

High energy photoemission from half-metallic ferromagnets.

Gerhard H. Fecher*, Benjamin Balke*, Claudia Felser*,
Keisuke Kobayashi**, Eiji Ikenaga**, Jung-Jin Kim**, and Shigenori Ueda**

* *Institut für Anorganische und Analytische Chemie,
Johannes Gutenberg - Universität, D-55099 Mainz, Germany*
** *Japan Synchrotron Radiation Research Institute (SPring-8/JASRI),
Kouto 1-1-1, Mikaduki-cho, Sayou-gun, Hyogo, 679-5198, Japan*

This work reports on the bulk properties of the quaternary Heusler alloy $\text{Co}_2\text{Mn}_{1-x}\text{Fe}_x\text{Si}$ with varying Fe concentration x . The electronic structure was explored by means of high energy photo emission spectroscopy at about 8 keV photon energy. This ensures true bulk sensitivity of the measurements. The experimental findings are discussed on the hand of self-consistent calculations of the electronic structure. To achieve good agreement with experiment, the calculations indicate that on-site electron-electron correlation must be taken into account.

The measurements were performed at the beamline BL47XU of the synchrotron SPring-8 (Hyogo, Japan). For the here reported experiments, a photon energy of 7939.15 eV has been employed. Under the present experimental conditions an overall resolution of 150-250 meV has been reached. The samples were comprehensively characterized by XRD, SQUID-magnetometry, and Mößbauer spectroscopy. The electronic structure was calculated by means of Wien2k using an LDA+U scheme to account for correlation.

High energy photoemission was taken from polycrystalline samples with $x=0, 0.5, \text{ and } 1$, as well as from a Co_2FeSi single crystal. Overall, the measured photoelectron spectra agree well with the calculated density of states and principally verify the use of the LDA+U scheme. In particular, the shape of the spectra close to the Fermi Energy can be explained by the occurrence of a gap in the minority states and thus points indirectly on the half-metallic state of the compounds investigated here by photo emission. Both, valence band spectra and measurement of the magnetic properties indicate an increase of the effective Coulomb exchange parameters with increasing Fe concentration.