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Ab initio calculations of spin polarization at Co_2CrAl/GaAs interfaces

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Abstract

We investigate the structural and electronic properties of Co_2CrAl/GaAs (100) and (110) interfaces using density functional theory within the generalized gradient approximation. Adhesion energy is calculated for various interfacial structures, and it is found that the (100) CrAl-terminated surface, which was theoretically predicted to be highly spin polarized, shows weaker adhesion to GaAs than the (100) Co-terminated surface. We then examine the spatial behaviour of local spin polarization at the Fermi level for the (100) and (110) interfaces, choosing the interfacial structures which give rise to relatively large adhesion energy. The (110) interface turns out to have very high spin polarization at the interface, while such behaviour is not observed in the (100) interface.

Studying the electronic properties of interfaces between magnetic materials and semiconductors is of considerable importance chiefly in relation to spin-polarized current injection into semiconductors [1–4]. According to the work of Schmidt *et al* [5], the efficiency of spin injection from ferromagnetic metals into normal semiconductors is significantly lowered because of their conductivity mismatch unless the spin polarization at the Fermi level of the ferromagnet is very close to unity. Although the analysis in [5] does not take account of the effects stemming from interfacial resistance which could alter the circumstances mentioned above [6, 7], half-metallic ferromagnets, where the spin polarization is unity, are still worth considering as possible candidates for spin-injecting sources.

A full Heusler alloy Co_2CrAl was theoretically predicted to be half metallic, and its Curie temperature is known to be beyond room temperature ($T_c \sim 334$ K) [8]. Besides, recent first-principles calculations predicted that the half-metallic properties of Co_2CrAl are robust against Cr–Al substitutional disorder [9], suggesting that Co_2CrAl is favourable for industrial applications [10]. Hence, in this paper, we investigate the structural and electronic properties of Co_2CrAl/GaAs interfaces, where GaAs is chosen as a typical semiconductor.

Table 1. Adhesion energy W (ideal work of separation) of the Co_2CrAl/GaAs interface (see text for the interfacial structure).

(100) interface		(110) interface	
Structure	W (J m^{-2})	Structure	W (J m^{-2})
As–Co–Al	2.86	As–Al(Ga–Co–Al)	1.70
Ga–Co–Al	2.63	Ga–Al(As–Co–Al)	1.64
As–Co–Cr	2.63	As–Cr(Ga–Co–Cr)	1.55
Ga–Co–Cr	2.52	Ga–Cr(As–Co–Cr)	1.22
As–Cr	1.59		
As–Al	1.44		
Ga–Al	1.40		
Ga–Cr	1.06		

Calculations are done by utilizing the Vienna *ab initio* simulation package [11, 12], where the projector augmented wave method is used [13].

Co_2CrAl consists of four sublattices, namely two fcc-Co lattices, an fcc-Cr lattice, and an fcc-Al lattice. In other words, it is comprised of two zinc-blende (ZB) structures, ZB–CoCr and ZB–CoAl, and one of them is located at the vacancy sites of the other. As initial conditions of Co_2CrAl/GaAs interfacial structure, we take the atomic configurations where the ZB structure of GaAs is connected to one of ZB–CoCr and ZB–CoAl inside Co_2CrAl. Accordingly, we here consider eight interfacial structures for the (100) interface and four for the (110) interface, and we name them from the elements which appear when the ZB-like track is followed through the interface. For example, 'As–Co–Al' denotes that the ZB structure of GaAs is connected to the ZB–CoAl, and that the As and Co atoms are neighboured at the interface.

To assess the stability of these interfaces, we calculate the adhesion energy defined as the ideal work of separation, namely, $W \equiv (E_{\mathrm{CCA}} + E_{\mathrm{GA}} - E_{\mathrm{CCA/GA}})/S$, where E_{CCA}, E_{GA} and $E_{\mathrm{CCA/GA}}$ are the energies of isolated Co_2CrAl, isolated GaAs and Co_2CrAl/GaAs interface slabs in the supercell, respectively, and S is the area of the interface. When we calculate E_{GA} for the (100) slab, we make use of a 1×2 supercell in order to dimerize the surface atoms. The resulting adhesion energy is listed in table 1. It is clearly observed that in the case of the (100) interface, Co-terminated Co_2CrAl tends to stick to GaAs more strongly than in the CrAl-terminated case. Recent theoretical work predicted that the CrAl-terminated free surface has very high spin polarization [14], but the results shown here suggest that the highly spin-polarized CrAl-terminated surface is chemically inert and brings about a less stable interface[1]. This adhesive tendency is also reflected in the interlayer distance at the interface, and the Co-terminated cases *do* have smaller interlayer distance than the CrAl-terminated cases. (For example, the interlayer distance at the (100) As–Co–Al interface is 1.27 Å while that at the (100) As–Cr is 1.59 Å.)

There are two major factors determining adhesion, one of which is the atomic species creating the interface and the other is the orientation of the interface. As to the former factor, we can bring up the marked trend of Co atoms toward adhesion. Regarding the latter factor, we mention that the number of bonds coming out of the GaAs plane per area is smaller in the (110) plane than in the (100) plane; from this viewpoint, the (110) interface is less adhesive. In the present case the former factor is more significant than the latter, and therefore the (110) interfaces, which always contain Co atoms, show slightly stronger adhesion than in the (100) CrAl-terminated interfaces as a whole.

[1] Moreover, the CrAl-terminated Co_2CrAl no longer leads to high spin polarization when it is attached to GaAs.

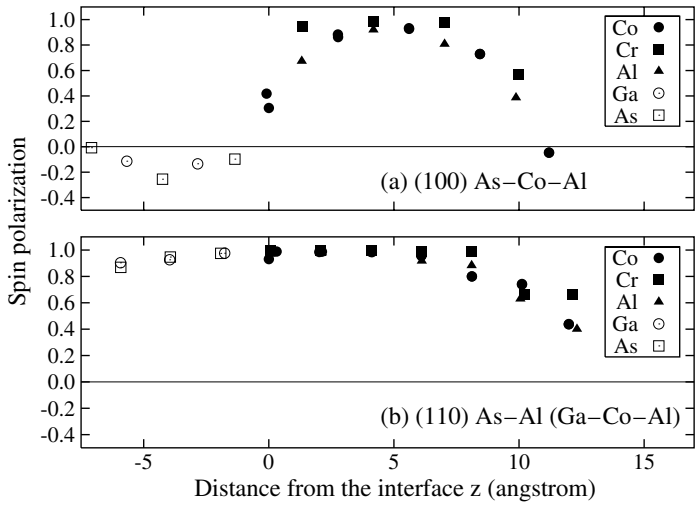

Figure 1. Local spin polarizations of the (100) As–Co–Al interface and the (110) As–Al(Ga–Co–Al) interface (see text for the interfacial structure) as a function of the distance from the interfacial atomic layer.

We then investigate the spatial behaviour of spin polarization defined by $P \equiv (D_\uparrow - D_\downarrow)/(D_\uparrow + D_\downarrow)$, where $D_\uparrow$ ($D_\downarrow$) is the local density of states (DOS) at the Fermi level for the majority (minority) spin. Here we focus our attention on the (100) As–Co–Al interface and the (110) As–Al(Ga–Co–Al) interface, which possess the largest adhesion energy in each orientation of the interfaces studied here.

Figure 1(a) presents the local spin polarization around the (100) As–Co–Al interface as a function of the distance from the interface. The spin polarization is found to be lowered significantly at the interfacial Co atomic layer (at $z = 0$ Å), though the value is slightly higher than that at the free surface (at $z = 11$ Å). Only Cr atoms show a rapid increase of spin polarization inside Co_2CrAl; indeed, the Cr atoms in the sub-interface layer already have spin polarization of more than 0.9. This rapid increase, however, most probably has little contribution to the spin polarization of the *current* because the increase comes from a sharp peak in the DOS just located at the Fermi level which originates in strongly-localized 3d orbitals. Spin polarization is also calculated inside GaAs where the gap states are induced. Although the gap states are still observed in the region where the interface is a few ångströms away, they do not show any significant spin polarization in this case.

By contrast, in the (110) As–Al(Ga–Co–Al) interface, the spin polarization remains very high at the interfacial atomic layer (see figure 1(b)), which is similar to the ZB–CrAs/GaAs interface [15]. This high spin polarization is preserved even without the contribution from d orbitals, and therefore is expected to be relevant to the transport properties. It is interesting to note that the gap states inside GaAs are also strongly spin polarized, that is, there is almost no gap state with minority spin around the Fermi level. As a matter of fact, the local DOS at the (110) surface of GaAs tends to have a dip at the Fermi level, and this tendency is not sensitive to the detailed surface structure though the DOS itself is. Regarding the behaviour of the majority-spin states, however, it should be noticed that Co_2CrAl is metallic for the majority spin, and furthermore that its band dispersion is quite significant in the [110] direction. Accordingly, the tails of those delocalized states penetrate into GaAs through the interface, and bring about appreciable gap states resulting in the high spin polarization.

In summary, using first-principles calculations, we have investigated the adhesive properties and spin polarization at the Co_2CrAl/GaAs interface. Our results have shown that the spatial behaviour of spin polarization is sensitive to the orientation of interfacial plane, and that very high spin polarization is expected at the (110) interface.

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