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To cite this article: G Isi et al 2010 J. Phys.: Conf. Ser. 242 012008

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A quantum transport model for the double-barrier nonmagnetic spin filter

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Abstract. A model for calculating the current and spin polarization in a double-barrier InGaAs resonant tunnelling structure is described with the aim to account for phase-breaking scattering. It is based on the nonequilibrium Green’s function method with both elastic and inelastic (LO-phonon) scattering described within the self-consistent first Born approximation. It has been found that the maximum current spin polarization of around 0.45 in the ballistic limit decreases to around 0.25 for scattering transport with scattering-induced broadening of quasi-bound states of around 4meV.

1. Introduction

Recently, it has been suggested that resonant tunnelling structures (RTS) [1] based on III-V semiconductor heterostructures are a promising candidate for a nonmagnetic spin filter, [2, 3, 4, 5]. The mechanism is based on electron tunnelling through quasi-bound states which are spin-split due to the spin-orbit interaction, manifested as Rashba [6] and Dresselhaus [7] effects.

Numerical estimates of the attainable spin polarization reported so far ignored the detrimental effects of carrier scattering. Here we use the method of nonequilibrium Green’s functions [8] adapted for modeling quantum transport in nanodevices, [9, 10, 11].

2. The model

The spin-dependent transport through the InGaAs double-barrier resonant tunneling structure (RTS) shown in Figure 1 is a consequence of the Rashba spin-orbit interaction (RSOI)

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

where \( k_x \) and \( k_y \) are the components of the lateral (perpendicular to the growth direction, denoted as the \( z \) axis) wave vector \( \mathbf{k} \). \( \sigma_x, \sigma_y \) are the Pauli matrices and \( \alpha \) is the Rashba parameter [12]

\[ \alpha = eE_{\text{ext}}\hbar^2 \frac{(2E_g + \Delta_{SO})\Delta_{SO}}{2mE_g(E_g + \Delta_{SO})(3E_g + 2\Delta_{SO})}, \]  

\( E_{\text{ext}} \) being the externally applied electric field while \( m = 0.023m_0, E_g = 356\text{meV} \) and \( \Delta_{SO} = 410\text{meV} \) are the InAs band parameters. RSOI creates the energy difference \( \Delta E(|k|) = 2\alpha|k| \)
between the two resonant energy levels denoted by $E_R^+$ and $E_R^-$ in Figure 1. The value of $\alpha$

Figure 1. The effective electron potential profile in a biased InGaAs RTS. The conduction band offset is taken to be $\Delta E_c = 792$meV, $m_{GaAs} = 0.067m_0$, the barrier and well width $L_b = 3$nm and $L_w = 6$nm, respectively, as in [2] while the Fermi energies in the contacts are $E_{F,E} = E_{F,C} = 20$meV.

obtained from (2) for $E_{ext} = 20$mV/nm (corresponding to the current peak in the $J(V_{CE})$ curves shown in Figure 2) has an order-of-magnitude agreement with values found experimentally in [13]. For $k = k_F$ ($E_F = 20$meV) it yields $\Delta E(k_F) = 2$meV. Since the spin splitting has the same order of magnitude as the scattering-induced broadening of the resonant energy levels [1], we conclude that to model the spin polarization in a RTD, one has to go beyond the ballistic transport picture.

The quantities describing the electronic system are the greater ($G^>(E)$) and lesser ($G^<(E)$), Green’s functions. Once $G^>(E)$ and $G^<(E)$ are found, it is straightforward to obtain the electron concentration, density of states and current density, [11]. The interaction with InAs optical phonons ($\omega_{LO} = 29$meV) and elastic phase breaking are calculated within the self-consistent first Born approximation, the procedure for which we briefly outline here.

We start by finding the retarded ($\Sigma^R(E)$), lesser ($\Sigma^<(E)$) and greater ($\Sigma^>(E)$) self-energies. They are obtained by adding up the contributions of various interactions. In particular, we have

$$\Sigma^\gamma(E) = \Sigma^\gamma_E(E) + \Sigma^\gamma_{el}(E) + \Sigma^\gamma_{ph}(E) + \Sigma^\gamma_{\alpha}(E), \quad \gamma = R, <, > . \quad (3)$$

The indices $E$ and $C$ refer to terms due to interaction with emitter and collector reservoirs, respectively, [11]. $\Sigma^\gamma_{ph}(E)$ and $\Sigma^\gamma_{\alpha}(E)$ describe the LO phonon and elastic phase breaking. In the first iteration, these two are assumed zero. At the end of each iteration, new values for the scattering self-energies are obtained and compared with previous ones. Typically, 10 to 30 iterations were required to obtain a relative error below $10^{-5}$.

Then, we find $G^R(E)$ according to

$$G^R(\sigma, |k|, z, z'; E) = \left( E - H(\sigma, |k|) - \Sigma^R(z, z'; E) \right)^{-1}, \quad (4)$$

$$H(\sigma, |k|) = -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + \frac{\hbar^2 k^2}{2m} + \sigma \alpha|k| + V(z). \quad (5)$$

$V(z)$ comprises the band-edge potential and the linear term due to the external field, see Figure 1. $\sigma = \pm$ denotes the spin subband. For calculations we use the $|k, z|$ basis with $N$ grid points for the $z$ axis and the finite difference approximation. Thus, for fixed values of $\sigma$, $|k|$ and $E$, $G^R(\sigma, |k|, z, z'; E)$ becomes a $N \times N$ matrix. The lesser and greater Green’s functions are found from the kinetic equation

$$G^A(\sigma, |k|, z, z'; E) = \int dz_1 \int dz_2 G^R(\sigma, |k|, z, z_1; E) \Sigma^A(z_1, z_2; E) G^A(\sigma, |k|, z_2, z'; E), \quad (6)$$

where $G^A(E)$ is the Hermitian conjugate of $G^R(E)$ and the $z$-integration goes from the emitter to the collector contact (left and right end of the structure shown in Figure 1).
New values of the lesser and greater scattering self-energies are given by the first Born approximation ($\varphi = \text{ph}', \text{el}'$)

$$\Sigma_\varphi^\lambda(z, z'; E) = \frac{U_\varphi^2}{8\pi^2} \delta(z - z') \int dk \left( G^\lambda(+,|k|, z, z; E \pm \hbar \omega_\varphi) + G^\lambda(-,|k|, z, z; E \pm \hbar \omega_\varphi) \right)$$

(7)

± in front of the phonon energy $\hbar \omega_\varphi$ means + for $\lambda \leq <$ (electron relaxation from $E + \hbar \omega_\varphi$ to $E$) and − for $\lambda \geq >$ (hole relaxation from $E - \hbar \omega_\varphi$ to $E$). The above expression accounts only for spontaneous phonon emission, which is appropriate for low temperatures such that the average number of phonons $n_B(\hbar \omega_{LO}) = (\exp(\hbar \omega_{LO}/kT) - 1)^{-1}$ is much smaller than 1. For elastic scattering, we put $\omega_\text{el} = 0$.

Finally, the imaginary part of the retarded scattering self-energy is given by:

$$\Sigma_R^\varphi(z, z'; E) = \frac{1}{2} \left( \Sigma_\varphi^>(z, z'; E) - \Sigma_\varphi^<(z, z'; E) \right),$$

(8)

while the real part of $\Sigma_R^\varphi(E)$ is neglected since it merely shifts the energy levels in the system. The self-energies found from (7) and (8) are local ($\sim \delta(z - z')$) due to the assumption that the coupling to scatterers is independent on $k$. It is exact for the deformation potential coupling to optical phonons, but not for polar coupling in which case the effective local scattering strength $U^2$ can be found by averaging, see Appendix C of [14]. In this work $U_{\text{ph}}^2 = 2500 \text{meVÅ}/D_{\text{InAs}}$ and $U_{\text{el}}^2 = 250 \text{meVÅ}/D_{\text{InAs}}$ with $D_{\text{InAs}} = m/2\pi\hbar^2$ (local density of states of a spin subband in a InAs two-dimensional electron gas) have been used. These gave average elastic and phonon scattering rates of around $10^{12} \text{s}^{-1}$ at the current main peak shown in Figure 2 inset ($V_{CE} \approx 270 \text{mV}$) and the enhanced value for phonon scattering of around $10^{13} \text{s}^{-1}$ at the phonon peak ($V_{CE} \approx 320 \text{mV}$), which is comparable to values reported in Ref. [10]. For $V_{CE} \approx 270 \text{mV}$ it has been found that the quasi-bound state broadening is $0.8 \text{meV}$ in the ballistic limit, $4.5 \text{meV}$ with only elastic scattering and $4.9 \text{meV}$ when both elastic and inelastic scattering are taken into account. Thus the scattering-induced broadening of quasi-bound states found using the above scattering strengths is consistent with typical values found in the literature [1].

The energy resolved spin-subband current density entering the system through contact $\gamma = E, C$ (emmitter and collector) is given by [11]

$$i_\gamma(\sigma, E) = \frac{e}{4\pi^2\hbar} \int dz \int dz' \int dk \left( \Sigma_\gamma^>(z, z'; E)G^>(\sigma, |k|, z', z; E) - \Sigma_\gamma^<(z, z'; E)G^<(\sigma, |k|, z', z; E) \right).$$

(9)

The total spin-subband current densities flowing through the device are obtained by integrating $i_\gamma(\sigma, E)$ over energy

$$J(\sigma) = \int dE i_E(\sigma, E) = - \int dE i_C(\sigma, E),$$

(10)

while the total current density is $J = J(+) + J(-)$. In absence of a lateral electric field, the Kramers degeneracy implies a zero spin polarization of the total current. Thus, the one-sided collector geometry is assumed, [4], in which case the spin polarization is given by

$$P = \frac{2 J(+)-J(-)}{\pi J(+)+J(-)}.$$  

(11)
3. Results

Figure 2 shows the dependence of $P$ and current density $J$ (inset) on the external bias. For reasons of compactness, curves for $J(+)$ and $J(-)$ separately are not shown. They have a shape similar to $J$ (multiplied by a factor of 0.5) and are mutually displaced in voltage by approximately $\Delta V_{CE} = 2\text{mV} \sim \Delta E(k_F)/e$. Maxima in $P$ occur at places where there is a sudden change of the magnitude of either $J(+)$ or $J(-)$: around the current turn-on ($V_{CE}^{on} \approx 245\text{mV}$) the $J(-)$ component suddenly rises leading to a negative peak in $P$; the positive peak in $P$ occurs at the current turn-off voltage ($V_{CE}^{off} \approx 285\text{mV}$) where $J(-)$ goes to zero before $J(+)$. The polarization is reduced by the broadening of features in $J(V_{CE})$, which is the main effect of carrier scattering. The maximal value of $P$ for the fully ballistic transport ($U_{ph} = 0, U_{el} = 0$) of around 0.4 is reduced to around 0.1 when elastic scattering is present. LO-phonon scattering causes the phonon-peak at $V_{CE} \approx 320\text{mV}$ in both subband currents, but it is so wide that no feature in $P(V_{CE})$ is observed. Compared to the case when only the elastic scattering is taken into account ($U_{ph} = 0, U_{el} \neq 0$), the case with LO-phonon scattering does not create a significant difference in $P(V_{CE})$ because when $V_{CE}$ is large enough to make the resonant transmission with phonon emission possible, there are no carriers that can be resonantly transmitted (without scattering) hence no sharp features in $J(V_{CE})$ exist.

![Spin polarization and current density](image)

Spin polarization

Figure 2. Calculated values of the spin polarization and current density (inset) for the InGaAs RTS described in Figure 1 at $T = 4.2K$. Three cases have been considered: ballistic transport (diamonds), elastic scattering only (stars) and both elastic and LO-phonon scattering (circles).

In summary, we have described a model to account for effects of carrier scattering on spin polarization of the current. By choosing numerical values of scattering strengths that yield average relaxation times of around 1ps (and around 0.1ps for resonant LO-phonon emission), the peak in spin polarization is found to decrease from 0.4 in the ballistic case to around 0.1 when carrier scattering is present.

Acknowledgments

Authors acknowledge the support of NATO Collaborative Linkage Grant (reference CBP.EAP.CLG 983316). G. I. is grateful for the support from ORSAS (UK), University of Leeds, the School of Electronic and Electrical Engineering and the Serbian Ministry of Science project No. 141047. V. M. and J. R. acknowledge the support from the Serbian Ministry of Science project No. 141006.

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