Resonance spin filtering due to overbarrier reflection in a single barrier contact

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Spin-polarized transmission is calculated for electrons that experience interface elastic and spin-orbit impurity scattering. It is shown that the spin-orbit part of impurity scattering enhances the spin polarization of transmitted electrons and that overbarrier reflection results in resonant spin-polarized transmission. Applied voltage dependence of spin transmission is calculated. This is the prerequisite for the electrically controlled in-plane spin current in a semiconductor structure.

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I. INTRODUCTION

Since spintronics has become an important part of solid-state physics, various aspects of spin injection into nonmagnetic semiconductors have been discussed. Electrical spin polarization in semiconductors has been studied mostly in metal-semiconductor contacts where electron injection from a ferromagnetic metal takes place.[1–3]

Spin-orbit interaction in cubic semiconductors with no inversion symmetry makes spin injection possible without the use of an applied magnetic field and (or) magnetic materials.[4–6] This approach to spin injection relies on tunneling through a single nonmagnetic barrier[7,8] or resonant transmission through a double-barrier structure.[9–11] The spin polarization originates from the momentum-dependent energy splitting of electrons with opposite spins. The sources of spin splitting are the intrinsic Dresselhaus and the interface-induced Rashba spin-orbit interaction terms in an electron energy spectrum.

To date, tunneling through a single III-V semiconductor barrier has been studied in Refs. 7, 8, and 12. In these references, only the Dresselhaus term was taken into account. This consideration is adequate if the material is of cubic symmetry, the interface orientation excludes polarization fields, and no voltage is applied, thus providing a symmetric barrier for which the Rashba term equals zero. In more complex case of wurtzite AlGaN quantum wells, symmetry allows intrinsic linear k-dependent spin splitting to exist, and the polarization fields distort the band structure, making the extrinsic Rashba term nonzero as the structure becomes asymmetric. One more difference between cubic and wurtzite structures is that the Dresselhaus and Rashba terms in wurtzite structures have the same momentum-dependent spin symmetry.[13]

As for spintronic applications, GaN-based devices may deliver performance comparable to their GaAs-based counterparts: spin splitting and Rashba coupling in GaN heterostructures have been calculated theoretically[14,15] and studied experimentally.[16–18] In-plane spin current induced by a vertical tunneling across the wide band-gap double-barrier structure has been studied in Ref. 19.

It is known that interface elastic impurity scattering plays an important role in transmission through metal-metal,[20] semiconductor-superconductor,[21] and metal-semiconductor[22] contacts. The elastic scattering affects electron transmission, current-voltage characteristics, and could even change the type of conductivity from metallic to a tunnel one. Since we are discussing spin polarization, it is important to take into account spin-orbit part of impurity scattering as it might influence the discrimination between transmission amplitudes in two spin channels.

In this paper, we calculate spin-polarized tunnel transmission through a biased GaN/AlGaN/GaN barrier in the presence of interface elastic scattering. Both mechanisms of electron-spin splitting, Dresselhaus and Rashba, are taken into account. The voltage-dependent spin-tunnel transmission is calculated and it is shown that impurity spin-orbit scattering increases the spin polarization. Also, it is shown that due to overbarrier electron reflection, even single barrier structures may deliver resonances in spin filtering. This makes single barrier ballistic contacts competitive with double-barrier structures where resonances stem from resonance tunneling.

II. HAMILTONIAN

We start with an effective Hamiltonian for a conduction electron at the $z=0$ interface between a thick GaN layer and an AlGaN barrier assuming the spin axis is along the growth direction $(0Z)$,[13]

$$H=\frac{\hbar^2k_\parallel^2}{2m_\parallel}+k_z\left[\frac{\hbar^2}{2m_z}+\alpha_D(\sigma_xk_y-\sigma_yk_x)\right]k_z+W_0(\vec{\rho})\delta(z)+V(z)$$
$$+\left[W_1(\vec{\rho})\delta(z)+\left(\lambda+\frac{1}{2}\frac{\partial\beta}{\partial z}+\frac{\beta}{2}\frac{\partial}{\partial z}\right)\right](\sigma_xk_y-\sigma_yk_x),$$

$$\beta(z)=\frac{P_1P_2\Delta_3}{[E_g+2\Delta_2-V(z)][E_g+\Delta_1+\Delta_2-V(z)]-2\Delta_3^2},$$

$$k_z=-i\frac{\partial}{\partial z};\quad \vec{\rho}=(x,y), \qquad (1)$$

where we use the notation of Ref. 14, α_D is the Dresselhaus spin-orbit coupling constant, λ is the linear spin-orbit

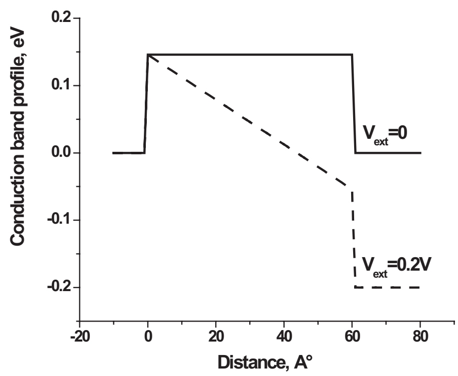

FIG. 1. Conduction-band profile in $Al_{0.2}Ga_{0.2}N$.

coupling parameter in a bulk wurtzite material, $V(z)$ is the heterostructure potential-energy profile that may include an external bias V_{ext} as shown in Fig. 1,

$$V(z)=\begin{cases} 0 & \text{left GaN } (l) \\ \Delta E_c - eFz & \text{AlGaN barrier } (b) \\ -eV_{ext} & \text{right GaN } (r), \end{cases}$$

$$F = V_{ext}/l, \tag{2}$$

ΔE_c is the conduction-band offset and l is the barrier width.

In contrast to cubic GaAs-based structures, the momentum-dependent spin invariant of the Dresselhaus term is similar to that of the Rashba term [term proportional to $\partial\beta/\partial z$ in Eq. (1)]. Matrix elements W_0 and W_1 describe spin-independent and spin-orbit parts of impurity-scattering amplitude. The impurity potential $W_{imp}(\vec{r})$ is an addition to the lattice periodic potential, thus generating matrix elements similar to those generated by the periodic potential resulting in the effective Hamiltonian (1). The Hamiltonian contains the matrix elements written below,

$$W_1(\vec{\rho}) = P_1P_2\frac{\partial}{\partial z} \times \frac{\langle iY|W_{imp}^{s.o.}(\vec{r})|Z\rangle}{[E_g+2\Delta_2-V(z)][E_g+\Delta_1+\Delta_2-V(z)]-2\Delta_3^2},$$

$$W_0(\vec{\rho}) = \langle S|W_{imp}(\vec{r})|S\rangle, \quad W_{imp}(\vec{r}) = \Sigma_i w(\vec{r}-\vec{R}_\iota), \tag{3}$$

where $|Z\rangle$, $|iY\rangle$, and $|S\rangle$ are atomic basis wave functions. Integration in matrix elements is over the unit cell defined by an in-plane vector $\vec{\rho}$, and $w(\vec{r})$ is the potential of a single impurity located at point $\vec{R}_\iota$, and $\Delta_{1,2,3}$ are the crystal-field and spin-orbit parameters in the bulk material, respectively. Amplitudes W_0 and W_1 vary slowly with $\vec{\rho}$ on the scale of the average distance between impurities. In addition, the amplitudes can be considered as random variables.

Unitary rotation u to a new spin axis in the x-y plane transforms eigenspinors and diagonalizes the Hamiltonian,

$$u = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i \\ i\ e^{i\alpha} & e^{i\alpha}\end{pmatrix}, \quad \tan(\alpha) = \frac{k_y}{k_x},$$

$$\Phi_\pm(\vec{\rho},z) = \frac{1}{\sqrt{2}}\chi(z)\varphi_\pm e^{i\vec{k}_\parallel\vec{\rho}}; \quad \varphi_\pm = \begin{pmatrix} 1 \\ \pm ie^{i\alpha}\end{pmatrix},$$

$$H_\pm = \frac{\hbar^2k_\parallel^2}{2m_\parallel} + k_z\left[\frac{\hbar^2}{2m_z^\pm}\right]k_z \mp \left(\lambda + \frac{1}{2}\frac{\partial\beta}{\partial z} + \frac{\beta}{2}\frac{\partial}{\partial z}\right)k_\parallel + W_0(\vec{\rho})\delta(z) \mp W_1(\vec{\rho})\delta(z)k_\parallel + V(z),$$

$$m_z^\pm = m_z(1 \mp 2\alpha_D m_z k_\parallel/\hbar^2)^{-1}. \tag{4}$$

Since we are considering scattering on nonmagnetic impurities, in a new basis there are no spin-flip processes, i.e., the spin-orbit scattering amplitude W_1 does not mix up the spin states $\Phi_\pm$.

Electron wave functions in layers, numbered in Eq. (2), can be represented as follows:

$$\chi_{l\pm} = e^{ik_lz} + r_\pm e^{-ik_lz}, \quad \chi_{b\pm} = A_2Ai(s_\pm) + B_2Bi(s_\pm),$$

$$\chi_{r\pm} = t_\pm e^{ik_r(z-a)}, \tag{5}$$

where $Ai(s)$, $Bi(s)$ are the Airy functions, $r_\pm, t_\pm$ are the reflection and transmission amplitudes, respectively,

$$\hbar k_l = \sqrt{2m_z\left(E - \frac{\hbar^2k_\parallel^2}{2m_\parallel}\right)}; \quad \hbar k_r = \sqrt{2m_z\left(E - \frac{\hbar^2k_\parallel^2}{2m_\parallel} + eV_{ext}\right)},$$

$$s_\pm = \left(\frac{2m_z^\pm}{\hbar^2e^2F^2}\right)^{1/3}(\Delta E_c - eFz - E). \tag{6}$$

III. BOUNDARY CONDITIONS AND SPIN-SELECTIVE TUNNEL TRANSMISSION

In order to account for the random field pinned to the interface, one has to obtain generic boundary conditions for the electron flux at the interface $z=0$ from the z integration of the Hamiltonian (3): $\int_{0_-}^{0_+}H_\pm\Phi_\pm dz=0$. Multiplying this equation by a conjugate $\Phi_\pm^*$ and averaging over the interface area A, $(1/A)\int\ldots e^{-(i\vec{k}_\parallel+\vec{k}_\parallel')\vec{\rho}/2}d\vec{\rho}$, one comes to the full set of matching conditions for wave functions and fluxes. Averaging the matching wave functions over the interface results in equal transverse momenta on both sides of the interface $\vec{k}_\parallel=\vec{k}_\parallel'$, and the boundary conditions follow:

$$\frac{1}{k_{Fl}}\frac{\partial\chi_l}{\partial z}\bigg|_{z=0} - \frac{m_l}{2m_r^\pm k_{Fl}}\frac{\partial\chi_b}{\partial z}\bigg|_{z=0} + \chi_l(0)[Z_0 \mp q(R+Z_1)] = 0,$$

$$\chi_l(0) = \chi_b(0), \tag{7}$$

where $q=k_\parallel/k_{Fl}$, $Z_0=\frac{2m_lV_0}{\hbar^2k_{Fl}}$, $Z_1=2m_1V_1/\hbar^2$, and $R=m_1\beta/\hbar^2$.

Here the potential and spin-orbit scattering parameters $V_{0,1}$ are zero Fourier components of random scattering fields

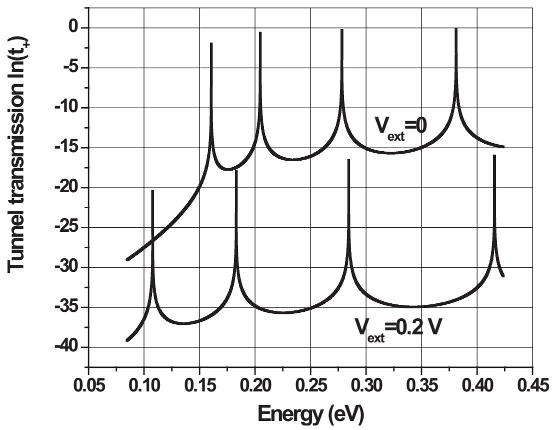

FIG. 2. Tunnel transmission as a function of an energy, $k_{\parallel}=0.3k_F$, $\langle Z_0\rangle=3$; $\langle Z_1\rangle=0.003$.

$W_{0,1}: V_{1,0}=(1/A)\int W_{1,0}(\vec{\rho})d\vec{\rho}$. Z_0 was introduced as a phenomelogical parameter in Ref. 20. It is assumed that the random variables $Z_{0,1}$ have Gaussian distribution with the root mean square of $\Delta_{0,1}=0.1\langle Z_{0,1}\rangle$, where $\langle\cdots\rangle$ is the average over the random field distribution.

The tunnel transparency of the structure is found using the transfer matrix method. The transfer matrix is composed of a set of four boundary conditions, Eq. (7), for interfaces at $z=0$ and $z=a$ (see Fig. 1).

Numerical calculations have been performed for a 60-Å-wide barrier with 20% Al content assuming the Dresselhaus coupling constant $\alpha_D\approx 2\times 10^{-31}$ eV m^3 (Ref. 23) and the Fermi energy $E_F=85$ meV. Bulk k-linear spin-orbit λ has been neglected as its role in tunneling is much less important than that of the Dresselhaus term that renormalizes the masses of tunneling electrons. Interband matrix elements are taken from Ref. 14: $\frac{P_{1,2}^2}{2m_0}=20$ eV. The parameter $R\approx 10^{-3}$ has been estimated from β Eq. (1). One can obtain an order of magnitude estimation of parameters $Z_{0,1}$ assuming Coulomb impurity potential-energy scale of $C_0\approx 1$ eV and spin-orbit characteristic energy of $C_1\approx 1$ meV. Based on Eq. (4), we have $V_0/a\approx C_0$ and $V_1k_{F1}/a\approx C_1$, where a is the lattice constant. Estimated parameters follow from Eq. (7): $Z_0\approx 3$, $Z_1\approx 3\times 10^{-3}$.

Figure 2 illustrates the averaged transmission $\langle t_+\rangle$ calculated for the structure shown in Fig. 1. Overbarrier electron reflection is at the origin of resonances in the transmission coefficient, making two barrier boundaries act as a semi-transparent Fabri-Perot resonator with a quality factor that depends on reflection coefficients. Transmission resonances are illustrated in Fig. 2. The first resonance in an unbiased structure occurs at $E=0.16$ eV, just above the top of the barrier. Finite bias makes the shape of the barrier triangular and then shifts resonance to lower energies.

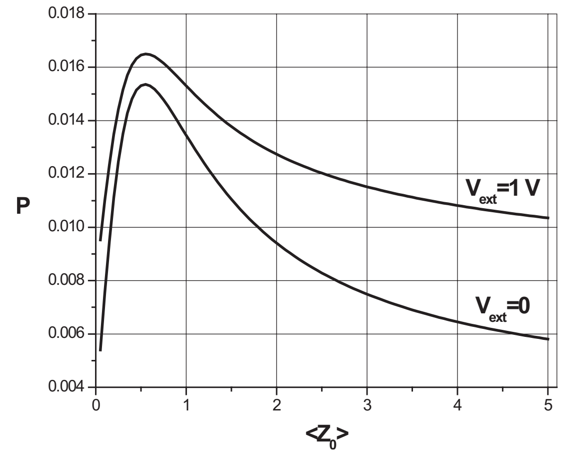

FIG. 4. Dependence of spin polarization on a potential scattering parameter, $E=1.5E_F$, $K_{\parallel}=1.1k_F$, and $\langle Z_1\rangle=0.003$.

Single-mode tunnel spin polarization is defined as $P=\frac{\langle t_+\rangle-\langle t_-\rangle}{\langle t_+\rangle+\langle t_-\rangle}$. Single-mode spin polarization is shown in Fig. 3 as a function of the applied voltage. Resonances in transmission (Fig. 2) and spin polarization (Fig. 3) originate from overbarrier electron reflection and look similar to those that occur in double-barrier structures, where they stem from resonance tunneling. The examples of spin polarization dependent on scattering parameters $\langle Z_0\rangle$ and $\langle Z_1\rangle$ are illustrated in Figs. 4 and 5, respectively. The spin-orbit scattering parameter represents an addition to the Rashba spin-splitting term in Eq. (7), i.e., it affects the spin polarization through boundary conditions.

The spin polarization by itself does not mean that spin injection occurs when the tunnel current flows across the barrier: in equilibrium the summation over all in-plane wave vectors makes the total spin polarization zero. Spin injection

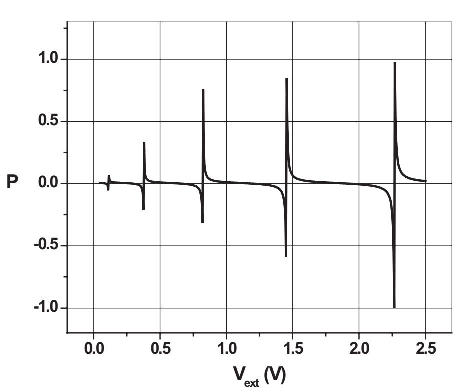

FIG. 3. Spin polarization vs applied voltage, $E=1.5E_F$, $k_{\parallel}=1.1k_F$, $\langle Z_0\rangle=3$; $\langle Z_1\rangle=0.003$.

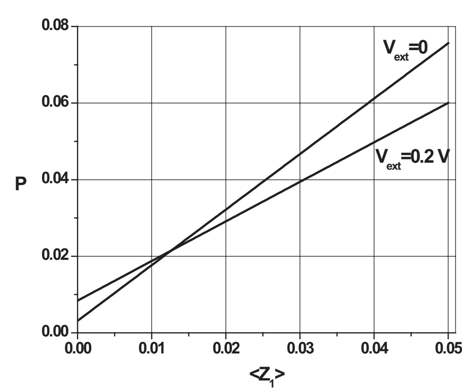

FIG. 5. Dependence of spin polarization on a spin-orbit scattering parameter, $E=1.5E_F$, $k_{\parallel}=1.1k_F$, and $\langle Z_0\rangle=3$.

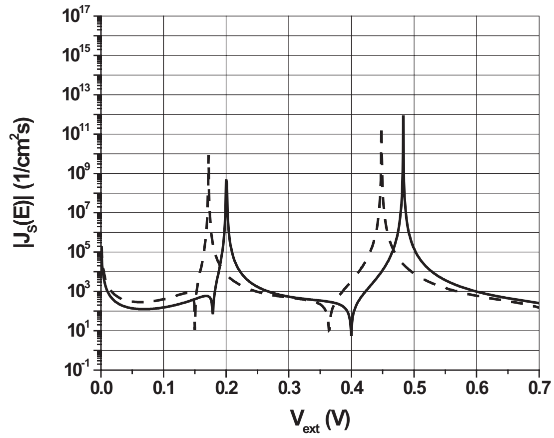

FIG. 6. Spin flux as a function of applied voltage. $\langle Z_0 \rangle = 3$, $\langle Z_1 \rangle = 0.003$; solid line: $E = 0.9 E_F$, dashed: $E = E_F$.

occurs if some nonequilibrium process violates in-plane symmetry [for instance, in-plane electric current in the region (r) or (l) (Refs. 10, 11, and 19)]. Resulting in-plane spin current is perpendicular to a lateral electric field F_L.

The magnitude of spin current, produced by tunneling electrons of energy E, can be written as

$$J_S(x) = \frac{q\tau F_L k_{Fl}^3}{32\pi^2 m_1} \int_0^{Q_{max}(x)} q^2 dq \frac{\partial f_1}{\partial x} (\langle t_+ \rangle - \langle t_- \rangle), \qquad (8)$$

where $x = E/E_F$, f_l is the equilibrium electron distribution function in the region (l). The upper limit $Q_{max}(x)$ is determined by the region where both incident and outgoing electron wave vectors are real. Assuming a momentum relaxation time of $\tau = 10^{-13}$ s and a lateral field of $F_L = 10^4$ V/cm, the spin current calculated with Eq. (8) is shown in Fig. 6.

In conclusion, the spin-orbit part of interface impurity scattering plays an important role in spin-selective electron transmission and may enhance spin-polarization efficiency. The resonance spin transmission, controlled by an applied voltage, which usually occurs in double-barrier structures, can be observed even in a single barrier contact. This is especially important in spintronic applications of wide band-gap semiconductors, where high-quality double-barrier resonant tunneling diodes have not yet been reported (see review Ref. 24).

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