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Towards half-metallic interfaces: Co_2CrAl/InP contacts

Iosif Galanakis

Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

E-mail: I.Galanakis@fz-juelich.de

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Abstract

Although the interest in half-metallic Heusler alloys, likely to be usable in spintronic applications, has grown considerably, their interfaces with semiconductors show very low spin polarization. I identify mechanisms which can keep high spin polarization at the interface (more than 80% of the electrons at the Fermi level of majority spin) although the half-metallicity is lost. The large enhancement of the Cr moment at the interface between a CrAl-terminated $Co_2CrAl(001)$ spacer and the InP(001) semiconductor weakens the effect of the interface states, resulting in this high spin polarization. On the other hand, the Co_2CrAl/InP interfaces made up by a Co layer and either an In or a P one show a severe decrease of the Co spin moment, but Cr in the subinterface layer is bulklike and the resulting spin polarization is similar to that of the CrAl-based interfaces.

1. Introduction

A central problem in the field of magnetoelectronics or spin electronics [1] is the spin injection from a metal into a semiconductor [2]. In principle it is possible to achieve 100% spin polarized injected current if the magnetic lead is a half-metallic material. These compounds are ferromagnets where there is a band gap at the Fermi level (E_F) for the minority spin band while the majority spin band is metallic. In such a compound the behaviour of the interface between the half-metal and the semiconductor is of great importance since interface states can kill the half-metallicity. Although from the point of view of transport a single interface state does not affect the magnetoconductance since the wavefunction is orthogonal to all bulk states incident on the interface, its interaction with other defect states makes the interface states conducting.

NiMnSb, a member of the Heusler alloys group, was the first material to be predicted to be a half-metal in 1983, by de Groot and his collaborators [3]. There exist several other *ab initio* calculations on NiMnSb reproducing the results of de Groot [4] and Galanakis *et al* showed that the gap arises from the hybridization between the d orbitals of the Ni and Mn atoms [5]. Its

half-metallicity seems to be well established experimentally in the case of single crystals [6]. Also the so-called full-Heusler alloys such as Co_2MnGe or Co_2CrAl were predicted to be half-metals [7] and the gap in the case of these materials arises from states located exclusively at the Co states which are non-bonding with respect to the other atoms [8].

Although films of both half- and full-Heusler alloys attracted a lot of experimental attention [9–11], theoretical calculations for the interfaces of these materials with semiconductors are few. All *ab initio* results agree that half-metallicity is lost at the interface between the Heusler alloy and the semiconductor [12–14] but the interface dependence of the spin polarization has not been studied in detail. Even if half-metallicity is lost, it is possible that a high degree of spin polarization remains at the interface, as will be shown in this contribution, and these structures remain attractive for realistic applications.

In this communication I study the (001) interfaces of the half-metallic Co_2CrAl Heusler alloy with InP. This Heusler alloy has the same experimental lattice constant as InP within 1%. I take into account all possible interfaces and show that in all cases a high degree of spin polarization remains at the interface. In section 2 I discuss the structure of the interface and the computational details and in section 3 I present and analyse my results. Finally in section 4 I summarize and conclude.

2. Computational method and structure

In the calculations I used the full-potential version of the screened Korringa–Kohn–Rostoker (KKR) Green function method [15, 16] in conjunction with the local spin-density approximation [17] for the exchange–correlation potential [18]. The results of Picozzi *et al* [14] and Debernardi *et al* [13] have shown that atomic positions scarcely change at the interface and the dominant effect is the expansion or the contraction of the lattice along the growth axis, to account for the in-plane change of the lattice parameter. In the case of the interfaces presented here the compounds have similar lattice parameters and thus perfect epitaxy can be assumed. To simulate the interface I used a multilayer consisting of 15 layers of the half-metal and 9 semiconductor layers. This thickness is enough to ensure that the layers in the middle of both the half-metallic part and the semiconducting one exhibit bulk properties. I have also converged the **k**-space grid, the number of energy points and the tight binding cluster so that the properties of the interfaces do not change (similar DOS and spin moments). So I have used a $30 \times 30 \times 4$ **k**-space grid to perform the integrations in the first Brillouin zone. To evaluate the charge density one has to integrate the Green function over an energy contour in the complex energy plane; for this, 42 energy points were needed. A tight binding cluster of 65 atoms was used in the calculation of the screened KKR structure constants [19]. Finally, for the wavefunctions I took angular momentum up to $\ell_{\max} = 3$ into account and for the charge density and potential up to $\ell_{\max} = 6$.

Co_2CrAl crystallizes in the $L2_1$ structure. The structure of the interface is shown in figure 1. $L2_1$ structure is similar to the zinc-blende structure and thus perfect epitaxy at the interface can be considered. There are several combinations at the interface; e.g. at the Co_2CrAl/InP contact the interface can be either a Co/In one, Co/P, CrAl/In or CrAl/P. I will keep this definition throughout the paper to denote different interfaces. Finally, I should mention that since my multilayer contains 15 half-metal and 9 semiconductor layers, I have two equivalent surfaces on either side of the half-metallic spacer.

3. Results and discussion

Interfaces with respect to simple surfaces are more complex systems due to the hybridization between the orbitals of the atoms of the metallic alloy and the semiconductor at the interface.

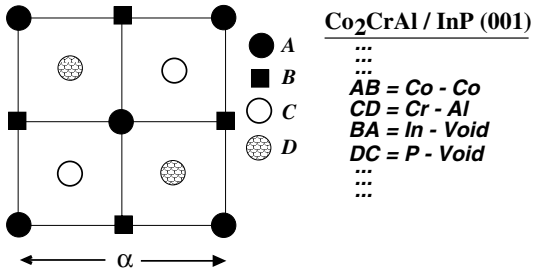

Figure 1. A schematic representation of the (001) interface between Co_2CrAl and InP. There are several different combinations at the interface which can be either Co/In, Co/P, CrAl/In (shown in the figure) or CrAl/P. Note that there are two inequivalent cobalt atoms at the interface layer or the subinterface layer. One is sitting at the 'bridge' site, continuing the zinc-blende structure of the semiconductor, and the other at the 'antibridge' site.

Thus results obtained for surfaces such as the ones in [21] cannot be easily generalized for interfaces since for different semiconductors different phenomena can occur. In Heusler alloy (001) surfaces, the appearance of surface states kills the half-metallicity [21], but there are cases such as the CrAl-terminated (001) surface of Co_2CrAl where the spin polarization is as high as 84%. The case of the multilayers made of half-metallic zinc-blende CrAs or CrSe compounds and binary semiconductors is simpler since for these interfaces the large enhancement of the Cr spin moment kills the interface states [20].

In the discussion which follows, the spin polarization, P, at the Fermi level is simply defined with respect to the density of states $n(E)$ as $P = \frac{n^{\uparrow}(E_F)-n^{\downarrow}(E_F)}{n^{\uparrow}(E_F)+n^{\downarrow}(E_F)}$ where $\uparrow$ stands for the majority electrons and $\downarrow$ for the minority electrons. This definition is adequate to represent results of experiments based on inverse photoemission [22] where only the density of states is scanned. On the other hand, when experiments involve transport, as is the case in superconducting point contact ones based on Andreev reflection, the situation is more complicated due to the fact that the current is largely dependent on the s electrons which have a very small weight at the Fermi level with respect to the d electrons. A detailed discussion of the different definitions of spin polarization and their connection can be found in [23].

3.1. CrAl/In and CrAl/P interfaces

Firstly I will concentrate my study on the case of the CrAl-terminated Co_2CrAl(001) film. In a previous article (see [21]) I showned that the CrAl(001)-terminated surface was showing a very high degree of spin polarization compared to all other surfaces. The mechanism was quite simple: Cr was losing four out of the eight first-neighbouring Co atoms and regained the charge that it was giving away to cobalts in the bulk case. Most of this charge filled up Cr majority states (in figure 3 the majority peak at the Fermi level moves lower in energy), its spin moment was strongly enhanced and, due to the stronger exchange splitting at the surface, the unoccupied Cr states were pushed higher in energy and only the surface state due to the Al atoms survived. Actually a similar phenomenon happens at the interface, but now the increase of the spin moment is smaller since Cr d orbitals hybridize also with the In or P p states at the interface. This is clearly seen in figure 2 where I have gathered the spin moments for the Cr and Co atoms for both interfaces, with In and P. Cr spin moments at the interface are enhanced and reach 2.8 μ_B in the case of the interface with In and 2.6 μ_B in the case of the P interface as compared with the 3.1 μ_B of the Cr in the CrAl-terminated surface. The Cr atoms deeper in the half-metallic spacer have bulklike spin moments. In the case of the Co atoms the situation is

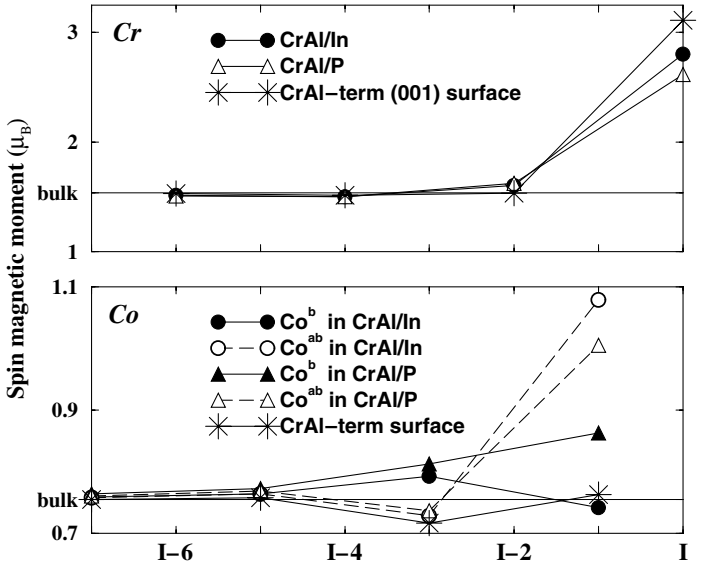

Figure 2. Atom-resolved spin moments in μ_B for Cr at the interface (I) and Co at the subinterface (I-1) layer and their variation in the film compared with the CrAl-terminated (001) surface. Co atoms can sit either at a 'bridge' site (Co^b) or at an 'antibridge' site (Co^{ab}). The straight horizontal line shows the bulk values.

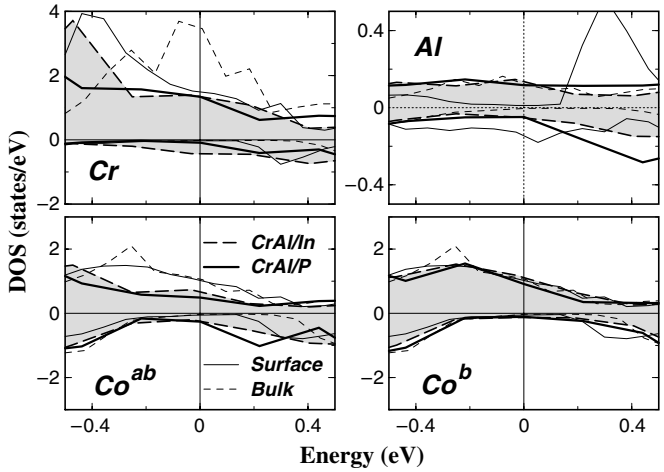

Figure 3. The spin-and atom-resolved DOS for the Cr and Al atoms at the interface with In (long dashed curve filled with grey) or P (thick solid curve) and the Co atoms at the subinterface layer. The solid line shows the (001) CrAl surface and the dashed line the bulk results, from [21] and [8], respectively. The zero of energy is chosen to correspond to the Fermi level. Positive values of the DOS correspond to the majority spin and negative to the minority.

more complicated. There are two inequivalent Co atoms: the one at the 'bridge' site (Co^b) and the one at the 'antibridge' site (Co^{ab}). At the subinterface layer, in general, Co spin moments are strongly enhanced and the moments are larger for the Co atoms at the 'antibridge' sites. If I add the spin moments of the two inequivalent Co atoms I notice that the sum is the same for both the CrAl/In and CrAl/P interfaces and around 2 μ_B. If I take into account the band structure analysis for the bulk Co_2CrAl presented in [8], that means that both majority e_u states are occupied leading to a total Co spin moment of 2 μ_B, while these non-bonding states are unoccupied for the minority band. In the case of the I-3 layer the average Co spin moment is equal to the bulk one and deeper in the film one finds again the bulk values.

Table 1. The number of states at the Fermi level in units of states eV^{-1} for the atoms at the interface for the case of the CrAl/In and CrAl/P interfaces as ratios between majority (↑) and minority (↓) spins, together with the results for the CrAl-terminated (001) surfaces. The last line is the spin polarization P taking into account the interface layers and the subinterface ones.

	CrAl/In	CrAl/P	CrAl surface
Co^b (↑ / ↓)	1.18/0.13	0.91/0.10	1.03/0.06
Co^{ab} (↑ / ↓)	0.72/0.12	0.49/0.26	1.03/0.06
Cr (↑ / ↓)	1.39/0.43	1.34/0.09	1.48/0.03
Al (↑ / ↓)	0.15/0.05	0.12/0.05	0.01/0.15
In (↑ / ↓)	0.09/0.25	0.07/0.06	—
Void (↑ / ↓)	0.09/0.08	0.02/0.01	—
P (↑ / ↓)	0.15/0.08	0.11/0.08	—
Void (↑ / ↓)	0.02/0.10	0.07/0.02	—
P ($\frac{\uparrow-\downarrow}{\uparrow+\downarrow}$)	63%	65%	84%

The next question which arises is that of whether this enhancement of the spin moment of Cr is enough to guarantee a high degree of spin polarization. In figure 3 I have plotted the DOS for the Cr and Al atoms at the interface and the Co atoms at the subinterface layer for both CrAl/In (dashed line filled with grey) and CrAl/P (thick solid line) contacts with respect to the surface (solid line) and bulk calculations (dashed line). At the Cr site the spin polarization is almost 100% for the CrAl/P case and there is a small DOS for the CrAl/In. For the other three atoms the differences are small between the two different interfaces. The Al atom shows a much higher spin polarization at the Fermi level with respect to the surface results, while Co^{ab} shows the inverse behaviour. Notice that the scale along the DOS axis for the Al atom is different to that for the other three. To make all this clearer, in table 1 I have gathered the densities of states at the Fermi level for all atoms at the interface for both CrAl/In and CrAl/P interfaces together with the results for the CrAl surface. Cobalt has different behaviours depending on which site it sits at and the ones at the 'bridge' site behave like in the surface, showing a higher spin polarization. As already mentioned, the Cr spin polarization is higher for the case of the contact with P than for that with In. In the semiconductor film the only noticeable effect is when the In atom is at the interface and it has a large negative spin polarization, while when it sits at the subinterface layer in the case of the CrAl/P contact its net spin polarization is almost zero. In total, the CrAl/In interface shows a spin polarization of 63% and the CrAl/P interface one of 65% as compared to the 84% for the CrAl surface case. This means that in both interfaces more than 80% of the electrons at the Fermi level are of majority spin character and the interface holds a very high degree of spin polarization.

3.2. Co/In and Co/P interfaces

In the second part of my study I will discuss the case of the interfaces made up by Co and either an In or a P layer. In figure 4 I have gathered the atomic spin moments for the Co atoms at the interface and the Cr atoms at the subinterface layers and their variation in the film. Spin moments at the interface are strongly reduced, especially for the Co atoms sitting at the ideal zinc-blende positions, the so-called 'bridge' sites. The Co^b spin moment decreases to $\sim 0.3\ \mu_B$ for the Co/P interface and the quenching of the Co^b spin moment is almost complete in the case of the Co/In interface. On the other hand, the Co^{ab} atoms show a more modest decrease of their spin moment by ~ 0.15–$0.2\ \mu_B$ with respect to the bulk value denoted by a straight line in the figure. The Cr atoms at the interface layer (I-1) follow through hybridization the behaviour

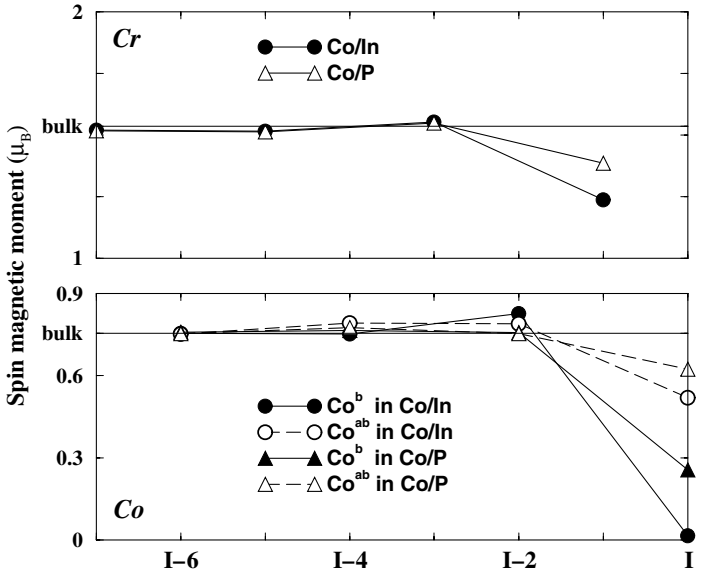

Figure 4. Atom-resolved spin moments in μ_B for Co at the interface (I) and Cr at the subinterface (I-1) layer and their variation in the spacer. Co atoms can sit either at a 'bridge' site (Co^b) or an 'antibridge' site (Co^{ab}). The straight horizontal line shows the bulk values.

of the Co spin moments and their spin moment is ∼0.15–0.25 μ_B smaller than the bulk value. As soon as one reaches the second layer below the interface, atoms regain a bulklike behaviour and moments are close to their bulk values.

The behaviour of the Co spin moments at the interface has also been observed in the case of the Co_2MnGe/GaAs contacts studied by Picozzi and collaborators [14]. For this compound, Co in the bulk has a spin moment of ∼1 μ_B, but at the Co/Ga or Co/As interfaces the decrease of Co^b is as much as 0.8 μ_B, while for Co^{ab} atoms the reduction of the spin moment is only 0.2 μ_B. It seems that the reduction of the Co spin moment depends strongly on the hybridization between the Co d orbitals and the p orbitals of the semiconductor. Already for Co at the 'bridge' site, the orbitals hybridize much more strongly than in the case of the Co at the 'antibridge' site, resulting in a larger decrease of the spin moment. Also, in the system which I study, hybridization is much more important in the case of an In interface layer than that of a P one, leading to the complete quenching of the Co^b spin moment. Similar results have been obtained in the case of an Fe film capped by GaAs [24]. In this case an ad-layer of Ga or As on top of the Fe film suppresses the Fe magnetic moments, the effect being particularly pronounced in the As-capped case, due to the stronger covalent bonding between the As and the Fe atoms.

Finally, I will discuss the atom-resolved DOS at the interface. The hybridization of the Co d states with the p states of either In or P at the interface not only reduces the spin moment but also kills half-metallicity at the Co sites, as can be seen for both Co^b and Co^{ab} in figure 5. Cr and Al atoms at the subinterface layer have an environment very similar to the bulk case and, although the spin moment of Cr is slightly decreased, as I have already mentioned above, its DOS remains similar to the bulk one and it keeps a very high majority DOS at the Fermi level similar to the bulk DOS. This effect largely compensates the loss of half-metallicity of the Co atoms, and the spin polarization at the Fermi level, if I take into account the layers close to the interface (as in table 1), is ∼56% for the Co/In interface and ∼74% for the Co/P interface. Thus 78% of the electrons at the Fermi level for the Co/In interface and 87% for the Co/P one are of majority character.

In the case of the CrAl interfaces the high spin polarization was due to the large enhancement of the Cr spin moment which weakened the effect of interface states, although

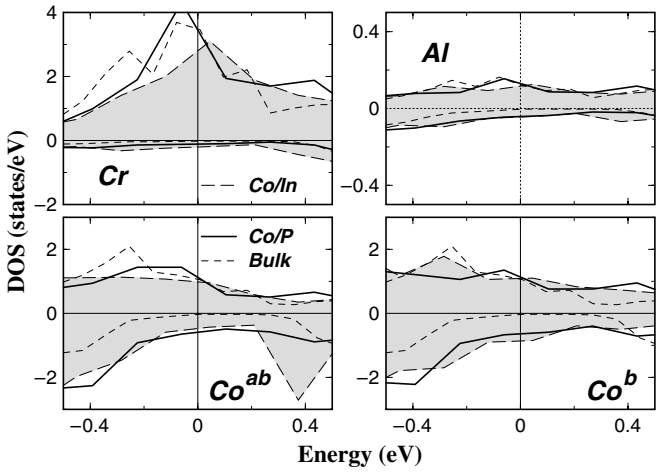

Figure 5. The spin-and atom-resolved DOS for the Co atoms at the interface with In (long dashed curve filled with grey) or P (thick solid curve) and the Cr and Al atoms at the subinterface layer. The dashed line shows the bulk results from [8].

the Cr majority DOS at the Fermi level was considerably smaller than in the bulk case; the peak moved lower in energy to accommodate the extra electrons (see figure 3). In the case of the Co interfaces, although the Co atoms themselves present almost a zero net spin polarization at the Fermi level, Cr atoms in the subinterface layer keep the high majority DOS of the bulk (see figure 5) and the resulting spin polarization is similar to that of the CrAl interfaces.

4. Summary and conclusions

I have studied the electronic and magnetic properties of the (001) interfaces between the half-metal Co_2CrAl and the binary semiconductor InP using a full-potential *ab initio* technique. When the interface is made up from a CrAl layer, the Cr spin moment is strongly enhanced at the interface, as was the case for the CrAl-terminated (001) surfaces. This enhancement limits the effect of the interface states and in both types of contact (In or P as the interface layer) the interface presents a very high spin polarization of ∼63–65%; thus more than 80% of the electrons at the Fermi level are of majority spin character. On the other hand, interfaces made up of Co layers present a large decrease of the Co spin moments but, due the bulklike density of states of the Cr atoms in the subinterface layer, they keep a high degree of spin polarization: 56% for the Co/In interface and 74% for the Co/P one.

The results on the CrAl-terminated half-metallic spacer should in principle remain valid not only in the case of interfaces made up of half-metallic Heusler alloys containing Cr but also when V is used instead of Cr. The mechanism for achieving the high spin polarization should remain the same (the large enhancement of the Cr or V spin moment at the interface reduces the effect of the interface states). Similar results have been obtained in the case of interfaces between binary semiconductors and Cr- or V-based pnictides and chalcogenides crystallizing in the zinc-blende structure [20]. Such structures can be realized experimentally with techniques such as molecular beam epitaxy which enable one to have a tight control on the growth of the interfaces. But one should keep in mind that in realistic applications point defects, stacking faults, chemical disorder, temperature effects etc could destroy this high spin polarization.

Interface states are important because their interaction with defects makes them conducting and lowers the efficiency of devices based on spin injection. Thus, building up interfaces with the highest spin polarization possible, such as the ones proposed here, is a prerequisite but not a guarantee of getting highly spin polarized current in spin injection experiments.

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