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Angle resolved photoemission study of CrP(100)

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It is well known that 3d transition metal monopnictides show various structural and magnetic properties. Among them, some compounds show structural phase transitions between NiAs-type structure to orthorhombic MnP type structure. The structural properties have been considered to be related to the magnetic properties. The present study is devoted to the Pauli paramagnetic compound CrP, which forms the MnP type crystal structure as shown in Fig.1(a). Recently, high quality single crystal of CrP has been successfully grown by a chemical vapour transport technique [1], which makes possible to observe the de Haas-van Alphen (dHvA) effect. Ten branches of dHvA frequency in the (010) plane have been found in the dHvA effect measurement. These branches are partially explained by the calculated Fermi surface. The electronic structures related to their magnetism and the structural phase transition are needed to be investigated. In order to study the whole features of the valence band electronic states, the angle-resolved photoemission was carried out for the single crystalline CrP(100).

The experiment was done at BL-18A. The clean surface was obtained by the repeated cycles of Ar ion bombardment and annealing up to 800K. The angle resolved photoemission spectra were measured at hν=21.2eV on the Γ(X)-Y(S) and Γ(X)-Z(U) planes in the orthorhombic Brillouin zone as shown in Fig.1 (b). Besides the spectra along Γ-X axis changing the incident photon energy was likewise measured. Fig.2 shows the experimental energy band structure as a function of a parallel component along the [100] direction of the wave vector ($k_{//}$), corresponding to the Γ(X)-Z(U) direction in the Brillouin zone. The normal emission spectrum excited by the photon energy of 21.2eV shows the structures just below E_F and E_B = 3.8eV and the small hump around 7eV, which are recognized at $k_{//}$ = 0 (Å^{-1}) in Fig.2. With increasing the emission angle, the structure around 3.8eV at $k_{//}$ = 0 (Å^{-1}) becomes broader and separates each other as clearly observed in the spectra above 30° ($k_{//} > 0.5$Å^{-1}). The weak structure at E_B=7eV at $k_{//}$ = 0 (Å^{-1}) shifts toward the lower binding energy with increasing the emission angle up to 26° ($k_{//} \sim 0.5$Å^{-1}) and again go back toward the higher binding energy. Although the sharp structure just below E_F seems to stay at the same E_B at any emission angles, the intensity of this peak is gradually suppressed (*not shown*). Comparing the experimental energy band structure with those calculated by LMTO method, we have found that the experimentally observed feature of the structure for Cr3d-P3p bonding state is well explained by the calculation.

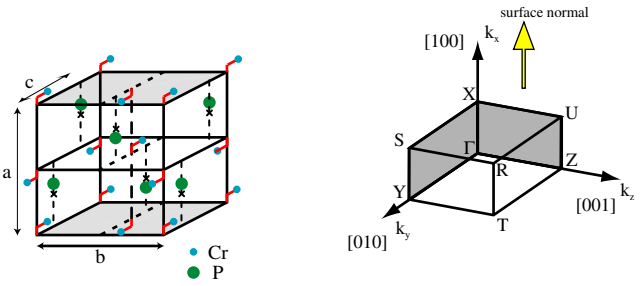

Fig.1 (a) Crystal structure of CrP. (b) Orthorhombic Brillouin zone of CrP.

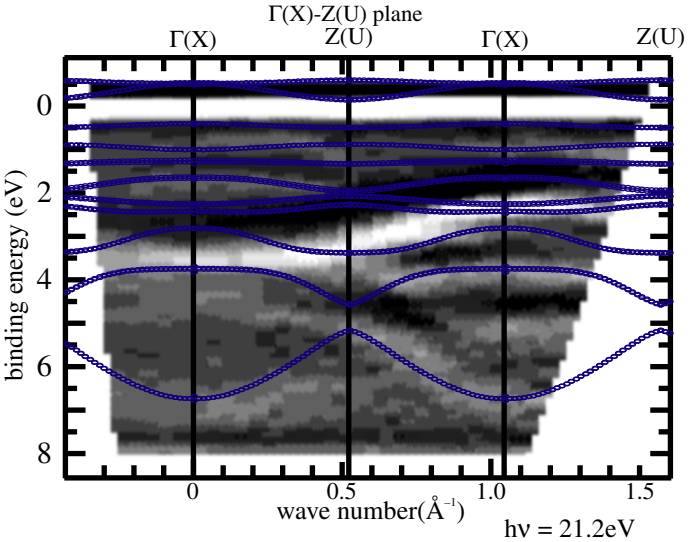

Fig.2 Experimental band structure of CrP(100) in Γ(X)-Z(U) plane in the orthorhombic Brillouin zone. The theoretical band structures calculated by LMTO method along X-U line are also shown for comparison.

References

[1] T. Nozue, et al, J. Magn. Soc. Japan **23**, 430 (1999).

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