

ELECTRONIC STRUCTURES OF NOBLE METAL DISORDERED BINARY ALLOYS

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Electronic structures of disordered alloys are interesting from the viewpoints of both fundamental physics and technological applications. The effects of disorder and of the lack of periodicity upon physical properties of solids are still much unexplored area. Especially the breakdown of translational symmetry and the consequent inapplicability of Bloch's theorem poses a very difficult problem in calculating electronic structures of alloys. It is now generally agreed that the coherent potential approximation (CPA) gives the most consistent picture which agrees with many experimental data, particularly for split-band systems such as Ni-Cu and Ag-Pd alloys.

For alloys whose d bands overlap each other strongly, there has been little effort to separate the spectra into the partial spectral weights (PSW's) and to compare the PSW's with the calculated partial DOS's. There have been some controversy over the most studied systems such as Cu-Pd and Cu-Au alloys as to whether these systems are of common-band type or of split-band type. It has been shown by the band calculations that the d bands of these alloys mix strongly with each other for Cu rich alloys, but the PES results generally gave the opposite results.¹ Thus it was postulated that the disagreement between the experiment and the band calculation results from the neglect of the lattice relaxation effect.² To resolve this controversy, we have studied systematically on the electronic structures of some disordered noble metal alloys Cu-Pd, Cu-Au, Au-Pd, and Cu-Pt with photoemission spectroscopy (PES).

The PES spectra were taken with synchrotron radiation, ultra-violet PES (UPS), and x-ray PES (XPS). In order to separate the spectra into the PSW's, we took advantage of Cooper minimum phenomena of the d state photoionization cross sections occurring at soft x-ray regime. The PSW's were extracted at various compositions for the systematic study on the variational change of partial DOS's.

We find in the soft x-ray regime the photoionization matrix element strongly suppresses structures at the high binding energy side of the valence band spec-

tra where CPA calculations on Cu-Pd alloys predicts appreciable bonding states between Cu 3*d* and Pd 4*d* levels. This binding energy dependent matrix element is found very important for extracting PSW's of alloys. After taking this matrix element effect into account, we find that the experimental Pd PSW of Cu₇₅Pd₂₅ determined from XPS spectra is in good agreement with theoretical predictions.³ The lattice relaxation effect does not seem very important for the suppression of bonding states. From the comparison with the Pd PSW's of Au-Pd alloys, it is clear that there should be a large amount of bonding states for Cu-Pd alloys.

Since the hybridization between the Pt impurity *d* state with the Cu host *d* band will be stronger than between the Pd impurity with the Cu host, we also expect strong Cu-Pt bonding states in Cu-Pt alloys. In this case, we find that the matrix element of Pt does not suppress bonding states severely, and we can compare the Pt PSW with the band calculation more correctly. The previous photoemission studies have insisted on the presence of the virtual bound states for the Pt and the Pd impurity in Cu host, but we found from the Pt PSW of Cu rich alloy that due to strong hybridization, there is no virtual bound state.

Finally, the lattice relaxation effect on the total bandwidths is studied with Cu-Au alloys. It is found that the reduction of the total bandwidth due to the lattice relaxation amounts only ~ 0.2 eV for Cu₇₅Au₂₅, which is not very important in determining the overall shape of the electronic structure. Also, the common-band behavior of this alloys system is clearly confirmed from the Au PSW's.

In summary, we have studied the electronic structures of some noble metal alloys extracting PSW's of both components. The PSW's are in good agreement with the CPA calculation results, and the lattice relaxation effect once proposed as an important factor in determining the electronic structure of disordered alloys is found to be a minor factor.

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