Origin of the difference in the magneto-optical Kerr effect between PtMnSb and NiMnSb

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The differences in electronic structure between PtMnSb and NiMnSb are investigated using the augmented-spherical-wave method. It is found that the large differences in magneto-optical behavior between the two compounds are due to the mass-velocity and Darwin terms, and not to the spin-orbit interaction.

The ferromagnetic compound PtMnSb, which crystallizes in the Heusler $C1_b$ structure, shows the highest magneto-optical Kerr rotation at room temperature.[1] The isostructural, isoelectronic compound NiMnSb shows only a modest magneto-optical Kerr effect (hereafter referred to as MOKE).

Generally, the origin of the MOKE is the incomplete cancellation of optical transitions for left and right circularly polarized light.[2] Two conditions have to be fulfilled in first order to obtain a MOKE: the occurrence of a net magnetization (either spontaneous or induced), and the spin-orbit interaction. It is tempting to attribute the large MOKE in PtMnSb, with respect to NiMnSb, to the much higher nuclear charge and thus to the much larger spin-orbit interaction of Pt vs Ni.

The electronic structure of both PtMnSb and NiMnSb is quite unusual.[3,4] Both compounds are so-called half-metallic ferromagnets, in which the energy bands for minority spin electrons have a gap at the Fermi level, whereas the Fermi level intersects the bands for majority spin electrons. Therefore, the compounds are metallic for electrons with one spin direction, and semiconducting for electrons of opposite spin. Other half-metallic magnets are CoMnSb,[5] FeMnSb,[6] Fe_3O_4,[7] CrO_2,[8] $KCrSe_2$,[9] and possibly CrMnSb and Mn_2Sb.

The band structures of PtMnSb and NiMnSb for majority and minority spin electrons are shown in Figs. 1 and 2, respectively. The band structures were calculated using the self-consistent augmented-spherical-wave method (ASW) of Williams, Kübler, and Gelatt.[10] The local-density approximation was used, as given by Hedin and Lundqvist.[11] Scalar relativistic effects (mass-velocity and Darwin terms) were included as described by Methfessel and Kübler,[12] but spin-orbit interaction was not taken into account.

There is a contradiction between the calculated band structures and the *ad hoc* assumption that the large spin-orbit interaction of Pt is responsible for the large MOKE in PtMnSb. The observed peak in the Kerr rotation of PtMnSb occurs at 1.7 eV. The position of the Pt $5d$ states in PtMnSb and the Ni $3d$ states in NiMnSb are more than 4 eV below the Fermi level. The empty $4p$ states of Ni and the empty $6p$ states of Pt are so high in energy that they are off the panel in Figs. 1 and 2. Thus there are no states depending in first order on the spin-orbit interaction of Pt or Ni in the spectroscopic range of the MOKE. The positions of Ni $3d$ and Pt $5d$ states obtained from the band-structure calculations are in very good agreement with photoemission measurements.[13]

The large MOKE of PtMnSb has been attributed to the peculiar electronic structure of this compound.[4] The top of the valence band Γ_4 for the minority spin direction is located just below the Fermi energy (see Fig. 1). The states at the top of the valence band are of primarily Sb $5p$ character. Under the influence of spin-orbit interaction this triply degenerate Γ_4 state splits into three equidistant

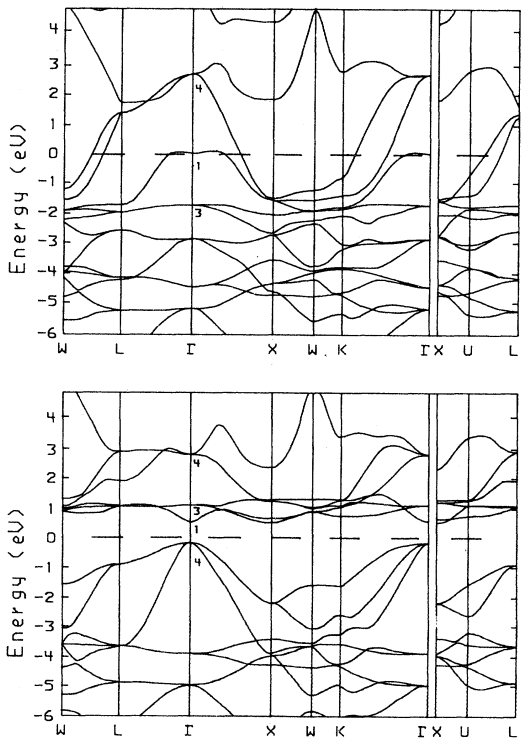

FIG. 1. Band structure of PtMnSb for majority (upper part) and minority spin electrons (lower part), calculated with the ASW method including the scalar relativistic effects.

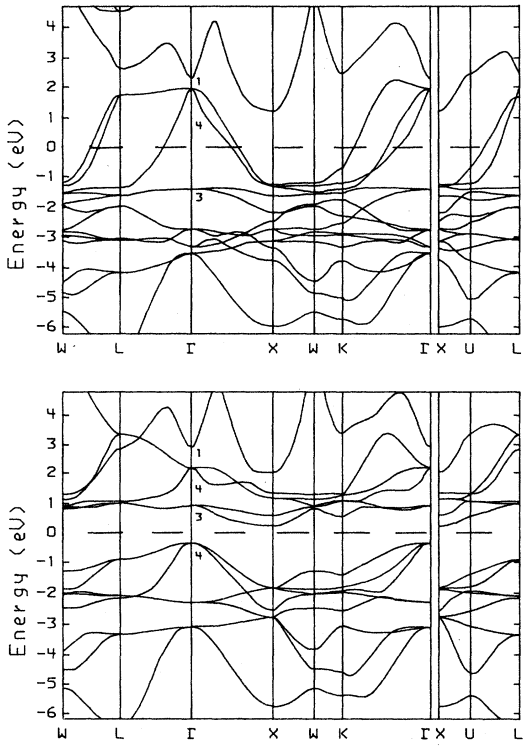

FIG. 2. Band structure of NiMnSb for majority (upper part) and minority spin electrons (lower part), calculated with the ASW method including the scalar relativistic effects.

singlets, with orbital quantum numbers $m = -1$, 0, and $+1$ (orbital quantization with respect to the direction of magnetization). The highest singlet state $m = +1$ is located above the Fermi level, and therefore cannot serve as an initial state for optical excitations. Thus the excitations from Γ_4 to the empty Γ_1 level (mainly Pt $6s$ character) are magneto-optically uncompensated. The oscillator strength of these transitions is large; the excitation energy coincides with the onset of the observed peak in the off-diagonal part of the dielectric tensor.[4] In addition, the behavior of the diagonal part of the dielectric tensor leads to an enhancement of the MOKE at the plasma energy, which also falls in this energy range.[14] The combination of the two effects explains quite well the observed peak with a large MOKE at about 1.7 eV in PtMnSb. Thus, the two requirements for a large MOKE, a magnetic moment and spin-orbit interaction, are due in PtMnSb to the spontaneous magnetic moment (which is localized mainly on the Mn atom) and the spin-orbit interaction of the top of the valence band (which is of Sb character) for the minority spin direction. As a consequence, in the first instance one would not expect large differences in MOKE between PtMnSb and NiMnSb, contrary to the observations.

However, in comparing the band structures of PtMnSb and NiMnSb, a striking difference is the position of the first unoccupied Γ_1 state for the minority spin electrons (Figs. 1 and 2). This state is located at about 1 eV above the top of the valence band in PtMnSb, but in NiMnSb it is about 4.2 eV above the top of the valence band. The ob-

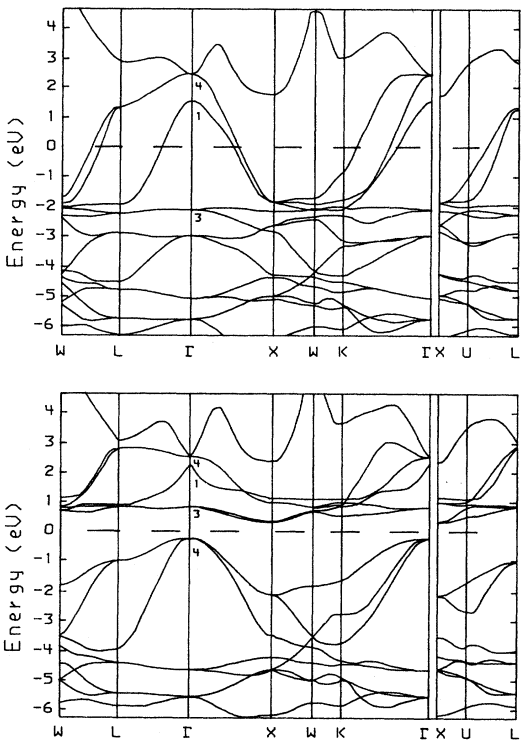

FIG. 3. Band structure of PtMnSb for majority (upper part) and minority spin electrons (lower part), calculated with the ASW method without the scalar relativistic effects.

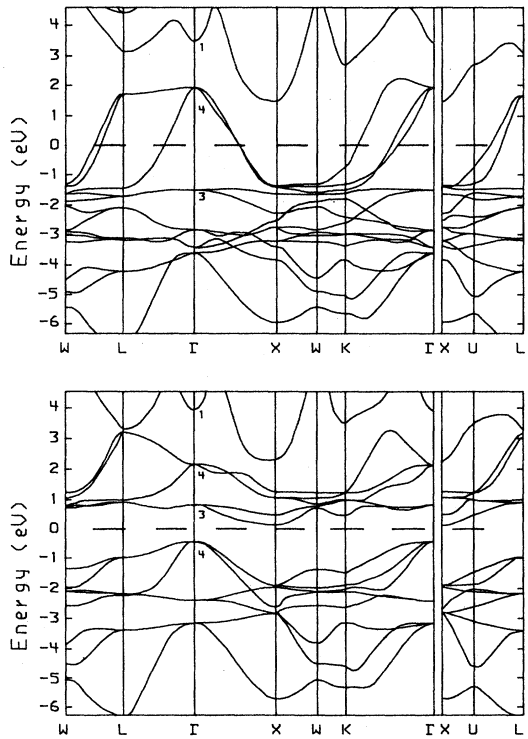

FIG. 4. Band structure of NiMnSb for majority (upper part) and minority spin electrons (lower part), calculated with the ASW method without the scalar relativistic effects.

served intensity of the excitation in NiMnSb is much lower, due to joint density of states or oscillator strength effect. In NiMnSb, a (weaker) peak in the off-diagonal part of the dielectric tensor is observed near 4 eV. Thus the key question is why the final states in PtMnSb are so favorable and in NiMnSb are so unfavorable for the MOKE.

The main difference between PtMnSb and NiMnSb is the higher nuclear charge of Pt with respect to Ni. The character of the wave function of the final Γ_1 state is rather delocalized, with Pt $6s$ (or Ni $4s$) character as dominant contributors. Relativistic effects can be separated into spin-orbit contributions and scalar relativistic effects, the so-called mass-velocity and Darwin terms. The latter two terms do not lead to splitting of energy levels, but produce energy shifts which are largest for s levels because of the finite value of the s wave function at the nucleus.

The band structures shown in Figs. 1 and 2 were calculated with the ASW method, including mass-velocity and Darwin terms. In order to explicitly find the influence of these relativistic terms we also performed a completely nonrelativistic calculation of PtMnSb and NiMnSb. For these calculations, the ASW method described by Williams, Kübler, and Gelatt was again employed.[10] The results are shown in Figs. 3 and 4. The main difference with the relativistic calculations is a shift of the Γ_1 level for minority spin electrons by 1.8 eV in PtMnSb; the corresponding shift in NiMnSb is much smaller. Moreover, the strong interaction of this Γ_1 level with the empty Γ_4 level in NiMnSb (of primarily Mn $3d$ character) leads to a strong dispersion away from Γ_1, and a corresponding decrease of the strength of the magneto-optical transitions, due to a smaller joint density of states.

In summary, the large difference in MOKE between PtMnSb and NiMnSb is relativistic in origin, but it is not caused by spin-orbit interaction. Darwin and mass-velocity terms play an essential role in MOKE and should not be neglected in any work on MOKE.

In order to obtain more information about the differences in electronic structure and MOKE of PtMnSb and NiMnSb, the MOKE and band structures of mixed crystals $Pt_{1-x}Ni_xMnSb$ were investigated. The results are planned to be presented in a forthcoming publication.[15]

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