CONNECTION BETWEEN THE ANOMALOUS HALL EFFECT AND THE STRUCTURE OF THE FERMI SURFACE

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We consider the connection between the anomalous Hall field in transition metals and the structure of the Fermi surfaces. It is established that the sign of the constant characterizing the anomalous field depends significantly not only on the shapes of these surfaces, but also on the predominance of some particular spin orientation in the phase volumes in which they are enclosed. Thus, in the case of nickel, a negative sign of the constant of the anomalous Hall field is the result of the fact that the average component M_z of the magnetic moment of the electrons of the unfilled bands is oriented against the resultant magnetic moment (which is directed along the z axis). It is shown that the predominance of the positive or negative M_z spin components on the Fermi surfaces can be established from the experimental data on the magnitude and signs of the anomalous and normal Hall fields.

UNTIL recently, the Fermi surfaces of ferromagnetic and many antiferromagnetic metals were unknown and it was necessary to consider in the theories of the anomalous Hall effect (see[1-8]) very simple models, which in the majority of cases were quite crude. As a result, the theoretical calculations were sufficiently rigorous only when intermediate formulas were obtained, containing parameters which could not be measured. Any concretization was achieved at the expense of rough approximations, which made the conclusions of the theory hypothetical. Thus, in[1-6] the calculations of the off-diagonal components of the electric conductivity tensor, and consequently of the Hall constants, were made in the effective-mass approximation. In [1,2] and [4,5], devoted to the anomalous Hall effect connected with polarized conduction electrons, each such electron was ascribed the same component M_z of the magnetic moment in the direction of the average magnetization. Obviously, all effects that can result from different signs of M_z in different conduction bands were thereby excluded. It is easy to show that neglect of these effects could lead to an error even in the estimate of the sign of the anomalous Hall-effect constant R_a.

During the last three–four years, following experimental investigations of the magnetoresistance and Hall effect of nickel in strong magnetic fields[9] and of the magnetooptic parameters of ferromagnetic metals[10-12], a real opportunity of constructing the Fermi surfaces arose. Thus, several sufficiently satisfactory variants of the Fermi surface of nickel, which are quite close to one another, have by now been proposed[13-16]. Models were proposed for the Fermi surface of iron[17]. Although there are still no Fermi-surface models for the rare-earth metals, there are sufficiently reliable data on the Hall effects of these metals. In this connection a possibility arises of a new approach in the theory of the anomalous Hall effect.

In the present article we consider briefly, for the most part, qualitative conclusions concerning the signs of the anomalous Hall effect, which can be drawn from the existing concepts, with allowance for new data on the Fermi surface.

1. DEPENDENCE OF THE SIGN OF THE ANOMALOUS HALL CONSTANT ON THE PREDOMINANT SPIN ORIENTATION ON THE FERMI SURFACE

The sign of the anomalous part of the Hall field, as well as the sign of its normal part, is influenced by the predominance of the positive or negative curvature on the Fermi surface, or more accurately the predominance of the electron or hole conductivity. This was precisely the basis of the first attempts at explaining the cause of the differences between the signs of the anomalous Hall effect constant R_a in different metals. Agreement of the signs of the normal and anomalous Hall constants R_0 and R_a in iron, nickel, and gadolinium has contributed to the opinion that the change of the character of the carriers is the main cause of the change in the sign of R_a, although opposite signs of R_0 and R_a in cobalt and in a few ferromagnetic alloys pointed to the existence of other causes. Thus, it was emphasized in our earlier paper[5] that the sign of R_a depends also on which of the contributions do the anomalous current is larger, the contribution from the intrinsic spin-orbit interaction (SOI) or from the SOI with other electrons.

There is, however, one more cause affecting the sign of the constant R_a. Namely, if the appearance of the anomalous Hall field is connected principally with the polarization of the electrons in the thick part in the conductivity, then the sign of R_a depends on the sign of the mean value of the component M_z of the magnetic moment of these electrons, as can be seen directly, for example, from formulas (26), (27), and (19)–(21) of the second of our articles in[5]. As mentioned earlier, in[1,2] and[4,5], each of the electrons was assigned a certain average positive component M_z (the z axis is directed parallel to the magnetization of the metal), thus excluding in a number of cases the possibility of correctly estimating the sign of R_a. Indeed, exchange splitting takes place in the ferromagnetic state, and the bands of the electrons with spins "upward" and "downward" are unequally filled. If, for example, the bands with the "downward" spin are completely filled, and the bands with the "upward" spin are partly filled, then the contribution to the anomalous Hall field is made only by the electrons of the bands with the "upward" spin, whose component M_z is directed opposite the magnetization of the metal. In this case the sign of the anomalous Hall field will be opposite the sign calculated under the assumption that the component M_z is positive.

We shall henceforth base ourselves on the assumption that the main part of the anomalous Hall field in pure ferromagnetic transition metals above the Debye temperatures T_D is produced as a result of the intrinsic SOI of the electrons of the conduction band in scattering by phonons or by spin inhomogeneities. This assumption follows from the presently accepted point of view that the main carriers of the spontaneous magnetization in these metals are the conduction electrons of the d-, d—s-, and d—p-like bands. We assume, in addition, the general premises advanced in the already cited papers[1] and[4,5], but will forego the effective-mass approximation, and will take the sign of the spin into account in the estimates of the contributions to the anomalous Hall current from the different bands. It is known that the lifetime of an electron with a specified spin is much longer, when $T > T_D$, than its lifetime in the state with a specified quasimomentum vector and band number n, as a result of which it is possible to separate in the system two weakly-interacting subsystems of electrons with opposite spins. We shall take into account henceforth only collisions in which the electron conserves the spin.

It was shown earlier[7] that from experimental data obtained in the investigation of the Hall effect in the region of magnetic saturation, where the spin inhomogeneities decrease with increasing magnetic field, it follows that in transition ferromagnetic metals above the Debye temperatures the scattering by the spin inhomogeneities makes a smaller contribution to the anomalous Hall current than the scattering by phonons. We shall therefore consider henceforth in first approximation the contribution from the scattering of the electrons by the phonons.

In order to estimate the influence of the structure of the Fermi surface on the anomalous Hall current, we should transform the formula for the density j_β of the anomalous Hall current in such a way, that it contains integrals over the Fermi surface. For the case of scattering by phonons, a formula for j_β was derived in[2,4,5] and has the following form (see (22) in[5]):

$$j_\beta = ie^2 E_\alpha \sum_l \frac{d\rho_l}{d\varepsilon_l} v_{\alpha l}^l J_\beta^n + j_\beta^{(q)} = j_\beta^{(0)} + j_\beta^{(q)}, \tag{1}$$

where l combines the indices k and n, the summation is carried out over the states with quasimomentum k and band numbers n, the bands with spins "upward" and "downward" being numbered separately, E_α—electric field intensity, ρ_l—Fermi function, $\epsilon_l = \epsilon_{kn}$—electron energy, J_β^n—a correction, linear in the spin and caused by the SOI, to the diagonal matrix element of the coordinate x_β. In the derivation of formula (1), account is taken of the main periodic part of the SOI operator. In such a case, its matrix elements in the l representation are diagonal in k. We then have for crystal lattices with symmetry centers (see[2], formulas (31) and (34))

$$J_{\beta^n} = -i \frac{\nu_n'}{\Delta^2} [\mathbf{k}\mathbf{M}_n]_\beta, \tag{2*}$$

where M_n—average magnetic moment of the electron of the n-th band ($M_n = \pm \mu_\beta$), Δ^{-2}—value of $(\epsilon_{nk}^0 - \epsilon_{n'k}^0)^{-2}$ averaged over the conduction bands, ϵ_{nk}^0—unperturbed SOI value of the energy, and ν_n'—negative parameter that depends on the distribution of the ion charge[1)].

The quantity $j_\beta^{(q)}$ in (1) combines the terms obtained from renormalization of the velocity by introducing in the Hamiltonian the electron-phonon interaction operator, and the terms resulting from the correction of the second order to the Born scattering cross section. A formula for $j_\beta^{(q)}$ was derived by Gurevich and Yassievich[4] (formula (19) of [4]). Luttinger[1] derived a similar formula for the case of scattering of electrons by impurities, and showed that if the crystal lattice has a symmetry center, then it is possible to separate from $j_\beta^{(q)}$ the sum of terms $j_{\beta_1}^{(q)}$, which differs from the first sum in (1) by a constant positive factor

$$j_{\beta 1}^{(q)} = q_1 j_\beta^{(0)}. \tag{3}$$

The remaining sum $j_{\beta_2}^{(q)}$, just as in $j_{\beta_1}^{(q)}$, contains terms proportional to the corrections $C_{qll'}^1$ to the matrix elements of the electron-phonon interaction; these corrections are linear in the SOI. As shown in[4], the $C_{qll'}^1$ are diagonal in the spin and are thus proportional to M_n (in our case, when only transitions with spin conservations are taken into account, this result is obtained automatically). Consequently, $j_{\beta_2}^{(q)}$ can be written in the following general form:

$$j_{\beta 2}^{(q)} = e^2 E_\alpha \sum_{n,k} M_n \frac{\partial \rho_l}{\partial \varepsilon_l} v_{\beta^l} k_{\beta^l} F_l, \tag{4}$$

where F_l is a parameter that depends in the general case on the vector **k** and the band number n.

*$[\mathbf{k}\mathbf{M}_n] \equiv \mathbf{k} \times \mathbf{M}_n$.

1)The parameter ν'_n coincides, apart from a constant positive factor, with the parameter ν_n which enters in formulas (35) and (36) of [2]. In the case of p- and d-like conduction bands, this parameter is negative, since the values of the corresponding Bloch functions at the nuclei are zero. We note that for the same reason allowance for the interaction of the spins of the p- and d- like electrons with orbits of other electrons leads to corrections $\Delta J_\beta{}^n$ of the same sign as the quantity $J_\beta{}^n$ itself, calculated with allowance for the intrinsic SOI. From this it follows, as can be readily seen, that in the case of the anomalous Hall and Nernst-Ettingshausen fields under consideration, which are connected with the scattering of electrons by phonons, it is impossible to ascertain from the signs of these fields whether the main carriers of the spontaneous magnetization of the ferromagnetic metals are the electrons of the conduction bands or the electrons connected with the ions, as was indicated earlier in our articles [5] and [18].

In calculating the contributions to $j_{\beta_2}^{(q)}$ from different bands in the isotropic approximation, it is found that the signs of the terms of the sum (4) in n coincide with the signs of the corresponding terms of the first sum in (1). We shall henceforth assume that the terms of the sum (4) make either contributions of equal signs with the terms of the first sum of (1), or a smaller contribution as a whole. The correctness of such an assumption can be verified so far only by comparison with experiment, as will be done later.

We choose the x axis along the electric-field vector and the z axis along the spontaneous-magnetization vector of the metal. Then, substituting (2)—(4) in (1) and transforming the sums over k into intervals over ϵ_l and over the Fermi surface, we obtain for cubic lattices

$$j_y = \frac{\bar{\nu}/\Delta^2}{(2\pi)^3} e^2 E_\alpha \sum_n M_n \int_{S_n} \left(q_l \frac{\partial \varepsilon_l}{\partial k_x} k_x / |\operatorname{grad} \varepsilon_l| \right)_{\varepsilon_l = \varepsilon_F} dS_n, \tag{5}$$

where $q_l = 1 + q_1 - \Delta^2 F_l/\bar{\nu}$ is a dimensionless parameter and $\bar{\nu}$ is the value of ν_n averaged over the conduction bands. The integral has positive values for the electronic parts of the Fermi surface of the band and negative for the whole parts.

It follows from (5) that the anomalous Hall constant equals

$$R_a = -\frac{\sigma_{yx}}{4\pi I_s \sigma^2} = C \frac{1}{I_s \sigma^2} \sum_n M_n K_n S_n,$$

$$K_n = \overline{\left(q_l \frac{\partial \varepsilon_{kn}}{\partial k_x} k_x \Big/ |\operatorname{grad} \varepsilon_{kn}| \right)_{\varepsilon_{kn} = \varepsilon_F}},$$

$$C = -\frac{\bar{\nu} e^2}{32\pi^4 \Delta^2} > 0, \tag{6}$$

where I_s is the spontaneous magnetization of the metal, $\sigma = \sigma_{xx}$ is the electric conductivity. The bar denotes averaging over the surface S_n. We note that in the case of closed surfaces enclosing phase volumes in approximately equal transverse dimensions, the quantities $K_n S_n$ are roughly proportional to these values.

A relation similar to formula (6) can also be obtained for the constant Q_a characterizing the anomalous Nernst-Ettingshausen field in transition ferromagnetic metals. To this end it is necessary to transform formula (23) of article[5] for the density of the anomalous Nernst-Ettingshausen current $j_\beta^{(0)}$, resulting from the intrinsic SOI in scattering of electrons by phonons. After transformations similar to those made above, we obtain for the part of Q_a that is independent of the thermal emf

$$Q_a^{(0)} = -C' \frac{T}{I_s \sigma} \sum_n M_n |K_n S_n|, \tag{7}$$

where C' is a positive parameter and t is the absolute temperature.

We shall find it convenient to introduce the following definitions: we agree that the main carriers of the anomalous Hall current are electrons (holes) if the quantity $\sum_n K_n S_n$ for the electronic parts of the Fermi surface is appreciably larger (smaller) than the quantity $\sum_n |K_n S_n|$ for the hole parts of this surface. In exactly the same manner, we agree to say that the positive (negative) sign of the average value of M_z of the conduction-band electrons predominates if $\sum_n M_n | K_n S_n |$ has a positive (negative) sign. Inasmuch as $| M_n | = \mu_B$ = const for all bands, it follows from (6) that if the positive (negative) sign of M_z predominates and the carriers of the anomalous Hall current are electrons, then R_a has a positive (negative sign, and if these carriers are holes, it has a negative (positive) sign. The table lists the signs of R_a and Q_a obtained from (6) and (7) with either sign of M_z predominating and for different types of main carriers of the anomalous Hall and Nernst-Ettingshausen currents.

Signs of the Hall constant R_a and of the Nernst-Ettingshausen constant Q_a, obtained from theoretical formulas (6) and (7) for ferromagnetic transition metals

Predominant sign of the component M_z of the electrons of the conduction band (z axis parallel to the magnetization of the the metal)	Main type of carriers of anomalous Hall current	Sign of R_a from formula (6)	Sign of Q_a from formula (7)
+	Electrons	+	—
+	Holes	—	—
—	Electrons	—	+
—	Holes	+	+

We shall consider below concrete cases when, knowing the structure of the Fermi surface, we can explain the appearance of any particular sign of the constant R_a or Q_a, or can assess the singularities of the Fermi surface from the experimentally known values of these constants.

2. ANOMALOUS HALL EFFECT IN TRANSITION METALS AND STRUCTURE OF THE FERMI SURFACE

a) Nickel. Figure 1 shows the arrangements of the bands and Fermi level of ferromagnetic nickel as given

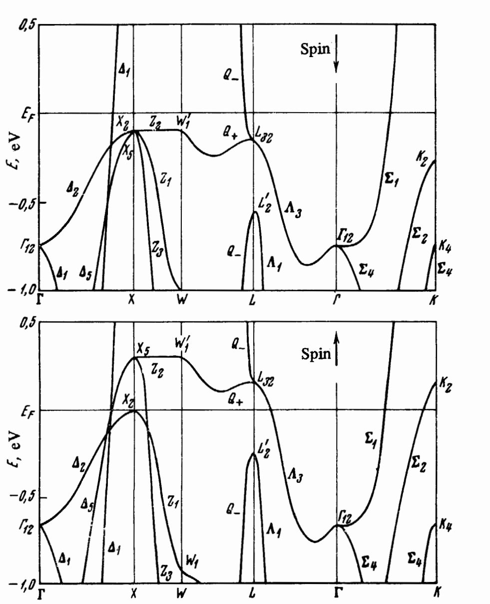

FIG. 1. Arrangement of bands and Fermi level of nickel, after [15].

in[15]. The arrangement of the curves $QL_2'\Lambda_1$ and $Q_1'L_{32}\Lambda_3$ indicated in Fig. 1 was first proposed by Krinchik and Gan'shina[11] to explain the results of an experimental investigation of the Kerr effect. The arrows show the direction of the spins in the bands. It is seen from Fig. 1 that in the ferromagnetic state the d-, d—s-, and d—p-like bands with "downward" spin are filled. (The Δ_2, Z_2, Q_+, Λ_3, and Σ_2 curves lie below the Fermi level.) Only the s-like band remains unfilled (the Δ_1, Q_-, and Σ_1 curves cross the Fermi level), and give a small contribution to the magnetization. The band with spin "upward" is unfilled. The electronic Fermi surface of this band has a spheroidal form with "nipples" in the direction of the points L, and the hole surface around the point X has the form of pockets with small volume. The electronic part of the Fermi surface of bands with "upward" spin, i.e., with M_z oriented opposite to the magnetization, has a larger area than the hole surface, and encloses a larger phase volume. Thus, in ferromagnetic nickel the electrons of the unfilled bands, which contribute to the current, have on the average a negative value of M_z and positive effective masses (owing to the hybridization of the d-, s-, and p-like bands, the effective masses of their electrons are not so large). It follows from the foregoing that the case of nickel corresponds to the third row of the table. Formulas (6) and (7) lead in this case to a negative sign for R_a and a positive sign for $Q_a^{(0)}$. The experimental data confirm this conclusion: at nitrogen temperatures and above, we have $R_a < 0$ and $Q_a^{(0)} > 0$ for nickel.

b) Iron. Investigations of the magnetoresistance of iron in strong magnetic fields leads to the conclusion that iron is among the metals in which the number of holes n_d equals the number of electrons n_e. However, in ferromagnetic compensated metals the numbers $n_d^{\pm}$ and $n_e^{\pm}$, i.e., the numbers of holes and electrons with specified spin direction, may differ. In the case of iron, as shown by Wakoh and Yamashita[17], $n_d^+ > n_e^+$ and $n_d^- < n_e^-$.

Figure 2 shows a diagram of the Fermi surfaces of iron for bands with "upward" and "downward" spins, as proposed in[17]. The Fermi surface of the less filled band with "upward" spin consists of small electronic "lenses," an electron surface around Γ, large hole cavities near H, and hole pockets around N. The total phase volume of the sections contained in the hole parts of this surface exceeds the phase volume located inside its electronic parts. The Fermi surface of the more filled band with "downward" spin consists of a large d—s electronic surface around Γ, small hole "pockets" near H and hole "sleeves" from H to N, but the phase volume enclosed in these sleeves inside one cell is smaller than the phase volume enclosed inside the d—s electron surface of the same band and the hole parts of the Fermi surface of the band with "upward" spin. This follows also from Table V of the article of Wakoh and Yamashita[17], which gives the cross sections of the indicated phase volumes and the ratios of the effective masses at different parts of the Fermi surface of iron.

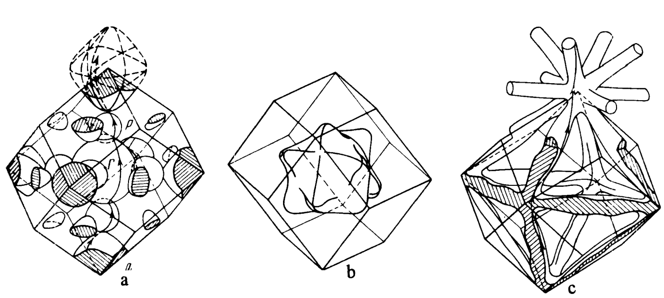

FIG. 2. Fermi surface of iron after [17]: a – for band with "upward" spin (less filled); b – electronic Fermi surface of band with spin "downward"; c – hole "sleeves" of band with "downward" spin.

Thus, the predominant current carriers of the polarized electrons of iron are electrons with positive M_z components and holes with negative components, corresponding to the first and fourth lines of the table. As seen from formula (6), both types of carrier give contributions of equal sign to the anomalous Hall current, corresponding to a positive sign of R_a. It is known from the experimental data that the constant R_a of iron is positive at nitrogen temperatures and above, thus confirming the theory.

The sign of the constant $Q_a^{(0)}$ of the anomalous Nernst-Ettingshausen effect, after subtracting the part connected with the Hall effect as a result of the thermal emf, as seen from formula (7), does not depend on the type of carrier, but depends on the predominant sign of the mean value of M_z of the conduction electrons. In the case of iron, as we have already seen, there are two predominant types of carrier with opposite signs of M_z. According to (7), these carriers should make contributions of different sign to the anomalous Nernst-Ettingshausen field, namely positive as a result of the holes of the less-filled band with "upward" spin (Fig. 2a) and negative as a result of electrons and holes of the more-filled band with "downward" spin (Figs. 2b and c). Thus, the theory leads to the conclusion that different signs of $Q_a^{(0)}$ can be observed in iron, depending on the degree of filling of the bands. This conclusion is confirmed by experiment. Experiment shows (see[18]) that negative $Q_a^{(0)}$ are observed in iron at lower temperatures and positive $Q_a^{(0)}$ at higher temperatures.

c) Cobalt. At present there are no reliable experimental data which make it possible to determine the structure of the Fermi surface of cobalt, and therefore we cannot explain the observed signs of R_a and $E_a^{(0)}$ by starting from the form of this surface. We can proceed to do the opposite, however, i.e., to attempt to reveal certain features of the Fermi surface of cobalt by starting with the known experimental data on R_a and $Q_a^{(0)}$.

It is known from experiment that in cobalt with face-centered lattice there are observed positive values of the constants R_a and $Q_a^{(0)}$, which means, in accordance with formulas (6) and (7) (see the table) that the negative sign of the component M_z predominates in the electrons of the conduction bands of cobalt if the main carriers of the anomalous Hall current are holes. Thus, the experimental data on the values of R_a and $Q_a^{(0)}$ lead to the conclusion that in cobalt with face-centered lattice, just as in nickel, there is a strong filling of bands with "downward" spin (with positive values of M_Z), but, unlike nickel, the hole Fermi surfaces of the less filled bands with negative components of M_Z prevail over the electronic ones.

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