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Model of intrinsic anomalous Hall effect in polycrystalline ferromagnets

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A method for estimating the coefficient of the dissipation-independent anomalous Hall effect for polycrystalline samples of pure ferromagnetic metals is proposed. The transverse resistivity characterizing the intrinsic anomalous Hall effect has been calculated for iron, cobalt and nickel. It is shown that the sign of the calculated anomalous Hall resistance always coincides with the experimental one. For nickel and cobalt, the results within the measurement error are in agreement with the experimental data. The experimental value for iron exceeds the calculated value by 2.7 times.

Keywords: anomalous Hall effect, spin-orbit interaction, strong coupling approximation, nearest neighbors approximation, ideal Fermi gas approximation, Hartree–Fock method, effective charge.

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Introduction

The anomalously high value of transverse conductivity in ferromagnetics was noted by E. Hall already in 1881 [1] when systematically studying electron transport in various metals in the external magnetic field. The anomalous Hall effect (AHE) is characterized by dependence of transverse resistivity both on magnetic induction **B** and magnetization **M** as well:

$$\rho_{xy} = \rho_H = R_0 B_z + R_s \mu_0 M_z, \tag{1}$$

where μ_0 is the magnetic constant. Here, as in the classic Hall effect, the coefficient R_0 is mainly determined by the concentration of carriers, whereas R_s is intricately related to many material parameters, in particular, it depends on longitudinal resistivity $\rho_{xx} = \rho$. The microscopic theory that explains the AHE by means of spin-orbit interaction of polarized conductivity electrons was developed in 1954 by R. Karplus and D. Lattinger [2].

Presently, the AHE is described by three competing mechanisms [3–5], which manifest themselves or get weaker depending on conductivity of the material and presence of foreign impurities therein. It is known that the same mechanisms are responsible for origin of the spin Hall effect (SHE) in non-magnetic materials [6]. When the metal contains impurities, the AHE can occur due to side jump perpendicular to a direction of electron momentum after scattering of any type. This mode is characterized by low longitudinal conductivity ($\sigma_{xx} < 10^6\,(\Omega \cdot \mathrm{m})^{-1}$), while the transverse conductivity depends almost quadratically on the longitudinal one.

In pure metals, when $\sigma_{xx} > 10^6\,(\Omega \cdot \mathrm{cm})^{-1}$, the basic mechanism of AHE origination is nonsymmetrical scattering on magnetic moments (skew-scattering) due to spin-orbit interaction [7]. It is quite difficult to experimentally study this mode, since the magnetic field H that is necessary for saturation of magnetization M, greatly contributes to the common Hall effect, while R_0 is about R_s [8], i.e. the common Hall effect with high conductivity is approximately the same as the anomalous one or higher.

The mode when longitudinal conductivity is within the range $10^6 < \sigma_{xx} < 10^8\,(\Omega \cdot \mathrm{m})^{-1}$ is an intrinsic (internal) or dissipation-independent one. The AHE of this mode is determined by a band structure of the material and transverse conductivity weakly depends on the longitudinal one. In the modern model of intrinsic AHE, the material band structure is analyzed in terms of an integral of the electron Berry curvature across an occupied part of the Brillouin zone. It has been shown in the paper [9] that in the strong coupling approximation and in the Vanier representation this integral could be reduced to the integral across the Fermi surface only. The illustrative calculation of anomalous Hall conductivity by this method provided the results that qualitatively match the experimental ones [10–12]. However, the studies [10,11] have measured not the anomalous Hall conductivity σ_{xy}, but rather the AHE coefficient R_S, $[\Omega \cdot \mathrm{cm/G}]$. The study [12] includes only temperature dependences of the anomalous Hall conductivity without any initial magnetic-field dependences.

It should be noted that the studies [10–12] do not identify contribution of the intrinsic AHE. The paper [9] does not list a method of such identification. The studies of the paper [11] were on nickel of technical purity within the temperature range $-200-360\,^\circ$C. The paper [10] investigated single-crystal iron whiskers. In this geometry, there is an additional AHE mechanism — charge carrier scattering on the sample surface [13], whose contribution to AHE does not depend on longitudinal conductivity in the same way as for the intrinsic mode. It is impossible to identify the intrinsic AHE by the temperature dependence of transverse conductivity within a range of the helium temperatures for thin films. That is why, despite existence of the developed theoretical description of the mechanism of the intrinsic AHE, it is difficult to experimentally substantiate it. The study [14] dedicated to it was not further confirmed [5].

By comparing the magnetic-field and temperature dependences of an anomalous component of Hall resistance with the temperature dependence of longitudinal resistance, the study [5] has obtained experimental confirmation of an essential role of the intrinsic AHE mechanism in the two-dimensional heterosystem. It seems that the two-dimensional nature of charge carriers' motion excludes influence of scattering on the film surface. In the 3D-structures, it is advisable to experimentally confirm the intrinsic AHE on macroscopic polycrystalline samples. The model of the intrinsic AHE in these structures can be presumably obtained by supplementing the strong coupling approximation and the Vanier representation used in [9] with taking into account specific features of the Fermi surface through a constant of the normal Hall effect [15,16].

1. Dynamics of conductivity electron in single-domain ferromagnetic

A spin-orbit additive to the single-energy electron in the defined electric field with the potential $\Phi(\mathbf{r})$ is as follows [17]:

$$\hat{V} = -\frac{\hbar e}{2m^2c^2}\,\varepsilon_{\beta\gamma\delta}\,\hat{s}_\beta\,\frac{\partial\Phi}{\partial r_\gamma}\,\hat{p}_\delta. \tag{2}$$

Here, m — the mass of electron with the charge $-e$, $\hbar$ — the reduced Planck constant, c — the speed of light in vacuum, $\varepsilon_{\alpha\beta\gamma}$ — the unit antisymmetric Levy–Civita tensor. The formula (2) and further on implies summing with respect to repeated indices over the entire range of their variation. The electron momentum dynamics induced by disturbance (2) is characterized by the following equation for the averages [18]:

$$\frac{dp_\alpha}{dt} = \frac{i}{\hbar}\,\langle[\hat{V},\hat{p}_\alpha]\rangle = \frac{\hbar e\varepsilon_{\beta\gamma\delta}}{2m^2c^2}\,\langle\psi|\hat{s}_\beta\,\frac{\partial^2\Phi}{\partial r_\alpha\partial r_\gamma}\,\hat{p}_\delta|\psi\rangle. \tag{3}$$

A crystallite of pure metal can be regarded as a homonuclear macromolecule with a metallic bond. Within the framework of the single-electron Hartree–Fock approximation, each collectivized electron is in a self-consistent field created by ion residues and other collectivized electrons [18]. The self-consistent field is usually constructed by the method of successive approximations. In the initial approximation, the wave function of the collectivized electron is considered to be a molecular spin-orbital and represented as a linear combination of the atomic spin-orbitals.

In any given spin state of an electron, one may choose such a direction of the axis z that the projection of its spin onto this axis assumes a specific value s_z, i.e. $\psi(\mathbf{r},\sigma) = \psi(\mathbf{r})\delta(\sigma, s_z)$. In doing so, the vector of the average value of the spin $\mathbf{s} = \langle\hat{\mathbf{s}}\rangle$ will be directed along the axis z [8]. In the strong coupling approximation, such a combination for a coordinate part of the wave function $\psi(\mathbf{r})$ may be the Vanier function [19]:

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{n=1}^{N}\Psi_C(\mathbf{r}-\mathbf{R}_n)\exp(i\mathbf{k}\mathbf{R}_n), \tag{4}$$

where $\Psi_C(\mathbf{r})$ — the atomic function of the external electron, $\mathbf{R}_n$ — the translation vector, N — the number of nodes in the crystallite.

The model potential of the initial approximation is taken by us to be a potential of the crystal field of the ionic residuals with the effective charge $+Ze$ and the coordinates $\mathbf{r}_k$:

$$\Phi(\mathbf{r}) = \frac{eZ}{4\pi\varepsilon_0}\sum_{k=1}^{N}\frac{1}{|\mathbf{r}-\mathbf{r}_k|}. \tag{5}$$

Here ε_0 is the electric constant.

If as the initial approximation, the atomic wave function $\Psi(\mathbf{r})$ in the relationship (4) is considered to be a hydrogen-like one, then the magnitude Z may be evaluated by equating the coordinate of the maximum of a radial component of this function to the atom radius. The effective charge in the model potential (5) together with the strong coupling approximation (4) means that construction of the self-consistent field for the collectivized electron takes into account only its interaction with the nuclei and localized electrons of the ion residues.

Within the framework of the Hartree–Fock, electron identity, i.e. exchange interaction of the conductivity electron with the localized electrons is taken into account by representing the wave function of the equation (3) as a Slater determinant that is composed of spin-orbitals of the conductivity electron and all the localized crystallite electrons. In this approximation, the exchange interaction energy of the conductivity electron with all the localized electron is disintegrated into a sum of pairwise exchange interactions of the conductivity electron with each of the localized electrons separately [20]. The similar conclusion can be made about the right-hand side of the equation (3), too. The following approximation shall take into account interaction (including the exchange interaction) of the collectivized electron with other conductivity electrons.

For pairwise interaction of the first and second electrons the average of the formula (3) is in the state

$$\psi(\mathbf{r}_1,\sigma_1,\mathbf{r}_2,\sigma_2) = \big(\psi_1(\mathbf{r}_1,\sigma_1)\psi_2(\mathbf{r}_2,\sigma_2) - \psi_1(\mathbf{r}_2,\sigma_2)\psi_2(\mathbf{r}_1,\sigma_1)\big)/\sqrt{2}.$$

We assume that (3) describes the dynamics of momentum of the first conductivity electron, while the second electron is a localized one. Then, taking into account the Hermitian quality of the momentum operator, we obtain

$$\langle\psi|\hat{s}_\beta \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi\rangle = \langle\psi_1|\hat{s}_\beta \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi_1\rangle - \mathrm{Re}\left\{\langle\psi_1|\hat{s}_\beta \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi_2\rangle\langle\psi_2|\psi_1\rangle\right\}.$$

Here, the quantum average means integration across the coordinates and summation over the spin variables. By assuming that

$$\psi_1(\mathbf{r},\sigma) = \psi_1(\mathbf{r})\delta(\sigma, s_{z1}),$$
$$\psi_2(\mathbf{r},\sigma) = c_+\psi_{2+}(\mathbf{r})\delta(\sigma, s_{z1}) + c_-\psi_{2-}(\mathbf{r})\delta(\sigma, -s_{z1}),$$
$$|c_+|^2 + |c_-|^2 = 1,$$

we obtain

$$\langle\psi|\hat{s}_\beta \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi\rangle = s_{1\beta}\langle\psi_1| \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi_1\rangle - |c_+|^2 s_{1\beta}\,\mathrm{Re}\left\{\langle\psi_1| \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi_{2+}\rangle\langle\psi_{2+}|\psi_1\rangle\right\}.$$

Taking into account that $|c_+|^2 = 1/2 + 2\mathbf{s}_1\mathbf{s}_2$ and neglecting that the coordinate part of the wave function of the localized electron depends on its spin state, we transform this formula:

$$\langle\psi|\hat{s}_\beta \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi\rangle = s_{1\beta}\left[\langle\psi_1| \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi_1\rangle - \frac{1}{2}\right] \times \mathrm{Re}\left\{\langle\psi_1| \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi_2\rangle\langle\psi_2|\psi_1\rangle\right\} - 2s_{1\beta}s_{1\sigma}s_{2\sigma} \times \mathrm{Re}\left\{\langle\psi_1| \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi_2\rangle\langle\psi_2|\psi_1\rangle\right\}. \quad (6)$$

In the formula (6), the quantum average is calculated by integration across the coordinates. The formula (3) is written for the momentum dynamics of one conductivity electron. In order to find the dynamics of the average momentum for an assembly of the conductivity electrons, the formula (6) shall be averaged along the spin states of these electrons. If the conductivity electrons are not polarized, then in a macroscopically isotropic medium $\langle s_{1\beta}\rangle = 0$, $\langle s_{1\beta}s_{1\sigma}\rangle = \delta_{\beta\sigma}/4$. Then

$$\frac{dp_\alpha}{dt} = -\frac{\hbar e\varepsilon_{\beta\gamma\delta}}{4m^2c^2} s_{2\beta}\,\mathrm{Re}\left\{\langle\psi_1| \frac{\partial^2\Phi}{\partial r_\alpha \partial r_\gamma} \hat{p}_\delta|\psi_2\rangle\langle\psi_2|\psi_1\rangle\right\}. \quad (7)$$

The left-hand side of relation (7) is equal to the force acting on an electron. It may be presented as a result of influence of the foreign electric field $\mathbf{E}_{AH}$ on the electron. The right-hand side of the relationship (7) is associated with pairwise interaction of the conductivity electron with one localized electron. In order to find the full field $\mathbf{E}_{AH}$, the formula (7) shall be summated over all the localized electrons taking into account their spins. In the ferromagnetic, the spins of the localized electrons of magnetization are oriented similarly within a domain due to exchange interaction, and it can be assumed for them that all $s_{2\beta} = s_\beta$. The spins of the other localized electrons are arbitrarily oriented and their total contribution to the field $\mathbf{E}_{AH}$ is zero.

Let each node have only one localized electron with the wave function $\psi_2(\mathbf{r}) = \Psi_L(\mathbf{r} - \mathbf{r}_i)$. Here $\mathbf{r}_i$ is the coordinate of the i-th node, the starting point is a node with the collectivized conductivity electron with the wave function like in (4). Then, for the potential of the effective field like in (5), by substituting the variables $\mathbf{r} - \mathbf{r}_k \to \mathbf{r}$, we obtain

$$E_{AH\alpha} = \frac{\hbar eZs_\beta}{16\pi\varepsilon_0 m^2c^2N}\,\mathrm{Re}\Big\{\exp\big(i\mathbf{k}(\mathbf{R}_n - \mathbf{R}_m)\big)\langle\Psi_C(\mathbf{r}+\mathbf{r}_k-\mathbf{R}_n)| \times \left(3\frac{\varepsilon_{\beta\gamma\delta}r_\alpha r_\gamma}{r^5} + \frac{\varepsilon_{\alpha\beta\delta}}{r^3}\right)\hat{p}_\delta|\Psi_L(\mathbf{r}+\mathbf{r}_k-\mathbf{r}_i)\rangle \times \langle\Psi_L(\mathbf{r}-\mathbf{r}_i)|\Psi_C(\mathbf{r}-\mathbf{R}_m)\rangle\Big\}. \quad (8)$$

The atomic functions are exponentially small when $r > R_a = na_\mathrm{B}/Z$, n is the principal quantum number. At the same time, the distance between atoms in the crystal is substantially higher than R_a. Therefore, in the first approximation only the summands with $\mathbf{r}_i = \mathbf{r}_k$ can be left in the relationship (8). The different atomic wave functions are orthogonal so when $\mathbf{R}_m - \mathbf{r}_k = 0$ the right-hand side of (8) is zero. The operator

$$\left(3\frac{\varepsilon_{\beta\gamma\delta}r_\alpha r_\gamma}{r^5} + \frac{\varepsilon_{\alpha\beta\delta}}{r^3}\right)\hat{p}_\delta$$

in the right-hand side of the relationship (8) is odd. If the wave functions Ψ_L and Ψ_C have the same parity ($s-d$-interaction), then when $\mathbf{R}_n - \mathbf{r}_k = 0$ the right-hand side of (8) is zero. It is possible to limit by a nearest neighbors approximation and to restrict the right-hand side only with summands for which $\mathbf{R}_n - \mathbf{r}_k = \mathbf{a}_i$, and $\mathbf{R}_m - \mathbf{r}_k = \mathbf{a}_j$, where $\mathbf{a}_i$ — the vector from the considered atom with a center in the point $\mathbf{r} = 0$ to the nearest neighbor. Thein, in the relationship (8) in the first order of smallness for $\mathbf{ka}_i$ we obtain:

$$E_{AH\alpha} = \frac{\hbar Zes_\beta k_\mu}{8\pi\varepsilon_0 m^2c^2}(a_{i\mu} - a_{j\mu})\,\mathrm{Im}\Big\{\langle\Psi_C(\mathbf{r}-\mathbf{a}_i)| \times \left(3\frac{\varepsilon_{\beta\gamma\delta}r_\alpha r_\gamma}{r^5} + \frac{\varepsilon_{\alpha\beta\delta}}{r^3}\right)\hat{p}_\delta|\Psi_L\rangle\langle\Psi_L|\Psi_C(\mathbf{r}-\mathbf{a}_j)\rangle\Big\}. \quad (9)$$

Considering the AHE only in metals, we will use the ideal Fermi gas approximation for conductivity electrons. Applicability of this model for the conductivity electrons in the metals is justified by the fact that thermodynamics of the Fermi system is determined by its microscopic structure only near the Fermi surface and is completely irrelevant of what is happening outside blur of the order of $k_\mathrm{B}T$, where k_B — the Boltzmann constant, T — the temperature. As a result, the denser Fermi gas in the metal, the more ideal it is [21]. The experimental studies of the temperature dependence of the electron heat capacity in the metals show that it well corresponds to the model of the ideal Fermi gas with the scalar effective mass m^*.

2. Dissipation-independent AHE in a polycrystalline ferromagnetic

Let us consider a homogeneous and isotropic macroscopic area of the polycrystalline ferromagnetic, within which the current density and magnetization may be considered to be constant. Assume within the framework of the effective mass method in (9) $\mathbf{k} = -\mathbf{j}m^*/(\hbar e n_e)$, where $\mathbf{j}$ — the density of the charge current, n_e — the concentration of the conductivity electrons. Within this area we average the equation (8) along the spin momentums of the localized electrons. Each crystallite is split into domains magnetized to saturation $M_S = B_S/\mu_0$, where B_S — the saturation induction, and within the crystallite it can be assumed that $\langle \mathbf{s} \rangle = -\mathbf{M}/(\mu_B n_a)$, where μ_B — the Bohr magneton, n_a — the atom concentration. Then

$$E_{AH\alpha} = \frac{Zm^* M_\beta j_\mu (a_{i\mu} - a_{j\mu})}{8\pi\varepsilon_0 m^2 c^2 \mu_B n_e n_a} \operatorname{Im}\Big\{ \langle \Psi_C(\mathbf{r}-\mathbf{a}_i)| \times \left(3\frac{\varepsilon_{\beta\gamma\delta} r_\alpha r_\gamma}{r^5} + \frac{\varepsilon_{\alpha\beta\delta}}{r^3} \right) \hat{p}_\delta |\Psi_L\rangle \langle \Psi_L | \Psi_C(\mathbf{r}-\mathbf{a}_j)\rangle \Big\}. \quad (10)$$

The energy of the electron in the atom in the electric field depends on a projection of its orbital moment to the field direction [8]. Therefore, orientation of the atom orbitals is determined by a position of crystallophysical axes of the crystallite and it may be assumed that the relationship (10) is written in the system of coordinates that is associated with the crystallite symmetry axes. Let us introduce a laboratory coordinate system associated with the instruments that set the conductivity current and magnetization and measure components of the electric field. That is why the vectors of the current density, magnetization and the electric field shall be assumed to be defined in the laboratory coordinate system. The components of vectors and tensors in the laboratory system will be denoted by hatched indices, and the components of vectors and tensors in the coordinate system associated with the domain crystal axes will be denoted by non-hatched indices.

Let us transform, within the crystallite, the vector of the current density and the magnetization vector from the laboratory system into the system of the crystallophysical axes, $j_\mu = p_{\mu\mu'} j_{\mu'}$, $M_\beta = p_{\beta\beta'} M_{\beta'}$, and transform the vector of the Hall electric field from the system of the crystallophysical axes into the laboratory one $E_{H\alpha'} = p^{-1}_{\alpha'\alpha} E_{H\alpha}$, where $p_{\alpha'\alpha}$ — the unitary rotation matrix. By inserting this conversion into the equation (10), we average the vector $\mathbf{E}_{AH}$ in the macroscopic area over random orientations of the crystallites. The rotation matrix is convenient to express through Euler angles:

$$p_{ij} = \begin{bmatrix} \begin{matrix}\cos(\alpha)\cos(\gamma)- \\ \sin(\alpha)\cos(\beta)\sin(\gamma)\end{matrix} & \begin{matrix}-\cos(\alpha)\sin(\gamma)- \\ \sin(\alpha)\cos(\beta)\cos(\gamma)\end{matrix} & \sin(\alpha)\sin(\beta) \\ \begin{matrix}\sin(\alpha)\cos(\gamma)+ \\ \cos(\alpha)\cos(\beta)\sin(\gamma)\end{matrix} & \begin{matrix}-\sin(\alpha)\sin(\gamma)+ \\ \cos(\alpha)\cos(\beta)\cos(\gamma)\end{matrix} & -\cos(\alpha)\sin(\beta) \\ \sin(\beta)\sin(\gamma) & \sin(\beta)\cos(\gamma) & \cos(\beta) \end{bmatrix},$$

where $0 \le \alpha \le 2\pi$ — the precession angle, $0 \le \beta \le \pi$ — the nutation angle, $0 \le \gamma \le 2\pi$ — the angle of intrinsic rotation. Then for the macroscopically isotropic polycrystalline ferromagnetic averaging over the random orientations of the crystallite is reduced to averaging over the random uniformly-distributed Euler angles.

$$E_{H\alpha'} = \frac{Zm^*\mu_0 M_{\beta'} j_{\mu'} \overline{p^{-1}_{\alpha'\alpha} p_{\beta\beta'} p_{\mu\mu'}}}{8\pi m^2 \mu_B n_e n_a} (a_{i\mu} - a_{j\mu}) \times \operatorname{Im}\Big\{ \langle \Psi_C(\mathbf{r}-\mathbf{a}_i)| \left(3\frac{\varepsilon_{\beta\gamma\delta} r_\alpha r_\gamma}{r^5} + \frac{\varepsilon_{\alpha\beta\delta}}{r^3} \right) \times \hat{p}_\delta |\Psi_{L0}\rangle \langle \Psi_{L0} | \Psi_C(\mathbf{r}-\mathbf{a}_j)\rangle \Big\}. \quad (11)$$

Here

$$\overline{p} = \frac{1}{8\pi^2} \int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} \sin(\beta) p(\alpha,\beta,\gamma) d\alpha d\beta d\gamma. \quad (12)$$

With analytical averaging of the equation (11), the integrals of the type (12) were calculated in a coordinate form, and then the result was transformed into an invariant form. As a result, we obtain

$$\mathbf{E}_{AH} = R_1[\mathbf{j} \times \mu_0 \mathbf{M}],$$

$$R_1 = \frac{\hbar e Z}{48\pi m \mu_B n_a} \frac{m^*/m}{e n_e} \operatorname{Re}\Big\{ \langle \Psi_C(\mathbf{r}-\mathbf{a}_i)| \times \frac{3\mathbf{r}\big(\mathbf{r}(\mathbf{a}_i - \mathbf{a}_j)\big) - (\mathbf{a}_i - \mathbf{a}_j) r^2}{r^3} \frac{\partial}{\partial \mathbf{r}} \times |\Psi_{L0}\rangle \langle \Psi_{L0} | \Psi_C(\mathbf{r}-\mathbf{a}_j)\rangle \Big\}. \quad (13)$$

3. Calculation of AHE coefficient

The first relationship (13) is similar in a form wit the expression for the classic Hall effect if the vector $\mu_0\mathbf{M}$ is replaced by the vector of magnetic induction $\mathbf{B}$. Therefore, it can be expected that the intrinsic AHE coefficient R_1 also depends on the effective mass of the conductivity electrons including its sign and on their concentration as does the coefficient R_0 of the classic Hall effect. Then the second part of the formula (13) can be written as

$$R_1 = \frac{\hbar e Z R_0}{48\pi m \mu_{\mathrm{B}} n_a} \operatorname{Re}\Big\{ \langle \Psi_C(\mathbf{r}-\mathbf{a}_i)| \times \frac{3\mathbf{r}\big(\mathbf{r}(\mathbf{a}_i-\mathbf{a}_j)\big)-(\mathbf{a}_i-\mathbf{a}_j)r^2}{r^3}\frac{\partial}{\partial \mathbf{r}} \times |\Psi_L\rangle\langle\Psi_L|\Psi_C(\mathbf{r}-\mathbf{a}_j)\rangle \Big\}. \quad (14)$$

We transform the double sum of the formula (14) in curly brackets into a product of the sums:

$$3\left(\sum_{\mu=1}^{3}\sum_{i=1}^{N} A_{i\mu}\right)\left(\sum_{i=1}^{N} C_i\right) - \left(\sum_{\mu=1}^{3}\sum_{i=1}^{N} B_{i\mu}\right)\left(\sum_{i=1}^{N} C_i\right) - 3\left(\sum_{i=1}^{N}\mathbf{D}_i\right)\left(\sum_{i=1}^{N}\mathbf{a}_i C_i\right) + \left(\sum_{i=1}^{N}\mathbf{E}_i\right)\left(\sum_{i=1}^{N}\mathbf{a}_i C_i\right). \quad (15)$$

Here

$$A_{i\mu} = \langle a_{i\mu}\Psi_C(\mathbf{r}-\mathbf{a}_i)|\frac{r_\mu}{r^5}\left(\mathbf{r}\frac{\partial}{\partial\mathbf{r}}\right)|\Psi_L\rangle,$$

$$B_{i\mu} = \langle a_{i\mu}\Psi_C(\mathbf{r}-\mathbf{a}_i)|\frac{1}{r^3}\frac{\partial}{\partial r_\mu}|\Psi_L\rangle,$$

$$C_i = \langle\Psi_L|\Psi_C(\mathbf{r}-\mathbf{a}_i)\rangle,$$

$$\mathbf{D}_i = \langle\Psi_C(\mathbf{r}-\mathbf{a}_i)|\frac{\mathbf{r}}{r^5}\left(\mathbf{r}\frac{\partial}{\partial\mathbf{r}}\right)|\Psi_L\rangle,$$

$$\mathbf{E}_i = \langle\Psi_C(\mathbf{r}-\mathbf{a}_i)|\frac{1}{r^3}\frac{\partial}{\partial\mathbf{r}}|\Psi_L\rangle. \quad (16)$$

Let's proceed to the spherical system of coordinates and direct in each of the averages (15) the polar axis z along the vector $\mathbf{a}_i$. Then, there is only one non-zero component of this vector $a_{iz} = a_i = |\mathbf{a}_i|$ in each of the summands in (15). At the same time, the first and second summands of the formula (15) have only

$$A_{iz} = A_i = a_i\langle\Psi_C(\mathbf{r}-\mathbf{a}_i)|\frac{\cos(\theta)}{r^3}\frac{\partial}{\partial r}|\Psi_L\rangle$$

and

$$B_{iz}=B_i=a_i\langle\Psi_C(\mathbf{r}-\mathbf{a}_i)|\frac{1}{r^3}\left(\cos(\theta)\frac{\partial}{\partial r}-\frac{1}{r\sin(\theta)}\frac{\partial}{\partial\theta}\right)|\Psi_L\rangle.$$

Let us consider interaction of the 4s conductivity electron with the wave function

$$W_C(\boldsymbol{\rho})=R_{40}(\rho)=\frac{1}{768}(-\rho^3+24\rho^2-144\rho+192)\exp\left(-\frac{\rho}{4}\right),$$

where $\boldsymbol{\rho} = \frac{\mathbf{r}Z}{a_B}$, and the 3$d$ magnetization electron with the wave function

$$W_L(\boldsymbol{\rho}) = \sum_{m=-2}^{2} c_m W_{Lm}(\boldsymbol{\rho}),$$

$$W_{Lm}(\boldsymbol{\rho}) = R_{32}(\rho)Y_{2m}(\theta)\exp(im\varphi),$$

$$R_{32}(\rho) = \frac{4}{81\sqrt{30}}\rho^2\exp\left(-\frac{\rho}{3}\right).$$

Here m is the magnetic quantum number. Then

$$\Psi_C(\mathbf{r}-\mathbf{a}_i) = R_{40}(\rho_i),$$

$$\rho_i = \sqrt{\rho^2+b_i^2-2\rho b_i\cos(\theta)}, \quad b_i = Za_i/a_B,$$

and all the magnitudes (16) are provided with a non-zero contribution only by the state

$$W_{L0}(\boldsymbol{\rho}) = \sqrt{5/16\pi}\,R_{32}(\rho)\big(1-3\cos^2(\theta)\big).$$

In this state the vectors $\mathbf{D}_i$ and $\mathbf{E}_i$ are directed along the vector $\mathbf{a}_i$.

The experimental values of a portion of the orbital component of the magnetic moment of the magnetization electron at 300 K are $(0.0918 \pm 0.003))$ for iron; are (0.1472 ± 0.003) for cobalt; and are (0.0507 ± 0.0027) for nickel [22,23]. Therefore, it can be assumed that the states with different values of a projection of the orbital moment to the arbitrary axis of quantization are equally probable and that a portion of the states Ψ_{L0} with the magnetic quantum number $m = 0$, which contribute to (15), is 1/5. Then in the formulas (16) we obtain

$$A_i = \frac{2\pi Z^3 b_i}{a_B^3\sqrt{16\pi}}\int_0^\infty\int_{-1}^{1}\frac{dR_{32}(\rho)/d\rho}{\rho}R_{40}(\rho_i)(1-3y^2)y\,d\rho\,dy,$$

$$\mathbf{D}_i = \frac{\mathbf{a}_i}{a_i^2}A_i,$$

$$B_i = \frac{2\pi Z^3 b_i}{a_B^3\sqrt{16\pi}}\int_0^\infty\int_{-1}^{1}\left\{\frac{(1-3y^2)dR_{32}(\rho)/d\rho}{\rho}-\frac{6R_{32}(\rho)}{\rho^2}\right\} \times R_{40}(\rho_i)y\,d\rho\,dy, \quad \mathbf{E}_i = \frac{\mathbf{a}_i}{a_i^2}B_i,$$

$$C_i = \frac{2\pi}{\sqrt{16\pi}}\int_0^\infty\int_{-1}^{1}R_{32}(\rho)R_{40}(\rho_i)(1-3y^2)\,d\rho\,dy. \quad (17)$$

Here, $y = \cos(\theta)$. It is clear from the formulas (17) that the magnitudes A_i, B_i and C_i like in (16), which are included in the sums (15) depend only on the distance from the considered atom to the nearest neighbor. Therefore, during their calculation the nearest neighbors of the considered atom can be divided into groups with the same distances thereto. If the lattice is symmetrical and each neighbor with the coordinate $\mathbf{a}_i$ is matched with the neighbor with the coordinate — $\mathbf{a}_i$, then the third and fourth summands of the formula (15) are zero. Let us note that $n_a = N_A/v_m$, where v_m — the molar volume, $N_A = 6.02214 \cdot 10^{23}$ — the Avogadro's number. The formula (14) then takes the following form

$$\frac{R_1}{R_0} = \frac{\hbar e Z v_m}{48\pi m\mu_{\mathrm{B}} N_A}\left(\sum_i m_i(3A_i - B_i)\right)\left(\sum_i m_i C_i\right). \quad (18)$$

Here m_i is the number of the nearest neighbors of the considered atoms at the distance of a_i thereto.

For nickel $Z = 10.5$; $\upsilon_m = 6.6 \cdot 10^{-6}\,\mathrm{m}^3$. The numerical calculation of the relationship R_1/R_0 by the formulas (17) and (18) gives the value 0.16. For cobalt $Z = 10.42$; $\upsilon_m = 6.7 \cdot 10^{-6}\,\mathrm{m}^3$; $R_1/R_0 = 0.35$. For iron $Z = 10.3$; $\upsilon_m = 7.1 \cdot 10^{-6}\,\mathrm{m}^3$; $R_1/R_0 = 0.33$.

4. Comparison with experiment

From the formula (1), assuming that $M(B \gg B_S) = M_S$, we obtain

$$R_0 = \lim_{B \gg B_S}\left(\frac{d\rho_H}{dB}\right),$$

$$R_S = \frac{\rho_H(B = 0, M = M_S)}{B_S} = \frac{\lim\limits_{B \gg B_S}\big(\rho_H(B) - R_0 B\big)}{B_S}. \quad (19)$$

The graphs illustrating the formulas (19) are provided in the paper [24]. In the study [25], the AHE coefficient was calculated by the formula $R_S = \lim\limits_{B\to 0}(d\rho_H/dB) - R_0$ in assuming that $\lim\limits_{B\to 0}(\mu_0 M/B) = 1$. For ferromagnetics in the Rayleigh region this condition may not be satisfied. So, the values of R_S were recalculated by the data of the paper [25] on Fig. 2, 3, 6 and 7.

When $T = 4.2\,\mathrm{K}$ for nickel

$$R_0 = -0.34 \cdot 10^{-10}\,\mathrm{m}^3/\mathrm{C},$$

$$\rho_H(B = 2.08\,\mathrm{T}) = -0.73 \cdot 10^{-10}\,\Omega \cdot \mathrm{m},$$

$$B_S = 0.61\,\mathrm{T}.$$

Then

$$R_S = -0.035 \cdot 10^{-10}\,\mathrm{m}^3/\mathrm{C},$$

$$R_S/R_0 = 0.11.$$

For cobalt

$$R_0 = -1.0 \cdot 10^{-10}\,\mathrm{m}^3/\mathrm{C},$$

$$\rho_H(B = 2.5\,\mathrm{T}) = -2.96 \cdot 10^{-10}\,\Omega \cdot \mathrm{m},$$

$$B_S = 1.7\,\mathrm{T},$$

$$R_S = -0.27 \cdot 10^{-10}\,\mathrm{m}^3/\mathrm{C},$$

$$R_S/R_0 = 0.27.$$

For iron

$$R_0 = 0.052 \cdot 10^{-10}\,\mathrm{m}^3/\mathrm{C},$$

$$\rho_H(B = 2.84\,\mathrm{T}) = 0.25 \cdot 10^{-10}\,\Omega \cdot \mathrm{m},$$

$$B_S = 2.15\,\mathrm{T},$$

$$R_S = 0.048 \cdot 10^{-10}\,\mathrm{m}^3/\mathrm{C},$$

$$R_S/R_0 = 0.92.$$

For nickel $\rho_{292}/\rho_{4.2} = 57.2$; for cobalt $\rho_{292}/\rho_{4.2} = 66.3$. For nickel and cobalt the conductivity when $T = 4.2\,\mathrm{K}$ is about $10^9\,\mathrm{S/m}$, and within the measurement error it can be assumed that $R_S \approx R_1$. The calculated values of the ratio R_1/R_0 exceed the measured values of R_S/R_0 approximately by 25%. This discrepancy agrees with the measurement error, since according to the second formula (18) the value of R_S is found as a small difference of two close values. For iron $\rho_{292}/\rho_{4.2} = 11.45$; the conductivity when $T = 4.2\,\mathrm{K}$ is $1.2 \cdot 10^8\,\mathrm{S/m}$, while the AHE constant and the calculated value of the intrinsic AHE coefficient are in 20 times less than those for cobalt. The measured value of the ratio R_S/R_0 exceeds the calculated ratio R_1/R_0 in 2.7 times. For pure iron $\rho_{292}/\rho_{10} \approx 10^4$ [26], and it can be presumed that with iron purity of 99.998% contribution to AHE by impurity-dependent dissipation substantially exceeds the dissipation-independent one, so R_S is substantially higher than R_1.

Conclusion

A promising field for implementing a new generation of devices of information and sensor technologies is antiferromagnetic spintronics based on AHE [27]. Substantiation of methods of designing the spintronics systems, calculating and optimizing their characteristics requires additional assumptions about the system. These assumptions include the representation of the wave function of the collectivized conductivity electron in the form of the Vanier function, the effective charge approximation and the nearest neighbors approximation in the relationship (8) as well as the model of the ideal Fermi gas for the conductivity electrons and taking into account the structure of the Fermi surface by the constant of the normal Hall effect. The SHE coefficients calculated within the framework of these models comply with the measured ones [15,16].

For AHE analysis, these assumptions are supplemented with an assumption that it is possible to regard the ferromagnetic crystallite as the homonuclear macromolecule within framework of the single-electron Hartree–Fock method. The magnetic structure of the planar antiferromagnetic can be presented as two sublattices that are shifted by a lattice vector and magnetized to saturation in opposite directions. The magnetic structure of a helimagnetic can be presented as a result of twisting of the centrally-symmetrical lattice of the saturation-magnetized ferromagnetic around a chirality axis [28]. Compliance of the AHE coefficients in the ferromagnetics calculated in these assumptions with the measured ones makes it possible to use the proposed method for constructing the AHE model in antiferromagnetics.

Presently, the AHE is actively studied in Heusler-type alloys, which belong to a group of the Weyl semimetals, including with a Kagome structure, and together with metal antiferromagnetics are regarded as promising materials for the spintronics elements. In the volume single crystal of the Weyl ferromagnetic semimetal ferromagnetic (SMFM) Co_2MnAl at the room temperature the anomalous Hall conductivity (AHC) of $1.3 \cdot 10^5\,\mathrm{S/m}$ was recorded with the record value $\tan(\theta_{AH}) = 0.21$. By comparing the temperature dependences of longitudinal resistivity and

AHC, it is shown that the AHE is an intrinsic one [29]. The SMFM $LiMn_6Sn_6$ with the Kagome structure has exhibited the intrinsic AHC of $3.8 \cdot 10^4$ S/m when $T = 50$ K. At the room temperature, the AHC decreases approximately in two times [30]. The authors explain the large AHE by the fact that the band structure of $LiMn_6Sn_6$ has several band intersections, including a spin-polarized Dirac point in the point K close to the Fermi energy. In the Weyl antiferromagnetic semimetal HoAgGe with the Kagome distorted lattice, the AHC of $2.8 \cdot 10^5$ S/m was recorded when $T = 45$ K [31]. The authors believe that distortion of the ideal Kagome lattice by oppositely rotating the triangles results in formation of a noncentrosymmetric structure. As a result, a doubly-degenerate Dirac cone of the Kagome lattices turns into a pair of the Weyl points that can generate the large Berry curvature and, therefore, the large intrinsic AHE.

A review of theoretical and experimental studies for the SMFM properties is given in the paper [32]. It is noted that one of the causes of a non-trivial topology of the electron band structure of the Weyl semimetals manifested in the gigantic AHE is spin-orbit interaction [33]. The gigantic AHE in combination with SHE and the Nernst spin effect is found in manganese-based semimetals that are promising for spintronics [34]. It can be assumed that the intrinsic AHE in the SMFM as well as AHE in the metal ferromagnetics and SHE in the non-magnetic conductors is of a spin-orbit nature. The topology of the electron band structure determines all the SMFM transport properties, including its longitudinal and transverse conductivities. The experimental temperature and magnetic-field dependences of longitudinal and transverse conductivity for the SMFM given in the papers [29–31] are similar to respective dependences for the metal ferromagnetic [10–13,24,25]. This suggests that the proposed method can be used for constructing the AHE model in the SMFM. In doing so, it is necessary to modify the formula (7) obtained in an assumption, valid for the metal ferromagnetics, that the conductivity electrons are not polarized. Vice versa, in the SMFM at the low temperatures, the conductivity electrons are highly polarized [32,35]. Besides, presence of non-quasiparticle states in the SMFM can bring about some complexity.

The SMFM crystal lattice, especially with the Kagome structure, is much more complicated than that of the metals. It is advisable to regard it as a superposition of several homonuclear sublattices Thus, the presentation of the complex lattice A15 of β-tungsten as the superposition of two simple sublattices made it possible to analyze the gigantic SHE in it with satisfactory accuracy [16]. Here, an approach developed in the paper [36] can be promising.

Conflict of interest

The authors declare that they have no conflict of interest.

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