Interface-Induced Electron Spin Splitting in SiGe Heterostructures

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Spin splitting of conduction electron states has been analyzed for all possible point symmetries of SiGe quantum well structures. A particular attention is paid to removal of spin degeneracy caused by the rotoinversion asymmetry of a (001) heterointerface between two diamond-lattice materials. Consequences of the spin splitting on the electron spin relaxation time is discussed.

I. INTRODUCTION

Spin properties attract the great attention in recent years due to attempts to realize an electronic device based on the spin of carriers. Conduction electrons are obvious candidates for such devices, particularly in nanostructures where electron energy spectrum and shape of the envelope functions can be effectively engineered by the growth design, application of electric or magnetic fields as well as by illumination with light.

Various semiconductor materials are being involved in the spintronics activities. SiGe quantum well structures are among them. Although bulk Si and Ge have a center of symmetry, quantum-well structures grown from these materials can lack such a center and allow the spin splitting of the electronic subbands.

The quantum engineering of spintronics devices is usually focused on the Rashba spin-dependent contribution to the electron effective Hamiltonian in heterostructures. This contribution appears due asymmetry of the heterostructure (the so-called structure inversion asymmetry, or SIA) and has no relation to the properties of a bulk semiconductor. It is commonly believed that the Dresselhaus contribution caused by bulk inversion asymmetry (BIA) is absent in structures grown from centrosymmetric materials. In the present work we show for the first time that the Dresselhaus-like spin splitting is possible in heterostructures made of Si and Ge, as an alternative to the Rashba effect, and it occurs due to the anisotropy of chemical bonds at interfaces.

II. SYMMETRY OF Si/Ge QUANTUM WELLS AND LINEAR-IN-k SPIN SPLITTING

We consider quantum well (QW) structures grown along the axis $z$ || [001], and introduce two orthogonal directions in the interface plane, $x$ || [100] and $y$ || [010]. Depending on the properties of an interface between Si$_{1-x}$Ge$_x$ and Si, its symmetry on average can be $C_{2v}$ or $C_{4v}$. The former point group describes the symmetry of an ideal heterointerface with the interfacial chemical bonds lying in the same plane. A nonideal interface containing monatomic fluctuations has two kinds of flat areas with interfacial planes shifted with respect to each other by a quarter of the lattice constant. The local symmetry of each area is $C_{2v}$ as well. However if the both kinds are equally distributed, the interface overall symmetry increases up to $C_{4v}$. It follows then that the symmetry of a Si$_{1-x}$Ge$_x$/Si quantum well structure containing two interfaces is described by one of five point groups: $D_{2d}$ or $D_{2h}$ in case of two ideal interfaces with odd or even number of monolayers between them; $C_{2v}$ for a pair of ideal and rough interfaces; $C_{4v}$ or $D_{4h}$ for two non-ideal interfaces of the overall symmetry $C_{4v}$ each — see Fig. 1.

The lowest conduction band in (001)-SiGe/Si QWs is located near the $X$ point of the Brillouin zone. At this point, the bulk electron states form projective representations of the point group $D_{4h}$. All five above-mentioned groups are subgroups of $D_{4h}$. Two of them, $D_{4h}$ and $D_{2h}$, contain the space inversion operation and forbid the spin splitting of electronic states. Three remaining groups allow the spin-dependent linear-in-$k$ term $H_k = \gamma_{\alpha\beta} \sigma_\alpha k_\beta$. Here $\sigma_\alpha$ are the Pauli matrices and $k = (k_x, k_y)$ is the in-plane electron wave vector. Note that in the following we consider the electronic states attached to the $X_z$ valley which lies lower than $X_x$ and $X_y$ valleys.

In the group $D_{2d}$, the Dresselhaus-like term $\sigma_x k_x - \sigma_y k_y$ is an only invariant which can be constructed from the products $\sigma_\alpha k_\beta$. In particular, the Rashba term $\sigma_x k_y - \sigma_y k_x$ is forbidden. On the contrary, in the group $C_{4v}$, the only invariant combination is $\sigma_x k_y - \sigma_y k_x$. The analysis shows that both combinations $\sigma_x k_x - \sigma_y k_y$ and $\sigma_x k_y - \sigma_y k_x$ are invariants of the group $C_{4v}$. Hence the latter allows both Dresselhaus- and Rashba-like spin-dependent terms.

III. SPIN SPLITTING: MICROSCOPIC MODEL

Microscopically, a linear-in-$k$ correction to the conduction-band effective Hamiltonian is given by the second order of the perturbation theory

$$\Delta H_i' = \sum_n \frac{\langle ci|H_{SO}|n\rangle\langle n|H_{kp}|ci'\rangle + \langle ci|H_{kp}|n\rangle\langle n|H_{SO}|ci'\rangle}{E_c - E_v},$$

Here $H_{kp}$ and $H_{SO}$ are the $k\cdot\hat{p}$ and spin-orbit interaction Hamiltonians, respectively. We take into consideration only the coupling of the conduction states $(c, X_1, i)$ with the valence states $n = (v, X_1, j)$, where the indices $i, j$ enumerate the degenerate states. The symmetry properties of the Bloch functions at the $X$ point of a diamond-lattice semiconductor crystal coincide with those of the
\[ X_1\text{-states} : \left\{ \begin{array}{l} S = \cos (2\pi z/a) \\ Z = \sin (2\pi z/a) \end{array} \right. , \quad (2) \]

\[ X_4\text{-states} : \left\{ \begin{array}{l} X = \sin (2\pi x/a) \cos (2\pi y/a) \\ Y = \cos (2\pi x/a) \sin (2\pi y/a) \end{array} \right. , \quad (3) \]

where \( a \) is the lattice constant. For the bulk states \( X_1, X_4 \) in the bases (2), (3), the interband matrix elements can be presented as

\[ H_{kp} = \mathcal{P} \begin{pmatrix} k_x & k_y \\ -k_y & -k_x \end{pmatrix}, \quad H_{SO} = \mathcal{U} \begin{pmatrix} \sigma_x & -\sigma_y \\ -\sigma_y & \sigma_x \end{pmatrix}. \quad (4) \]

where \[ \mathcal{P} = (\hbar/m_0) \langle S|\hat{p}_x|X \rangle, \quad \mathcal{U} = \langle S|U_x|X \rangle, \quad \hat{p} \] is the momentum operator, and \( U_x \) is the \( x \)-component of the pseudovector \( \hat{\mathbf{U}} \) which enters into the spin-orbit Hamiltonian \( H_{SO} = \vec{\sigma} \cdot \hat{\mathbf{U}} \).

The substitution of (4) into (1) gives a spin-dependent matrix \( \Delta H \) proportional to

\[ (\sigma_x k_x - \sigma_y k_y) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

which however does not lead to removal of the degeneracy of the \( X_1 \)-states in the bulk centrosymmetric material as expected. The splitting can be achieved if one takes into account the anisotropy of chemical bonds at the interfaces which results in \( \delta \)-functional contributions to \( H_{kp} \) and \( H_{SO} \) of the form

\[ \Delta H_{kp} = \hat{V}_{kp} \delta(z - z_{if}), \quad \Delta H_{SO} = \hat{V}_{SO} \delta(z - z_{if}), \quad (5) \]

where \( z_{if} \) is the interface coordinate, and the matrices \( \hat{V}_{kp}, \hat{V}_{SO} \) have few linearly independent components. In the case of the lowest symmetry under study, \( C_{2v} \), each matrix is determined by four linearly-independent parameters

\[ \hat{V}_{kp} = \begin{pmatrix} P_1 k_x + P_2 k_y & P_1 k_y + P_2 k_x \\ P_3 k_y + P_4 k_x & P_3 k_x + P_4 k_y \end{pmatrix}, \quad (6) \]

\[ \hat{V}_{SO} = \begin{pmatrix} U_1 \sigma_x - U_2 \sigma_y & -U_1 \sigma_y - U_2 \sigma_x \\ -U_3 \sigma_y + U_4 \sigma_x & U_3 \sigma_x - U_4 \sigma_y \end{pmatrix}. \quad (7) \]

In the bases (2), (3), the parameters \( P_l \) and \( U_l \) (\( l = 1 \div 4 \)) are purely imaginary.

According to Eq. (1), the linear in \( k_{x,y} \) correction to the conduction-band Hamiltonian for a single interface of the \( C_{2v} \)-symmetry, is given by

\[ \Delta H_{C_{2v}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} H_{if} \delta(z - z_{if}), \quad (8) \]

where \( H_{if} \) is a linear combination of the Pauli matrices. Treating the perturbation (5) in the first-order approximation, one can obtain

\[ H_{if} = \frac{\mathcal{P}}{E_0} \begin{pmatrix} (\sigma_x k_x - \sigma_y k_y)(U_1 - U_3) + (\sigma_x k_y - \sigma_y k_x)(U_2 - U_4) \\ -\mathcal{U} \end{pmatrix} \]

\[ -\frac{\mathcal{U}}{E_0} \begin{pmatrix} (\sigma_x k_x - \sigma_y k_y)(P_1 + P_3) + (\sigma_x k_y - \sigma_y k_x)(P_2 + P_4) \end{pmatrix}, \]

where \( E_0 \) is the energy separation between \( X_1 \) and \( X_4 \) states.

The electron effective Hamiltonian in an ideal QW contains a sum of two contributions (8) related to the left- and right-hand-side interfaces. The corresponding parameters \( U_{1l}, U_{3l}, P_{1l}, P_{3l} \) are interconnected by

\[ [U_1, U_2, U_3, U_4]_R = [U_3, U_4, U_1, U_2]_L, \quad (10) \]

\[ [P_1, P_2, P_3, P_4]_R = [-P_3, -P_4, -P_1, -P_2]_L, \]

if the QW contains an even number of monoatomic layers (\( D_{2h} \) symmetry), and

\[ [U_1, U_2, U_3, U_4]_R = [U_1, -U_2, U_3, -U_4]_L, \quad (11) \]

\[ [P_1, P_2, P_3, P_4]_R = [P_1, -P_2, P_3, -P_4]_L, \]

if the QW contains an odd number of monoatomic layers (\( D_{2d} \) symmetry). It readily follows from here that, in the former case, the electronic states in Si/Ge QWs are spin-degenerate \((H_{if} = 0)\) and, in the latter, the spin degeneracy is removed by a Dresselhaus-like linear-in-\( k \) terms. The similar analysis can be carried out for non-ideal Si/Ge QW structures of the \( C_{2v} \) and \( C_{4v} \) symmetry.
IV. CONCLUSION

In this work, we have analyzed spin splitting of electron states in Si/Ge heterostructures of all possible symmetries. This opens a possibility to discuss the recent spin relaxation times measurements in these heterostructures. The work on estimation of the interface parameters $U_l$ and $P_l$ in the microscopic tight-binding model is in progress.

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