The efficient spin injector scheme based on Heusler materials.

Stanislav Chadov\textsuperscript{1}, Tanja Graf\textsuperscript{1}, Kristina Chadova\textsuperscript{2}, Xuefang Dai\textsuperscript{1}, Frederick Casper\textsuperscript{1}, Gerhard H. Fecher\textsuperscript{1}, Claudia Felser\textsuperscript{1}

\textsuperscript{1}Institut für Anorganische und Analytische Chemie, Johannes Gutenberg - Universität, 55099 Mainz, Germany
\textsuperscript{2}Dept. Chemie und Biochemie, Ludwig Maximilians - Universität, 81377 München, Germany

We present the rational design scheme intended to provide the stable high spin-polarization at the interfaces of the magneto-resistive junctions by fulfilling the criteria of structural and chemical compatibilities at the interface. This can be realized by joining the semiconducting and half-metallic Heusler materials with similar structures. The present first-principal calculations verify that interface remains half-metallic if the nearest interface layers effectively form a stable Heusler material with the properties intermediate between the surrounding bulk parts. This leads to a simple rule for selecting the proper combinations.

PACS numbers: 71.20.-b,75.47.Np,85.75.-d
Keywords: magneto-resistance, half-metal, spin polarization

New spintronic devices as magneto-resistive (MR) random access memory or read-out heads of hard disk drives \cite{1, 2} require materials exhibiting thermally stable high degree of the spin-polarization needed for the efficient spin injection \cite{3, 4}. Rich source are the half-metals (HM) provided the family of Co\textsubscript{2}MnSi thin film where the HM state is preserved to the strong surface-subsurface coupling \cite{10}. In this context the importance of studies focusing on half-metallic properties of the interface is crucial for designing new efficient spin-injecting devices.

The extremely wide range of electronic properties and rather similar geometry exhibited by the Heusler family provide the straightforward way to construct the whole spintronic device by using only Heusler building blocks. For example, the first-principle calculations \cite{10} for Co\textsubscript{2}CrAl(Si)/Co\textsubscript{2}CrAl(001) Heusler GMR junctions predicted the spin-polarization of about 80%. In the following we propose the systematic scheme to search for such proper pairs of Heusler materials for TMR/GMR junctions and justify it by the first-principle band structure calculations.

The suitable combinations can be derived from the same parent material. By making various mixtures one can produce the series of new Heusler materials with smoothly varying electronic properties ranging from half-metallic to semiconducting and non-magnetic. Much helpful in such design is the so-called Slater-Pauling rule \cite{21, 22} which states the linear dependency of the unit cell magnetic moment as a function of the valence electron number.

We will sketch our idea in details on example of the well-known Heusler Co\textsubscript{2}MnAl \cite{22} which fulfills the basic requirements of the efficient spin-injecting material. Band structure calculations \cite{23, 24} characterize it as the HM ferromagnet with magnetic moment of 4 \mu\textsubscript{B} in agreement with experiment. Its measured Curie temperature is T\textsubscript{C} = 698 K \cite{23, 25}. In order to derive a SC material with a similar lattice it is enough to substitute one Co atom by V. It can be synthesized, for example, by 50\% mixing of Mn\textsubscript{2}VAl \cite{27} and Co\textsubscript{2}VAl \cite{28}. The resulting CoMnVAl (SC) compound with 24 valence electrons is non-magnetic in agreement with the Slater-Pauling rule. The calculated bulk band structures of both Co\textsubscript{2}MnAl and CoMnVAl are shown in Figure 1(a).

To verify which sequence of stacking layers conserves...
Figure 1. (color online) (a) Calculated bulk band structures of the typical candidate materials: the half-metallic ferromagnet Co$_2$MnAl and the nonmagnetic semiconductor CoMnVAl. In case of Co$_2$MnAl the bands of the gapped minority-spin channel are made thicker. The Fermi level is marked by the dashed line. (b) Structure of the supercell. Subsections marked as HM (half-metal) or SC (semiconductor) represent the complete Heusler blocks each containing four atomic layers.

As it follows from the spin-resolved DOS curves (Figure 2) the spin polarization indeed depends critically on the way of stacking: independently on the system size the half-metallicity is preserved for the system with Co-Co/V-Al and Co-Mn/Mn-Al interfaces and in case of Co-Co/Mn-Co and Mn-Al/Al-V interfaces it is destroyed. The substantially higher total energy (by about 3 mRy) of the supercell with “destructive” interfaces indicates their relative instability. In the “destructive” case the minority-spin DOS at the Fermi level for the larger supercell (HM) is noticeable lower than for the smaller one, (HM). This obviously tells that the “destructive” states originate locally from the interface layers. This can be viewed in more details by considering the layer-resolved DOS($E_F$) and the magnetization profiles (Figure 3).

At Co-Co/V-Al (a), and Co-Mn/Mn-Al (b) interfaces, the spin polarization increases. At the same time at Co-Co/Mn-Co (c) and Al-V/Mn-Al (f) interfaces it is destroyed. The reason can be qualitatively understood by comparing the materials effectively formed on the interfaces with their ideal bulk equivalents, since the properties of Heuslers in a large extent originate from the nearest neighbor coupling. Indeed, Co-Co/V-Al and Co-Mn/Mn-Al interfaces correspond to the existing Heusler compounds with 2 $\mu_B$ magnetic moment and high spin polarization: Co$_2$VAL [24, 27] and Mn$_2$CoAl [31]. As it follows from Figure 2, except of the overall demagnetization, the magnetic structure of these interfaces is rather...
FIG. 3. (color online) Black solid line (with opened circles) represent the layer-resolved DOS at the Fermi energy with positive values referring to the majority-spin, negative to the minority-spin channels (a, b, e, f) and the magnetic moments (c, d, g, h) calculated for HM/SC-supercells (HM = CoMnAl, SC = CoMnVAl). Gray bars show the corresponding values calculated for the bulk HM and SC materials. Colored bars mark the atom-projected contributions within the first nearest and next-nearest interface layers (each layer contains two atoms). Vertical red dashed lines mark the interface borders.

The atomic moments are approximately 2.5, 0.78 and −0.68 µB, comparing to 3, 1 and −2 µB for Mn, Co and the second Mn atom respectively.

The other two compounds, AlVMnAl and CoCoMnCo which form the “destructive” interfaces, are equivalent to MnVAl\(_2\) and Co\(_3\)Mn which to our knowledge do not exist in the Heusler structure. Indeed, as we mentioned above, their calculated total energies are noticeably higher than for “constructive” interfaces and they exist mainly due to the coupling with the outer layers.

Thus we can conclude that the “constructive” interface (preserving the half-metallicity) can be formed if the effective interface composition would correspond to the stable bulk material with the intermediate properties between the left- and right-side materials, as in the sequence of Co\(_2\)MnAl/Co\(_2\)VAl/CoMnVAl which exhibit the bulk magnetic moments of 4, 2 and 0 µB, respectively. The experimentally suitable method to obtain the 24-electron SC material would be through a mixture of two stable HM ferromagnets with numbers of valence electrons larger and smaller than 24.

This situation is rather general. By applying similar first-principle analysis we have justified the analogous situation for the series of other Co\(_2\)-based Heusler materials. The pairs of “constructive” and “destructive” interfaces were found also for Co\(_2\)MnZ/CoMnTiZ (Z=Si, Ge, Sn) and Co\(_2\)FeZ/CoFeTiZ (Z=Al, Ga) (more details can be found in Ref. [32]). For the “constructive” case the effective interface compounds will correspond to Co\(_2\)TiZ group of half-metallic ferromagnets with magnetic moments of 1 µB.

The particularly selected (001)-orientation of the interfaces is also not unique. For example, we have verified that the same rules apply for (111)-orientation as well. This goes in line with the general idea that the most important condition is the relative smooth change of properties while going from the ferromagnetic half-metallic to a non-magnetic semiconducting Heusler system.

ACKNOWLEDGMENTS

Financial support by DFG Research unit FOR 559 (projects P01, P07), the Bundesministerium für Bildung und Forschung BMBF (Project MultiMag), the Graduate School of Excellence MAInZ and the DFG/ASPI-MATT project (unit 1.2-A) are gratefully acknowledged.

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