Spectroscopy of the valence band by high energy photoemission

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This work reports on the bulk properties of the quaternary $C1_b$ compounds $CoTi_{1-x}Fe_xSb$ with varying Fe concentration *x*. The electronic structure was explored by means of high energy photoemission spectroscopy at 2 – 6 keV photon energy. This results in an increase of the bulk sensitivity of the measurements. The experimental findings are discussed on the hand of self-consistent calculations of the electronic structure.

The experiment was carried out at the high-energy KMC-1 beamline at BESSY (Berlin, Germany) using a new developed hemispherical analyzer with a mean radius of 225 mm (SPECS, Berlin). For the here reported experiments, variable photon energies in the range of 2 keV to 6 keV were exploited. The resolution ranges from 200 meV to 3 eV using a Si(111) double crystal monochromator. Using a Si(422) double crystal, the resolution is 300 meV at about 6 keV. Under the present experimental conditions an overall resolution (monochromator plus analyzer) of 450 meV has been reached at 6 keV measured at the Au 4f and 240 meV at 2 keV measured at the Au Fermi edge at room temperature. The latter reveals the high resolution of the analyzer. The samples were comprehensively characterized by XRD, SQUID-magnetometry, and Mößbauer spectroscopy. The electronic structure was calculated by means of Wien2k as well Munich SPRKKR with a CPA scheme to allow for a random distribution of the Fe atoms.

High energy photoemission spectra were taken from polycrystalline $CoTi_{1-x}Fe_xSb$ samples with x=0 and 0.05, as well as from several X_2YZ Heusler compounds. Overall, the measured photoelectron spectra agree well with the calculated density of states. The emission from the low lying *sp* bands shows a less pronounced decrease of the intensity with increasing photon energy compared to the emission from the *d* bands. The energy range close to the Fermi energy is strongly enhanced at low photon energies, giving advice on life-time effects. At 2.5 keV, however, the complete *d*-band is already detectable, in contrast to the emission excited by Al K_{alpha} radiation. The results prove, in comparison to emission from the core-level, the high bulk sensitivity of high energy photo emission in valence band spectroscopy.