Spin-orbit effects on the band structure and Fermi surface of ErAs and $Er_xSc_{1-x}As$

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(Received 16 October 1996)

Band structures of ErAs and $Er_xSc_{1-x}As$ alloys (treated in virtual crystal approximation) calculated by the linear muffin-tin orbital method including spin-orbit coupling as well as spin polarization are presented. Corrections to the local spin density approximation are included by a constant upwards shift of the Er-5*d* derived conduction bands adjusted to yield the observed carrier concentration. Fermi-surface and effective mass parameters are presented and used to simulate the Shubnikov–de Haas spectrum which is shown to be in good agreement with the experimental spectrum. [S0163-1829(97)05215-6]

ErAs and related materials (e.g., $Er_xSc_{1-x}As$ alloys) have recently been grown epitaxially on GaAs (Ref. 1) and incorporated in novel semiconductor/semimetal device structures.[2,3] The magnetotransport properties of these materials which are semimetals were studied in several papers.[4–9] The electronic band structure of these materials was studied by Petukhov, Lambrecht, and Segall[10–12] and used to interpret these data. An important result from those studies[10,11] was that the local spin density approximation (LSDA) (Refs. 13 and 14) overestimates the overall dimensions of the Fermi surface. It was shown that this could be corrected for by a small rigid upwards shift of the lowest mostly unoccupied Δ_2' Er-5*d* derived band. This is analogous to the ''gap'' correction required for semiconductors. Although fairly good agreement with the reported Shubnikov–de Haas (SdH) frequencies[6] was thereby obtained, the agreement involved a different assignment of some of the experimental frequencies to hole (near Γ) and electron (near X) orbits from the one given originally by the experimentalists. Subsequent studies[7,8] have in fact lent support to the original interpretation, and, in addition, found an extra peak at $\sim$600 T. The purpose of the present paper is to show that this issue is resolved by including spin-orbit interaction, as was suggested earlier.[11] The spin-orbit interaction was also found to be crucial in understanding resonant tunneling through ErAs.[12]

The band-structure calculations were performed within the LSDA as parametrized by von Barth and Hedin.[14] The linear muffin-tin orbital (LMTO) method was used in the atomic sphere approximation (ASA).[15] The essential difference from the previous work is the inclusion here of the spin-orbit coupling.[16] The spin-orbit interaction parameter is obtained by solving the intrasphere Dirac relativistic equation as discussed by Andersen.[17] As in our previous work, the Er-4*f* bands are treated as corelike states, an approximation which was justified in detail in Ref. 11. The Fermi-surface orbit areas were calculated using a linear interpolation of the bands on a triangular mesh in the appropriate planar cross sections, i.e., using an approach similar in spirit to the tetrahedron method[18,19] for the Fermi-surface volume. The Sc alloying effects were incorporated by averaging the LMTO potential parameters in the appropriate proportions. The bandwidth parameters[15] Δ_{Rl} were averaged multiplicatively $(\Delta_{Rl}(Er_xSc_{1-x}As)=[\Delta_{Rl}(ErAs)]^x[\Delta_{Rl}(ScAs)]^{1-x})$ while the center of the band C_{Rl} and band shape γ_{Rl} and p_{Rl} parameters were additively mixed, e.g., $C_{Rl}(Er_xSc_{1-x}As)=xC_{Rl}(ErAs)+(1-x)C_{Rl}(ScAs)$. Here, R stands for the various atomic sites and l the angular momentum components. The experimental lattice constants were used in the present work. The metal *d* potential parameters were shifted up so as to yield an effective quasiparticle self-energy correction of $\sim$0.4 eV to the LSDA gap as discussed in Ref. 10.

We recall that in this material spin-polarization effects are important because an external magnetic field **B** orients the localized 4*f* moments, which in turn polarize the valence and conduction states by the exchange mechanism. When the spin-orbit interaction is switched on, the hole exchange splittings depend strongly on the relative orientation of the spins

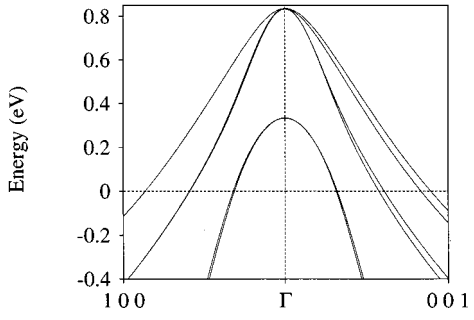

FIG. 1. ErAs hole bands along the [100] and [001] directions for a magnetic field (or spin-polarization direction) parallel to [001].

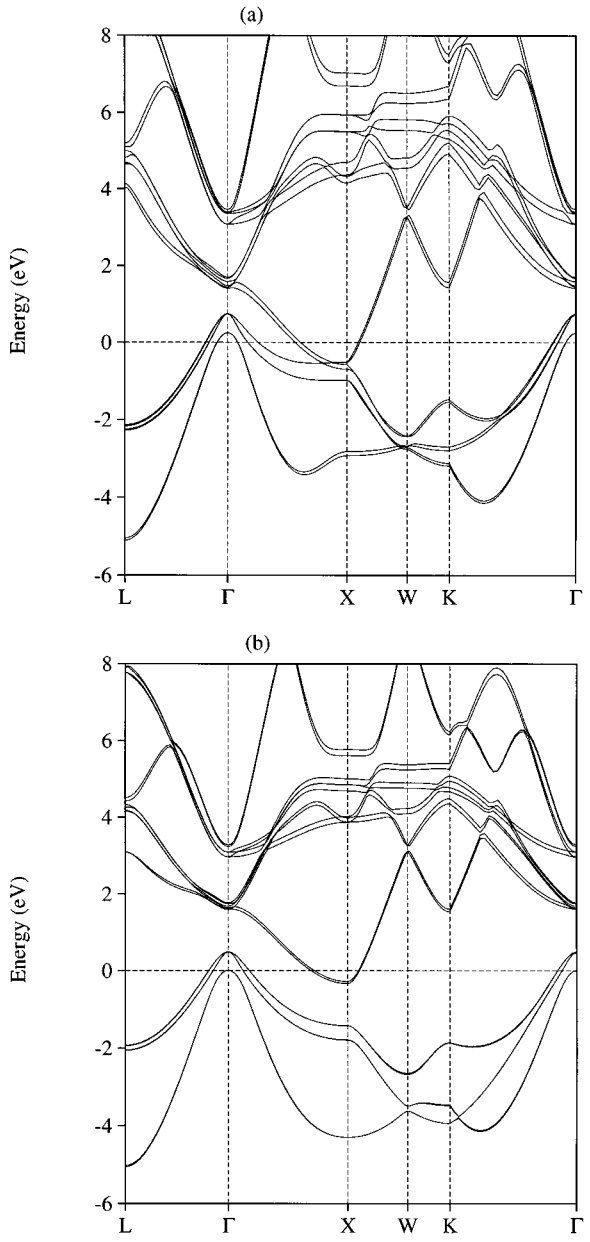

FIG. 2. LSD band structure of ErAs (a), and adjusted band structure of $Er_{0.6}Sc_{0.4}As$ (b). The symmetry labels (neglecting magnetic-field-dependent spin polarization but including double group representations) following notation of Elliott (Ref. 21) for the lower bands in increasing energy order are at L, $6+$, $(4+,5+)$ (time reversal degenerate), $6+$, $6+$,$(4+,5+)$, $6+$; at Γ, $(6+$, $8+)$ derived from Γ_{15} As-p-like, $(8+, 7+)$ derived from Γ'_{25} Er-d-like, $8+$ derived from Γ_{12} Er-d-like, $6+$ derived from Γ_1 Er-s-like; at X, $6+, 7+, 7+, 6+, 7+$. The labels for Λ and Δ are the same as for L or X, respectively, but without the $\pm$ distinction.

(or **B**) and the **k** vector. This was shown previously using the Kohn-Luttinger Hamiltonian in the spherically symmetric approximation.[12] In particular, it was found that the exchange splitting of the light-hole bands is significantly lower for $\mathbf{B}\perp\mathbf{k}$ than for $\mathbf{B}\|\mathbf{k}$. This is consistent with the observation of a spin-dependent and magnetic-field-orientation-dependent resonant tunneling[12] and with the SdH measurements discussed here. In fact, a sizable spin splitting in the tunneling resonance was observed only for the magnetic field

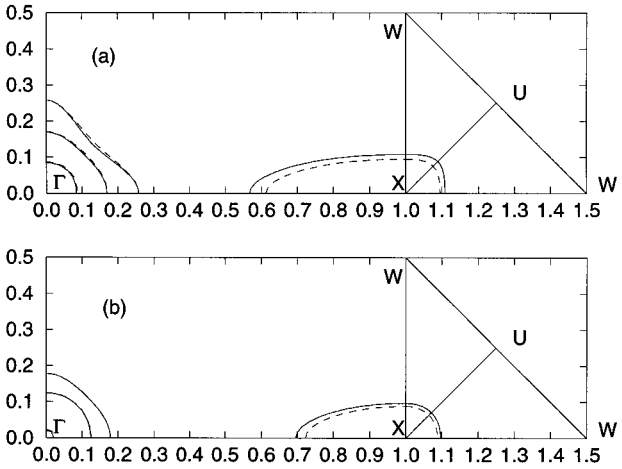

FIG. 3. Fermi surface of ErAs in LSD appromixation (a) and of $Er_{0.6}Sc_{0.4}As$ with adjusted band structure (b). Solid and dashed lines correspond to different spin. Wave vectors along the axes are in units of $2\pi/a$.

parallel to the quantization axis of the wave vector, i.e., perpendicular to the interface of the ErAs quantum well in the tunneling device. In the SdH experiments,[9] where the magnetic field is always perpendicular to the quantized hole orbit, only a small exchange splitting (10.9 ± 0.6 meV) of the hole bands was detected.

The band structures along [001] and [100] directions with $\mathbf{B}\|[001]$ are displayed in Fig. 1. It shows that the exchange splitting of the hole states for $\mathbf{B}\|\mathbf{k}$ (40 meV at the Fermi level) is indeed much larger than for $\mathbf{B}\perp\mathbf{k}$ (4 meV). The latter is even smaller than suggested by the experiment,[9] but we note that the experiments do not pertain to bulk samples.

The band structures presented in Fig. 2 correspond to $\mathbf{B}\|\hat{z}$ while the $\Delta\equiv\Gamma-X$ axis displayed is in the xy plane. The considerable splitting of the hole bands (e.g., along the $\Lambda=\Gamma-L$ direction) is mostly due to the $\mathbf{B}\|\mathbf{k}$ component. The corresponding extremal Fermi-surface cross sections are shown in Fig. 3. The orbits shown are perpendicular to the **B** field so as to correctly represent the spin splittings for the hole states appearing in SdH measurements. For the electron orbits near X we are concerned with the large ''longitudinal'' cross section in the ΓXW plane labeled B, and the small ''transverse'' cross section in the XWU plane labeled A. The spin polarization for both can readily be observed. For the hole orbits near Γ, we are concerned with the heavy-, light-, and spin-orbit split-off-hole band orbits. As can be seen, the spin splitting of the hole sheets of the Fermi surface is rather small, as discussed in the preceding paragraph.

The top panel of Fig. 2 presents the bands for ErAs in the LSDA while the bottom panel shows the adjusted band structure of $Er_{0.6}Sc_{0.4}As$. We note in Fig. 3 the overall reduction in Fermi-surface dimensions introduced by our correction to the LSDA as well as the shape change in the electron surface which becomes more ellipsoidal as a result of the reduction of hybridization between the crossing bands near X.

The SdH frequencies are proportional to the areas A of the extremal cross sections. The oscillating part of the transverse magnetoconductivity was calculated following Adams and Holstein[20] as

TABLE I. Fermi-surface parameters of ErAs and $Er_{0.6}Sc_{0.4}As$.

	ErAs		$Er_{0.6}Sc_{0.4}As$		
	LSDA	Adjusted[a]	LSDA	Adjusted[b]	Expt.[c]
	Shubnikov–de Haas frequencies (Tesla)				
e_{A+}	550	486	510	388	386
e_{A-}	414	360	386	323	328
e_{B+}	1887	1581	1570	1206	1111
e_{B-}	1477	1213	1202	1018	941
hh_+	1926	1635	1480	1246	1273
hh_-	1875	1604	1477	1237	1222
lh_+	1071	846	888	645	612
lh_-	1044	826	876	637	589
sh_+	333	165	239	44	150
sh_-	317	158	235	43	150
	Cyclotron masses (electron mass)[d]				
e_{A+}	0.17	0.16	0.19	0.16	0.17
e_{A-}	0.15	0.14	0.18	0.15	0.17
e_{B+}	0.45	0.42	0.50	0.43	0.47
e_{B-}	0.42	0.39	0.47	0.42	0.47
hh_+	0.50	0.47	0.40	0.41	1.0
hh_-	0.49	0.46	0.39	0.41	1.0
lh_+	0.32	0.28	0.27	0.25	0.5
lh_-	0.31	0.28	0.26	0.25	0.5
sh_+	0.14	0.16	0.14	0.17	
sh_-	0.13	0.15	0.13	0.16	
	Carrier concentrations (10^{20} cm^{-3})[e]				
total $n=p$	5.54	4.14	4.89	2.795	3.3 (3.33)[e]
$e-$	3.38	2.57	3.05	1.625	
$e+$	2.16	1.57	1.84	1.173	
hh_+	1.96	1.55	1.74	1.03	2.5
hh_-	1.70	1.38	1.48	0.98	2.5
lh_+	0.88	0.62	0.79	0.40	0.83
lh_-	0.79	0.57	0.70	0.39	0.83
sh_+	0.11	0.01	0.09	0.00	
sh_-	0.10	0.01	0.08	0.00	

[a]Er-5d shifted up by 0.82 eV as for $Er_xSc_{1-x}As$.
[b]Er-5d–Sc-3d shifted upwards so as to adjust e_A SdH frequencies.
[c]Deduced by a fit of Eq. (1) to the experiment for a 71 monolayer sample of $Er_{0.57}Sc_{0.43}As$. (Ref. 9).
[d]Note that $m_B=\sqrt{m_t m_l}$ and $m_A=m_t$ in an ellipsoidal model.
[e]The value in parentheses is p, the other is n.

$$\frac{\Delta\sigma}{\sigma_0}=5\pi\sum_i\sum_{r=1}^{\infty}(-1)^r\sqrt{\frac{B}{2\pi r f_i}}\times\exp\left(-\frac{2\pi^2 m_i kT_{Di}r}{\hbar eB}\right)\frac{2\pi^2 r m_i kT/\hbar eB}{\sinh(2\pi^2 r m_i kT/\hbar eB)}\times\cos\left(\frac{2\pi r f_i}{B}-\frac{\pi}{4}\right), \quad (1)$$

where i labels the various orbits whose SdH frequencies are given by $f_i=A_i\hbar/e$ and masses m_i by $m_i=(\hbar^2/2\pi)(\partial A_i/\partial E)_{E_F}$, B is the magnetic field, and T the temperature. The f_i and m_i are obtained from our band-structure calculations. The remaining parameters which describe the broadenings of the various peaks are the Dingle temperatures $T_{Di}=\hbar/2\pi k\tau_i$ which are determined by the lifetimes τ_i. Approximate values for the lifetimes are given by $\tau_i=m_i\mu_i/e$ with mobilities μ_i deduced from Hall measurements.[8] The values used in the simulation corresponding to $T=4.2$ K were $\mu_{e\perp}=969$, $\mu_{e\parallel}=126$, $\mu_{lh}=767$, and $\mu_{hh}=856$ cm^2/V s.[8]

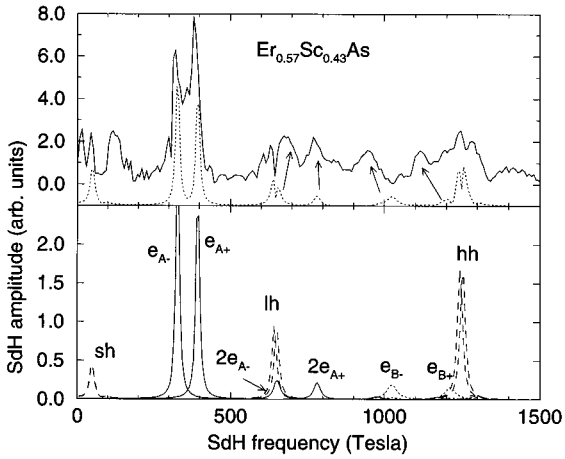

FIG. 4. Shubnikov–de Haas Fourier transform spectrum for $Er_{0.6}Sc_{0.4}As$ alloy. Upper panel: experiment (solid line) compared to theory (dotted line); bottom panel: separate electron A (solid line), B (dotted line), and hole (dashed line) orbit contributions to theory.

The calculated SdH frequencies, cyclotron masses, and carrier concentrations are given in Table I for pure ErAs and for $Er_{0.6}Sc_{0.4}As$ with and without the corrections to the LSDA along with experimental values.[8] The Fourier transform of Eq. (1), which is nearly periodic in $1/B$, for the calculated parameters for $Er_xSc_{1-x}As$ is shown in Fig. 4 along with its decomposition into separate contributions and the experimental spectrum. The agreement between theory and experiment is quite good considering that the only adjusted parameters in the theory are the rigid upward shifts of (minority) spin-up (+) and majority spin-down (−) Er-5d bands. The poorest agreement occurs for the electron B-orbit SdH frequencies which are overestimated by the theory by about 100 T. We note that this is sensitive to the precise shape of the Er-d derived Δ_7 band (Δ_2' in single group notation) which is slightly more susceptible to error in our calculations because of the uncertainties in the quasiparticle correction.

The present calculations strongly support the original interpretation of the experiment which assigns the highest frequency (above 1200 T) to the heavy-hole orbit and the spin-split peaks at 930 T and 1110 T to the B cross sections of the electron pockets. The spin-orbit split-off band (sh) can be seen to barely contribute any carriers. Its contribution is expected to disappear completely in thinner samples due to size quantization effects which would further lower the corresponding energy levels relative to the Fermi level. Experimentally,[9] a peak at 150 T was assigned to the spin-orbit split-off band. It is more pronounced in Hall data and indeed only detectable in sufficiently thick samples. The adjusted calculation underestimates the corresponding SdH fre-

quency. This and the remaining small discrepancies for the other SdH frequencies perhaps indicate the need for nonuniform shift and mass corrections for the hole bands beyond local spin density approximation (LDA).

The major change from our earlier work resulting from the inclusion of the spin-orbit interaction involves the hole surfaces. In particular, the area of the heavy- (split-off) hole orbit is significantly increased (decreased) while the difference between the hh and lh areas is increased. These changes can easily be understood in terms of the lowering of the split-off band and the increased interaction between the hh and lh bands. The former requires a shift of the Fermi level versus the top of the As-p bands at Γ in order to maintain the same Fermi volume as without spin-orbit coupling. The latter results from the lifting of degeneracies along symmetry lines in the double group.

The hole mass parameters extracted independently from the experiment[8] for which the discrepancy appears to be quite large were noted earlier[8] to be rather uncertain because the experimental derivation is based on the temperature dependence of the SdH signal over a very narrow temperature range (1.4 – 4.2 K). The ratio of the light- to heavy-hole contribution to the carrier concentration $p_{\mathrm{lh}}/p_{\mathrm{hh}}$ ($=0.40$ calculated) is in good agreement with the experiment (0.33–0.38). In a parabolic band model this determines the light- to heavy-hole density of states mass ratio through $m_{\mathrm{lh}}/m_{\mathrm{hh}}=(p_{\mathrm{lh}}/p_{\mathrm{hh}})^{2/3}$. The directly calculated value for $m_{\mathrm{lh}}/m_{\mathrm{hh}}$ is 0.60 while the above relation yields 0.54.

In conclusion, the present band-structure study including spin-orbit coupling resolves the difference in the interpretations of the Shubnikov–de Haas spectra of $\mathrm{Er}_x\mathrm{Sc}_{1-x}\mathrm{As}$. It supports the original interpretation[6–9] rather than the interpretation of Ref. 10 in which heavy-hole and longitudinal electron assignments were interchanged. The main conclusion from the earlier work that the overall Fermi-surface dimensions are overestimated by the LSDA remains unchanged. With the introduction of a constant energy ''gap correction'' our calculations for $\mathrm{Er}_{0.6}\mathrm{Sc}_{0.4}\mathrm{As}$ yield Fermi-surface parameters which are in excellent agreement with experiment. A similar gap correction in the calculations for ErAs provides corresponding predictions for that material.

This work was supported by the Air Force Office of Scientific Research under Grants No. F49620-95-1-0043 at CWRU and No. F49620-96-1-0383 at SDSM&T. R.B. acknowledges support from the Belgian National Fund for Scientific Research.

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