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# Spin splitting of conduction subbands in GaAs-$Ga_{0.7}Al_{0.3}As$ heterostructures

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The spin splitting of conduction subbands in GaAs-$Ga_{0.7}Al_{0.3}As$ heterostructures is calculated using a five-level $\mathbf{k}\cdot\mathbf{p}$ model and taking fully into account both bulk and structural inversion asymmetry of the system. The role of the boundary conditions for the structural inversion asymmetry is emphasized and it is shown (in contradiction to previous work) that this mechanism is of decisive importance for the spin splitting. Our theory is in agreement with the recent Raman data.

Spin splitting of electric subbands in GaAs-$Ga_{1-x}Al_xAs$ heterostructures has attracted in recent years a considerable amount of theoretical and experimental interest. The problem goes back to the well-known property of bulk semiconductors: in a material with bulk inversion asymmetry (BIA) the energy bands are spin split for a given direction of the wave vector $\mathbf{k}$. In heterostructures the spin splitting may also occur as a result of structure inversion asymmetry (SIA), which was first pointed out by Bychkov and Rashba.[1] The history of the subject is quite controversial. An early theory of Ohkawa and Uemura[2] showed that in a system with an asymmetric potential $V(z)$ the spin splitting is proportional to $\partial V/\partial z$. However, as remarked by Darr, Kotthaus, and Ando,[3] in bound states the average value of $\partial V/\partial z$ vanishes. Lassnig[4] considered the effect of SIA in GaAs-$Ga_{1-x}Al_xAs$ heterostructures within an incomplete five-level $\mathbf{k}\cdot\mathbf{p}$ model, taking into account a mass discontinuity at the interface and assuming that the average electric field in the structure vanishes. In an often quoted work, Malcher, Lommer, and Rossler[5] took into account both BIA and SIA and pointed out that the mass discontinuity in a heterostructure results in an additional force. Since it is the mean value of the force that vanishes in a bound state, the average electric field is nonzero. Sobkowicz[6] treated SIA in narrow-gap heterostructures and showed that boundary conditions involve terms not considered in Ref. 5 (cf. also Bastard, Brum, and Ferreira[7]). Eppenga and Schurmann[8] calculated an anisotropy of the subband splitting due to BIA in GaAs/AlAs quantum wells. In a recent paper Andrada e Silva, La Rocca, and Bassani[9] followed the approach of Ohkawa and Uemura. On the experimental side there exists an attempt to measure the spin splitting in GaAs-$Ga_{1-x}Al_xAs$ at $B=0$ by means of spin resonance (Stein, von Klitzing, and Weimann[10]), an observation of the spin precession using antilocalization by Dresselhaus *et al.*,[11] and a direct measurement of the spin splitting with the use of Raman scattering by Jusserand *et al.*[12] The conclusion of the last two papers is that in GaAs-$Ga_{1-x}Al_xAs$ heterostructures the spin splitting is dominated by the BIA mechanism, which follows the theoretical result of Ref. 5. There has been also some controversy concerning a reduction of the bulk spin splitting to that in two-dimensional (2D) systems (cf. Santos and Cardona[13]).

Here we present a theory of the subband spin splitting in heterostructures due to both BIA and SIA mechanisms. Compared to the previous work our approach fully accounts for BIA of the crystal and demonstrates the decisive importance of the boundary conditions in SIA mechanism. The formalism is applied to GaAs-$Ga_{1-x}Al_xAs$ heterostructures and the results are compared with available experimental data. Our conclusions contradict those mentioned above.

We begin with the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian written in the five-level model of $\Gamma_7^v,\Gamma_8^v,\Gamma_6^c,\Gamma_7^c,\Gamma_8^c$ levels, as derived by Pfeffer and Zawadzki[14] (PZ). The resulting $14\times14$ matrix is completed by the external potential $V(z)$ on the diagonal. This potential is characterized by a jump at the interface (at $z=0$). Also the band parameters have different values on both sides of the interface. Because of the translational symmetry in the $x$-$y$ plane, $k_x$ and $k_y$ are good quantum numbers. Using the perturbation theory up to the third order we obtain the following eigenvalue problem for the two spin states of the $\Gamma_6$ conduction band:

$$\begin{pmatrix} \hat{A}+\hat{B}-\lambda & \hat{K} \\ \hat{K}^\dagger & \hat{A}-\hat{B}-\lambda \end{pmatrix}\begin{pmatrix} \Phi_1(z) \\ \Phi_2(z) \end{pmatrix}=0, \tag{1}$$

where

$$\hat{A}=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}-\frac{\hbar^2F}{2}\frac{\partial}{\partial z}+\frac{\hbar^2k_\perp^2}{2m^*}+V(z), \tag{2}$$

$$\hat{B}=i(k_x^2-k_y^2)\gamma\frac{\partial}{\partial z},$$

$$\hat{K}=-i\frac{k_-}{\sqrt{2}}M-ik_xk_yk_-\sqrt{2}\gamma-\sqrt{2}k_+ \times\left[\gamma\frac{\partial^2}{\partial z^2}+\delta(z)(\gamma_r-\gamma_l)\frac{\partial}{\partial z}\right], \tag{3}$$

in which

 

$$F=\frac{1}{3}\frac{2m_0}{\hbar^2}\frac{\partial V(z)}{\partial z}\left\{P_0^2\left(\frac{2}{E_0^2}+\frac{1}{G_0^2}\right)+P_1^2\left(\frac{2}{G_1^2}+\frac{1}{E_1^2}\right)+\frac{4\tilde{\Delta}P_0P_1}{3}\left(\frac{1}{E_1G_0^2}+\frac{1}{E_1^2G_0}-\frac{1}{E_0^2G_1}-\frac{1}{E_0G_1^2}\right)\right\}, \quad (4)$$

for $z\neq 0$, and $F=\delta(z)(1/m_r^*-1/m_l^*)$ for $z=0$,

$$\eta=\frac{2}{3}\left\{P_0^2\left(\frac{1}{E_0}-\frac{1}{G_0}\right)+P_1^2\left(\frac{1}{G_1}-\frac{1}{E_1}\right)-\frac{2\tilde{\Delta}P_0P_1}{3}\left(\frac{1}{E_0G_1}+\frac{2}{E_1G_0}\right)\right\}, \quad (5)$$

$$M=-\frac{2}{3}\frac{\partial V(z)}{\partial z}\left\{P_0^2\left(\frac{1}{E_0^2}-\frac{1}{G_0^2}\right)+P_1^2\left(\frac{1}{G_1^2}-\frac{1}{E_1^2}\right)-\frac{2\tilde{\Delta}P_0P_1}{3}\left(\frac{1}{E_0G_1^2}+\frac{1}{E_0^2G_1}+\frac{2}{E_1G_0^2}+\frac{2}{E_1^2G_0}\right)\right\}, \quad (6)$$

for $z\neq 0$, and $M=\delta(z)(\eta_r-\eta_l)$ for $z=0$. Here $m^*$ is the effective mass of conduction electrons at the band edge, $\gamma$ is proportional to the spin splitting of the conduction band in the bulk crystal (both defined in PZ), and $k_\pm=(k_x\pm ik_y)/\sqrt{2}$. The matrix elements of momentum $P_0,P_1,Q$, the energy gaps $E_0,E_1$, the spin-orbit energies $\Delta_0,\Delta_1,\tilde{\Delta}$, and their combinations $G_0,G_1$ have been defined in PZ, subscripts $r$ and $l$ denote the corresponding values at the right and left side of the interface, and $\delta(z)$ is the Dirac delta function. The above expressions contain some simplifications having negligible effect on the final results. Generally speaking, the terms involving $\gamma$ are related to BIA, while those involving $\eta$ and $M$ are related to SIA. The inspection of the final results shows that the $\hat{B}$ terms in (1) have a negligible influence on the spin splitting. Hence we omit them in the following considerations.

To solve the set (1) one can use general methods applicable to $2\times 2$ eigenvalue matrices. After some manipulations we obtain

$$K^2(\hat{A}-\lambda)\Phi_1+C(\hat{G}_R-i\hat{G}_I)\Phi_2=0, \quad (7a)$$

$$(\hat{G}_R+i\hat{G}_I)\Phi_1+C(\hat{A}-\lambda)\Phi_2=0, \quad (7b)$$

where $K\hat{K}^\dagger=\hat{G}_R+i\hat{G}_I$ and $K^\dagger\hat{K}=\hat{G}_R-i\hat{G}_I$, while $K^2=\langle\Phi_1|\hat{K}|\Phi_2\rangle\langle\Phi_2|\hat{K}^\dagger|\Phi_1\rangle$, and $C=(\varepsilon_{12}^2+K^2)^{1/2}-\varepsilon_{12}$, in which $\varepsilon_{12}=\varepsilon_1^0-\varepsilon_2^0$. Energies $\varepsilon_1^0$ and $\varepsilon_2^0$ are eigenvalues of the equations $\hat{A}\Phi_1=\varepsilon_1^0\Phi_1$ and $\hat{A}\Phi_2=\varepsilon_2^0\Phi_2$. If the terms $\hat{K}$ in (1) did not contribute to the boundary conditions for the functions $\Phi_1$ and $\Phi_2$, the latter would be identical. This is, however, not the case. The set (7) is equivalent to four coupled differential equations for real and imaginary parts of $\Phi_1$ and $\Phi_2$. In addition, these functions are coupled by complicated boundary conditions. In order to simplify the problem we average over the angle $\varphi$ in the $k_x$-$k_y$ plane. The averaged coefficients of (7) have the form

$$\hat{G}_R^{k_\perp^2}=\bar{G}_R=\frac{k_\perp^2}{4}\left[\langle M\rangle M+4\left\langle\gamma\frac{\partial^2}{\partial z^2}\right\rangle\gamma\frac{\partial^2}{\partial z^2}+\frac{k_\perp^4}{2}\langle\gamma\rangle\gamma+k_\perp^2\left(\langle\gamma\rangle\gamma\frac{\partial^2}{\partial z^2}+\left\langle\gamma\frac{\partial^2}{\partial z^2}\right\rangle\gamma\right)\right], \quad (8)$$

$$\hat{G}_I^{k_\perp^2}=0, \quad (9)$$

where the symbol $\langle I\rangle$ means $\langle\Phi_1|I|\Phi_2\rangle$. Thus the averaged coefficients in (7) are real. We now add and subtract Eqs. (7a) and (7b), which gives

$$\left(\hat{A}-\lambda+\frac{\bar{G}_R}{|K|}\right)F_1=0, \quad (10a)$$

$$\left(\hat{A}-\lambda-\frac{\bar{G}_R}{|K|}\right)F_2=0, \quad (10b)$$

where $F_1=|K|\Phi_1+C\Phi_2$ and $F_2=|K|\Phi_1-C\Phi_2$. In the set (10) the functions $F_1$ and $F_2$ are decoupled and the eigenvalue problems can be solved separately for the two states and energies.

The boundary conditions are found by integrating Eqs. (10) across the interface at $z=0$. For $F_1$ we obtain

$$F_1|_{+0}=F_1|_{-0}, \quad (11)$$

$$\left.\frac{\partial F_1}{\partial z}\right|_{+0}=\left(\frac{\hbar^2}{2m_l^*}\left.\frac{\partial F_1}{\partial z}\right|_{-0}+R\right)\left(\frac{\hbar^2}{2m_r^*}-S\right)^{-1}, \quad (12)$$

where

$$R=\frac{k_\perp^2}{4|K|}\left[\langle M\rangle(\eta_r-\eta_l)F_1|_{-0}-\left.\frac{\partial F_1}{\partial z}\right|_{-0}\times\left(4\left\langle\gamma\frac{\partial^2}{\partial z^2}\right\rangle+k_\perp^2\langle\gamma\rangle\right)\gamma_1\right], \quad (13)$$

$$S=\frac{k_\perp^2}{4|K|}\left(4\left\langle\gamma\frac{\partial^2}{\partial z^2}\right\rangle+k_\perp^2\langle\gamma\rangle\right)\gamma_r \quad (14)$$

in which, again, the subscripts $r$ (and $l$) mark the values to the right (and left) of the interface. In expressions (13) and (14) we have omitted negligible terms. The boundary conditions for $F_2$ have the form similar to (11) and (12), the difference being the change of signs in front of $R$ and $S$ in (12). In principle the total wave function has a multicomponent character and the boundary conditions should take this feature into account (cf. Marques and Sham[15] and Sobkowicz[6]), but since we are interested in medium-gap materials of GaAs type the conditions for the dominant $\Gamma_6^c$ component of the wave function provide a very good approximation.

We apply the above formalism to the GaAs-$Ga_{0.7}Al_{0.3}As$ heterojunction by specifying the potential and the band parameters on both sides of interface. The potential is found in a self-consistent way by taking a parametrized $V(z)$ dependence and the generalized Fang-Howard subband function (penetrating the $Ga_{1-x}Al_xAs$ region to the left, as described by Bastard;[16] cf. also Ando[17]). Generalizing slightly this approach by taking the decaying penetration in the form

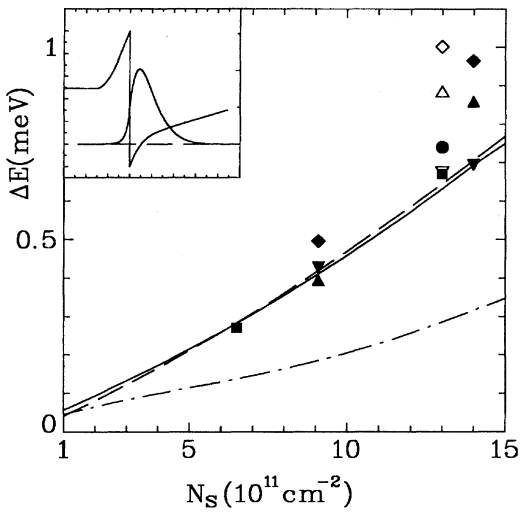


FIG. 1. Spin splitting of the lowest subband in GaAs-$Ga_{0.7}Al_{0.3}As$ heterojunction vs electron density ($N_{depl}=8\times10^{10}$ $cm^{-2}$). Dashed-dotted line, theory for bulk inversion asymmetry alone; dashed line, structural inversion asymmetry alone; solid line, the effect of both mechanisms. Experimental values: Jusserand *et al.* (Ref. 12): ● (averaged over $\mathbf{k}_F$ directions); Jusserand *et al.* (Ref. 21): ◇, $\mathbf{k}_F\|[100]$, △, $\mathbf{k}_F\|[1\bar{1}0]$, ▽, $\mathbf{k}_F\|[110]$; Richards *et al.* (Ref. 22): ◆, $\mathbf{k}_F\|[100]$, ▲, $\mathbf{k}_F\|[1\bar{1}0]$, ▼, $\mathbf{k}_F\|[110]$; ■, $\mathbf{k}_F$ direction unknown. The inset shows self-consistent potential of the heterojunction and the wave function for the ground electric subband as calculated for $N_s=6\times10^{11}$ $cm^{-2}$.

$\exp(-k_bz)$, where $k_b=2[(V_b-E)2m_l^*/\hbar^2]^{1/2}$, in which $V_b$ is the offset and $E$ is the subband energy, we find complete agreement with the fully self-consistent results of Stern and Das Sarma.[18]

We take the following band parameters for GaAs (cf. PZ): $m^*=0.0660m_0$, $\eta=-9.131$ eV Å$^2$, $\gamma=24.12$ eV Å$^3$, $E_0=-1.519$ eV, $G_0=-1.86$ eV, $E_1=2.969$ eV, $G_1=3.14$ eV, $\bar{\Delta}=-0.061$ eV, $E_{P_0}=2m_0P_0^2/\hbar^2=27.86$ eV, $E_{P_1}=2.36$ eV, $E_Q=15.56$ eV. For $Ga_{0.7}Al_{0.3}As$ we take $m^*=0.0880m_0$, $\eta=-5.844$ eV Å$^2$, $\gamma=18.03$ eV Å$^3$, $E_0=-1.921$ eV, $G_0=-2.242\,86$ eV, $E_1=2.671$ eV, $G_1=2.842$ eV (the values of matrix elements and $\bar{\Delta}$ are taken to be the same as for GaAs). The offset value is $V_b=0.240$ eV.

The spin splitting of the first electric subband due to both BIA and SIA mechanisms is shown in Fig. 1 as a function of the electron density $N_s$ (solid line). The dashed-dotted line shows the spin splitting caused by BIA alone (obtained by neglecting in the theory the terms $\eta$ and $M$). On the other hand, the SIA mechanism alone gives almost the same splitting as the combined effect of BIA and SIA. Thus, we find that the two mechanisms are strongly nonadditive (in contradiction to the conclusion of Ref. 5). This is due to the strong influence of the complete boundary conditions for the SIA mechanism [i.e., the conditions which account for both diagonal and nondiagonal terms in (1)]. Malcher, Lommer, and Rossler[5] used for the boundary conditions only the diagonal terms in (1) and treated the nondiagonal terms as a perturbation (which for $2\times2$ matrix can be done exactly). This approximation gives good results for the BIA mechanism, as stated by Eppenga and Schurmann[8] and confirmed by our calculation. (Thus for the BIA mechanism alone we calculate roughly the same as Ref. 5, apart from some differences in the band parameters.) On the other hand, for the SIA mechanism this is a very poor approximation, which results in a considerable underestimation of the splitting. Applying those oversimplified boundary conditions to the SIA mechanism we would get for $N_s=10^{12}$ $cm^{-2}$ the splitting $\Delta E(\mathrm{SIA})=0.17$ meV, whereas the complete calculation gives $\Delta E(\mathrm{SIA})=0.46$ meV. The results of Ref. 5 in addition underestimate the splitting due to SIA by taking it to be proportional to the average electric field in the structure. As stated above, the average field is nonzero only due to the difference of electron effective masses in GaAs and $Ga_{0.7}Al_{0.3}As$. Since this difference is small, the resulting average field and consequently the SIA splitting are also small. (According to this approach in the limit of $m_l^*-m_r^*\to0$ there would be no SIA splitting.) However, in the multiband scheme the SIA splitting is *not* proportional to the average electric field, since the band discontinuities in different bands are *not* the same. This was first pointed out by Lassnig,[4] and recently recognized by Winkler and Rossler.[19] In our formulas this is seen from the fact that the quantity $M$ at $z=0$ is not proportional to $\partial V/\partial z$. All in all, our results show that the SIA mechanism plays a considerable role for the spin splitting in GaAs-$Ga_{0.7}Al_{0.3}As$ heterojunctions, in contradiction to the conclusion of Ref. 5.

The weakest point in our treatment of the SIA mechanism is the band parameters of $Ga_{0.7}Al_{0.3}As$ alloy. We have taken the known values of energy gaps, but in the evaluation of $\gamma$ and especially $\eta$ for this material the momentum matrix elements and the interband spin-orbit energy $\bar{\Delta}$ have been taken to be the same as in GaAs, which is certainly not quite true.

As to the comparison of our theory with experiment, the antilocalization transport data of Dresselhaus *et al.*[11] measure the spin precession of conduction electrons, which can be related to the energy spin splitting via the Dyakonov-Perel theory.[20] However, as stated by the authors, the precession is related to only a part of the splitting. Using Eq. (5) of Ref. 11 one obtains $\Delta E=2\gamma(\pi N_s)^{3/2}$. Taking their determined value of $\gamma=26.1$ eV Å$^3$ we get roughly 70% of our splitting (the solid line in Fig. 1) and a similar dependence on $N_s$ in the range of interest. However, the transition from the measured values of the spin-orbit magnetic field $H_{so}$ to the above expression for $\Delta E$ is based on the hypothesis that the spin splitting is described only by the BIA formula in which one puts $k_z=0$. Both these assumptions are highly questionable (as to putting $k_z=0$, cf. Ref. 13). Also the measured $H_{so}\sim N_s^2$ dependence, emphasized in Ref. 11, is not conclusive for the predominance of the BIA mechanism, as the considerations are based from the very beginning on the considerable underestimation of the SIA mechanism.[5]

Jusserand *et al.*[12] measured the spin splitting of the first subband in GaAs-$Ga_{0.7}Al_{0.3}As$ modulation-doped quantum wells much more directly using Raman scattering. The ex-

periments with nonpolarized light yield the spin splitting averaged over the $k_x$-$k_y$ plane, which is directly comparable with our theory. The value published in Ref. 12 is quoted in Fig. 1. Very recent data of Jusserand *et al.*[21] and Richards *et al.*[22] are also included. These data have been obtained with the use of polarized light, which differentiates between various directions of $\mathbf{k}_F$ in the plane perpendicular to the [100] direction. Our theory averages over $\mathbf{k}_F$ directions in the same plane. Since, as seen in Fig. 1, the spin splitting due to the BIA mechanism alone (dashed-dotted line) is considerably smaller than the splitting due to combined SIA+BIA mechanisms (solid line), this agreement signifies that in the investigated GaAs-$Ga_{0.7}Al_{0.3}As$ structures both inversion asymmetries are of importance. This conclusion is corroborated by the results of Jusserand *et al.*[21] on the directional dependence of the spin splitting in similar structures.

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