Effective one-band approach for the spin splittings in quantum wells

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The spin-orbit interaction of 2D electrons in the quantum wells grown from the III-V semiconductors consists of the two parts with different symmetry: the Bychkov-Rashba and the Dresselhaus terms. The last term is usually attributed to the bulk spin-orbit Hamiltonian which reflects the $T_d$ symmetry of the zincblende lattice. While it is known that the quantum well interfaces may also contribute to the Dresselhaus term, the exact structure and the relative importance of the interface and the bulk contributions are not well understood yet. To compare the bulk contribution with the interface one, we perform tight-binding calculations of the spin splittings of the electron levels in [100] GaAs/AlGaAs quantum wells and analyze the obtained spin splittings within the one-band effective mass electron Hamiltonian containing the two interface contributions to the Dresselhaus term. We show that the dependencies of the spin splittings on the quantum well width and the electric field along the growth direction are perfectly reproduced by the analytical one-band calculations and the magnitude of the interface contribution to the spin-orbit interaction for sufficiently narrow quantum wells is of the same order as the contribution from the bulk Dresselhaus Hamiltonian.

INTRODUCTION

The spin-orbit interaction of two-dimensional (2D) electrons in the heterostructures based on the non-centrosymmetric cubic semiconductors has been extensively investigated during the last three decades [1, 2]. However, there is still no complete understanding of the physical nature and magnitudes of different contribution to the spin-orbit interaction even in the conventional GaAs/AlGaAs heterostructure systems.

For the bulk III-V semiconductors the one-band effective mass electron Hamiltonian with the spin-orbit terms and the effective-mass anisotropy can be derived from the 14-band Kane $\mathbf{k}\cdot\mathbf{p}$-Hamiltonian [3]. The magnitude of the spin-orbit term in the one-band electron Hamiltonian can be obtained from the gaps between the different bands of a semiconductor and the interband matrix elements of the momentum operator between the different bands in the $\mathbf{k}\cdot\mathbf{p}$-Hamiltonian.

The spin-orbit interaction of 2D electrons in the heterostructures grown from the III-V semiconductors consists of the two parts with different symmetry: Bychkov-Rashba and Dresselhaus terms. The isotropic part of the spin-orbit interaction (the Bychkov-Rashba contribution) is induced by electric field along the growth direction. It consists of the two contributions: the bulk contribution, associated with the smooth part of the electric field along the normal, and the interface contribution, associated with the strong atomic field at the well interfaces (i.e., the electric fields due discontinuities of the band edges at the interfaces) [4]. Analogously, the anisotropic part of the spin-orbit interaction of 2D electrons (the Dresselhaus term) contains the bulk contribution, related with the spin interaction in the zincblende lattice, and the interface contribution, determined with the atomic structure of the interfaces.

For the first time, the interface anisotropic terms in the effective mass Hamiltonian were proposed in Refs. [5, 6] for the case of the hole Hamiltonian in [100] quantum wells in order to describe the unusual optical properties of that structures. In the papers [7, 8] it was shown that the Hamiltonian of Refs. [5, 6] leads to a spin-orbit interface anisotropic term in the effective electron Hamiltonian, which induces a contribution to the electron spin splittings, additional to the bulk contribution. More recently, the two interface anisotropic spin-dependent terms were introduced in the electron effective Hamiltonian in Refs. [9, 10] in an attempt to describe lateral anisotropy of 2D electron $g$-factor recently observed in the [100] GaAs quantum wells [11–13]. Similar interface terms were derived in Ref. [14] from the $\mathbf{k}\cdot\mathbf{p}$-Hamiltonian containing infinite number of bands. The analysis of the experimental data from Refs. [11–13] shows that the contributions to the $g$-factor anisotropy from the quantum well interfaces and from the bulk regions are of the same order of magnitude [9]. Recently, it was demonstrated within the framework of the 14-band Kane model that the interface spin-orbit terms are substantial in the Luttinger $4 \times 4$ Hamiltonian for 2D holes in GaAs quantum wells [15].

It should be mentioned that, at present, there is a strong controversy concerning the value of the bulk spin-orbit constant $\gamma$ in various semiconductors [3, 16–19]. For example, it was concluded in Ref. [16] from measurements of the spin splittings of the electron dispersion in GaAs quantum wells that the bulk spin-orbit constant $\gamma$ in GaAs is approximately half of the value which was previously accepted in literature [3, 17]. However, in the interpretation of the experimental data in Ref. [16], the presence of anisotropic spin-orbit terms localized at the interfaces of the wells was not taken into account. Some novel ways of determining the bulk spin-orbit Dresselhaus parameter from the experiments on bulk semiconductors subjected in homogeneous and inhomogeneous magnetic field were discussed in Refs. [20–23].

The tight-binding approach is the method which is able
to take into account both the bulk and the interface contribution to the spin-orbit interaction of 2D electrons by a rigorous uniform way [24]. Tight-binding calculations of the spin splittings of 2D electron in the [110] quantum wells grown from III-V semiconductors were recently performed in Refs. [25, 26].

In this paper we perform the tight-binding calculations of the spin splittings of the electron energy spectrum in the [100] GaAs quantum wells subjected in an electric field along the growth direction. We compare the obtained dependencies of the spin splittings on the quantum well width and the electric field with the analytic expressions derived within the one-band electron Hamiltonian containing the bulk [3] and the two interface [9, 10] spin-orbit terms. From the comparison, we extract the values of the bulk and the interface parameters in the effective electron Hamiltonian. The analytical one-band calculations perfectly reproduce the results of tight-binding numerical calculations for different quantum wells. As a result, we estimate the interface terms and prove the importance of the interface contributions to the spin splitting of 2D electron spectrum in GaAs quantum wells.

**TIGHT-BINDING CALCULATIONS**

Electron states in the quantum well structure are calculated in the extended basis $sp^d$ tight-binding approach which is known as an efficient empirical-parameter full-band representation of semiconductor electronic properties [27]. The coordinate system is chosen in such a way that the cation atom is located at the origin and one of its neighbors is located in [111] direction. This choice results in the opposite sign of cubic spin splitting constant $\gamma$ and the constants of linear spin splitting in comparison with the “anion in the origin” convention.

We consider GaAs quantum well between Ga$_{0.7}$Al$_{0.3}$As barriers. The alloys are treated in the virtual crystal approximation: all tight-binding parameters are taken as weighted linear combination of the corresponding GaAs and AlAs parameters, which means that we neglects possible effects of bowing and disorder. This is a good approximation for GaAs/AlGaAs heterostructures, but for other alloys a more sophisticated approximation might be necessary [28].

The tight-binding parameters are taken from Ref. 27. To calculate the spin splitting we choose small wave vector $k$ and change its direction in the (001) plane. At finite $k$, the (double) degeneracy of quantum-confined electron states is lifted, with the splitting proportional to $|k|$. For each lateral direction of $k$, we calculate the splitting $\Delta(k)$ and the vector $s$ of the mean value of electron spin for the lower spin branch. The typical splitting is of the order of meV. We note that the tight-binding method provides high accuracy of the spin splitting near the band edge [29–31] since $\Delta(k)$ is determined by the difference between the energies of spin subbands and possible inaccuracy in the band positions does not affect its value significantly. The electric field $E_z$, applied along the growth direction and causing the quantum well asymmetry, is taken into account in the framework of standard procedure [32] by shifting of the diagonal energies due to the local potential at atomic sites.

The effective Hamiltonian for an electron in quantum well can be written as:

$$ H_{\text{eff}}(k) = \beta (k_x \hat{\sigma}_x - k_y \hat{\sigma}_y) + \alpha (k_y \hat{\sigma}_x - k_x \hat{\sigma}_y) . $$  \hspace{1cm} (1)

The solution of this one-band Hamiltonian gives us the splitting between the two states:

$$ \Delta(k) = 2\sqrt{\left(\beta^2 + \alpha^2\right)k^2 + 4\alpha\beta k_x k_y} , $$  \hspace{1cm} (2)

and the mean value of spin projection for the lower energy state:

$$ s^{\text{eff}}_x = -\frac{\beta k_x + \alpha k_y}{\Delta(k)} , $$

$$ s^{\text{eff}}_y = \frac{\beta k_y + \alpha k_x}{\Delta(k)} . $$  \hspace{1cm} (3)

The splittings and spin direction as functions of the lateral wave vector angle are extracted from tight-binding calculations are fitted with equations (2), (3). The fit is shown in Fig. 1. This allows us to extract the Dresselhaus and Rashba constants $\beta$ and $\alpha$ directly from the tight-binding calculations.
In accordance with symmetry consideration, the parameter $\alpha$ vanish at zero electric field, when the quantum well is symmetric, and then increase linearly with $E_z$. The Dresselhaus parameter $\beta$ depends on the electric field $E_z$ in a more weak manner: it starts to deviate significantly from zero-field value only when the variation of electrostatic potential $-eE_zz$ from the electric field $E_z$ in the interface regions is comparable with the quantum confinement energy.

Repeating the calculation procedure for different quantum wells, we obtain the dependence of the spin-orbit coupling parameters on the quantum well width. The dependence of the Dresselhaus parameter $\beta$ on the quantum well width is non-monotonic. This is expected for $k$-linear splitting caused only by $k$-cubic terms in the bulk crystal. We discuss this point in more details below within the one-band electron Hamiltonian containing the bulk as well as the interface spin-orbit terms.

**SPIN SPLITTINGS WITHIN THE ONE BAND APPROACH**

The cubic term in the Hamiltonian of zincblende semiconductor [3] in a quantum well grown along [001] direction may be written in linear in the lateral wavevector order as:

$$\hat{H}_{BIA} = \frac{d}{dz} \gamma(z) \frac{d}{dz} (k_x \sigma_x - k_y \sigma_y), \quad (4)$$

Here $\gamma(z)$ is the bulk spin-orbit parameter, which depends on the layer material. Analysis of the experimental data for bulk GaAs yield the value of $\gamma$ around 25 eVÅ$^3$ [3].

The interface contributions to the spin-orbit interaction of 2D electrons in a quantum well have the same symmetry relative to the symmetry operations in the $xy$ plane, but instead the operator $d^2/dz^2$ contains the delta-function and its derivative localized at the well interfaces [8–10, 14]:

$$\hat{H}_{int} = \sum_{\nu=l,r} \left( \hat{H}_{int,0,\nu} + \hat{H}_{int,1,\nu} \right),$$

$$\hat{H}_{int,0,\nu} = \zeta_\nu \delta(z - z_\nu)(k_x \sigma_x - k_y \sigma_y), \quad (5)$$

$$\hat{H}_{int,1,\nu} = \xi_\nu \delta'(z - z_\nu)(k_x \sigma_x - k_y \sigma_y).$$

The parameters $\zeta_{l,r}$ and $\xi_{l,r}$ are determined by the structure of the chemical bonds of the atom at the interface. Comparison of the results of tight-binding calculation and the analytical expressions (5) allows us to determine $\zeta$ and $\xi$.

The equations (5) assumes continuity of the wave function derivative at the interfaces of the quantum well. If we use the one-band electron Hamiltonian with different values of the effective mass in the barrier and in the well, then the wave function derivative at the quantum well interfaces is discontinuous, and we should modify the form of the interface contribution (5).

The equations (5) also assumes some fixed form of the bulk spin-orbit term containing discontinuities of the bulk Dresselhaus parameter $\gamma(z)$ at the well interfaces. Other forms of the Hamiltonian (4) are allowed. For example, one can take them proportional to $[\gamma(z) d^2/dz^2 + d^2/dz^2\gamma(z)]/2$ or $\gamma^{1/2}(z) d^2/dz^2\gamma^{1/2}(z)$. Our choice is based only on the reason of most simplicity of Eq. (4). Of course, this freedom of choice is limited by the requirement that Eq. (4) should be an Hermitian operator.

Let $u(z)$ be the electron wavefunction of the first level of space quantization within the one-band electron Hamiltonian. Projection of the operators (4) and (5) onto the first subband, corresponding to the wave function $u(z)$, leads to the following form of the bulk and the surface contributions to the anisotropic spin-orbit interaction of 2D electrons:

$$\hat{H}_D = \beta (k_x \sigma_x - k_y \sigma_y),$$

$$\beta = -\int_{-\infty}^{\infty} dz \gamma(z)|u'(z)|^2 +$$

$$+ \sum_{\nu=l,r} \left\{ \zeta_\nu u(z_\nu)^2 + \xi_\nu [u(z_\nu)^2]' \right\}. \quad (6)$$

We consider a rectangular quantum well. The parameter $\gamma(z)$ in this structure is a step-like function with the two different values in the well and in the barrier layers:

$$\gamma(z) = \begin{cases} \gamma_b, & z < 0, \ z > a \ \\ \gamma_w, & 0 < z < a \end{cases}. \quad (7)$$

Without an electric field the symmetry of the quantum well $D_{2h}$ leads to relations between the coefficients $\zeta_\nu$ and $\xi_\nu$ for the left and right interfaces: $\zeta_l = \zeta_l$, $\xi_l = -\xi_r$. The wave function $u(z)$ is symmetric with respect to reflection plane in the center of the well, and we obtain

$$\beta = -\int_{-\infty}^{\infty} dz \gamma(z)|u'(z)|^2 + 2\zeta u(z_r)^2 + 2\xi [u(z_r)^2]' \quad (7)$$

If an electric field $E_z$ is applied along the normal to the quantum well, the relationships $\zeta_l = \zeta_l$, $\xi_l = -\xi_r$ are retained, but the wave function $u(z)$ is not symmetric.
with respect to the quantum well center. In this case,
\[
\beta = \beta_b + \beta_{\text{int},0} + \beta_{\text{int},1},
\]
\[
\beta_b = -\int_{-\infty}^{\infty} dz \gamma(z)[u'(z)]^2, \tag{8}
\]
\[
\beta_{\text{int},0} = \zeta [u(z_i)]^2 + u(z_r)^2],
\]
\[
\beta_{\text{int},1} = \xi \{[u(z_i)]^2' + [u(z_i)]^2'\}.
\]

The potential energy of an electron in an empty rectangular quantum well in a homogenous electric field \(E_z\) is:
\[
U(z) = eE_z z + \begin{cases} 0, & 0 < z < a \\ \overline{U}, & z < 0, \ z > a \end{cases} \tag{9}
\]

Here \(e > 0\) is the absolute value of the electron charge. In order to calculate the wave function \(u(z)\) analytically we substitute the real potential (9) of the quantum well by the model potential
\[
\overline{U}(z) = \begin{cases} eE_z z, & 0 < z < a \\ U_0, & z < 0 \\ U_0 + eE_z a, & z > a \end{cases}. \tag{10}
\]

The electron ground level \(E_0\) is resonant for the true potential \(U(z)\) (9), but turns into actually stationary level for the model potential \(\overline{U}(z)\) (10). We assume that the well is deep: \(E_0 \ll U_0\). The approximation of Eq. (10) is valid in the electric fields \(E_z\), for which the condition \(eE_z/\kappa \ll U_0\) is fulfilled, where \(\kappa = \sqrt{2m(U_0 - E_0)/\hbar}\) is the reciprocal length of decay of the electron wave function in the barrier.

The wavefunction \(u(z)\) of the ground state corresponding to the model potential \(\overline{U}(z)\) is expressed via the Airy functions in the well region:
\[
u(z) = c_A \text{Ai} \left(\frac{z - E_0/eE_z}{d}\right) + c_B \text{Bi} \left(\frac{z - E_0/eE_z}{d}\right) \tag{11}\]
and the exponents in the barriers:
\[
u(z) = c_t e^{\kappa t z}, \ z < 0,
\]
\[
u(z) = c_t e^{-\kappa_r (z-a)}, \ z > a. \tag{12}\]

Here \(d = (2meE_z/h^2)^{-1/3}, \kappa_t = \kappa = \sqrt{2m(U_0 - E_0)/\hbar}, \kappa_r = \sqrt{2m(U_0 + eE_z a - E_0)/\hbar}\). The coefficients \(c_A, c_B, c_t, c_r\), and the eigenenergy \(E_0\) were calculated as the functions of the quantum well width and the electric field \(E_z\) by use of the standard methods.

In Fig. 2 we present the bulk and the interface contributions to the 2D electron spin-orbit interaction calculated by Eqs. (8), (11), and (12). In this paper we consider quantum wells in the typical heterostructures Ga\(_{0.7}\)Al\(_{0.3}\)As/GaAs/Ga\(_{0.7}\)Al\(_{0.3}\), for which we take the following electron band parameters: \(U_0 = 300\) meV and \(m = 0.067m_0\). The panel (a) of Fig. 2 presents the dependencies of the bulk and the interface contributions to the spin-orbit parameter \(\beta\) on the quantum well width in the absence of electric field \(E_z\) along the \(z\) direction. We see that all the contribution have maximums at the well widths \(a \sim 2 - 3\) nm and tend to zero at very small and very large \(a\). The endings of the curves in the region of small widths \(a\) correspond to the one-monolayer quantum well for which \(a \sim a_0\) and the effective mass method and the spin-orbit Hamiltonians (4) and (5) are not applicable surely (here \(a_0\) is the lattice constant). The dependencies \(\beta_b(a)\) and \(\beta_{\text{int},1,2}(a)\) exhibit the power behavior in the region of large widths \(a\):
\[
\beta_b \sim a^{-2}, \ \beta_{\text{int},0} \sim a^{-3}, \ \beta_{\text{int},1} \sim a^{-3}, \tag{13}\]
as well as in the region of small widths \(a\):
\[
\beta_b \sim a^2, \ \beta_{\text{int},0} \sim a, \ \beta_{\text{int},1} \sim a^2. \tag{14}\]

However we must keep in mind that Eq. (14) imply that the quantum well width is large enough, as minimum \(a \gtrsim a_0\).

The panel (b) in Fig. 2 shows the dependencies of the bulk and the interface contributions to the spin-orbit pa-
We plotted the pairs \( \beta, \delta \beta \) which has some uncertainty. We have in hand the experimental or the numeric (e.g., infinitely large quantum well width, \( E_z = 0 \)), and continuously varying quantum well width, \( E_z \rightarrow \infty \), for the con- tinuously varying electric field \( E_z \) and infinitely large quantum well width, \( a \rightarrow \infty \).

Parameter \( \beta \) on the magnitude of the electric field \( E_z \) for the infinitely large quantum well width. The absolute values of \( \beta_\text{b} \) and \( \beta_{\text{int},0,1} \) increase with the electric field \( E_z \) in the region from \( E_z = 0 \) up to \( E_z \sim U_0 \kappa/e \), where the approximate electron potential (10) is yet applicable. At small electric fields the values \( \beta_\text{b} \) and \( \beta_{\text{int},0,1} \) depends on electric field \( E_z \) as:

\[
\beta_\text{b} \sim (E_z^{2/3}), \quad \beta_{\text{int},0} \sim E_z, \quad \beta_{\text{int},1} \sim E_z. 
\]

At larger electric fields, \( E_z > U_0 \kappa/e \), the energy level \( E_0 \) becomes resonant to a large extent. This is illustrated in Fig. 1(b) by blur and broadening of the graphic lines.

To compare the dependences of the bulk and the interface contributions on the quantum well width and the electric field we have drawn the parametric plots of the values \( \beta_{\text{int},0}, \beta_{\text{int},1} \), and \( \beta_\text{b} \). In the panels (a,b) of Fig. 3 we plotted the pairs \([\beta_\text{b}, \beta_{\text{int},0}]\) and \([\beta_\text{b}, \beta_{\text{int},1}]\) for continuously varying values of the the quantum well width \( a \) at zero electric field \( E_z = 0 \). We see that all contributions \( \beta_{\text{int},0}(a), \beta_{\text{int},1}(a) \), and \( \beta_\text{b}(a) \) are approximately proportional each other in the wide intervals of the values of quantum well width \( a \). This implies that if we have in hand the experimental or the numeric (e.g., tight-binding) dependence \( \beta(a) \) of the total spin splitting, which has some uncertainty \( \delta \beta(a) \), we can establish the relative magnitudes of the bulk \( \beta_\text{b}(a) \) and the interface \( \beta_{\text{int},0,1}(a) \) contributions in this dependence \( \beta(a) \) only for rather small values of the uncertainty, \( \delta \beta(a) \ll \beta(a) \). Otherwise, if the uncertainty \( \delta \beta(a) \) is large, one cannot designate the contributions \( \beta_\text{b}(a), \beta_{\text{int},0}(a), \beta_{\text{int},1}(a) \) in it as the set of the functions \( \beta_\text{b}, \beta_{\text{int},0}, \beta_{\text{int},1} \) is close to be a linearly dependent set. For example, for large \( a, a \rightarrow \infty \) one obtains from Eq. (13) that \( \beta_\text{b} \rightarrow 0, \beta_{\text{int},0,1} \rightarrow 0, \) and \( \beta_{\text{int},0,1} \sim b^3 \), see Fig. 2(a,b).

In the panels (c) and (d) of Fig. 3 we show the parametric plots of the pairs \([\beta_\text{b}, \beta_{\text{int},a}]\) and \([\beta_\text{b}, \beta_{\text{int},b}]\) for the infinitely wide quantum well and continuously varying values of the electric field \( E_z \) from zero up to the limit value \( \sim U_0 \kappa/e \). We again see that the functions \( \beta_\text{b}(E_z), \beta_{\text{int},0}(E_z), \) and \( \beta_{\text{int},b}(E_z) \) are almost proportional. At small \( E_z \), \( E_z \rightarrow 0 \), one obtains from Eq. (15) that \( \beta_\text{b} \rightarrow 0, \beta_{\text{int},0,1} \rightarrow 0, \) and \( \beta_{\text{int},0,1} \sim b^3 \), see Fig. 2(c,d).

It should be mentioned also that for a quantum well with a substantial concentration of electrons, the electron potential energy \( U(z) \) is strongly modified by the presence of electron charge inside quantum well. The potential \( U(z) \) should be calculated simultaneously with the energy levels in a self-consistent procedure of a joint solution of the Poisson and Schrödinger equations. At the edges of the quantum well the resulting wavefunction has the values, which are significantly greater by their absolute values than for the wave function in the quantum well with the same width and depths, but containing no electrons (for example, see Ref. [9]). This means that the large electron concentration in a quantum well leads to an increase of the role of the interface contributions to the spin-orbit interaction compared with an empty quantum well.

**ANALYSIS OF RELATIVE IMPORTANCE OF DIFFERENT CONTRIBUTIONS**

With the help of the tight-binding approach, we have calculated the absolute values of the spin splitting constants as functions of the well width in the range from 1 to 20 nm, and the electric fields \( E_z \) in the range from 0 up to \( 10^5 \) V/cm. The results of these calculation for \( E_z = 0 \) and \( E_z = 10^5 \) V/cm are shown in Fig. 4.

The character electric field \( E_{z,\text{max}} \) in which the center of the wavefunction \( u(z) \) becomes substantially shifted from the quantum well center should be calculated from the equality \( eE_z a \sim E_0 |_{E_z=0} \). For the quantum well with the parameters \( a = 10 \) nm and \( U_0 = 300 \) meV we obtain

\[
E_{z,\text{max}} \sim 3 \cdot 10^3 \text{ V/cm}
\]

We fitted the obtained dependence \( \beta(a) \) for \( E_z = 10^5 \) V/cm by the analytical dependence (8) by the least square method. We take into account that the bulk spin-orbit Dresselhaus parameter \( \gamma \) is different in the well and in the barrier regions of the heterostructure. As we consider the heterostructure with the barriers grown from the compound \( \text{Al}_{0.3}\text{Ga}_{0.7}\text{As} \), we adopted the following estimation of the ratio of the spin-orbit bulk parameters in
the well and in the barrier: $\gamma_{\text{bar}}/\gamma_{\text{w}} = 0.7$. It is seen from the Fig. 5(a) that the numerical dependence $\beta(a)$ can be very well reproduced by the analytical formula (8) with the three parameters $\gamma$, $\xi$, $\zeta$. From the fitting procedure we obtained the following values of the bulk and interface parameters: $\gamma_{\text{GaAs}} = -23$ eV$\cdot$Å$^2$, $\xi = -1.5$ eV$\cdot$Å$^3$, $\zeta = 6.5 \cdot 10^{-6}$ eV$\cdot$Å$^2$.

We checked that, for the obtained parameters $\gamma$, $\xi$, $\zeta$, the analytical one-band dependencies $\beta(a)$ for all the electric fields $E_z$ in the interval from 0 up to $10^5$ V/cm well coincides with the results of the tight-binding calculations of $\beta(a)$. In the Fig. 5(b) we show the numeric tight-binding and the analytical one-band functions $\beta(a)$ for $E_z = 0$. These two curves almost coincide. The obtained result proves that the description of the electron spin-orbit interaction in the GaAs quantum well with sharp interfaces within the one-band Hamiltonians (4) and (5) is adequate.

The obtained value of the coefficient $\zeta$ in the interface term $H_{\text{int},1,\nu}$ for GaAs quantum wells corresponds by the order of magnitude to the value of the interface contribution in linear spin splitting which has been estimated within the framework of multi-band $k\cdot p$-Hamiltonian in Refs. [8, 33].

**CONCLUSION**

In conclusion, we show that the results of atomistic calculations of spin splittings of the 2D electron spectrum in GaAs quantum wells can be perfectly reproduced in the framework of one-band effective-mass model by adding the interface terms in the one-band Hamiltonian. By introducing the two independent parameters in the interface terms, the microscopic atomistic calculations are reproduced with the correct functional dependencies of spin-dependent terms on the quantum well width and the electric field applied.

The effective one-band description allows us to conclude that the interface-induced anisotropy contributes significantly to the value of the coefficient in the Dresselhaus term in the electron Hamiltonian in quantum wells.

We have also demonstrated that the separation of bulk and interface terms in the experiments is complicated by the fact that both terms contribute to the linear spin splitting of the same symmetry and have very similar functional dependency on quantum well width and electric field applied.
It should be noted that, in the real quantum wells, there also exists a contribution to the observed magnitude of the spin-orbit interaction from the electron-electron interaction [34]. The strength of this interaction inducing renormalization of the constant $\beta$ depends on the geometry of the quantum well and the electron density. This fact more complicates the interpretation of the experimental data on the absolute value of the spin-orbit coupling in quantum wells.

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[1] R. Winkler, Spin-Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems (Springer, Berlin, 2003).
[2] I. Žutić, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004).
[3] G. E. Pikus, V. A. Maruschkak, and A. N. Titkov, Sov. Phys. Semicond. 22, 115 (1988), [Fiz. Tekh. Poluprovodn. 22, 185 (1988)].
[4] E. A. de Andrade e Silva, G. C. La Rocca, and F. Bassani, Phys. Rev. B 55, 16293 (1997).
[5] E. L. Ivchenko, A. Y. Kaminski, and U. Rössler, Phys. Rev. B 54, 5852 (1996).
[6] O. Krebs, D. Rondi, J. L. Gentner, L. Goldstein, and P. Voisin, Phys. Rev. Lett. 80, 5770 (1998).
[7] L. Vervoort, R. Ferreira, and P. Voisin, Semicond. Sci. Technol. 14, 227 (1999).
[8] U. Rößler and J. Kainz, Solid State Commun. 121, 313 (2002).
[9] P. S. Alekseev, JETP Lett. 98, 84 (2013), [Pis’ma v Zh. Exp. Teor. Fiz. 92, 92 (2013)].
[10] P. S. Alekseev, Semiconductors 47, 1241 (2013), [Fiz. Tekh. Polupr. 47, 1253 (2013)].
[11] Yu. A. Nefyodov, A. A. Fortunatov, A. V. Shchepetilnikov, and I. V. Kukushkin, JETP Lett. 91, 357 (2010), [Pis’ma v Zh. Exp. Teor. Fiz. 91, 385 (2010)].
[12] Yu. A. Nefyodov, A. V. Shchepetilnikov, I. V. Kukushkin, et al., Phys. Rev. B 83, 041307 (2011).
[13] Yu. A. Nefyodov, A. V. Shchepetilnikov, I. V. Kukushkin, et al., Phys. Rev. B 84, 233302 (2011).
[14] Zh. A. Devizorova and V. A. Volkov, JETP Lett. 98, 101 (2013), [Pis’ma v Zh. Exp. i Teor. Fiz. 98, 110 (2013)].
[15] M. V. Durnev, M. M. Glazov, and E. L. Ivchenko, Phys. Rev. B 89, 075430 (2014).
[16] M. P. Walser, U. Siegenthaler, V. Lechner, et al., Phys. Rev. B 86, 195309 (2012).
[17] J.-M. Jancu, R. Scholz, E. A. de Andrade e Silva, and G. C. La Rocca, Phys. Rev. B 72, 193201 (2005).
[18] A. N. Chantis, M. van Schilfgaarde, and T. Kotani Phys. Rev. Lett. 96, 086405 (2006).
[19] A. N. Chantis, M. Cardona, N. E. Christensen, et al., Phys. Rev. B 78, 075208 (2008).
[20] P. S. Alekseev, M. V. Yakunin, and I. N. Yassievich, Semiconductors 41, 1092 (2007), [Fiz. Tekh. Polupr. 41, 1110 (2007)].
[21] P. S. Alekseev, JETP 107, 854 (2008), [Zh. Exp. Teor. Fiz. 134, 996 (2008)].
[22] P. S. Alekseev, JETP Lett. 90, 102 (2009), [Pis’ma v Zh. Exp. Teor. Fiz. 90, 111 (2009)].
[23] P. S. Alekseev, JETP 121, 491 (2015), [Zh. Exp. Teor. Fiz. 148, 564 (2015)].
[24] The $k\cdot p$-method, in principle, can be applied to calculate the magnitudes of the spin-orbit interaction in quantum wells. For rectangular quantum wells, discontinuities of the energy gaps at the interfaces lead to the interface terms in the one-band electron and hole Hamiltonians. However, using the $k\cdot p$-Hamiltonian containing a finite number of bands is not a mathematically rigorous procedure as a strong mixing of the states from all the bands takes place due to the sharpness of the interfaces.

[25] M. O. Nestoklon, S. A. Tarasenko, J.-M. Jancu, and P. Voisin, Phys. Rev. B 85, 205307 (2012).
[26] M. O. Nestoklon, S. A. Tarasenko, R. Benchamekh, and P. Voisin, arXiv:1605.08942 (2016).
[27] J.-M. Jancu, R. Scholz, F. Beltram, and F. Bassani, Phys. Rev. B 57, 6493 (1998).
[28] M. O. Nestoklon, R. Benchamekh, and P. Voisin, J. Phys.: Condens. Matter 28, 305801 (2016).
[29] M. O. Nestoklon, E. L. Ivchenko, J.-M. Jancu, and P. Voisin, Phys. Rev. B 77, 155328 (2008).
[30] M. O. Nestoklon, L. E. Golub, and E. L. Ivchenko, Phys. Rev. B 73, 235334 (2006).
[31] J.-M. Jancu, R. Scholz, E. A. de Andrade e Silva, and G. C. La Rocca, Phys. Rev. B 72, 193201 (2005).
[32] M. Graf and P. Vogl, Phys. Rev. B 51, 4940 (1995).
[33] M. V. Durnev and M. M. Glazov, private communication.
[34] S. S. Krishtopenko, Semiconductors 49, 174 (2015), [Fiz. Tekh. Polupr. 49, 179 (2015)].