RELATIVISTIC ENERGY BAND OF LaSb

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§ 1. Introduction

The La and Ce pnictides with the NaCl crystal structure belong to a large group of rare-earth pnictides (Hulliger 1979). Among them, the Ce pnictides have recently attracted particular interest, because they show various anomalies due to the valence-fluctuating states of the 4f electrons (Kasuya 1981). The La pnictides can serve as a proper reference for the study of the Ce pnictides.

To understand their ground state properties quantitatively, the energy band structures for a series of the La pnictides, LaX, where X means N, P, As or Sb, has recently been calculated with the local-density approximation (Hasegawa 1980). It can explain reasonably well a transition from semiconductors to metals in the series from LaN to LaSb. The calculated density of states for the valence band agrees well with the XPS spectrum. Though this previous calculation can thus explain well the conducting property and the density of states, it may be inadequate to explain detailed Fermi surface property of the La pnictides with heavy pnictogens, because it neglected the spin-orbit interaction. Since the spin-orbit splitting of an outer p shell in heavy pnictogen atoms is comparable with the Fermi energy, E_F, measured from the top of the valence band, the energy band structure near E_F may be modified appreciably.

In the present work, the energy band structure for LaSb is recalculated by a fully relativistic APW method to investigate how the Fermi surface should be modified by the introduction of the spin-orbit interaction. As a result of the calculation, it is found that one of the three hole Fermi surfaces centred at the Γ point predicted by the non-relativistic calculation should disappear. The narrow 4f bands lying a few eV above E_F tend to push down the valence band near the Γ point, and thus can strengthen the effect of the spin-orbit interaction on the Fermi surface. The de Haas-van Alphen effect measurement by Suzuki et al (1981) confirms this calculated result.

For comparison, relativistic energy bands for YSb, which has no f state near E_F, is also calculated. In contrast to LaSb, *three* hole Fermi surfaces remain existing.

§ 2. Method of calculation

In the previous calculation (Hasegawa 1980), the one-electron potentials for YSb and La pnictides were determined by a self-consistent APW method with the

local-density approximation. The spin-orbit interaction term was eliminated from the Hamiltonian. Therefore, relativistic energy shifts were taken into account, and the spin-orbit splittings were neglected. In the present calculation the logarithmic derivatives of the electron radial wave function in a relativistic approximation are generated from the one-electron potential determined previously. Eigenvalues are evaluated by a standard, fully relativistic APW method. About 80 plane waves are used, and the convergence is sufficiently good.

§ 3. Energy band structure and the Fermi surface

Figure 1 shows relativistic energy band structure for LaSb along three symmetry axes in the Brillouin zone. As was explained previously, the electron wave function of the valence band has the Sb p character dominantly, and the La d states mix in the valence band appreciably. The conduction and valence bands overlap each other around the X point; the band structure is metallic. The narrow 4f bands lie a few eV above E_F. They are omitted in Fig. 1.

The effects of the spin-orbit interaction on the energy band near E_F are different from state to state. The absolute magnitude of the splitting of the Γ_{15} and X_5' states is about 0.6 eV, comparable with the spin-orbit splitting of the 5p state in the Sb atom (Herman and Skillman 1963). It is remarkable that the splitting of the Δ_5 and Λ_3 states near the centre of the zone is appreciably large. In contrast, the splitting of the crossing of the third and fourth bands in the middle of the Δ axis is extremely small, because the wave functions of the two states have large amplitude within constituent atoms of a different kind.

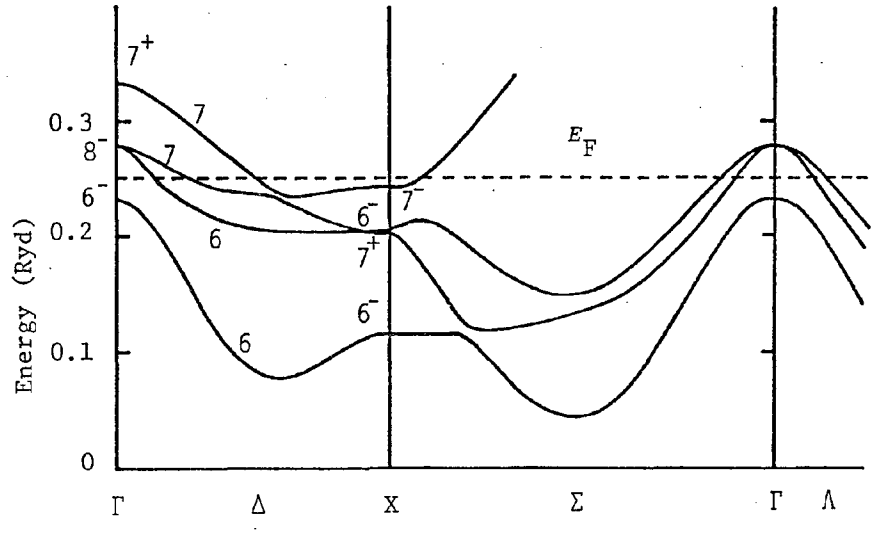

Figure 1. Relativistic energy band structure for LaSb.

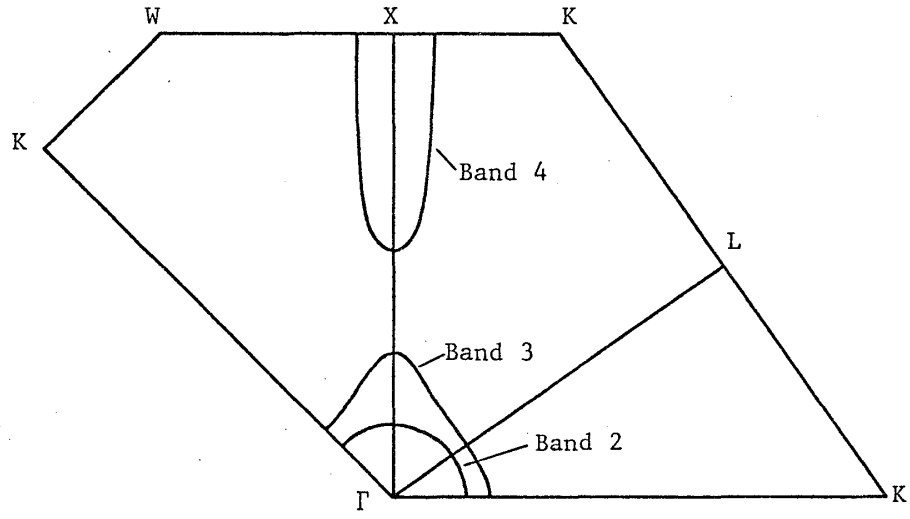

Figure 2. Fermi surface for LaSb.

Since the top of the non-relativistic valence band near Γ is much depressed by the 4f bands, E_F measured from the valence band top becomes smaller than the spin-orbit splitting of the Γ_{15} state. Therefore, the spin-orbit interaction can easily cause the whole lowest band to lie below E_F; the smallest hole Fermi surface may disappear.

Figure 2 shows the cross sections of the Fermi surface on the {100} and {110} planes in the Brillouin zone. There are two hole sheets centred at Γ as well as three equivalent electron sheets centred at X. The small hole sheet is nearly spherical and the large one is stretched along the Δ axis. Carriers are 0.027 electrons per cell and the compensating number of holes; 0.008 in the small sheet and 0.019 in the large sheet. The average effective mass of holes is $0.2m$ and $0.5m$ for the small and large sheets, respectively, where m is the free-electron mass.

§ 4. Comparison with experiment

The validity of the predicted Fermi surface can be tested by the recent de Haas-van Alphen effect measurement by Suzuki et al (1981). Extremal cross-sectional areas of the Fermi surface in the <100> and <110> directions of magnetic field are calculated and summarised in Table 1, in which the experimental results of Suzuki et al (1981) are also included.

It is obvious that the origin of the experimental branch β is the small hole sheet, because the branch β is observed in the whole range of angles measured and is nearly independent of the magnetic-field direction. The calculated magnitude is, however, larger by 50% than the experimental one.

The origin of the experimental branches α_1 and α_2 may be ascribed reason-

Table 1. Calculated and experimental cross-sectional area, in units of $(2\pi/a)^2$, of the Fermi surface for LaSb. The experimental results are taken from Suzuki et al (1981).

Magnetic field direction		<100>		<110>	
		cal.	exp.	cal.	exp.
Band 2	hole	0.07	0.046 (β)	0.07	0.048 (β)
Band 3	hole	0.18		0.13	
Band 4	electron	0.03	0.023 (α_1)	0.04	0.032 (α_1,α_2)
		0.14	0.12* (α_2)		

* an extrapolated value

ably to the fourth-band electron sheet. The agreement between theory and experiment is reasonably good, though the calculated magnitude of the areas is larger than the experimental one in all directions. In the experiment, any branches whose absolute magnitude is larger than $0.07(2\pi/a)^2$ have not been observed, because of the low purity of samples. Therefore, the validity of the large hole sheet can not be confirmed at present. Measurements with samples of high purity by the magnetic-field direction on both {100} and {110} symmetry planes are highly desirable.

Details of the calculation including results for YSb and other pnictides will be published elsewhere.

References

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