

## Hole spin relaxation during the tunneling between coupled quantum dots

A. F. Zinovieva,\* A. V. Nenashev, and A. V. Dvurechenskii

*Institute of Semiconductor Physics, Siberian Branch of the Russian Academy of Sciences, 630090 Novosibirsk, Russia*

(Received 24 May 2004; revised manuscript received 13 September 2004; published 24 January 2005)

We investigate theoretically the spin transport in an array of Ge/Si quantum dots. In the frame of the tight-binding approach we calculate the probability of hole spin-flip for resonant tunneling between localized states in neighboring quantum dots. The tunneling between hole ground states occurs mainly with conservation of the spin. For excited states the probability of the spin-flip is higher. We find that the main source of the spin-flip is the structure-inversion asymmetry (SIA) of the Ge quantum dot. Every tunneling event is accompanied by the small rotation of the angular momentum and this provokes the spin-flip. Simple estimations of the time of spin relaxation caused by the SIA-mechanism give  $\tau_{\text{SIA}} \sim 10^{-5}$  s.

DOI: 10.1103/PhysRevB.71.033310

PACS number(s): 72.25.Rb, 73.21.La, 71.70.Ej

The recent proposals of quantum computing and spin devices based on the manipulation with spin of carriers in quantum dots (QDs) (Refs. 1–3) caused a great interest to the problem of spin relaxation in QDs. The Ge/Si system is one of the most attractive systems for exploiting in spintronics, because the spin relaxation mechanisms caused by bulk-inversion-asymmetry (the Dresselhaus term in electron effective Hamiltonian<sup>4</sup>) do not work in these semiconductors. But other additional mechanisms of spin relaxation can appear in the SiGe structures with reducing dimensionality of the system. The asymmetry of heterostructures results in the appearance of the Rashba spin-orbit coupling.<sup>5</sup> Recently it has been shown that the Dresselhaus-type contribution is also possible in the two-dimensional SiGe heterostructures.<sup>6</sup> The kind of spin-orbit coupling is defined by the symmetry of quantum well structures. The structures with symmetry  $D_{4d}$  and  $D_{2h}$  have the center of the space inversion and the additional terms do not appear in the Hamiltonian. In the case of group  $D_{2d}$  the Hamiltonian contains only the Dresselhaus-type term. In the case of group  $C_{4v}$  only the Rashba coupling is allowed, whereas in the structures with  $C_{2v}$  symmetry both Dresselhaus-type and Rashba terms are possible.

Here we show that the additional mechanism of spin relaxation appears also in the Ge/Si structures with self-assembled QDs. This mechanism is caused by the structure-inversion-asymmetry (SIA) and can be considered as an analog of the Rashba term.

We consider a typical Ge QD embedded in the Si matrix. The Ge QD layers are usually fabricated by molecular beam epitaxy in the Ge/Si heteroepitaxial system (lattice mismatch  $\sim 4\%$ ). The experimental results show that the shape of Ge/Si QD is close to the square pyramid with the height  $h$  one order smaller than the length of the base side  $l$  ( $h/l \sim 1/10$ ).<sup>7</sup> The Ge nanocluster represents a quasi-two-dimensional object with principal symmetry axis  $Z$  coinciding with growth direction. The symmetry of the Ge QD is described by group  $C_{2v}$ . The main symmetry property of Ge QDs is the absence of top-bottom symmetry. The large ( $\sim 0.7$  eV) valence-band offset characteristic of the Ge/Si heterojunction leads to an effective confinement of holes in Ge clusters.<sup>8</sup>

We consider the spin-polarized hole state created by optical or electrical injection in any Ge QD in zero magnetic

field. In our calculations we focus on the spin behavior when hole moves through the array of coupled Ge QDs. Essentially we investigate the spin transport via the resonance tunneling between coupled QDs in Ge/Si heterostructures. We will show that the spin relaxation due to SIA-mechanism occurs during the resonant tunneling between neighboring coupled QDs even at zero temperature (without phonon assistance).

Our studies are based on the calculation of the energy spectrum of holes and their wave functions in the tight-binding (TB) approach.<sup>9,10</sup> The spin-orbit (SO) interaction was added to the Hamiltonian following Chadi<sup>11</sup> as  $\hat{H}_{\text{SO}} = \sum_i \hat{H}_{\text{SO}}^{(i)}$  with  $\hat{H}_{\text{SO}}^{(i)} = (2\Delta/3)\hat{\mathbf{I}}\hat{\mathbf{s}}$ ,  $\hat{\mathbf{s}} = \frac{1}{2}\hat{\sigma}$ . Here  $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$  denotes the Pauli spin matrices,  $i$  is the number of atom,  $l$  is the orbital momentum, and  $\Delta$  is the SO gap between the bulk valence bands  $\Gamma_7^v$  and  $\Gamma_8^v$ . The localized states in the Ge QD can be characterized by the angular momentum  $\mathbf{J}$  and its projection  $J_z$  on the growth direction  $Z$ . The ground hole state in Ge QD is formed mainly from heavy hole states (the angular momentum projection  $J_z = \pm 3/2$ ) and has a small admixture of light hole states and split off band states ( $J_z = \pm 1/2$ ). The excited states contain more admixture of hole with  $J_z = \pm 1/2$  (Ref. 10). We will demonstrate below that this changes the spin behavior significantly.

We consider the projection of the angular momentum  $J_z$  as an analog of electron spin for hole states. From now on we will refer to  $J_z$  as the “spin of holes.”

We calculate the probability of hole spin-flip for resonant tunneling between localized states in neighboring QDs. A probability of tunneling event is defined by the integral of overlapping between states in neighboring QDs:  $W_{ij} = (2\pi/\hbar)|I_{ij}|^2\delta(\varepsilon_i - \varepsilon_j)$ , where  $I_{ij}$  is the overlapping integral,  $\varepsilon_i$ ,  $\varepsilon_j$  are the energy of holes in  $i$  and  $j$  QDs.

For the tunneling without spin-flip the overlap integral is calculated for the states with equal directions of spins in neighboring QDs. The following procedure was used to determine the overlap integrals. We consider an infinite well-ordered chain of coupled QDs. The neighboring QDs adjoin each other. We calculate the energies of hole states in this one-dimensional crystal, where Ge QDs serve as atoms. The equivalent problem is the calculation of the energy spectrum in a model structure, that represents a Si building block containing one Ge QD, with periodic boundary conditions (Fig.

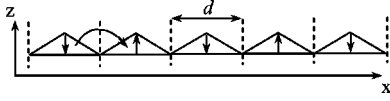


FIG. 1. The schematic sketch of the tunneling process with spin-flip.

1). The width of the energy band is determined by the magnitude of the overlap integral between artificial atoms. It is defined as  $I_{ij} = |E_+ - E_-|/4$ , where  $E_+$  and  $E_-$  are the hole energies of bonding and antibonding states correspondingly. To calculate  $E_{\pm}$  we use the boundary conditions  $|\psi\rangle_{x=0} = \pm |\psi\rangle_{x=d}$ , where  $d$  is the building block size in the  $x$  direction,  $|\psi\rangle$  is the hole wave function. The details of the calculations in TB approach are presented in our previous papers.<sup>9,10</sup>

For the tunneling with spin-flip the overlap integral is calculated for states with spin *up* and spin *down* in neighboring QDs. In this case we use the boundary condition

$$|\psi\rangle_{x=0} = \hat{K}|\psi\rangle_{x=d}, \quad (1)$$

where  $\hat{K}|\psi\rangle$  is the Kramers conjugate state. A problem with this boundary condition has the same eigenvalues as a problem with the boundary condition

$$|\psi\rangle_{x=0} = i|\psi\rangle_{x=d}. \quad (2)$$

The proof of this statement is the following. Let the function  $|\psi\rangle = u_1(x)\exp(ikx)$  be the eigenfunction of the problem (2) with energy  $E$ . This function corresponds to the point  $k = \pi/2d$  in the Brillouin zone of our artificial crystal. Then  $\hat{K}|\psi\rangle = u_1^*(x)\exp(-ikx)$  is the function with  $k = -\pi/2d$  and the same energy  $E$ . Let us construct the function  $|\varphi\rangle$  in the following way:

$$|\varphi\rangle = (|\psi\rangle + i\hat{K}|\psi\rangle)/\sqrt{2}.$$

One can see that this function is the superposition of two Bloch functions with opposite spin and quasimomentum directions. At the translation by  $d$  this function transforms as

$$|\varphi\rangle \rightarrow (i|\psi\rangle + \hat{K}|\psi\rangle)/\sqrt{2}.$$

It is easy to check that the transformed wave function is the Kramers conjugate function,  $|\varphi\rangle_{x=0} = \hat{K}|\varphi\rangle_{x=d}$ . So, the wave function  $|\varphi\rangle$  satisfies to the boundary conditions (1) and has the same energy  $E$  as the wave function  $|\psi\rangle$ . Therefore by solving problem (2) we find the eigenvalues for problem (1). The problem with the boundary condition (2) has two eigenvalues  $E_{1*}$  and  $E_{2*}$ . The difference between them gives the spin splitting of the energy band. The origin of this spin splitting is the same as in the noncentrosymmetric crystals like GaAs. Our artificial crystal has no inversion center due to asymmetrical shape of QDs and this results in the spin splitting of the energy band at  $k \neq 0$ . This spin splitting is equivalent to the presence of effective internal magnetic field, so called SIA-field, in our artificial crystal. The overlap integral is defined as

$$I_{ij} = |E_{1*} - E_{2*}|/4. \quad (3)$$

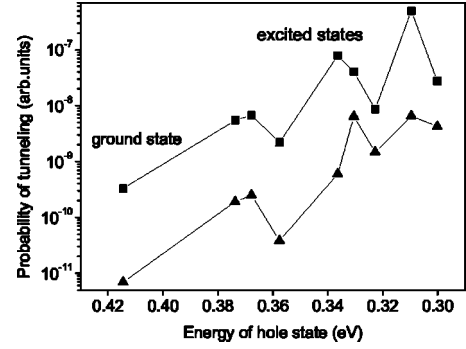


FIG. 2. The probabilities of tunneling processes with spin-flip ( $\blacktriangledown$ ) and without it ( $\blacksquare$ ) for the ground and excited hole states in Ge QD. The height of the Ge nanocluster  $h = 1.5$  nm, lateral size  $l = 15$  nm.

So, having the values of overlap integrals, we can calculate the probabilities of the tunneling with spin-flip and without it.

The results of these calculations demonstrate that the tunneling between hole ground states in the neighboring Ge QDs occurs with conservation of spin mainly. More exactly, only one spin-flip happens every hundred tunneling events. The probability of the spin-flip during the tunneling between excited states is higher. One spin-flip event happens every 5–10 tunneling events on average. Our calculations show the increase in the spin-flip probability with the number of states (see Fig. 2). This relationship is not described by a smooth function, but consists of oscillations. These oscillations can be explained by the dependence of overlap integrals on the symmetry of the wave function,<sup>10</sup> for example, the overlap integral is smaller for *s*-like and *d*-like states and bigger for *p*-like states.

We investigate the probability of the tunneling with spin-flip and without it for different sizes and shapes of QDs. At fixed height of QDs both probabilities decrease with increasing lateral size of QDs (see Fig. 3). But the probability of the tunneling with spin-flip ( $P_1$ ) is always lower than the probability of the tunneling without it ( $P_2$ ). The ratio  $P_2/P_1$  increases with decreasing lateral size of QDs (Fig. 3, inset) (with decreasing  $l$  from 20 nm to 12 nm this ratio changes

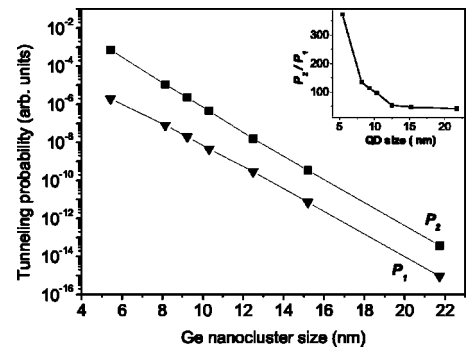


FIG. 3. Size dependence of probabilities  $P_1$  and  $P_2$  of the tunneling with spin-flip ( $\blacktriangledown$ ) and without it ( $\blacksquare$ ) correspondingly for the ground hole state in Ge QD ( $h = 1.5$  nm,  $l$  is changed). Inset, size dependence of the  $P_2/P_1$  ratio.

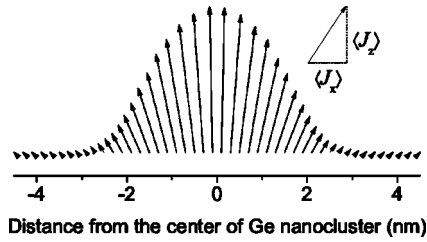


FIG. 4. The distribution of the angular momentum for the ground state. The arrows schematically show the direction and magnitude of the vector  $\langle \psi | \hat{\mathbf{J}} | \psi \rangle$  along the line passing through the center of the QD base. For better representation we multiply the deviation angle by 5.

weakly, for smaller QDs the ratio drastically rises: for  $l=6$  nm it runs up to  $\approx 360$ ). In general one can conclude that the spin transport in array of small QDs can occur mainly without spin-flip (if phonon-assisted process can be neglected,  $T \leq 4$  K).

We find that the probability of spin-flip event is lower for more flat QDs. We compare two Ge QDs with base side  $l=15$  nm and different heights ( $h=4.5$  nm and  $h=1.5$  nm). In the first case the probability of the tunneling with spin-flip is only two times smaller than the one without it. While in the second case the ratio  $P_2/P_1$  is approximately 50. This is the evidence of strong dependence of spin-flip event on the aspect ratio  $h/l$ . In addition we must note that the overlap integral (3) is larger in the case of QDs with high aspect ratio  $h/l$ . Then the spin splitting of the energy band is greater, that is equivalent to a greater SIA-field.

The action of the SIA-field on the spin is presented in Fig. 4. Here we consider the distribution of the vector with components  $\langle \psi | \hat{J}_x | \psi \rangle$ ,  $\langle \psi | \hat{J}_y | \psi \rangle$ ,  $\langle \psi | \hat{J}_z | \psi \rangle$  across the QD for the ground state. One can see that the absence of top-bottom symmetry leads to a fanlike distribution of the angular momentum. Based on these results we can conclude that during the tunneling of carrier through QD, the hole angular momentum gradually turns by the small angle. After several events of the tunneling this can provoke the spin-flip.

To understand the nature of the SIA-field we consider the different model structures that contain from 3 to 14 atoms. These structures are molecules with structure-inversion-asymmetry and without it. Four of them, the most simple ones, are presented in Fig. 5. The upper molecules (a) and (b) have the same symmetry property as the Ge QD (the absence of top-bottom symmetry). Lower molecules (c) and (d) have the higher symmetry.

We solve the eigenvalue problem for these structures in two-center TB approximation, including only  $p$ -orbitals in the consideration. For simplicity we assume that the interaction between neighboring atoms does not depend on the distance between them. The spin-orbit interaction is included in the same way as above. We consider the spin  $up$  state. We calculate the components of the angular momentum and their distribution at each atom. One can see in Fig. 5 that the absence of top-bottom symmetry leads to the deviation of the angular momentum from the direction  $Z$ .

This consideration demonstrates the crucial role of the microscopical arrangement of atoms in the appearance of the

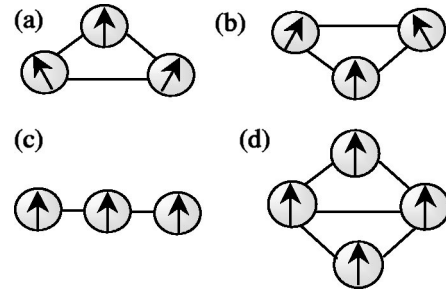


FIG. 5. Model structure of molecules. Upper molecules (a), (b) have a structure-inversion-asymmetry. Lower molecules (c), (d) are without it. The arrows schematically show the direction of the angular momentum.

SIA-field. If we come back to real Ge QD, we can say that the SIA-field does not appear in the QD with equal upper and lower sides as in the low molecules (c) and (d).

Now we discuss a mechanism that increases the probability of spin-flip. The spin-flip occurs due to the rotation of hole angular momentum in the transverse SIA-field. The heavy hole angular momentum rotation is negligible because the transverse component of heavy hole  $g$ -factor is very small. While the rotation of light hole spin is much greater because its transverse  $g$ -factor is  $\sim 4k$ , where  $k$  is the Luttinger parameter ( $k=3.41$  for Ge<sup>13</sup>). Then the admixture of  $|1/2\rangle$ -states enhances the probability of spin-flip. For excited states the admixture of  $|1/2\rangle$ -states is greater, therefore the probability of spin-flip is more probable in this case (Fig. 2).

In order to find the reason for the drastic decrease of the spin-flip probability for ultrasmall QD with  $l < 10$  nm (Fig. 3) one needs to consider the structure of the hole wave function. The tails of the wave function mainly consist of the light hole with  $J_z = \pm 1/2$  and the core of the wave function consists of the heavy hole with  $J_z = \pm 3/2$  (Fig. 6). The SIA-field effectively acts on the spin only in the Ge region (the large value of Luttinger parameter  $k$ ). For sufficiently large QD ( $l \approx 15$  nm) almost all parts of the wave function, even its tails, are enclosed in QD. For QD with  $l < 10$  nm the tails of the wave function penetrate in the Si environment. Here the action of the SIA-field is not so effective as in the Ge region. Then the spin-flip event has low probability and the

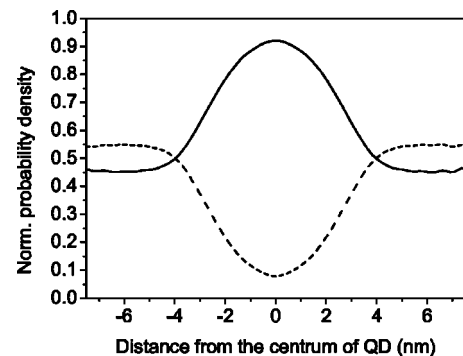


FIG. 6. The probability density profiles for light hole part ( $J_z=1/2$ , dashed line) and heavy hole part ( $J_z=3/2$ , solid line) for the ground state inside the Ge quantum dot ( $h=1.5$  nm,  $l=15$  nm). Each curve was normalized to full probability density.

difference between tunneling processes with spin-flip and without it is high.<sup>12,13</sup>

Finally we estimate the spin-flip rate during the tunneling by using the properties of real Ge QD array. We refer to the recent experiments where two-dimensional hopping conductance in Ge QDs array was investigated.<sup>14</sup> The SIA-field effectively perturbs the spin of hole only when carrier is located inside Ge QD. The time spent by the carrier inside the QD is a reciprocal of the rate of hopping between centers  $i$  and  $j$  in QD array, that is  $\tau_{\text{hopping}} \sim 1/\Gamma_{ij}$ . The conductance between centers  $i$  and  $j$  is defined as  $G_{ij} \sim e^2\Gamma_{ij}/kT$  (Ref. 15). The conductance of the typical Ge/Si heterostructure with Ge QDs was obtained in experiments at the helium temperature ( $T \approx 4$  K) and was near  $\sim 10^{-4}(e^2/h)$ . Using this value we obtain  $\tau_{\text{hopping}} \sim 10^{-7}$  s. Since the spin-flip probability is 100 times smaller than the tunneling probability, we can estimate the time of spin relaxation as  $\tau_{\text{SIA}} \sim 10^{-5}$  s.

In conclusion, our results show that the tunneling between coupled QDs is accompanied by the rotation of hole spin. This rotation results in the spin-flip after several tunneling events. The probability of spin-flip is defined by aspect ratio  $h/l$  of QD and the admixture of states with  $J_z = \pm 1/2$ . The origin of the spin-flip is the structure-inversion-asymmetry. This leads to the appearance of effective magnetic field (SIA-field), which turns the spin of the hole. The effect of spin rotation due to the shape asymmetry of QD can appear not only in the Ge/Si system with QDs, but also in all systems with self-assembled QDs, which have this type of asymmetry.

This work has been supported by the Russian Foundation of Basic Research (Grant No. 05-02-16285), INTAS-2001-0615 and Program RAS and SB RAS (No. 27) for young scientists.

---

\*Electronic address: aigul@isp.nsc.ru

<sup>1</sup>D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).

<sup>2</sup>G. Burkard, D. Loss, and D. P. DiVincenzo, Phys. Rev. B **59**, 2070 (1999).

<sup>3</sup>P. Recher, E. V. Sukhorukov, and D. Loss, Phys. Rev. Lett. **85**, 1962 (2000).

<sup>4</sup>G. Dresselhaus, Phys. Rev. **100**, 580 (1955).

<sup>5</sup>Yu. L. Bychkov and E. I. Rashba, J. Phys. C **17**, 6039 (1984).

<sup>6</sup>L. E. Golub and E. L. Ivchenko, Phys. Rev. B **69**, 115333 (2004).

<sup>7</sup>A. I. Yakimov, A. V. Dvurechenskii, Yu. Yu. Proskuryakov, A. I. Nikiforov, O. P. Pchelyakov, A. S. Teys, and A. K. Gutakovskii, Appl. Phys. Lett. **75**, 1413 (1999).

<sup>8</sup>A. I. Yakimov, A. V. Dvurechenskii, A. I. Nikiforov, and O. P.

Pchelyakov, Thin Solid Films **336**, 332 (1998).

<sup>9</sup>A. V. Dvurechenskii, A. V. Nenashev, and A. I. Yakimov, Nanotechnology **13**, 75 (2002).

<sup>10</sup>A. V. Nenashev, A. V. Dvurechenskii, and A. F. Zinovieva, Phys. Rev. B **67**, 205301 (2003).

<sup>11</sup>D. J. Chadi, Phys. Rev. B **16**, 790 (1977).

<sup>12</sup>M. V. Entin and L. I. Magarill, Phys. Rev. B **64**, 085330 (2001).

<sup>13</sup>J. C. Hensel and K. Suzuki, Phys. Rev. Lett. **22**, 838 (1969).

<sup>14</sup>A. I. Yakimov, A. V. Dvurechenskii, A. I. Nikiforov, and A. A. Bloshkin, JETP Lett. **77**, 376 (2003).

<sup>15</sup>B. I. Shklovskii and A. L. Efros, *Electronic Properties of Doped Semiconductors* (Springer, Berlin, 1984).