A.10: Electronic structure of Co_2MnSn Heusler alloy investigated by RPES using Indus-1 and *ab-initio* calculations

Half metallic ferromagnets are important for spintronic device applications because of their metal like band structure in one spin states and a band gap in the other one. Among various classes of half-metals, Co-based full Heusler alloys have attracted interest due to their structural matching with standard semiconductor substrates and high Curie temperature (Tc). Co_2MnSn, which is a member of this family of half-metals, crystallizes in cubic structure with lattice parameters a = b = c = 6Å, T_C= 829 K and total magnetic moment of 5.08 μ_B/f.u. The experimental value of spin polarizations (P) measured at 4.2 K is reported to be 60% in this system, which is smaller than the calculated value of 75%. The motivation of the present work is to understand the reasons for the reported experimental low value of P in this system. Since P is mainly governed by the electrons at the Fermi level (E_F), the valence band (VB) electronic structure of Co_2MnSn has been investigated using Resonant Photoemission Spectroscopy (RPES) across Mn and Co 3p-3d resonances, to determine the partial density of Co and Mn 3d states in the VB. The detailed analysis of the RPES results and its comparison with the *ab-initio* GGA + U level calculations indicate the presence of extra e- - e- Coulomb correlation "U" on the Mn 3d states, which in turn results in reduction of the spin polarization at the E_F.

Polycrystalline sample of Co_2MnSn was prepared by arc melting technique. X-ray diffraction studies showed ordered $L2_1$ (FCC) structure and low temperature magnetic measurement using SQUID showed total magnetic moment of 5.05 μ_B/f.u. RPES measurements were carried out at AIPES beamline (BL-2) of Indus-1. Core level XPS spectra of in-situ scraped sample showed negligible contribution from oxygen and carbon.

The VB PES spectra were recorded at excitation energies in the range of 45 eV to 70 eV. VB spectra at excitation energies close to Mn 3p and Co 3p threshold are shown in Fig.A.10.1. VB features at fixed binding energies (BE) in the spectra are marked as A, B, C, D, E and F. Due to the change in photoemission cross-section of the VB states (mostly the 3d states of Mn and Co) with excitation energies, the spectral shape changes. In order to locate the positions and the nature of the Mn and Co 3d partial density of states (PDOS) in the VB, the intensity of the features at fixed BE positions is plotted as a function of excitation energy, which is referred to as Constant Initial State (CIS) plot and is shown in Fig.A.10.2. The CIS plots are fitted with Fano line profiles of the form $f = (q+\varepsilon)^2/1+\varepsilon^2$ *and* $\varepsilon = (h\nu - E_0)/\Gamma$, where q is Fano asymmetry parameter, Γ is spectral width and E_0 is the Fano resonance energy. Analysis of the CIS plots along with the fitted Fano parameters show the absence of Mn 3d states at E_F, and these states are localized at ~ - 3 eV below E_F. In contrast, the Co states are itinerant in nature and present at E_F and extend up to ~ - 2.5 eV.

The experimentally observed PDOS and magnetic moments were compared with the *ab-initio* calculations within the GGA and GGA + U formalism. Our experimental results show good matching with the GGA + U approach. With an increase in U on the Mn site in the calculations, the Mn 3d PDOS shifts towards higher BE and for U = 3 eV, the energy position matches well with the experiment. At the same time, the Co 3d PDOS increases at E_F. Moreover, theoretically obtained total magnetic moment of 5.12 μ_B/f.u. and the spin polarization of 65% for U = 3 eV are in good agreement with the experimental value of total magnetic moment of 5.05 μ_B/f.u. and the spin polarization of 60% at 4.2 K as reported in literature. Thus the combined results of the RPES measurements and *ab-initio* calculations help in understanding the reduced spin polarization in this system.

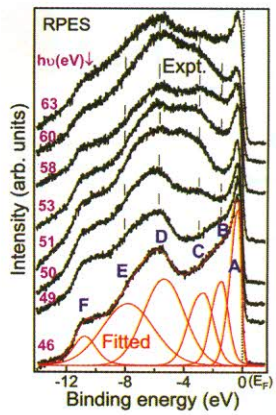

Fig. A.10.1: The PES spectra of Co_2MnSn recorded at different excitation energies across 3p threshold along with the fitting (red solid lines).

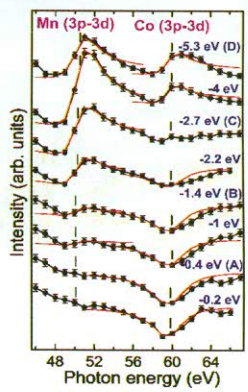

Fig. A.10.2: The CIS spectra of the VB features as a function of photon energy. The red line shows the fitting with the Fano line shape.

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