High energy, high resolution photoelectron spectroscopy of $Co_2Mn_{1-x}Fe_xSi$.

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This work reports on high resolution photoelectron spectroscopy from the valence band of $Co_2Mn_{1-x}Fe_xSi$ (x = 0, 0.5, 1) excited by photons of about 8 keV energy. The measurements show a good agreement to calculations of the electronic structure using the LDA+U scheme. It is shown that the high energy spectra reveal the bulk electronic structure better compared to low energy XPS spectra. The high resolution measurements of the valence band close to the Fermi energy indicate the existence of the gap in the minority states for all three alloys. The results of this work are published in: Balke et al; Phys. Rev. B ***74*** (2006) 104405

The electronic structure of Co_2Mn_1-xFe_xSi was explored experimentally by means of high energy X-ray photoemission spectroscopy (HXPS). The measurements were performed at the beamline BL47XU and BL22XU of the synchrotron SPring-8 (Hyogo, Japan). The energy of the photoemitted electrons was analysed using Gammadata - Scienta R 4000-12kV electron spectrometers.

The electronic structure of the substitutional series of the quaternary Heusler compound $Co_2Mn_{1-x}Fe_xSi$ was investigated for x = 0, 0.5, 1 by means of photoelectron spectroscopy. All samples exhibit an $L2_1$ order, independent of the Fe concentration. In agreement with the expectation from the Slater-Pauling curve for half-metallic ferromagnets, the magnetic moment increases linearly with x from 5 μB to 6 μB. True bulk sensitive, high energy photoemission bearded out the inclusion of electron-electron correlation in the calculation of the electronic structure and gave an indirect advise on the gap in the minority states. The valence band spectra indicate an increase of the effective Coulomb exchange parameters with increasing Fe concentration.

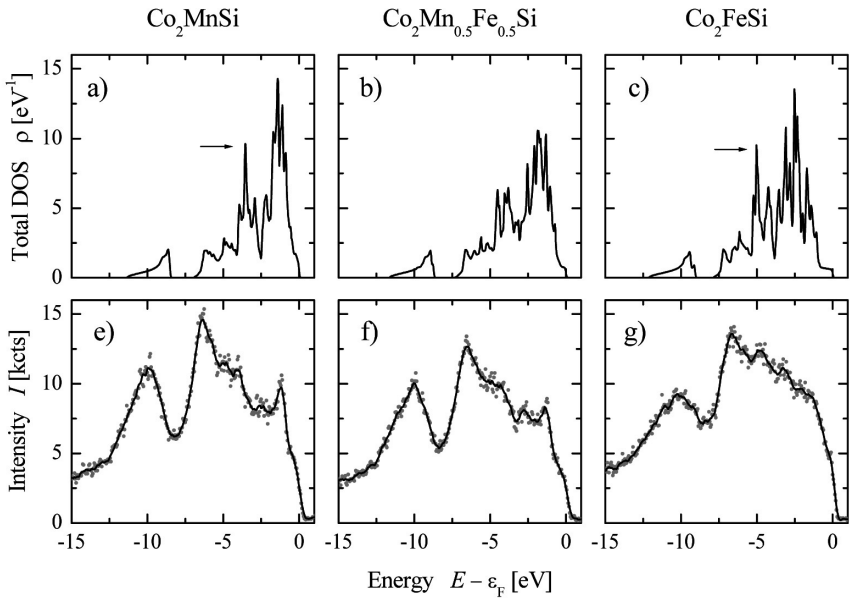

Figure 1. Density of states and high energy valence band spectra of $Co_2Mn_{1-x}Fe_xSi$.

The density of states is shown in panels (a)-(c) for x = 0, 0.5, and 1. The arrow points on a state contributing to a localised moment. The valence spectra are shown in panels (e) - (g). The spectra were excited by synchrotron radiation with 7.939 keV photon energy