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XPS Study of Mn 2*p* and 3*s* Satellite Structures of Heusler Alloys: NiMnSb, PdMnSb, PtMnSb

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ABSTRACT - Half-metallic Heusler alloys (NiMnSb, PdMnSb, PtMnSb) have attracted much attention due to their unique electronic and magnetic structures. Spin-polarized band structure calculation predicts metallic behavior for the majority spin states and semiconductor behavior for the minority spin states. We have studied the electronic structures of these half-metallic Heusler alloys by core-level photoemission spectroscopy of Mn 2*p* and 3*s* XPS spectra. We found large intensities of Mn 2*p* satellites and 3*s* exchange splitting compared with other metal Mn-alloys. These satellite structure can be understood by applying Anderson impurity model. This fact supports the calculated spin projected partial density of states which suggests that the valence electrons be highly spin polarized near Fermi level and that the electrons involved with charge-transfer be mainly minority spin ones which have semiconducting band structure. The trend of charge transfer energies Δ from ligands (Sb 5*p*) to Mn 3*d*, obtained from our model fitting, is consistent with that calculated from spin projected partial density of state. Also the trend of *d*-*d* electron correlation energies U calculated from Mn Auger line L_3VV by Mg Kα source is compatible with that resulted from our model fitting. We fitted the Mn 3*s* curve in the same way as for insulating Mn compounds by using the same parameters calculated from Mn 2*p* curve fitting except for the Coulomb interaction energy *Q* between core hole and *d*-electrons. The 3*s* spectra were analyzed by combining the charge transfer model and a simple model taking into account the configuration mixing effect due to the intra-shell correlation. We found that the exchange interaction between 3*s* hole and 3*d* electrons is mainly responsible for the satellite of Mn 3*s* spectra. This is consistent with the neutron scattering data, which suggests local 3*d* magnetic moment. We find that the XPS analysis results of Mn 2*p* and 3*s* satellite structures of half-metallic Heusler alloys are very similar to those of insulating transition metal compounds.