Spin diffusion in Si/SiGe quantum wells: Spin relaxation in the absence of D'yakonov-Perel' relaxation mechanism

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In this work, the spin relaxation accompanying the spin diffusion in symmetric Si/SiGe quantum wells without the D'yakonov-Perel' spin-relaxation mechanism is calculated from a fully microscopic approach. The spin relaxation is caused by the inhomogeneous broadening from the momentum-dependent spin precessions in spatial domain under a magnetic field in the Voigt configuration. In fact, this inhomogeneous broadening together with the scattering lead to an irreversible spin relaxation along the spin diffusion. The effects of scattering, magnetic field, and electron density on spin diffusion are investigated. Unlike the case of spin diffusion in the system with the D'yakonov-Perel' spin-orbit coupling such as GaAs quantum wells where the scattering can either enhance or reduce spin diffusion depending on whether the system is in the strong or weak scattering limit, the scattering in the present system has no countereffect on the inhomogeneous broadening and suppresses the spin diffusion monotonically. The increase in magnetic field reduces the spin diffusion, while the increase in electron density enhances the spin diffusion when the electrons are degenerate but has a marginal effect when the electrons are nondegenerate.

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I. INTRODUCTION

The study of semiconductor spintronics has attracted a great deal of attention for its potential application to spin-based devices.[1–3] Among different prerequisites for realizing these devices, such as efficient spin injection[4,5] and suitable spin lifetime,[6,7] long spin-diffusion or transport length[8–10] is required sometimes, especially for the design of spin transistors and spin valves. Therefore, it is important to investigate the spin diffusion/transport in semiconductors.

In the study of spin diffusion or transport, the two-component drift-diffusion model is widely used in the literature.[9,11–16] In this model the spin-diffusion length L_s is connected to spin-relaxation time τ_s through spin-diffusion coefficient D_s: $L_s=\sqrt{D_s\tau_s}$,[9,11–13] with D_s usually assumed to be equal to the charge-diffusion coefficient D_c.[11,13–16] This equation implies infinitely long spin-diffusion length when the spin-relaxation time τ_s goes to infinity. In bulk Si, there is no D'yakonov-Perel' (DP) spin-orbit coupling[17] due to the bulk inversion symmetry. Thus the DP spin-relaxation mechanism[17] is absent and the spin-relaxation time in bulk Si is infinite when the other spin-relaxation mechanisms (such as the Elliott-Yafet mechanism[18]) are ignored. Therefore, an extremely long or even infinite spin-diffusion length is expected in bulk Si. However, this is not the case in the presence of a magnetic field. Very recently, Appelbaum *et al.*[19] studied the spin transport in bulk Si with a magnetic field perpendicular to both directions of spin transport and spin polarization. It has been shown that the spin-diffusion length is very small when the magnetic field becomes slightly strong (typically the spin-diffusion length is about several microns when the magnetic field is in the order of 0.1 T).[19] To account for the experimental spin relaxation and dephasing (R&D) along spin transport as well as the small spin-diffusion length, the drift-diffusion model was utilized and the interference among different spin-precession angles when reaching the same distance due to distinct transit times was suggested to be important.[14] In fact, this spin R&D along spin diffusion due to the magnetic field in the absence of the DP spin-relaxation mechanism was predicted from a fully microscopic approach, i.e., the kinetic spin Bloch equation (KSBE) approach,[20–26] back in 2002.[23] In this approach, the momentum-dependent spin precessions give rise to the inhomogeneous broadening.[20,21] In the presence of the inhomogeneous broadening, any scattering (including the spin-conserving scattering) leads to an irreversible spin R&D.[20–22] In spin diffusion or transport, it has been shown that the inhomogeneous broadening is determined by the spin-precession frequency $\boldsymbol{\omega}_{\mathbf{k}}=\frac{m^*}{\hbar^2 k_x}(\boldsymbol{\Omega}_{\mathbf{k}}+g\mu_B\mathbf{B})$ when the spin diffusion or transport is along the x axis.[26] Here $\boldsymbol{\Omega}_{\mathbf{k}}$ is the DP term.[17] It was shown in Ref. 23 that even when $\boldsymbol{\Omega}_{\mathbf{k}}=0$, the k_x dependence in $\boldsymbol{\omega}_{\mathbf{k}}$ still causes spin R&D. This is exactly the case in the experimental work on Si. The present work is to investigate the spin diffusion in Si/SiGe quantum wells (QWs) by means of the KSBE approach, in order to gain a deeper insight into the spin relaxation along spin diffusion in the absence of the DP spin-relaxation mechanism. The QWs are symmetric with an even number of monatomic Si layers and ideal heterointerfaces to exclude the Rashba spin-orbit coupling.[27] In addition, the study of spin relaxation in asymmetric Si/SiGe QWs has been carried out theoretically[28] and experimentally,[29,30] showing that the Rashba spin-orbit coupling[31] is very small (typically about three orders of magnitude smaller than that in QW structures based on III–V semiconductors[29]) and the spin-relaxation time is quite long (in the order of $10^{-7}\sim10^{-5}$ s).[28–30] Thus even for asymmetric Si/SiGe QWs, the present study still makes senses as long as the DP term $\boldsymbol{\Omega}_{\mathbf{k}}$ is weak enough compared to the magnetic-field term $g\mu_B\mathbf{B}$.

II. MODEL AND KSBES

We start our investigation from an n-type symmetric Si/SiGe QW with its growth direction along the $z \| [001]$ direction. The lowest conduction band in bulk Si is located near the X points of the Brillouin zone. Due to the quantum confinement along the z direction, the two degenerate X_z valleys lie lower than X_x and X_y valleys. The well width a is set as small as 5 nm and the temperature is lower than 80 K; thus with the moderate electron concentration, only the lowest subband of the X_z valley is occupied. The spin polarization is injected constantly from one side of the sample ($x=0$ plane) with polarization P and diffuses along the x axis, while the spatial distribution of spin in the y direction is uniform. The magnetic field $\mathbf{B}$ is applied in the x-y plane. It can be along an arbitrary direction without inducing any essential difference in the absence of the DP spin-orbit coupling. However, for the sake of convenience, the magnetic field is set to be along the y axis.

As the two X_z valleys are degenerate, only one of them needs to be considered. However, both the intravalley and intervalley scatterings have to be taken into account. The KSBEs for one valley read[23–26]

$$\frac{\partial \rho_{\mathbf{k}}(x,t)}{\partial t} = -\frac{e}{\hbar}\frac{\partial \Psi(x,t)}{\partial x}\frac{\partial \rho_{\mathbf{k}}(x,t)}{\partial k_x} - \frac{\hbar k_x}{m_t}\frac{\partial \rho_{\mathbf{k}}(x,t)}{\partial x} - \frac{i}{\hbar}\left[\frac{g\mu_B B \sigma_y}{2} + \Sigma_{\mathbf{k}}(x,t), \rho_{\mathbf{k}}(x,t)\right] + \left.\frac{\partial \rho_{\mathbf{k}}(x,t)}{\partial t}\right|_{\text{scat}}^{\text{intra}} + \left.\frac{\partial \rho_{\mathbf{k}}(x,t)}{\partial t}\right|_{\text{scat}}^{\text{inter}}. \quad (1)$$

Here $\rho_{\mathbf{k}}(x,t)$ represent the density matrices of electrons with two-dimensional momentum $\mathbf{k}$ (referring to the bottom of the X_z valley under investigation) at position x and time t. Their diagonal terms $\rho_{\mathbf{k},\sigma\sigma} \equiv f_{\mathbf{k},\sigma}$ ($\sigma = \pm 1/2$) represent the electron-distribution functions and the off-diagonal ones $\rho_{\mathbf{k},1/2,-1/2} = \rho^*_{\mathbf{k},-1/2,1/2}$ describe the inter-spin-band correlations for the spin coherence. $\Sigma_{\mathbf{k}}(x,t)$ is the Hartree-Fock term from the Coulomb interaction.[23–25] $-e$ is the electron charge, $m_t = 0.196 m_0$ is the transverse effective mass in the x-y plane, and $g \approx 2$ is the effective g factor for electrons in X valleys of Si.[32] $\Psi(x,t)$ is the electric potential determined by the Poisson equation $\frac{\partial^2 \Psi(x,t)}{\partial x^2} = e[n(x,t) - N_0]/(4\pi\varepsilon_0 \kappa_0 a)$ with $n(x,t) = \Sigma_\sigma n_\sigma(x,t)$ standing for the electron density at position x and time t. N_0 is the background positive charge density, and $n(x,0) = N_0$ denoting the initial uniform spatial distribution of electron density. $\kappa_0 = 11.9$ is the relative static dielectric constant.[33] $\left.\frac{\partial \rho_{\mathbf{k}}(x,t)}{\partial t}\right|_{\text{scat}}^{\text{intra}}$ and $\left.\frac{\partial \rho_{\mathbf{k}}(x,t)}{\partial t}\right|_{\text{scat}}^{\text{inter}}$ originate from the intravalley and intervalley scatterings, respectively. They are composed of the electron-phonon, electron-impurity, and electron-electron Coulomb scatterings (see also the Appendix).

Before numerically solving the KSBEs, a much simplified situation with the elastic electron-impurity scattering only is investigated analytically. Based on this simplified investigation, some properties of spin diffusion in Si/SiGe QWs can be speculated. Assuming $\mathbf{k} = k(\cos\theta, \sin\theta)$, in the steady state the Fourier components of the density matrix with respect to angle θ obey the following equation:

$$\frac{\hbar k}{2m_t}\frac{\partial}{\partial x}[\rho_k^{l+1}(x) + \rho_k^{l-1}(x)] = -i\frac{g\mu_B B}{2\hbar}[\sigma_y, \rho_k^l(x)] - \frac{\rho_k^l(x)}{\tau_k^l}, \quad (2)$$

with $\rho_k^l(x) = \frac{1}{2\pi}\int_0^{2\pi} d\theta \rho_{\mathbf{k}}(x) e^{-il\theta}$. Here $\frac{1}{\tau_k^l} = \frac{m^* N_i}{2\pi\hbar^3}\int_0^{2\pi} d\theta (1-\cos l\theta) U_{\mathbf{q}}^2$ is the lth-order momentum-relaxation rate, with $|\mathbf{q}| = \sqrt{2k^2(1-\cos\theta)}$. $U_{\mathbf{q}}^2$ is the electron-impurity scattering potential and N_i represents the impurity density. It is noted that $\frac{1}{\tau_k^l} = \frac{1}{\tau_k^{-l}}$ and $\frac{1}{\tau_k^0} = 0$. From the above equation one can obtain a closed group of first-order differential equations for $\rho_k^{\pm 1}$ and ρ_k^0 by neglecting higher orders of ρ_k^l with $|l| > 1$. From these equations the following second-order differential equation about ρ_k^0 is obtained:

$$\frac{\partial^2}{\partial x^2}\rho_k^0(x) = -2\left(\frac{m_t g\mu_B B}{2\hbar^2 k}\right)^2 [\sigma_y, [\sigma_y, \rho_k^0(x)]] + \frac{ig\mu_B B}{\hbar \tau_k^1}\left(\frac{m_t}{\hbar k}\right)^2 [\sigma_y, \rho_k^0(x)]. \quad (3)$$

Defining the "spin vector" as $\mathbf{S}_k^0(x) = \mathrm{Tr}[\rho_k^0(x)\boldsymbol{\sigma}]$ and using the boundary conditions (i) $\mathbf{S}_k^0(0) = (0,0,S_{kz}^0)^T$ and (ii) $\mathbf{S}_k^0(+\infty) = 0$, $\mathbf{S}_k^0(x)$ is found to be

$$\mathbf{S}_k^0(x) = S_{kz}^0 \begin{pmatrix} \sin\left[\frac{m_t}{\hbar k \tau_k^1}\left(\sqrt{1 + \frac{1}{(\tau_k^1 \omega_p)^2}} - 1\right)^{-1/2} x\right] \\ 0 \\ \cos\left[\frac{m_t}{\hbar k \tau_k^1}\left(\sqrt{1 + \frac{1}{(\tau_k^1 \omega_p)^2}} - 1\right)^{-1/2} x\right] \end{pmatrix} \times e^{-m_t \omega_p (\sqrt{1 + [1/(\tau_k^1 \omega_p)]^2} - 1)^{1/2} x/\hbar k}, \quad (4)$$

with $\omega_p = g\mu_B B/\hbar$ being the spin-precession frequency in the time domain under magnetic field $\mathbf{B} = B\hat{y}$. The total spin signal in the z direction (including two valleys) reads $S_z(x) = 2\Sigma_{\mathbf{k}}\mathrm{Tr}[\rho_{\mathbf{k}}(x)\sigma_z] = \int_0^{+\infty}\frac{dk}{\pi} k S_{kz}^0(x)$. To get $S_z(x)$, S_{kz}^0 in boundary condition (i) is assumed to be $S_{kz}^0 = f_{k,1/2} - f_{k,-1/2}$ with $f_{k,\sigma} = \frac{1}{e^{\beta(\hbar^2 k^2/2m_t - \mu_\sigma)} + 1}$. Here μ_σ is determined by $\int_0^{+\infty}\frac{dk}{\pi} k(f_{k,1/2} + f_{k,-1/2}) = N_0$ and $\int_0^{+\infty}\frac{dk}{\pi} k(f_{k,1/2} - f_{k,-1/2}) = PN_0$ with P the spin polarization at the $x=0$ plane.

It is noted from Eq. (4) that during the spin diffusion, $\mathbf{S}_k^0(x)$ on one hand precesses around the direction of magnetic field, and on the other hand decays in magnitude. However, when τ_k^1 becomes infinity, i.e., in the limit of zero electron-impurity scattering, Eq. (4) becomes $\mathbf{S}_k^0(x) = S_{kz}^0(\sin\frac{\sqrt{2}m_t\omega_p}{\hbar k}x, 0, \cos\frac{\sqrt{2}m_t\omega_p}{\hbar k}x)^T$. This solution clearly indicates the momentum dependence of spin precession in the spatial domain under magnetic field, which leads to the inhomogeneous broadening.[23] This inhomogeneous broadening alone leads to a reversible decay of the total spin signal $S_z(x)$ along the x direction. However, in the presence of scattering, this decay becomes irreversible, as shown in the exponential damping term for each $S_{kz}^0(x)$ in Eq. (4). Therefore, even without the DP term, there is spin relaxation accompanying the spin diffusion. Due to the factor S_{kz}^0 included in Eq. (4), the main contribution to $S_z(x)$ comes from k states near the Fermi surface at the $x=0$ plane, especially when the temperature is low. Thus

$$S_z(x) \propto \cos\left[\frac{m_t}{\hbar k_f \tau^1_{k_f}}\left(\sqrt{1+\frac{1}{(\tau^1_{k_f}\omega_p)^2}}-1\right)^{-1/2} x\right] \times e^{-m_t\omega_p(\sqrt{1+[1/(\tau^1_{k_f}\omega_p)]^2}-1)^{1/2}x/\hbar k_f}, \quad (5)$$

indicating that the spin diffusion can be suppressed by the scattering strength and the magnetic field, based on the increase in the exponential damping rate with $1/\tau^1_{k_f}$ and ω_p. It has been shown earlier that, in systems with the DP spin-orbit coupling, the scattering on one hand provides the spin-R&D channel in the presence of the inhomogeneous broadening from the DP term but, on the other hand, can have a countereffect on the inhomogeneous broadening.[21,22,26] In the strong scattering limit, the countereffect dominates and thus increasing scattering strength results in a suppression of spin R&D in the time domain[21,22] or an enhancement of spin diffusion or transport in spatial domain.[26] However, for the current case without the DP spin-orbit coupling, the scattering shows *no* countereffect on the inhomogeneous broadening but just suppresses the spin diffusion. Except for the above analysis based on the simplified model, to gain a complete picture of the problem of spin diffusion, one must solve the KSBEs taking into account the electron-phonon and electron-electron Coulomb scatterings, both of which play an important role on spin R&D.

III. NUMERICAL RESULTS

To numerically solve the KSBEs, the double-side boundary conditions are used.[26] These conditions assume a steady spin polarization P for electrons with $k_x>0$ at boundary $x=0$ and a vanishing spin polarization at finite sample length $x=L$ for electrons with $k_x<0$.[26] For the Poisson equation, the boundary conditions are set to be $\Psi(0,t)=\Psi(L,t)=0$. The numerical scheme for solving the KSBEs is given in Ref. 26. Once the KSBEs are numerically solved, the steady-state distribution of electrons $N_\sigma(x)=n_\sigma(x,+\infty)=2\Sigma_{\mathbf{k}} f_{\mathbf{k},\sigma}(x,+\infty)$ (factor 2 comes from the two degenerate X_z valleys) is calculated and thus the spin signal $S_z(x)=N_{1/2}(x)-N_{-1/2}(x)$ can be derived to analyze the spin-diffusion properties. In the calculation, the electron density N_0 is set to be 4×10^{11} cm^{-2} except otherwise specified, and the impurity density N_i is assumed to be $0.1N_0$ when the impurities are present. Furthermore, the initial spin polarization P at the $x=0$ plane is set to be 5%. The effects of scattering, magnetic field, and electron density on spin diffusion are investigated, with the main results given in Figs. 1–3.

We first investigate the effects of scattering and magnetic field on spin diffusion. The steady-state spatial distributions of spin signal calculated with different scatterings are shown in Fig. 1. In order to show the property of spin diffusion clearly, we also plot the absolute value of S_z vs x on a logarithmic scale in the same figure. All these curves indicate obvious spin relaxation along spin diffusion without the DP spin-relaxation mechanism. By comparing the curves labeled

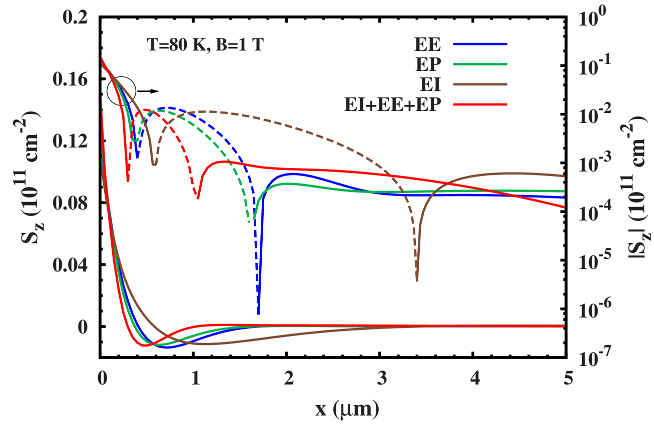

FIG. 1. (Color online) The steady-state spatial distributions of spin signal S_z with different scatterings included. The curve labeled "EE," "EP," or "EI" stands for the calculations with the electron-electron, electron-phonon, or electron-impurity scattering, respectively, while the curve labeled "EI+EE+EP" stands for the calculation with all the scatterings. In order to get a clear view of the decay and precession of S_z, we also plot the corresponding absolute value of S_z against x on a logarithmic scale (note the scale is on the right hand of the frame). The dashed curves correspond to the part with $S_z<0$.

as "EE" and "EI," one finds that the electron-electron Coulomb scattering can suppress spin diffusion effectively. In fact, the Coulomb scattering plays an important role in both spin R&D (Refs. 21, 22, and 34) and spin diffusion or transport.[24–26] In a system with the DP spin-orbit coupling, the Coulomb scattering not only contributes to the total momentum-relaxation time τ_k,[34] but also has a countereffect to the inhomogeneous broadening.[21,22,24–26] Therefore, in the strong scattering limit, adding Coulomb scattering may suppress the spin relaxation and enhance the spin diffusion or transport.[22,25] For the current situation without the DP spin-orbit coupling, the Coulomb scattering affects the spin diffusion only through τ_k and thus only suppresses the spin diffusion or transport. Similarly, the electron-phonon scatterings, including both the intravalley and intervalley scatterings, also contribute to the momentum relaxation and suppress

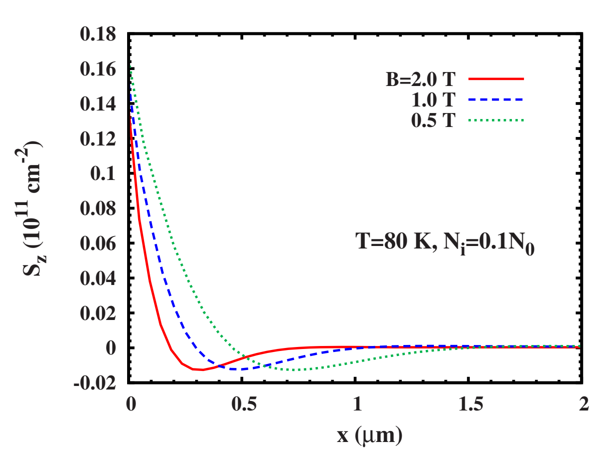

FIG. 2. (Color online) S_z vs x in the steady state for different magnetic-field strengths. Solid curve: $B=2$ T; dashed curve: $B=1$ T; dotted curve: $B=0.5$ T. $T=80$ K and $N_i=0.1N_0$.

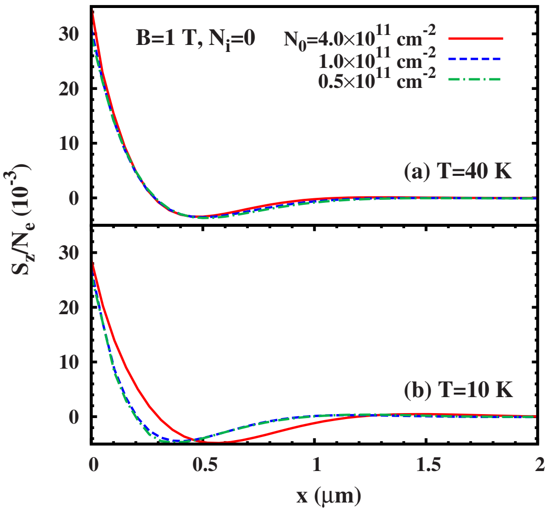

FIG. 3. (Color online) S_z/N_0 vs x in the steady state with different electron densities at (a) $T=40$ K and (b) $T=10$ K. $B=1$ T and $N_i=0$.

spin diffusion effectively, as shown by the "EP" curve. For the case of stronger scattering strength (i.e., with all the different scatterings included), the spin-diffusion length becomes much smaller. It is also noted that with the increase in scattering strength, the spatial spin-precession period decreases. This is because the spin-precession frequency increases with $1/\tau_{k_f}^{1}$ as shown in Eq. (5). The magnetic-field dependence of spin diffusion is investigated as well, with the results corresponding to different magnetic fields shown in Fig. 2. It is revealed that both the spin-diffusion length and the spin-precession period decrease with an increase in magnetic-field strength B. This is because both the damping rate and the spin-precession frequency increase with ω_p and thus B, as shown in Eq. (5). These studies indicate a suppression of spin diffusion due to the scattering and magnetic field, just as obtained earlier with the simplified model.

The density dependence of spin diffusion is also investigated. The steady-state spatial distributions of spin signal with three different electron densities under temperature $T=40$ and 10 K are plotted in Figs. 3(a) and 3(b), respectively. The spin signal is rescaled by the corresponding electron density to be S_z/N_0 for comparison. It is noted that when $T=40$ K, the spin diffusion is *insensitive* to the electron density. That is because the electrons are nondegenerate in the studied electron-density regime when $T=40$ K, due to the large transverse effective electron mass in X valleys of Si. However, when T decreases to 10 K, the effect of electron density on the spin diffusion can be seen, as shown in Fig. 3(b). In the large density regime where the electrons become degenerate, the spin-diffusion length increases with the electron density (compare the situations with $N_0=4.0\times10^{11}$ and 1.0×10^{11} cm^{-2}). This is mainly due to the decrease in the damping rate with k_f, as shown in Eq. (5). In addition, in the low-density regime it is shown that the density again has a marginal effect on spin diffusion (compare the situations with $N_0=1.0\times10^{11}$ and 0.5×10^{11} cm^{-2}), as the electrons remain nondegenerate there. It is noted that the density dependence of spin diffusion in Si is very different from the density dependence of the spin relaxation in GaAs QWs where nonmonotonic density dependence was predicted[22] and realized experimentally very recently.[35] This is due to the fact that in GaAs QWs the inhomogeneous broadening comes from the DP term which is, however, absent in the symmetric Si/SiGe QWs.

IV. SUMMARY

In summary, the present work investigates the spin diffusion in symmetric Si/SiGe (001) QWs at low temperature. There is no DP spin-relaxation mechanism due to the absence of the DP spin-orbit coupling in this system. However, a magnetic field in the Voigt configuration is present. Our simulations were performed in a fully microscopic way based on the KSBE approach, with all the relevant scatterings included. It was shown that, even without the DP spin-relaxation mechanism, the electron spins relax effectively along the spin diffusion. This spin relaxation is caused by the inhomogeneous broadening from the momentum-dependent spin precessions in the spatial domain. The effects of scattering, magnetic field, and electron density on spin diffusion were investigated. It was shown that, unlike the case of spin diffusion in the system with the DP spin-orbit coupling,[26] in Si/SiGe (001) QWs any scattering suppresses the spin diffusion without any countereffect on the inhomogeneous broadening. The magnetic field reduces spin diffusion also. It was further revealed that the increase in electron density enhances the spin diffusion when the electrons are degenerate but has a marginal effect when the electrons are nondegenerate.

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APPENDIX: THE SCATTERING TERMS OF THE KSBE

The scattering terms are analogous to those shown in Ref. 36, except the following differences. The two valleys are degenerate here, thus the multivalley KSBEs similar to those shown in Ref. 36 can be simplified to obtain the KSBEs of a "single" valley [i.e., Eq. (1)]. The intravalley scatterings consist of those due to longitudinal-acoustic (LA) and transverse-acoustic (TA) phonons, while the intervalley scatterings are the g-type scatterings involving LA, TA, and longitudinal-optical (LO) phonon branches.[37] However, due to the low temperature, the scattering due to the LO phonon is neglected. $M^2_{\alpha,\mathrm{intra},\mathbf{Q}}=\frac{\hbar D_\alpha^2 Q^2}{2d\Omega_{\alpha,\mathrm{intra},\mathbf{Q}}}|I_{\mathrm{intra}}(iq_z)|^2$ is the matrix element for the intravalley scattering, and $M^2_{\alpha,\mathrm{inter},\mathbf{Q}}=\frac{\hbar\Delta_\alpha^2}{2d\Omega_{\alpha,\mathrm{inter},\mathbf{Q}}}|I_{\mathrm{inter}}(iq_z)|^2$ for the intervalley scattering. $\alpha=\mathrm{LA/TA}$ stands for the LA/TA phonon mode. $d=2.33$ g/cm^3 is the mass density of Si.[38] $D_{\mathrm{LA}}=6.39$ eV and $D_{\mathrm{TA}}=3.01$ eV.[37] $\Omega_{\alpha,\mathrm{intra},\mathbf{Q}}=v_\alpha Q$ with phonon velocities $v_{\mathrm{LA}}=9.01\times10^5$ cm/s and $v_{\mathrm{TA}}=5.23\times10^5$ cm/s.[37] Δ_{LA}

$=1.5\times10^8$ eV/cm and $\Delta_{\rm TA}=0.3\times10^8$ eV/cm.[37] The phonon energies for the intervalley scattering are approximately fixed to be $\hbar\Omega_{\rm LA,inter,\mathbf{Q}}=0.019$ eV and $\hbar\Omega_{\rm TA,inter,\mathbf{Q}}=0.01$ eV.[37] $|I_\gamma(iq_z)|^2=\frac{\pi^4\sin^2 y}{y^2(y^2-\pi^2)^2}$ (γ=intra/inter) is the form factor with $y\equiv aq_z/2$ for the intravalley scattering and $y\equiv a(q_z-2K^z_{X_z})/2$ for the intervalley scattering. Here $K^z_{X_z}=0.85\times\frac{2\pi}{a_0}$ with a_0 being the Si lattice constant is the z component of the coordinate of the bottom of the X_z valley.

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