Spin-dependent tunneling in double-barrier semiconductor heterostructures

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(Received 21 September 1998)

Spin-dependent tunneling in symmetric and asymmetric double-barrier semiconductor heterostructures is studied. The effective one-band Hamiltonian approximation and spin-dependent boundary conditions approach are used for a theoretical investigation of the influence of electron spin on the tunneling probability. It is shown that spin-orbit splitting in the dispersion relation for electrons in $A_{\mathrm{III}}B_{\mathrm{V}}$ semiconductors can provide the dependence of the tunneling transmission probability on the electron-spin polarization without additional magnetic field. The dependence can be controlled by an external electric field, and may be significant for realistic models of double-barrier semiconductor heterostructures. [S0163-1829(99)02320-6]

I. INTRODUCTION

Resonant double-barrier tunnel (DBT) structures have attracted considerable attention since the pioneering work of Tsu and Esaki.[1] These structures are not only rich in physics but also useful for various device applications.[2–5] However, up to the present time, the electron motion parallel to the tunnel structure boundary has been overlooked in the total electronic current of the structures.[1,6] This neglect of the motion is the main assumption of present day resonant tunneling theories.[7] Almost all theoretical calculations are done with a one-dimensional approach for determining the tunneling transmission probability. Recently a few articles have called attention to some peculiarities in the dependence of the tunneling transmission probability on parallel (''in-plane'') electron wave-vector components for symmetric tunnel heterostructures.[8–10] It was found that for structures with an electronic effective mass dependent on space position (as is usually the case for tunnel structures), the in-plane component can play a well-defined role in the transmission processes. The main condition for this is the existence of a discontinuity in the electronic band parameters at the tunnel structure interfaces.[9,10]

Another interesting problem linked to the in-plane electron motion is the well-known spin-orbit coupling and electronic bands splitting in $A_{\mathrm{III}}B_{\mathrm{V}}$ quantum heterostructures.[11–14] It is known that there is a coupling between the in-plane electron motion and the electron-spin polarization. This can happen in asymmetric heterostructures or heterostructures with an external electric field.[15,16] Two contributions to the spin-splitting effect can be distinguished which play different roles: band-edge discontinuity at the structure interfaces, and additional electrostatic potential. The former brings about spin-dependent boundary conditions, and the latter gives a spin-dependent term in the effective-mass Hamiltonian.[15–18] The spin-orbit splitting effect has been discussed theoretically,[11–18] and already investigated experimentally in quantum-well structures.[19–23]

We have recently found that this effect can be also significant in tunneling barrier structures.[24] In this work, the spin-dependent effect on a more interesting structure, a double-barrier resonant tunneling structure, is studied. Present day molecular-beam-epitaxy and metal-organic chemical-vapor deposition technologies give us the opportunity to construct quantum tunneling barrier heterostructures with a wide range of possible discontinuities of the semiconductor band parameters.[25,26] The theoretically predicted effects of the in-plane motion of tunneling electrons have now became experimentally researchable. As presented below, this effect can be very strong, and may provide a fast spin-dependent transport device.

The effect we are expecting should be most clear for DBT heterostructures with a significant discontinuity in the spin-splitting parameters at the boundaries — asymmetric heterostructures. The asymmetry can also be produced by an external electric field. Therefore, we can in principle control the spin polarization of the tunneled electron current only by an electric field applied to the structure.

In this paper we calculate the tunneling transmission probability for DBT heterostructures with a space-dependent electronic effective mass and spin-splitting parameters. We use mass- and spin-dependent boundary conditions and the Rashba coupling term to describe the external electric-field effect.[15–17] A considerable effect can be achieved in DBT structures with narrow gap A_{III}-B_{V} semiconductors (where the spin-splitting effect is strong). We found it is important to take nonparabolicity into account in the electron dispersion relation.[17,24] In our calculation we use the nonparabolic approximation for the energy and space dependencies of the electronic effective mass, proposed in Refs. 15–17. We obtained a dependence of the transmission probability on the in-plane electron wave vector and polarization of the electron spin, and demonstrated that the consideration of spin in tunneling processes can considerably change the tunnel transmission probability in DBT structures with and without external electric field.

This paper is organized as follows. In Sec. II we describe details of the calculation of the electron spin-dependent tun-

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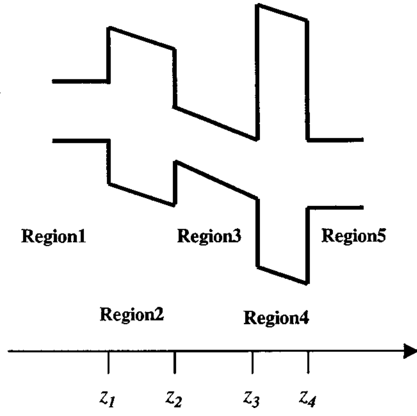

FIG. 1. Variation of the semiconductor band parameters in DBT heterostructures with an external electric field.

neling transmission probability in DBT structures. In Sec. III, results of calculations for different kinds of DBT structures with narrow-gap $A_{\rm III}$-$B_{\rm V}$ semiconductors are presented. Possible ways to investigate the effect experimentally are discussed in Sec. IV. There we also summarize the work results.

II. SPIN-DEPENDENT TUNNELING TRANSMISSION PROBABILITY

The variation of the band-structure parameters for a DBT structure with an external electric field is shown in Fig. 1. The layers of the structure are perpendicular to that z axis, and the in-plane electron's wave vector is k [if k is put along an arbitrary x direction, the spin polarization is set along y-axis in a layer plane $\rho=(x,y)$]. With the above-mentioned assumptions we can write the effective quasi-one-dimensional one-electronic-band Hamiltonian as follows:[17]

$$H=-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m(E,z)}\frac{d}{dz}+\frac{\hbar^2k^2}{2m(E,z)}+E_c(z)-\sigma\frac{d\beta(E,z)}{dz}k+V(z), \tag{1}$$

where

$$\frac{1}{m(E,z)}=\frac{P^2}{\hbar^2}\left[\frac{2}{E-E_c(z)+E_g(z)+V(z)}+\frac{1}{E-E_c(z)+E_g(z)+\Delta(z)+V(z)}\right], \tag{2}$$

$$\beta(E,z)=\frac{P^2}{2}\left[\frac{1}{E-E_c(z)+E_g(z)+V(z)}-\frac{1}{E-E_c(z)+E_g(z)+\Delta(z)+V(z)}\right]. \tag{3}$$

$\sigma=\pm 1$ refers to the spin polarization, E denotes the total electron energy in the conduction band, and $V(z)=-eFz$ is the potential due to the external electric field F (e is the electronic charge). The matrix element P does not depend on z,[27] and $E_c(z)$, $E_g(z)$, and $\Delta(z)$ stand for the corresponding z dependencies of the conduction-band edge, the main band gap, and the spin-orbit splitting profiles. We use the envelope-function approximation for the total wave function of the electron $\Phi_\sigma(z,\rho)$, and can write it as

$$\Phi_\sigma(z,\rho)=\Psi_{j\sigma}(z)\exp(i\mathbf{k}\cdot\rho),$$

where $\Psi_{j\sigma}(z)$ satisfies the z component of the Schrödinger equation in the jth region. We assume that the electronic effective mass does not depend on a coordinate within jth region, and the equation for $\Psi_{j\sigma}(z)$ becomes

$$H_{j\sigma}\Psi_{j\sigma}(z)=E_\sigma\Psi_{j\sigma}(z), \tag{4}$$

where

$$H_{1\sigma}=-\frac{\hbar^2}{2m_1(E_\sigma)}\frac{d^2}{dz^2}+\frac{\hbar^2k^2}{2m_1(E_\sigma)}+E_{1c} \quad \text{when} \quad j=1,$$

$$H_{j\sigma}=-\frac{\hbar^2}{2m_j(E_\sigma)}\frac{d^2}{dz^2}+\frac{\hbar^2k^2}{2m_j(E_\sigma)}+E_{jc}-eF(z-z_1)-\sigma\alpha_jkF \quad \text{when} \quad j=2\text{–}4,$$

$$H_{5\sigma}=-\frac{\hbar^2}{2m_5(E_\sigma)}\frac{d^2}{dz^2}+\frac{\hbar^2k^2}{2m_5(E_\sigma)}+E_{5c}-eFd \quad \text{when} \quad j=5.$$

In Eq. (4), E_{jc} is the energy of the electronic band bottom in the jth region without external electric field ($E_{1c}=0$, conventionally), $d=z_4-z_1$ is the total thickness of regions 2–4, and α_j is the Rashba spin-orbit coupling parameter:[17]

$$\alpha_j=\frac{\hbar^2}{2m_j(0)}\frac{\Delta_j}{E_{jg}}\frac{2E_{jg}+\Delta_j}{(E_{jg}+\Delta_j)(3E_{jg}+\Delta_j)}. \tag{5}$$

We can use the expressions above in barrier and well regions ($j=2-4$) when the electric fields satisfy the well-understandable conditions

$$E_{jg} \gg eF(z_j - z_{j-1}).$$

The coefficient α_j presets the ''second'' contribution to the Rashba spin-orbit splitting.[17] The ''first'' one — the electronic band-edge discontinuity — provides the boundary conditions for $\Psi_{j\sigma}(z)$ at an interface plane $z=z_j$ between j and $j+1$ regions that follow from Eq. (1)–(3)

$$\frac{1}{m_j(E_\sigma)}\left\{\frac{d}{dz}\ln[\Psi_{j\sigma}(z)]\right\}_{z=z_j} - \frac{1}{m_{j+1}(E_\sigma)}\left\{\frac{d}{dz}\ln[\Psi_{j+1\sigma}(z)]\right\}_{z=z_j} = \frac{2\sigma k[\beta_{j+1}(E_\sigma)-\beta_j(E_\sigma)]}{\hbar^2},$$

$$\Psi_{j\sigma}(z_j) - \Psi_{j+1\sigma}(z_j) = 0. \tag{6}$$

The boundary conditions above were obtained in Refs. 17 and 28–31.

The general solution of Eq. (4) in a given jth region has the form

$$\Psi_{j\sigma}(z) = a_{j\sigma}\Phi^{+}_{j\sigma}(z) + b_{j\sigma}\Phi^{-}_{j\sigma}(z), \tag{7}$$

where $\Phi^{\pm}_{j\sigma}(z)$ is a pair of linearly independent solutions of Eq. (4) within the region.

The boundary conditions (5) then determine the coefficients set $\{a_{j\sigma}, b_{j\sigma}\}$ for Eq. (6). The coefficient set in neighboring regions are related by the well-known transfer matrix M:[6]

$$\begin{pmatrix} a_{j\sigma} \\ b_{j\sigma} \end{pmatrix} = M^{j}_{\sigma}\begin{pmatrix} a_{j+1\sigma} \\ b_{j+1\sigma} \end{pmatrix}. \tag{8}$$

The matrix M^{j}_{σ} can be written as

$$M^{j}_{\sigma} = \frac{1}{\Delta_j}\begin{pmatrix} \Lambda^{-}_{j+} & \Lambda^{+}_{j+} \\ -\Lambda^{-}_{j-} & -\Lambda^{+}_{j-} \end{pmatrix} \tag{9}$$

with

$$\Delta_j = \Delta^{+}_{j} - \Delta^{-}_{j},$$

$$\Delta^{\pm}_{j} = \left\{\frac{d}{dz}\ln[\Phi^{\pm}_{j\sigma}(z)]\right\}_{z=z_j} - \frac{2\sigma m_j k[\beta_{j+1}(E_\sigma)-\beta_j(E_\sigma)]}{\hbar^2},$$

$$\Lambda^{\pm}_{j+} = \left(\frac{m_j}{m_{j+1}}\left\{\frac{d}{dz}\ln[\Phi^{\pm}_{j+1\sigma}(z)]\right\}_{z=z_j} - \Delta^{+}_{j}\right)\frac{\Phi^{\mp}_{j+1\sigma}(z_j)}{\Phi^{+}_{j\sigma}(z_j)},$$

$$\Lambda^{\pm}_{j-} = \left(\frac{m_j}{m_{j+1}}\left\{\frac{d}{dz}\ln[\Phi^{\pm}_{j+1\sigma}(z)]\right\}_{z=z_j} - \Delta^{-}_{j}\right)\frac{\Phi^{\mp}_{j+1\sigma}(z_j)}{\Phi^{-}_{j\sigma}(z_j)}.$$

The potential profile in the DBT problem (Fig. 1) consists of four interfaces, and, therefore, the total transfer matrix can be written as

$$M_\sigma = \prod_{j=1}^{4} M^{j}_{\sigma}. \tag{10}$$

For the regions with $j=1$ and 5, which we assume to be the regions with a flat electronic band edge ($F=0$), the pair of the linearly independent solutions are a plane wave set

$$\Phi^{\pm}_{1\sigma}(z) = \exp(\pm ik_1 z),$$

$$\Phi^{\pm}_{5\sigma}(z) = \exp(\pm ik_5 z),$$

$$k_1(E_z,k) = \frac{1}{\hbar}\sqrt{2m_1(E_z,k)E_z}, \tag{11}$$

$$k_5(E_z,k) = \frac{1}{\hbar}\sqrt{2m_5(E_z,k)(E_z-E_{5c}+eFd) - \hbar^2\left[1-\frac{m_5(E_z,k)}{m_1(E_z,k)}\right]k^2},$$

where E_z is the longitudinal component of the total energy in the first region:

$$E = E_z + \frac{\hbar^2 k^2}{2m_1(E,k)}. \quad (12)$$

We use this expression, along with Eqs. (2) and (3), to find the dependence of $E(E_z,k)$ and, through that, the $m_j(E_z,k)(j=2–5)$, and $\beta_j(E_z,k)(j=1–5)$ dependencies.

For regions $j=2–4$, with the external electric field F, we choose solutions in the form of the Airy functions[32]

$$\Phi^+_{j\sigma}(z) = \mathrm{Bi}(Z_{j\sigma}), \quad \Phi^-_{j\sigma}(z) = \mathrm{Ai}(Z_{j\sigma}). \quad (13)$$

Argument $Z_{j\sigma}$ is a function of the coordinate z and other parameters of the regions

$$Z_{j\sigma}(E_z,k,z) = \left[\frac{2em_j(E_z,k)F}{\hbar^2}\right]^{1/3}\left[\frac{A_{j\sigma}(E_z,k)}{eF} - z\right],$$

$$A_{j\sigma}(E_z,k) = E_{jc} - E_z + \frac{\hbar^2 k^2}{2m_j(E_z,k)}\left[1 - \frac{m_j(E_z,k)}{m_1(E_z,k)}\right] - (\sigma\alpha_j k - ez_1)F. \quad (14)$$

The electron is incident from the left only from the region $j=1$. A transmitted wave will appear in the region $j=5$, and, therefore, $b_{5\sigma}=0$. With this condition the tunneling transmission probability is given by

$$T_\sigma(E_z,k) = \frac{m_1(E_z,k)k_5(E_z,k)}{m_5(E_z,k)k_1(E_z,k)}\left|\frac{a_{5\sigma}}{a_{1\sigma}}\right|^2 = \frac{m_1(E_z,k)k_5(E_z,k)}{m_5(E_z,k)k_1(E_z,k)}\left|\frac{1}{M_{\sigma 11}}\right|^2. \quad (15)$$

We used this equation to calculate the spin-dependent tunneling probability of the DBT structures.

III. CALCULATION RESULTS

In symmetric DBT structures without an external electric field we cannot observe any difference in the tunneling characteristics between spin up and spin-down electrons in accordance with the general features of the spin-splitting effect.[16] However, for structures with a sharp discontinuity of the band-structure parameters at the structure interfaces, we can find a difference between the traditional description and a description that accounts for the in-plane wave-vector dependency.[10,24]

To gain a qualitative feeling about the k-vector dependence of the tunneling probability, let us consider a DBT structure consisting of two identical InAs-GaAs-InAs barriers with the barriers width $z_2-z_1=z_5-z_4=30$ Å and a distance between the barriers of $z_2-z_3=60$ Å. The results of the calculation of $T_\sigma(E_z,k)$ for this symmetric structure are presented in Fig. 2. It can be found from the three-dimensional plot in Fig. 2 that two sharp peaks (corresponding to two resonant levels in the well) shift as the in-plane wave vector increases. Even the first resonant peak has a well-pronounced dispersion in the (E_z,k) plane.

To demonstrate the role of spin splitting in symmetric

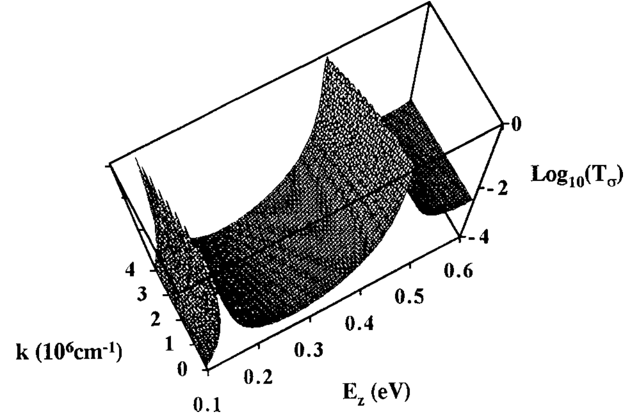

FIG. 2. The tunnel transmission probability as a function of the longitudinal energy E_z and the in-plane wave vector k in an symmetric InAs-GaAs-InAs-GaAs-InAs DBT structure (parameters are obtained from Refs. 33 and 34): $E_{2c}=E_{4c}=0.792$ eV,$E_{3c}=E_{5c}=0.0$ eV, $E_{1g}=E_{3g}=E_{5g}=0.418$ eV, $E_{2g}=E_{4g}=1.52$ eV, $\Delta_1=\Delta_3=\Delta_5=0.38$ eV, $\Delta_2=\Delta_4=0.341$ eV, $m_1(0)=m_3(0)=m_5(0)=0.023m_0$, $m_2(0)=m_4(0)=0.067m_0$ (m_0 is the free electron's mass), $z_2-z_1=z_5-z_4=30$ Å, and $z_3-z_2=60$ Å.

DBT structures, we use an external electric field that provides an asymmetry to the symmetric tunneling structure and, through that, a spin-polarization dependence of the tunneling transmission probability. In Fig. 3(a) we show the normalized differential spin-dependent tunneling probability

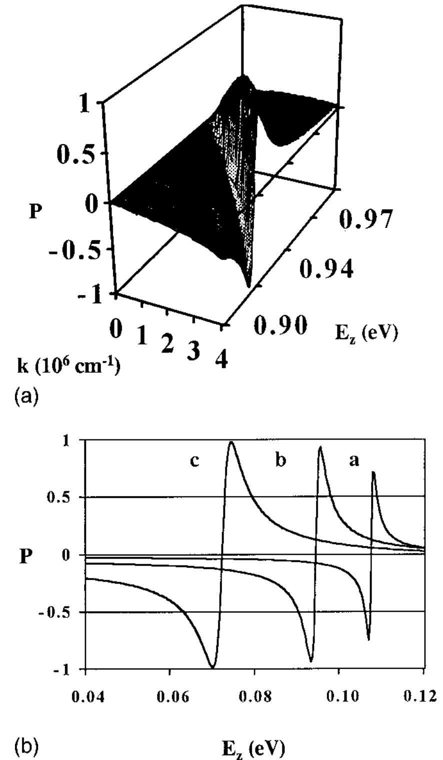

FIG. 3. The normalized differential spin-dependent tunneling probability **P** for the structure of Fig. 2. (a) Three-dimensional plot for the external electric field $F=5\times10^4$ V cm^{-1}. (b) $\mathbf{P}(E_z,k=4\times10^6$ cm$^{-1})$ intersections of three-dimensional plots. Curves a–c correspond to the cases $F=2\times10^4$, $F=5\times10^4$, and $F=1\times10^5$ V cm^{-1}, respectively.

$$\mathbf{P}=\frac{T_+-T_-}{T_++T_-} \tag{16}$$

for a InAs-GaAs-InAs-GaAs-InAs DBT structure with an external electric field. It is evident that the spin-orbit splitting effect with the transverse (in-plane) motion of the electron provides a dependence of the transmission probability on the tunneling electron-spin polarization. From the plot of Fig. 3(a), it can be found that the polarization changes sign along the lines of the (E_z,k) plane when we cross a line corresponding to the resonant peak position in the traditional description with $\sigma=0$. The magnitude of the polarization obviously depends on the electric-field magnitude. Curves a, b, and c in Fig. 3(b) show the $\mathbf{P}(E_z)$ relation at three different values of the external electric field, when $k=4\times10^6$ cm^{-1}, and clearly demonstrate the last dependence. We can note that the polarization for electrons with E_z and k near the resonant line in the (E_z,k) plane can reach about 100%, and rapidly change its sign.

Contrary to the case of symmetric DBT structures, asymmetric structures manifest a dependence of the transmission probability on the electron-spin sign even without any external electric fields. With the field we can control the effect magnitude.

First we pay attention to a fact of the spin-polarization dependency of the tunnel transmission probability in asymmetric structures without an external electric field. A noticeably large output electron polarization was observed in the structure with parameters of InAs-GaAs-InAs-AlAs-InAs.[33,34] This is demonstrated in Fig. 4(a). The built-in asymmetry in the spin-splitting parameters provides a high magnitude of **P**. From Fig. 4(b) it is clear that the external electric field can increase the amplitude of **P** near the resonant line. The polarization can be suppressed by reversing the electric field. For the described structure we can totally suppress $\mathbf{P}(\mathbf{P}=0)$ with the reversed electric field $F\approx-1.3\times10^4$ V cm^{-1}. We can even change the sign of it with a stronger reversed field, as shown in the inset of the Fig. 4(b). In view of these results we can say that asymmetric DBT structures provide wider room for experimental investigation and practical applications of the effect.

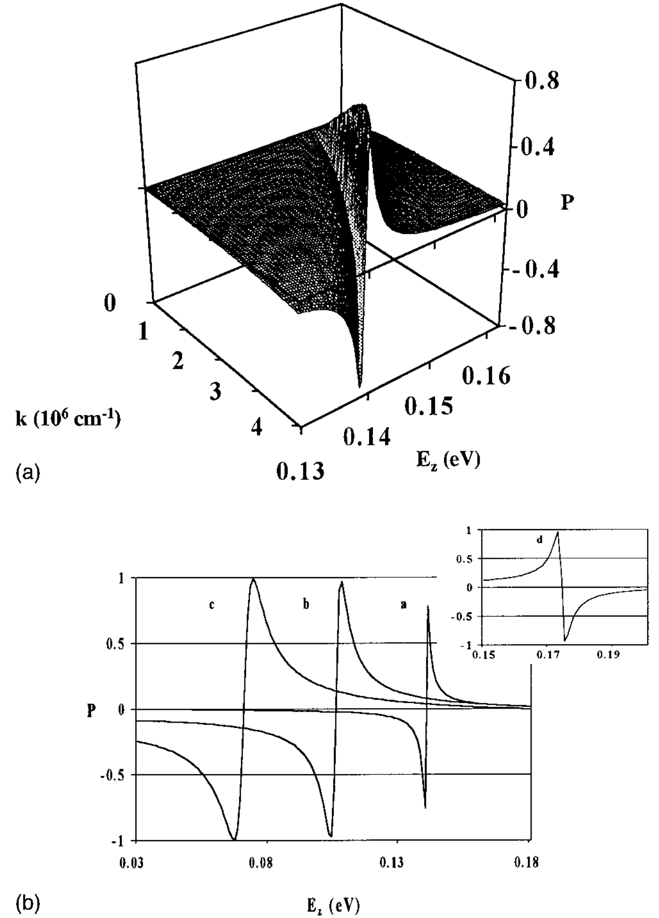

FIG. 4. The normalized differential spin-dependent tunneling probability **P** for an asymmetric InAs-GaAs-InAs-AlAs-InAs DBT structure (parameters are obtained from Refs. 33 and 34): $E_{2c}=0.792$ eV, $E_{4c}=1.86$ eV, $E_{3c}=E_{5c}=0.0$ eV, $E_{1g}=E_{3g}=E_{5g}=0.418$ eV, $E_{2g}=1.52$ eV, $E_{4g}=3.13$ eV, $\Delta_1=\Delta_3=\Delta_5=0.38$ eV, $\Delta_2=0.341$ eV, $\Delta_4=0.28$ eV, $m_1(0)=m_3(0)=m_5(0)=0.023m_0$, $m_2(0)=0.067m_0$, $m_4(0)=0.15m_0$, $z_2-z_1=30$ Å, $z_3-z_2=60$ Å, and $z_4-z_3=15$ Å. (a) Three-dimensional plot for the structure without external electric field. (b) $\mathbf{P}(E_z,k=4\times10^6$ cm$^{-1})$ intersections of three-dimensional plots. Curves $a-c$ correspond to the cases $F=0$, $F=5\times10^4$, and $F=1\times10^5$ V cm^{-1}, respectively. The inset (curve d) corresponds to the case of the reverse external electric field $F=-5\times10^4$ V cm^{-1}.

IV. DISCUSSION AND CONCLUSION

The well-defined spin dependence of the tunneling probability $T_\sigma(E_z,\mathbf{k})$ described above allows us to discuss possible ways to investigate experimentally a polarization effect in the electronic tunnel current in the structures. Tunneling coupling in double quantum wells[35] and tunneling transmission processes through barriers between wells, considered the electron's in-plane motion,[36] are also fields of possible spin-orbit splitting effect investigation and implementations.

The result, which is very important, is a spin splitting of the resonant peak in the (E_z-k) plane in DBT structures, with a well-recognized peak position dependence on k: $E_z^\sigma(k)$ (see Fig. 2). Those spin-split peaks correspond to quasistationary levels with different electronic spin polarizations in the DBT structure well.[15–17] The spin-split resonant tunneling probability provides a difference in resonance conditions for tunneling electrons with different directions of the electron spin. We can expect that the split resonant peaks can give different contributions to the total electronic tunneling current in the structures. Therefore, the spin-polarized output electronic current can be obtained.

The total electron tunnel current is

$$J=J_+-J_-,$$

where

$$J_\sigma=\frac{e}{8\pi^3}\int T_\sigma(E_z,\mathbf{k})[f_1(\mathbf{k},k_z)-f_5(\mathbf{k},k_z)]u_{1z}d\mathbf{k}dk_z$$

is the tunneling current for electrons with σ polarization, $f_j(\mathbf{k},k_z)$ is the electronic distribution function in three-dimensional $(\mathbf{k},k_z)$ space in the emitter $(j=1)$ and collector $(j=5)$ regions, and u_{1z} is the z component of the electron velocity

$$\mathbf{u}_1(\mathbf{k}) = \frac{1}{\hbar}\frac{\partial E}{\partial \mathbf{k}}$$

in the emitter region.

According to the general features of the spin-orbit interaction (1) and (4) the spin-dependent tunneling probability $T_\sigma(E_z;\mathbf{k})$ satisfies the following relation of symmetry:

$$T_\sigma(E_z;\mathbf{k}) = T_{-\sigma}(E_z;-\mathbf{k}).$$

In the low-temperature regime, when the Fermi distribution $f_0(E)$ for electrons in the electrode regions ($j=1$ and 5) and the Fermi-level line $E_z^f(k) = E^f - [\hbar^2 k^2/2m_1(E^f,k)]$ are symmetric in the (k_x,k_y) plane $[f_1(\mathbf{k},k_z) = f_0(E)$, $f_5(\mathbf{k},k_z) = f_0(E+eV)$, E_f is the Fermi energy, and $V = F_z d$ is applied along the z direction], there is no polarization in the total output current. We can obtain the polarized output current only when the electron distribution in the emitter region has an asymmetry in the (k_x,k_y) in-plane intersection of the $\mathbf{k}$ space.

Let us assume that the total external electric field has an additional in-plane component F_x. Under the additional x component of the electric field, the electron distribution becomes asymmetric in the (k_x,k_y) plane. We can expect a highly polarized output electronic current in this situation, when the electric-field Fermi level crosses the lowest spin-split quasistationary level [for instance, $E_z^-(k)$]. We also can expect a reverse of the polarization when the highest spin-split level [then $E_z^+(k)$] crosses the bottom of the electronic band in the emitter region. Polarization in DBT structures with sharp peaks of the tunneling probability (well defined by the quasistationary levels) in principle can gain nearly 100%.

The history of the investigation of resonant tunneling current in DBT structures shows us that the implementation and optimization procedures demand very complicated investigation.[2] Certainly, spin-dependent resonant tunneling currents, taking account of all accompanying processes (elastic and inelastic), also need special theoretical and experimental investigations. Here we only briefly described the main points of the investigation.

In short, we have presented a study of spin-dependent resonant tunneling in double-barrier heterostructures. The effective one-band Hamiltonian approximation with spin-dependent boundary conditions was employed to describe and evaluate this effect in symmetric and asymmetric double-barrier tunnel heterostructures. The calculation results show a considerable influence of the spin-splitting effect on the tunneling transmission characteristics. The dependence can be controlled by an external electric field. In addition, the coupling between components of the electron motion in directions parallel and perpendicular to the interfaces can manifest itself in a strong dependence of the tunneling transmission probability on the in-plane wave vector component and spin polarization.

ACKNOWLEDGMENTS

This work was supported by the Ministry of Education of R.O.C. under Grant No. B87002, and by the National Science Council under Contract No. NSC 87-2215-E009-010.

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