Transverse thermo-magnetic effect in double-periodic semiconductor superlattice at the lack of inversion symmetry

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The surface density of charge current in two-dimensional double-periodic *n*-type semiconductor superlattices is calculated in the one-electron approximation in an external magnetic field in the presence of a temperature gradient. The magnetic field was assumed to be constant, uniform, applied perpendicular to the plane of the electron gas. The joint solution of the Schrödinger equation and the kinetic Boltzmann equation is shown that the dependence of the transverse surface density of the current about temperature and module temperature gradient are significantly non-linear in nature, there are areas with negative differential conductivity. The dependence of the relaxation time on the quasi-momentum of the electron is taken into account in the model phenomenologically through the dispersion law of carrier in magnetic subbands. At the lack of inversion symmetry the dispersion laws of magnetic subbands are not even functions of the quasimomentum defined in magnetic Brillouin zone. As a result, the transverse surface thermo-magnetic current increases in many times in comparison with symmetric case

Keywords: thermo-magnetic effect, two-dimensional doubly periodic semiconductor superlattices.

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1. Introduction

It is known that magnetic field quantizes the transversal motion of the charged particle, while the crystal lattice field leads to formation of energy areas. As a result, the conductivity bands and the valence band of the semiconductors form „ladders" of the Landau levels in the magnetic field. In fact, as it is shown by the results of the first theoretical studies in the middle of the last century [1,2], the Landau levels in the crystals are widened to areas of an exponentially small width. It is caused by removal of degeneracy of the states within the magnetic field in the orbit center due to the interaction of the charged particle with the electrostatic periodic field of the crystal.

The nonparabolicity of the carrier dispersion law in the materials leads to non-trivial behavior of the thermomagnetic [3–6], magnetotransport [7] and magneto-optical [8] effects. Thus, the study [3] has calculated the Nernst-Ettingshausen (NE) coefficient in single-dimensional superlattices with a cosine dispersion law. When scattering the carriers on the polar optical phonons, the NE coefficient has changed its sign in strong magnetic fields oriented within the plane of the superlattice layer. In mercury selenide crystals with the impurities of gallium and ferrum atoms, the transverse NE effect was with changing of its sign, if changing the concentration of the impurity atoms of gallium, which define a degree of ordering of the ferrum atoms in the sample [4]. The study [5] has investigated oscillations of the Nernst coefficient in the gap and gapless graphene with taking into account the dependence of the position of the Landau levels on the value of the electric field. The recent study [6] has made up a quantum kinetic theory of thermoelectric transport within the magnetic field. By taking into account a topological Berry phase of the magnetic subbands, resulting to appearance of an anomalous velocity of the carriers, the authors could calculate the Nernst effect, thereby confirming that the Onsager relations are true within their developed kinetic theory.

Our study is focused on a two-dimensional electron gas within the semiconductor heterojunction with a surface doubly periodic superlattice with a period a, which is placed in the constant uniform perpendicular magnetic field. Fig. 1 shows a typical diagram of such a structure. With the temperature gradient in the heterojunction plane, a thermomagnetic surface current occurs in the direction perpendicular to the magnetic field and ∇T. The present study has used a simple model of the sign-alternating periodic electrostatic potential of the superlattice, which, in our opinion, can reflect fundamental properties of the electron spectrum and features of occurrence of the transverse thermomagnetic current in the studied structures. The effect of occurrence of the Nernst current is not new in itself, but previously, in the literature, it has been neither publicized nor discussed for the studied model structures without the inversion center of the superlattice field.

The superlattices created by the electron lithography are preferred in terms of magnetotransport experiments, first of all, due to a high degree of their periodicity. It is also possible to create the superlattices with a various symmetry of the lattice cell, disrupt the inversion symmetry, building a two-dimensional non-centrosymmetric artificial crystal. When applying the external magnetic field, the laws of dispersion of the charge carriers in the magnetic Bloch subbands already are not even functions of the quasi-

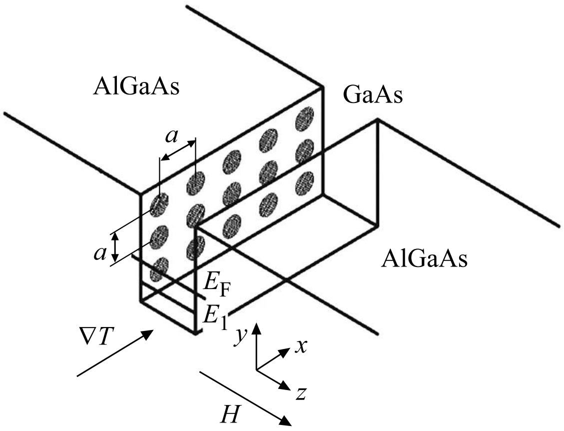

Figure 1. Diagram of the semiconductor heterojunction with a surface superlattice, which is placed in the perpendicular magnetic field **H**.

pulse, which, in our opinion, should be definitely reflected in the progress of the NE effect in the two-dimensional electron gas of such structures. Undoubtedly, it will require development of the available experimental technologies of forming the superlattices of a low periodicity and the magnetotransport measurements. Besides, the experimental samples must be quite clean so that the widening of the magnetic subbands of the electron spectra does not exceed values of energy gaps splitting them.

For actual parameters of semiconductor superlattices [9–11] for the up-to-date experiments and magnetic field strengths of about several tens of thousands of Oersteds, the typical splitting in the carrier spectrum due to the action of the electrostatic field of the superlattice upon the electron turns out to be much less than the typical Landau energy $\hbar\omega_c$. That is why it is possible to perform the simulation calculations of the electron quantum states in a single-level approximation, when it is possible to neglect the impurity of the Landau states in the states of magnetic Bloch subbands of the given level $E_S = \hbar\omega_c(S + 1/2)$ with a specified value of the number S. Besides, as the typical period of the superlattices of several dozens of nanometers exceeds by two orders the scale of natural periodicity of the crystal, it is justified to use an approximation of the isotropic effective mass in the Gamma-point.

2. Theoretical model and the calculation method

Classification of the electron states in the external constant uniform magnetic and doubly periodic electrostatic fields by irreducible design representations of the group of magnetic translations is possible only when the magnetic field is oriented perpendicular to the carrier gas plane [12]. At the same time, it is also necessary that a number of magnetic flux quantums penetrating the crystal lattice cell is a rational number $\Phi/\Phi_0 = eHa^2/2\pi\hbar c = p/q$. As a result, the electron wave function is also an eigen function of the magnetic translation operator and satisfies the generalized Bloch conditions in the magnetic field [13] (the Bloch−Peierls conditions).

The Hamiltonian describing the quantum-mechanical motion of the electron in the systems under consideration takes the form

$$\hat{H} = \hat{H}_0 + V_1(\cos 2\pi x/a + \cos 2\pi y/a)\hat{E} + V_2(\sin 2\pi x/a + \sin 2\pi y/a)\hat{E}, \quad (1)$$

where $V_{1,2}$ — the amplitudes of the model periodic potential of the superlattice ($V_1 = 1\,\text{meV}$, $V_2 = \gamma V_1$), $\hat{H}_0$ — the Hamiltonian of the electron in the constant uniform magnetic field, $\hat{E}$ — a unit operator. It is suggested that the lowest level of dimensional quantization E_1 within the heterojunction is occupied (Fig. 1). The effective mass of the electron m^* in GaAs is taken to be $0.067m_e$, while the superlattice period is $a = 50\,\text{nm}$. With the values $\gamma = 0$, the potential of the superlattice field becomes a centrosymmetric one: $V(\mathbf{r}) = V(-\mathbf{r})$.

The electron wave function in the μ-magnetic subband ($\mu = \overline{1, p}$), which satisfies the generalized boundary Bloch conditions in the magnetic field is represented as a symmetrized linear combination of the basis states of Landau φ_0 of the main level in the constant magnetic field:

$$\Psi^{\mu}_{\mathbf{k}}(x, y) = \sum_{n=1}^{p} C^{\mu}_n(\mathbf{k}) \sum_{l=-\infty}^{+\infty} \exp\big(ik_x a(lq + nq/p) + 2\pi iy(lp + n)/a\big) \exp(ik_y y) \times \varphi_0\big((x - x_0 - lqa - nqa/p)/l_H\big), \quad (2)$$

where l_H — the magnetic length, $x_0 = c\hbar k_y/eH = k_y l_H^2$. The wave functions (2) are a p-dimensional stratification above a two-dimensional torus — the Brillouin magnetic zone (BMZ): $-\pi/qa \le k_x \le \pi/qa$, $-\pi/a \le k_y \le \pi/a$. We have numerically solved the eigenproblem and the eigen functions for the Hamiltonian (1) by unitary basis transformations, which retain a vector norm.

3. Results and discussion

The study has calculated the positions of the magnetic Landau subbands of the zero energy level in the magnetic field in dependence on the quantum number of the magnetic flux through the lattice cell of the superlattice. In the calculations, the amplitudes of the non-centrosymmetric periodic potential of the superlattice are accepted to be $V_1 = 1\,\text{meV}$, $V_2 = \gamma V_1$ at the values $\gamma = 0.0$, 0.1, 0.3. The number of the magnetic subbands coincides with a numerator of the fraction p/q. Fig. 2 show the results of the corresponding calculations for the centrosymmetric potential of the superlattice at $\gamma = 0.0$.

The carrier dispersion law in the lowest magnetic subband of the Landau zero level is shown on Fig. 3 at the flux

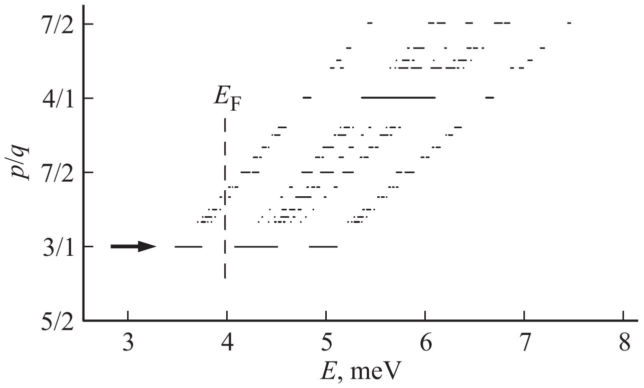

Figure 2. Dependence of the position of the magnetic Bloch subbands related to the main Landau level, on the quantum number of the magnetic flux through the lattice cell in the AlGaAs/GaAs/AlGaAs model structure at the parameters: $V_1 = 1$ meV, $\gamma = 0$, $m^* = 0.067m_0$, $a = 50$ nm.

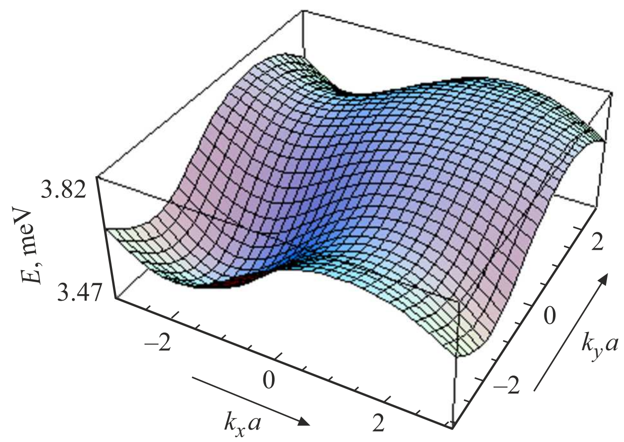

Figure 3. The dispersion law in the lowest magnetic subband related to the main Landau level, at $p/q = 3/1$ in the AlGaAs/GaAs/AlGaAs model structure with the parameters: $V_1 = 1$ meV, $\gamma = 0.1$, $m^* = 0.067m_0$, $a = 50$ nm.

quantum number of $p/q = 3/1$. With the above-said values of the superlattice periods and the above-said quantum number of the magnetic flux, the magnitude of the magnetic field strength vector is $H = 4.97 \cdot 10^4$ Oe. At the same time, the width of the split band structure is much less than the typical Landau energy $\hbar\omega_c = 2\pi\hbar^2 p/m^* a^2 q \approx 8.6$ meV. The Fermi level in the model is located so as to occupy the lowest magnetic Landau subband ($\mu = 1$), and to ensure that the charge carrier concentration is about $n = 1.3 \cdot 10^{11}$ cm^{-2}. Since the model periodic potential of the superlattice has no inversion center at $\gamma = 0.1$, then as per the Kramers theorem, in the magnetic field the subband electron dispersion laws are not even functions of quasi-pulse projections in BMZ.

The calculations of the surface density of the thermomagnetic transverse current (along the y-direction)

$$j_y^\mu = (2e/h^2) \int v_y^\mu f^\mu(\mathbf{k}, \xi) dp_x dp_y \qquad (3)$$

within the lowest magnetic Landau subband ($\mu = 1$) were preceded by a numerical solution of the quasi-classical uniform Boltzmann's kinetic equation in the relaxation approximation ($\tau > 2\pi\hbar/kT$):

$$(|e|\alpha\xi/\hbar) \frac{\partial f^\mu(\mathbf{k}, \xi)}{\partial k_x} = -\big(f^\mu(\mathbf{k}, \xi) - F^\mu(\mathbf{k})\big)/\tau, \qquad (4)$$

where $F^\mu(\mathbf{k}) = f^\mu(\mathbf{k}, 0)$ — the equilibrium function of the Fermi–Dirac distribution, $\xi = (\nabla T)_x$, α — the Seebeck constant (for GaAs $\alpha \cong 3 \cdot 10^{-6}$ $C\Gamma C_V/K$ [14]).

The dependence of the pulse relaxation time on the electron quasi-pulse has been phenomenologically taken into account by us through the law of dispersion of the two-dimensional carriers $\varepsilon(\mathbf{p})$ within the most suitable model of weakly interacting quantum wells, which is developed in the study [15]: $\tau(\mathbf{p}) \sim (kT)^\beta \varepsilon(\mathbf{p})^{\alpha+0.5}$. The transverse current has been calculated by us for electron scattering on the neutral impurities ($\alpha = 0$, $\beta = 0$) and on the longitudinal acoustic phonons creating a deformation potential for the charge carriers (DA-scattering) ($\alpha = -0.5$, $\beta = -1$). It is important to note that a piezoelectric scattering (PA-scattering) existing regardless of the deformation-acoustic scattering is typical for crystals with a zinc blende structure, while the piezopotenial for the electrons in the Gamma-valley is created both by the transverse and longitudinal phonons [16]. At the same time, the pulse relaxation of the charge carriers at the low temperatures is mainly determined, of course, by elastic scattering on the impurity ions and the neutral atoms.

The projection of the electron velocity vector $v_y^\mu(\mathbf{k})$ and its effective mass in the μ-the Landau subband substantially depend on a point in the Brillouin magnetic zone due to the nonparabolicity of the spectrum and the presence of the inversion asymmetry of the superlattice field. Fig. 4, *a* and *b* show the results of the calculations of the y-projection of the surface current density in the studied model structure in dependence on the temperature gradient in cases of the charge carriers scattering on the impurity neutral atoms and the acoustic phonons, respectively. In the simulation calculations, the temperature of the electron gas within the heterojunction with the superlattice is accepted to be $T = 2$ K. At small temperature gradients, the Boltzmann's kinetic equation can be solved analytically [17]. In this case, the non-equilibrium correction for the distribution function is linear by $|\nabla T|$, which is confirmed by the numerical calculation. With increase in the temperature gradient, the initial linear rise of the function $j_y^1(\xi)$ is replaced by its decreasing portion, while the thermomagnetic current density has a maximum. As the temperature gradient is increasing, the distribution function is changing so as to increase the contribution in (3) by the states of the carriers

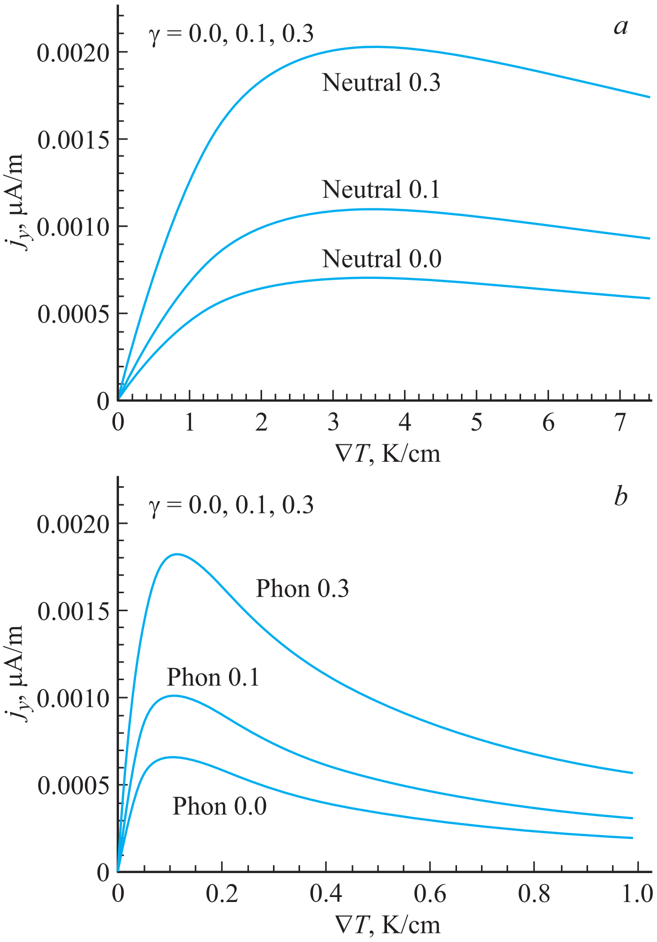

Figure 4. Dependence of the y-projection of the surface density of the thermomagnetic current in the lower magnetic subband ($\mu = 1$) on the temperature gradient at $T = 2$ K at the three values of the asymmetry parameter γ: *a* — the scattering on the neutral atoms of the impurity; *b* — the scattering on the acoustic phonons.

with the positive projection of the velocity in the Landau subband. It results in the increase in the value $j_y^1(\xi)$ up to the maximum one on each of the dependences. With further increase in the magnitude of the temperature gradient, the function of distribution of the carriers to pulses has no pronounced maximum in the BMZ and equally takes into account the contribution to the current by the states of both the positive and negative y-projection of the velocity. There is a section with a negative transverse differential conductivity. In the phonon scattering, it is quite justified to see the shift of the current density maximum towards the lesser temperature gradients. The relaxation time becomes dependent on the gas absolute temperature and the area of the temperature gradients, which corresponds to the portion with the negative different transverse conductivity, is widening (Fig. 4, *b*). The typical width of the current density peak of Fig. 4, *b* becomes smaller in comparison with a case of the impurity scattering only. Thus, in our study, the results of the simulation calculations of the surface density of the transverse thermomagnetic current indicate quite high sensitivity of the NE effect to the carrier scattering mechanism.

With the increase in the γ ratio, the thermomagnetic current increases at the fixed magnitude of the temperature gradient. It is correlated to disruption of the parity of the carrier dispersion law in the magnetic field and, as a consequence, an additional nontrivial contribution to the transverse velocity. With the said γ ratios, there is triple amplification of the Nernst-Ettingshausen effect at the maximum of the thermomagnetic current.

One can qualitatively discuss the contribution to the thermomagnetic current by the effect of spin and spin-orbit splitting in the carrier spectrum. Previously, within the models equivalent to the one examined in this study, we had calculated the quantum states of the electrons in the doubly periodic superlattices in the perpendicular magnetic filed, taking into account the electron spin (see, for example, [7,8]). The spin-orbit (SO) interaction in the electron gas was taken into account both by the Rashba type, and by the Dresselhaus type for the two-dimensional systems. In both the cases, the spin polarization of the carrier quantum states in the Brillouin magnetic zone had a vortex structure in the gas plane. The values of the spin, spin-orbit splittings in the spectrum, as well as of the splitting defined by the action of the periodic electrostatic field of the superlattice on the electron, having the parameters of the present study, are mutually comparable in the magnetic fields of about tens of thousands of Oersteds. Due to the bond of the spin and coordinate degrees of freedom of the electron, its velocity, for example, along the y-direction in some quantum state will be determined by the projection of the spin polarization of this state onto the x-direction (SO-Rashba interaction) and the y-direction (SO-the Dresselhaus interaction). The qualitative evaluations and the preliminary calculations show that it is possible to expect some slight contribution to the thermomagnetic current $j_y^\mu(\xi)$ (determined by the SO-interaction constant) by the projections of the spin polarization of the states in the linear region of the transfer phenomenon in the presence of the spin-orbit interaction in the electron gas. At the same time, the Boltzmann's distribution function is little different from the equilibrium one, and the contribution to the thermomagnetic current is mainly determined a carrier velocity field in the subband. With increase in the magnitude of the temperature gradient, the results of the numerical solution of the problem indicate a significant compensation of the contributions to the current by the carrier states in the Brillouin magnetic zone: the Boltzmann's distribution function almost equally takes into account the states with the v_y^μ projections of the opposite signs. Finally, the density of the thermomagnetic current decreases and, correspondingly, the contributions to the current by the spin polarization of the states becomes negligible against the background of the values of the decreasing function $j_y^\mu(\xi)$.

4. Conclusion

A range of the materials used to theoretically and experimentally study the thermomagnetic effects in the gas of the charge carriers is unusually wide. The doubly periodic semiconductor superlattices belong to a class of the materials, in which the investigation of the carrier transport is interesting not only in terms of the fundamental science, but of applications thereof as well. The present paper has performed the required calculations and specified the areas of the magnetic fields and parameters of the lattice structures, when it is possible to experimentally study the NE effect in such superlattices. The dependences of the current surface density on the temperature gradient, which are calculated within the frame of the model, exhibit a substantially non-linear behavior. There is an effect of negative differential transverse conductivity. It has found the causes of such nonlinearity due to the various contribution to the current by the magnetic Bloch states of the electron in the subband. As a result, the disruption of the parity of the carrier dispersion law in the Landau subband in the magnetic field due to no inversion center of the periodic electrostatic potential of the superlattice field leads to the additional nontrivial contribution to the transverse velocity. With the said γ ratios, there is multiple amplification of the NE effect at the maximum of the transverse thermomagnetic current.

Generally speaking, the time of the relaxation carrier pulse in the systems with an arbitrary dispersion law is an unsolvable problem. In the two-dimensional semiconductor superlattices, in the external perpendicular uniform magnetic field, the dependence of the electron energy on its quasi-pulse in the Brillouin magnetic zone is substantially non-parabolic, while the number of the magnetic Bloch subbands is determined by the number of magnetic flux quantums through the lattice cell of the superlattice. Thus, the magnetic field does not only quantize the transversal motion of the charged carrier, but it is also a control parameter, and the total number of the spectrum magnetic subbands depends on its value. At the same time, it is known that the Nernst-Ettingshausen effect in the semiconductors is present due to the fact that the charge carriers with various pulses are differently scattered in interaction with the impurities and the lattice oscillations. That is why in the context of the usability of results of our study in formulation of the corresponding transport experiments with the electron gas, it is necessary to mention the importance of the results obtained within the model designated in this study as an reference point for studying the scattering mechanisms for the two-dimensional electrons of the doubly periodic superlattices in the magnetic field.

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Conflict of interest

The authors declare that they have no conflict of interest.

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