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Controlling the dynamics of spin polarization of conduction electrons by electrical and mechanical action

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Abstract: A quantum model for the interaction of a collectivized conduction electron with a crystal field in a homogeneous and isotropic deformed polycrystalline sample, taking into account the spin-orbit interaction, is proposed. A dynamic equation of motion of the conduction electron spin in a stress-strained metal is obtained. It is shown that under conditions of inhomogeneous torsion in the stationary case, the average spin of conduction electrons is oriented predominantly along the current density vector. The maximum value of the spin-orbit interaction is observed when the torsion axis is orthogonal to the current density vector.

Keywords: spin-orbit interaction, transition metals, Wannier functions, torsion distortion PACS: 67.57.Lm, 72.25.Ba, 75.76.+j

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1. INTRODUCTION

One of the directions of modern spintronics is the study of spin fluxes in conductors and semiconductors in order to use these in various kinds of microelectronic devices [1, 2]. In recent decades, a new scientific direction in condensed matter physics has been formed – straintronics, which uses physical effects in matter due to

deformations that occur in micro-, nano- and hetero-structures under the action of external controlling fields, leading to a change in the electronic structure, electrical, magnetic, optical and other properties of materials [3]. One of the branches of straintronics is aimed at studying the effect of mechanical stresses on the electronic properties of a substance.

Earlier, within the framework of the created models of a stress-strain ferromagnet, a solution of Landau-Lifshitz-Gilbert type equations was obtained in the form of a dynamic hysteresis loop [4] and it was shown that the crystal field effectively interacts with the spin moments of localized electrons [5], and taking into account the spin-orbit interaction can effectively polarize

conduction electrons in the macroscopic region [6].

In the paper the dynamic control of a polarization by conduction current and torsional strain, which are variable in magnitude and direction, is considers. The novelty of the proposed approach lies in taking into account the interaction with the crystal field of a deformed metal in the model Hamiltonian of collective conduction electrons using relativistic spin-orbit corrections of the second order. Previously, this interaction was not taken into account, since in an unde-formed crystal it does not create a macroscopic coherent polarization of spin currents.

2. MODEL BUILDING

Let us consider the mechanically induced spin polarization of the conduction electron in a homogeneous and isotropic polycrystalline. The interaction of the collective electron with the crystal field is chosen in the form of a spin-orbit interaction with lattice ions, that is, relativistic corrections in the second order of a magnitude $1/\epsilon$, where ϵ is the speed of light. The energy of the Coulomb interaction of conduction electrons with each other, as well as with the other electrons of the crystallite, both collective and localized in the ions of the lattice, that is, with the crystal in the framework of the selfconsistent field method, is taken into account by replacing its mass with the effective mass m.

Let there are N sites in the crystallite, each of which contains identical ions with an effective charge +Ze. Such lattice creates a perturbation of the potential energy of an electron at a point with a radius vector **r** and the corresponding electric field

$$\mathbf{E}(\mathbf{r}) = -\frac{eZ}{4\pi\varepsilon_0} \sum_{k=1}^{N} \frac{\mathbf{r} - \mathbf{r}_k}{\left|\mathbf{r} - \mathbf{r}_k\right|^3},$$

where ε_0 is the electrical constant, e is the elementary charge, \mathbf{r}_{k} is the radius vector of the k-th node of the lattice. The value of the effective charge Z can be estimated by equating the coordinate of the maximum of the hydrogenlike radial wave function to the covalent radius of the atom. For example, for platinum the atomic radius is 1.39·10⁻¹⁰ m, which for a 6s shell corresponds to $Z \approx 22.45$.

The spin-orbital addition to the electron energy has the form [7]

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

where *m* is the effective mass of an electron with charge -e, where \hbar is the Dirac constant, ρ and sare the electron momentum and spin operators respectively.

The dynamics of the electron spin, created by perturbation (1), is described by the equation for averages [8]

$$\begin{aligned}
\frac{ds_{\alpha}}{dt} &= \frac{i}{\hbar} \left\langle \left[\hat{V}, \hat{s}_{\alpha} \right] \right\rangle = \\
&= -\frac{e^{2} Z \varepsilon_{\alpha\beta\gamma}}{8\pi\varepsilon_{0} m^{2} c^{2}} \sum_{k=1}^{N} \left\langle \left[\frac{\mathbf{r} - \mathbf{r}_{k}}{\left| \mathbf{r} - \mathbf{r}_{k} \right|^{3}} \times \hat{\mathbf{p}} \right]_{\beta} \hat{s}_{\gamma} \right\rangle, \end{aligned}$$

where $\varepsilon_{\alpha\beta\nu}$ is the unit asymmetric Levi-Civita tensor. Here and below greek indices denote spatial variables.

We choose the wave function of the collective conduction electron in the form of the Wannier function [9]:

$$\Psi(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \Psi(\mathbf{r} - \mathbf{R}_{n}) \exp(i\mathbf{k}\mathbf{R}_{n}),$$

where $\Psi(\mathbf{r})$ is the hydrogen-like function of an electron, \mathbf{R}_{n} is the lattice vector.

After summing over the spin variables, setting $\langle \hat{\mathbf{s}} \rangle = \mathbf{s}$ and performing the change of variables $\mathbf{r} - \mathbf{r}_k \rightarrow \mathbf{r}$, we obtain the equation

$$\frac{ds_{\alpha}}{dt} = -\frac{\hbar e^{2} Z \varepsilon_{\alpha\beta\gamma}}{8\pi\varepsilon_{0} m^{2} c^{2} N} s_{\gamma} \sum_{n,m,k=1}^{N} \exp(i\mathbf{k} (\mathbf{R}_{n} - \mathbf{R}_{m})) \times \left\langle \Psi(\mathbf{r} + \mathbf{r}_{k} - \mathbf{R}_{m}) | \frac{\hat{I}_{\beta}}{r^{3}} | \Psi(\mathbf{r} + \mathbf{r}_{k} - \mathbf{R}_{n}) \right\rangle, \tag{2}$$

where $\hat{m{I}}$ is the electron orbital momentum operator.

Hydrogen-like functions are small at r > $na_{\rm B}/Z$, where $a_{\rm B}=5.29\cdot10^{-11}~m$ is the Bohr

radius and n is the principal quantum number. Therefore, the average on the right side of expression (2) is non-zero only when $\mathbf{R}_{p} - \mathbf{r}_{p} = 0$ or a_{v} and $\mathbf{R}_{m} - \mathbf{r}_{k} = 0$ or \mathbf{a}_{v} , where \mathbf{a}_{v} is a vector drawn to the nearest neighbouring site. Then, taking into account that the orbital momentum operator is Hermitian, we obtain

$$\begin{split} &\frac{ds_{\alpha}}{dt} = -\frac{\hbar e^{2}Z\epsilon_{\alpha\beta\gamma}}{4\pi\epsilon_{0}m^{2}c^{2}}s_{\gamma}\times\\ &\times \left\{\cos\left(\mathbf{ka}_{v}\right)\operatorname{Re}\left\langle\Psi_{v}^{+}\left|\frac{\hat{l}_{\beta}}{r^{3}}\right|\Psi\right\rangle + \sin\left(\mathbf{ka}_{v}\right)\operatorname{Im}\left\langle\Psi_{v}^{-}\left|\frac{\hat{l}_{\beta}}{r^{3}}\right|\Psi\right\rangle\right\}. \end{split}$$

 $\Psi_{\nu}^{\pm}(\mathbf{r}) = \Psi(\mathbf{r} + \mathbf{a}_{\nu}) \pm \Psi(\mathbf{r} - \mathbf{a}_{\nu})$ functions with parity coinciding (index "+") and with opposite (index "-") parity of the function $\Psi(\mathbf{r})$. The equation implies summation over the index v over pairs of symmetrically located nearest neighbouring sites.

Introducing the wave vector $\mathbf{k} = -\mathbf{j}m/(e\hbar n_e)$, where **j** is the charge current density, n_{ij} is the concentration of conduction electrons, we obtain in the first order of smallness in ka the equation of motion of the conduction electron spin:

$$\frac{d\mathbf{s}}{dt} = \left[\left\{ \mathbf{I} - \mathbf{J} \right\} \times \mathbf{s} \right],$$

$$\mathbf{I} = \frac{\hbar e^{2} Z}{4\pi\epsilon_{0} m^{2} c^{2}} \sum_{\mathbf{v}} \operatorname{Re} \left\langle \Psi_{\mathbf{v}}^{+} \middle| \frac{\hat{\mathbf{l}}}{r^{3}} \middle| \Psi \right\rangle,$$

$$J_{\alpha} = \frac{eZ j_{\beta}}{4\pi\epsilon_{0} m c^{2} n_{e}} \sum_{\mathbf{v}} a_{\mathbf{v}\beta} \operatorname{Im} \left\langle \Psi_{\mathbf{v}}^{-} \middle| \frac{\hat{l}_{\alpha}}{r^{3}} \middle| \Psi \right\rangle.$$
(3)

In a non-deformed crystallite, due to the orbital momentum unquench [10], the value J = 0.

3. EQUATION OF SPIN DYNAMICS IN STRESS-STRAIN CRYSTAL

Let us consider an inhomogeneous distortion, in which a point, including a crystal site with coordinate r, is transferred to a new position with coordinate r' by the displacement vector u, related to the original by known relations [11]

$$r_{\alpha}' = r_{\alpha} + u_{\alpha}, \quad dr_{\alpha}' = \left(\delta_{\alpha\beta} + u_{\alpha\beta}\right) dr_{\beta}, \quad u_{\alpha\beta} = \partial_{\beta}u_{\alpha},$$

with the help of which it is easy to obtain shift derivatives:

$$\begin{split} dr_{\beta} &= \left(\delta_{\alpha\beta} + u_{\beta\alpha}\right)^{-1} dr_{\alpha}' \approx \left(\delta_{\alpha\beta} - u_{\beta\alpha}\right) dr_{\alpha}', \\ \frac{\partial}{\partial r_{\alpha}'} &= \frac{\partial r_{\beta}}{\partial r_{\alpha}'} \frac{\partial}{\partial r_{\beta}} = \partial_{\alpha} - u_{\beta\alpha} \partial_{\beta}. \end{split}$$

Using shift derivatives, the orbital momentum operator and wave function can be repre-sented

$$\hat{l}'_{\alpha} = -i\varepsilon_{\alpha\beta\gamma}r'_{\beta}\frac{\partial}{\partial r'_{\gamma}} = \hat{l}_{\alpha} - i\varepsilon_{\alpha\beta\gamma}\left(u_{\beta}\partial_{\gamma} - r_{\beta}u_{\delta\gamma}\partial_{\delta}\right),
\Psi(\mathbf{r}') = \Psi(\mathbf{r}) + \partial_{\alpha}\Psi \cdot u_{\alpha\beta}r_{\beta}.$$
(4)

Correspondingly, the orientations of the crystal axes and orbitals of valence electrons change under deformation. With sample torsion strain along the **n** axis of the form $\Omega(\mathbf{r}) =$ $\mathbf{n}(\mathbf{r}\mathbf{n})\omega$, where ω is an angle of torsion per unit length, rad/m, limited to the first degrees of deformation, we obtain

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

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

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

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

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

$$\Psi (\mathbf{r}') = \Psi (\mathbf{r}) + i \Omega (\mathbf{r}) \hat{\mathbf{I}} \Psi (\mathbf{r}) =$$

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

In the approximation linear in ω , taking into account the Hermiticity of the orbital momentum operator and the commutation relations

$$\begin{split} & \left[\hat{l}_{\alpha},\hat{l}_{\beta}\right] = i\epsilon_{\alpha\beta\gamma}\hat{l}_{\gamma}, \quad \left[\hat{l}_{\alpha},r_{\beta}\right] = i\epsilon_{\alpha\beta\gamma}r_{\gamma} \\ \text{we obtain expressions for the averages} \\ & \left\langle\Psi_{\nu}'\right|\Psi'\right\rangle - \left\langle\Psi_{\nu}\right|\Psi\right\rangle = i\omega n_{\beta}n_{\delta}\left\langle\Psi_{\nu}\right|r_{\delta}\hat{l}_{\beta} - \hat{l}_{\beta}r_{\delta}\right|\Psi\right\rangle = \\ & = \omega\epsilon_{\beta\delta\gamma}n_{\beta}n_{\delta}\left\langle\Psi_{\nu}\right|r_{\gamma}\left|\Psi\right\rangle = 0, \\ & \left\langle\Psi_{\nu}'\right|\hat{l}_{\alpha}'\left|\Psi'\right\rangle - \left\langle\Psi_{\nu}\right|\hat{l}_{\alpha}\left|\Psi\right\rangle = \\ & = \omega n_{\beta}n_{\delta}\left\langle\Psi_{\nu}\right|\hat{l}_{\alpha}r_{\delta}\hat{l}_{\beta} - \hat{l}_{\beta}r_{\delta}\hat{l}_{\alpha} + \epsilon_{\alpha\beta\gamma}r_{\delta}\hat{l}_{\gamma} + \epsilon_{\alpha\beta\gamma}r_{\gamma}\hat{l}_{\delta}\left|\Psi\right\rangle = \\ & = 2\omega\epsilon_{\alpha\beta\gamma}n_{\beta}n_{\delta}\left\langle\Psi_{\nu}\right|\hat{r}_{\nu}\hat{l}_{\delta}\right|\Psi\right\rangle. \end{split}$$

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Let us substitute these relations into the formula for the operator I in the equation (3):

$$J_{\alpha'} = \frac{\omega eZ}{2\pi\epsilon_0 mc^2 n_e} \epsilon_{\alpha'\beta'\gamma'} n_{\beta'} n_{\delta'} j_{\sigma'} \sum_{\nu} a_{\nu\sigma'} \operatorname{Im} \left\langle \Psi_{\nu}^- \middle| \frac{r_{\gamma'} \hat{l}_{\delta'}}{r^3} \middle| \Psi \right\rangle. \quad (5)$$

The relation (5) is written in the coordinate system associated with the axes of the crystallite. Let us introduce a laboratory coordinate system associated with instruments that set the conduction current and distortion and measure the spin components. The components of vectors and tensors in the laboratory system will be denoted by non-primed indices, but in the coordinate system, associated with the crystal axes, by prime marks.

Let us transform the vectors of current density and torsion axes from the laboratory system into the system of crystal axes $j_{\sigma'} = p_{\sigma'\sigma}j_{\sigma}$, $n_{\delta'} = p_{\delta'\delta}n_{\delta}$, and the vectors ${f I}$ and ${f J}$ from the system of crystal axes into the laboratory one $J_{\alpha} = p_{\alpha\alpha'}^{-1} J_{\alpha'}$, where $p_{a'a}$ is a unitary rotation matrix, which is conveniently expressed in terms of Euler angles. Substituting this transformation into equation (3) and averaging the vector \mathbf{s} in the macroscopic region over random orientations of crystallites:

$$\frac{d\overline{\mathbf{s}}}{dt} = \left[\left\{ \overline{\mathbf{I}} - \overline{\mathbf{J}} \right\} \times \overline{\mathbf{s}} \right] + \left[\overline{\left\{ \delta \mathbf{I} - \delta \mathbf{J} \right\}} \times \delta \overline{\mathbf{s}} \right]
\delta \overline{\mathbf{I}} = \overline{\mathbf{I}} - \overline{\mathbf{I}}, \quad \overline{\delta \overline{\mathbf{I}}} = 0, \quad \delta \overline{\mathbf{J}} = \overline{\mathbf{J}} - \overline{\overline{\mathbf{J}}}, \quad \overline{\delta \overline{\mathbf{J}}} = 0.$$
(6)

Here the overline means averaging over random orientations of crystallites,

$$\overline{I}_{\alpha} = \frac{\hbar e^{2} Z}{4\pi \varepsilon_{0} m^{2} c^{2}} \overline{p_{\alpha\alpha'}^{-1}} \sum_{\nu} \operatorname{Re} \left\langle \Psi_{\nu}^{+} \middle| \frac{\hat{l}_{\alpha'}}{r^{3}} \middle| \Psi \right\rangle,$$

$$\overline{J}_{\alpha} = \frac{\omega e Z}{2\pi \varepsilon_{0} m c^{2} n_{e}} \varepsilon_{\alpha'\beta'\gamma'} \overline{p_{\alpha\alpha'}^{-1} p_{\beta'\beta} p_{\sigma'\sigma} p_{\delta'\delta}} n_{\beta} n_{\delta} j_{\sigma} \times$$

$$\times \sum_{\nu} a_{\nu\sigma'} \operatorname{Im} \left\langle \Psi_{\nu}^{-} \middle| \frac{r_{\gamma'} \hat{l}_{\delta'}}{r^{3}} \middle| \Psi \right\rangle.$$
(7)

Analytical averaging of equations (7) leads to

$$\bar{\mathbf{I}} = 0, \quad \bar{\mathbf{J}} = \omega K \left[\mathbf{n} \times \left[\mathbf{n} \times \mathbf{j} \right] \right],$$

$$K = \frac{eZ}{12\pi\epsilon_0 mc^2 n_e} \sum_{\mathbf{v}} \operatorname{Im} \left\langle \Psi_{\mathbf{v}}^{-} \middle| \mathbf{a}_{\mathbf{v}} \frac{\left[\mathbf{r} \times \hat{\mathbf{l}} \right]}{r^3} \middle| \Psi \right\rangle. \tag{8}$$

The maximum value of J is obtained when the torsion axis is orthogonal to the current density vector. In this case

$$\overline{\mathbf{J}} = -\omega K \mathbf{j}. \tag{9}$$

It follows from Eq. (3) that the spin modulus of a single electron is conserved in a nondeformed crystallite. Equation (6) shows that in the presence of inhomogeneous distortion, the modulus of the spin averaged over the sample is not conserved due to the second term on the right side. Therefore, it can be considered as a relaxation one and, by analogy with the Bloch-Bloembergen equation, can be written as

$$\left[\overline{\left\{\delta\mathbf{I} - \delta\mathbf{J}\right\} \times \delta\mathbf{s}}\right] = -\frac{\overline{\mathbf{s}} - \overline{\mathbf{s}}_{e}}{\tau},\tag{10}$$

where $\overline{\mathbf{s}}_{e}$ is the equilibrium value of the spin averaged over the sample, τ is the longitudinal relaxation time. In this case, the steady state in (6) corresponds to the orientation of the average spin parallel or antiparallel to the vector $\overline{\mathbf{J}}$. Averaging the perturbation (1) over the quantum state and over random orientations of crystallites, similarly to the averaging of its commutator, we obtain that the energy of the states when the average spin is oriented parallel or antiparallel to the vector $\overline{\mathbf{J}}$ is $\pm \hbar |\overline{\mathbf{J}}|/2$, respectively.

Then, at a finite temperature T, taking into account the formula (9), we write the equilibrium value of the spin averaged over the sample in the equation (10) in the form:

$$\overline{\mathbf{s}}_{e} = -\frac{\mathbf{j}}{2j} \operatorname{th} \left(\frac{\hbar \omega K j}{2k_{B}T} \right),$$

where $k_{\rm B}$ is the Boltzmann constant. Thus, the equation for the dynamics of the average electron spin (6) takes the form

$$\frac{d\overline{\mathbf{s}}}{dt} = -\omega K \left[\mathbf{j} \times \overline{\mathbf{s}} \right] - \tau^{-1} \left(\overline{\mathbf{s}} + \frac{\mathbf{j}}{2j} \operatorname{th} \left(\frac{\hbar \omega K j}{2k_B T} \right) \right). \tag{11}$$

In the steady-state case, the average spin of the conduction electrons over a polycrystalline sample will be oriented predominantly along the current density vector **j**, as was shown earlier in [6].

For an s-electron with l = 0 in the relation (8), all integrals are equal to zero. In transition metals, the s and p bands overlap [10]. Therefore, collective conduction electrons can be formed from p-state electrons. In a crystallite, the axis of localization of the maximum electron density of the *p*-electron will be oriented in the direction of the v-pair of nearest neighbours, that is, along the vector $\mathbf{a}_{\mathbf{y}}$. Let us direct the polar axis \mathbf{z} along the vector a and count the azimuthal angle φ from the plane a.r. Then the wave function of the electron can be represented as:

$$\Psi(\mathbf{r}) = i\sqrt{\frac{3}{4\pi}}R_{n1}(r)\cos(\theta),$$

where $R_{n1}(r)$ is is the *p*-electron radial wave function, θ is the polar angle. Then from the formula (8) follows the form of the coefficient *K*:

$$K = \frac{\hbar e Za}{24\pi\varepsilon_0 mc^2 n_e} \int_0^\infty R_{n1}(x) dx \times$$

$$\times \int_{0}^{1} \left\{ R_{n1}(x_{1}) - R_{n1}(x_{2}) \right\} (1 - y^{2}) dy,$$

where \mathbf{a} is the distance to the nearest neighbours, $x = Zr/a_R$, $b = Za/a_R$, $y = \cos \theta$,

$$x_1 = \sqrt{x^2 + b^2 + 2xby}, \quad x_2 = \sqrt{x^2 + b^2 - 2xby}.$$

4. CONCLUSION

The resulting equation of motion demonstrates the dynamic effect of controlling the spin polarization of conduction electrons with the inhomogeneous deformation of the metal. The resulting equations are valid for a wide class of crystals with strong spin-orbit interaction, for example, for platinum, etc. The effect can find application in a number of branches of modern spintronics.

Thus, over last 3 years, it have appeared a number of experimental works in which the discovered effects of spintronics and spincaloritronics have not yet been explained: controlling the direction of the heat flux by the magneto-thermoelectric effect in a deformed metal magnet [12], expansion of the temperature range of heat pumping using elastocaloric effect [13], anomalous Righi-Leduc effect in ferromagnetic materials [14]. The dynamic effect presented in this paper can form the basis of the theory of new effects of strain spintronics.

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