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Charge transfer in ion-beam-mixed Au-Pd alloys studied by XPS and XAS

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1. Introduction

The formation of the metastable transition metal alloys using ion-beam-mixing has been extensively studied for many years because of their specific properties that differ from those of bulk materials. In ion-beam-mixing, the alloy or compound is formed due to the atomic interaction between different species during ion bombardment.

We studied the electronic structure change in ion-beam-mixed Au-Pd alloys by XPS and XAS which can provide detailed information concerning the bonding-induced changes in the density of states. Therefore, we show that a charge compensation model can explain the XPS and XANES data with accuracy. From this study, we are undertaking a set of fundamental studies of charge redistribution upon alloying and formation of intermetallic compounds such as how alloying affects the hybridization between neighboring atoms or how it changes the valence-band density of states.

2. Experimental

The multi-layer films were deposited on a wet-oxidized Si(100) substrate by sequential electron beam evaporation at a pressure of less than 5×10^{-7} Torr during deposition. These comprise 4 pairs of Au and Pd layers, where thicknesses of each layer were varied in order to change the alloy composition.

Ion-beam-mixing was carried out with 80 keV Ar^+ ions with a dose of 1.5×10^{16} Ar^+/cm^2 at room temperature.

Core and valence level energy shift in these system were investigated by x-ray photoelectron spectroscopy(XPS). Photoelectrons were excited by monochromatized Al Kα(1486.6 eV). The pass energy of the hemispherical analyzer was set at 17.5 eV. Core-level binding energies were referenced to the Fermi level.

Au and Pd L_3-edge XANES spectra were measured at the X!9A beam line of the NSLS at Brookhaven National Laboratory. To avoid the thickness effect, the spectra were collected in the total electron yield mode which is particularly suitable for thin film materials.

3. Results and discussion

In Au and Pd L_3-edges XANES spectra for ion-beam-mixed Au-Pd alloys, we show that Au WL area is increasing and Pd WL area is decreasing upon alloying. From these results, we can see that Au *5d* bands are reduced as the Pd content is increased upon alloying. On the other hand, Pd *4d* bands are increased with decreasing Pd concentration.

In XPS spectra, we can see that upon alloying by ion-beam-mixing, Pd $3d_{3/2}$ core level shifts are positive and Au $4f_{7/2}$ shifts are negative, in contrast to arc-melted Au-Pd alloys.

From these results, we can calculate the charge transfer in Au-Pd alloys. From these calculations, we can see that Au gains *sp* and loses an almost compensating number of *d* electrons in ion-beam-mixed Au-Pd alloys.

References

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