PERGAMON

Solid State Communications 125 (2003) 381–385

solid state communications

www.elsevier.com/locate/ssc

Spin-dependent electron single and double scattering from quantum dots and antidots

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Received 24 October 2002; received in revised form 2 December 2002; accepted 6 December 2002 by H. Takayama

Abstract

We present a theoretical study of the spin-dependent electron scattering from spherical quantum dots (antidots) embedded into III–V semiconductors. To calculate the elastic scattering cross-section we use the effective one electron band Hamiltonian and spin-dependent boundary conditions generated by the spin–orbit interaction in the structures. It is demonstrated that the spin–orbit interaction can lead to a recognizable magnitude of polarization for single and double scattering at zero magnetic field.

PACS: 72.20.Dp; 72.25.Dc; 73.63.Kv

Keywords: A. Nanostructures; A. Semiconductors; D. Electronic transport; D. Spin–orbit effects

The asymmetric scattering of polarized electrons in gas and metallic systems has been extensively studied for decades (see Refs. [1–3] and references therein). The relaxation of electron and hole spin polarization due to spin-dependent scattering in semiconductor structures was also of great interest and has been studied both experimentally and theoretically [4–6]. Recently it was discovered that most of the scattering events conserve spin and the electron spin-relaxation time can become surprisingly long in III–V semiconductors (as 100 ns [6]). The spin-diffusion length is much longer than the electron mean free path, and in some III–V semiconductor nano-structures it may be of the order of the sample dimensions (100 μm [7]).

In semiconductors the most important interaction, which causes spin-dependent processes is the spin–orbit interaction [8,9]. The Rashba spin–orbit coupling [9] is an essential element of the spin field effect transistor proposed by Datta and Das [10]. A new branch of semiconductor electronics so called spintronics [11] became under an extensive development recently. For this reason, the spin-dependent kinetics of electrons in traditional III–V semiconductor heterostructures becomes a topic of a great.

This paper describes a model of the spin-dependent electron scattering from nano-scale semiconductor quantum dots (antidots). Recent advances in semiconductor nano-technology allow us to consider small spherical dots (antidots) of III–V semiconductors [12] as 'artificial defects' with controllable parameters. We calculate the polarization (the Sherman function [2,3]) after a single scattering and investigate how the polarization changes after the second scattering. In our calculation we use the effective one band Hamiltonian with the spin-dependent boundary conditions [13–15]. The rectangular hard-wall potential of the dots (antidots) is induced by the discontinuity of the conduction band edge of the system.

For three-dimensional semiconductor quantum dots (antidots) the approximate one electronic band effective

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PII: S0038-1098(02)00850-5

Hamiltonian is given in the form [13]

$$\hat{H} = -\frac{\hbar^2}{2}\nabla_{\mathbf{r}}\frac{1}{m(E,\mathbf{r})}\nabla_{\mathbf{r}} + V(\mathbf{r}) + V_{\mathrm{so}}(\mathbf{r}), \tag{1}$$

where $\nabla\mathbf{r}$ stands for the spatial gradient, $m(E,\mathbf{r})$ is energy and position-dependent electron effective mass

$$\frac{1}{m(E,\mathbf{r})} = \frac{2P^2}{3\hbar^2} \times\left[\frac{2}{E+E_{\mathrm{g}}(\mathbf{r})-V(\mathbf{r})} + \frac{1}{E+E_{\mathrm{g}}(\mathbf{r})-V(\mathbf{r})+\Delta(\mathbf{r})}\right],$$

$V(\mathbf{r})$ is the hard-wall confinement potential of the dots or hard core repulsive potential of the antidots, $E_{\mathrm{g}}(\mathbf{r})$ and $\Delta(\mathbf{r})$ stand for position-dependent band gap and the spin–orbit splitting in the valence band, P is the momentum matrix element. The spin–orbit interaction $V_{\mathrm{so}}(\mathbf{r})$ for conducting band electrons is described by [9,14,15]

$$V_{\mathrm{so}}(\mathbf{r}) = \mathrm{i}\nabla_{\mathbf{r}}\beta(E,\mathbf{r})\cdot[\hat{\boldsymbol{\sigma}}\times\nabla_{\mathbf{r}}], \tag{2}$$

where

$$\beta(E,\mathbf{r}) = \frac{P^2}{3} \times\left[\frac{1}{E+E_{\mathrm{g}}(\mathbf{r})-V(\mathbf{r})} - \frac{1}{E+E_{\mathrm{g}}(\mathbf{r})+\Delta(\mathbf{r})-V(\mathbf{r})}\right], \tag{3}$$

is the spin–orbit coupling parameter, and $\hat{\boldsymbol{\sigma}} = \{\sigma_x, \sigma_y, \sigma_z\}$ is the vector of the Pauli matrices.

For systems with a sharp discontinuity of the conduction band edge between the dot (antidot) (material 1) and the crystal matrix (material 2) the scattering potential can be presented as

$$V(\mathbf{r}) = \begin{cases} -V_0, & \mathbf{r}\in 1 \\ 0, & \mathbf{r}\in 2, \end{cases} \tag{4}$$

where the potential barrier is chosen as $V_0 \geq 0$ for dots and $V_0 \leq 0$ for antidots. From integration of the Shrödinger equation with Hamiltonian (1) along direction perpendicular to the interface ($\mathbf{r}_n$) we obtain the spin-dependent Ben Daniel–Duke boundary conditions for the electron wave function $\Psi(\mathbf{r})$

$$\begin{aligned} &\Psi_1(\mathbf{r}_{\mathrm{s}}) = \Psi_2(\mathbf{r}_{\mathrm{s}}); \\ &\left\{\frac{\hbar^2}{2m(E,\mathbf{r})}\nabla_{\mathbf{r}} - \mathrm{i}\beta(E,\mathbf{r})[\hat{\boldsymbol{\sigma}}\times\nabla_{\mathbf{r}}]\right\}_n \Psi_1(\mathbf{r}_{\mathrm{s}}) \\ &= \left\{\frac{\hbar^2}{2m(E,\mathbf{r})}\nabla_{\mathbf{r}} - \mathrm{i}\beta(E,\mathbf{r})[\hat{\boldsymbol{\sigma}}\times\nabla_{\mathbf{r}}]\right\}_n \Psi_2(\mathbf{r}_{\mathrm{s}}), \end{aligned} \tag{5}$$

where $\mathbf{r}_{\mathrm{s}}$ denotes the position of the system interface.

Considering dots (antidots) with spherical shapes we choose the solution of the scattering problem in spherical coordinates (r,θ,ϕ) as [1,16,17]

$$\Psi(\mathbf{r}) = (4\pi)^{1/2}\sum_{l,s=\pm 1}\mathrm{i}^l[l+(1+s)/2]^{1/2}R_l^s(r)\mathbf{Y}_l^s(\theta,\varphi), \tag{6}$$

where

$$\mathbf{Y}_l^s(\theta,\varphi) = s\sum_{s'=\pm 1}\mathbf{C}[l+s/2,1/2; \times(1-s')/2, s'/2]\cdot Y_{l,(1-s')/2}(\theta,\varphi)\chi^{s'},$$

$\mathbf{C}[x,y;z,w]$ are the Clebsh–Gordan coefficients [1], $Y_{l,m}(\theta,\varphi)$ are the spherical harmonics, $s=\pm 1$ refers to the electron spin polarization, and χ^s is a spin function upon which the Pauli matrix vector operates:

$$\chi^{+1} = \begin{pmatrix}1\\0\end{pmatrix}, \qquad \chi^{-1} = \begin{pmatrix}0\\1\end{pmatrix}.$$

Substituting Eq. (6) into the Schrödinger equation, we obtain

$$\begin{aligned} &-\frac{\hbar^2}{2m_1(E)}\left[\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}r^2\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2}\right]R_{1l}^s(r) \\ &= (E+V_0)R_{1l}^s(r), \quad r\geq r_0, \\ &-\frac{\hbar^2}{2m_2(E)}\left[\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}r^2\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2}\right]R_{2l}^s(r) = ER_{2l}^s(r), \\ &r<r_0, \end{aligned} \tag{7}$$

where r_0 is the radius of the sphere. The spin-dependent boundary conditions (5) for the spherical quantum dot (antidot) can be written as

$$\begin{aligned} &R_{1l}^s(r_0) = R_{2l}^s(r_0), \\ &\frac{\hbar^2}{m_1(E)}\frac{\mathrm{d}}{\mathrm{d}r}R_{1l}^s(r)\bigg|_{r0} - \frac{\hbar^2}{m_2(E)}\frac{\mathrm{d}}{\mathrm{d}r}R_{2l}^s(r_0)\bigg|_{r0} + \frac{2[\beta_1(E)-\beta_2(E)]}{r_0} \\ &\times\left[j(j+1) - l(l+1) - \frac{3}{4}\right]R_{1l}^s(r_0) \\ &= 0, \end{aligned} \tag{8}$$

where $j = |l+s/2|$.

The method of partial waves is convenient in this specific case of spherical quantum dots (antidots) with short-range potentials (4), when we can solve the scattering problem without additional assumptions. The proper solution of Eq. (7) behaves like

$$\begin{aligned} &R_{1l}^s(r) = A_l^s g_l(\kappa r), \\ &R_{2l}^s(r) = B_l^s[j_l(kr) - \tan\delta_l^s\eta_l(kr)], \end{aligned} \tag{9}$$

where δ_l^s is the phase shift due to spin-dependent scattering, j_l and η_l are the spherical Bessel functions of the first and

second kind, respectively

$$k(E) = \frac{\sqrt{2m_2(E)E}}{\hbar},$$

and g_l is a solution in the dot (antidot) region. For the dot case:

$$g_l(\kappa r) = j_l(\kappa r),$$

where

$$\kappa(E) = \frac{\sqrt{2m_1(E)(E+V_0)}}{\hbar},$$

while for the antidot case:

$$g_l(\kappa r) = \sqrt{\frac{\pi}{2\kappa r}} I_{l+1/2}(\kappa r),$$

$$\kappa(\varepsilon) = \frac{\sqrt{2m_1(E)(|V_0| - E)}}{\hbar}.$$

($I_{l+1/2}(z)$ is the modified Bessel function of the first kind). The phase shift δ_l^s can be obtained from the values of the wave functions $R_l^s(r)$ at the dot boundary ($r = r_0$)

$$\tan \delta_l^s = \frac{kj_l'(kr_0) - \gamma_l^s j_l(kr_0)}{k\eta_l'(kr_0) - \gamma_l^s \eta_l(kr_0)}, \tag{10}$$

where

$$\gamma_l^s = \kappa \frac{m_2}{m_1} \frac{g_l'}{g_l} + \frac{2m_2(\beta_1 - \beta_2)}{r_0\hbar^2}\left[j(j+1) - l(l+1) - \frac{3}{4} \right],$$

and primes denote the first derivatives with respect to the function argument.

The complex scattering amplitude [17] is defined as

$$\mathbf{F}^s = [f^s(\theta) + (\hat{\boldsymbol{\sigma}} \cdot n_1) g^s(\theta)]\chi^s, \tag{11}$$

where

$$f^s(\theta) = \frac{1}{k} \cdot \sum_{l=0}^{\infty} [(l+1)\exp(\mathrm{i}\delta_l^+)\sin\delta_l^+ + l\exp(\mathrm{i}\delta_l^-)\sin\delta_l^-]P_l(\cos\theta),$$

and

$$g^s(\theta) = \frac{\mathrm{i}}{k} \cdot \sum_{l=1}^{\infty} [\exp(\mathrm{i}\delta_l^+)\sin\delta_l^+ - \exp(\mathrm{i}\delta_l^-)\sin\delta_l^-]P_l^1(\cos\theta),$$

are the direct amplitude and the spin-flip amplitude, correspondingly, (is the scattering angle between initial $\mathbf{k}_\mathrm{i}$ and final $\mathbf{k}_\mathrm{f}$ wave vectors,

$$\mathbf{n}_1 = \frac{\mathbf{k}_\mathrm{i} \times \mathbf{k}_\mathrm{f}}{|k_\mathrm{i} \times k_\mathrm{f}|},$$

is a unit vector perpendicular to the scattering plane, $P_l(\cos\theta)$ and $P_l^1(\cos\theta)$ are the Legendre polynomial and Legendre associated function, respectively.The Mott scattering cross-section for spin-polarized electrons can be written in terms of the incident electron spin-polarization vector $\mathbf{P}_\mathrm{i}$

$$\sigma(\theta) = I(\theta)[1 + S(\theta)\mathbf{P}_\mathrm{i} \cdot \mathbf{n}_1], \tag{12}$$

where

$$I(\theta) = |f^s(\theta)|^2 + |g^s(\theta)|^2,$$

is the differential cross-section for an un-polarized incident beam and

$$S(\theta) = \frac{f^{s*}g^s + f^s g^{s*}}{|f^s(\theta)|^2 + |g^s(\theta)|^2}, \tag{13}$$

is the Sherman function [2,3]. The Sherman function characterizes the left–right asymmetry in the scattering cross-section for initially polarized electron beams and the average polarization after a single scattering $\mathbf{P}_l$ for an initially unpolirazed beam

$$\mathbf{P}_1 = S(\theta)\mathbf{n}_1.$$

It follows from the equations above that the spin–orbit interaction influences the phase shifts with angular momentum $l > 0$. The effect is stronger for pairs of materials with a lager difference in the spin–orbit coupling parameters. Fig. 1

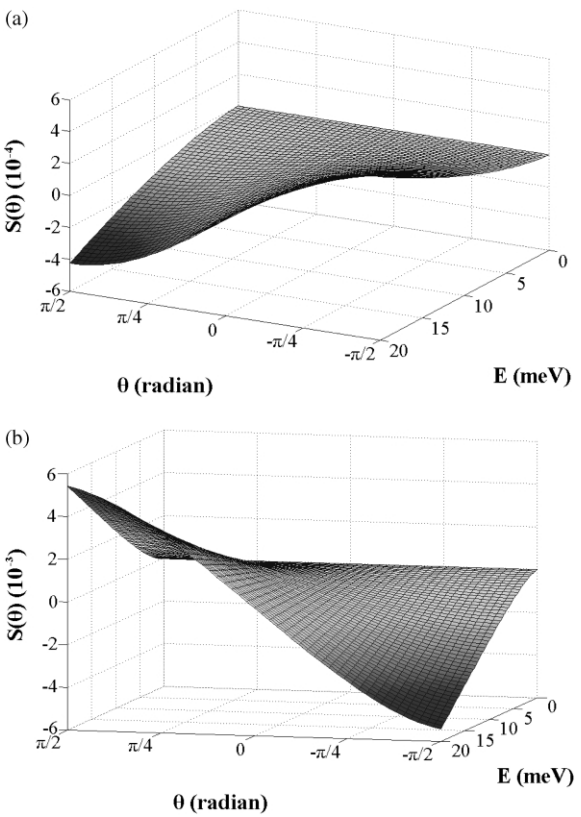

Fig. 1. The Sherman function for (a) spherical InAs/GaAs quantum dot with $r_0 = 1.3$ nm and (b) spherical GaAs/InAs antidot with $r_0 = 6$ nm. $E_{\mathrm{gInAs}} = 0.42$ eV, $E_{\mathrm{gGaAs}} = 1.52$ eV, $|V_0| = 0.77$ eV, $\Delta_{\mathrm{InAs}} = 0.38$ eV, $\Delta_{\mathrm{GaAs}} = 0.34$ eV, $m_{\mathrm{InAs}}(0) = 0.023m_0$, $m_{\mathrm{GaAs}}(0) = 0.067m_0$ (m_0—the free electron mass) [13].

presents the Sherman function versus the scattering angle and the energy of the incoming electrons calculated for a nano-scale quantum dot (InAs/GaAs) and antidot (GaAs/InAs). In the case of quantum dots (Fig. 1(a)) we avoided an additional complexity by neglecting the interaction of the scattered electrons with charges bound in the dots and the resonance effects. This restricts us to use dot sizes, which do not allow any bound states in the dots. The electron energy is adjusted to the electron band edge of GaAs. In the dot region the denominators of the spin–orbit coupling parameter (see Eq. (3)) are relatively large ($V_0 = 0.77$ eV, $E_{1g} = E_{gInAs} = 0.42$ eV, $\Delta_1 = \Delta_{InAs} = 0.38$ eV) that makes β_1, the total difference $\beta_1 - \beta_2$ and the effect rather small. For the antidot case, the situation is quite different. In antidot region the dominators are relatively small, so the parameter $\beta_1 - \beta_2$ is large. The Sherman function amplitude becomes much lager than that for the quantum dot case (see Fig. 1(b)).

Polarization produced by scattering of an unpolarized electron beam affects subsequent scattering processes. The first scattering generates a polarization that in the second scattering results in the left–right asymmetry in the scattering cross-section. If the azimuthal asymmetry after the second scattering can be measured, the scattering induced polarization can be found [1,16,17]. We consider double scattering in the same x–y plane as it is presented in Fig. 2. The polarization $\mathbf{P}_2$ in the double scattering process is parallel to $\mathbf{n}_l$ and it is described by

$$P_2^l(\theta_1, \theta_2) = \frac{S_1(\theta_1) + S_2(\theta_2)}{1 + S_1(\theta_1)S_2(\theta_2)},$$

when the second scattering occurs to the left of an observer standing to $\mathbf{n}_l$ and

$$P_2^r(\theta_1, \theta_2) = \frac{S_1(\theta_1) - S_2(\theta_2)}{1 - S_1(\theta_1)S_2(\theta_2)},$$

when the second scattering occurs to the right of the observer.

In Fig. 3 we present the calculated result of the left polarization for the double scattering from GaAs/InAs antidotes. The results demonstrate a well recognizable polarization after the second scattering. In addition, Fig. 4

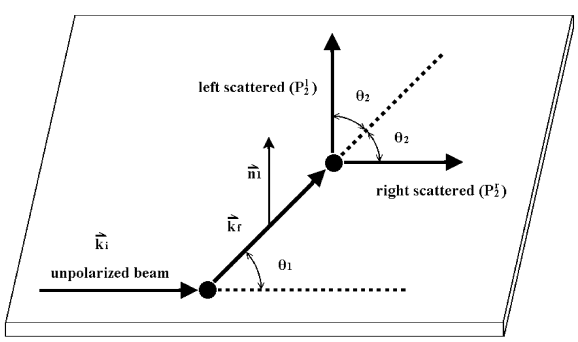

Fig. 2. Schematic diagram of single and double scattering.

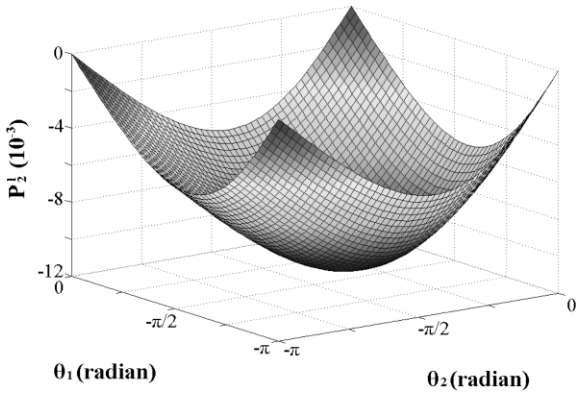

Fig. 3. Polarization of double scattering to the left ($P_2^l(\theta_1, \theta_2) = P_2^r(\theta_1, -\theta_2)$) induced by scattering from GaAs/InAs antidotes with $r_0 = 6$ nm and $E = 20$ meV.

shows the energy dependence of the polarization of the double scattering process with a fixed direction of the first scattering.

Subsequent scatterings (more than double) generate more complicated angular dependencies of the polarization [1,2] and could be investigated theoretically one after another [2,17]. But in reality, the intensity of the polarized electrons is small. In addition the background scattering processes (phonons, impurities, defects, plural scatterings, etc.) should substantially randomize the subsequent polarization process [2]. From other side, this randomization in higher order scatterings provides some grounding in the kinetic theory of the anomalous Hall effect [18–21].

Following the method from [18–21], for degenerated electronic system and a random three dimensional array of the quantum dots (antidots) at zero magnetic field the anomalous Hall angle can be estimated as

$$|\theta_H| = \frac{\tau_0}{\tau_H}, \tag{14}$$

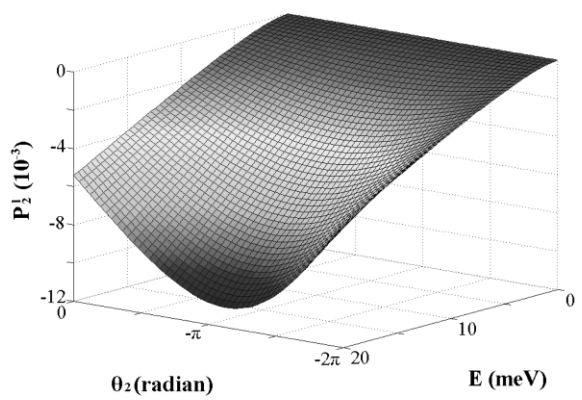

Fig. 4. Energy dependence of the left–right double scattering polarizations induced by scattering from GaAs/InAs antidotes with $r_0 = 6$ nm and $\theta_1 = -\pi/2$.

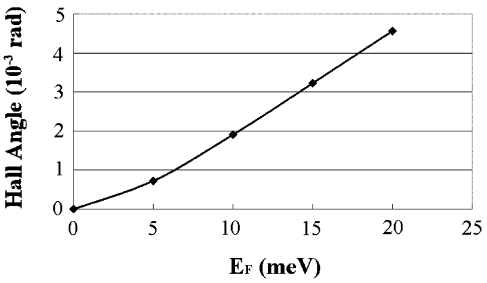

Fig. 5. The absolute value of the anomalous Hall angle for a random array of GaAs/InAs antidots with radius $r_0 = 6$ nm.

where

$$\frac{1}{\tau_0} = 2\pi N_d v_F \int_0^{\pi} d\theta\, I(\theta)(1 - \cos\theta)\sin\theta, \tag{15}$$

is the elastic scattering rate, and

$$\frac{1}{\tau_H} = 2\pi N_d v_F \int_0^{\pi} d\theta\, I(\theta)S(\theta)(1 - \cos\theta)\sin^3\theta, \tag{16}$$

is the spin-flip scattering rate. All functions are taken at the Fermi shell, N_d is the concentration of the dots (antidotes), v_F is the Fermi velocity, and it is assumed that the electron current is completely polarized. In Fig. 5 we present the result calculated for the anomalous Hall angle as a function on the Fermi energy for an array of GaAs/InAs antidotes. It should be noted, the anomalous Hall effect produced by quantum antidots has a measurable magnitude.

In summary, we discussed the influence of the spin–orbit interaction on the electron scattering from semiconductor quantum dots and antidots. The one electron band effective Hamiltonian and the spin-dependent boundary conditions for spherical quantum dots (antidots) allowed us to calculate a spin asymmetry in the electron scattering cross-section. We found a polarization produced by single and double scattering of unpolirazed electron beams due to the spin–orbit interaction. We would like to stress that, the polarization is caused by non-magnetic GaAs/InAs semiconductor structures without external magnetic fields. We should mention, that in the anomalous Hall effect the Hall angle is proportional to the Sherman function at the Fermi energy shell [18,19]. Our calculation results suggest a small but measurable magnitude of the Hall angle for antidots. The anomalous Hall effect produced by quantum antidots is expected to be reduced by the electron impurity scattering, but should still have a significant magnitude. This effect is potentially useful in integrated electron spin-polarization devices based on all-semiconductor heterostructures.

Acknowledgements

This work was supported by the National Science Council of Taiwan under contracts NSC-90-2215-E-009-022 and NSC-91-2219-M-009-003.

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