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Electric-field-induced ferroelectricity of electron gas

G M Shmelev and I I Maglevanny

Volgograd State Pedagogical University, 27 Prospekt Lenina, Volgograd 400013, Russia

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Abstract. Under the action of a high applied electric field, the non-equilibrium electron gas in a lateral superlattice exhibits the properties of a ferroelectric. That it is in principle possible for a transverse electric field to appear spontaneously as a result of a non-equilibrium phase transition is established. A theory of electron ferroelectricity taking into account the interaction of charge carriers with acoustic phonons is constructed.

1. Introduction

The main feature of the new kinetic effect considered in this paper consists in the following. If the sample is open-circuited in the OY-direction and the constant current (j_x) flows in the OX-direction, then, upon lowering the temperature (T), a spontaneous transverse electric field (E_y) appears. It is seen that $E_y \sim \pm\sqrt{T_C - T}$, where the 'Curie temperature' T_C is determined by the value of the applied field $|E_x|$. Under these conditions, second-order non-equilibrium phase transitions (NPTs) occur. If the sample is closed-circuited in series with some finite resistor in the OY-direction, then, upon lowering the temperature, first-order NPTs (accompanied by jumps in the value of E_y) are also possible. This situation is quite similar to that of the appearance of spontaneous polarization in ferroelectrics. Thus, from the phenomenological point of view, the non-equilibrium electron gas represents a peculiar ferroelectric. The necessary condition for the existence of such ferroelectricity is the non-additivity and the boundedness of the electron energy spectrum. Examples of materials in which this effect is possible include the lateral (quasi-two-dimensional) superlattices (SLs) [1, 2].

When one uses a tight-binding approximation, the electron energy spectrum with respect to the principal axes ('1' and '2') of a simple quadratic SL has the form

$$\varepsilon(\boldsymbol{p}) = \Delta - \frac{\Delta}{2}\left(\cos\frac{p_1 a}{\hbar} + \cos\frac{p_2 a}{\hbar}\right) \tag{1}$$

where 2Δ is the allowed miniband width, p_1 and p_2 are the Cartesian components of the carrier crystal momentum ($\boldsymbol{p}$), and a is the lattice constant.

When using a reference frame with coordinate axes which are at an angle (θ) to the principal axes of the SL, the spectrum becomes non-additive: $\varepsilon(\boldsymbol{p}) \neq \varepsilon(p_x) + \varepsilon(p_y)$, i.e. the condition given above holds.

In papers [3–5], applying to the spectrum (1) and $\theta = 45^\circ$, the field E_y as a function of E_x has been calculated, the sample temperature being fixed. Note also the papers [6, 7], in which the influence of a magnetic field on the spontaneous transverse field for $T =$ fixed was investigated. In [3–7], the problems have been solved by using the Boltzmann kinetic

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equation with the τ-approximation, and also the simplest case, that with τ = constant, has been considered. In the present paper, devoted to the calculation of the temperature dependence $E_y = E_y(T)$ in a lateral SL for E_x = fixed, we go beyond the limits of the τ-approximation and consider a non-equilibrium electron gas with spectrum (1) interacting with acoustic phonons at low temperatures $T \ll \hbar\omega_D$ (where ω_D is the Debye phonon frequency, and T is the temperature in energy units) in an arbitrary electric field. We assume that $2\Delta \ll \hbar\omega_D$.

2. Current density in a lateral superlattice

As is known from the theory of small-radius polarons [8], for conductors with narrow electron energy bands the linear (with respect to displacements) interaction of electrons with the acoustic phonons proves to be significantly weakened because of the smallness of the parameter $\Delta/\hbar\omega_D \ll 1$. Under these conditions, the dominant role is taken by the quadratic interaction [9, 10]. For $T \ll \hbar\omega_D$, the probability of electron scattering is small, and the mobility is described by a kinetic equation which, under the condition $T \ll s|\boldsymbol{p}|$ (where s is the sound velocity), leads to the Fokker–Plank equation. For the system considered, this equation has the form [10]

$$\gamma \boldsymbol{E}\frac{\partial f}{\partial \boldsymbol{p}} = \frac{\hbar}{a}\frac{\partial}{\partial \boldsymbol{p}}\left(\frac{1}{T}\boldsymbol{v}f + \frac{\partial f}{\partial \boldsymbol{p}}\right) \tag{2}$$

where $f(\boldsymbol{p})$ is the distribution function, e is the electron charge, $\boldsymbol{v} = \partial\varepsilon/\partial\boldsymbol{p}$ is the electron velocity, and

$$\gamma^{-1} = \frac{(2\pi)^5}{60ae}\hbar\omega_D(q_D a)^8\left(\frac{C_2}{Ms^2}\right)^2\left(\frac{T}{\hbar\omega_D}\right)^9. \tag{3}$$

Here $q_D = \omega_D/s$ is the Debye phonon wave vector, M is the mass of the elementary cell, and C_2 is the deformation potential for the quadratic interaction.

Because of the additivity of spectrum (1), the variables in equation (2) may be separated; thus we find its solution in the form

$$f = g(p_1)g(p_2) \tag{4}$$

where $g(p)$ is the solution of the equation

$$\gamma E\frac{\mathrm{d}g}{\mathrm{d}p} = \frac{\hbar}{a}\frac{\mathrm{d}}{\mathrm{d}p}\left(\frac{1}{T}vg + \frac{\mathrm{d}g}{\mathrm{d}p}\right) \tag{5}$$

with

$$v(p) = \frac{\Delta a}{2\hbar}\sin\frac{pa}{\hbar}. \tag{6}$$

Following [10], we assume that

$$g = \chi(p)\exp\left(\frac{\Delta}{2T}\cos\frac{pa}{\hbar}\right).$$

This substitution leads to an equation for the function χ:

$$\gamma E\chi - \frac{\hbar}{a}\frac{\mathrm{d}\chi}{\mathrm{d}p} = C\exp\left(-\frac{\Delta}{2T}\cos\frac{pa}{\hbar}\right). \tag{7}$$

The periodic solution of (7) may be found in terms of Fourier series. The resulting solution of equation (5) has the form

$$g(p) = A\exp\left(\frac{\Delta}{2T}\cos\frac{pa}{\hbar}\right)\sum_{m=-\infty}^{+\infty}\frac{(-1)^m}{\gamma E - \mathrm{i}m}I_m\left(\frac{\Delta}{2T}\right)\exp\left(\mathrm{i}m\frac{pa}{\hbar}\right). \tag{8}$$

Here $I_m(z)$ is the modified Bessel function, and $A = A(E, T)$ is the normalizing constant which may be found from the condition

$$\sum_{\boldsymbol{p}} f(\boldsymbol{p}) = n \tag{9}$$

where n is the carrier density. Note that as $\boldsymbol{E} \to 0$ the function $f(\boldsymbol{p})$ takes on the form of the equilibrium distribution function

$$f_0(\boldsymbol{p}) = nI_0^{-2}\left(\frac{\Delta}{2T}\right)\exp\left\{\frac{\Delta}{2T}\left(\cos\frac{p_1a}{\hbar} + \cos\frac{p_2a}{\hbar}\right)\right\}. \tag{10}$$

The current density is defined by the expression

$$\boldsymbol{j} = e\sum_{\boldsymbol{p}}\boldsymbol{v}(\boldsymbol{p})f(\boldsymbol{p}). \tag{11}$$

Taking into account (4), the formula for the α-component of the current density ($\alpha = 1, 2$) takes the form [10]

$$\begin{aligned} j_\alpha = j_\alpha(E_\alpha, T) &= \frac{ea}{2\pi\hbar}\int_{-\pi\hbar/a}^{\pi\hbar/a} v(p)g(p)\,\mathrm{d}p \\ &= \frac{enaT}{\hbar}\sum_{m=-\infty}^{+\infty}\frac{(-1)^m\mathrm{i}m}{\gamma E_\alpha - \mathrm{i}m}I_m^2\left(\frac{\Delta}{2T}\right)\Big/\sum_{m=-\infty}^{+\infty}\frac{(-1)^m}{\gamma E_\alpha - \mathrm{i}m}I_m^2\left(\frac{\Delta}{2T}\right). \end{aligned} \tag{12}$$

From (12) it follows in particular that for $E \ll E_0$ and $\Delta \ll T$ the electron mobility $\sim T^{-10}$. This asymptotics has been obtained in [11] by another method.

Let us introduce the reference frame with the coordinate axes OX and OY which are at an angle 45° with the principal axes of the SL. In such a reference frame, the electron energy spectrum becomes non-additive:

$$\varepsilon(\boldsymbol{p}) = \Delta - \Delta\cos\frac{p_xd}{\hbar}\cos\frac{p_yd}{\hbar} \qquad \left(d = \frac{a}{\sqrt{2}}\right). \tag{13}$$

Using the formulae for coordinate transformations affected by the rotation of the coordinate axes, we get the expression for the current density $\boldsymbol{j} = (j_x, j_y)$ in the new reference frame. In the following, we go over to dimensionless variables: $T/\Delta \to T$, $\hbar\boldsymbol{j}/en\,\Delta d \to \boldsymbol{j}$, $\boldsymbol{E}/E_0 \to \boldsymbol{E}$, where

$$E_0 = \frac{(2\pi)^5\sqrt{2}\Delta}{60ae}\left(\frac{C_2}{Ms^2}\right)^2\left(\frac{a\Delta}{\hbar s}\right)^8. \tag{14}$$

Using (12) and the identity

$$I_0^2(z) + 2\sum_{m=1}^{\infty}(-1)^m I_m^2(z) = 1 \tag{15}$$

we finally get

$$j_{\substack{x\\y}} = \frac{T}{2}\left[j_0\left(\frac{E_x + E_y}{T^9}, T\right) \pm j_0\left(\frac{E_x - E_y}{T^9}, T\right)\right]. \tag{16}$$

Here

$$j_0(x,T) = x\left(1 - \frac{1}{\psi(x,T)}\right) \tag{17}$$

and

$$\psi(x,T) = I_0^2\left(\frac{1}{2T}\right) + 2x^2\sum_{m=1}^{\infty}\frac{(-1)^m}{m^2+x^2}I_m^2\left(\frac{1}{2T}\right). \tag{18}$$

3. Non-equilibrium phase transitions

Let the sample be closed-circuited in series with some finite resistor R in the OY-direction. For this electric circuit we have

$$j_{yr} \equiv j_y + rE_y = 0 \tag{19}$$

where

$$r^{-1} = SRen\,\Delta d/(\hbar L E_0). \tag{20}$$

Here L is the sample length in the OY-direction, and S is its cross-sectional area.

For given E_x, T, and r, condition (19) represents an equation for the function $E_y = E_y(E_x, T)$. In addition to the trivial solution ($E_y = 0$), this equation also has non-trivial ones ($E_y \neq 0$).

It is useful to investigate the stability of the transverse field E_y (i.e. of the solutions of equation (19)) with respect to small fluctuations, using the function (the synergetic potential) [3, 4]

$$\Phi(E_x, E_y, T) = \int_0^{E_y} j_{yr}(E_x, E_y', T)\ \mathrm{d}E_y' + \text{constant} \tag{21}$$

by means of which the Kirchhoff condition (19) and the stability condition $\partial j_y/\partial E_y > 0$ (see, e.g., [12]) may be written in the forms

$$\frac{\partial\Phi}{\partial E_y} = 0 \qquad \frac{\partial^2\Phi}{\partial E_y^2} > 0. \tag{22}$$

Thus, the stable solutions of equation (19) for fixed E_x, T correspond to minima of the synergetic potential Φ. Note that $j_x = \partial\Phi/\partial E_x$, $j_{yr} = \partial\Phi/\partial E_y$.

Now we will discuss briefly the meaning of the synergetic potential Φ (independently, Epshtein [13] has come to analogous conclusions). The function Φ, equation (21), is the power density which, as is known [14], is proportional to the velocity of entropy generation (here, at given E_x and T). Thus we have established that the minima of the synergetic potential, i.e. the minima of entropy production (independently of the degree of deviation from equilibrium), correspond to stationary stable states. So, in the present paper, a model demonstrating the feasibility of, in principle, entropy production minima [15] leading to stable stationary states, without any restriction on the degree of deviation from equilibrium, has been established. Note that for the stationary (but unstable) states, the entropy production attains its maximum.

The Curie temperature $T_C = T_C(E_x, r)$ may be found from the condition

$$(j_{yr}/E_y)_{E_y=0} = 0$$

which leads to the following equation:

$$rT_C^8 + \left.\frac{\partial j_0(x,T_C)}{\partial x}\right|_{x=E_x/T_C^9} = 0. \tag{23}$$

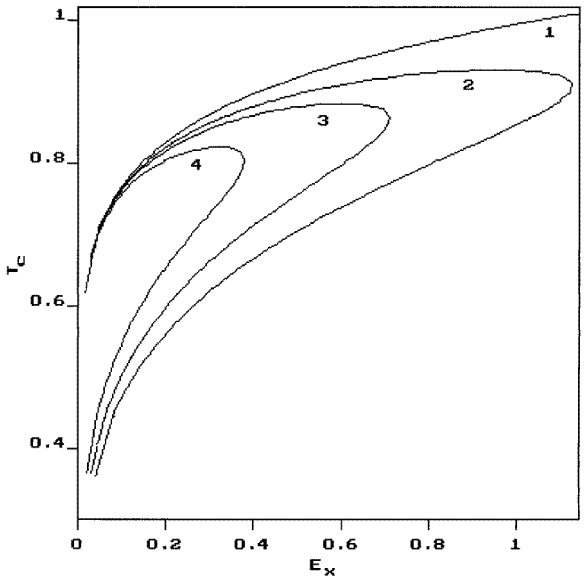

Figure 1. The dependence of the Curie temperature T_C on the applied field E_x. The curves correspond to the following (normalized) values of the parameters: (1) $r = 0$; (2) $r = 0.03$; (3) $r = 0.05$; (4) $r = 0.1$.

The numerical solution of this equation for different values of the parameter r is presented in figure 1. In figure 2 the results of the numerical solution of equation (19) at $|E_x| = 0.6$ and for different values of r are presented.

At $r = 0$ (when the sample is open-circuited in the OY-direction), every value of $|E_x|$ corresponds to just one value of T_C. In this case, the character of the solutions of equation (19) may be clarified at high temperatures $T \gg 1$. Using (16)–(18) and the approximations $I_0^2(0.5T^{-1}) \approx 1 + 1/8T^2$ and $I_1^2(0.5T^{-1}) \approx 1/16T^2$, we get

$$j_y = \frac{T^8}{8} \frac{E_y(T^{18} - E_x^2 + E_y^2)}{(T^{18} + E_x^2 + E_y^2)^2 - 4E_x^2E_y^2}. \tag{24}$$

Then, substituting (24) in (19), we find that, at $r = 0$, the non-trivial solutions have the form

$$E_y = \pm\sqrt{E_x^2 - T^{18}}. \tag{25}$$

Substituting (24) in (21), we find the synergetic potential for the case considered:

$$\Phi(E_x, E_y, T) = \frac{T^8}{32} \ln[(T^{18} + E_x^2 + E_y^2)^2 - 4E_x^2E_y^2] + \text{constant}. \tag{26}$$

From (26) and the conditions (22), it follows that for $E_x^2 > T^{18}$ (T = fixed) or for $T^{18} < E_x^2$ (E_x = fixed) the solutions (25) are stable with respect to small fluctuations of the field, and hence that the solution $E_y = 0$ is unstable. Writing $E_x^2 = T_C^{18}$, we find that $E_y \sim \pm\sqrt{T_C - T}$. This situation is similar to that for ferroelectric second-order NPTs, for which the spontaneous polarization $P \sim \pm\sqrt{T_C - T}$. In our case the quantity $T_C = \sqrt[9]{E_x}$ (E_x = fixed) plays the role of the Curie temperature. Note that the transverse field (25) coincides exactly with the expression for E_y calculated independently by using the Boltzmann kinetic equation with the τ-approximation ($\tau = \tau_0 T^{-9}$) for the collision

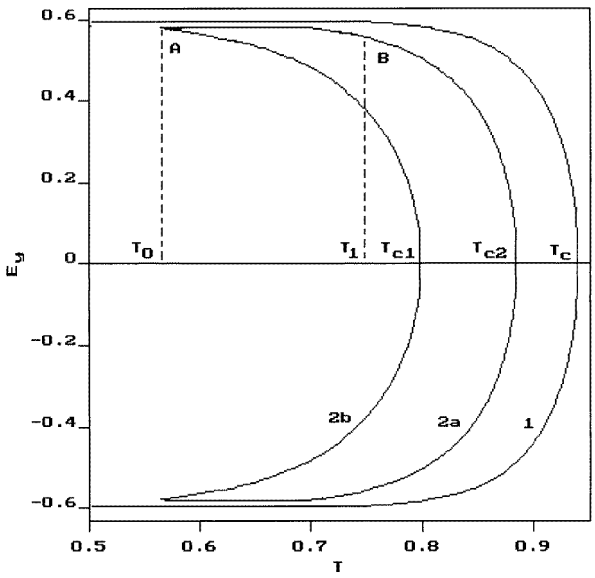

Figure 2. The dependence of the transverse field E_y on the temperature T for $E_x = 0.6$ (normalized). The curves correspond to the following values of the parameters: (1) $r = 0$; (2) $r = 0.05$. The branches 2a and 2b of curve 2 show the stable and unstable states respectively. The dashed lines define the limits of the region of first-order NPTs and near to them. The region from T_0 to T_1 ($T_0 = 0.57$, $T_1 = 0.744$) (B $\Leftrightarrow$ $T_0 = 0.57$, A $\Leftrightarrow$ $T_1 = 0.744$) defines the corresponding values of T, and the region from A to B on the stable branch corresponds to the metastable states of E_y.

integral. Numerical experiments show that formula (25) gives a good approximation for $T > 2$. In the general case, the same experiments, with formulae (16)–(18), confirm the conclusion that a transverse field appears spontaneously of as a result of a second-order NPT. In figure 2, curve 1 illustrates this conclusion for $|E_x| = 0.6$.

For $r \neq 0$, first-order NPTs are also possible. In this case, every admissible value of E_x corresponds to two values of the Curie temperature, T_{C1} and T_{C2} (see figure 1). The numerical analysis shows that a non-zero solution exists in the region $T \in [T_0, T_{C2}]$ ($T_0 < T_{C1}$) and has two branches, one of them being stable and the other being unstable (the analysis of the stability was performed with the help of potential (21)). In the region $T \in [T_0, T_{C1}]$, there is a temperature $T = T_1$ at which the local minima of the potential for two different phases (with $E_y = 0$ and $E_y \neq 0$) are, by conditions (22), equal:

$$\Phi(E_x, E_y, T_1) = \Phi(E_x, 0, T_1). \tag{27}$$

This means that at $T = T_1$, first-order NPTs occur. For $T \in [T_0, T_1]$, the local minimum of the corresponding potential curve for $E_y \neq 0$ is larger then the minimum for $E_y = 0$. Therefore, the interval $[T_0, T_1]$ defines the region of first-order NPTs and their neighbourhood, and the corresponding values $E_y \neq 0$ on the stable branches of the solution of equation (19) define the metastable states.

In figure 2, curve 2 represents the results of the numerical calculation of equation (19) at $|E_x| = 0.6$ and $r = 0.05$. The region $[T_0, T_1]$ defines the temperature values corresponding to metastable states of E_y. For temperatures inside the metastable region, the hysteresis associated with first-order NPTs occurs. For example, the transverse-field behaviour may

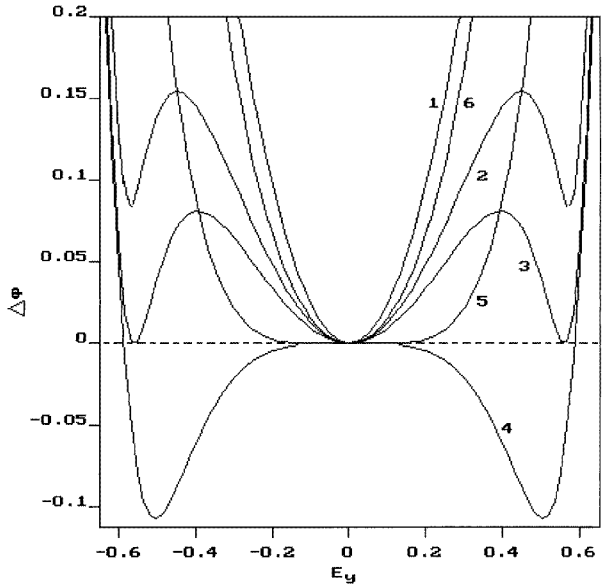

Figure 3. The potential curves $\Delta\Phi = 10^2(\Phi - \Phi|_{E_y=0})$ for $r = 0.05$, $E_x = 0.06$ (normalized). The curves correspond to the following values of the controlling parameter T: (1) $T = T_0 = 0.57$; (2) $T = 0.72$; (3) $T = T_1 = 0.744$; (4) $T = T_{C1} = 0.8$; (5) $T = T_{C2} = 0.8815$; (6) $T = 0.92$. The local maxima and minima correspond to the points of intersection of the $T =$ constant lines with the unstable and stable branches shown in figure 2.

follow the path T_0T_1BA. In terms of the synergetic potential, the situation is illustrated in figure 3.

Let us make an approximate numerical estimate of the value of E_0. For $\Delta = 1$ meV, $a = 10^{-7}$ cm, $s = 5 \times 10^5$ cm s^{-1}, and $(C_2/(Ms^2))^2 \simeq 1$, we get $E_0 \approx 170$ V cm^{-1}. Together with the results presented in the figures, these values indicate that the conclusions of this paper are realistic.

Hence, the results presented reflect a number of typical features of the ferroelectricity of non-equilibrium electron gas.

4. Conclusions

The spontaneous appearance of a transverse EMF is not merely interesting for its own sake. It also has a number of consequences, influencing, for example, the behaviour of galvanomagnetic [16, 17, 6, 7] and optical [18] effects, in high electric fields. Experimental investigation of the effects including the spontaneous transverse field E_y could make a contribution to the physics of NPTs and give useful information about the parameters of appropriate materials to use in electronic devices. In support of this statement, we note the recent paper [19] in which a transverse EMF in lateral superlattices on a substrate of GaAs/Al$_x$Ga$_{1-x}$As with a unidirectional potential modulation has been detected and measured experimentally (the applied field was directed at an angle to the lattice axis). The experiments described in [19] will also stimulate further theoretical analysis of the problem.

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