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# Model of the Peltier spin effect in nonmagnetic chiral conductors

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It is shown that in a polycrystalline conductor with a helicity chiral structure and a strong spin-orbit interaction, the generation of a longitudinally polarized spin current and the heat flux associated with it are possible. At a given density of the charge current, the heat flux density depends on the local temperature, but not on its gradient, and is proportional to the lattice thermal conductivity coefficient.

**Keywords:** spin caloritronics, spin thermohalvanic effects, spin-orbit interaction, spin-phonon Hamiltonian, locally quasi-equilibrium distribution, helicity chiral crystal, polycrystalline conductor.

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## Introduction

Spin Peltier Effect (SPE) that refers to the heat flux generation caused by spin current was initially discovered in magnetic dielectrics [1]. One of the grounds for the SPE possibility was its mutuality with the Spin Seebeck Effect (SSE) referring to the generation of spin current caused by the temperature gradient and earlier found in magnetic dielectrics [2]. In the study [1] the temperature gradient caused by heat flux was registered by microthermocouples. SSE and SPE mutuality ratios were qualitatively verified by using numerical simulation.

We succeeded in significant improvement of spatial resolution and the sensitivity threshold of the temperature changes by means of the use of the local intensive thermography (LIT) when studying SPE [3], in particular, the mutuality ratios for it, which were justified analytically [4]. Further improvement of the resolution and sensitivity of local thermography by passive thermorefraction [5–8] allowed experimental verification of the mutuality ratio between SSE and SPE in magnetic dielectrics [9].

It should be noted that SSE was initially discovered in conductive ferromagnetic metals [10]. The authors explained that effect by magnon and phonon degrees of freedom [11]. The magnon theory was proposed also for SPE in magnetic dielectrics [12,13]. The model of magnon thermal conductivity based on the analysis of magnon-phonon interaction within the Boltzmann theory allowed to get a good correlation of the calculated and experimental data on SSE and SPE in magnetic dielectrics [14]. Thereafter, SSE was found in non-magnetic materials [15,16]. Theoretical model of SSE in paramagnetic dielectric was experimentally confirmed [17]. SSE and SPE symmetry justified experimentally by non-equilibrium Green's function and non-equilibrium thermodynamics [18] and confirmed experimentally [9] allows to assume that SPE, the same as SSE, is possible also in conductive magnetics, where spin moment is carried by conductivity electrons [19].

Efficient use of the interaction between spin current and heat flux is one of the main questions of the spin caloritronics. New capabilities for it are opened by experimentally found activation of SSE in non-magnetic materials by chiral phonons flux [20]. In the authors' opinion, chiral phonons having the angle moment disturb the material symmetry and enable the spin current generation in case of the temperature gradient. Such symmetry disturbance exists without external impacts in enantiopure crystals with helicoid chirality. At the present time application of chiral media and waves is considered as main area of the spintronics development [21]. Crystallographic chirality (according to terminology in [22]) can be accompanied by helimagnetic chirality, e.g. due to Dzyaloshinski–Moriya interaction. These effects were analyzed in the studies [23,24].

Experimentally studied SSE and SPE, generally, are magnetic thermogalvanic. These are manifested in paramagnetics in the external magnetic field or in magnetized ferromagnetics. The magnetic induction vector or residual magnetization defines the distinguished direction in isotropic substance. In chiral structures such direction can define the chirality axis. This is why materials with crystallographic helicoid chirality can be perspective material for non-magnetic spin caloritronics. For efficient control of large heat fluxes the control component must not be a thin-film, but massive one, therefore the SPE model in polycrystalline chiral structures is of the interest.

Many inorganic materials have chiral crystalline structures. Chirality of crystalline materials is determined by the symmetry of directions (symmetry of the second nature) [25]. Of 32 crystallographic dotted groups only 11 (1, 2, 3, 4, 6, 222, 422, 32, 622, 23 and 432), where no second nature symmetry operation (inversion, reflection, rotoinversion and sliding reflection), are enantiomorphous. These enantiomorphous dotted groups can define geometrically chiral classes of local symmetry of crystals. Integration of Bravais lattices with enantiomorphous dotted groups gives 65 space groups, which can form chiral crystalline structures, these are called Sohncke groups [26].

However, only 22 out of Sohncke groups are enantiomorphous space groups (11 enantiomosphous pairs) may contain a helicoid structure [27]. This is why inorganic crystalline materials having helicoid chirality in atom arrangement are related to these enantiomorphous space groups. In the rest of 43 groups the remote ordination of atoms is basically achiral, but every asymmetrical unit has local chirality and therefore it can also form chiral crystalline structures. Inorganic crystalline materials having chiral crystalline structure can easily create asymmetrical and enantioselective surfaces, because chiral atom arrangement continues on the surface [28]. Such crystalline faces provide asymmetrical chemical reactivity of the material and the possibility of biological recognition. For example, asymmetrical adsorption of enantiomers of amino acids and enantioselective catalysis with the use of quartz crystals were noted [29].

3D structures of pure metals have no chiral properties, except for manganese in $\beta$-modification [30]. In the study [31] the example of pure aluminum shows that formation of a distinguished direction in macroscopic metals is possible in case of quenching the sample in presence of deformation. Spirality is not round, but a broken line formed by the ribs of the system planes 111. The study [32] gives an overview of existing works on the synthesis of chiral nanostructures based on precious metals. The basis for such metamaterials are nanoparticles of metals manufactured, e.g., by nanolithography. The experiments show efficiency of synthesized chiral metamaterials in optics. The study [33], where the method of production of self-organizing chiral structures based on gold nanoparticles is presented, is potentially applicable to the spintronics problems.

## 1. Spin Hamiltonian of a conductivity electron in a helicoid-chiral metal

Let a crystallite with the volume of $V$ contain $N$ nodes, each of which includes similar ions with effective charge $+Ze$. Such a lattice creates an electric field

$$\mathbf{E}(\mathbf{r}) = -\frac{eZ}{4\pi\varepsilon_0}\sum_{l=1}^{N}\frac{\mathbf{r}-\mathbf{r}_l}{\left|\mathbf{r}-\mathbf{r}_l\right|^3}. \tag{1}$$

The spin-orbital addition to the electron energy has the form [34]:

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

Here $m$ — is the mass of an electron with charge — $e$.

Let us build effective Hamiltonian of the conductivity electron for disturbance (2) in the field (1), by averaging the operator (2) by coordinates of electron wave function, by replacing variables $\mathbf{r}-\mathbf{r}_l \to \mathbf{r}$ and taking into consideration that the moment operator commutates with any central potential

$$\hat{V}_e = -\frac{\hbar^2e^2Z}{8\pi\varepsilon_0m^2c^2}\,\hat{\mathbf{s}}\left\langle\psi(\mathbf{r}+\mathbf{r}_l)\middle|\frac{\hat{\mathbf{l}}}{r^3}\middle|\psi(\mathbf{r}+\mathbf{r}_l)\right\rangle. \tag{3}$$

Hereafter the summation by repeated indices is meant.

The wave function of the collectivized conductivity electron is written down in the form of the Vanier function [35]

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

where $\Psi(\mathbf{r})$ — is the atomic function of electron, $\mathbf{R}_n$ — is the translation vector. Then

$$\hat{V}_e = -\frac{\hbar^2e^2Z}{8\pi\varepsilon_0m^2c^2N}\,\hat{\mathbf{s}}\left(i\mathbf{k}\left(\mathbf{R}_\mathbf{n}-\mathbf{R}_m\right)\right)$$

$$\times\left\langle\psi\left(\mathbf{r}+\mathbf{r}_l-\mathbf{R}_m\right)\middle|\frac{\hat{\mathbf{l}}}{r^3}\middle|\Psi\left(\mathbf{r}+\mathbf{r}_l-\mathbf{R}_n\right)\right\rangle. \tag{5}$$

In the approximation of the nearest neighbors the quantum mean in the right side (5) differs from zero only at $\mathbf{R}_n-\mathbf{r}_k=0$ or $\mathbf{a}_\nu$ and $\mathbf{R}_m-\mathbf{r}_k=0$ or $\mathbf{a}_\nu$, where $\mathbf{a}_\nu$ — is the vector drawn to the nearest neighbor.

$$\hat{V}_e = -\frac{\hbar^2e^2Z}{8\pi\varepsilon_0m^2c^2}\,\hat{s}_\alpha\left\{\mathrm{Re}\left\langle\Psi\middle|\frac{\hat{l}_\alpha}{r^3}\middle|\Psi\right\rangle + 2\cos(\mathbf{k}\mathbf{a}_\nu)\right.$$

$$\left.\times\mathrm{Re}\left\langle\Psi_\nu^+\middle|\frac{\hat{l}_\alpha}{r^3}\middle|\Psi\right\rangle + 2\sin(\mathbf{k}\mathbf{a}_\nu)\mathrm{Im}\left\langle\Psi_\nu^-\middle|\frac{\hat{l}_\alpha}{r^3}\middle|\Psi\right\rangle\right\}.$$

Here $\Psi_\nu^\pm(\mathbf{r}) = \Psi(\mathbf{r}+\mathbf{a}_\nu)\pm\Psi(\mathbf{r}-\mathbf{a}_\nu)$.

Considering SPE only in metals, we will use the approximation of an ideal fermi gas for conductivity electrons. The applicability of this model is justified by the fact that the thermodynamics of a fermi system is determined by its microscopic structure only near the Fermi surface [36]. Experimental studies of the temperature dependence of the electron heat capacity in metals show that it corresponds well to the model of an ideal fermi gas. At that, for the most of metals effective mass of conductivity electron $m^*$ is close to the mass of free electron. This is why $\mathbf{k} = -m^*\mathbf{j}/(\hbar e n_e)$, where $\mathbf{j}$ — is the density of charge current, $n_e$ — is the concentration of conductivity electrons.

In the first order of smallness by $(\mathbf{j}\mathbf{a}_\nu)$ we get

$$V_e = \frac{\hbar^2e^2Z}{8\pi\varepsilon_0m^2c^2}\left(-\mathbf{I}_0-\mathbf{I}_1+\mathbf{J}\right)\hat{\mathbf{s}}, \tag{6}$$

$$\mathbf{I}_0 = \mathrm{Re}\left\langle\Psi\middle|\frac{\hat{\mathbf{l}}}{r^3}\middle|\Psi\right\rangle,\quad \mathbf{I}_1 = 2\mathrm{Re}\left\langle\Psi_\nu^+\middle|\frac{\hat{\mathbf{l}}}{r^3}\middle|\Psi\right\rangle,$$

$$\mathbf{J} = \frac{2m^*}{\hbar e n_e}(\mathbf{j}\mathbf{a}_\nu)\mathrm{Im}\left\langle\Psi_\nu^-\middle|\frac{\hat{\mathbf{l}}}{r^3}\middle|\Psi\right\rangle. \tag{7}$$

Here the summation in (7) and next by $\nu$ by pairs of symmetrically arranged nearest neighbors is meant.

In centrally symmetrical crystallite $\mathbf{J} = 0$, since the function $\Psi_\nu^-(\mathbf{r})$ has the parity, which is opposite to the parity of the function $\Psi(\mathbf{r})$.

Let us consider the crystallite with helicoid chirality. Its crystalline lattice can be represented as a result of twisting centrally symmetrical lattice around the chirality axis. Thus, twisting transforms centrally symmetrical crystallite $P\bar{3}1m$ into helicoid chiral one $P6_322$.

Twisting along the chirality axis can be described by axial vector $\Omega(\mathbf{r}) = (\mathbf{rn})\omega\mathbf{n}$. Here $\mathbf{n}$ — is the single vector oriented along the chirality axis, $\omega$ — is the pseudoscalar, linear twisting. Twisting operations correspond to transformation of coordinates $r'_\alpha = r_\alpha + u_\alpha(\mathbf{r})$, where $\mathbf{u}(\mathbf{r}) = [\Omega(\mathbf{r}) \times \mathbf{r}] = (\mathbf{rn})\omega[\mathbf{n} \times \mathbf{r}]$.

In coordinates transformation the wave function and the moment operator in (7) are transformed according to the law

$$dr'_\alpha = dr_\alpha + \frac{\partial u_\alpha}{\partial r_\beta}\, dr_\beta,$$

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

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

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

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

Here $\varepsilon_{\alpha\beta\gamma}$ — is the single antisymmetric Levi-Chivita tensor. In the approximation, which is linear by $\omega$ we get

$$\delta r_\alpha = r'_\alpha - r_\alpha = \omega\varepsilon_{\alpha\beta\gamma} n_\beta n_\delta r_\gamma r_\delta,$$

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

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

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

$$\delta I_{0\alpha'} = \frac{2m^*\omega}{\hbar e n_e}\, \varepsilon_{\alpha'\beta'\gamma'} n_{\beta'} n_{\delta'} \mathrm{Re}\left\langle \Psi \middle| \frac{r_{\gamma'} \hat{l}_{\delta'}}{r^3} \middle| \Psi \right\rangle,$$

$$\delta I_{1\alpha'} = \frac{2m^*\omega}{\hbar e n_e}\, \varepsilon_{\alpha'\beta'\gamma'} n_{\beta'} n_{\delta'} \mathrm{Re}\left\langle \Psi_\nu^+ \middle| \frac{r_{\gamma'} \hat{l}_{\delta'}}{r^3} \middle| \Psi \right\rangle,$$

$$\delta J_{\alpha'} = \frac{2m^*\omega}{\hbar e n_e}\, \varepsilon_{\alpha'\beta'\gamma'} n_{\beta'} n_{\delta'} j_{\sigma'} a_{\nu\sigma'} \mathrm{Im}\left\langle \Psi_\nu^- \middle| \frac{r_{\gamma'} \hat{l}_{\delta'}}{r^3} \middle| \Psi \right\rangle. \tag{9}$$

The value $a_\nu\omega$ in the formula (8) is the rotation angle of its crystallographic plane perpendicular to the chirality axis relative to the neighboring one. The operator in quantum mean in the ratios (9) is odd, and the function $\Psi_\nu^+(\mathbf{r})$ has the parity which coincides the parity of the function $\Psi(\mathbf{r})$. Therefore $\delta\mathbf{I}_0 = \delta\mathbf{I}_1 = 0$.

In crystalline field (1) the position of axes, in which the wave functions of electrons are written, is defined by the position of crystallophysical axes. This is why one can consider that the ratios (9) are recorded in the coordinates system related with the crystallite axes. Let us introduce a laboratory coordinate system associated with the instruments that set the conductivity current and measure the spin and energy flux components. The components of vectors and tensors in the laboratory system will be denoted by non-hatched indices, and the components of vectors and tensors in the coordinate system associated with the crystallophysical axes, — by hatched indices, as in the formula (9). The vector $\mathbf{n}$, the same as vectors $\mathbf{a}_\nu$, is set in the system of crystallophysical axes, and the vector $\mathbf{j}$, the same as the vector $\mathbf{s}$, in the formula (6) — is set in the laboratory system.

Let us transform the current density vector from the laboratory system into the system of crystallophysical axes $j_{\sigma'} = p_{\sigma'\sigma} j_\sigma$, and the vectors $\mathbf{I}$ and $\mathbf{J}$ from the system of crystalline axes — into the laboratory system $J_\alpha = p^{-1}_{\alpha\alpha'} J_{\alpha'}$ where $p_{\alpha'\alpha}$ — is the unitary rotation matrix. Let us put that transformation into the equation (6) and average the vectors $\mathbf{I}$ and $\mathbf{J}$ in microscopic region by random orientations of crystallites. The rotation matrix is convenient to express through Euler angles. Then the averaging in macroscopically isotropic region is limited to the averaging by random uniformly distributed Euler angles. Wherein the quantum mean in the formula (8) is the scalar, which depends only on the crystal properties, can be derived in the system of crystallophysical axes and is not changed when averaging by random orientations of crystallites.

$$\overline{\mathbf{I}_0} = \overline{\mathbf{I}_1} = 0, \quad \overline{\delta\mathbf{J}} = \mathbf{J}_h = \mathbf{j}\, \frac{m^*\omega}{3\hbar e n_e}\, \mathrm{Im}\left\langle \Psi_\nu^- \middle| \mathbf{a}_\nu\, \frac{\lfloor \mathbf{r} \times \hat{\mathbf{l}} \rfloor}{r^3} \middle| \Psi \right\rangle. \tag{10}$$

Here, the index $h$ denotes contribution caused by helicoid chirality of the medium.

## 2. Effective spin-phonon Hamiltonian

Let the harmonic wave with the wave vector $\mathbf{K}$ and the frequency of $\Omega(\mathbf{K})$ as $\mathbf{u}(t, \mathbf{r}) = \mathbf{a}(t, \mathbf{r}) + {} + \mathbf{a}^*(t, \mathbf{r})$, $\mathbf{a}(t, \mathbf{r}) = \mathbf{e}a\exp(i\Omega t - i\mathbf{Kr})$ propagates along the vector e in the crystallite with helicoid chirality. For the deformation created by that wave, in a similar way to the ratios (8), we get

$$\begin{aligned}\delta\hat{l}_\alpha = {} & \hat{l}'_\alpha - \hat{l}_\alpha = \varepsilon_{\alpha\beta\gamma}\Big(\left(a_\beta + a^*_\beta\right)\hat{p}_\gamma \\ & + iK_\gamma\left(r_\beta + a_\beta + a^*_\beta\right)\left(a_\delta - a^*_\delta\right)\hat{p}_\delta\Big).\end{aligned}$$

Considering that the pulse operator is imaginary, we get

$$\delta\hat{\mathbf{l}} = \delta_1\hat{\mathbf{l}} - \delta_1\hat{\mathbf{l}}^* + \delta_2\hat{\mathbf{l}} - \delta_2\hat{\mathbf{l}}^* + \delta_3\hat{\mathbf{l}} - \delta_3\hat{\mathbf{l}}^*,$$

$$\delta_1\hat{\mathbf{l}} = a\exp\left(i\Omega t - i\mathbf{Kr}\right)\left\{[\mathbf{e} \times \hat{\mathbf{p}}] + i[\mathbf{r} \times \mathbf{K}](\mathbf{e}\hat{\mathbf{p}})\right\},$$

$$\delta_2\hat{\mathbf{l}} = -ia^*a(\mathbf{e}\hat{\mathbf{p}})[\mathbf{e} \times \mathbf{K}],$$

$$\delta_3\hat{\mathbf{l}} = ia^2\exp(i2\Omega t - i2\mathbf{Kr})(\mathbf{e}\hat{\mathbf{p}})[\mathbf{e} \times \mathbf{K}].$$

Here, the component $\delta_2\hat{\mathbf{l}}$ is not explicitly dependent on the time and coordinates. The same

$$\psi' - \psi = \frac{\partial u_\alpha}{\partial r_\beta} r_\beta \frac{\partial \psi}{\partial r_\alpha} = \delta\psi + \delta\psi^*,$$

$$\delta\psi = \frac{a}{\hbar}\exp(i\Omega t - i\mathbf{Kr})(\mathbf{Kr})(\mathbf{e}\hat{\mathbf{p}})\psi.$$

For the components of each member of the sum not explicitly dependent on the time in (3) we get

$$\begin{aligned}\mathbf{A} =& \left\langle \psi' \middle| \frac{\hat{\mathbf{l}}}{r^3} \middle| \psi' \right\rangle - \left\langle \psi \middle| \frac{\hat{\mathbf{l}}}{r^3} \middle| \psi \right\rangle = \left\langle \psi \middle| \frac{\delta_2\hat{\mathbf{l}} - \delta_2\hat{\mathbf{l}}^*}{r^3} \middle| \psi \right\rangle \\ &+ \left\langle \delta\psi \middle| \frac{\hat{\mathbf{l}}}{r^3} \middle| \delta\psi \right\rangle + \left\langle \delta\psi^* \middle| \frac{\hat{\mathbf{l}}}{r^3} \middle| \delta\psi^* \right\rangle + \left\langle \delta\psi \middle| \frac{\delta_1\hat{\mathbf{l}}}{r^3} \middle| \psi \right\rangle \\ &- \left\langle \delta\psi^* \middle| \frac{\delta_1\hat{\mathbf{l}}^*}{r^3} \middle| \psi \right\rangle + \left\langle \psi \middle| \frac{\delta_1\hat{\mathbf{l}}}{r^3} \middle| \delta\psi^* \right\rangle - \left\langle \psi \middle| \frac{\delta_1\hat{\mathbf{l}}^*}{r^3} \middle| \delta\psi \right\rangle \\ &+ \left\langle \delta\psi \middle| \frac{\delta_3\hat{\mathbf{l}}}{r^3} \middle| \delta\psi^* \right\rangle - \left\langle \delta\psi^* \middle| \frac{\delta_3\hat{\mathbf{l}}^*}{r^3} \middle| \delta\psi \right\rangle.\end{aligned}$$

To build effective spin-phonon Hamiltonian in representation of the secondary quantization let us replace $a \to \hat{a}_{\mathbf{K}}\sqrt{\frac{\hbar}{2wV\Omega}}$, $a^* \to \hat{a}^+_{\mathbf{K}}\sqrt{\frac{\hbar}{2wV\Omega}}$, where $w$ — is the body density, $V$ — is its volume and, subject to the commutation rules $[\hat{a}, \hat{a}^+] = 1$, let us distinguish the components, which are proportional to the density operator of the phonon number with the wave vector $\mathbf{K}$ $\hat{c}_{\mathbf{K}} = \hat{a}^+_{\mathbf{K}}\hat{a}_{\mathbf{K}}/V$, and build the operator

$$\hat{\mathbf{A}}_{\mathbf{K}} = \frac{\hat{c}_{\mathbf{K}}}{2\hbar\Omega w}(\mathbf{e}\hat{\mathbf{p}})(\mathbf{Kr})\frac{\hat{\mathbf{l}}}{r^3}(\mathbf{Kr})(\mathbf{e}\hat{\mathbf{p}}).$$

For the ensemble of equilibrium thermal phonons let us average that operator by random orientations of vectors $\mathbf{K}$ and $\mathbf{e}$:

$$\left\langle \hat{\mathbf{A}}_{\mathbf{K}} \right\rangle = \frac{\langle \hat{c}_{\mathbf{K}} \rangle}{2\hbar\Omega w}\left\langle e_\alpha e_\gamma \right\rangle \left\langle K_\beta K_\delta \right\rangle \hat{p}_\alpha r_\beta \frac{\hat{\mathbf{l}}}{r^3} r_\delta \hat{p}_\gamma.$$

If in macroscopically isotropic medium all directions of vectors $\mathbf{K}$ and $\mathbf{e}$ are equally probable and independent, then $\langle e_\alpha e_\gamma \rangle = \delta_{\alpha\gamma}/3$, $\langle K_\beta K_\delta \rangle = \delta_{\beta\delta}K^2/3$ In isotropic medium one can consider the phonon frequency $\Omega$ as unambiguous monotone function of the modulus of its wave number and put $K = \Omega/v_\Omega$, where $v_\Omega$ — is the phase speed of the phonon, $\langle \hat{c}_{\mathbf{k}} \rangle = \hat{c}_\Omega$. Then, subject to commutation ratios between the operators of coordinates, pulse and moment components, we get

$$\left\langle \hat{\mathbf{A}}_{\mathbf{K}} \right\rangle = \hat{\mathbf{A}}_\Omega = \frac{\hat{h}_\Omega}{18\hbar^2 w v_\Omega^2}\hat{p}_\alpha r_\beta \frac{\hat{\mathbf{l}}}{r^3} r_\beta \hat{p}_\alpha. \tag{11}$$

Here $\hat{h}_\omega = \hbar\Omega\hat{c}_\Omega$ — is the density operator of Hamiltonian of the phonons with the frequency of $\Omega$.

In harmonic approximation the phonons do not interact. We will treat interaction of phonons conditioned by anharmonicity as one of possible mechanisms of relaxation. Then we can introduce the density operator of undisturbed Hamiltonian of the system of phonons as the sum of Hamiltonians of subensembles of phonons with the frequency of $\Omega$: $\hat{h}_{0p} = \sum_\Omega \hat{h}_\Omega$, where summation is performed for all frequencies of the phonon spectrum. Let us introduce the average in terms of phonon spectrum phase speed $v$. Then, from (11) we get

$$\hat{\mathbf{A}}_{\mathbf{K}} = \sum_\Omega \hat{\mathbf{A}}_\Omega = \frac{\hat{h}_{0p}}{18\hbar^2 w v_\Omega^2}\hat{p}_\alpha r_\beta \frac{\hat{\mathbf{l}}}{r^3} r_\beta \hat{p}_\alpha. \tag{12}$$

Formulas (9) for the deformation of centrally symmetrical crystallite, which is caused only be phonons, will be

$$\delta\mathbf{l}_0 = \frac{m^*}{\hbar e n_e}\operatorname{Re}\left\langle \Psi \middle| \hat{\mathbf{A}} \middle| \Psi \right\rangle, \quad \delta_1 = \frac{2m^*}{\hbar e n_e}\operatorname{Re}\left\langle \Psi_\nu^+ \middle| \hat{\mathbf{A}} \middle| \Psi \right\rangle,$$

$$\delta\mathbf{J} = \frac{2m^*(\mathbf{j}\mathbf{a}_\nu)}{\hbar e n_e}\operatorname{Im}\left\langle \Psi_\nu^- \middle| \hat{\mathbf{A}} \middle| \Psi \right\rangle. \tag{13}$$

Since the operator (12) is even, $\delta\mathbf{l}_0 \neq 0$ and $\delta\mathbf{l}_1 \neq 0$, but when averaging by random orientations of crystals we get $\overline{\delta\mathbf{l}_0} = \overline{\delta\mathbf{l}_1} = 0$. In case of deformation conditioned only by phonons $\delta\mathbf{J} = 0$. If a phonon propagates in helicoid chiral medium, then the last formula (13) turns into

$$\begin{aligned}\delta\mathbf{J} =& \frac{2m^*(\mathbf{j}\mathbf{a}_\nu)}{\hbar e n_e}\operatorname{Im}\left\{ \left\langle \Psi_\nu^- \middle| \delta\hat{\mathbf{A}} \middle| \Psi \right\rangle + \left\langle \delta\Psi_\nu^- \middle| \hat{\mathbf{A}} \middle| \Psi \right\rangle \right. \\ &\left. + \left\langle \Psi_\nu^- \middle| \hat{\mathbf{A}} \middle| \delta\Psi \right\rangle \right\} = \frac{m^*\omega j_{\sigma'} a_{\nu\sigma'}\hat{h}_0}{9wv^2\hbar^3 e n_e}\operatorname{Im}\left\{ \left\langle \Psi_\nu^- \middle| \hat{\mathbf{B}} \middle| \Psi \right\rangle \right\},\end{aligned}$$

$$\begin{aligned}\delta\hat{\mathbf{A}} =& \frac{\hat{h}_0/\hbar^2}{18wv^2}\left\{ \hat{p}_\alpha r_\beta \frac{\delta\hat{\mathbf{l}}}{r^3} r_\beta \hat{p}_\alpha + \delta\hat{p}_\alpha r_\beta \frac{\hat{\mathbf{l}}}{r^3} r_\beta \hat{p}_\alpha + \right. \\ &\left. + \hat{p}_\alpha r_\beta \frac{\hat{\mathbf{l}}}{r^3} r_\beta \delta\hat{p}_\alpha + \hat{p}_\alpha \delta r_\beta \frac{\hat{\mathbf{l}}}{r^3} r_\beta \hat{p}_\alpha + \hat{p}_\alpha r_\beta \frac{\hat{\mathbf{l}}}{r^3}\delta r_\beta \hat{p}_\alpha \right\}.\end{aligned} \tag{14}$$

$$\begin{aligned}\hat{B}_{\alpha'} =& \varepsilon_{\alpha'\beta'\gamma'} n_{\beta'} n_{\delta'} \hat{p}_{\mu'} r_\chi \frac{r_{\delta'}\hat{l}_{\gamma'} + r_{\gamma'}\hat{l}_{\delta'}}{r^3} r_{\chi'} \hat{p}_{\mu'} \\ &+ \varepsilon_{\chi'\beta'\gamma} n_{\beta'} n_{\delta'} \hat{p}_{\mu'} r_\gamma \left( r_{\delta'} \frac{\hat{l}_{\alpha'}}{r^3} r_{\chi'} \hat{p}_{\mu'} + \frac{\hat{l}_{\alpha'}}{r^3} r_{\chi'} r_{\delta'} \hat{p}_{\mu'} \right) \\ &- n_{\eta'} \left( \varepsilon_{\beta'\eta'\mu'} n_{\delta'} r_{\delta'} + \varepsilon_{\beta'\eta'\gamma'} n_{\mu'} r_{\gamma'} \right) \hat{p}_{\beta'} r_{\chi'} \frac{\hat{l}_{\alpha'}}{r^3} r_{\chi'} \hat{p}_{\mu'} \\ &- n_{\eta'} \hat{p}_{\mu'} r_{\chi'} \frac{\hat{l}_{\alpha'}}{r^3} r_{\chi'} \left( \varepsilon_{\beta'\eta'\mu'} n_{\delta'} r_{\delta'} + \varepsilon_{\beta'\eta'\gamma'} n_{\mu'} r_{\gamma'} \right) \hat{p}_{\beta'} \\ &+ i n_{\beta'} n_{\delta'} r_{\delta'} \left( \hat{p}_{\mu'} r_{\chi'} \frac{\hat{l}_{\alpha'}}{r^3} r_{\chi'} \hat{p}_{\mu'} \hat{l}_{\beta'} - \hat{l}_{\beta'} \hat{p}_{\mu'} r_{\chi'} \frac{\hat{l}_{\alpha'}}{r^3} r_{\chi'} \hat{p}_{\mu'} \right).\end{aligned} \tag{15}$$

By substituting the expression (15) in the right side of the formula (14) and by averaging it by random orientations of crystallites, we obtain that the averaged vector $\delta\mathbf{J}$ is proportional to the density vector of the charge current. The coefficient of proportionality has a quite cumbersome structure. By limiting only to the contribution from the first member of sum in the formula (15), we get

$$\overline{\delta\mathbf{J}} = \mathbf{J}_{ph} = \frac{m^*\omega\hat{h}_{0P}}{27\hbar^3 e n_e w v^2}\mathbf{j}\mathrm{Im}\Big\langle\Psi_\nu^-\Big|\hat{p}_\alpha r_\beta \mathbf{a}_\nu$$

$$\times\left\{(\mathbf{nr})\left[\mathbf{n}\times\frac{\hat{\mathbf{l}}}{r^3}\right]+[\mathbf{n}\times\mathbf{r}]\left(\mathbf{n}\frac{\hat{\mathbf{l}}}{r^3}\right)\right\}r_\beta\hat{p}_\alpha\Big|\Psi\Big\rangle. \qquad (16)$$

Here, the index *ph* denotes contribution caused by phonons propagating in chiral medium.

Let us substitute formulas (10) and (16) in the equation (6). To analyze the spin subsystem dynamics we build efficient spin Hamiltonian, by averaging the ratio (6) by variables of the phonon subsystem:

$$\hat{V}_S = (\mathbf{j}\hat{\mathbf{s}})(D_S + D_P h_{0P}),$$

$$D_S = \frac{\hbar e Z m^*\omega}{24\pi\varepsilon_0 m^2 c^2 n_e}\mathrm{Im}\Big\langle\Psi_\nu^-\Big|\mathbf{a}_\nu\,\frac{\lfloor\mathbf{r}\times\hat{\mathbf{l}}\rfloor}{r^3}\Big|\Psi\Big\rangle,$$

$$D_P = \frac{eZm^*\omega}{216\pi\varepsilon_0\hbar m^2 c^2 n_e w v^2}\,\mathrm{Im}\Big\langle\Psi_\nu^-\Big|\hat{p}_\alpha r_\beta \mathbf{a}_\nu$$

$$\times\left\{(\mathbf{nr})\left[\mathbf{n}\times\frac{\hat{\mathbf{l}}}{r^3}\right]+[\mathbf{n}\times\mathbf{r}]\left(\mathbf{n}\frac{\hat{\mathbf{l}}}{r^3}\right)\right\}r_\beta\hat{p}_\alpha\Big|\Psi\Big\rangle. \qquad (17)$$

Accordingly, for description of the dynamics of the phonon subsystem we build efficient phonon Hamiltonian, by averaging (6) by variables of the spin subsystem:

$$\hat{V}_P = D_P(\mathbf{js})\hat{h}_{0P}. \qquad (18)$$

The ratios (17) and (18) are written for one electron interacting with the system of phonons. Let us distinguish a physically small volume with the center in the point with the coordinate $\mathbf{r}$, containing sufficient number of conductivity electrons, within which the conductivity current density, the phonons density and other parameters of formulas (17) and (18) can be considered as constant, and introduce the densities of spin moment $\hat{\mathbf{s}}(\mathbf{r}, t)$, undisturbed Hamiltonian of electrons $\hat{h}_{0S}(t, \mathbf{r})$, effective spin perturbation $\hat{u}_S(\mathbf{r}, t)$ and effective phonon perturbation $\hat{u}_P(t, \mathbf{r})$ so that

$$\hat{\mathbf{S}}(t) = \int\limits_V \hat{\mathbf{s}}(t, \mathbf{r})d^3r,$$

$$\hat{V}_S(t) = \int\limits_V \hat{u}_S(t, \mathbf{r})d^3r, \quad \hat{V}_P(t) = \int\limits_V \hat{u}_P(t, \mathbf{r})d^3r,$$

$$\hat{H}_{0P}(t) = \int\limits_V \hat{h}_{0P}(t, \mathbf{r})d^3r, \quad \hat{H}_{0S}(t) = \int\limits_V \hat{h}_{0S}(t, \mathbf{r})d^3r. \qquad (19)$$

Here $\hat{\mathbf{S}}(t)$ — is the operator of total spin of conductivity electrons, $\hat{H}_{0P}(t)$ and $\hat{H}_{0S}(t)$ — are undisturbed Hamiltonians of phonons and electrons in the volume $V$, accordingly.

Density operators of phonon Hamiltonian $\hat{h}_P(t, \mathbf{r})$ and spin moment $\hat{\mathbf{s}}(\mathbf{r}, t)$ in representation of interaction satisfy the ratios [37]

$$\frac{\partial\hat{h}_P(t, \mathbf{r})}{\partial t} = -div\hat{\mathbf{q}}(t, \mathbf{r}),$$

$$i\hbar\frac{\partial\hat{s}_\alpha(t, \mathbf{r})}{\partial t} = \left[\hat{S}_\alpha(t), \hat{h}_{0S}(t, \mathbf{r})\right] - i\hbar\frac{\partial\hat{\upsilon}_{\alpha\beta}(t, \mathbf{r})}{\partial r_\beta},$$

$$\alpha, \beta = 1, 2, 3, \qquad (20)$$

where $\hat{\mathbf{q}}(t, \mathbf{r})$ is the density operator of the flux of phonons Hamiltonian, $\hat{\upsilon}_{\alpha\beta}(t, \mathbf{r})$ — are the operator components of pseudotensor of the spin current density. From the formulas (18) and (19) for the phonons Hamiltonian we get

$$\hat{H}_P(t) = \hat{H}_{0P} + V_{0P}(t) = \int\limits_V \hat{h}_P(t, \mathbf{r})d^3r,$$

$$\hat{h}_P(t, \mathbf{r}) = \hat{h}_{0P}(t, \mathbf{r})\Big\{1 + D_P(\mathbf{j}(t, \mathbf{r})\mathbf{s}(t, \mathbf{r}))\Big\}. \qquad (21)$$

## 3. Locally quasi-equilibrium distribution

Application of Boltzmann theory allowed to obtain a good correlation of the calculated and experimental data for SSE and SPE in magnetic dielectrics [14]. Quantum generalization of such approach is the concept of locally quasi-equilibrium distribution of the density operator [38].

In absence of fluxes, locally quasi-equilibrium distribution with the density operator is established in the phonon subsystem

$$\hat{\rho}_P^q(t) = \exp\Big\{-\Phi(t) - \int\limits_V \theta(t, \mathbf{r})\hat{h}_P(\mathbf{r}, t)d^3r\Big\},$$

$$\Phi(t) = \ln\mathrm{Sp}\exp\Big\{-\int\limits_V \theta(t, \mathbf{r})\hat{h}_P(t, \mathbf{r})d^3r\Big\}. \qquad (22)$$

Here $\Phi(t)$ — is the functionality of Massier-Planck, $\theta(t, \mathbf{r}) = 1/(k_B T(t, \mathbf{r}))$, $k_B$ — is the Boltzmann constant, $T(t, \mathbf{r})$ — is the local temperature.

We will consider that in absence of fluxes the distribution (22) is established in the phonon subsystem. In phonon subsystem brought out of the locally quasi-equilibrium state (22) into the state with density operator $\hat{\rho}_P(t)$, the energy flux occurs with density

$$\mathbf{q}(t, \mathbf{r}) = \mathrm{Sp}(\hat{\mathbf{q}}(t, \mathbf{r})\hat{\rho}_P(t)) = \mathbf{q}_{mn}(t, \mathbf{r})\rho_{Pnm}(t). \qquad (23)$$

Hereinafter the matrix elements of operators are derived in the basis of eigen functions of undisturbed phonon Hamiltonian $\hat{H}_{0P}$ and the summation by repeated indices is implied. The energy flux (23) is one of the mechanisms of the system relaxation to locally quasi-equilibrium state (22). In the approximation of Markov's relaxation the density operator dynamics can be described by using the equation

$$\frac{\partial\rho_{Pnm}(t)}{\partial t} = \frac{\rho_{Pnm}^q(t) - \rho_{Pnm}(t)}{\tau_{nm}},$$

which is equivalent to integral equation

$$\rho_{Pnm}(t) = \left(\rho_{Pnm}^0 + \rho_{Pnm}^q(t)\right)\exp\left(\frac{t_0 - t}{\tau_{nm}}\right) - \rho_{Pnm}^q(t)$$

$$+ \int\limits_{t_0}^{t}\exp\left(\frac{t - t'}{\tau_{nm}}\right)\frac{d\rho_{Pnm}^q(t')}{dt'}\,dt'. \qquad (24)$$

Here $\tau_{nm}=\tau_{mn}$ — are real positive times of relaxation, and, it is adopted that at the moment of time $t_0$ the system was in quasi-equilibrium state with the density operator $\hat{\rho}_P^0$.

It follows from the equations (20)–(22) that for steady-state distribution of local temperature, density of charge current and spin polarization

$$\frac{d\hat{\rho}_P^q(t)}{dt} = -\hat{\rho}_P^q(t)\int\limits_V \hat{q}_\alpha(t,\mathbf{r})\frac{\partial}{\partial r_\alpha}\{\theta(\mathbf{r}) + D_P\theta(\mathbf{r})(\mathbf{j}(\mathbf{r})\mathbf{s}(\mathbf{r}))\}d^3r + \int\limits_\Sigma \hat{q}_\alpha(\mathbf{r},t)\theta(\mathbf{r}) \times \{1 + D_P(\mathbf{j}(\mathbf{r})\mathbf{s}(\mathbf{r}))\}d\Sigma. \tag{25}$$

Here $\Sigma$ — is the surface limiting the body $V$. If the surface $\Sigma$ is isothermal and no heat emission inside the body, the second member of sum in the right part (25) is equal to zero.

Let moment of time $t_0$ in the formula (24) tend to $-\infty$, then the first member of sum on the right-hand side is zero. Let us introduce a new variable $\tau = t - t'$. Subject to the formula (25) the equation (18) will be

$$\rho_{Pnm}(t) = -\rho^q_{Pnm}(t) - \int\limits_V\int\limits_0^\infty \exp\left(\frac{-\tau}{\tau_{nm}}\right)\left(\rho^q_{Pnl}(t-\tau)q_{\alpha lm}(\mathbf{r}',t-\tau)\right)d\tau \times \frac{\partial}{\partial r'_\alpha}\left\{\theta(\mathbf{r}') + D_p\theta(\mathbf{r}')((\mathbf{j}(\mathbf{r}')\mathbf{s}(\mathbf{r}'))\right\}d^3r'. \tag{26}$$

Considering that there are no fluxes in quasi-equilibrium state, from the formulas (23) and (26) we get

$$q_\alpha(t,\mathbf{r}) = \int\limits_V\int\limits_0^\infty \exp\left(\frac{-\tau}{\tau_{nm}}\right)\rho^q_{Pnl}(t-\tau)q_{\alpha mn}(t,\mathbf{r})q_{\beta lm}(t-\tau,\mathbf{r}')d\tau \times \frac{\partial}{\partial r'_\alpha}\left\{D_p\theta(\mathbf{r}')((\mathbf{j}(\mathbf{r}')\mathbf{s}(\mathbf{r}')) + \theta(\mathbf{r}')\right\}d^3r'. \tag{27}$$

Quasi-equilibrium distribution is a quasi-steady-state, this is why we can ignore the change of matrix elements of quasi-equilibrium density operator for typical time of relaxation of non-equilibrium operator. If the typical scale of space correlation of ensemble of non-interacting thermal phonons is small versus the distance, at which the gradient in the subintegral expression (27) changes, we may assume

$$\begin{aligned}\rho^q_{Pnl}(t-\tau)q_{\alpha mn}(t,\mathbf{r})q_{\beta lm}(t-\tau,\mathbf{r}') &= \mathrm{Sp}\left\{\hat{\rho}^q_P\hat{q}_\alpha(t,\mathbf{r})\hat{q}_\beta(t-\tau,\mathbf{r}')\right\} \\ &= \left\langle\hat{q}_\alpha(t,\mathbf{r})\hat{q}_\beta(t-\tau,\mathbf{r}')\right\rangle^q \\ &= \left\langle\hat{\mathbf{q}}(t,\mathbf{r})\hat{\mathbf{q}}(t-\tau,\mathbf{r})\right\rangle^q\delta(\mathbf{r}-\mathbf{r}')\delta_{\alpha\beta}/3.\end{aligned}$$

Then the formula (27) takes the form

$$\mathbf{q}(t,\mathbf{r}) = \frac{1}{3k_BT^2(t,\mathbf{r})}\int\limits_0^\infty \exp\left(\frac{-\tau}{\tau_{nm}}\right)\rho^q_{Pnl}(t-\tau)q_{\alpha mn}(t,\mathbf{r}) \times q_{\alpha lm}(\mathbf{r},t-\tau)d\tau\,\frac{\partial T(t,\mathbf{r})}{\partial\mathbf{r}} + \frac{D_P}{3k_B}\int\limits_0^\infty \exp\left(\frac{-\tau}{\tau_{nm}}\right)\rho^q_{Pnl} \times (t-\tau)q_{\alpha mn}(t,\mathbf{r})q_{\alpha lm}(t-\tau,\mathbf{r})d\tau\,\frac{\partial}{\partial\mathbf{r}}\frac{\mathbf{j}(t,\mathbf{r})\mathbf{s}(t,\mathbf{r})}{T(t,\mathbf{r})}. \tag{28}$$

If no charge current flows through the body, then the second member of sum in the equation (28) is equal to zero, and the first one describes the lattice thermal conductivity with the coefficient

$$W_l = -\frac{1}{3k_BT^2(t,\mathbf{r})}\int\limits_0^\infty \exp\left(\frac{-\tau}{\tau_{nm}}\right)\rho^q_{Pnl}(t-\tau)q_{\alpha mn}(t,\mathbf{r}) \times q_{\alpha lm}(t-\tau,\mathbf{r})d\tau.$$

If there is spin current, then the second member of sum in (28) describes the thermal flux caused by spin-phonon interaction

$$\mathbf{q}_{SP}(t,\mathbf{r}) = -D_PW_1T(t,\mathbf{r})\frac{\partial}{\partial\mathbf{r}}\left\{\mathbf{j}(t,\mathbf{r})\mathbf{s}(t,\mathbf{r})\right\} + D_PW_1\left\{\mathbf{j}(t,\mathbf{r})\mathbf{s}(t,\mathbf{r})\right\}\frac{\partial T(t,\mathbf{r})}{\partial\mathbf{r}}. \tag{29}$$

The first member on the right-hand side of the formula (29) describes SPE — thermal flow created by spin current in absence of the temperature gradient. The same as for Electron Peltier Effect this flux is proportional to the temperature. The second member of sum describes the impact of spin current on thermal conductivity similarly to the Righi&ndash;Leduc effect describing the magnetic field impact on thermal conductivity.

## 4. Dynamics of spin polarization and heat flux

In representation of secondary quantization

$$\hat{h}_{0S}(t,\mathbf{r}) = -\frac{\hbar^2}{2m}\hat{\psi}^+_\sigma(t,\mathbf{r})\Delta\hat{\psi}_\sigma(t,\mathbf{r}),$$

$$\hat{\mathbf{s}}(t,\mathbf{r}) = \hat{\psi}^+_\sigma(t,\mathbf{r})\mathbf{s}_{\sigma\sigma'}\hat{\psi}_{\sigma'}(t,\mathbf{r}). \tag{30}$$

Here $\hat{\psi}_\sigma(t,\mathbf{r})$ — is the field operator of electron, $\sigma$ — is the spin variable, $\mathbf{s}_{\sigma\sigma'}$ — is the spin matrix. Commutation relations for field operators of electrons can be written as $\hat{\psi}_{\sigma'}(t,\mathbf{r}')\hat{\psi}^+_\sigma(t,\mathbf{r}) + \hat{\psi}^+_\sigma(t,\mathbf{r})\hat{\psi}_{\sigma'}(t,\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma\sigma'}$. Other anticommutators are equal to zero. Moreover, $\hat{\psi}^+_{\sigma'}(t,\mathbf{r}')\Delta_\mathbf{r}\hat{\psi}_\sigma(t,\mathbf{r}) = \Delta_\mathbf{r}\left(\hat{\psi}^+_{\sigma'}(t,\mathbf{r}')\hat{\psi}_\sigma(t,\mathbf{r})\right)$. Then, subject to the ratios (19) and (30) $\left[\hat{S}_\alpha(t), \hat{h}_{0S}(t,\mathbf{r})\right] = 0$, the second equation (20) also turns to continuity equation

$$\frac{\partial \hat{s}_\alpha(t,\mathbf{r})}{\partial t} = -\frac{\partial \hat{\upsilon}_{\alpha\beta}(t,\mathbf{r})}{\partial r_\beta}. \tag{31}$$

The components of the operator of the pseudotensor of density of spin current are [39]

$$\hat{\upsilon}_{\alpha\beta}(t,\mathbf{r}) = -\frac{i\hbar}{2m}\left(\hat{\psi}^+_\sigma(t,\mathbf{r})s_{\alpha\sigma\sigma'}\frac{\partial}{\partial r_\beta}\hat{\psi}_{\sigma'}(t,\mathbf{r}) - \frac{\partial}{\partial r_\beta}\hat{\psi}^+_\sigma(t,\mathbf{r})s_{\alpha\sigma\sigma'}\hat{\psi}_{\sigma'}(t,\mathbf{r})\right). \tag{32}$$

The equation of dynamics of the operator of pseudotensor of the spin current density (32) in representation of interaction [40] subject to ratios (19) and (30) is

$$i\hbar\frac{\partial \hat{\upsilon}_{\alpha\beta}(t,\mathbf{r})}{\partial t} = \left[\hat{\upsilon}_{\alpha\beta}(t,\mathbf{r}), \hat{H}_{0S}\right] = \int\limits_V \left[\hat{\upsilon}_{\alpha\beta}(t,\mathbf{r}), \hat{h}_{0S}(t,\mathbf{r}')\right]d^3r' = 0, \tag{33}$$

i.e. in the representation of interaction the operator of pseudotensor of density of spin current is not explicitly dependent on time.

The equations of dynamics of average components of the spin moment density $s_\alpha(t,\mathbf{r}) = \langle\hat{s}_\alpha(t,\mathbf{r})\rangle = \mathrm{Sp}\left(\hat{s}_\alpha(t,\mathbf{r})\hat{\rho}_s\right)$ and tensor of spin current density $\upsilon_{\alpha\beta}(t,\mathbf{r}) = \langle\hat{\upsilon}_{\alpha\beta}(t,\mathbf{r})\rangle = \mathrm{Sp}\left(\hat{\upsilon}_{\alpha\beta}(t,\mathbf{r})\hat{\rho}_s\right)$ subject to equations (31) and (32) are

$$\frac{\partial s_\alpha(t,\mathbf{r})}{\partial t} = \mathrm{Sp}\left(\hat{s}_\alpha(t,\mathbf{r})\frac{d\hat{\rho}_s}{dt}\right) - \frac{\partial \upsilon_{\alpha\beta}(t,\mathbf{r})}{\partial r_\beta},$$
$$\frac{\partial \upsilon_{\alpha\beta}(t,\mathbf{r})}{\partial t} = \mathrm{Sp}\left(\hat{\upsilon}_{\alpha\beta}(\mathbf{r})\frac{d\hat{\rho}_s}{dt}\right), \tag{34}$$

where $\hat{\rho}_s$ — is the density operator of spin subsystem. In the approximation of Markov's relaxation, Neumann equation for the matrix of density of spin subsystem is

$$\frac{d\rho_{Smn}}{dt} = -\frac{\rho_{Smn} - \rho^e_{Smn}}{\tau_{mn}} - \frac{i}{\hbar}\left[\hat{V}_S, \hat{\rho}_S\right]_{mn}, \tag{35}$$

where $\rho^e_{Smn}$ — are the matrix elements of equilibrium density operator of spin subsystem, $\tau_{mn}$ — are the relaxation times.

Let us assume that when calculating the first member of sum on the right-hand side of the equation (35) we can replace the relaxation times with an averaged value $\tau_r$. Then the equations of spin dynamics (34) subject to rearrangement of operators under diagonal sum will be

$$\frac{\partial s_\alpha(t,\mathbf{r})}{\partial t} = -\frac{s_\alpha(t,\mathbf{r}) - s^e_\alpha(t,\mathbf{r})}{\tau_r} - \frac{i}{\hbar} \times \int\limits_V \mathrm{Sp}\left(\hat{\rho}_s\left[\hat{s}_\alpha(t,\mathbf{r}), \hat{u}_s(t,\mathbf{r}')\right]\right)d^3r' - \frac{\partial \upsilon_{\alpha\beta}(t,\mathbf{r})}{\partial r_\beta}, \tag{36}$$

$$\frac{\partial \upsilon_{\alpha\beta}(t,\mathbf{r})}{\partial t} = -\frac{\upsilon_{\alpha\beta}(t,\mathbf{r}) - \upsilon^e_{\alpha\beta}(t,\mathbf{r})}{\tau_r} - \frac{i}{\hbar}\int\limits_V \mathrm{Sp}\left(\hat{\rho}_s\left[\hat{\upsilon}_{\alpha\beta}(t,\mathbf{r}), \hat{u}_s(t,\mathbf{r}')\right]\right)d^3r'. \tag{37}$$

Here,

$$s^e_\alpha(t,\mathbf{r}) = \mathrm{Sp}\left(\hat{s}_\alpha(t,\mathbf{r})\hat{\rho}^e_s\right),\ \upsilon^e_{\alpha\beta}(t,\mathbf{r}) = \mathrm{Sp}\left(\hat{\upsilon}_{\alpha\beta}(t,\mathbf{r})\hat{\rho}^e_s\right)$$

equilibrium components of density of spin moment and pseudotensor of density of spin current, accordingly. In steady-state equilibrium state, in a first approximation we can assume that there is no pure spin current. Within the framework of Dyakonov-Perel model [41] it implies that the effects of spin diffusion and spin-orbit interaction compensate each other, and $\upsilon^e_{\alpha\beta}(t,\mathbf{r}) = -\frac{s^e_\alpha(t,\mathbf{r})j_\beta(t,\mathbf{r})}{en_e(t,\mathbf{r})}$ can be accepted. Here $n_e(t,\mathbf{r}) = \left\langle\hat{\psi}^+_\sigma(t,\mathbf{r})\hat{\psi}_\sigma(t,\mathbf{r})\right\rangle$ — is the concentration of conductivity electrons, whose energy is within the interval of the order $k_BT$ near to Fermi level.

Effective spin Hamiltonian $\hat{V}_S$ in the first equation (17) — is a single-particle operator, its density is derived by a standard method [37]: $\hat{u}_S(t,\mathbf{r}) = (\mathbf{j}\hat{\mathbf{s}}(t,\mathbf{r}))(D_S + D_P h_{0P}(t,\mathbf{r}))$. Let us assume $h_{0P} = c_lT$, where $c_l$ — is a specific volumetric lattice thermal capacity averaged by the temperature interval. By calculating relevant commutators in the equations (36) and (37), we get

$$\frac{\partial s_\alpha(t,\mathbf{r})}{\partial t} = -\frac{s_\alpha(t,\mathbf{r}) - s^e_\alpha(t,\mathbf{r})}{\tau_r} + \frac{\varepsilon_{\alpha\beta\gamma}(D_S + c_lD_PT(t,\mathbf{r}))j_\beta(t,\mathbf{r})s_\gamma(t,\mathbf{r})}{\hbar} - \frac{\partial \upsilon_{\alpha\beta}(t,\mathbf{r})}{\partial r_\beta}, \tag{38}$$

$$\frac{\partial \upsilon_{\alpha\beta}(t,\mathbf{r})}{\partial t} = \frac{s^e_\alpha(t,\mathbf{r})j_\beta(t,\mathbf{r}) - en_e(t,\mathbf{r})\upsilon_{\alpha\beta}(t,\mathbf{r})}{en_e(t,\mathbf{r})\tau_r} + \frac{n_e(t,\mathbf{r})}{4m}\frac{\partial}{\partial r_\beta}\left(\left(D_S + c_lD_PT(t,\mathbf{r})\right)j_\alpha(t,\mathbf{r})\right). \tag{39}$$

By averaging the perturbation (17) by quantum state, we will get that the energy of states, when average spin is oriented parallel or antiparallel to the vector $\mathbf{j}$, is $\pm j(D_S + D_Ph_{0P})/2$, accordingly. Then, at the temperature of $T$:

$$\mathbf{s}^e(t,\mathbf{r}) = \frac{\mathbf{j}(t,\mathbf{r})n_e(t,\mathbf{r})}{2|\mathbf{j}(t,\mathbf{r})|}\mathrm{th}\left(|\mathbf{j}(t,\mathbf{r})|\frac{D_S + D_Pc_lT}{2k_BT}\right). \tag{40}$$

The second member of sum on the right-hand side (38) describes precession of spin moment around the vector of density of charge current. The only distinguished direction is caused by isotropic behavior of polycrystalline model with random orientations of chirality axes of crystallites. There is the second distinguished direction for single-crystal sample — chirality axis, and this member of sum has more complicated structure. If spin polarization is parallel to the current density, then the precession member of sum disappears. If the equilibrium spin polarization (40) can be ignored, then the equation (38) coincides the first equation of Dyakonov-Perel [41]. However, subject to spin-phonon interaction phenomenological relation of spin and electric current is dynamic and is described not by the second equation of Dyakonov-Perel, but the system of equations (38)−(40).

Quasi-steady-state distribution of current density in homogeneous isotropic conductor with the conductivity $\sigma$, constrained by closed surface $\Sigma$, is the solution for internal Neumann problem.

$$\mathbf{j} = -\sigma\frac{\partial\varphi}{\partial\mathbf{r}},\ \Delta\varphi = 0,\ \left.\frac{\partial\varphi}{\partial n}\right|_{\Sigma} = -\frac{j_n(\mathbf{r}\in\Sigma)}{\sigma},\ \oiint\limits_{\Sigma} j\,d\Sigma = 0. \tag{41}$$

The equation (41) has single solution and jointly with the equations (29), (38), (39) and (40) unambiguously defines the dynamics of distribution of spin polarization, spin current and heat flux at specified dynamics of distribution of normal component of current density over the conductor surface.

Let us consider homogeneous semi-space $x \geq 0$, on which homogeneously distributed charge current with the density of $j_x = -j$ is flowing towards axis $x$. Then, in steady-state mode the equation (38) for longitudinal component of density of spin moment of conductivity electrons turns to

$$\frac{ds_x}{dx} + \frac{en_e}{j\tau_r}s_x = \frac{en_e^2}{2j\tau_r}\,\mathrm{th}\left(j\,\frac{D_S + D_P c_l T}{2k_B T}\right). \tag{42}$$

Solution of equation (42) with boundary condition $s_x(0) = 0$ is

$$s_x(x) = \frac{n_e}{2}\mathrm{th}\left(j\,\frac{D_S + D_P c_l T}{2k_B T}\right)\left\{\exp\left(-\frac{en_e}{j\tau_r}x\right) - 1\right\}.$$

Accordingly

$$\frac{\partial}{\partial\mathbf{r}}\left\{\mathbf{j}(\mathbf{r})\mathbf{s}(\mathbf{r})\right\} = -j\,\frac{ds_x}{dx} = \frac{en_e^2}{2\tau_r}\,\mathrm{th}\left(j\,\frac{D_S + D_P c_l T}{2k_B T}\right)$$
$$\times\exp\left(-\frac{en_e}{j\tau_r}x\right).$$

Then, from the equation (29) we get

$$q_x(x) = -D_P W_l T\,\frac{en_e^2}{2\tau_r}\,\mathrm{th}\left(j\,\frac{D_S + D_P c_l T}{2k_B T}\right)\exp\left(-\frac{en_e}{j\tau_r}x\right). \tag{43}$$

According to the equation (43), $|q| \leq en_e^2 D_p W_l T/(2\tau_r)$. Wherein heat flux generated by spin current depends on the temperature, but not on its gradient. It corresponds to the general conclusion [42]. If $D_p c_l T \gg D_s$, then we get that in linear mode with $j \ll j_p = k_B/(D_p c_l)$ at the distance of $x \ll l_p = j\tau_r/(en_e)$ from the conductor surface the thermal flux is proportional to the charge current density

$$q = -\frac{en_e^2 D_p^2 W_l T}{4\tau_r k_B}\,j.$$

## Conclusion

According to the solution (43), if non-polarized charge current flows into a non-magnetic helicoid-chiral polycrystalline conductor with heavy spin-orbit interaction, then the maximum longitudinal spin polarization is reached at the distance of about $l_p$ from the surface. The heat fluxes control by means of spin current described by the equation (29), was experimentally demonstrated in the study [43].

SPE analysis in non-magnetic helicoid-chiral conductors was performed by using the model of ideal Fermi gas for conductivity electrons in metals and representation of their wave function as the Vanier function, approximation of the nearest neighbors in Hamiltonian (5) and the model of isotropic polycrystalline conductor with random orientations of crystallites. The applicability of these models for a specific task should be justified experimentally. Reliable experimental data on the spin Hall effect in metals are currently available. Therefore, the coefficients of the spin Hall effect of 19 non-magnetic metals of the 3th−6th periods were calculated using the described approximations [44]. The results of the calculations are consistent with the experimental ones within the margin of error.

In the metals with a high value of spin-Hall specific conductivity, e.g., in platinum, no crystallographic helicoidity was found. Therefore, the promising and relevant area for spin caloritronics is formation of metallic chiral surfaces on the structural substrates [28]. In the study [45] it was demonstrated that deposition of platinum and copper onto strontium titanate substrate (621) allows producing films completed with low-symmetrical chiral surface with a high Miller index. Such demonstration of homochiral heteroepitaxial growth has shown that deposition of metals onto chiral minerals, such as quartz, even as particles, can be used for production of chiral metals in morphology with a large surface area. The surfaces of produced films have no helicoidal symmetry, but have a distinguished direction laying in the film plane.

Compounds of transition metals with crystalline non-centrally symmetrical structure manifest non-trivial electrical and magnetic properties, a part of which has been discovered for the recent time. The study [24] has shown that CoSi is a non-magnetic semi-metal crystallizing in chiral structure B20, whose space group P$2_1$3 does not contain the inversion center. The study [46] demonstrated that semi-metal CoGe, RhSi and RhGe alloys also have chiral crystalline structure B20. Wherein a high value of spin-Hall specific conductivity and helicoidity of chiral structure are correlated.

It can be expected that the optimum material for achievement of macroscopic coherency of spin currents and their effective interaction with intensive fluxes of heat can be binary conductors with chiral helicoidal structure, whose crystalline lattice belongs to space groups of the symmetry $P6_122$, $P6_222$, $P6_422$, $P6_522$ [30,47], such as, $WAl_2$ [30]. Metal shall be transition one from the 6th period or a lanthanide with heavy spin-orbit interaction. The compound in terms of its magnetic properties must be antiferromagnetic, helimagnetic or ferrimagnetic. So, in the study [48] with the combination of $TaSi_2$ and $NbSi_2$ materials, the length of spin coherency of 60 mm was reached.

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## Conflict of interest

The author declares that he has no conflict of interest.

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