Valley Splitting and Spin Lifetime Enhancement in Strained Thin Silicon Films

D. Osintsev[1], V. Sverdlov[1], N. Neophytou[2], and S. Selberherr[1]
[1]Institute for Microelectronics, TU Wien, Gußhausstraße 27–29/E360, 1040 Wien, Austria
[2]School of Engineering, University of Warwick, CV4 7AL Coventry, United Kingdom
E-mail: {Osintsev|Sverdlov|Neophytou|Selberherr}@iue.tuwien.ac.at

***Abstract*—Spintronics attracts much attention because of the potential to build novel spin-based devices which are superior to nowadays charge-based microelectronic devices. Silicon, the main element of microelectronics, is promising for spin-driven applications. We investigate the surface roughness and electron-phonon limited spin relaxation in silicon films taking into account the coupling between the relevant valleys through the Γ-point. We demonstrate that applying uniaxial stress along the [110] direction considerably suppresses the spin relaxation.**

I. INTRODUCTION

Electron spin properties in silicon and other semiconductors have attracted a significant attention in recent theoretical and experimental studies. Silicon is an ideal material for spintronic applications due to its long spin lifetime in the bulk [1]. However, large spin relaxation in gated silicon structures was experimentally observed. Understanding the details of spin propagation in ultra-scaled MOSFETs is urgently needed [2].

We investigate the spin relaxation in (001) silicon structures by taking into account surface roughness and electron-phonon interaction. The two interfaces of the film are assumed to be independent. The surface roughness scattering matrix elements are proportional to the product of the corresponding subband wave functions' derivatives at each interface [3].

The subband energies and wave functions were obtained from a $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian [4], [5] generalized to include the spin degree of freedom [2], [6]. The Hamiltonian is written in the vicinity of the X-point along the k_z-axis in the Brillouin zone and includes the two relevant valleys of the conduction band [7]. After a unitary basis transformation it is written as

$$H = \begin{bmatrix} H_1 & H_3 \\ H_3 & H_2 \end{bmatrix}, \qquad (1)$$

with

$$H_{1,2} = \left[\frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2\left(k_x^2+k_y^2\right)}{2m_t} + U(z) \pm \delta\right] I, \quad (2)$$

$$H_3 = \begin{bmatrix} \dfrac{\hbar^2 k_0 k_z}{m_l} & 0 \\ 0 & \dfrac{\hbar^2 k_0 k_z}{m_l} \end{bmatrix}. \qquad (3)$$

Here I is the identity 2×2 matrix, $U(z)$ is the confinement potential, m_t and m_l are the transversal and the longitudinal silicon effective masses, $k_0 = 0.15\times 2\pi/a$ is the position of the valley minimum relative to the X-point in unstrained silicon, $\delta = \sqrt{\left(D\varepsilon_{xy} - \frac{\hbar^2 k_x k_y}{M}\right)^2 + \Delta_{so}^2\left(k_x^2+k_y^2\right)}$, ε_{xy} denotes the shear strain component, $M^{-1} \approx m_t^{-1} - m_0^{-1}$, $D = 14$eV is the shear strain deformation potential, and $\Delta_{so} = 1.27$meVnm.

II. RESULTS AND DISCUSSION

In the two valleys' plus two spin projections' basis the subband wave functions possess four components. These wave functions are written as ($k_x = 0$)

$$\Psi_1 = \begin{pmatrix} \Psi_{1,1} \\ \Psi_{1,2} \\ \Psi_{1,1}^* \\ -\Psi_{1,2}^* \end{pmatrix} \Psi_2 = \begin{pmatrix} -\Psi_{1,2} \\ \Psi_{1,1} \\ \Psi_{1,2}^* \\ \Psi_{1,1}^* \end{pmatrix}$$
$$\Psi_3 = \begin{pmatrix} \Psi_{2,2} \\ \Psi_{2,1} \\ -\Psi_{2,2}^* \\ \Psi_{2,1}^* \end{pmatrix} \Psi_4 = \begin{pmatrix} -\Psi_{2,1} \\ \Psi_{2,2} \\ -\Psi_{2,1}^* \\ -\Psi_{2,2}^* \end{pmatrix}, \qquad (4)$$

where $\Psi_{1(3)}$ and $\Psi_{2(4)}$ are the up- and down-spin wave functions for the first (second) subband. Wave functions with opposite spin in the same subband are orthogonal and correspond to the same energy. The wave functions

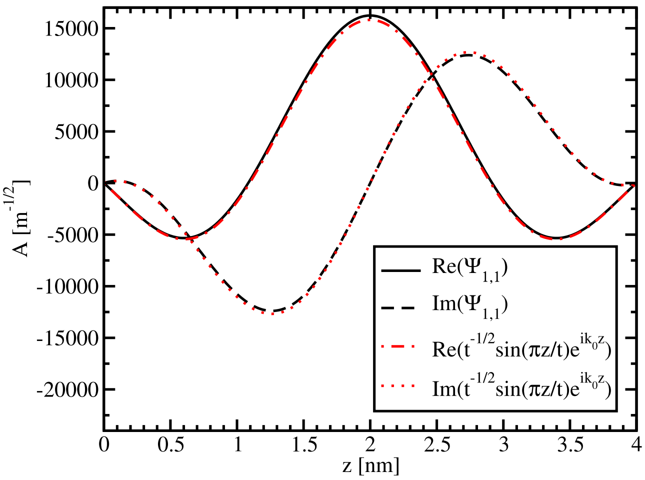

Fig. 1. The large component of the wave function of the lowest unprimed subband in an unstrained film located in the valley centered at k_0.

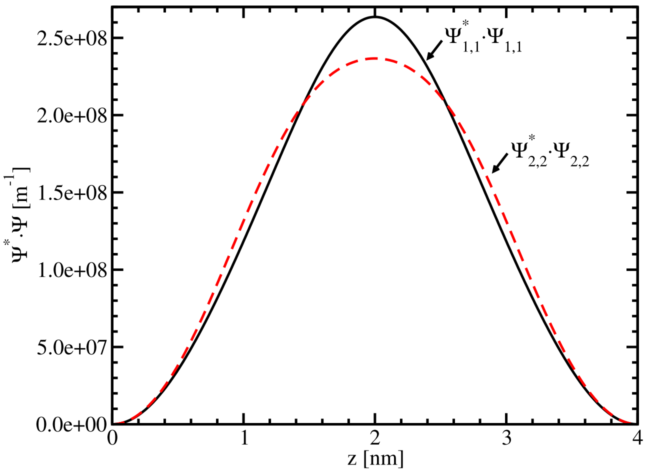

Fig. 2. The large components of the two unprimed subbands with ε_{xy}=0.05%.

are chosen such that only the average z-axis spin projection is nonzero. Then the dominant components are $\Psi_{1,1}$ and $\Psi_{2,2}$ for $\Psi_{1(2)}$ and $\Psi_{3(4)}$, respectively. Thus, Ψ_1 and Ψ_3 are considered as up-spin wave functions, while Ψ_2 and Ψ_4 are the down-spin wave functions. The small components of the wave functions are the result of the spin-orbit interaction taken into account with the $\tau_y \otimes \Delta_{SO}(k_x\sigma_x - k_y\sigma_y)$ term, where τ_y is the y-Pauli matrix in the valley degree of freedom, and σ_x and σ_y are the spin Pauli matrices.

Without spin-orbit interaction properly included the wave function with the spin projection assumed along the OZ-axis does not contain the small components. The large components of the wave functions are well described by $\Psi_{1,1(2,2)} = e^{ik_0z}\sin\left(\frac{\pi z}{t}\right)$ (Figure 1) and their conjugates corresponding to the usual envelope quantization function located at the valley minima. Under shear strain ε_{xy} the degeneracy between the two unprimed subbands is lifted which results in slightly different envelope functions $\Psi_{1,1}$ and $\Psi_{2,2}$ (Figure 2).

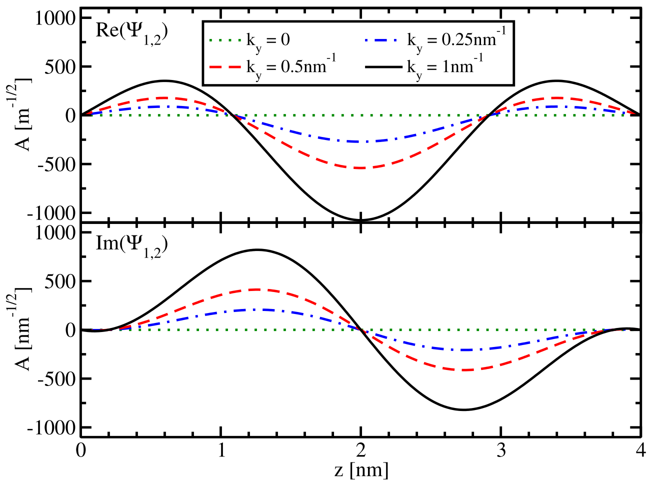

Fig. 3. The small components are proportional to the strength of the spin-orbit interaction.

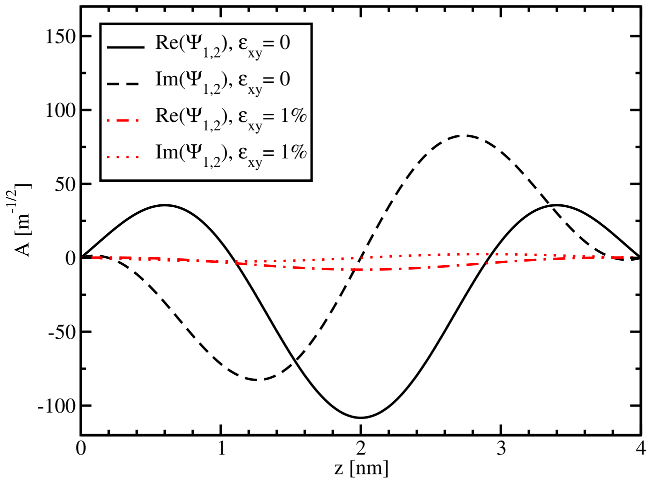

Fig. 4. The small components are considerably suppressed by tensile shear strain.

The small components of the four-components' wave function are proportional to the spin-orbit interaction strength. Indeed, the amplitude of these components shown in Figure 3 for an unstrained film of 4nm thickness for $k_x = 0$ linearly depends on the value of k_y. For $k_y = 1\text{nm}^{-1}$ the small components of the wave functions are pronounced, while decreasing k_y makes the small components vanishing.

Shear strain ε_{xy} considerably suppresses the small components as shown in Figure 4. $\Psi_{1,2}$ for the strain

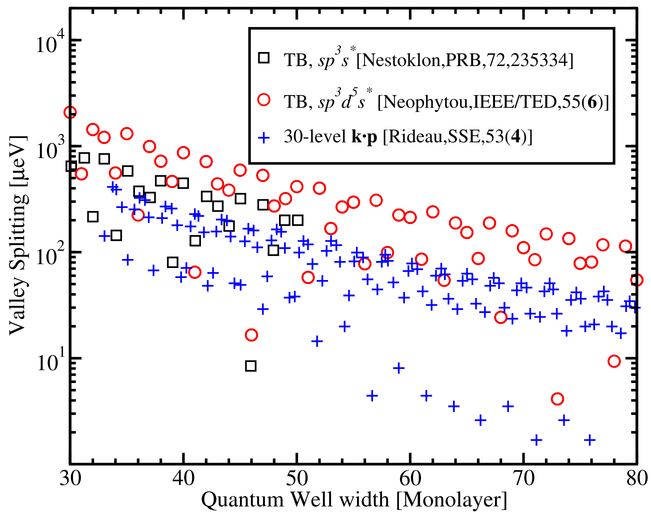

Fig. 5. Valley splitting in a Si quantum well at zero strain as a function of the quantum well width including results from literature [2], [8], [12].

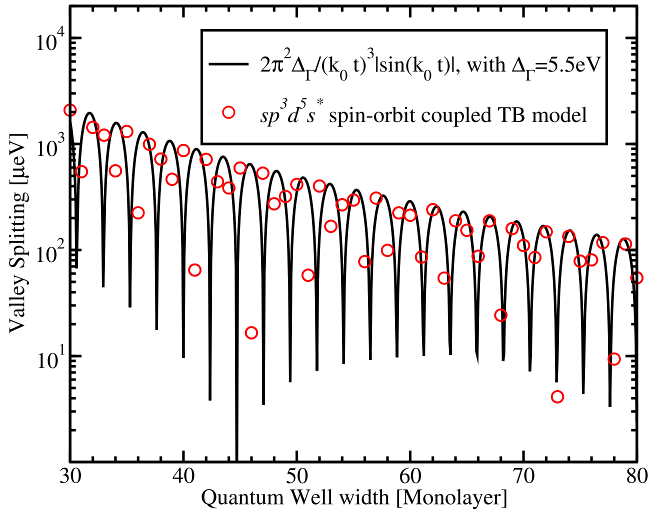

Fig. 6. Dependence of the valley splitting on the quantum well width from the tight binding (TB) model and the analytical expression with Λ_Γ=5.5eV.

value of 1% is almost vanished, while for the unstrained film the wave function component is significant (Figure 4). Vanishing values of the small components decrease the spin mixing between the states with the opposite spin projections, which results in longer spin lifetime.

The calculation of the conduction electron spin relaxation due to surface roughness and electron-phonon scattering in (001) silicon films starts from properly taking into account the valley degeneracy lifting in unstrained films. The [001] equivalent valley coupling through the

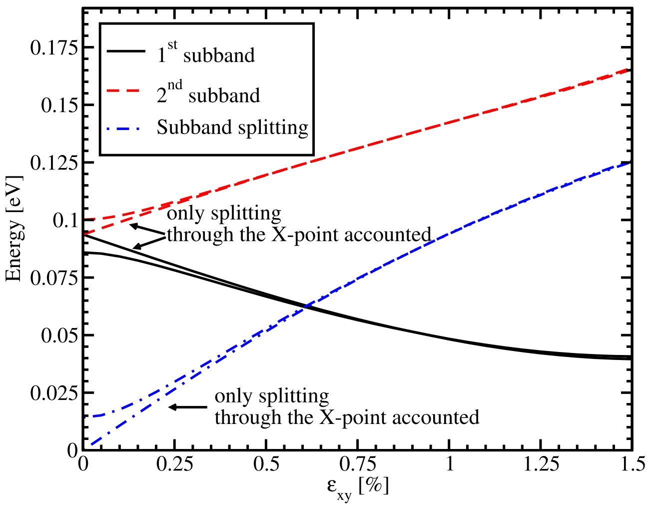

Fig. 7. Dependence of the energy of the 1^{st} and the 2^{nd} subbands together with the subband splitting on shear strain for the film thickness 2.1nm.

Γ-point results in a subband splitting in confined electron structures [9]. The values of the valley splitting obtained from a 30-band $\mathbf{k}\cdot\mathbf{p}$ model [10], an atomistic tight-binding model from [11], and from [12] are shown in Figure 5. Although looking irregular, the results follow a certain law. Figure 6 demonstrates a good agreement of the results of the tight-binding calculations with the analytical expression for the subband splitting [5]

$$\Lambda_\Gamma = \frac{2\pi\Delta_\Gamma}{(k_{0\Gamma}t)^3}\sin(k_{0\Gamma}t), \tag{5}$$

where Δ_Γ is the splitting at Γ-point, $k_{0\Gamma} = 0.85\frac{2\pi}{a}$, a is the lattice constant, and t is the film thickness. The good agreement is found for the value Δ_Γ=5.5eV. Then, the valley splitting of an infinite potential square well [7] is generalized by including the Λ_Γ term

$$\begin{aligned}\Delta E_n = &\frac{2y_\mathrm{n}^2\delta}{k_0t\sqrt{\left(1-y_\mathrm{n}^2-\eta^2\right)\left(1-y_\mathrm{n}^2\right)}}\times\\ &\left|\sin\left(\sqrt{\frac{1-y_\mathrm{n}^2-\eta^2}{1-y_\mathrm{n}^2}}k_0t\right)\right|,\end{aligned} \tag{6}$$

with $y_\mathrm{n} = \frac{\pi}{k_0t}$, $\eta = \frac{m_\mathrm{l}B}{k_0^2\hbar^2}$, and $\delta = \sqrt{\Delta_\mathrm{so}^2\left(k_\mathrm{x}^2+k_\mathrm{y}^2\right)+\left(D\varepsilon_\mathrm{xy}-\frac{\hbar^2k_\mathrm{x}k_\mathrm{y}}{M}\right)^2+\Lambda_\Gamma^2}$.

Figure 7 shows the dependence of the lowest unprimed subbands' energies and their splitting on shear strain with and without accounting for the Λ_Γ term. The unprimed subbands are degenerate at zero strain without the Λ_Γ term. The Λ_Γ term lifts the degeneracy while shear strain gives the major contribution to the splitting at high strain

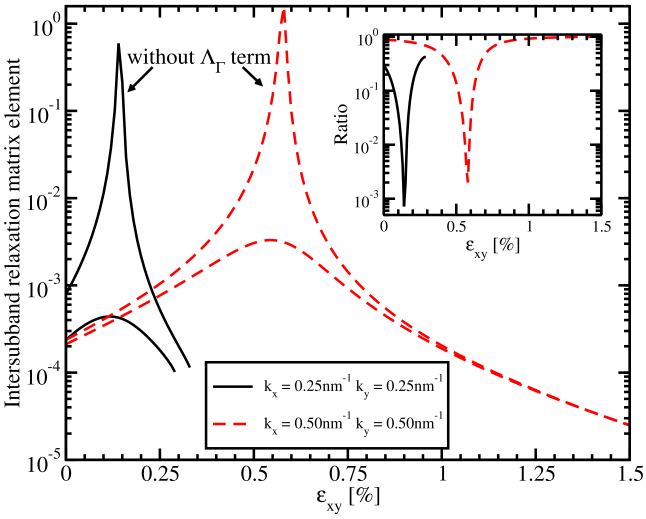

Fig. 8. Dependence of the normalized intersubband relaxation matrix elements on shear strain for the film thickness 2.1nm. The inset shows the ratio of the matrix elements with the Λ_Γ term to the matrix elements without the Λ_Γ term.

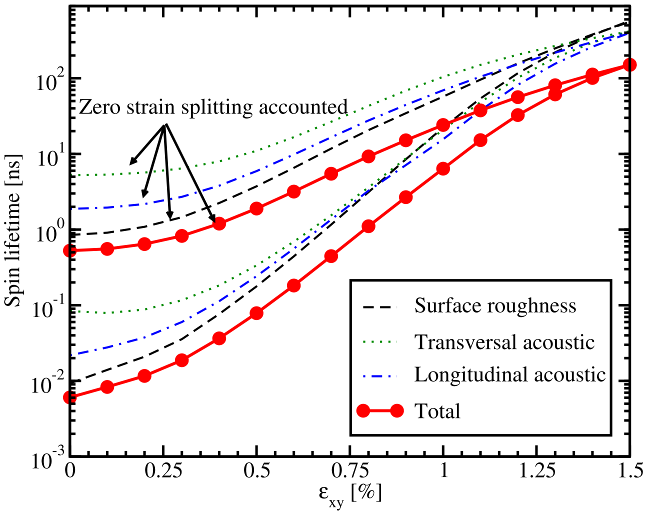

Fig. 9. Dependence of spin lifetime on shear strain for T=300K and film thickness 2.1nm.

values. The surface roughness scattering matrix elements are taken to be uncorrelated at both interfaces. The surface roughness intersubband spin relaxation matrix elements with and without the Δ_Γ term are shown in Figure 8. The difference in the matrix elements' values calculated with and without the Δ_Γ term (inset Figure 8) can reach two orders of magnitude. Hence, the valley coupling through the Γ-point must be taken into account for accurate spin lifetime calculations.

Electron-phonon scattering is taken into consideration in the deformation potential approximation [13]. A strong increase of the spin lifetime is demonstrated in Figure 9. The increase is less pronounced, if the term responsible for the valley splitting in relaxed films is taken into account. However, even in this case the spin lifetime is boosted by almost two orders of magnitude.

III. CONCLUSION

We have used a $\mathbf{k} \cdot \mathbf{p}$ approach to evaluate the spin lifetime in strained thin silicon films. It is shown that the small components of the four-component wave functions vanish with strain. We have demonstrated that coupling through the Γ-point must be taken into account. Tensile shear strain boosts the spin lifetime by almost two orders of magnitude.

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