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The effect of the spin polarization control of conduction electrons through the deformation of a ferromagnet

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A model of the exchange interaction of collectivized conduction electrons with magnetization electrons in a deformed ferromagnet with taking into account spin–orbit corrections is proposed. Under the conditions of inhomogeneous torsion distortion, the conduction electron spin in the domain is oriented along the exchange interaction vector. If the conduction current density vector is orthogonal to the torsion axis, then the average conduction electron spin will be oriented predominantly along the current density vector.

Keywords: spin–orbit interaction, transition metals, Wannier functions, torsion distortion.

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The state–of–the–art spintronics deals with studying effects in which an essential role is played by spin degrees of freedom. One of its directions is studying spin fluxes in conductors and semiconductors in order to reveal the ways of using them in various microelectronic devices [1]. Spin dynamics of collectivized conduction electrons in the spintronics systems is conventionally simulated by the Rashba and Drosselhaus Hamiltonians accounting for the energy of the conduction electron spin–orbit interaction [2]. Estimates show that interaction of this kind can ensure the spin polarization coherence at the distances of about $0.1\,\mu$m; however, it is insufficient for efficient macroscopic (about 1 mm) polarization of spin currents in polycrystals. In recent decades there has been formed such a new research direction of the Condensed Matter Physics as straintronics employing physical effects in matter caused by deformations induced in micro—, nano— and heterostructures by external control fields that lead to variations in the material electronic structure and electrical, magnetic, optical and other properties [3]. The objective of one of the straintronics branches is studying the effect of mechanical stresses on the substance electronic properties.

In the framework of previously created authorial deformed–ferromagnet models, it was shown that the crystal field efficiently interacts with spin moments of localized electrons [4], and spin–orbit interaction leads to efficient polarization of conduction electrons in the macroscopic area [5].

The novelty of the proposed approach is that the model Hamiltonian of the exchange interaction between collectivized conduction electrons and magnetization electrons in the deformed ferromagnet crystal field accounts for the second–order relativistic spin–orbit corrections. Such an interaction was not previously taken into account since it does not create macroscopic coherent polarization of spin currents in a strain–free crystal.

Let us consider the exchange interaction between two electrons, a collectivized and a localized ones, in a domain of a homogeneous and isotropic ferromagnet with taking into account the spin–orbit interaction, i. e. relativistic second–order corrections by $1/c$, where c is the light speed. In the framework of the self–consisted field method, the energy of the Coulomb interaction of the considered electrons with each other and also with other domain electrons, both collectivized and localized in ions, namely, with the crystal, is accounted for by substituting their mass m with effective mass m^*.

Spin–orbit additions to the energy of two electrons located at the points with radius–vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ are conventionally defined as follows [6]:

$$\hat{V} = \frac{\hbar e}{2m^{*2}c^2}\left(\Big[\mathbf{E}_1(\mathbf{r}) \times \hat{\mathbf{p}}_1\Big]\hat{\mathbf{s}}_1 + \Big[\mathbf{E}_2(\mathbf{r}) \times \hat{\mathbf{p}}_2\Big]\hat{\mathbf{s}}_2\right), \quad (1)$$

where $\hbar$ is the Diracś constant, $\mathbf{p}_i$ and $\mathbf{s}_i$ are the i-th electron momentum and spin operators. Field argument $\mathbf{E}$ is the same as that of the wave function under the operator.

Considering sum (1) as a perturbation, find its mean value V in the state

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

composed of single–particle spin–orbitals $\psi(\mathbf{r}_i, \sigma_i)$, σ_i is the i-th electron spin variable. Assume that the first electron is a collectivized conduction electron of the i-th domain lattice site, while the second electron is localized in the j-th site, and write the collectivized electron wave function in the form of the Wannier function:

$$\psi_1(\mathbf{r}) = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} W_C(\mathbf{r} - \mathbf{r}_i - \mathbf{R}_n)\exp(i\mathbf{k}\mathbf{R}_n),$$
$$\psi_2(\mathbf{r}) = W_L(\mathbf{r} - \mathbf{r}_j), \quad (2)$$

where $W_C(\mathbf{r})$ and $W_L(\mathbf{r})$ are the hydrogen–like functions of the collectivized and localized electrons; $\mathbf{R}_n$ is the translation vector; linear combination of lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$; $\mathbf{r}_i$ and $\mathbf{r}_j$ are coordinates of the i-th and j-th lattice sites.

Assume that, due to the exchange interaction, all the spins of electrons localized in the domain are oriented identically (for instance, along the easiest magnetization axis) and, hence, all $\mathbf{s}_j = \mathbf{s}_L$. Assuming the energy of exchange interaction between a collectivized conduction electron and all localized magnetization electrons to be a sum of those of its binary interactions like (1), substitute into (1) relations (2) ignoring the dependence of the hydrogen–like functions on the spin–spin interaction. After summation over spin variables, obtain

$$V = \left(\mathbf{J}_C\mathbf{s}_i\right)\left(\mathbf{s}_i\mathbf{s}_L\right) + \left(\mathbf{J}_L\mathbf{s}_L\right)\left(\mathbf{s}_i\mathbf{s}_L\right). \tag{3}$$

Formula (3) includes the following designations:

$$\mathbf{J}_L = -\frac{2DZ}{\hbar N}\sum_{j=1}^{N}\sum_{n=1}^{N}\sum_{m=1}^{N} e^{i\mathbf{k}(\mathbf{R}_n-\mathbf{R}_m)} \times \left\langle \Psi_C^*\left(\mathbf{r}-\mathbf{R}_m+\mathbf{r}_j-\mathbf{r}_i\right)\frac{\hat{\mathbf{l}}}{r^3}\Psi_L(\mathbf{r})\right\rangle \times \langle \Psi_L^*(\mathbf{r})\Psi_C(\mathbf{r}-\mathbf{R}_n+\mathbf{r}_j-\mathbf{r}_i)\rangle, \tag{4}$$

$$\mathbf{J}_C = -\frac{2DZ}{\hbar N}\sum_{j=1}^{N}\sum_{n=1}^{N}\sum_{m=1}^{N} e^{i\mathbf{k}(\mathbf{R}_m-\mathbf{R}_n)} \times \left\langle \Psi_L^*(\mathbf{r})\frac{\hat{\mathbf{l}}}{r^3}\Psi_C(\mathbf{r}-\mathbf{R}_m+\mathbf{r}_j-\mathbf{r}_i)\right\rangle \times \left\langle \Psi_C^*(\mathbf{r}-\mathbf{R}_n+\mathbf{r}_j-\mathbf{r}_i)\Psi_L(\mathbf{r})\right\rangle = \mathbf{J}_L^*. \tag{5}$$

Here Z is the effective charge of the ion residue, $\mathbf{l}$ is the electron orbital moment operator. It may be estimated by setting the coordinate of the maximum of the hydrogen–like wave function radial component to the ion residue radius Me^{3+}. For iron and cobalt, the ion residue radius is $6.3 \cdot 10^{-11}\,\mathrm{m}$ which corresponds to effective charge $Z \approx 5.2$. Parameter D is $D = \hbar^2 e^2/(8\pi\varepsilon_0 m^{*2} c^2) \approx 2 \cdot 10^{-51}\,\mathrm{J}\cdot\mathrm{m}^3$ at $m^* \approx 0.3m$. The crystal field orients the electron orbitals along the crystal symmetry axes. Therefore, it is possible to assume that coordinate axes within which integrals (4), (5) and next ones are calculated are closely associated with the crystal basis vectors $\mathbf{a}_\nu$.

The hydrogen–like functions have low values at $r > na_\mathrm{B}/Z$, where $a_\mathrm{B} = 5.3 \cdot 10^{-11}\,\mathrm{m}$ is the Bohr radius, n is the principal quantum number. This is why the first integral in (4) and (5) is non–zero only at either $\mathbf{r}_j - \mathbf{r}_i - \mathbf{R}_m = 0$ or $\pm\mathbf{a}_\nu$, while the second one is non–zero at either $\mathbf{r}_j - \mathbf{r}_i - \mathbf{R}_n = 0$ or $\pm\mathbf{a}_\nu$. When $\mathbf{r}_j - \mathbf{r}_i - \mathbf{R}_n = 0$ or $\mathbf{r}_j - \mathbf{r}_i - \mathbf{R}_m = 0$, the relevant integrals in a strain–free crystallite are zero since different atomic functions of one and the same atom are orthogonal. In transition metals, s- and p-zones are overlapped [7]. Therefore, conduction electrons may be formed from p-orbitals. In the case of the $p{-}d$-interaction, formula (4) takes the following form:

$$\mathbf{J}_L = -2DZ\langle\Psi_P(\mathbf{r})\Psi_D^*(\mathbf{r})\rangle\left\langle\Psi_P^*(\mathbf{r})\frac{\hat{\mathbf{l}}}{r^3}\Psi_D(\mathbf{r})\right\rangle - 4DZi\sum_{\nu=1}^{3}\sin(\mathbf{k}\mathbf{a}_\nu) \times \left\{\langle\Psi_P(\mathbf{r}+\mathbf{a}_\nu)\Psi_D^*(\mathbf{r})\rangle\left\langle\Psi_P^*(\mathbf{r})\frac{\hat{\mathbf{l}}}{r^3}\Psi_D(\mathbf{r})\right\rangle + \langle\Psi_P(\mathbf{r})\Psi_D^*(\mathbf{r})\rangle\left\langle\Psi_P^*(\mathbf{r}+\mathbf{a}_\nu)\frac{\hat{\mathbf{l}}}{r^3}\Psi_D(\mathbf{r})\right\rangle\right\}. \tag{6}$$

Here in the integrals containing functions $\Psi_P(\mathbf{r}-\mathbf{a}_\nu)$, the $\mathbf{r} \to -\mathbf{r}$ variable substitution was performed taking into account the function $\Psi_P(\mathbf{r})$ oddity, and the term of the second order of smallness with respect to $\exp(-|\mathbf{a}_\nu|/a_\mathrm{B})$ was omitted. In the strain–free crystallite, $\mathbf{J}_L = 0$.

In the ferromagnet, the energy of exchange interaction between the conduction electron and magnetization electrons is approximately equal to the energy of exchange interaction between neighboring localized electrons and significantly exceeds the magnetic anisotropy energy. Thus, it is possible to assume that in formula (3) $\mathbf{s}_i = \mathbf{s}_L$ and $\mathbf{s}_L\mathbf{s}_i = 3/4$. Then, introducing designation $\mathbf{J} = \mathrm{Re}\mathbf{J}_L$ obtain

$$V = 3\mathbf{J}\mathbf{s}_i/2. \tag{7}$$

In the case of a non–uniform distortion, a point, e.g. a lattice site with coordinate $\mathbf{r}$, is displaced to a new position with coordinate $\mathbf{r}'$ by vector $\mathbf{u}$ [7]:

$$r'_\alpha = r_\alpha + u_\alpha(\mathbf{r}), \quad dr'_\alpha = \left(\delta_{\alpha\beta} + \frac{\partial u_\alpha}{\partial r_\beta}\right)dr_\beta,$$

$$dr_\beta = \left(\delta_{\alpha\beta} + \frac{\partial u_\beta}{\partial r_\alpha}\right)^{-1} dr'_\alpha \approx \left(\delta_{\alpha\beta} - \frac{\partial u_\beta}{\partial r_\alpha}\right)dr'_\alpha,$$

$$\frac{\partial}{\partial r'_\alpha} = \frac{\partial r_\beta}{\partial r'_\alpha}\frac{\partial}{\partial r_\beta} = \frac{\partial}{\partial r_\alpha} - \frac{\partial u_\beta}{\partial r_\alpha}\frac{\partial}{\partial r_\beta},$$

$$\hat{l}'_\alpha = -i\varepsilon_{\alpha\beta\gamma} r'_\beta \frac{\partial}{\partial r'_\gamma} = \hat{l}_\alpha - i\varepsilon_{\alpha\beta\gamma}\left(u_\beta\frac{\partial}{\partial r_\gamma} - r_\beta\frac{\partial u_\delta}{\partial r_\gamma}\frac{\partial}{\partial r_\delta}\right),$$

$$\Psi(\mathbf{r}') = \Psi(\mathbf{r}) + \frac{\partial\Psi}{\partial r_\alpha}u_{\alpha\beta}r_\beta,$$

where $\varepsilon_{\alpha\beta\gamma}$ is the unit antisymmetric Levi–Civita tensor, $u_{\alpha\beta} = \partial_\beta u_\alpha$ is the distortion tensor, $\alpha, \beta, \gamma = x, y, z$. Orientations of the crystal axes and valence–electron orbitals change accordingly. Consider the case of distortion of the sample torsion along axis $\mathbf{n}$ defined as $\Omega(\mathbf{r}) = \mathbf{n}(\mathbf{r}\mathbf{n})\omega$, where ω is the linear torsion; restricting ourselves to the first–order distortion, obtain

$$u_\beta = \omega\varepsilon_{\beta\sigma\nu}n_\sigma n_\mu r_\nu r_\mu,$$

$$u_{\gamma\delta} = \omega\varepsilon_{\delta\sigma\nu} n_\sigma n_\mu (r_\nu \delta_{\mu\gamma} + r_\mu \delta_{\nu\gamma})$$

$$= \omega\varepsilon_{\delta\sigma\nu} n_\sigma n_\gamma r_\nu + \omega\varepsilon_{\delta\sigma\gamma} n_\sigma n_\mu r_\mu,$$

$$\hat{\mathbf{l}}' = \hat{\mathbf{l}} + \omega(\mathbf{nr})\big[\mathbf{n} \times \hat{\mathbf{l}}\big] + \omega\big(\mathbf{n}\hat{\mathbf{l}}\big)[\mathbf{n} \times \mathbf{r}],$$

$$\hat{l}'_\alpha = \hat{l}_\alpha + \omega\varepsilon_{\alpha\beta\gamma} n_\beta n_\delta \big(r_\delta \hat{l}_\gamma + r_\gamma \hat{l}_\delta\big),$$

$$\Psi(\mathbf{r}') = \Psi(\mathbf{r}) + i\boldsymbol{\Omega}(\mathbf{r})\hat{\mathbf{l}}\Psi(\mathbf{r}) = \Psi(\mathbf{r}) + i\omega n_\beta n_\delta r_\delta \hat{l}_\beta \Psi(\mathbf{r}). \tag{8}$$

Taking into account the moment operator hermiticity and commutation relations $\big[\hat{l}_\alpha, \hat{l}_\beta\big] = i\varepsilon_{\alpha\beta\gamma}\hat{l}_\gamma$, $\big[\hat{l}_\alpha, r_\beta\big] = i\varepsilon_{\alpha\beta\gamma} r_\gamma$, obtain from relations (8) in the approximation linear in ω:

$$\langle \Psi'_C | \Psi'_L \rangle - \langle \Psi_C | \Psi_L \rangle = \omega n_\beta n_\delta \big\{ i \langle \Psi_C | r_\delta \hat{l}_\beta \Psi_L \rangle$$

$$- i \langle r_\delta \hat{l}_\beta \Psi_C | \Psi_L \rangle \big\} = \omega\varepsilon_{\beta\delta\gamma} n_\beta n_\delta \langle \Psi_C | r_\gamma | \Psi_L \rangle = 0,$$

$$\langle \Psi'_C | \hat{l}'_\alpha | \Psi'_L \rangle - \langle \Psi_C | \hat{l}_\alpha | \Psi_L \rangle = \omega n_\beta n_\delta \big\{ i \langle \Psi_C | \hat{l}_\alpha | r_\delta \hat{l}_\beta \Psi_L \rangle$$

$$- i \langle r_\delta \hat{l}_\beta \Psi_C | \hat{l}_\alpha | \Psi_L \rangle + \varepsilon_{\alpha\beta\gamma} \langle \Psi_C | r_\delta \hat{l}_\gamma + r_\gamma \hat{l}_\delta | \Psi_L \rangle \big\}$$

$$= 2\omega\varepsilon_{\alpha\beta\gamma} n_\beta n_\delta \langle \Psi_C | r_\gamma \hat{l}_\delta | \Psi_L \rangle.$$

Substitute these relations into (6); then, in the first–smallness–order approximation in ω and $\mathbf{ka}_\nu$, obtain:

$$J_{\alpha'} = \varepsilon_{\alpha'\beta'\gamma'} n_{\beta'} n_{\delta'} k_{\sigma'} a_{\nu\sigma'} B_{\nu\gamma'\delta'},$$

$$B_{\nu\gamma'\delta'} = 4ZD\omega \operatorname{Im}\left\{ \langle \Psi_P(\mathbf{r}+\mathbf{a}_\nu) \Psi^*_D(\mathbf{r}) \rangle \left\langle \Psi^*_P(\mathbf{r}) \frac{r_{\gamma'} \hat{l}_{\delta'}}{r^3} \Psi_D(\mathbf{r}) \right\rangle \right\}. \tag{9}$$

Relation (9) is written in the frame of reference associated with the domain axes. From equation (7) it follows that the mean conduction electron spin in the domain is oriented along vector $\mathbf{J}$. Consider a macroscopic region of a multi–domain ferromagnet that is homogeneous and isotropic in the absence of deformations. Introduce a laboratory frame of reference bound to the instruments setting strains and measuring spin components. Let us designate the vector and tensor components by indices without primes in the laboratory frame of reference and by indices with primes in the frame of reference associated with the domain crystal axes. In the laboratory system, let us prescribe the torsion by angle $\Omega(\mathbf{r})$.

Now let us transform the torsion vector and wave vector from the laboratory system to the crystal axes system: $n_{\beta'} = p_{\beta'\beta} n_\beta$, $k_{\sigma'} = p_{\sigma'\sigma} k_\sigma$, where $p_{\beta'\beta}$ is the unitary rotation matrix. Substituting this transformation into (9), convert components of vectors $\mathbf{J}$ and $\mathbf{l}_L$ from the crystal axis system to the laboratory system:

$$J_\alpha = m^* p^{-1}_{\alpha\alpha'} p_{\beta'\beta} p_{\delta'\delta} p_{\sigma'\sigma} j_\sigma \varepsilon_{\alpha'\beta'\gamma'} n_\beta n_\delta a_{\nu\sigma'} B_{\nu\gamma'\delta'} / (ne\hbar), \tag{10}$$

where j is the conduction current density, n is the conduction electron concentration.

Let us average vector $\mathbf{J}$ (10) in the macroscopic region over random crystallite orientations. It is convenient to express the rotation matrix via Euler angles. The analytical averaging provides the expression for the averaged vector $\mathbf{J}$ in the following form:

$$\bar{\mathbf{J}} = \frac{2m^* ZD\omega}{3ne\hbar} \operatorname{Im}\bigg\{ \langle \Psi_P(\mathbf{r} + \mathbf{a}_\nu) \Psi^*_D(\mathbf{r}) \rangle$$

$$\times \left\langle \Psi^*_P(\mathbf{r}) \frac{\mathbf{a}_\nu [\mathbf{r} \times \hat{\mathbf{l}}]}{r^3} \Psi_D(\mathbf{r}) \right\rangle \bigg\} \big[\mathbf{n} \times [\mathbf{n} \times \mathbf{j}]\big]. \tag{11}$$

The scalar in curly brackets in formula (11), where summation over ν is implied, depends only on the strain–free crystal properties. It may be calculated in the crystal symmetry axes. The triple vector product in (11) consists of vectors that are preset in the laboratory frame of reference and describe the impact on the polycrystalline sample. Its modulus is maximal when the vector of the conduction current density is orthogonal to the torsion axis. In this case, the average conduction electron spin will be oriented predominantly along the current density vector.

During recent years there were published a number of experimental studies where the revealed spintronics and spin–caloritronics effects have not yet been explained: strain–induced switching of the heat flux direction due to magneto–thermoelectric effect in a magnetic metal [8], extension of the heat pump temperature range due to the elastocaloric effect [9], and anomalous Righi-Leduc effect in ferromagnetic materials [10]. The model presented in this paper may be used as a basis for theoretical description of those new effects.

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Conflict of interests

The authors declare that they have no conflict of interests.

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