Spin dependent transmission probabilities in double- and triple-barrier Al$_x$Ga$_{1-x}$Sb heterostructures

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Abstract — The impact of bulk inversion asymmetry (Dresselhaus effect) of Al$_x$Ga$_{1-x}$Sb alloys, and structure inversion asymmetry (Rashba effect) of heterostructures based on them, on spin-dependent transmission probabilities is investigated for spin-filtering purposes. The transmission probabilities, calculated for double-barrier and triple-barrier heterostructures, indicate that if the applied electric field is small enough, the structure inversion asymmetry effects may be neglected. The interplay between the two effects is expected to be important for efficient spin filtering, hence we conclude that the investigated structures have limited spin-filtering prospects.

Keywords — Bulk inversion asymmetry, Rashba effect, resonant tunneling.

I. INTRODUCTION

The extra degree of freedom provided by the electron spin is expected to be of paramount importance in future electronic devices [1], [2]. Recent results on spin-injection from magnetic semiconductors [3], [4] suggest that tunneling phenomena may be used to significantly enhance the degree of spin polarization. From the practical point of view, the feasibility of spin injection within the existing semiconductor technologies presents an important issue. The concept of nonmagnetic spin-filters based on exploitation of the structure inversion asymmetry (SIA)-induced spin splitting in resonant tunneling structures originated from Voskoboynikov et al. [5]. Subsequently, the idea was refined by the use of triple-barrier resonant tunneling diode (TB-RTD) proposed by T. Koga et al. [6] and the asymmetric resonant interband tunneling diode proposed by Y. Ting and X. Cartoixa [7]. Papers [5]-[7] considered only the SIA, neglecting the impact of bulk inversion asymmetry (BIA). Theoretical considerations, such as in Ref. [8], showed that BIA effects can be quite strong, and must therefore be included into the model. There have been some papers dealing with BIA only, [9], as well as coupled BIA and SIA [10] contributions to the transmission probabilities, but none have presented a unified approach.

In this paper we investigate the coupled BIA and SIA effects in Al$_x$Ga$_{1-x}$Sb heterostructures under small external electric fields, used to obtain a highly efficient subband filtering in a TB-RTD. In section II we describe the theoretical model used in calculating the transmission probabilities, while in section III we present the numerical results and discuss their impact on the overall spin polarization.

II. SPIN-DEPENDENT EFFECTS

We shall discuss the spin-dependent transport in the conduction band of heterostructures grown along the z∥[001] direction by adopting the envelope function approximation and the Kane model for the bulk. The conventional, spin-independent form of the Schrödinger equation, for an electron with the in-plane wave vector $k_{||}$ reads:

$$
\begin{pmatrix}
H_0 & 0 \\
0 & H_0
\end{pmatrix}
\begin{pmatrix}
\eta_+ \\
\eta_-
\end{pmatrix} = E
\begin{pmatrix}
\eta_+ \\
\eta_-
\end{pmatrix},
$$

where $H_0$ represents the effective Hamiltonian given by:

$$
H_0 = -\frac{\hbar^2}{2m(E,z)} \frac{d^2}{dz^2} + \frac{d}{dz} + U_{\text{eff}}(E,k_{||},z).
$$

The nonparabolic effective mass, $m(E,z)$, is calculated according to:

$$
\frac{1}{m(E,z)} = \frac{P^2}{\hbar^2}
\begin{pmatrix}
1 \\
E - E_g - V(z) + E_g
\end{pmatrix}
\begin{pmatrix}
1 \\
E - E_g - V(z) + E_g + \Delta
\end{pmatrix},
$$

where $P$, $E_g$ and $\Delta$ are the interband momentum matrix element, the main band gap and the spin-orbit splitting, respectively. $V(z) = eF_{\perp}(z-z_0)$ is the potential due to the external electric field $F_{\perp}$ pointed along the [001] direction. $U_{\text{eff}}(E,k_{||},z)$ in equation (2) is the effective potential seen by the electron.
\[ U_{\text{eff}}(E, k_\parallel, z) = \frac{\hbar^2 k_\parallel^2}{2m(E, z)} + E_c + V(z). \]  

(4)

The two components, \( \eta_+ \) and \( \eta_- \), of the wave function in Eq. (1) describe the \"spin-up\" and \"spin-down\" state of the Pauli spin operator \( \sigma \), i.e. the spin state along the \( z \)-direction.

The inclusion of spin-dependent effects is performed in two steps. First, we consider the BIA effect described by the \( k^7 \) Dresselhaus Hamiltonian [11]

\[ H_D = (\sigma_x k_x - \sigma_y k_y) \frac{d}{dz} - \frac{d}{dz}, \]  

(5)

with \( \sigma_x \) and \( \sigma_y \) being the Pauli spin operators and \( k_x \) and \( k_y \) being the components of \( k \) along \( x ||[100] \) and \( y ||[010] \) directions, respectively. Parameter \( \sigma \) in (5) is a material constant \[8\]. By expressing \( k_x \) and \( k_y \) as \( k_x = k_0 \cos \varphi \) and \( k_y = k_0 \sin \varphi \) we find that \( H_D \) is diagonalized by the spinors

\[ \chi_\sigma(\varphi) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{-i \varphi} \end{pmatrix}, \sigma = \pm, \]  

(6)

and that the energy eigenstates \( \psi \) may be decomposed to eigenstate basis \( \psi_\sigma = \eta_\sigma \chi_\sigma(\varphi) \). In other words, the Schrödinger equation may be written as

\[ \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix} \begin{pmatrix} \eta_+ \\ \eta_- \end{pmatrix} = E \begin{pmatrix} \eta_+ \\ \eta_- \end{pmatrix}, \]  

(7)

with

\[ H_\sigma = \frac{\hbar^2}{2} \frac{d}{dz} - \frac{d}{dz} + U_{\text{eff}}(E, k_\parallel, z) + m_\sigma(z) \frac{2}{d \sigma}, \]  

(8)

where the spin-dependent effective mass \( m_\sigma(E, k_\parallel, z) \) is obtained in the form

\[ m_\sigma(E, k_\parallel, z) = m(E, z) \left( 1 - \sigma 2 m(E, z) k_\parallel^2 / \hbar^2 \right)^{-1}. \]  

(9)

Hence, the BIA effect merely modifies the effective mass along the \( z \)-direction. The diagonal form of (7) denotes that the spin state in bulk is a conserved quantity, thus we may view the conduction band as an union of two spin-subbands - the \"+\" and \"-\" subband corresponding to spinors \( \chi_+ \) and \( \chi_- \). Since \( \langle \chi_+(\varphi) | \sigma_x | \chi_-(\varphi) \rangle = 0 = \langle \chi_+(\varphi) | \sigma_y | \chi_-(\varphi) \rangle \) all the electrons have their spin in the \(x\)-plane with the direction defined by \( \langle \chi_+(\varphi) | \sigma_z | \chi_-(\varphi) \rangle = \cos \varphi \) and \( \langle \chi_+(\varphi) | \sigma_y | \chi_-(\varphi) \rangle = \sin \varphi \). Note that Eq. (6) implies that the spin direction doesn't depend on \( k_\parallel \).

The second part of spin-dependence is due to SIA and it is described by the Rashba Hamiltonian [12]

\[ H_R = \alpha \left( \sigma_x k_x - \sigma_y k_y \right), \]  

(10)

where \( \alpha = e \beta / \hbar \) is the Rashba parameter and \( \beta \) is given by

\[ \beta(E, z) = \frac{\alpha^2}{2} \left[ \frac{1}{E - E_c - V(z) + E_g} \right] + \frac{1}{E - E_c - V(z) + E_g + \Delta}. \]  

(11)

Since \( H_D \) and \( H_R \) don't commute, \( H_D + H_R \) cannot be diagonalized and there is no diagonal Schrödinger equation available so we write it down with respect to spinors \( \chi_\sigma(\varphi) \):

\[
\begin{pmatrix} H_+(\varphi) & iQ(\varphi) \\ -iQ(\varphi) & H_-(\varphi) \end{pmatrix} \begin{pmatrix} \eta_+ \\ \eta_- \end{pmatrix} = E \begin{pmatrix} \eta_+ \\ \eta_- \end{pmatrix},
\]

(12)

with

\[ H_\sigma(\varphi) = \frac{\hbar^2}{2} \frac{d}{dz} - \frac{d}{dz} + U_{\text{eff}}(E, k_\parallel, z) + \sigma k_\parallel \alpha \sin 2\varphi, \]  

(13)

and

\[ Q = -k_\parallel \alpha \cos 2\varphi, \]  

(14)

where the dependence on \( E, k_\parallel \) and \( z \) has been left out to reduce the complexity of the expressions.

III. TRANSMISSION PROBABILITIES

Consider a GaSb-AlSb-GaSb-AlSb-GaSb-AlSb-GaSb-GaSb-AISb-GaSb double barrier heterostructure whose conduction-band edge profile is shown in Fig. 1.

![Fig. 1. GaSb-AlSb-GaSb-AlSb-GaSb-AlSb-GaSb-GaSb double barrier structure. Parameters for AlSb and GaSb are obtained from [8], while the values for alloy Al0.5Ga0.5Sb are calculated by linear interpolation; z0=-20Å, z1=120Å, z2=136Å, z3=156Å, m0(0)=m1(0)=m2(0)=m3(0)=m4(0)=m5(0)=0.041m0, m5(0)=m5(0)=0.12m0, m4(0)=0.08m0, E1(0)=E2(0)=E3(0)=E4(0)=0.956eV, E1=-0.478eV, E2=-E3=-0.813eV, E3=-E2=-2.219eV, E4=1.516eV, \Delta_1=\Delta_2=\Delta_3=\Delta_4=0.8eV, \Delta_5=\Delta_6=0.75eV, \Delta_7=0.775eV, \gamma_1=\gamma_2=\gamma_3=187eVÅ^2, \gamma_4=\gamma_5=\gamma_6=32.7eVÅ^2. The conduction band is tilted by \( F_c=8.8\times10^5\text{V/m}\).]

In this structure, the SIA effect originates from the presence of Al0.5Ga0.5Sb layer and the non-zero external electric field \( F_c \) which tilts the conduction-band edge profile. The latter is hardly visible in the above figure, since \( F_c \) is taken to be very small (less than \( 10^5\text{V/m}\)). GaSb layers labeled 1 (the emitter) and 6 (the collector) represent the leads, i.e. they are assumed to be highly doped, so when an external bias \( V_{CE} \) is applied the electric field therein is vanishingly small. Consequently, we may form an \"exact\" solution of Eq. (12) yielding \[ \psi_j = \begin{pmatrix} A_{j+} \exp(i k j z) + B_{j+} \exp(-i k j z) \\ A_{j-} \exp(i k j z) + B_{j-} \exp(-i k j z) \end{pmatrix} \chi_\sigma(\varphi), \quad j = 1, 6, \]  

(15)

so the transmission probabilities from emitter to collector may easily be defined by
\[ T_{\sigma\delta} = \frac{k_{\sigma,\delta}}{k_{\delta,\sigma}} \left( \frac{m_{\sigma,\delta}}{m_{\delta,\sigma}} \right) \frac{\mathbf{A}_{\sigma,\delta}^2}{\mathbf{A}_{\delta,\sigma}^2}, \]  

(16)

with \( \sigma \) and \( \delta \) denoting the spin states in layers 1 and 6, respectively. \( k_{\sigma,\delta} \) are the spin-dependent wave vectors along the z-axis given by

\[ k_{j,\sigma} = \frac{1}{\hbar} \sqrt{2m_{j,\sigma} \left( E - U_{\text{eff},j}(E,k_{||}) \right)}, \]  

(17)

for \( j=1,6 \) and \( \sigma = \pm \).

In the previous section we showed that \( H_0 = 0 \) leads to a diagonalized form of the Schrödinger equation with the conservation of the spin state along the z-axis. That is exactly what happens in the leads so we may associate an electrical current density, \( J_0 \), with each of the two spin-subbands in the collector lead

\[ J_\sigma = \frac{e}{(2\pi)^7} \int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \left( T_{\sigma,\varphi} + T_{\sigma,-\varphi} \right) \times \left[ f(E - f(E + eV_{\text{CE}})) \right] dE_k dk_d d\varphi, \]  

(18)

where \( f(E) \) is the Fermi distribution in the emitter lead.

To obtain these transmission probabilities we have to solve (12) which, in general, has to be done numerically.

The term \( Q \), given by (14), drops to zero whenever \( \varphi = \varphi_\text{m} + \pi/4 + m\pi/2 \) with \( m \) being an integer value. This implies that for angles \( \varphi_\text{m} \) the Rashba and the Dresselhaus Hamiltonians become "aligned", yielding a diagonal Hamiltonian with respect to spinors \( \chi_\pm (\varphi) \). Hence, electrons with \( k_{||} \) along \( \varphi_\text{m} \) have their spin conserved in the heterostructure. At the same time, the term \( k_0 \sin 2\varphi \) which describes the SIA-induced splitting between \( H_1 \) and \( H_2 \) in (12) reaches its peak.

A typical spin-split transmission spectra of a double barrier heterostructure is shown in Fig. 2. Consider \( \varphi = \pi/4 \). The BIA part raises the effective mass of the "+" electrons while lowering it for "-" electrons. Therefore, the "+" quasibound state in layer 3 (the well) will have a smaller energy than the "-" quasibound state if only the BIA effect is considered. The SIA part lowers the effective potential \( U_{\text{eff}}^{-} + \alpha k_{||} \) seen by "+" subband electrons because \( \alpha \) is negative in the well (\( \beta \) reduces continuously due to \( F_z \) and has an abrupt decrease at the GaSb-AlAs-GaAs interface). Since for \( \varphi = \pi/4 \) both SIA and BIA tend to decrease (increase) the energy of the "+" ("-") quasibound state, the spin splitting will be largest for this angle. The opposite stands for \( \varphi = -\pi/4 \). Hence we may estimate the relative magnitudes of SIA and BIA effects by examining the transmission spectra for these two values of \( \varphi \).

The reason why we are interested in this particular range of values of \( F_z \) becomes clear by investigating the structure shown in Fig. 3. It represents a triple-barrier resonant tunneling diode used in [6] as a spin filter by exploiting the Rashba effect. Here we apply a slightly different approach by taking into account the BIA effects as well.

![Graph 2](image2.png)

Fig. 2. The calculated transmission spectra for the structure described in Fig. 1. for \( k_{||} = 0.01 \AA^{-1}, \varphi = \pi/4, F_z = 8.8 \times 10^4 \text{V/m} \). Solid line represents \( T_+ \) and the dashed line \( T_- \). The inset shows the \( \varphi = \pi/4 \) case (dashed line) compared to the \( \varphi = \pi/4 \) case (solid line).

![Graph 3](image3.png)

Fig. 3. GaSb-AlSb-GaSb-AlAs-GaAs-GaAs-GaSb symmetric triple-barrier structure. \( z_0 = 0, z_1 = 20 \AA, z_2 = 120 \AA, z_3 = 136 \AA, z_4 = 156 \AA, z_5 = 172 \AA, z_6 = 272 \AA, z_7 = 292 \AA \).

The structure parameters are same as in Fig. 1. except for \( \gamma_0 = -\gamma_4 \) and \( \gamma_4 = -\gamma_0 \).
The solid and dashed lines in well regions of the structure in Fig. 3. schematically represent the energies of quasibound states for the "+" and "-" spin-subband, respectively. A positive $F_t$ tilts the conduction band edge so the two "+" quasibound states eventually become aligned. The opposite order of spin-splitting in this structure is obtained by growing layers 6-9 along [00 T], while layers 1-5 are grown along [001] as in the case of previously considered double-barrier structure.

The transmission probabilities for this structure are much below unity, unless an exact alignment of the two corresponding quasibound states is achieved by $F_t$. In Fig. 4, we display the transmission spectra when the above condition is fulfilled. The improvement offered by this concept is that the two "+" quasibound states are closer to each other than the two "-" states thus enabling much higher transmission probabilities for "+" spin-subband. A distinctive feature of TB-RTDs is that the highest subband filtering efficiency, $\eta_{(J+J)}(J+J)$ [14], is obtained at the peak of the $IV$ curve, while the polarization peaks of resonant tunneling devices (i.e. double barrier structures) appear when the total current is nearly zero.

The inset of Fig. 4. offers comparison between segments of $T$ spectra obtained for $\varphi=\pi/4$, $F_t=8.8 \times 10^{6}$V/m$^2$. Solid line represents $T_+$ and the dashed line $T_-$. The inset shows that $\varphi=\pi/4$ case (dashed line) compared to the $\varphi=\pi/4$ case (solid line). The two arrows indicate the resonances of $T_+$. 

![Fig. 4. The calculated transmission spectra for structure described in Fig. 3. for $k_z=0.01 \AA^{-1}$, $\varphi=\pi/4$, $F_t=8.8 \times 10^{6}$V/m$^2$. Solid line represents $T_+$ and the dashed line $T_-$. The inset shows that $\varphi=\pi/4$ case (dashed line) compared to the $\varphi=\pi/4$ case (solid line). The two arrows indicate the resonances of $T_+$.](image)

The inset of Fig. 4. offers comparison between segments of $T_+$ spectra obtained for $\varphi=\pm \pi/4$. We see that the differences are negligible just as in the case of double barrier structure. The problem with $\varphi$-independent transmissions is that the transmitted electrons, which all may fall into one subband if a TB-RTD is used, have their spins directed along angles in the range $[-3\pi/4, \pi/4]$ (if a one-sided collector is placed at angle $\varphi_c=\pi/4$ and $\eta=1$). It is simple to show that when $T_+$ do not depend on $\varphi$, the current polarization is given by $P=2\eta /\pi$. This problem may be solved by using a TB-RTD with a more pronounced SIA effect. One approach would be to use $p$-type doping to create a mountain-like conduction-band edge profile like in [6]. The other possibility is to balance the SIA and BIA effects by tailoring a TB-RTD from materials which have a greater difference of $\beta$ than the GaSb-AlSb combination.

IV. SUMMARY

We have demonstrated that the BIA effect in Al$_x$Ga$_{1-x}$Sb triple-barrier heterostructures may be used in a similar manner as the SIA in previously investigated TB-RTDs. The spin-polarization efficiency of TB-RTDs with balanced SIA and BIA effects is expected to significantly exceed the $P_{\max}=2/\pi$ limit in the one-sided collector configuration of the spin filter device.

REFERENCES