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## Study of Unoccupied Pd 4*d* State of Cu-Pd Alloys by Bremstrahlung Isochromat Spectroscopy

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Fuggle *et al.*[1] reported that the Ni or Pd valence *d* band centroid shifts to higher binding energy with respect to Fermi level($E_F$) when they form alloys with electropositive metal. It was also found that the density of states at $E_F$ reduces severely and Ni or Pd *d* bandwidth tends to be come narrow with alloying. These facts led them to expect that Ni or Pd valence *d* band is being filled as alloying with electropositive metals. It is very controversal question wheather or not Ni or Pd valence *d* band is completely filled so that there exists no *d* state in the unoccupied level when Ni or Pd is very dilute in such alloys. However, there have been few studies on the unoccupied level in contrast to abundant theoretical and experimental studies on the occupied level. We chose Cu-Pd alloy as a sample because their electronic structures of occupied level had been well known[2-4] but very little had been understood about the unoccupied level so far. We have measured the unoccupied spectrum by Bremsstrahlung Isochromat Spectroscopy(BIS) to see the change of the unoccupied *d* state upon alloying.

The polycrystalline $Cu_{1-x}Pd_x$ (x=0,0.1,0.25,0.5,0.75,0.9,and 1) alloys were made by arc melting method with high purity metallic Cu and Pd wires under argon atmosphere in arc furnace. We checked weight loss after arc-melting process and found that there was no severe change of the total weights. We also measured the x-ray diffraction and obtained the simple peaks resulting from the fcc crystal structure. In BIS experiment we used X-ray monochromator which had been set at 1486.6 eV to detect a fixed frequency of photons. So, we used electron beams whose kinetic energy was close to 1500 eV. The total resolution was about 1.0 eV(full width at half maximum:FWHM) as measured by the spectrum width near the fermi level.

The BIS spectra of alloys shown in the Figure reveals the reduction of DOS upon alloying at $E_F$ clearly, which is consistent with the results of x-ray photoemission spectroscopy(XPS)[3]. They are normalinzed at 20 eV above $E_F$ because Cu or Pd *d* state edge does not exist at that high energy and that the contribution from the inelastically scattered background is dominant since the photoionization cross section of Cu 4*sp* (Pd 5*sp*) is much smaller than that of Cu 3*d* (Pd 4*d*)[5]. We are interested in whether or not the unoccupied 4*d* state of Pd atom exists at some energy above $E_F$. So, we have to obtain Pd partial BIS spectra from the total BIS spectra by proper subtraction procedure. We assume the partial DOS of Cu does not change upon alloying, while the partial DOS of Pd changes very severely. And we neglected the contribution from the difference of photoionization cross section between Cu 4*sp* and Pd 5*sp* since they are nearly the same[5]. With these assumptions we are able to obtain the Pd partial BIS spectra of $Cu_{1-x}Pd_x$ alloy by subtracting $x$ fraction of pure Cu BIS spectra from alloy BIS spectra.

By this method, we found that the Pd partial DOS at the Fermi level is reduced clearly

upon alloying compared with the pure Pd metal.


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