Detection of the Valence Band in Buried Co_2MnSi-MgO Tunnel Junctions by Means of Hard X-Ray Photoemission Spectroscopy

The Co_2YZ (Y = transition metal, Z = main group element) Heusler compounds have attracted scientific and technological interest for their potential use as materials for magneto-electronic devices [1]. From *ab initio* calculations it was concluded that these compounds have peculiar transport properties because the minority-spin density at the Fermi energy ε_F vanishes, wherefore they are called half-metallic ferromagnets. One major technology where Co_2 based Heusler compounds are used is on tunneling magneto resistive (TMR) junctions. High TMR ratios of 179% at room temperature and 683% at 4.2 K were demonstrated for fully epitaxial magnetic tunnel junctions with Co_2MnSi films as both lower and upper electrodes and MgO tunnel barrier [2]. To develop high performance spintronic devices with Heusler compound based thin films as ferromagnetic electrodes, it is essential to clarify the electronic structures of these films interms of the half-metallic nature.

For the present study [3], multi component thin film arrangements were used (see [2,3] and references there for details). Polycrystalline bulk material was used for comparison (see [4] for details). The HAXPES (hard X-ray photoemission spectroscopy) experiments were performed at beamline **BL15XU**. The photon energy was fixed at 5.94677 keV using a double crystal monochromator and a Si(333) post monochromator. The photo emitted electrons were analyzed for their kinetic energy and detected by means of a hemispherical analyzer (Scienta). The overall energy resolution (monochromator plus analyzer) was set to 250 meV, as verified by spectra of the Au valence band at ε_F. Spectra close to ε_F were taken with a resolution of 150 meV. The angle between the electron spectrometer and photon propagation is fixed at 90°. The photons are p-polarized. For the thin films, a near normal emission ($\theta = 2°$) detection angle was used.

A wide energy scan photoelectron spectrum of the Co_2MnSi/MgO thin film system is shown in Fig. 1. It demonstrates the demanding task of high energy valence band spectroscopy. The intensity of the valence band is about 200 times lower compared to the dominant emission from the Co 2*p* states and becomes only weakly visible in the spectrum taken with reduced energy and intensity scales.

Figure 2 compares valence band spectrum of bulk Co_2MnSi to spectra from a Co_2MnSi layer buried underneath MgO/AlO_x with different thickness of the MgO interlayer. The spectrum of the thin film in Fig. 2(b) agrees well with the bulk sample. However, the emission is strongly suppressed in the film with the 20 nm thick MgO layer. In particular, the peak in the density of states at -1.3 eV is clearly resolved. The low lying *s*-band below -8 eV is only seen in Fig. 2(a) and 2(b). This part, in addition to the lower parts of the *p*- and *d*-bands, is covered by the emission from oxygen 2*p* states of MgO in Fig. 2(c) where the oxide is 20 nm thick. The similar structure of the valence band close to ε_F in the thin films and the bulk material is obvious.

In Fig. 3, the valence band spectra for different MgO thicknesses are directly compared by scaling

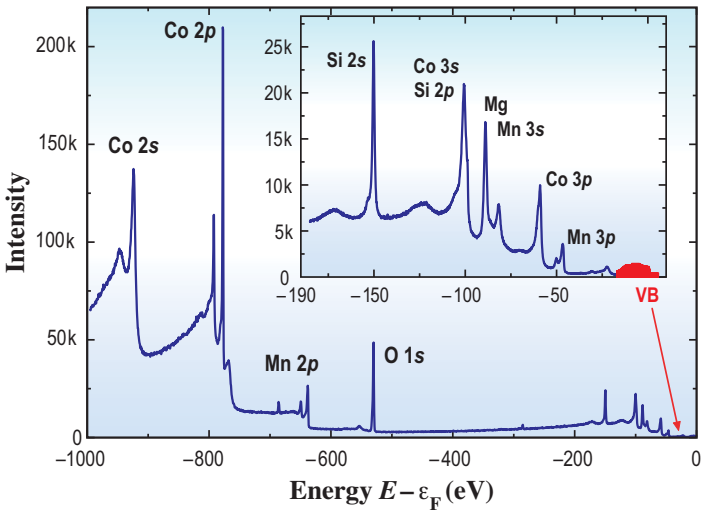

Fig. 1. High kinetic energy survey spectrum of Co_2MnSi/2 nm MgO/1 nm AlO_x. The inset shows the energy range of the semi-core level and the valence band.

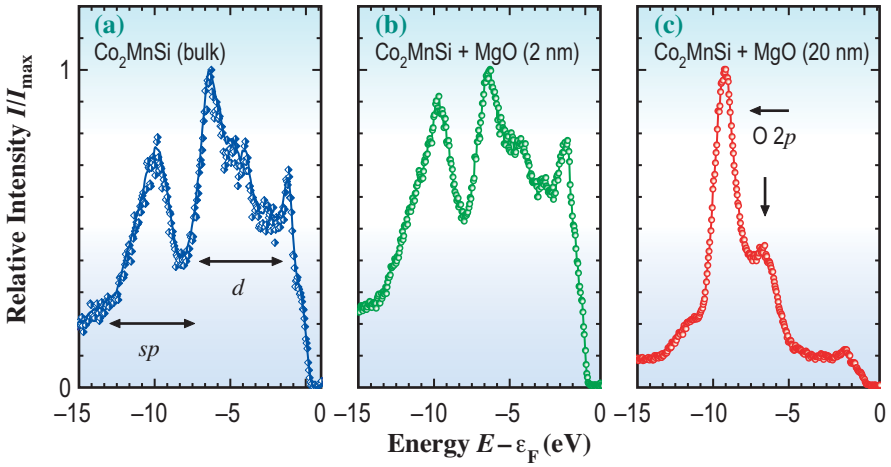

Fig. 2. High kinetic energy photoemission spectra of buried Co_2MnSi. The spectrum from bulk material **(a)** is compared to thin films with different thickness 2 nm **(b)**, 20 nm **(c)** of the MgO interlayer. Co_2MnSi valence bands and oxygen 2*p*-states are indicated by arrows in **(a)** and **(c)**, respectively.

up the intensity of the 20 nm layer. The identical structure of the spectra, in particular close to the Fermi energy, is easily recognized. The high intensity with a center at about -1.3 eV is due to emission from flat *d*-bands belonging to minority states localized in the Co planes and the highly localized Mn *d* majority states (e_g). The Co t_{2g} like states mainly define the upper energy of the minority valence bands, whereas the lower intensity at the Fermi energy arises from steep delocalized majority *d*-bands with t_{2g} character.

The obtained result confirms the promise of an epitaxial, single-crystalline Co_2-based Heusler compound film as a ferromagnetic electrode for spintronic devices. In particular it was shown that buried Co_2MnSi films exhibit the same valence density of states like bulk samples that is typical for halfmetallic ferromagnets for spintronic applications. In summary, the present study demonstrates the feasibility of HAXPES to explore the valence band electronic structure in metallic layers deeply buried under oxide films.

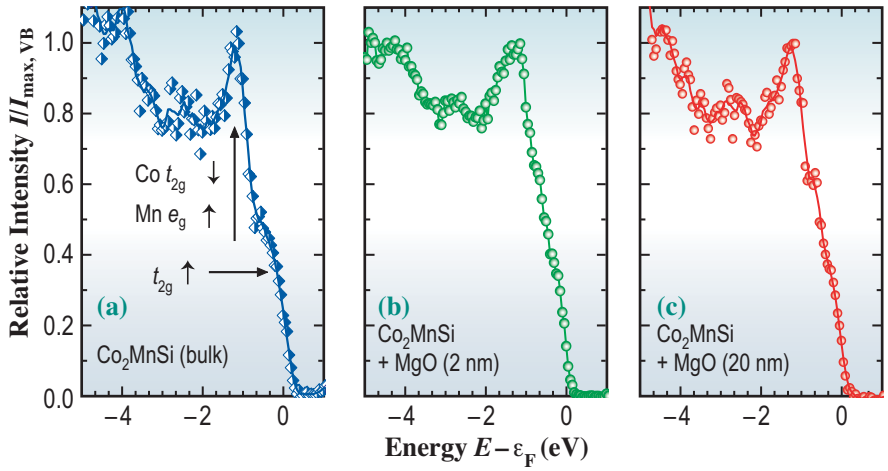

Fig. 3. Comparison of the Co_2MnSi valence band spectra close to ε_F. *d*-states with different character are indicated by arrows.

Gerhard H. Fecher [a,*], Claudia Felser [a] and Keisuke Kobayashi [b]

[a] Institute of Inorganic and Analytical Chemistry, The Johannes Gutenberg University, Germany
[b] Dept. of Materials Infrastructure, Beamline Station, NIMS

*E-mail: fecher@uni-mainz.de

References

[1] C. Felser *et al.*: Angew. Chem. Int. Ed. **46** (2007) 668.
[2] T. Ishikawa *et al.*: J. Appl. Phys. **103** (2008) 07A919.
[3] *G.H. Fecher, B. Balke, A. Gloskowskii, S. Ouardi, C. Felser, T. Ishikawa, M. Yamamoto, Y. Yamashita, H. Yoshikawa, S. Ueda, K. Kobayashi: Appl. Phys. Lett.* ***92*** *(2008) 193513.*
[4] B. Balke *et al.*: Phys. Rev. B **74** (2006) 104405.