Rashba effect in inversion layers on *p*-type InAs MOSFET's

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For electrons in the inversion layer on bulk *p*-type InAs, the Rashba spin-orbit parameter is computed self-consistently as a function of areal electron density *Ns*. The spin splitting increases with *Ns* but is not a linear function of in-plane wave vector *k* and the corresponding Rashba parameter increases with increasing electric field but decreases very strongly with *k*. For the ground subband, and at the fermi level, this decrease with *k* combined with subband occupation yields a decreasing Rashba parameter α for $Ns < 1.97\times10^{12}\,\mathrm{cm}^{-2}$ and a nearly constant average value of 1.46×10^{-11} eV m above. At the doping level considered here ($1.8\times10^{17}\,\mathrm{cm}^{-3}$) the highest achievable value of $\alpha \cong 1.92\times10^{-11}$ eV m. Moreover α is a nonlinear function of *Ns*. Our results are compared to recent experimental work by Matsuyama *et al.* [Phys. Rev. B **61**, 15 588 (2000)] and previous theoretical treatments.

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With the potential for technological applications in new electronic devices, recent years witnessed a large amount of experimental[1–4] and theoretical[5–7] investigations of spin-related phenomena in artificial structures. The use of the spin degree of freedom in the semiconductor technology is a most attractive idea and for this goal, narrow-gap semiconductors such as InAs are serious candidates.[4] These materials are characterized by strong spin-orbit interaction and bulk inversion asymmetry[6] (BIA) that combine to lift the spin degeneracy of the energy spectrum. In heterostructures with structural inversion asymmetry[6] (SIA) as well such as heterojunctions, asymmetric quantum wells, and MOSFET's (metal-oxide-semiconductor field-effect transistor) where the surface potential is asymmetric, another spin-splitting mechanism adds. This is the so-called Rashba effect given by[8]

$$H_{SO} = \alpha(\vec{k}\times\hat{x})\cdot\vec{\sigma}, \tag{1}$$

where α is the Rashba spin-orbit parameter, while $\vec{\sigma}$ and $\hat{x}$ are the Pauli spin matrices and unit vector along the *x* axis, respectively. Theoretical[5,6] as well as experimental[1] work on quantum wells and heterojunctions established SIA to be dominant. Despite much effort, however, no general agreement has so far been reached as far as the dependence of α on the two-dimensional (2D) electron density *Ns* is concerned. As a case in hand, recently Matsuyama *et al.*[4] investigated the Rashba effect in still another system, a MOSFET on *p*-type InAs, and found a different behavior for α as a function of *Ns*. Beatings in the Shubnikov-de Haas oscillations were observed and taken to be a signature for a spin-split ground subband. To interpret their results, these authors[4] used a simple model for the band structure and adopted the triangular well approximation; to account for spin they then added a term $\pm\alpha k$ in their energy dispersion. Their results for α show at low electron density a slight decrease (to within a 20% relative error), followed by a steady increase and "saturation" at higher densities. Strictly increasing behavior may, however, be expected from a low order approximate theoretical expression[7] for α. The results of Ref. 4 also differ in trend and magnitude with results found in asymmetric quantum wells[2,3] where, for instance, the constant α of Heida *et al.*[2] and the decreasing trend of Nitta *et al.*[3] need clarifications.

In the light of these remarks, we believe that α depends on the surface potential in a more complex way than has hitherto been thought and in the following, for electrons in inversion layers on *p*-type bulk InAs, we address this problem numerically and self-consistently taking full account of the strong nonparabolicity of the bulk band structure with the aim being twofold: First to find quantitatively the size as well as the trend of α as a function of *Ns* by adopting a more realistic model and second to provide accurate numerical results against which tests of accuracy for approximate analytic expressions of α can be made.

We utilize the three-band Kane model[9] including the lowest conduction band Γ_6^c and topmost valence bands Γ_8^v as well as the split-off Γ_7^v band. For simplicity the oxide/semiconductor interface is considered to be perfect. In addition an infinite potential barrier at the interface is assumed and the Hartree approximation is adopted. Note that these

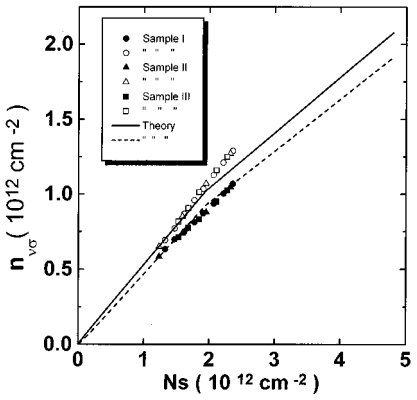

FIG. 1. Occupancy of the spin-split ground subband with solid (——) dashed (– – –) lines for $\sigma=+$ and $\sigma=-$, respectively. Experimental data inferred from Ref. 4.

assumptions have already been employed without serious errors.[10]

Because the experiments[4] were carried out at low temperatures, we also let $T=0$ K, then a Fermi level is sharply defined. Let the x axis be normal to the interface and choose y along the in-plane wave vector $\vec{k}=k\hat{j}$, then with the spin σ being quantized along the z axis and using the effective-mass approximation, the Schrödinger equation for spin up reads

$$\begin{pmatrix} E_g/2+V(x) & \frac{P}{\sqrt{2}}\left(i\frac{\partial}{\partial x}-ik\right) & \frac{P}{\sqrt{6}}\left(-i\frac{\partial}{\partial x}-ik\right) & \frac{P}{\sqrt{3}}\left(-i\frac{\partial}{\partial x}-ik\right) \\ \frac{P}{\sqrt{2}}\left(i\frac{\partial}{\partial x}+ik\right) & -E_g/2+V(x) & 0 & 0 \\ \frac{P}{\sqrt{6}}\left(-i\frac{\partial}{\partial x}+ik\right) & 0 & -E_g/2+V(x) & 0 \\ \frac{P}{\sqrt{3}}\left(-i\frac{\partial}{\partial x}+ik\right) & 0 & 0 & -E_g/2-\Delta+V(x) \end{pmatrix} \times \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \varphi_4 \end{pmatrix} = E \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \\ \varphi_4 \end{pmatrix}, \tag{2}$$

where E_g, Δ, P, and $V(x)$ denote, respectively, the forbidden gap, the bulk spin-orbit splitting, Kane's-momentum matrix element,[9] and the surface potential. For spin down, reverse the sign of k in Eq. (2). In the Hartree approximation, $V(x)$ satisfies the Poisson equation where the right-hand side includes contributions from ionized impurities and electrons in bound states. At $x=0$, the components of the wave function satisfy the boundary condition

$$\varphi_1(0)=i\left(-\frac{\sqrt{3}}{2}\varphi_2(0)+\frac{1}{2}\varphi_3(0)+\frac{1}{\sqrt{2}}\varphi_4(0)\right) \tag{3}$$

corresponding to a nil current at the interface. With $+(-)$ standing for the two eigenstates (up and down for a given direction of **k**), the solution of this set of equations yields a spin-split subband structure $\varepsilon_{\pm}(k)$ from which the Rashba effect is assessed. The following parameters are used:[11] $E_g=418$ meV, $\Delta=380$ meV, moreover, we take $m_0^*=0.0239m_e$ and $\varepsilon_s=15.15$ for the band-edge mass and static dielectric constant, respectively; P is deduced from the expression of the bulk effective mass,[12] and the density of ionized impurities is taken from Ref. 4 as $1.8\times10^{17}\,\mathrm{cm}^{-3}$ while *Ns* is swept from $0.1\times10^{12}\,\mathrm{cm}^{-2}$ up to $4.8\times10^{12}\,\mathrm{cm}^{-2}$, thus covering a wide interval. Figures 1–3 summarize our results.

The computed occupation numbers $n_{\nu\sigma}$ of the spin-split subbands are deduced from the fermi wave vectors $k_f^{\pm}$ for $(+)$ and $(-)$. Our results for $n_{\nu\sigma}$ along with the experimental values inferred from the Rashba parameter of Matsuyama *et al.*[4] are shown in Fig. 1 that shows excellent agreement up to about $Ns=2\times10^{12}\,\mathrm{cm}^{-2}$; beyond this point discrepancies start to grow slightly, the relative errors remain within ~9% however. Note that beyond this point, the first excited subband is populated and comparison with experiment is less conclusive because Ref. 4 states that up to $2.4\times10^{12}\,\mathrm{cm}^{-2}$ only the ground subband is occupied. However, these authors do not give the relative errors of their measurements, in InSb inversion layers[13] errors in *Ns* of ~5% are common. Add to this, the fact that the magnetic fields (up to ~6 T) involved in the experiment are quite moderate for a narrow-gap semi-

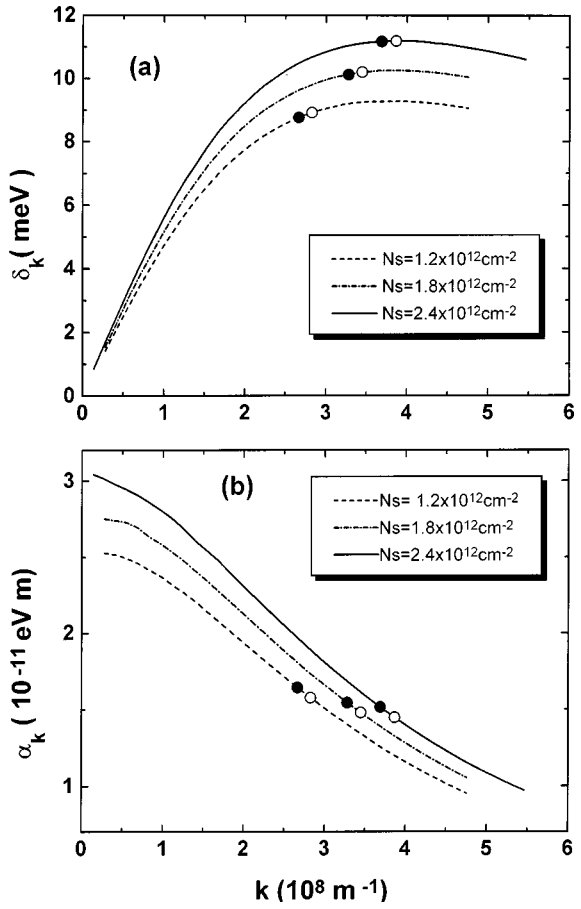

FIG. 2. (a) Spin splitting and (b) Rashba parameter in the ground subband as a function of in-plane wave vector; Open and solid circles mark the corresponding points on the fermi level, at k_f^+ and k_f^-, respectively.

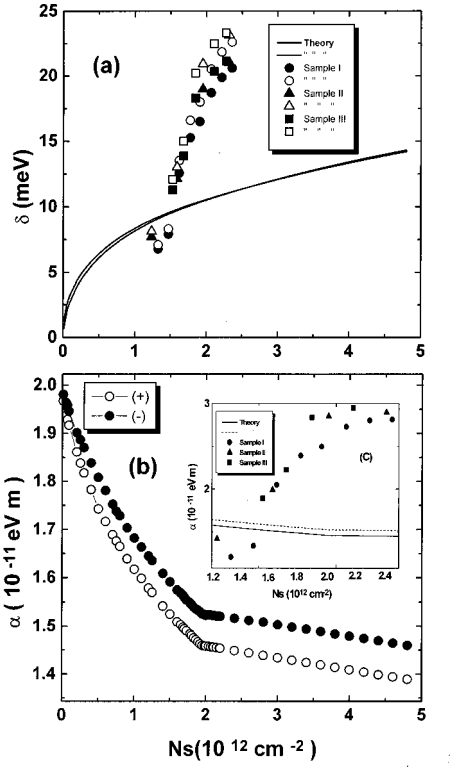

FIG. 3. (a) Theoretical (solid lines) and experimental [symbols: with open (filled) for $+(-)$] spin splitting at the fermi level as functions of areal electron density. (b) Theoretical values of the Rashba parameter at the fermi level as a function of electron density. Inset (c): Comparison of theoretical (solid and dashed lines) and experimental (symbols) values of the Rashba parameter at the fermi level. Experimental data taken from Ref. 4.

conductor like InAs. These fields are expected to affect the occupancies of the different subbands slightly when they have just begun to be populated; our values above $2\times10^{12}\,\mathrm{cm}^{-2}$ can, therefore, be considered satisfactory. In addition, we calculated the depletion charge density N_d that we found to vary from $1.3\times10^{12}\,\mathrm{cm}^{-2}$ for $Ns=1.2\times10^{12}\,\mathrm{cm}^{-2}$ to $1.4\times10^{12}\,\mathrm{cm}^{-2}$ for $Ns=2.4\times10^{12}\,\mathrm{cm}^{-2}$, in very good agreement with the reported experimental[4] value of $1.1\times10^{12}\,\mathrm{cm}^{-2}$.

In Figs. 2(a), 2(b), we show our spin splitting $\delta_k=\varepsilon_-(k)-\varepsilon_+(k)$ and Rashba parameter $\alpha_k=\delta_k/2k$ as functions of wave vector k for three different electron sheet densities *Ns*. The values of these two quantities at the fermi level are also marked. The most striking feature is that δ_k does not depend linearly on wave vector. As a matter of fact at the values of k of interest for transport, the splitting has already reached its maximum and even begun to decrease. In Fig. 2(b) we show the Rashba parameter α_k as a function of wave vector for the same values of *Ns* as in Fig. 2(a). One clearly sees the very strong dependence of this parameter on k, indeed α_k attains its maximum value in the limit $k\to0$, then it decreases very rapidly as the wave vector increases. For a given value of k this parameter is an increasing function of *Ns*, furthermore as $k\to0$, α_k presents a vanishing derivative, which is consistent with symmetry.

Figure 3(a) shows the spin splitting $\delta_\pm$ at the Fermi level as a function of *Ns*; note that $\delta_\pm$ is deduced from $\varepsilon_\pm(k)$ by evaluating δ_k at $k_f^\pm$. The values of Ref. 4 as we deduced them from their reported results and adopted model are also shown for comparison. One first notes that for both eigenstates the theoretical splittings $\delta_\pm$ are nearly indistinguishable, furthermore the splitting is a nonlinear function of *Ns* especially if one considers it over a wide interval. In addition, one notes that the experimental data of Ref. 4 besides presenting a nonuniform trend are larger than ours. They also show $\delta_\pm$ to depend appreciably on $\sigma=\pm$. The discrepancies between both works can be traced back to the model used by these authors for the band structure and the surface potential along with their taking a constant value for the Rashba parameter. Such an assumption overestimates δ_k as it can easily be seen from Fig. 2(a).

In Fig. 3(b) we show the Rashba parameter $\alpha_\pm$ calculated at the fermi level as a function of the 2D electron density. Because of the slight difference between k_f^+ and k_f^-, $\alpha_\pm$ are slightly different for $(+)$ and $(-)$. The inset to Fig. 3(b) compares our theoretical results with the experimental ones of Ref. 4. One clearly sees that the experimental data, which the authors in Ref. 4 deduced, are too large and in addition do not show the same dependence on *Ns* as the present work. Indeed the model adopted by these investigators for the bulk band structure is too simple. Moreover a k-independent Rashba parameter is inappropriate for InAs and overestimates both the spin splitting and the Rashba parameter at the fermi level, besides it leads to errors in the fermi energy E_F and wave vectors $k_f^\pm$. In addition the use of the triangular approximation for the surface potential leads to errors even if one uses the full multiband Kane Hamiltonian.

At the doping level considered in our work, the theoretical curves show $\alpha_\pm$ to be slowly decreasing for densities below $\sim1.97\times10^{12}\,\mathrm{cm}^{-2}$ and beyond this value $\alpha_\pm$ is nearly constant. As a matter of fact the relative change of $\alpha_\pm$ for *Ns* between $1.97\times10^{12}\,\mathrm{cm}^{-2}$ and $4.8\times10^{12}\,\mathrm{cm}^{-2}$ never exceeds 5%. Moreover, although $\alpha_\pm$ is a continuous function of *Ns*, it is not differentiable at the point where its trend changes that within our accuracy coincides with the onset of occupation in the first excited subband. Furthermore, it is of interest to point out the similarity of the trend found here with that of Can-Ming Hu *et al.*[3] for a gated quantum well.

The behavior of $\alpha_\pm$ with respect to *Ns* is the result of two competing processes that have opposite effects on α_k: The first mechanism is the increase of α_k when *Ns* increases and the second is its decrease for a given *Ns* when k gets larger, these two effects can easily be seen in Fig. 2(b). Thus, as *Ns* gets larger the Rashba parameter α_k increases for all values of k, i.e., in Fig. 2(b) the curve representing α_k shifts upward, however at the same time the fermi wave vectors $k_f^\pm$ also increase as compared to their values for a lower *Ns*, i.e., the symbols in Fig. 2(b) shift to the right. Now, since for a given electron density *Ns* α_k decreases with k, it follows that as *Ns* varies the overall behavior of $\alpha_\pm$ as a function of density will depend on the precise balance of these two opposite tendencies [see symbols in Fig. 2(b)]. This fact makes

the overall dependence of $\alpha_{\pm}$ on *Ns* hard to predict without adequate computations or careful measurements.

It is of interest to note that as *Ns* increases, and because of the strong nonparabolicity of InAs, the decrease as well as the near constancy of $\alpha_{\pm}$ in the ground subband both do not follow the surface electric field,[7] they also do not obey conjectures found in the literature.[2,3] Moreover, the nearly constant value of $\alpha_{\pm}$ that is kept for a rather large interval corresponds to a minimum rather than a maximum, which *a priori* one intuitively expects.

For *Ns* larger than $\sim 1.97\times 10^{12}\,\mathrm{cm}^{-2}$, the near constancy of $\alpha_{\pm}$ can be traced to the first excited subband whose occupation affects the fermi wave vectors $k_f^{\pm}$ in the ground subband and thereby $\delta_{\pm}$ and $\alpha_{\pm}$. Indeed, by purposely assuming only one populated subband we found $\alpha_{\pm}$ to be strictly and planely decreasing. This means that even if the first excited subband is not populated appreciably its effect is nonetheless not negligible.

We also computed $\alpha_{\pm}$ for the first excited subband and found a strictly decreasing trend without abrupt slope changes and with values in the range 1.62×10^{-11}–$1.37\times 10^{-11}\,\mathrm{eV\,m}$. In addition we computed the product $m^*\alpha$ for the ground subband that, in atomic units, is found to increase from 3.47×10^{-4} to 5.58×10^{-4}.

In conclusion, compared to quantum wells, electrons in inversion layers on bulk *p* InAs exhibit larger spin-splittings and spin-orbit parameters α and experimental investigations using optical probes to measure directly the spin splitting are highly desirable in order to test the predictions of the present work.

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