Spin splitting and weak localization in (110) GaAs/Al_xGa_{1-x}As quantum wells

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We investigate both theoretically and experimentally the spin-orbit effects on the weak localization in a (110) GaAs two-dimensional electron gas. We analyze the role of two different terms in the spin splitting of the conduction band: the Dresselhaus terms, which arise due to the lack of inversion center in the bulk GaAs, and the Rashba terms, which are caused by the asymmetry of the quantum well. It is shown that in A_3B_5 quantum wells the magnetoresistance due to the weak localization depends qualitatively on the orientation of the well. In particular, it is demonstrated that the (110) geometry has a distinctive feature that in the absence of the Rashba terms the "antilocalization" effect, i.e., the positive magnetoresistance, does not exist. Calculation of the weak antilocalization magnetoresistance is found to be in excellent agreement with experiments. [S0163-1829(97)10316-2]

I. INTRODUCTION

The effect of the negative magnetoresistance observed in high-density 2d electron gas in semiconductor quantum wells is known to be caused by the weak localization, which results from the constructive interference of two electron waves propagating along a closed path in opposite directions, and leads to suppression of the conductivity. In a magnetic field the interference conditions are violated, which causes the effect of the *negative magnetoresistance*.¹

It was shown in Ref. 2 that triplet states with a total momentum of both electron wave functions J=1 make a positive contribution into the resistance, while the singlet state with J=0 makes a negative contribution (antilocalization). Then the interference conditions can also be changed by the spin relaxation, which, depending on the relaxation mechanism, can suppress the contribution of either triplet or (mainly) singlet states.^{2,3} In the noncentrosymmetric semiconductors and semiconductor structures, the dominant spin relaxation mechanism is the Dyakonov-Perel mechanism, which is caused by the spin splitting of the conduction band.^{4,5} If this splitting is not very small, in weak magnetic fields the antilocalization effect prevails, and the resistance increases with the magnetic field B. Therefore, the nature and strength of the spin relaxation determines not just the magnitude of the negative magnetoresistance effect, but even the qualitative behavior of the magnetoconductivity $\sigma(B)$. Furthermore, it was recently shown⁶⁻⁸ that if the conductionband spin splitting is linear in the wave vector, which is always the case in 2d structures, the theory of weak localization must take into account the correlation between the electron motion in coordinate and spin spaces. The effects of the spin relaxation on the magnetoresistance were recently investigated experimentally by Knap et al.⁸ and by Pedersen, Hassenkam, and Lindelof,⁹ and a very good agreement was obtained with the theory for the (100)-oriented GaAs quantum wells. In this paper we report on a study of magnetoresistance in (110)-oriented quantum wells, and present the theory of the weak localization for this particular case.

II. THEORY

In asymmetric A_3B_5 quantum wells the spin splitting of the conduction band has two terms. The first, Dresselhaus term,¹⁰ arises from the asymmetry of the crystal itself, and in the bulk crystal is described by Hamiltonian

$$\mathcal{H}_1 = \gamma \sum \sigma_i k_i (k_{i+1}^2 - k_{i+2}^2), \qquad (1)$$

where $i=x, y, z, i+3 \rightarrow i$; γ is the spin-orbit coefficient for the bulk semiconductor; σ_i are the Pauli matrices; and \vec{k} is the electron wave vector (in this paper we take $\hbar = 1$ everywhere except in final formulas). We take the coordinate system $z \| 110, x \| 1\overline{10}$, and $y \| 001$. In a (110) quantum well, k_z is quantized: $\langle k_z \rangle = 0$ and $\langle k_z^2 \rangle = \int |\nabla \psi|^2 dz$, where $\psi(z)$ is the electron wave function in the well. Consequently, Hamiltonian (1) becomes

$$\mathcal{H}_{1} = -\gamma \sigma_{z} k_{x} [\frac{1}{2} \langle k_{z}^{2} \rangle - \frac{1}{2} (k_{x}^{2} - 2k_{y}^{2})].$$
(2)

It is convenient to write this Hamiltonian as a sum of harmonics $^{6\!-\!8}$

$$\mathcal{H}_1 = \sigma_z(\Omega_{1z} + \Omega_{3z}), \tag{3}$$

where

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$$\Omega_{1z} = \Omega_1 \cos\phi, \quad \Omega_{3z} = \Omega_3 \cos 3\phi, \tag{4}$$

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$$\Omega_1 = -\frac{1}{2} \gamma k (\langle k_z^2 \rangle - \frac{1}{4} k^2), \quad \Omega_3 = \frac{3}{8} \gamma k^3,$$
$$k^2 = k_x^2 + k_y^2, \quad \tan \phi = \frac{k_y}{k_x}.$$

The other term in the conduction-band spin splitting, the Rashba term, is caused by the asymmetry of the quantum well.¹¹ Its Hamiltonian *does not depend on the orientation of the quantum well*,

$$\mathcal{H}_2 = (\vec{\sigma} \cdot \vec{\Omega}_2), \tag{5}$$

where $\Omega_{2_x} = \Omega_2 \sin\phi$, $\Omega_{2_y} = -\Omega_2 \cos\phi$, $\Omega_2 = \alpha k$. In a uniform electric field \mathcal{E} (triangular well) $\alpha = \alpha_0 e \mathcal{E}$; the coefficient α_0 may depend on the properties of the heterointerface.

Using the formalism similar to that of Refs. 6–8, one can show that the correction to the conductivity σ caused by the weak localization is determined by the zero harmonic of the Cooperon $\mathbb{C}_{0}(\vec{q})$, which obeys the equation

$$\mathcal{H}C_0 = \frac{1}{2\pi\nu_0\tau_0^2},$$
 (6)

where ν_0 is the density of states at the Fermi level, τ_0 is the elastic lifetime, and v is the Fermi velocity. In the basis of the eigenfunctions ϕ_0 (antisymmetric singlet state) and ϕ_l^m , with l=1 and m=-1,0,1 (symmetric triplet state) the operator \mathcal{H} consists of two blocks; \mathcal{H}_0 for the singlet states, and $\tilde{\mathcal{H}}$ for the triplet states:

$$\mathcal{H}_{0} = D(q_{x}^{2} + q_{y}^{2}) + \frac{1}{\tau_{\varphi}},$$

$$\widetilde{\mathcal{H}} = D(q_{x}^{2} + q_{y}^{2}) + \frac{1}{\tau_{\varphi}}$$

$$+ 2 \Big[2\Omega_{2}^{2} + J_{z}^{2} \Big(\Omega_{1}^{2} - \Omega_{2}^{2} + \Omega_{3}^{2} \frac{\tau_{3}}{\tau_{1}} \Big) - 2J_{y}J_{z}\Omega_{1}\Omega_{2} \Big] \tau_{1}$$

$$+ 2v \tau_{1} \Big[q_{x}(\Omega_{1}J_{z} - \Omega_{2}J_{y}) + q_{y}\Omega_{2}J_{x} \Big].$$
(7)

Here J_i are the matrices of the angular momentum operator with total momentum J=1; τ_{φ} is the phase-breaking time; $D=v^2\tau_1/2$ is the diffusion coefficient; τ_n , n=1,3, is the relaxation time of the respective component of the distribution function.

In a magnetic field $B||_z$ the wave vector **q** becomes an operator with the commutation relations

$$[q_+q_-] = \frac{\delta}{D}, \quad \delta = \frac{4eBD}{\hbar c}, \tag{8}$$

where $q_{\pm} = q_x \pm i q_y$. This allows us to introduce creation and annihilation operators a^{\dagger} and a, respectively, for which $[aa^{\dagger}] = 1$:

$$D^{1/2}q_{+} = \delta^{1/2}a, \quad D^{1/2}q_{-} = \delta^{1/2}a^{\dagger}, \quad Dq^{2} = \delta\{aa^{\dagger}\}.$$
 (9)

The weak localization correction to the conductivity in a magnetic field can now be written as

$$\Delta \sigma = -\frac{e^2 \delta}{4 \pi^2 \hbar} \sum_{n=0}^{n_{\text{max}}} \left(-\frac{1}{\mathcal{E}_{0n}} + \sum_{m=-1}^{1} \frac{1}{E_{mn}} \right), \quad (10)$$

where $n_{\text{max}} = 1/\delta \tau_1$. The eigenvalues \mathcal{E}_{0n} of \mathcal{H}_0 are given by the following equation:

$$\mathcal{E}_{0n} = \delta \left(n + \frac{1}{2} \right) + \frac{1}{\tau_{\varphi}}.$$
 (11)

The expression for the operator $\widetilde{\mathcal{H}}$, of which E_{mn} are the eigenvalues, follows from Eqs. (7) and (9),

$$\begin{aligned} \widetilde{\mathcal{H}} &= \delta \{ a a^{\dagger} \} + \frac{1}{\tau_{\varphi}} + 2 (\Omega_{1}^{2} \tau_{1} + \Omega_{3}^{2} \tau_{3}) J_{z}^{2} + 2 (2 - J_{z}^{2}) \Omega_{2}^{2} \tau_{1} \\ &- 4 \Omega_{1} \Omega_{2} \tau_{1} J_{y} J_{z} + 2 (\delta \tau_{1})^{1/2} \bigg[\frac{1}{\sqrt{2}} \Omega_{1} J_{z} (a^{\dagger} + a) \\ &+ i \Omega_{2} (a^{\dagger} J_{+} - a J_{-}) \bigg], \end{aligned}$$

$$(12)$$

where $J_{\pm} = (J_x \pm i J_y) / \sqrt{2}$.

If we keep only the Dresselhaus terms in Eq. (7), i.e., put $\Omega_2=0$, the matrix $\tilde{\mathcal{H}}$ becomes diagonal in the basis of the eigenfunctions of J_z , and its nonzero matrix elements for arbitrary n and m=-1,0,1 can be written as

$$\widetilde{\mathcal{H}}_{mm} = D[q_y^2 + (q_x + q_m)^2] + 2\Omega_3^2 \tau_3 m^2 + \frac{1}{\tau_{\varphi}}, \quad (13)$$

where $q_m = (2\Omega_1/v)m$. Since the shift by q_m does not change the commutation relations (8) for the operators q_y and $q'_x \equiv q_x + q_m$, the energies E_{mn} depend only on the cubic Dresselhaus term

$$E_{mn} = \delta(n + \frac{1}{2}) + 2\Omega_3^2 \tau_3 m^2 + \frac{1}{\tau_{\varphi}}, \qquad (14)$$

while the spin relaxation rate is determined by the sum of all terms: $\tau_s^{-1} = 2(\Omega_1^2 \tau_1 + \Omega_3^2 \tau_3)$. One can see from Eqs. (10), (11), and (14) that the term with m = 0 cancels the contribution of \mathcal{E}_{0n} in the conductivity, and, therefore, the magneto-conductivity $\Delta \sigma(B)$ is given by the expression²

$$\Delta\sigma(B) - \Delta\sigma(0) = \frac{e^2}{2\pi^2\hbar} \left\{ \Psi\left(\frac{1}{2} + \frac{H_{\varphi}}{B} + \frac{H_{\rm SO}^{(3)}}{B}\right) - \ln\frac{H_{\varphi}}{B} \right\},\tag{15}$$

where

$$H_{\varphi} = \frac{c\hbar}{4eD\tau_{\varphi}}, \quad H_{\rm SO}^{(3)} = \frac{c\hbar}{4eD} 2\Omega_3^2 \tau_3. \tag{16}$$

Therefore, in absence of the Rashba terms in a (110) quantum well the positive magnetoresistance cannot be observed.

When both Dresselhaus and Rashba terms are present, the eigenvalues of $\tilde{\mathcal{H}}$ can be found only numerically. In practice it is more convenient to compute directly the sum of the inverse eigenvalues, using the expression^{8,12}

$$\sum_{n} \sum_{m=-1}^{1} \frac{1}{E_{nm}} = \sum_{i} \frac{|D_{ii}|}{|D|}, \qquad (17)$$

where |D| is the determinant of the matrix \mathcal{H} , and $|D_{ii}|$ is the minor of its diagonal element *i*,*i*. The detailed description of the numerical procedure will be published elsewhere.

III. EXPERIMENT

The samples used in our work were grown by the molecular-beam-epitaxy technique. The layer sequence was of the standard high-mobility transistor type. The 2*d* electron gas was formed in GaAs at the (110) GaAs/Ga_{0.7} Al_{0.3} As interface. The sample was δ doped with silicon in two planes at 10 and 50 nm from the interface. The individual samples were mesa etched into rectangular Hall bars with the width of 0.2 mm, and the total length of 4.2 mm. Three voltage contacts on each side were placed at a distance of 0.8 mm to avoid perturbing significantly the four-point measurements. Ohmic contacts to the two-dimensional electron gas was made by an annealed Au_xGe_{1-x}NiAu composite film in 0.6×0.6 -mm² contact areas. The contacted areas were subsequently bonded to the legs of a nonmagnetic chip carrier.

Our four-point measurements of the resistivity were carried out by standard low-frequency lock-in technique. Typically the sample resistance was few $k\Omega$, and with an ac current amplitude below 200 nA we have avoided significant Joule heating of the sample at our lowest temperature, 0.3 K.

To generate low stable magnetic fields, we used two highly stable current sources (Keithley 220); the first was used to outcompensate the magnetic flux trapped in the superconducting magnet, whereas the second was used for the magnetic-field sweep around the zero value. The peak in the weak-localization resistivity (or, for antilocalization, conductance) defines the zero value. Incidentally, this method is accurate enough to determine this zero point within about 1 μT .¹³

IV. RESULTS AND DISCUSSION

In Fig. 1 we show the results of the magnetoconductivity measurements for a sample with electron density $n=5\times10^{11}$ cm⁻² and mobility $\mu=7\times10^4$ cm²/V s at T=0.36 K. Also shown are the best fits as obtained from our theory, and from the theory of Hikami, Larkin, and Nagaoka (HLN),² which assumes that all terms of the spin splitting make additive contributions to the magnetoconductivity. The fitting was done by weighted explicit orthogonal distance regression using the software package ODRPACK.¹⁴ The weights were selected to increase the importance of the low-field ($B \le 3$ Gs) part of the magnetoconductivity curve. Only the experimental points at $|B| \le H_{tr} = c\hbar/4eD\tau_1 = 4.5$ Gs we used for fitting, since the above theories use the diffusion approximation, and, therefore, are only valid for *B* small compared to H_{tr} .

The parameters of our theory are τ_{φ} and Ω_i , i = 1,2,3. It is convenient to convert them into characteristic magnetic fields H_{φ} , $H_{SO}^{(3)}$ [see Eq. (16)], and $H_{SO}^{(1,2)}$:

$$H_{\rm SO}^{(1)} = \frac{c\hbar}{4eD} 2\Omega_1^2 \tau_1, \quad H_{\rm SO}^{(2)} = \frac{c\hbar}{4eD} 2\Omega_2^2 \tau_1.$$
(18)

The parameters of the best fit are $H_{\varphi} = 0.02$ Gs, $H_{SO}^{(1)} = 0.12$ Gs, $H_{SO}^{(2)} = 1.3$ Gs, and $H_{SO}^{(3)} = 0.04$ Gs for



FIG. 1. Magnetoconductivity $\Delta \sigma(B) - \Delta \sigma(0)$ in a (110) quantum well. Experimental results are shown by the solid line, the theoretical best fit by the dashed line. The dots show the best fit by the Hikami-Larkin-Nagaoka theory. Sample characteristics and parameters of the theory are given in the text. The vertical lines show the interval $|B| \leq H_{tr} = 4.5$ Gs.

our theory, and $H_{\varphi}=0.014$ Gs and $H_{SO}=0.33$ Gs for the HLN theory. One can clearly see that the HLN theory is unable to describe the experimental data. The disagreement between the experiment and the HLN theory in our case is much more severe than for (001) quantum wells,^{7,8} since the effects of the correlations between the electron motion in coordinate and spin spaces is much stronger here: as we have shown above, in a (110) quantum well the linear Dresselhaus terms have no effect on the magnetoconductivity (in the absence of the Rashba term), whereas in a (001) well such a dramatic cancellation is only possible when both Rashba and Dresselhaus terms exist and are nearly equal.

From the above values of the parameters $H_{SO}^{(i)}$, we can determine the values of the constants γ and α_0 , using Eqs. (4), (16), and (18), $k_{\rm F} = \sqrt{2 \pi N_s}$, and the following expressions for $\langle k_z^2 \rangle$ (Ref. 15) and α , which are obtained using the standard variational wave function for electrons at the heterointerface,¹⁶

$$\langle k_z^2 \rangle = \frac{1}{4} \left(\frac{16.5 \pi e^2 m N_s}{\kappa \hbar^2} \right)^{1/3}, \quad \alpha = e \overline{\mathcal{E}} \alpha_0, \quad \overline{\mathcal{E}} = \frac{2 \pi e N_s}{\kappa},$$
(19)

where N_s is the electron density, κ is the dielectric constant, *m* is the effective electron mass, and $\overline{\mathcal{E}}$ is the average electric field in the well. The resulting values of the coefficients are $\gamma \approx 22$ eV Å³ and $\alpha_0 \approx 14$ Å². The value of γ is very close to the previously reported values, both measured and calculated,^{5,17–21,7,8} including those measured in weaklocalization experiments in (001) quantum wells.^{7,8} The value of α_0 was only measured in the latter experiments, and reported to be about 7.2 Å². However, unlike γ , which is the bulk material coefficient, α_0 may make contributions from the interface.^{22,23} Their magnitude is not reliably known; therefore, we view the discrepancy between our value of α_0 and the one measured in (001) wells as an experimental confirmation of the effects of interfaces on the value of α_0 . Also, from the value of $H_{SO}^{(3)}$ we can determine the ratio $\tau_3/\tau_1 \approx \frac{1}{8}$. This ratio can vary from 1 for short-range scattering to $\frac{1}{9}$ for scattering on remote impurities, and the experiment shows that in our samples those are practically the only source of scattering. Lastly, we can determine the phase relaxation time $\tau_{\varphi} \approx 6 \times 10^{-10}$ s.

V. CONCLUSIONS

In conclusion, we have presented interesting experimental and theoretical studies of magnetoconductivity caused by the weak localization in (110) GaAs quantum wells. It is demonstrated that if the spin splitting of the conduction band is linear in the wave vector, it is necessary to take into account the correlation between the electron motion in coordinate and spin spaces. This correlation leads to the special feature of the (110) geometry: in a perfectly symmetric quantum well, when the Rashba terms are absent, the weak antilocal-

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ization effect, which leads to positive magnetoresistance, does not exist. The presence of the positive magnetoresistance in our samples is a clear signature of the Rashba terms in the conduction-band spin splitting. We have also shown, experimentally, that the magnitude of the Rashba term depends on the orientation of the well. Our theory achieves a good agreement with the experiment, and gives values for the parameters of the spin splitting which are in agreement with previous optical and transport experiments and theoretical calculations.

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