The half-metallic ferromagnet $\text{Co}_2\text{Mn}_{0.5}\text{Fe}_{0.5}\text{Si}$. 

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Abstract

Electronic structure calculation were used to predict a new material for spintronic applications. $\text{Co}_2\text{Mn}_{0.5}\text{Fe}_{0.5}\text{Si}$ is one example which is stable against on-site correlation and disorder effects due to the position of the Fermi energy in the middle of the minority band gap. Experimentally the sample were made exhibiting $L2_1$ structure and a high magnetic order.

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I. INTRODUCTION

Half-metallic ferromagnets have been proposed as ideal candidates for spin injection devices because they have been predicted to exhibit 100% spin polarization at the Fermi energy ($\epsilon_F$) [1]. From the applications point of view, a high Curie temperature for a half-metallic ferromagnet may be an important condition. For this reason, Heusler alloys ($L2_1$ structure) have recently attracted great interest. Some of these alloys exhibit high Curie temperatures and, according to theory, should have a high spin polarization at the Fermi energy [2]. Calculations also show that anti-site disorder will destroy the high spin polarization [3], implying that precise control of the atomic structure of the Heusler alloys is required.

The Heusler alloy Co$_2$MnSi has attracted particular interest because it is predicted to have a large minority spin band gap of 0.4 eV and, at 985 K, has one of the highest Curie temperature, among the known Heusler compounds [4, 5]. Structural and magnetic properties of Co$_2$MnSi have been reported for films and single crystals [6, 7, 8]. From tunnelling magneto resistance (TMR) data with one electrode consisting of a Co$_2$MnSi film Sakuraba et al. [9] measured a TMR ratio of 159% at 2K and $\approx 70$% at 300K. If using Co$_2$FeSi as one electrode Inomata et al. [10] obtained TMR ratios of 60% at 5K and 41% at 300K.

An important quantity for the application of the half-metallic ferromagnets is the size of the gap in the minority states and the position of $\epsilon_F$ inside of the gap. Small gaps may be easily destroyed by temperature effects or quasi-particle excitations [11]. The half-metallicity may also be easily destroyed if $\epsilon_F$ is located close to the band edges, either of the minority valence or conduction bands.

The recent TMR results [9, 10] show that electrodes made of Heusler compounds result in high TMR ratios at low temperatures but the temperature dependence is still a challenge which has to be solved to use Heusler electrodes in applications. The present investigation focuses on searching for a mixed compound where the half-metallic behaviour is stable against temperature effects.

The self-consistent electronic structure calculations were carried out using the full potential linearized augmented plane wave method (FLAPW) as provided by Wien2k [12]. The LDA+$U$ method [13] was used to account for on-site correlation at the transition metal sites. Semi-empirical values corresponding to 7.5% of atomic values of Coulomb-exchange
FIG. 1: Dependence of the minority band gap on the Fe concentration $x$ in Co$_2$Mn$_{1-x}$Fe$_x$Si. The extremal energies of the gap involving states are shown. The shaded areas indicate the region of half-metallic ferromagnetism. Lines are drawn for clarity.

parameter have been used as suggested in our previous publication [14].

II. RESULTS AND DISCUSSION

A. Electronic properties

The size of the minority band gap and position of $\epsilon_F$ can be seen from the calculated energies displayed in Fig. 1 for the Heusler alloy Co$_2$Mn$_{1-x}$Fe$_x$Si. In Co$_2$MnSi, $\epsilon_F$ is close to the top of the valence band. In Co$_2$FeSi, the situation is different and $\epsilon_F$ is near to the bottom of the conduction band. Both of the compounds are at the two corners of the gap. In Co$_2$Mn$_{0.5}$Fe$_{0.5}$Si $\epsilon_F$ is directly in the middle of the minority band gap and therefore this compound should be more stable against temperature effects or quasi-particle excitations compared to pure Co$_2$MnSi and Co$_2$FeSi.
FIG. 2: (a) XRD spectra for Co$_2$Mn$_{0.5}$Fe$_{0.5}$Si. The spectra were excited by Mo K$_\alpha$ radiation. (b) $^{57}$Fe Mößbauer spectrum of Co$_2$Mn$_{0.5}$Fe$_{0.5}$Si. The spectrum was taken at 290K and excited by a $^{57}$Co(Rh) source. Solid lines are results of a fit to determine the sextet and singlet contributions and to evaluate the hyperfine field.

B. Structural and magnetic properties

Co$_2$Mn$_{0.5}$Fe$_{0.5}$Si samples were prepared by arc melting of stoichiometric amounts of the constituents in an argon atmosphere at $10^{-4}$ mbar. The polycrystalline ingots were then annealed in an evacuated quartz tube at 1273 K for 21 days. The samples exhibiting the Heusler type $L_2_1$ structure with a lattice parameter of 5.64 Å (see Fig. 2(a)). Another proof of the high order of the samples are the results from the $^{57}$Fe Mößbauer spectra taken of the samples (see Fig. 2(b)). The spectrum is dominated by an intense sextet with a line width of approximately (0.14 ± 0.01) mm/s. In addition to the sextet, a much weaker line at the centre of the spectrum is visible. Its contribution to the overall intensity of the spectrum is approximately 3.5 %. The origin of the singlet may be caused by anti-site disorder leading to a small fraction of paramagnetic Fe atoms. The hyperfine field (HFF) at the Fe sites amounts to 26.5 $\times$ $10^6$ A/m. For more details and other properties of the whole series of Co$_2$Mn$_{1-x}$Fe$_x$Si with the Fe concentration ranging from $x = 0$ to 1 in steps of 0.1 see Ref. 15.
III. SUMMARY

Electronic structure calculations predicted the Heusler compound Co$_2$Mn$_{0.5}$Fe$_{0.5}$Si due to the position of $\epsilon_F$ in the middle of the minority band gap as very stable against any kind of effects destroying the halfmetallicity and therefore well suited for spintronic applications. Polycrystalline samples were prepared exhibiting $L2_1$ structure and a high magnetic order.

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