

**Experiment title:**

Test of a hypothesis of "half-metallic ferromagnets" and study of spinsubsystems of valence electrons in Heusler alloys

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Report:

We have studied magnetic circular dichroism (MCD) in Mn $L_{2,3}$ X-ray emission and absorption for Heusler alloys NiMnSb and Co_2MnSb . Very intense resonance Mn L_3 emission is found at the Mn $2p_{3/2}$ threshold and is attributed to a peculiarity of threshold excitation in materials with half-metallic character. We have developed a theoretical model for the description of this resonance scattering of polarized x-rays. The model is based on the calculated partial Mn 3d-density of states for NiMnSb which has the following main features: (i) a strong exchange splitting (about 2 eV) which affects the valence states distribution, (ii) spin-down states have a strong peak above the Fermi level (spin-up states are absent in this region and located below the Fermi level). This peak can be used as a trap for an excited core electron with a spin selectivity and is responsible for the high intense re-emission peak in XES.

Mn 2p X-ray emission spectra (XES) measured at the L_3 threshold ($E_{\text{exc}}=640.5$ eV), L_2 threshold ($E_{\text{exc}}=652$ eV) and far above threshold ($E_{\text{exc}}=680$ eV) show quite different fine structures (see figure below). The Mn L_3 XES measured at $E_{\text{exc}}=640.5$ eV, which corresponds to the $3d\ 4s$ to $2p_{3/2}$ transition, has two subbands A and B located at 637.0 and 640.5 eV, respectively. Both subbands show dichroism with the same sign as is found for the Mn L_3 XAS. The MCD effect reaches its maximum at emission energy $E=640.5$ eV which exactly corresponds to the Mn L_3 threshold. The double peak structure revealed in Mn 2p XES can be a result of superposition of spectra of normal emission (A) and elastic x-ray scattering, known

as re-emission (B). The intensity of the B subband is found to be about 1.5 times higher than that of the A subband. The Fermi level (estimated from Mn2p_{3/2} core level photoemission), is at the intensity minimum between these two subbands which means that the B subband corresponds to re-emission from unoccupied 3d states which are populated during near-threshold excitation of the Mn 2p_{3/2} electron to the conduction band. X-ray re-emission is usually observed in spectra of insulators but in the case of a Heusler alloy, it have been never seen with so high intensity.

The MCD effects that we have found in x-ray emission and absorption of Heusler alloys is evidence of a strong exchange splitting of Mn 3d-states with different spin projections. Both the existence of an energy gap in the spin-down projected Mn 3d-states and weak hybridization of Mn 3d electrons with its nearest neighborhood conduce to the suppression of the excited electron relaxation. Therefore our findings can be considered as a spectroscopic evidence of the half-metallic character of electronic structure of Heusler alloys. Also the observed giant re-emission peak in the Mn XES at the L₃ threshold is assumed to be due to the half-metallic character of Heusler alloys. The long lifetime of the excited states (which is necessary for intense re-emission) is provided by the limitation of the radiationless relaxation of excited electrons at the Fermi level and their delay on the atom by the field of the core hole. In Heusler alloys with a large local magnetic moment there is a possibility of revealing such a suppression of the relaxation due to strong exchange splitting, typical for half-metallic systems.

