7/HiSOR and BL2C/PF, respectively, as well as in-house inverse-photoemission spectrum [4]. Solid curves in the figures show the Pd 4*d* partial density of states (DOS) estimated from the incident photon energy ($h\nu$) dependence of the PES spectra of (a) $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ glass together with (b) the reference $Pd_{40}Ni_{40}P_{20}$ glass, having a worse CCR of 1.6 K/s. The PES spectra at $h\nu = 50$ eV given as dashed lines for the comparison. The Ni 3*d* (triangles) and Cu 3*d* (circles) partial DOSs obtained from the SXES measurements are also given.



From these spectra in the figures, it was found that the Pd 4*d* partial DOS near the Fermi energy largely decreases and becomes localized by replacing the Ni atoms with the Cu atoms. They are largely different from X-ray PES spectra of polycrystal pure Pd metal given at the bottom of the figures. On the other hand, the Ni 3*d* partials remain unchanged in the shape. This may be closely related to the excellent GFA in the $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ bulk metallic glass due to a selective formation of Pd-P covalent bonds. This finding is strongly supported by a recent structural study using anomalous X-ray scattering technique [5].

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