Experimentally determined partial Density of States in disordered Au-Pd alloys

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There have been a great deal of efforts to understand the electronic structure of disordered binary alloys. In recent years many experiments and band calculations on alloys composed of transition metals and/or noble metals have been performed partly due to their useful catalytic behavior and partly due to the intrinsic physical interest in disordering effect. Since compositionally disoredered systems cannot have well-defined Bloch states, ordinary band calculations cannot be used to predict the electronic structure of these materials. The purpose of this work is to experimentally determine the partial density of states (DOS) of disordered Au-Pd alloy system using Cooper minimum phenomena in a systematic way taking the matrix element effect in full consideration.

The experiments were perfomed at National Synchrotron Light Source (NSLS) Beamline U4A in Brookhaven National Laboratory (Upton, NY, USA) equipped with toroidal grating monochrometer. The photon energies used ranged from 40eV to 200eV. The samples Au_xPd_{1-x} alloys (x=0.05, 0.25, 0.50, 0.75, 0.90) were prepared by arc melting of 99.99% Au and Pd wires. They were annealed at 950°C to ensure the homogeneity and X-ray diffraction result assured the f.c.c. solid solution.

The spectra at the photon energy of the Cooper minimum of one constituent element can be regarded as the experimental partial DOS of the other constituent at that photon energy. Then the careful consideration of matrix element effect in photoemission process makes it possible to obtain the experimental partial DOS of the latter constituent at another photon energy. We found that the changes of matrix elements at differnt photon energies should be properly considered to get accurate partial DOS, and it was accomplished by iteration procedure. We thus obtained partial DOS of constituent Au and Pd in Au_xPd_{1-x} (x=0.05, 0.25, 0.50, 0.75, 0.90). The result reveals the importance of the following two mechanisms in band forming of binary alloys, the band narrowing due to the decrease in the number of same kind of electronic states in adjacent sites and the band broadening due to the hybridization with different kind of atoms. The differences in Pd partial DOS of Au-Pd alloys and Cu-Pd alloys can be interpreted to arise from the differences in the strength of these two mechanisms.