Electron Momentum and Spin Relaxation in Silicon Films

D. Osintsev, V. Sverdlov, and S. Selberherr

Abstract Semiconductor spintronics is promising, because it allows creating microelectronic elements which are smaller and consume less energy than present charge-based devices. Silicon is the main element of modern charge-based electronics, thus, understanding the peculiarities of spin propagation in silicon is the key for designing novel devices. We investigate the electron momentum and the spin relaxation in thin (001) oriented SOI films using a $\mathbf{k} \cdot \mathbf{p}$-based approach with spin degree of freedom properly included. We demonstrate that shear strain routinely used to enhance the electron mobility can boost the spin lifetime by an order of magnitude.

Keywords Charge-based electronics • Semiconductor • Silicon films

1 Introduction

Growing technological challenges and soaring costs are gradually bringing MOSFET scaling to an end. This intensifies the search of alternative technologies and computational principles. The electron spin attracts attention as a possible candidate to be used in future electron devices for complementing or even replacing the charge degree of freedom employed in MOSFETs. The spin state is characterized by the two spin projections on a given axis and it thus has a potential in digital information processing. In addition, only a small amount of energy is needed to flip the spin orientation. Silicon is an ideal material for spintronic applications due to the long spin lifetime in the bulk. The spin lifetime is determined by spin-flip scattering between the valleys located on different crystallographic axes [1, 2]. This mechanism is suppressed in thin films; however, large spin relaxation in gated silicon structures was observed [3]. Understanding the spin relaxation mechanisms and identifying ways to boost the spin lifetime in confined electron systems is urgently needed.

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2 Model and Results

We investigate spin relaxation in (001) silicon structures by taking into account surface roughness and electron-phonon interaction induced momentum scattering and spin relaxation. 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 [4]. To find the wave functions and matrix elements we use the effective **k·p** Hamiltonian written at the X-point for the two relevant valleys along the OZ-axis with shear strain and the spin degree of freedom included [5]. We generalize the deformation potential based electron-phonon scattering theory to include the shear strain deformation potential and the deformation potential due to spin-orbit interaction responsible for spin relaxation in confined systems [6].

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

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

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 valley are orthogonal. 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 $\Delta_{SO} = 1.27$ meVnm [2, 5], 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 included the wave function conserves the spin projection which is assumed along the OZ-axis. The large components of the wave functions are well described by $\Psi_{1,1(2,2)} = e^{ik_0 z} \sin\left(\frac{\pi z}{t}\right)$ (Fig. 1) and their conjugates. This expression corresponds to the usual envelope quantization function. 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 $\Psi_{2,2}$ (Fig. 2).

The small components of the four-components' wave function are proportional to the spin-orbit interaction strength. The amplitude of these components shown in Fig. 3 for an unstrained film of 4 nm thickness for $k_x = 0$ strongly 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 value makes the small components vanish.

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

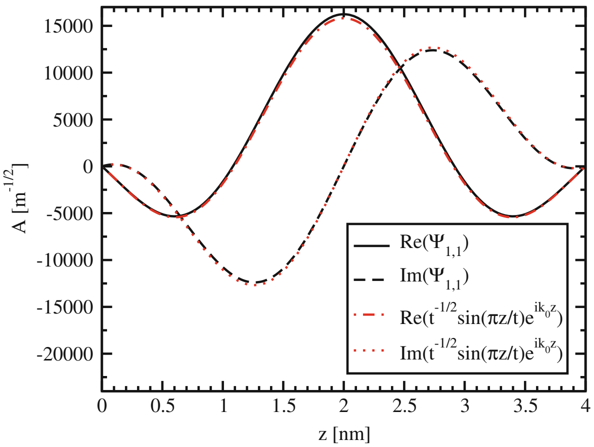
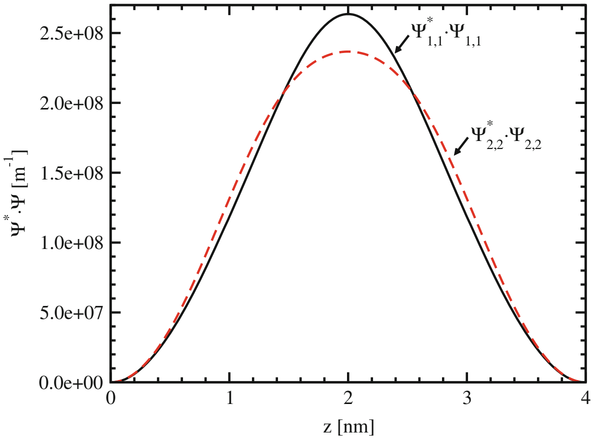


Fig. 2 The large components of the two unprimed subbands with ε_{xy}=0.05 %



Shear strain ε_{xy} greatly suppresses the small components as shown in Fig. 4. $\Psi_{1,2}$ for the strain value of 1 % is almost vanished, while for the film the wave function component is significant (Fig. 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.

Surface roughness limited spin lifetime and momentum relaxation time as a function of temperature are shown in Fig. 5. For the chosen electron concentrations the spin and momentum relaxation times decrease with temperature [1]. As a confirmation of the Elliot-Yafet spin relaxation mechanism, the spin lifetime remains proportional to the momentum relaxation time (Fig. 5).

Under shear strain the spin lifetime is enhanced much stronger than the momentum relaxation time (Fig. 6) due to the small components' suppression (Fig. 4). An

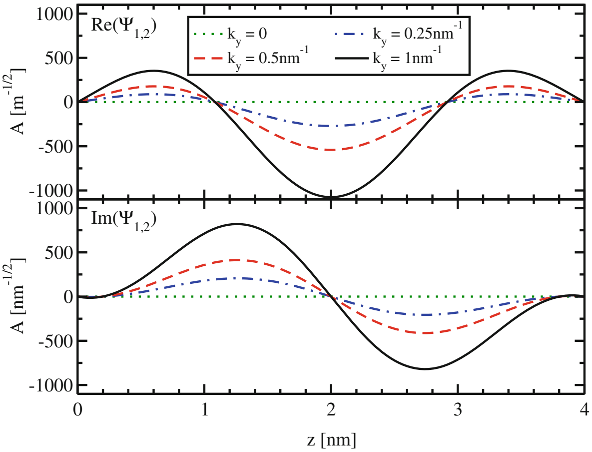


Fig. 3 The small components are proportional to the strength of the spin-orbit interaction

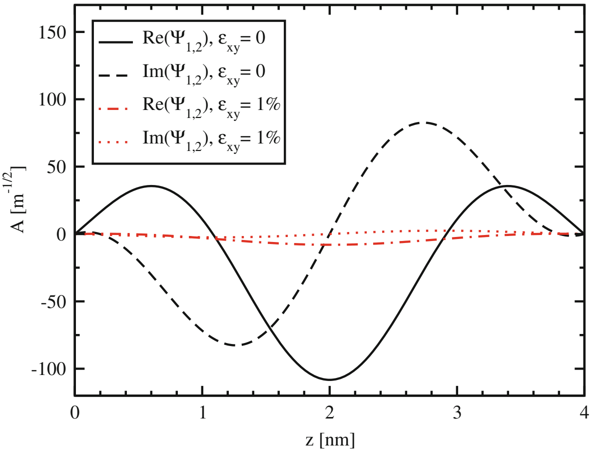


Fig. 4 The small components are considerably suppressed by tensile shear strain

extensive code parallelization and optimization allowed us to extend the method [6] for a larger set of parameters, including the film thickness and the electron concentration. The ratio of the spin to the momentum relaxation time (inset in Fig. 6) demonstrates the significant enhancement.

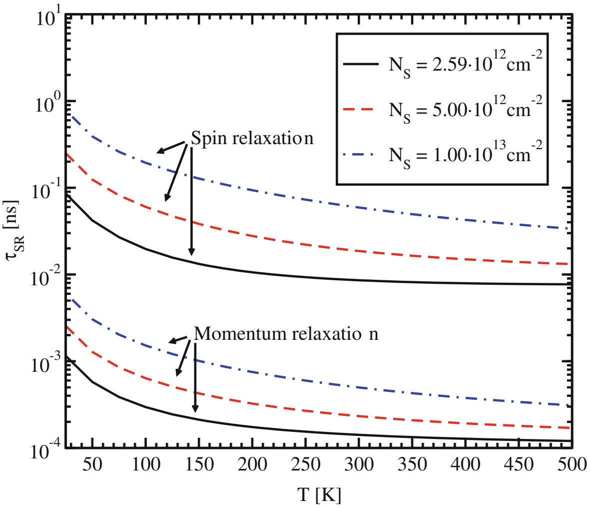


Fig. 5 The spin lifetime is proportional to the momentum relaxation time as function of temperature. This is an indication of the Elliot-Yafet spin relaxation mechanism [1]

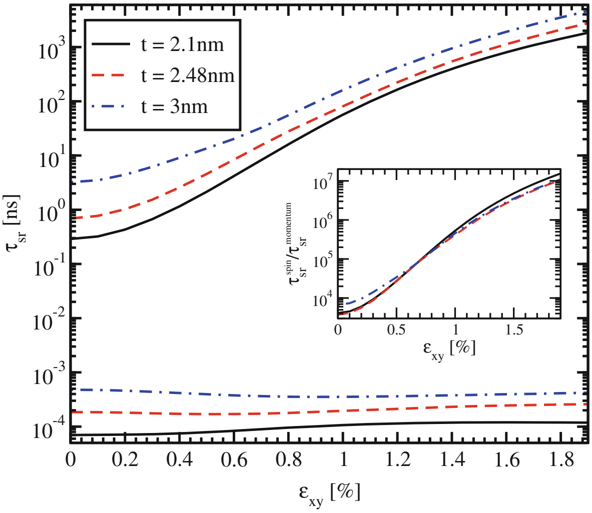


Fig. 6 Dependence of the spin lifetime and the momentum relaxation time on shear strain for different thicknesses. *Inset*: ratio of the spin to the momentum relaxation time

3 Conclusion

We have used a $\mathbf{k} \cdot \mathbf{p}$ approach to evaluate the momentum relaxation time and the spin lifetime in strained thin silicon films. We have shown that the small components of four-component wave functions vanish with strain. Thus, the spin lifetime is enhanced much stronger by shear strain than the momentum relaxation time. Tensile shear strain boosts both the electron mobility and the spin lifetime in silicon films.

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