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The influence of spin–orbit coupling on the band gap of Heusler alloys

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Abstract

The band gap of half-metallic ferromagnets can be affected by the spin–orbit coupling, which introduces there a small, but non-vanishing, density of states. We study this effect in the case of Heusler alloys. We find that, as a rule, the spin polarization in the middle of the gap decreases for compounds of heavier elements.

Half-metallic ferromagnets are spin-polarized materials with the exotic property that the density of states (DOS) of spins in one direction shows a gap around the Fermi level E_F , while the DOS of the others spin is metallic. The half-metallic property was first discovered by de Groot and co-workers in 1983 [1] in Heusler alloys. Since then, half-metals have been attracting increasing interest [2–5], even more so in recent years due to their potential application in spin-dependent transport and spintronics [6].

Although first-principles calculations show the presence of the half-metallic band gap, in reality a number of physical processes can introduce states within it. One can consider defects [7] and interface [8] or surface states [9], which destroy the perfect crystal periodicity and thus the covalent hybridization leading to the gap. But even in an ideally prepared sample, the spin–orbit coupling can introduce states in the half-metallic gap of the minority states (for the spin-down electrons), which are produced by spin-flip scattering of the majority states (with the spin-up direction).

In a recent paper [10], the effect of the spin–orbit coupling on the half-metallic band gap was investigated for a few half-metallic substances of different character, namely the Heusler alloy NiMnSb, the ordered zinc-blende compounds CrAs, CrSb, and MnBi, and the diluted magnetic semiconductors (Ga, Mn)As and (Ga, Mn)N. The main conclusion was that, within

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the gap, the spin-down DOS was a weak image of its spin-up counterpart. The presence of heavier elements, which are expected to cause stronger spin–orbit scattering, increased the effect. Thus the spin polarization at E_F , $P(E_F)$, varied between 99% for NiMnSb and 77% for MnBi, instead of the ideal 100%. In the present work we extend our calculations to more Heusler alloys: in addition to NiMnSb, we study the cases of FeMnSb, CoMnSb, PdMnSb, and PtMnSb. Although the last two are not half-metallic (a spin-down gap exists, but E_F enters slightly into the valence band), it is instructive to examine the DOS in the gap region and see how P decreases as one changes to heavier elements (Ni \rightarrow Pd \rightarrow Pt).

Our calculations employ density-functional theory within the local density approximation for the exchange and correlation potential. The Green function of the systems is calculated by the Korringa–Kohn–Rostoker (KKR) multiple-scattering Green function method, extended to a fully relativistic treatment by solving the Dirac equation for the cell-centred potentials [11]. Thus the spin–orbit coupling, which is a relativistic effect, is automatically taken into account. Note that, although the Green function $G(E)$ is evaluated at complex energies (using a very small, but nonzero, imaginary part), its analytical property allows us to extrapolate directly to the real energy axis, in order to calculate the DOS as $n(E) = -\text{Im} G(E)/\pi$, in a manner equivalent to the one described in [12]. In this way we avoid the artificial Lorentzian broadening of $n(E)$ which appears for complex energies, and which would drown an effect as small as the spin–orbit induced DOS in the gap. For more details we refer the reader to [10].

Although in our method the Dirac equation is solved, it is easier to understand the spin–orbit effect within perturbation theory using the Schrödinger equation. In this framework, we recall that the spin–orbit coupling of the two spin channels is related to the unperturbed potential $V(r)$ around each atom via the angular momentum operator \vec{L} and the Pauli spin matrix $\vec{\sigma}$:

$$V_{\text{so}}(r) = \frac{1}{2m^2c^2} \frac{\hbar}{2} \frac{1}{r} \frac{dV}{dr} \vec{L} \cdot \vec{\sigma} = \begin{pmatrix} V_{\text{so}}^{\uparrow\uparrow} & V_{\text{so}}^{\uparrow\downarrow} \\ V_{\text{so}}^{\downarrow\uparrow} & V_{\text{so}}^{\downarrow\downarrow} \end{pmatrix}. \quad (1)$$

The 2×2 matrix form is understood in the spinor basis. The two spin directions are denoted by \uparrow and \downarrow . The unperturbed crystal Hamiltonian eigenvalues for the two spin directions are $E_{n\vec{k}}^{0\uparrow}$ and $E_{n\vec{k}}^{0\downarrow}$, and the unperturbed Bloch eigenfunctions are $\Psi_{n\vec{k}}^{0\uparrow}$ and $\Psi_{n\vec{k}}^{0\downarrow}$. Then, noting that within the spin-down gap there exist no unperturbed solutions $\Psi_{n\vec{k}}^{0\downarrow}$ and $E_{n\vec{k}}^{0\downarrow}$, the first-order solution Schrödinger equation for the perturbed wavefunction $\Psi_{n\vec{k}}^{\downarrow}$ reads for states in the gap

$$\Psi_{n\vec{k}}^{(1)\downarrow}(\vec{r}) = \sum_{n'} \frac{\langle \Psi_{n'\vec{k}}^{0\downarrow} | V_{\text{so}}^{\downarrow\uparrow} | \Psi_{n\vec{k}}^{0\uparrow} \rangle}{E_{n\vec{k}}^{0\uparrow} - E_{n'\vec{k}}^{0\downarrow}} \Psi_{n'\vec{k}}^{0\downarrow}(\vec{r}). \quad (2)$$

Here, the summation runs only over the band index n' and not over the Bloch vectors \vec{k}' , because Bloch functions with $\vec{k}' \neq \vec{k}$ are mutually orthogonal. Close to the crossing point $E_{n\vec{k}}^{0\uparrow} = E_{n'\vec{k}}^{0\downarrow}$ the denominator becomes small and the bands strongly couple. Then one should also consider higher orders in the perturbation expansion. Since at the gap edges there exist spin-down bands of the unperturbed Hamiltonian, this effect can become important near the gap edges. Apart from that, the important result is that in the gap region the spin-down spectral intensity is a weak image of the spin-up one. Since the spin-down DOS is related to $|\Psi_{n\vec{k}}^{(1)\downarrow}|^2$, it is expected that within the gap the DOS has a quadratic dependence on the spin–orbit coupling strength: $n_{\downarrow}(E) \sim (V_{\text{so}}^{\downarrow\uparrow})^2$.

The main results of the present work are given in table 1. For the Heusler alloys CoMnSb, FeMnSb, NiMnSb, PdMnSb, and PtMnSb, three quantities are shown: the spin polarization at E_F , $P(E_F)$, and in the middle of the gap, $P(E_M)$, and the spin-down/spin-up DOS ratio in the middle of the gap, $(n_{\downarrow}/n_{\uparrow})(E_M)$. The last two quantities reflect the strength of the spin–orbit

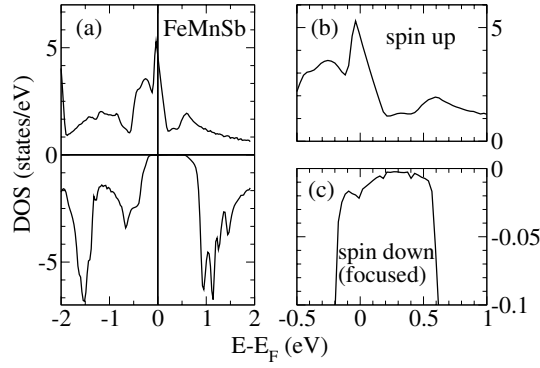


Figure 1. (a) The density of states of FeMnSb close to the gap region. ((b), (c)) The same, but more focused around the gap region. In (c), the DOS axis for spin down has been scaled to focus on the small but nonzero DOS within the half-metallic gap. The small peak at E_F reflects the analogous peak for spin up at the same energy. Negative numbers on the DOS axis correspond to spin down (minority spin).

Table 1. The calculated spin polarization at the Fermi level ($P(E_F)$) and in the middle of the spin-down gap ($P(E_M)$), and the spin-down/spin-up DOS ratio in the middle of the gap ($(n_{\downarrow}/n_{\uparrow})(E_M)$), for various Heusler alloys. The alloys PdMnSb and PtMnSb present a spin-down gap, but are not half-metallic, as E_F is slightly below the gap.

Compound	$P(E_F)$ (%)	$P(E_M)$ (%)	$(n_{\downarrow}/n_{\uparrow})(E_M)$ (%)
CoMnSb	99.0	99.5	0.25
FeMnSb	99.3	99.4	0.30
NiMnSb	99.3	99.3	0.35
PdMnSb	40.0	98.5	0.75
PtMnSb	66.5	94.5	2.70

induced spin-flip scattering, while the first is relevant to our considerations only when E_F is well within the gap (which is not the case for PdMnSb and PtMnSb). Clearly, the compounds including 3d transition elements (NiMnSb, CoMnSb, and FeMnSb) show high spin polarization and a low $n_{\downarrow}/n_{\uparrow}$ ratio, with a small variation as we move along the 3d row of the periodic table from Ni to Fe. In contrast, when we replace Ni with Pd (a 4d element), $(n_{\downarrow}/n_{\uparrow})(E_M)$ increases and $P(E_M)$ drops drastically, and much more so when we change Pd to Pt (a 5d element). This trend is expected, since it is known that heavier elements are characterized by stronger spin-orbit coupling. For example, in [13] it was shown from perturbation theory arguments that the spin-orbit cross section shows a quadratic dependence on the atomic number, times a modulation due to the form of the wavefunction and the DOS.

As an example, we show in figure 1 the DOS of FeMnSb in the vicinity of the gap. In panel (a) one cannot see the tiny DOS for spin down within the gap. But when we scale this, in panel (c), the nonzero DOS (of the order of 0.3% of the spin-up DOS, shown in panel (b)) becomes visible. Although PtMnSb has the highest spin-orbit effect among the materials examined here, we show results for FeMnSb because it is half-metallic and because of the peak of the spin-up DOS just below E_F , which is reflected in the spin-orbit induced spin-down DOS. This supports the conclusion following equation (2).

In summary, we have investigated the effect of the spin-orbit coupling to the spin-down band gap of Heusler alloys by means of *ab initio* calculations. We have examined the compounds CoMnSb, FeMnSb, and NiMnSb, to show that changing the transition element

within the 3d series makes only insignificant changes to the effect, and PdMnSb and PtMnSb, to demonstrate that heavier elements cause a much higher spin-orbit induced DOS within the gap. From perturbation theory arguments we have seen that this DOS depends quadratically on the spin-orbit coupling strength, and that it is a weak reflection of the spin-up DOS. We hope that our results will motivate further work in this field in the future.

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