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Spin relaxation of two-dimensional holes in strained asymmetric SiGe quantum wells

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We analyze spin splitting of the two-dimensional hole spectrum in strained asymmetric SiGe quantum wells (QWs). Based on the Luttinger Hamiltonian, we obtain expressions for the spin-splitting parameters up to the third order in the in-plane hole wave vector. The biaxial strain of SiGe QWs is found to be a key parameter that controls spin splitting. Application to SiGe field-effect transistor structures indicates that typical spin splitting at room temperature varies from a few tenths of meV in the case of Si QW channels to several meV for the Ge counterparts, and can be modified efficiently by gate-controlled variation of the perpendicular confining electric field. The analysis also shows that for sufficiently asymmetric QWs, spin relaxation is due mainly to the spin-splitting related D'yakonov-Pereĺ mechanism. In strained Si QWs, our estimation shows that the hole spin relaxation time can be on the order of 100 picoseconds at room temperature, suggesting that such structures are suitable for *p*-type spin transistor applications as well.

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I. INTRODUCTION

Recently, there has been considerable interest in the field of spintronic applications. They range from various approaches in logic and memory elements to quantum computation.[1] Many spintronic device concepts rely on the so-called Das-Datta spin transistor,[2] where the transfer of spins between the spin-polarized source and drain contacts is controlled by the gate bias through the perpendicular (i.e., confining) electric field in the quantum well (QW) channel. Experimentally, the efforts have concentrated mainly on *n*-type III-V devices; in particular, those with InGaAs QWs. The reasons for this preference are (1) easy control of electron spin states in this material[3] and (2) availability of III-V diluted magnetic semiconductors.[4] Much less attention has been paid to the hole-based spintronic applications, whose rationale actually originates from the considerations related to the bulk semiconductors. Indeed, in bulk cubic semiconductors the top of the valence band at the Brillouin zone center is fourfold degenerate (including spin), and hybridization of the hole states for finite wave vectors depends on the direction of the wave vector. As a result, hole scattering is supplemented by simultaneous change of spin, and the so-called Elliott-Yafet mechanism of spin relaxation is very effective.[5] In fact, the hole spin relaxation rate is close to the momentum relaxation rate; i.e., nonquilibrium spin relaxes too fast to allow control in any realistic device. This picture is not exactly correct in the case of two-dimensional (2D) holes confined in a QW, where the degeneracy at the zone center is partially lifted due to quantization. Moreover, the hole spectrum in a QW is in general completely nondegenerate for nonzero wave vectors, qualitatively resembling that of electrons. For the QWs based on the centrosymmetric crystals such as Si and Ge, the removal of degeneracy takes place due to the QW asymmetry, while for the compound material-based QWs the additional contribution arises due to the bulklike contributions to the Hamiltonian. The symmetry properties of the effective Hamiltonian of confined holes were analyzed previously, for example, in Refs. 6–9.

In this paper, we address the problem of the hole spectrum and spin relaxation in strained SiGe QWs. Previously, spin splitting in such QWs was estimated based on the observation of the circular photogalvanic effect[10] and transport measurements.[11] In Ref. 10, possible sources of spin splitting proportional to the in-plane hole wave vector were examined briefly. Here, we present quantitative calculations of spin splitting based on the Luttinger Hamiltonian approach. We take into account the biaxial strain inherent in the SiGe heterostructures which gives rise to stronger splitting of the hole subbands. We consider both the cases of tensile and compressive strain resulting in the light-hole (LH)-like and heavy-hole (HH)-like ground state, respectively. Based on the results for spin splitting, we analyze the spin-relaxation process for 2D holes. For asymmetric QWs, it is found that the D'yakonov-Pereĺ mechanism is more important than the Elliott-Yafet mechanism. According to our calculations, the hole spin mean-free path in a strained Si QW can be as large as a micron at room temperature. This estimate suggests the feasibility of *p*-type spintronic applications based on Si, particularly in view of recent advances in group-IV magnetic semiconductors.[12]

II. BASIC EQUATIONS

First, we need clarify what we mean by the term "spin." Due to the degeneracy at the zone center, the spin-orbit interaction leads to strong hybridization of the hole states and the total angular momentum must be considered. If some asymmetry is introduced such as the confinement in a QW, the degeneracy between the LH and HH states is lifted at least partly. When the resulting doublet is well separated

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energetically from the other states, it can be treated by using a spin Hamiltonian with the effective spin $1/2$. So, in speaking of spin states, we mean the states of this quasidegenerate doublet.

Let us describe the model used in our calculations. We consider the case of a QW grown along the [001] direction that is subject to biaxial strain. We start from the following 6×6 effective-mass Hamiltonian:

$$H = H_L^{(0)} + H_L^{(\|)} + H_\epsilon + U(z)I_6. \tag{1}$$

Here $H_L \equiv H_L^{(0)} + H_L^{(\|)}$ is the Luttinger Hamiltonian with $H_L^{(0)}$ corresponding to the part with $k_{x,y}=0$, H_ϵ is the contribution due to the biaxial strain, $U(z)$ is the confining potential which forms the QW, and I_6 is the 6×6 unity matrix. The explicit expression for H is not provided since it is readily available in the literature (see, for example, Ref. 13). Note, however, that in the following the top of the HH band is used as the reference energy. As in $\mathbf{k}\cdot\mathbf{p}$ theory, $H_L^{(\|)}$ is treated as a perturbation. Following the conventional notation,[13] we choose the zeroth-order (i.e., unperturbed) wave functions as

$$\Psi_{1ln} = \begin{pmatrix} 0 \\ \chi_n^{(l1)} \\ 0 \\ 0 \\ i\chi_n^{(l2)} \\ 0 \end{pmatrix}, \quad \Psi_{2ln} = \begin{pmatrix} 0 \\ 0 \\ \chi_n^{(l1)} \\ 0 \\ 0 \\ i\chi_n^{(l2)} \end{pmatrix},$$

$$\Psi_{1hn} = \begin{pmatrix} \chi_n^{(h)} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \Psi_{2hn} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \chi_n^{(h)} \\ 0 \\ 0 \end{pmatrix}, \tag{2}$$

$$\Psi_{1sn} = \begin{pmatrix} 0 \\ \chi_n^{(s1)} \\ 0 \\ 0 \\ i\chi_n^{(s2)} \\ 0 \end{pmatrix}, \quad \Psi_{2sn} = \begin{pmatrix} 0 \\ 0 \\ \chi_n^{(s1)} \\ 0 \\ 0 \\ i\chi_n^{(s2)} \end{pmatrix},$$

where the plane-wave factors $\exp[i(k_x x + k_y y)]$ are omitted for simplicity. In Eq. (2), the first subscript of Ψ (i.e., 1 or 2) denotes the doubly degenerate states for $k_{x,y}=0$, n is the subband number, and l, h, or s represents the LH, HH, or spin-split (SS) states, respectively. In fact, if the strain is strong enough such that the corresponding strain energy E_ϵ is comparable to the spin-orbital gap Δ in the bulk material, the so-called LH and SS states are hybridized even for $k_{x,y}=0$. Hereafter, we term the states "LH" and "SS" which take the genuinely light and spin-split nature in the limit $\Delta\to\infty$. This hybridization is evident from the eigenvalue equations for the LH and SS envelope functions χ,

$$H_2\begin{pmatrix} \chi_n^{(x1)} \\ \chi_n^{(x2)} \end{pmatrix} = E\begin{pmatrix} \chi_n^{(x1)} \\ \chi_n^{(x2)} \end{pmatrix},$$

$$H_2 = \begin{pmatrix} \frac{\hbar^2}{2m_0}(A+B)\frac{d^2}{dz^2} + E_\epsilon & -B\frac{\hbar^2}{\sqrt{2}m_0}\frac{d^2}{dz^2} - \frac{E_\epsilon}{\sqrt{2}} \\ -B\frac{\hbar^2}{\sqrt{2}m_0}\frac{d^2}{dz^2} - \frac{E_\epsilon}{\sqrt{2}} & \frac{\hbar^2}{2m_0}A\frac{d^2}{dz^2} - \Delta + \frac{E_\epsilon}{2} \end{pmatrix} + U(z)I_2. \tag{3}$$

Here x stands for l or s, A and B are parameters of the hole spectrum,[14] m_0 is the free electron mass, I_2 is the 2×2 unitary matrix, and the deformation energy mentioned previously is $E_\epsilon = b(2u_{zz} - u_{xx} - u_{yy})$, where b is the deformation potential constant and u is the strain tensor. The envelope functions for HH states $\chi_n^{(h)}$ are determined by the conventional Schrödinger equation with an effective mass $m^{(h)} = m_0/(A-B)$.

In general, further steps require numerical solution of Eq. (3) to obtain the spectrum and envelope functions of LH and SS states. Considerable simplification is possible, however, if the quantization energy is much less than E_ϵ or Δ, which is often the case for strained SiGe QWs. Under this approach, it is adequate to use an "effective mass" approximation for the solution of Eq. (3), which treats the nondiagonal part of H_2 containing the z derivatives as a perturbation. Subsequently, we obtain

$$\chi_n^{(l1)} = t_{11}\chi_{nl} + t_{12}\sum_{n'} \chi_{n's}\frac{w_{n'snl}}{E_n^{(l)} - E_{n'}^{(s)}},$$

$$\chi_n^{(l2)} = t_{21}\chi_{nl} + t_{22}\sum_{n'} \chi_{n's}\frac{w_{n'snl}}{E_n^{(l)} - E_{n'}^{(s)}},$$

$$\chi_n^{(s1)} = t_{12}\chi_{ns} + t_{11}\sum_{n'} \chi_{n'l}\frac{w_{n'lns}}{E_n^{(s)} - E_{n'}^{(l)}},$$

$$\chi_n^{(s2)} = t_{22}\chi_{ns} + t_{21}\sum_{n'} \chi_{n'l}\frac{w_{n'lns}}{E_n^{(s)} - E_{n'}^{(l)}}. \tag{4}$$

Here the spectrum $E_n^{(l,s)}$ and the envelope functions χ_{nl}, χ_{ns} are determined by the conventional Schrödinger equation with the effective masses,

$$m^{(l)} = m_0\left(A + B\left[\frac{1}{2} + \frac{9/4 + \Delta/(2E_\epsilon)}{\sqrt{9/4 + \Delta/E_\epsilon + (\Delta/E_\epsilon)^2}}\right]\right)^{-1},$$

$$m^{(s)} = m_0\left(A - B\left[\frac{9/4 + \Delta/(2E_\epsilon)}{\sqrt{9/4 + \Delta/E_\epsilon + (\Delta/E_\epsilon)^2}} - \frac{1}{2}\right]\right)^{-1}, \tag{5}$$

and

$$w_{n\alpha n'\beta} = -\frac{\hbar^2}{2m^*}\int dz\, \chi_{n\alpha}\frac{d^2\chi_{n'\beta}}{dz^2},$$

$$m^* = m_0\frac{\sqrt{9E_\epsilon^2/4 + \Delta E_\epsilon + \Delta^2}}{\sqrt{2}\Delta B}. \qquad (6)$$

In Eq. (4), t_{ij} are the elements of the unitary transformation matrix T that approximately diagonalizes H_2 (for $U=0$ and $d/dz=0$),

$$T = \begin{pmatrix} \frac{1}{\sqrt{N_l}} & \frac{1}{\sqrt{N_s}} \\ \sqrt{\frac{2}{N_l}}(1 - E^{(l)}/E_\epsilon) & \sqrt{\frac{2}{N_s}}(1 - E^{(s)}/E_\epsilon) \end{pmatrix}, \qquad (7)$$

where $E^{(l,s)}$ are the LH and SS states in a strained material with no confinement (i.e., $U=0$),

$$E^{(l,s)} = \tfrac{1}{2}\left(\tfrac{3}{2}E_\epsilon - \Delta \pm \sqrt{9E_\epsilon^2/4 + \Delta E_\epsilon + \Delta^2}\right) \qquad (8)$$

and

$$N_{l,s} = 1 + 2(1 - E^{(l,s)}/E_\epsilon)^2. \qquad (9)$$

These basis functions result in nondiagonal terms in the Hamiltonian H. Using the perturbation method,[13] it is possible to transform it to the quasidiagonal form in any desired order in $H_L^{(\parallel)}$. Under this approach, the effective Hamiltonian for the quasidegenerate ground subband can be written as

$$H_{\text{eff}}^{(l,h)} = -\frac{\hbar^2(k_x^2 + k_y^2)}{2m_\parallel^{(l,h)}}I_2 - \frac{\hbar}{2}\boldsymbol{\sigma\Omega}^{(l,h)}(k_x,k_y), \qquad (10)$$

where σ are Pauli matrices. Restricting $\boldsymbol{\Omega}$ to the terms proportional to k and k^3 and neglecting the corrections to the longitudinal effective mass, we obtain for the ground LH-like state

$$m_\parallel^{(l)} = m_0[A - B(\lambda_{00}^{l1l1}/2 - \sqrt{2}\lambda_{00}^{l1l2})]^{-1},$$

$$\boldsymbol{\Omega}^{(l)} = \boldsymbol{\Omega}_1^{(l)} + \boldsymbol{\Omega}_3^{(l)},$$

$$\boldsymbol{\Omega}_{1x,y}^{(l)} = \frac{\hbar}{m_0}\sqrt{6(3B^2 + C^2)}\kappa_{00}^{(l1l2)}k_{x,y}, \qquad (11)$$

$$\boldsymbol{\Omega}_{3x}^{(l)} = \Pi Bk_x(k_x^2 + k_y^2) + \Theta[3Bk_x(k_x^2 - k_y^2) + 2\sqrt{3(3B^2 + C^2)}k_y^2k_x],$$

$$\boldsymbol{\Omega}_{3y}^{(l)} = \Pi Bk_y(k_x^2 + k_y^2) + \Theta[-3Bk_y(k_x^2 - k_y^2) + 2\sqrt{3(3B^2 + C^2)}k_x^2k_y],$$

where C is a parameter of the hole spectrum[14] and

$$\Pi = \frac{\hbar^3}{m_0^2}\sqrt{\frac{3(3B^2 + C^2)}{2}} \times\sum_{n=0}^{\infty}\frac{1}{E_0^{(l)} - E_n^{(s)}}(\kappa_{0n}^{(l1s2)} - \kappa_{0n}^{(l2s1)}) \times[\sqrt{2}(\lambda_{0n}^{(l1s2)} + \lambda_{0n}^{(l2s1)}) - \lambda_{0n}^{(l1s1)}],$$

$$\Theta = \frac{\hbar^3}{m_0^2}\sqrt{\frac{3B^2 + C^2}{3}} \times\sum_{n=0}^{\infty}\frac{1}{E_0^{(l)} - E_n^{(h)}}\left(\kappa_{0n}^{(l1h)} - \frac{1}{\sqrt{2}}\kappa_{0n}^{(l2h)}\right) \times(\sqrt{2}\lambda_{0n}^{(l2h)} + \lambda_{0n}^{(l1h)}). \qquad (12)$$

In Eqs. (11) and (12), we use the following overlap integrals:

$$\lambda_{nn'}^{(\alpha\beta)} = \int dz\, \chi_n^{(\alpha)}\chi_{n'}^{(\beta)}, \quad \kappa_{nn'}^{(\alpha\beta)} = \int dz\, \chi_n^{(\alpha)}\frac{d\chi_{n'}^{(\beta)}}{dz}. \qquad (13)$$

For the ground HH state, we have

$$m_\parallel^{(h)} = m_0(A + B/2)^{-1},$$

$$\boldsymbol{\Omega}^{(h)} = \boldsymbol{\Omega}_3^{(h)},$$

$$\boldsymbol{\Omega}_{3x}^{(h)} = \Lambda[3Bk_x(k_x^2 - k_y^2) - 2\sqrt{3(3B^2 + C^2)}k_y^2k_x],$$

$$\boldsymbol{\Omega}_{3y}^{(h)} = \Lambda[3Bk_y(k_x^2 - k_y^2) + 2\sqrt{3(3B^2 + C^2)}k_x^2k_y], \qquad (14)$$

where

$$\Lambda = \frac{\hbar^3}{m_0^2}\sqrt{\frac{3B^2 + C^2}{3}} \times\Bigg[\sum_{n=0}^{\infty}\frac{1}{E_0^{(h)} - E_n^{(l)}}\left(\frac{1}{\sqrt{2}}\kappa_{0n}^{(hl2)} - \kappa_{0n}^{(hl1)}\right)(\sqrt{2}\lambda_{0n}^{(hl2)} + \lambda_{0n}^{(hl1)}) + \sum_{n=0}^{\infty}\frac{1}{E_0^{(h)} - E_n^{(s)}}\left(\frac{1}{\sqrt{2}}\kappa_{0n}^{(hs2)} - \kappa_{0n}^{(hs1)}\right)(\sqrt{2}\lambda_{0n}^{(hs2)} + \lambda_{0n}^{(hs1)})\Bigg]. \qquad (15)$$

For both the LH-like and HH-like states, the z component of $\boldsymbol{\Omega}$ is zero. It is important to note that $\boldsymbol{\Omega}$ is proportional to the product $\int dz\, \chi\, d^2\chi'/dz^2 \int dz\, \chi\, d\chi'/dz$ for the terms proportional to k and to the product $\int dz\, \chi\chi' \int dz\, \chi\, d\chi'/dz$ for those proportional to k^3, where χ and χ' are the envelope functions obtained as a solution of the Schrödinger equation with the potential $U(z)$ and appropriate effective masses. For a symmetric $U(z)$, the products of this kind are zero and the spin splitting vanishes in accordance with the general symmetry requirements.

Based on these results for hole spectrum, we can calculate the related spin relaxation rate. Basically, two mechanisms of relaxation must be addressed. The first is the D'yakonov-Perel' (DP) mechanism.[15] It is related to spin precession with a frequency $\boldsymbol{\Omega}(k_x,k_y)$, which changes randomly due to rapid electron transitions in the momentum space. For this mechanism, the spin relaxation times for the x, y, and z spin components obey the following relation $T_x=T_y=2T_z\equiv T_{\text{DP}}$. For nondegenerate carriers, it is given as

$$\frac{1}{T_{\text{DP}}} = \frac{\Sigma_{k_x,k_y}\Omega_x^2(k_x,k_y)f_0(k_x,k_y)}{\Sigma_{k_x,k_y}f_0(k_x,k_y)}\tau. \qquad (16)$$

In this equation, f_0 is the Boltzmann distribution function and τ is an average characteristic time of electron

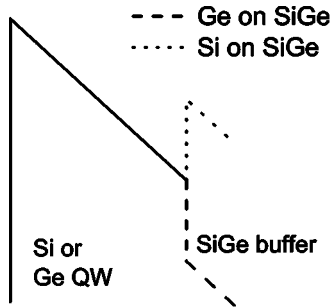

FIG. 1. Model valence band profile used for spin splitting calculations. Holes are assumed to be confined in a triangular well with an infinite barrier on the left-hand side. The band discontinuity at the SiGe interface depends on the structure type (Si/SiGe or Ge/SiGe) and was disregarded.

scattering;[15] in the following, we will assume it to be equal to the electron momentum relaxation time. Another dominant source of spin relaxation is the Elliott-Yafet (EY) mechanism. It is caused by hybridization of the hole states at the finite wave vectors. Using the results for hole wave functions, an order-of-magnitude estimate in a strongly asymmetric QW is obtained for the ratio of Elliott-Yafet relaxation time T_{EY} to T_{DP},

$$\frac{T_{\mathrm{EY}}}{T_{\mathrm{DP}}} \sim \left(\frac{E_Q \tau}{\hbar}\right)^2, \tag{17}$$

where E_Q is the characteristic energy of hole confinement, typically of the order of few tens of meV. The expression suggests that the D'yakonov-Pereĺ mechanism provides the major contribution to spin relaxation in the case of well-defined quantized energy levels. Of course, this is not true for weakly asymmetric QWs, where the D'yakonov-Pereĺ mechanism can become less important.

III. RESULTS AND DISCUSSION

As a specific example, we consider SiGe inversion layers. The first case corresponds to a thin Ge layer grown on SiGe, and the second a Si layer on SiGe; an insulator is placed on top in each case. Such structures have been studied extensively due to their perspective applications in *p*-type enhanced-mobility metal-oxide-semiconductor field-effect transistors.[14] Hole confinement in these devices is achieved by a strong perpendicular electric field and the insulator as schematically illustrated in Fig. 1. The barrier at the left-hand side is assumed to be infinitely high. The deformation energy in this case is $E_\epsilon = -2b(2c_{12}/c_{11}+1)\delta$, where c_{11} and c_{12} are the elastic constants of the QW material (i.e., Si or Ge), b is the deformation potential constant, and δ is the relative mismatch in the lattice parameters. For the case of a relaxed SiGe buffer, the ground state in the Si QW is LH-like with $E_\epsilon > 0$, while the Ge QW with $E_\epsilon < 0$ has a HH-like ground state. Note that the band discontinuity at the Si/SiGe or Ge/SiGe interface is not a well-defined quantity since not only the band gap but also the spin-orbit energy Δ are different across the interface. In our calculations, we assume that the confining electric field is strong enough to shift the holes away from the interface.

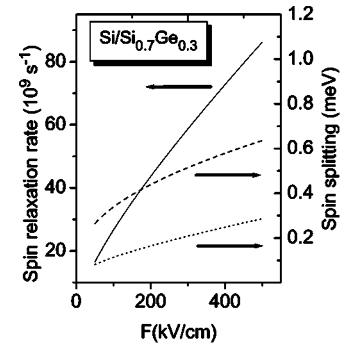

FIG. 2. Spin splitting and D'yakonov-Pereĺ spin relaxation rate for a strained Si QW grown on the $Si_{0.7}Ge_{0.3}$ buffer. Spin splitting is given for the hole kinetic energy of k_BT along the [100] (dotted line) and [110] (dashed line) directions.

In Figs. 2 and 3, we show the obtained spin splitting and spin relaxation rate $1/T_{\mathrm{DP}}$ as a function of the confining electric field at $T=300$ K. Figure 2 presents the case of a $Si/Si_{0.7}Ge_{0.3}$ structure, while Fig. 3 is for $Ge/Si_{0.3}Ge_{0.7}$. The momentum relaxation time τ of 5×10^{-14} s is used, which corresponds roughly to the reported values of hole mobility.[14,16] The material parameters are taken from Ref. 14. The spin splitting is calculated for the absolute value of the wave vector corresponding to the in-plane kinetic energy of k_BT along the [100] (dotted line) or [110] (dashed line) direction, respectively. For the case of a Si QW, the main contribution to Ω at room temperature is due to the terms proportional to k^3. This is because the k-linear term is proportional to B, which is small in the case of Si. On the other hand, the main contribution to Ω in the Ge QW is from the HH-LH coupling since the spin-orbital gap Δ in Ge is large. Note that the mixing between valence and conduction band states can noticably influence spin splitting in the latter case (i.e., the Ge QW).[10] For a Si QW, this is less likely to be important since the direct band gap is 3.5 eV, much larger than that for Ge (0.9 eV).[17]

As can be seen for the figures, the valence band of a Ge QW is characterized by spin splitting comparable to that for electrons in III-V QWs. Simultaneously, the hole spin relaxation time is quite short. In contrast, spin splitting and the

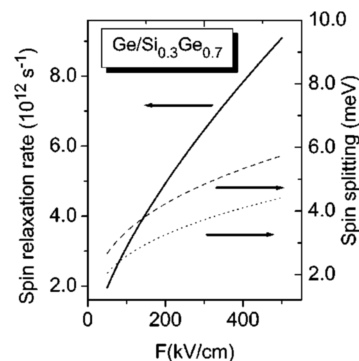

FIG. 3. Spin splitting and D'yakonov-Pereĺ spin relaxation rate for a strained Ge QW grown on the $Si_{0.3}Ge_{0.7}$ buffer. Spin splitting is given for the hole kinetic energy of k_BT along the [100] (dotted line) and [110] (dashed line) directions.

relaxation rate for holes in a strained Si QW are much smaller. The reason for this is a weak spin-orbit interaction in Si, which is characteristic for light elements. In particular, the k^3 contribution to Ω is proportional to Δ, which is as little as 44 meV for Si. Hence, it can be suggested that by applying a moderate longitudinal electric field, hole spin in a strained Si QW can be transferred over a distance of a micron or so without the loss of coherence. On the other hand, spin relaxation can be tuned effectively by modulating the confining electric field. It is important to note once more that in unstrained structures, say conventional p-type Si/SiO_2 inversion channels, spin relaxation is expected to be much faster due to relatively small subband separation and, as a result, strong hybridization of the hole states at finite wave vectors.

IV. CONCLUSION

We predict that spin splitting of 2D holes and the related spin relaxation time in strained SiGe QWs can be effectively controlled by the structure composition and the degree of QW asymmetry. For field-effect transistorlike structures,[18] spin splitting depends strongly on the value of the perpendicular electric field. In particular, the hole spin relaxation time in a strained Si QW channel can be in the hundred picosecond range at room temperature, making it suitable for spintronic applications.

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