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Partial Spectral Weights of Disordered Au-Pd Alloy Systems in Pd Dilute Limit

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The electronic properties of dilute alloys of Pd with noble metals are interesting subjects due to their technological importance in catalysis and material science. And these systems are also interesting test cases for experimental and theoretical studies of scattering, localization and correlation problems. But in these randomly substituted alloy systems, even a minute concentration of impurities destroys the translational periodicity of the crystal, and thus there is serious theoretical difficulty that the Bloch's theorem is not applicable. The concept of virtual bound state(VBS), proposed by Friedel and Anderson, well describes the transport phenomena and magnetic properties of some alloy systems such as dilute solutions of Ni, Co, Fe, Mn, Cr, V, etc., in Cu or Al. And there have been many photoemission works to observe the VBS directly. Au-Pd alloy system is expected to be intermediate in various Pd-dilute alloy systems, whose bands are not so split band as Ag-Pd, but do not form common band as Cu-Pd. We measured the photoemission spectra of valence band of $Au_{1-x}Pd_x$ alloy systems(x=0.1 and 0.05) in Pd dilute limit at two photon energies, $h\nu$=230 eV (at this photon energy the Au 5*d* photoemission cross section goes through the Cooper minimum) and $h\nu$ =130 eV. And we also obtained partial spectral weights(PSW's) of each constituent with the iteration scheme taking into account the matrix element effect.

All samples were prepared by arc-melting high purity materials in argon atmosphere. They were heated at about 950° C for 2 days to guarantee the uniformity and then quenched into liquid nitrogen to get disordered alloy. X-ray Diffraction measurements confirmed the homogeneity and no presence of the ordered phases. All photoemission spectra were taken at Pohang Light Source 2B1 beamline equipped with VG CLAM 2 analyser. Before the measurements the surface of the samples was sputtered mildly with 2 KeV Ne ions for 20 min. and then annealed at about 200° C for 20 min. in UHV.

The procedure to extract the PSW's of the valence band of each component is as follows. The valence band spectra taken at $h\nu$=230 eV where the cross section ratio of Au 5*d* is 0.3 times that of Pd 4*d* shows the Pd 4*d* PSW very prominently. First stage Pd 4*d* PSW is extracted by subtracting Au 5*d* PSW in this spectra which is assumed to be the valence band spectra of the same alloy taken at 130 eV. At this photon energy the cross section ratio of Pd 4*d* is 0.3 times that of Au 5*d* and the composition ratio of Pd is lower than 0.1, so the spectral area from the Pd component is negligible. In this process the matrix element with the kinetic energy is taken into account by .multiplying the Au 5*d* PSW with the ratio taken from that of the valence band spectra of pure Au at both photon energies. Next, subtracting the first stage Pd 4*d* PSW from the valence band spectra of the alloy at $h\nu$=130 eV, we can extract Au 5*d* PSW's which will be utilized again to obtain Pd 4*d* PSW's at $h\nu$=230 eV.

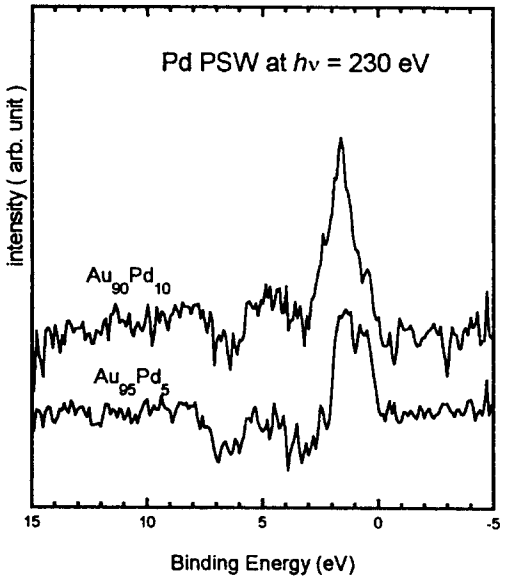

Fig. 1

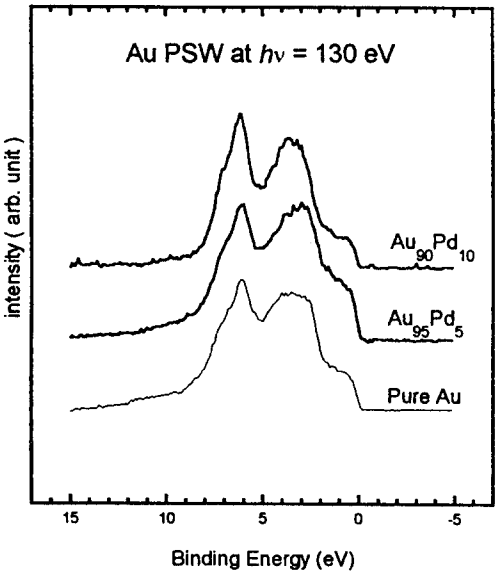

Fig. 2

The Iterations of 3 or 4 times as stated above were enough to obtain the convergence to self-consistent results. Fig. 1 and Fig. 2 show the result after ten iterations.

Fig. 1 shows very sharp peak at about E_B=1.6 eV which is in agreement with the result of earlier photoemission works and coherent potential approximation(CPA) calculations for Pd dilute alloys. This result suggests that the Pd impurity state forms a VBS in the Au host. A small structure at about E_B=4.5 eV is expected to be due to Au $5d_{5/2}$ - Pd $4d$ hybridization, which is also shown in the result of CPA calculations and model Hamiltonian calculations. The Au $5d_{3/2}$ states are little involved in this hybridization, since sharp structure around E_B=6 eV in Au PSW's due to the Au $5d_{3/2}$ states are not smeared out at all composition ratios as shown in Fig. 2. We can also see in Fig. 2 that the structure about E_B=3 eV due to the Au $5d_{5/2}$ states becomes narrower with the increase of the Pd content. This is expected to the band narrowing effect which results from the increase of disorder with the Pd content. This band narrowing of host metal pushes the bound state of impurity toward the band maximum of host, so VBS of $Au_{90}Pd_{10}$ is better formed than that of $Au_{95}Pd_5$.