Parameters of the spin-orbit interaction in a two-dimensional electron gas in surface layers of $Hg_{1-x}Cd_xTe$

V.F. Radantsev

Ural State University, Sverdlovsk (Submitted 10 March 1989; resubmitted 3 July 1989) Zh. Eksp. Teor. Fiz. **96**, 1793–1800 (November 1989)

Periodic (in terms of the reciprocal magnetic field) and close to π jumps in the phase of capacitance magneto-oscillations, observed in surface layers of Hg_{1-x} Cd_x Te, are interpreted using a model of the splitting of the spectrum of two-dimensional electrons by the spin-orbit interaction. The experimental values of the coefficients in front of the Hamiltonian term linear in respect of the quasiwave vector amount to $\alpha \sim 10^{-8} \text{ eV} \cdot \text{cm}$. These values are obtained from beat periods, subband populations, and cyclotron masses. They are more than an order of magnitude larger than the coefficients estimated for materials with quadratic dispersion laws. However, they agree with calculations based on semiclassical quantization in a surface well where the potential is calculated employing the Thomas–Fermi pseudorelativistic method. In the case of values of the band bending found experimentally the theory gives a universal expression for the phenomenological parameter α in narrow-gap semiconductors. This expression does not in fact contain any parameters of the pseudoultrarelativistic nature of the motion of surface electrons in such materials), in full agreement with the absence of significant dependences of the experimental values of α on the width of the band gap ($-0.1 < E_g < 0.1 \text{ eV}$) and of the surface density of electrons.

1.INTRODUCTION

A two-dimensional electron gas in surface channels of semiconductors is subject to an electric field (created by the space charge region and the potential barrier at the interface) directed perpendicular to the plane of two-dimensional motion. This disturbs the inversion symmetry and can modify significantly the energy spectrum because of the spin-orbit interaction (SOI).¹⁻⁷ The problem of the magnitude of the effects which occur in this case is still largely unsolved (and in the opinion of Därr et al.8 there should be no effect at all because of the mutual compensation of the contributions of the space charge region and of the interface barrier), so that the problem should be tackled primarily by experimental investigation. The SOI modifies the spectrum in a magnetic field, so that the SOI parameters can be determined from cyclotron and spin resonance experiments. It was shown in Refs. 2 and 5 that information on the SOI can be obtained using also such traditional (in studies of 2D systems) experimental methods as magneto-oscillation phenomena. This approach was adopted in an analysis of the experimental data in Ref. 9, where changes were observed in the sequence of the Landau levels in p-type channels in Si, manifested by characteristic jumps of the oscillation phase.

The most striking manifestations of the SOI effects can be expected in surface layers of narrow-gap semiconductors. This is related not only to the smallness of the effective masses and the major role of the relativistic effects in such materials, but also to a considerable asymmetry of the surface potential wells (because of the large values of the screening length compared with the dimensions of the interface barrier), which weakens the influence of the mechanism of suppression of the SOI effects discussed in Ref. 8. The phase jumps in 2D systems formed in narrow-gap semiconductors had been observed earlier in magneto-oscillations of the capacitance of surface layers, ^{10,11} but interpretation of

the results in the investigated lightly doped materials was difficult because several 2D subbands were found to be filled at surface carrier densities as low as $n_s \leq 10^{11}$ cm⁻². In this case the results (periodicity of the jumps in respect of the reciprocal magnetic field H^{-1} , the proximity of the periods to the periods of oscillations in excited subbands) can be explained also by a mechanism attributing the oscillation phase jumps to perturbations of the Fermi level in the course of filling of the Landau levels in the mixed (in accordance with its serial number) 2D subband. Investigations of surface layers of a material (InAs) with a wider gap¹² have failed to confirm this explanation (no oscillation phase jumps were observed, although the distribution of carriers between the subbands in InAs was similar to the distribution in $Hg_{1-x}Cd_{x}Te$), so that the nature of the jumps in narrowgap materials has remained unclear. The most rigorous method for solving the problem requires elimination of the influence of the excited subbands, i.e., the 2D system should be investigated at the electrical quantum limit which in the case of narrow-gap semiconductors can be reached in inversion layers formed near the surfaces of heavily doped materials.13

2. MAIN RESULTS

We investigated magneto-oscillations of the capacitance of inversion layers in Hg_{1-x} Cd_x Te with compositions corresponding to the direct (x = 0.22, $N_A - N_D$ = 1.7×10^{17} cm⁻³) and inverted ($x = 0.09, N_A - N_D = 6.0 \times 10^{17}$ cm⁻³) energy band structures. Anodic oxidation of plates of this material (with an oxide thickness ~ 1000 Å) followed by evaporation of gate electrodes of typical area $10^{-3}-10^{-4}$ cm² were used in the fabrication of between five and ten metal-oxide-semiconductor capacitors. Then, a method similar to that described in Ref. 11 was used to determine the capacitance-voltage



FIG. 1. Magneto-oscillations of the capacitance (a) and the fan diagram (b) for inversion layers in $Hg_{0.01}Cd_{0.09}$ Te.

characteristics and capacitance magneto-oscillations. The physical effects in the two investigated samples were nearly identical so that we shall confine our discussion to the sample with the inverted (zero-gap) composition.

Oscillations of the capacitance C(H), reproduced in Fig. 1 for one of the gate voltages V_g , exhibited changes in the phase close to π in the range of values of V_g before and after the start of filling of the first excited subband (the start voltages V_{si} for the *i*th subband are identified by arrows in



FIG. 2. Magneto-oscillations of the capacitance and positions of the oscillation extrema as a function of the reciprocal magnetic field for a sample with $n_s = n_0 = 1.02 \times 10^{12} \text{ cm}^{-2}$. Here, $N = chn_0/2eH_N$ is the oscillation number.



FIG. 3. Dependences of the oscillation numbers $N = (H_N \overline{\Delta})^{-1}$ corresponding to phase jumps on the surface carrier density in the subbands. Arrows are used to identify the start of filling of the next (in respect of the serial number) subbands.

Fig. 1). In the magnetic fields between the phase jumps the oscillations were periodic in H^{-1} and the periods of different intervals were equal within the limits of the experimental error (Fig. 2). The surface carrier densities deduced from the oscillation periods agreed with the density of the charge $Q_s = C_{\rm ox} (V_g - V_{s0})$ induced in the metal-oxide-semiconductor structure ($C_{\rm ox}$ is the specific capacitance of the oxide) on the assumption of a double degeneracy of the Landau levels manifested in the oscillations.

Figure 1 shows also the positions of the oscillation extrema which apply to the ground subband, plotted as a function of the applied magnetic fields for different gate voltages. A network of "Landau levels" can be seen to have a typical form of the fan diagrams if in neighboring sectors differing in respect of the phase (separated by dashed lines in Fig. 1) we plot the opposite extrema (the procedure used in plotting this diagram becomes clear if we compare it with the oscillation curve also shown in Fig. 1). The positions of the phase jumps are periodic in respect of V_g , which is manifested directly in an investigation of the oscillations of dC/dV_g when V_g is varied while keeping the magnetic field fixed. In view of the fan-like nature of the network corresponding to the phase jumps (dashed lines), these jumps are periodic in terms of the magnetic field, as illustrated well by the dependence of the oscillation numbers on H^{-1} plotted in Fig. 2. The results apply equally well to the oscillations in the first excited subband (i = 1). There are no changes in the behavior of the oscillations at the start of filling of the next subband (Fig. 3) and the periods of jumps in terms of H^{-1} in the range $V_g > V_{3i}$ are considerably less than the periods which apply to excited oscillation subbands. This is a consequence of the smallness of the ratios n_{i+1}/n_i of the surface densities to the densities in the next (in respect of the serial number) subbands in the investigated samples characterized by a high charge density in the depletion region.

Since the influence of the excited subbands in the investigated structures can be eliminated, the presence of phase jumps, as well as the periodicity of these jumps in terms of H^{-1} and the multiplicity of the oscillation degeneracy (v = 2) demonstrate that the oscillations are in the nature of beats due to two systems of the Landau levels differing in respect of the periods in terms of the reciprocal magnetic field. We shall show below that the presence of the SOI in the system should give rise to such a spectrum. The theory of Ref. 5, designed for wide-gap semiconductors, cannot be used directly in an analysis of the oscillation effects in narrow-gap materials because of the considerable deviation of the dispersion law from the quadratic form. The nonparabolicity effects in such materials with typical values of the surface band bending are so strong that they cannot be considered simply as corrections. In the two-band approximation within the framework of the k-p effective mass method the equation for the eigenvalues and wave functions of the electron states in narrow-gap semiconductors is formally analogous to the Dirac equation subject to the substitution $c \to s = (E_g/2m_b)^{1/2} \approx 10^8 \text{ cm/s} [E_g = |E(\Gamma_6) - E(\Gamma_8)|,$ m_b is the effective mass at the bottom of the conduction band]. Eliminating from the Dirac equation (in the standard representation) a spinor corresponding to the valence band and diagonalizing the resultant 2×2 -matrix equation, we readily obtain the following dispersion law $E(k_i)$ for the 2D subbands:

$$\left[E-V(z) - \frac{\hbar^2 s^2 k_s^2}{E-V+2m_b s^2} + \frac{\hbar^2 s^2 k_s^2}{E-V+2m_b s^2} + \frac{\hbar^2 s^2 k_s^2}{E-V+2m_b s^2} + \frac{\hbar^2 s^2 k_s dV/dz}{(E-V+2m_b s^2)^2} + i \frac{\hbar^2 s^2 k_s dV/dz}{(E-V+2m_b s^2)^2}\right] \psi^{\pm} = 0, \quad (1)$$

where $k_s = (k_x^2 + k_y^2)^{1/2}$ is the two-dimensional quasiwave vector (with the energies measured from the bottom of the conduction band). In view of the smallness of the contribution of the last two terms in Eq. (1) (at energies of the order of the Fermi energy this contribution is independent of n_i and does not exceed 5–15%), we can consider the SOI as a perturbation of the spectrum described by the first terms.

In the case of the unperturbed problem it follows from Refs. 12–15 that good results can be obtained by an approach based on semiclassical quantization in a surface potential well where the potential V(z) is calculated using the Thomas-Fermi pseudorelativistic method. The dispersion laws for the 2D subbands can then be approximated satisfactorily by the Dirac-type relationships with the effective mass *m* renormalized relative to its bulk value. The SOI can be allowed for, as is done in Ref. 5, by introduction of a term linear in k_i , which leads to the dispersion relationship

$$E_{i} = (\hbar^{2}k_{i}^{2}s^{2} \pm 2m_{i}s^{2}\alpha_{i}k_{i} + m_{i}^{2}s^{4})^{\prime \mu} - m_{i}s^{2}.$$
⁽²⁾

We can find the relationship between the phenomenological parameters of the SOI

$$\alpha_i \approx \hbar^2 \langle eF_i \rangle / s^2 (2m_i)^2 (1 + \mu_i / 2m_i s^2)$$
(3)

(here, $\langle F_i \rangle = \langle e^{-1}dV/dz \rangle$ is the suitably averaged effective field acting on carriers and μ_i is the Fermi energy in the *i*th subband) and the oscillation peak periods in a magnetic field can be found by a simple approach based on an analysis of the populations. The surface density of carriers in two branches of the spectrum (2) differing in respect of the density of states can be written in the following form when $\mu_i \gg kT$:

$$n_i^{\pm} = \frac{1}{2} n_i [1 \mp (2\lambda_i^2 - \lambda_i^4)^{\frac{1}{2}}], \qquad (4)$$

where $n_i = n_i^+ + n_i^- = m_i (\mu_i^* + 2\Delta_i) / \pi \hbar^2$ is the total surface density of carriers in the *i*th subband

$$\lambda_{i} = \left(1 + \frac{\mu_{i}}{2\Delta_{i}}\right)^{-\mu} = \frac{m_{i}\alpha_{i}}{\hbar^{2}(\pi n_{i})^{\mu_{i}}}$$
$$\mu_{i} = \mu_{i} \left(1 + \frac{\mu_{i}}{2m_{i}s^{2}}\right), \quad \Delta_{i} = \frac{m_{i}\alpha_{i}^{2}}{2\hbar^{2}}.$$
(5)

The values of the magnetic fields corresponding to the filling of the N th Landau level (a capacitance minimum) can be found for each of the branches using the condition $n_i^{\pm} = NeH_{iN}^{\pm}/ch$, which together with Eq. (4) gives

$$\frac{1}{H_{iN^{\pm}}} = \frac{2eN}{chn_i} \frac{1}{(1-\lambda_i^2)^2} \{1 \pm [1-(1-\lambda_i^2)^2]^{\frac{1}{2}}\}.$$
 (6)

It follows from the spectrum of the investigated system in a magnetic field that an allowance for the Zeeman splitting leads to the appearance of a factor $1 - \delta^2/N^2$ in front of the second term in the radicand in Eq. (6) (here, $\delta = 1/2 - m_i g_i/4m_0$, g_i is the g factor, and m_0 is the mass of a free electron) and to departure from periodicity. However, in the case of the investigated materials we have $g_i \sim m_0/m_i$ and $\delta \sim 0.25$, so that in an analysis of the experimental results which are normally characterized by N > 5 we can omit the term containing δ/N .

According to Eq. (6), the oscillations are periodic in H^{-1} and the periods differ for the different branches:

$$\Delta_i^{\pm} = (H_N^{\pm})^{-1} - (H_{N+1}^{\pm})^{-1},$$

so that we can expect beats in the case of a sufficiently strong broadening of the Landau levels when the singularities in the density of states are nearly sinusoidal.¹⁶ The beat periods

$$\Delta_{bi} = \Delta_i^+ \Delta_i^- / (\Delta_i^+ - \Delta_i^-),$$

are related—as demonstrated by Eq. (6)—to the parameters λi by

$$\begin{split} \bar{\Delta}_{i} / \Delta_{bi} &= 2 \left(2 \lambda_{i}^{2} - \lambda_{i}^{4} \right)^{\nu_{h}} \approx 2^{\nu_{h}} \lambda_{i}, \\ \bar{\Delta}_{i} &= 2 \Delta_{i}^{-} \Delta_{i}^{+} / \left(\Delta_{i}^{+} + \Delta_{i}^{-} \right) = 2e/chn_{i} \end{split}$$

$$(7)$$

(here, $\overline{\Delta}_i$ is the main period), which together with the first equation in the system (5) gives the required relationship between Δ_{bi} and the SOI parameters α_i .

These parameters α_i were determined using Eq. (7) and the experimental values of $\overline{\Delta}_{bi}$, $\overline{\Delta}_i$, n_i , and m_i (the effective "rest masses" in the subbands m_i were determined from the cyclotron masses $m_{ci}^2 = m_i^2 + 2\pi n_i \hbar^2/s^2$ deduced from the temperature dependences of the oscillation amplitudes); the parameters α_i are plotted in Fig. 4 as functions of n_i for the first two subbands.

From the viewpoint of the mechanisms responsible for the singularities in the spectrum of a 2D system associated with the SOI in narrow-gap semiconductors, considerable



FIG. 4. Plots of $\alpha_i(n_i)$ obtained for the first two subbands.

interest attaches not only to the carrier-density dependence of α_i , but also to the dependence of these parameters on the laws of dispersion of such semiconductors. Information on this topic can be obtained from an analysis of the magnetooscillations of the capacitance of lightly doped $Hg_{1-x} Cd_x$ Te samples of different compositions, partly reported in Refs. 10 and 11. Interpretation of the results¹⁾ on the jumps of the oscillation phases^{10,11} on the basis of the mechanism proposed here gives the values of α_i which, within the limits of the experimental error, are independent of n_i and in the interval $E_g = -100$ to 100 meV are independent of the band gap, and amount to $\alpha_0 = 1.1 \pm 0.2$, $\alpha_1 = 0.65 \pm 0.2$, $\alpha_2 = 0.55 \pm 0.1$ (in units of $10^{-8} \text{ eV} \cdot \text{cm}$) for the first three subbands.

3. DISCUSSION

The reported experimental values of α_i are more than one order of magnitude greater than the available estimates for wide-gap semiconductors,^{5,9} which is not unexpected because of the smallness of m_i in the investigated narrow-gap materials. Worth noting is the absence of significant changes in α_i on increase in the carrier density in the subbands. In the case of materials with a quadratic dispersion law such behavior can be used as an argument in support of the dominant contribution in the region of the surface barrier to α_i (Ref. 5). In the case of narrow-gap semiconductors the experimental observation of the constancy of α_i leads to the opposite conclusion. In fact, in the investigated range of n_i the effective masses m_i increase by almost one order of magnitude and the constancy of α_i represents—in accordance with Eq. (3)—simply a similar increase of the effective field acting on carriers in an inversion layer. In view of the fact that the field at the barrier interface cannot change significantly as a result of a change in n_i , the main contribution to α_i clearly comes from the field created by the space charge region in the semiconductor and the intensity of this field is proportional to the charge en, induced in the inversion layer.

Since the potential in the surface layer of a semiconductor and, consequently, the effective field $\langle F_i \rangle$ in Eq. (3) can be calculated (like the effective masses) for the materials under consideration, it should be possible to estimate theoretically also the values of α_i . These estimates are obtained particularly simply in the case when it is possible to ignore the influence of the charge eN_{dep} in the depletion layer (this can be done in the case of lightly doped samples and sufficiently high surface carrier densities $n_s > N_{dep}$). Under these conditions even a moderate surface band bending $\mu_s > m_b s^2$ makes it possible to use the pseudoultrarelativistic approximation¹³ according to which the surface chemical potential $\mu(z)$, Fermi energies μ_i , the Fermi quasimomentum p_{Fi} , and the semiclassical effective masses m_i are described by the following simple analytic approximations^{13,17}:

$$\mu(z) = \frac{\mu_s}{1 + z/z_s}, \quad \mu_i = c_i' \mu_s, \quad p_{Fi} s = c_i \mu_s, \quad (8)$$

$$m_{i} = \frac{\mu_{i}}{2s^{2}} \left[\left(\frac{c_{i}}{c_{i}'} \right)^{2} - 1 \right] = \frac{\hbar}{2s} \left(2\pi n_{i} \right)^{\frac{\mu_{i}}{2}} \left(\frac{c_{i}}{c_{i}'} - \frac{c_{i}'}{c_{i}} \right), \quad (9)$$

where

 $z_s=2\pi s\hbar/\mu_s\beta, \quad \beta=(8\pi\alpha/3)^{\nu_s}, \quad \alpha=e^2/sh\chi,$

 α is a modified fine-structure constant, χ is the permittivity, and the coefficients c_i and c'_i are described by the transcendental equations (5) and (6) in Ref. 13: if $\beta = 1$, then

$$c_0 = 0.55, c_1 = 0.32, c_2 = 0.19, c_{i>2} \approx 2 \exp \left[-(4i+11)/8\right];$$

 $c_0' = 0.36; c_1' = 0.19, c_2' = 0.1, c_{i>2} \approx c_i/2.$

The effective field $\langle E_i \rangle$ can be determined as the average from semiclassical wave functions, but calculations demonstrate that a satisfactory approximation for $\langle F_i \rangle$ is provided by the value of the field at $z = z_i/2$ (z_i is the classical turning point). The first two equations give

$$\langle F_i \rangle = F_i(z_i/2) = F(0) \left[\frac{2c_i'}{(1+c_i')} \right]^2$$

and if we express the field on the surface $F(0) = 4\pi e N_s / \chi$ in terms of the surface carrier density $n_i = 3N_s \beta c_i^2/2$ (Ref. 13), we finally obtain

$$\langle F_i \rangle = \frac{32\pi e n_i}{3\chi\beta} \left(\frac{c_i'}{c_i} \right)^2 \frac{1}{(1+c_i')^2}.$$
 (10)

It follows from Eqs. (9) and (10) that both m_i^2 and $\langle F_i \rangle$ are porportional to n_i and the densities n_i disappear from the final expression for α_i [the factor $1 + \mu_i/2m_i s^2$ is given by Eq. (9) and is independent of n_i], which gives the following universal expression

$$\alpha_{i} = a_{i}\beta s\hbar, \quad a_{i} = \frac{2}{\pi} \left(\frac{c_{i}}{c_{i}'}\right)^{3} (1 + c_{i}')^{-2} \left(\frac{c_{i}}{c_{i}'} - \frac{c_{i}'}{c_{i}}\right)^{-1}, \quad (11)$$

which in fact contains neither the parameters of the space charge region nor the parameters of the investigated semiconductor ($\beta \approx 1$ and $s \approx 10^8$ cm/s and the coefficients c_i and c'_i governed by them are practically the same for the whole class of the Kane semiconductors¹³), which—in the final analysis—is a consequence of the near-ultrarelativisitic nature of the motion of electrons in quantum wells present near surfaces of narrow-gap semiconductors.

In the case of heavily doped materials characterized by $|N_A - N_D| \sim 10^{17} \cdot 10^{18}$ cm⁻³ the analytic approximations represented by Eqs. (9) and (10) suffer from serious errors already in the range $n_i > 2 \times 10^{12}$ cm⁻², so that we have to carry out numerical calculations but these show that in the range of surface carrier densities $n_i > (2-4) \times 10^{11}$ cm⁻² (important in experiments) the ratios $\langle F_i \rangle / m_i^2$ and, consequently, the values of α_i do not differ greatly from the predictions of the ultrarelativistic approximation. Although the quantitative agreement cannot be taken too seriously because of the approximations adopted in the calculations, the qualitative agreement of the characteristic features of the behavior of α_i with the experimental results (such as the constancy of α_i when n_i and E_g are varied, or a reduction in α_i on increase in the subband number) can hardly be accidental and provides a serious argument in support of the dominant contribution of the space-charge region of a semiconductor to α_i in two-dimensional systems of carriers in narrow- and zero-gap semiconductors. The difference between the above results and the available data for Si is again not unexpected because of the much smaller thickness of the surface channels in Si and the consequently greater role of the surface barrier.

The SOI is clearly an important factor in the effects associated with the magnetic quantization of the energy spectrum of two-dimensional systems of carriers in narrowand zero-gap semiconductors. In materials of this kind the spin splitting is close to half the cyclotron value and in the absence of the SOI the density-of-states maxima of one spin branch correspond to the minima of the other branch. If the density-of-states singularities are nearly sinusoidal and the same for both branches, this phase shift by π results in compression of such singularities. Therefore, in the absence of the spin splitting of the spectrum in H = 0, we can expect the oscillation effects in a magnetic field to appear in the case of these materials solely because of the difference between the broadening of the levels belonging to different branches (this is precisely the behavior of the spin-split components of the oscillations that was reported in Ref. 11 for low numbers of the Landau levels in the range $N \leq 2$ in lightly doped $Hg_{1-x}Cd_{x}Te$) or deviations of the broadening from sinusoidal.

The parameter α introduced in Ref. 5 is most suitable as the characteristic of the spin-orbit splitting of the spectrum because the energy parameter Δ [see the third equation in the system (5)] depends on n_i in the case of a nonquadratic dispersion law, i.e., it is not universal.

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¹⁾ In the case of the samples investigated by Deryabina *et al.*¹⁰ and Radantsev *et al.*¹¹ the beats in the ground subband were manifested by an anomalous behavior of the oscillation amplitudes without clear changes in their phase. When measurements were repeated on metal-oxide-semiconductor structures made of samples 5 and 9 (see Table I in Ref. 11) with smaller areas of the field electrodes ($S = 10^{-4}$ cm²), we were able