EFFECTIVE SPIN-ORBIT INTERACTION IN NARROW QUANTUM WELLS

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Abstract. **Rashba and linear Dresselhaus interactions are believed to yield dominant contribution to the spin splitting of two-dimensional electrons in the quantum wells based on A_3B_5 compounds. We show that the interfacial spin-orbit interaction significantly renormalizes the value of the corresponding Rashba (α_{SIA}) and Dresselhaus (α_{BIA}) parameters. For this purpose, we solve the effective mass equation in a quantum well supplemented by the original boundary conditions on the atomically sharp interfaces and calculate the interfacial contributions to α_{SIA} and α_{BIA}. Our results explain a considerable spread in the experimental data on spin-orbit parameters in GaAs/ AlGaAs quantum wells. We also demonstrated that the non-equivalence of the interfaces leads to the anisotropy of the spin splitting even in quantum wells with zero average electric field.**

CONTENTS

I. INTRODUCTION

The conservation of the spin polarization is crucial for spintronic device applications. Due to the spin-orbit interaction (SOI), electrons in quantum wells (QWs) experience spin relaxation and dephasing by Dyakonov-Perel mechanism [3]. In the QWs based on A_3B_5 compounds there are two types of the SOI: Dresselhaus [1] and Rashba [2]. The Dresselhaus-type SOI is believed to originate from the lack of inversion symmetry in the bulk crystal and is proportional to the Dresselhaus parameter α_{BIA}. The Rashba-type SOI is due to the structural asymmetry and is proportional to the parameter α_{SIA}. If α_{BIA} and α_{SIA} are equal, the spin polarization of a helical spin state is conserved [4]. To achieve this regime, one should know and control the values of both parameters. In the envelope functions approximation they are determined by the following expressions $\quad \alpha_{BIA}^{(0)} = \gamma_c \left\langle \hat{p}_z^2 \right\rangle / \hbar^3, \alpha_{SIA}^{(0)} = a_{so} \left\langle \partial_z V(z) \right\rangle,$

where γ_c и a_{so} are bulk constants [18]. Thus, it is believed that the parameter α_{SIA} can be tuned by using the gate electrodes or by choosing the ratio between the dopant concentration on the two sides of QW, while the parameter α_{BIA} is determined by choosing the material and the width of QW. However, the experimental determination of the bulk constants γ_c and a_{SO} is still challenging. In spite of many experimental investigations in a wide range GaAs-based QWs, the precise value of γ_c is still being discussed controversially in the literature.

The parameter γ_c was measured by Marushchak with collaborators for bulk GaAs [5[and the value $\gamma_c = 24$ eV·Å³ was obtained which is in the good agreement with kp-theory and has not been revised yet. But since 1990th γ_c bas been measured not in bulk GaAs, but in QWs with the interfaces [4, 6-15]. There is a considerable spread in the data obtained (see **Fig. 1**), moreover, they are inconsistent with the theoretical results. As it was pointed out in Ref. [17], the possible reason of the spread is an incomplete account of the interfacial spin-orbit interaction (ISOI). Thus, not bulk values, but some effective quantities containing the information about the microscopic structure of the interfaces are obtained in the experiments. The theory of ISOI in the
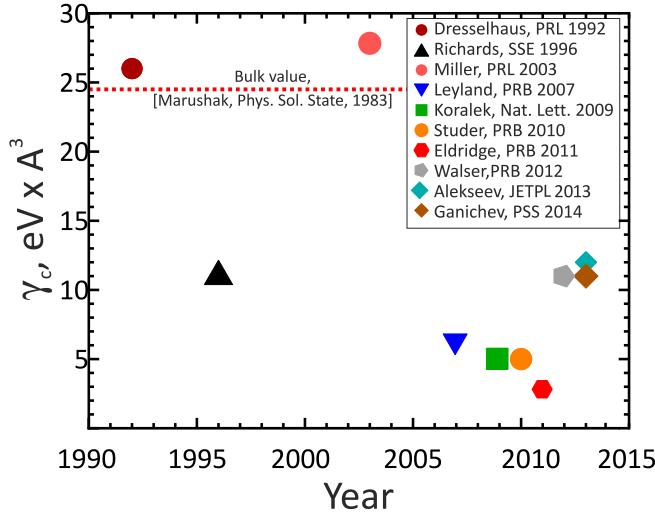
Fig. 1. *The values of the bulk spin-orbit constant γ_c extracted from the experimental data obtained by different groups in GaAs/AlGaAs quantum wells. There is a considerable spread in the data and inconsistency with the result of bulk measurements.*

wide unilaterally doped GaAs quantum well, where the electrons are pushed toward the (001) GaAs/AlGaAs heterointerface by the built-in electric field was developed in Refs. [16 and 17]. The interfacial contributions to the α_{BIA} and α_{SIA} were shown to be of the same order as bulk ones. However, in a more general situation the electrons interact with atomically sharp interfacial potentials of two heterointerfaces, and ISOI at both of them contribute to α_{BIA} and α_{SIA}. To take it into account, we develop the theory of the ISOI in the QWs with an arbitrary thickness and potential profile in the present paper.

2. GENERAL THEORY OF SPIN-ORBIT INTERACTION IN NARROW QUANTUM WELLS

In the QWs grown in $z\,||\,[001]$ direction, the spin splitting of the 2D electron spectrum has the general form

$$E_{SS} = 2p\sqrt{\alpha_{BIA}^2 + \alpha_{SIA}^2 + 2\alpha_{BIA}\alpha_{SIA}\sin 2\phi}, \quad (1)$$

where $p_x = p\cos\phi$, $p_y = p\sin\phi$ are the components of 2D momentum.

To derive the interfacial contributions to α_{BIA} and α_{SIA} we begin with 3D problem in which an effective wave function ϕ of the conduction electron obeys the effective mass equation inside the QW of the thickness d. The corresponding Hamiltonian $\hat{H}$ contains the terms $\hat{H}_{BIA}$ and $\hat{H}_{SIA}$ describing the spin splitting of the spectrum arising due to the lack of inversion symmetry in the bulk crystal and asymmetry of the structure, respectively:

$$\hat{H} = \frac{\hat{p}^2}{2m^*} + V(z) + \hat{H}_{BIA} + \hat{H}_{SIA}, \quad (2)$$

$$\hat{H}_{BIA} = \frac{\gamma_c}{\hbar^3}\left[\sigma_x p_x(p_y^2 - \hat{p}_z^2) + \sigma_y p_y(\hat{p}_z^2 - p_x^2) + \sigma_z \hat{p}_z(p_x^2 - p_y^2)\right], \quad (3)$$

$$\hat{H}_{SIA} = a_{so}(\sigma_x p_y - \sigma_y p_x)\partial_z V(z), \quad (4)$$

where σ_x, σ_y and σ_z are the Pauli matrices.

Aiming to take into account the microscopic structure of the interfaces, we introduce appropriate boundary conditions (BCs) for the effective wave function. The phenomenological BC for a single (001) GaAs/AlGaAs heterointeface with C_{2v} symmetry taking into account the spin-orbit interaction with atomically sharp interfacial potential was derived in Refs. [16 and 17] from the general physical requirements. Since the interfaces are, in general, non-equivalent we describe them by such BCs with different phenomenological parameters

$$\hat{\Gamma}_1\phi(z)\,|_{z=d/2} = 0, \quad \hat{\Gamma}_2\phi(z)\,|_{z=-d/2} = 0, \quad (5)$$

$$\hat{\Gamma}_{1(2)} = \left[\begin{array}{c} \hat{1} - i\dfrac{R_{1(2)}}{\hbar}\hat{\mathbf{p}}\mathbf{n} - i\dfrac{2m^*\gamma_c R_{1(2)}}{\hbar^4}(\sigma_y p_y - \sigma_x p_x)\hat{\mathbf{p}}\mathbf{n} + \\[2mm] + \dfrac{(\chi + \chi_{1(2)}^{int})R_{1(2)}}{\hbar}\boldsymbol{\sigma}(\hat{\mathbf{p}}\times\mathbf{n}) - \dfrac{2m^*\gamma_{c_{1(2)}}^{int}}{\hbar^3}(\sigma_y p_y - \sigma_x p_x) \end{array}\right]. \quad (6)$$

Here $\mathbf{n}$ is the unit vector directed along the external normal to the corresponding interface; R_1 (R_2) is a real quantity describing the spectrum of the Tamm's states near the right (left) boundary if they exist (for this sake the condition $R > 0$ must be fulfilled); χ is the bulk spin-orbit parameter ($\chi = 0.082$ for GaAs); $\gamma_{c_1}^{int}, \chi_1^{int}$ and $\gamma_{c_2}^{int}, \chi_2^{int}$ characterizes the spin-orbit interaction at the right and left heterointerfaces, respectively.

In the lowest order over the scalar contributions of the interfaces and the ISOI parameters, the operators $\hat{\Gamma}_{1(2)}$ in the BCs (5) can be transformed to the unitary form

$$\hat{\tilde{\Gamma}}_{1(2)} = \exp(i\hat{g}_{1(2)}\hat{p}_z/\hbar) \text{ with } \hat{g}_{1(2)} \text{ satisfying}$$

$$\begin{aligned} \hat{g}_{1(2)} = &-R_{1(2)}n_z - \frac{2m^*\gamma_c R_{1(2)}}{\hbar^3}(\sigma_y p_y - \sigma_x p_x)n_z - \\ &-\frac{(\chi + \chi_{1(2)}^{int})R_{1(2)}^2}{\hbar}(\sigma_x p_y - \sigma_y p_x) - \\ &-\frac{2m^*\gamma_{c_{1(2)}}^{int} R_{1(2)}}{\hbar^3}(\sigma_y p_y - \sigma_x p_x)n_z, \end{aligned} \quad (7)$$

where $n_z = 1$ for the right interface and $n_z = -1$ for the left one. To obtain $\hat{\tilde{\Gamma}}_{1(2)}$ we multiply $\hat{\Gamma}_{1(2)}$ by

the operator $\left\{1+\left[\left(\chi+\chi_{1(2)}^{\mathrm{int}}\right)R_{1(2)}/\hbar\right]\boldsymbol{\sigma}(\hat{\mathbf{p}}\times\mathbf{n})-\left[2m^*\gamma_{c_{1(2)}}^{\mathrm{int}}/\hbar^3\right](\sigma_y p_y-\sigma_x p_x)\right\}^{-1}$ from the left and neglect the terms nonlinear over the SOI parameters.

If the system allows to perform spin diagonalization, the operators $\hat{g}_1$ and $\hat{g}_2$ transform into scalar quantities $\varDelta d_1$ and $\varDelta d_2$, respectively, having the dimensionality of length. In this case the operator $\hat{\Gamma}_{1(2)}$ just shifts the right (left) boundary to the new position $z_r = d/2 + \varDelta d_1$ ($z_l = -d/2 + \varDelta d_2$) which depends on the spin projection $\sigma = \pm 1$ and the corresponding interfacial parameters. Such spin diagonalization is possible in the systems with only one type of SOI (Rashba or Dresselhaus).

We begin with the case when only Rashba SOI is present. The resulting problem reads as

$$\left(\frac{\hat{p}_z^2}{2m^*}+V(z)+a_{so}p\sigma\partial_z V\right)\psi_\sigma(z)=E_\sigma\psi_\sigma(z), \quad (8)$$

$$\psi_\sigma(z)|_{z=d/2+\Delta d_1}=0, \quad \psi_\sigma(z)|_{z=-d/2+\Delta d_2}=0, \quad (9)$$

$$\Delta d_{1(2)}=-R_{1(2)}n_z+\frac{\tilde{\chi}_{1(2)}R_{1(2)}^2}{\hbar}p\sigma, \quad (10)$$

where $\tilde{\chi}_{1(2)}=\chi+\chi_{1(2)}^{\mathrm{int}}$, p is the absolute value of 2D momentum.

The further analysis is organized as follows. At first we consider the simple problem

$$\left(\frac{\hat{p}_z^2}{2m^*}+V(z)\right)\psi^{(0)}=E^{(0)}\psi^{(0)}, \quad (11)$$

$$\psi^{(0)}(z)|_{z=z_r}=0, \quad \psi^{(0)}(z)|_{z=z_l}=0, \quad (12)$$

which allows an exact numerical solution for an arbitrary potential profile $V(z)$. Next we assume $\varDelta d_1$ and $\varDelta d_2$ to be much smaller than d and obtain the energy spectrum of the problem (8)-(10). In the lowest order over the SOI parameters it reads as

$$E_\sigma = E^{(0)} + a_{so}\left\langle\psi^{(0)}\,|\,\partial_z V\,|\,\psi^{(0)}\right\rangle p\sigma +$$
$$+\frac{\partial E^{(0)}}{\partial z_r}\bigg|_{-\frac{d}{2},\frac{d}{2}}\Delta d_1 + \frac{\partial E^{(0)}}{\partial z_l}\bigg|_{-\frac{d}{2},\frac{d}{2}}\Delta d_2. \quad (13)$$

Finally, we calculate the spin splitting $E_{SS}=(E_{+1}-E_{-1})$ and, comparing it with (1), obtain α_{SIA}

$$\alpha_{\mathrm{SIA}}=\alpha_{\mathrm{SIA}}^{(0)}+\frac{\tilde{\chi}_1 R_1^2}{\hbar}\frac{\partial E^{(0)}}{\partial z_r}\bigg|_{-\frac{d}{2},\frac{d}{2}}+\frac{\tilde{\chi}_2 R_2^2}{\hbar}\frac{\partial E^{(0)}}{\partial z_l}\bigg|_{-\frac{d}{2},\frac{d}{2}}. \quad (14)$$

Here the last two terms are the desired interfacial contributions. In the system with only Dresselhaus-type SOI we have

$$\Delta d_{1(2)}=-R_{1(2)}n_z-\frac{2m^*\tilde{\gamma}_{c_{1(2)}}R_{1(2)}}{\hbar^3}n_z p\sigma, \quad (15)$$

where $\tilde{\gamma}_{\tilde{n}_{1(2)}}=\gamma_{\tilde{n}}+\gamma_{\tilde{n}_{1(2)}}^{\mathrm{int}}$. Performing the similar analysis as before we obtain interfacial contributions to α_{BIA}

$$\alpha_{\mathrm{BIA}}=\alpha_{\mathrm{BIA}}^{(0)}-\frac{2m^*(\gamma_c+\tilde{\gamma}_{c_1})R_1}{\hbar^3}\frac{\partial E^{(0)}}{\partial z_r}\bigg|_{-\frac{d}{2},\frac{d}{2}}-$$
$$-\frac{2m^*\tilde{\gamma}_{c_1}R_1}{\hbar^3}\frac{\partial E_2^{(0)}}{\partial z_r}\bigg|_{-\frac{d}{2},\frac{d}{2}}+\frac{2m^*(\gamma_c+\tilde{\gamma}_{c_2})R_2}{\hbar^3}\frac{\partial E_1^{(0)}}{\partial z_l}\bigg|_{-\frac{d}{2},\frac{d}{2}}+ \quad (16)$$
$$+\frac{2m^*\tilde{\gamma}_{c_2}R_2}{\hbar^3}\frac{\partial E_2^{(0)}}{\partial z_l}\bigg|_{-\frac{d}{2},\frac{d}{2}},$$

where $E_1^{(0)}=\left\langle\psi^{(0)}(z)\,|\,\hat{p}_z^2/2m^*\,|\,\psi^{(0)}(z)\right\rangle$, $E_2^{(0)}=\left\langle\psi^{(0)}(z)\,|\,V(z)\,|\,\psi^{(0)}(z)\right\rangle$.

One can expect that since all spin-orbit constants are small in general case when both Rashba and Dresselhaus type terms are allowed in the effective spin Hamiltonian, the corresponding spin splitting has the form (1), where in the lowest order over SOI parameters, α_{SIA} and α_{BIA} are still determined by Eqs. (14) and (16), respectively. This assumption will be verified below on a simple example.

It is important to note that the interfacial contributions to α_{SIA} and α_{BIA} can be calculated in a QW with arbitrary doping level and potential distribution since one is always able to find $E^{(0)}$ and $\psi^{(0)}$ numerically. However, in some cases transparent analytical results can be obtained. As an example we now consider the "narrow" QW in which the size quantization energy much exceeds the energy of the electron interaction with the smooth (in the atomic scale) potential $V(z)$. Treating the potential $V(z)$ as a perturbation, we obtain from Eqs. (14) and (16) for the ground subband

$$\alpha_{\mathrm{SIA}}=\alpha_{\mathrm{SIA}}^{(0)}-\frac{2\tilde{E}_0}{\hbar}\frac{(\tilde{\chi}_1 R_1^2-\tilde{\chi}_2 R_2^2)}{d}+$$
$$+\frac{eFd}{2E_0}\frac{E_0}{\hbar}\frac{(\tilde{\chi}_1 R_1^2+\tilde{\chi}_2 R_2^2)}{d}, \quad (17)$$

$$\alpha_{\mathrm{BIA}}=\alpha_{\mathrm{BIA}}^{(0)}-\frac{2k_0^2}{\hbar}\left[\frac{\gamma_c(R_1+R_2)}{d}+\right.$$
$$\left.+\frac{\tilde{E}_0}{E_0}\frac{(\tilde{\gamma}_{c1}R_1+\tilde{\gamma}_{c2}R_2)}{d}+\frac{eFd}{4E_0}\frac{(\tilde{\gamma}_{c2}R_2-\tilde{\gamma}_{c1}R_1)}{d}\right], \quad (18)$$

where

$$k_0 = \pi / d, \quad eF = \langle \psi_0(z) | V'(z) | \psi_0(z) \rangle,$$

$$\psi_0(z) = \sqrt{2/d}\, \cos k_0 z, \quad E_0 = \frac{\hbar^2 k_0^2}{2m^*}, \tag{19}$$

$$\tilde{E}_0 = E_0 - \frac{1}{2}\langle \psi_0(z) | z V'(z) | \psi_0(z) \rangle.$$

It follows from Eqs. (17) and (18) that the ISOI not only renormalizes the values of α_{BIA} and α_{SIA}, but also affect the qualitative behaviour of the spin splitting. The spin splitting is anisotropic in the structures where both Dresselhaus- and Rashba-type SOIs are present. In the framework of the envelope functions approximation, α_{SIA} is commonly assumed to be nonzero only in the structures with built-in or external electric field. However, it is seen from the Eq. (17) that if the interfaces are non-equivalent, i.e. $\tilde{\chi}_1 R_1^2 \neq \tilde{\chi}_2 R_2^2$, the α_{SIA} is finite even in the QWs with zero average electric field. This effect gives rise to anisotropy of the spin splitting in such structures. Our theory naturally explains the results of Ref. [4] where significantly nonzero α_{SIA} was observed in the nominally symmetric QW with equally doped sides and zero average electric field. At the same time, the interfacial contribution to α_{BIA} is nonzero even for structures with identical boundaries, i.e. $\gamma_{c_1}^{\text{int}} = \gamma_{c_2}^{\text{int}}$ and $R_1 = R_2$.

Now we check if the above assumption regarding the additivity of the Rashba and Dresselhaus contributions in the lowest order over SOI constants is fulfilled in the "narrow" QW. For this purpose, we calculate the spin splitting starting from the 3D problem (2)-(5) with both types of SOI and compare obtained α_{SIA} and α_{BIA} with ones satisfying (17) and (18).

Aiming to analyse the effect of ISOI on the spin splitting, we take into account the interaction with the interfacial potential exactly. At the same time, bulk SOI $\hat{H}_{BIA} + \hat{H}_{SIA}$ and the smooth potential $V(z)$ which average value is assumed to be small in comparison with the size quantization energy are treated perturbatively. At first, we consider the following problem

$$\frac{\hat{p}_z^2}{2m^*}\phi^{(0)}(z) = \in^{(0)} \phi^{(0)}(z), \tag{20}$$

$$\hat{\Gamma}_1 \phi^{(0)}(z)|_{z=d/2} = 0, \quad \hat{\Gamma}_2 \phi^{(0)}(z)|_{z=-d/2} = 0. \tag{21}$$

Introducing the values

$$\alpha_{1(2)} = 2m^* \tilde{\gamma}_{c_{1(2)}} R_{1(2)} p / \hbar^3,$$

$$\beta_{1(2)} = \tilde{\chi}_{1(2)} R_{1(2)}^2 p / \hbar,$$

$$\Delta = (\alpha_1 + \alpha_2)e^{-i\phi} - i(\beta_1 - \beta_2)e^{i\phi},$$

$$\tilde{\Delta} = (\alpha_1 - \alpha_2)e^{-i\phi} + i(\beta_1 - \beta_2)e^{i\phi}$$

we obtain the eigenvalues and eigenfunctions of the problem (20)-(21) in the lowest order over the scalar contributions of the interfaces and the ISOI parameters $\in_\pm^{(0)} = E_0 [1 + 2(R_1 + R_2)/d \pm 2|\Delta|/d]$,

$$\phi_\pm^{(0)}(z) = \begin{pmatrix} C_1^\pm e^{-ik_\pm z} + C_3^\pm e^{ik_\pm z} \\ C_2^\pm e^{-ik_\pm z} + C_4^\pm e^{ik_\pm z} \end{pmatrix}, \tag{22}$$

where

$$k_\pm = k_0 [1 + (R_1 + R_2)/d \pm |\Delta|/d],$$

$$C_2^\pm = \mp \frac{\Delta^*}{|\Delta|}C_1^\pm, \quad C_3^\pm = \left[1 + ik_0(R_1 - R_2) \pm \frac{\tilde{\Delta}}{\Delta}|\Delta|\right]C_1^\pm, \tag{23}$$

$$C_4^\pm = \left[\mp \frac{\Delta^*}{|\Delta|} - ik_0 \tilde{\Delta}^*\right]C_1^\pm, \tag{24}$$

and $|C_1| = (1/4d)[1 - (R_1 + R_2)/d \mp |\Delta|/d]^{-2}$.

Next we find the spectrum of the problem (2)-(5) using the eigenfunctions (22) as a basis $\phi(z) = A\phi_+^{(0)} + B\phi_-^{(0)}$ and considering $\hat{\delta H} = \hat{H}_{BIA} + \hat{H}_{SIA} + V(z)$ as a perturbation

$$\begin{pmatrix} \in_+^{(0)} + \langle \phi_+^{(0)} | \delta\hat{H} | \phi_+^{(0)} \rangle & \langle \phi_+^{(0)} | \delta\hat{H} | \phi_-^{(0)} \rangle \\ \langle \phi_-^{(0)} | \delta\hat{H} | \phi_+^{(0)} \rangle & \in_-^{(0)} + \langle \phi_-^{(0)} | \delta\hat{H} | \phi_-^{(0)} \rangle \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} =$$

$$= E \begin{pmatrix} A \\ B \end{pmatrix}. \tag{25}$$

As it was expected, we obtain that the resulting spin splitting of the spectrum has the form (1) with α_{SIA} and α_{BIA} satisfying Eqs. (17) and (18), respectively.

The values of the interfacial parameters can be extracted from comparison with the experiment, as it was done for the wide one-side doped quantum well GaAs/AlGaAs in Ref.[17]. Let us, for example, evaluate the values $\tilde{\chi}_1 R_1^2$ and $\tilde{\chi}_2 R_2^2$ comparing Eq. (17) with the experimental data from Ref. [4]. Due to the fact that all quantum wells were grown under the same conditions we assume the interfacial parameters to be equal for all structures. However, in each quantum well the left interface is not equivalent to the right one. We also suppose $\tilde{E}_0 \approx E_0$. For the symmetrical sample with $F = 0$ and $d = 12$ nm the parameter $\alpha_{\text{SIA}} = (0.4 \cdot 10^{-3})v_F$ ($v_F = 4.11 \cdot 10^7$ sm/s is the Fermi velocity) is determined

from the difference between $\tilde{\chi}_1 R_1^2$ and $\tilde{\chi}_2 R_2^2$. Thus, we can estimate this difference as $\tilde{\chi}_1 R_1^2 - \tilde{\chi}_2 R_2^2 = 1.4\text{Å}^2$. Next we consider the sample with the same thickness and asymmetrical doping for which [4] $\alpha_{SIA} = (1.3 \cdot 10^{-3})\ v_F$. Performing the self-consistent solution of the Shrödinger and Poisson equations, we obtain $F = 2.085 \cdot 10^5\ V/sm$. Thus, we evaluate $\tilde{\chi}_1 R_1^2 + \tilde{\chi}_2 R_2^2 = 7.7\ 2$. Finally, we find $\tilde{\chi}_1 R_1^2 = 4.6\text{Å}^2$, $\tilde{\chi}_2 R_2^2 = 3.1\text{Å}^2$. The experimental data presented in Ref. [4] is not enough to calculate $\tilde{\chi}_1$, $\tilde{\chi}_2$, R_1 and R_2 separately. However, some estimates can be obtained. The typical value of R is in the order of $\sim$20Å [17]. Thus, we evaluate $\tilde{\chi}_1 \sim 0.012$ and $\tilde{\chi}_2 \sim 0.008$. The corresponding values $\tilde{\chi}_1^{int} \sim -0.07$ and $\tilde{\chi}_2^{int} \sim -0.74$ are the same order as bulk value $\chi = 0.082$.

3. CONCLUSION

In conclusion we developed the theory of ISOI in the narrow QWs. We have obtained the renormalization of the Dresselhaus and Rashba parameters arising from the SOI at two heterointerfaces. The considerable spread in the experimentally determined values of spin-orbit constants can originate from the dependence of α_{BIA} and α_{SIA} on the interfacial parameters and, thus, on the growth conditions. We also have demonstrated that the microscopic dissimilarity of the interfaces leads to the finite Rashba parameters even in the QWs with zero average electric field. This result explains the experimental data of Ref. [4] where nonzero α_{SIA} was obtained in the symmetric structure.

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