Influence of Surface Roughness Scattering on Spin Lifetime in Silicon

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Silicon is an ideal material for spintronic applications [1] due to long spin lifetime, however, considerable spin relaxation in gated silicon structures was experimentally observed [2]. Surface roughness scattering determines the transport in the channel at high carrier concentration N_s in thin silicon films [3].

Here we investigate the spin relaxation due to surface roughness. The surface roughness scattering matrix elements are proportional to the square of the product of the subband wave function derivatives at the interface [4, 5]. To find the corresponding matrix elements for spin relaxation we use the effective **k·p** Hamiltonian for the two relevant valleys along the *OZ*-axis [6, 7] with the spin degree of freedom properly included [8-10].

The relaxation time τ is calculated as a thermal average with the Fermi function $f(\varepsilon)$

$$\frac{1}{\tau} = \frac{\int \frac{1}{\tau(\mathbf{K_1})} f(\varepsilon)\big(1-f(\varepsilon)\big)\, d\mathbf{K_1}}{\int f(\varepsilon)\, d\mathbf{K_1}} \tag{1}$$

of the rate [4,8,9]

$$\frac{1}{\tau(\mathbf{K_1})} = \frac{4\pi}{\hbar} \sum_{i,j=1,2} \int_0^{2\pi} \pi\Delta^2 L^2 \frac{1}{\epsilon_{ij}^2(\mathbf{K_2}-\mathbf{K_1})} \frac{\hbar^4}{4m_l^2} \left[\frac{d\Psi^*_{i\sigma\mathbf{K_1}}}{dz}\frac{d\Psi_{j\sigma'\mathbf{K_2}}}{dz}\right]^2_{z=\pm\frac{t}{2}}$$
$$\times \exp\left(\frac{-(\mathbf{K_2}-\mathbf{K_1})^2 L^2}{4}\right) \frac{|\mathbf{K_2}|}{\left|\frac{\partial\varepsilon(\mathbf{K_2})}{\partial\mathbf{K_2}}\right|} \frac{1}{(2\pi)^2}\, d\varphi, \tag{2}$$

where ε is the electron energy, $\mathbf{K_{1,2}}$ are the in-plane wave vectors, σ, σ' are the spin projections on a chosen axis, ϵ_{ij} is the dielectric permittivity, L is the autocorrelation length, Δ is the mean square value of the surface roughness fluctuations. In case the wave vector dependence of the derivatives of the wave functions $\Psi_{i\sigma\mathbf{K}}$ on $\mathbf{K}$ can be ignored [4, 5], the rate (2) is approximated as

$$\frac{1}{\tau(\mathbf{K_1})} = \frac{2\pi\Delta^2 L^2}{\hbar} \sum_{i,j=1,2} \frac{\hbar^4}{4m_l^2} \left[\frac{d\Psi^*_{i\sigma\mathbf{K}\to\mathbf{0}}}{dz}\frac{d\Psi_{j\sigma'\,\mathbf{K}\to\mathbf{0}}}{dz}\right]^2_{z=\pm\frac{t}{2}}$$
$$\times \exp\left(\frac{-(\mathbf{K}_2^2+\mathbf{K}_1^2)L^2}{4}\right) \frac{m_t}{2\pi\hbar^2} 2\pi I_0\left(-\frac{L^2 K_1 K_2}{2}\right), \tag{3}$$

where I_0 is the modified Bessel function of the first kind.

Through all simulations we use a film thickness of 2.48nm. Fig. 1 shows the dependence of the surface roughness limited mobility on shear strain. A good agreement between the results calculated with (2) and (3) is observed confirming the standard approximation of neglecting the wave vector dependence in the matrix elements [4]. In the absence of strain the mobility is higher for higher electron concentrations N_s, in agreement with [3]. For $N_s = 10^{12}\text{cm}^{-2}$ the mobility increases with tensile shear strain because of the reduction of the transport effective mass [6]. For $N_s = 5 \cdot 10^{12}\text{cm}^{-2}$ an opposite trend is observed, because of the increase of intrasubband scattering with strain within the second subband (Fig. 2), which gets split from the first one due to strain-induced valley splitting (inset in Fig. 2). The occupation of the second subband remains substantial even at high strain as confirmed by the Fermi level dependence (inset in Fig. 2). This increase of the intrasubband scattering overcompensates the mobility enhancement due to the reduced transport mass, resulting in an overall decrease of the surface roughness limited mobility at high N_s (Fig. 1).

To evaluate the electron spin relaxation we take the matrix elements on the wave functions with the opposite spin projections $\sigma' = -\sigma$ corresponding to the spin flip events. Normalized spin relaxation matrix elements display sharp peaks at the same values of strain, where the intersubband splitting is reduced. These minima determine the positions of the narrow hot spots.

Fig. 4 shows the dependence of the spin lifetime on temperature for an unstrained film. While the temperature increases, the number of the hot spot points which lie in the energy range determined by the term $f(\varepsilon)\big(1-f(\varepsilon)\big)$ increases. In combination with the Fermi level lowering this results in the reduction of the spin lifetime with temperature due to increased surface roughness scattering, in complete analogy with the momentum relaxation time behavior [3].

For higher shear strain values the hot spots are pushed to higher energies (Fig. 5) away from the subband minima (inset in Fig. 5). This leads to a strong increase of the spin lifetime shown in Fig. 6. This also demonstrates that the approximation of the independence of the matrix elements on the wave vectors used to obtain (3) is inappropriate for evaluation of the spin lifetime. Indeed, while the momentum relaxation time changes insignificantly with strain, the spin relaxation time increases by orders of magnitude. Thus, shear strain used to enhance mobility can also be used to increase spin lifetime.

References

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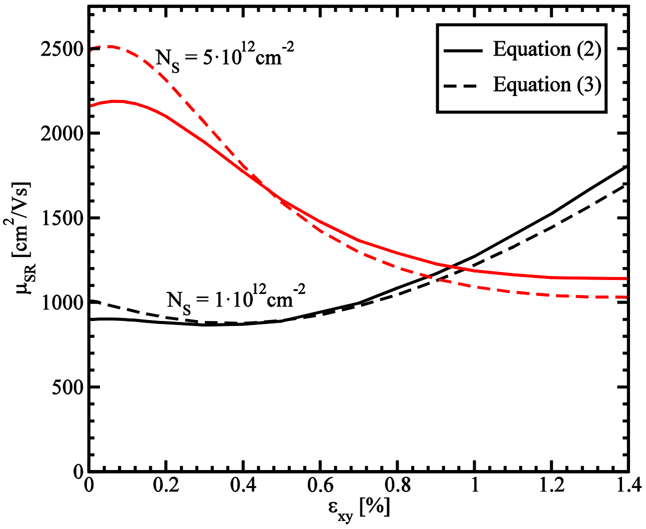

Fig. 1. Dependence of the surface roughness limited electron mobility calculated with (2) and (3) on shear strain for different values of the electron concentration.

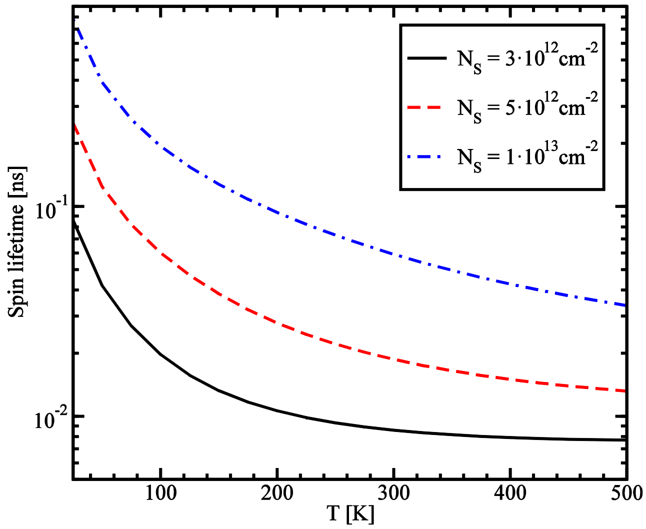

Fig. 4. Dependence of the spin lifetime on temperature for different values of the electron concentration in unstrained film.

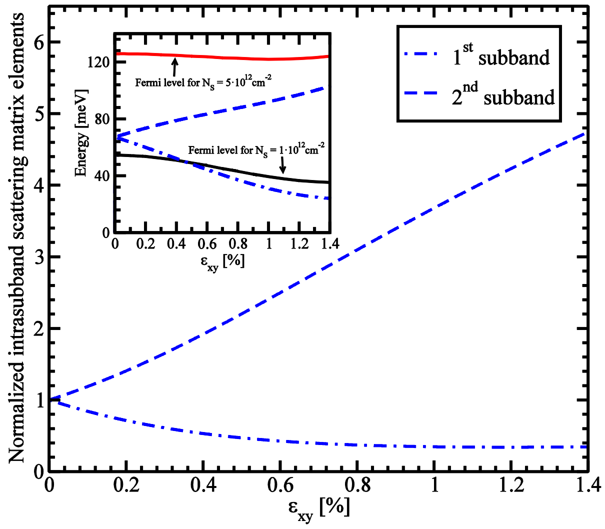

Fig. 2. Normalized intrasubband scattering matrix elements as a function of shear strain. The inset shows the dependence of subband energies and Fermi levels on shear strain.

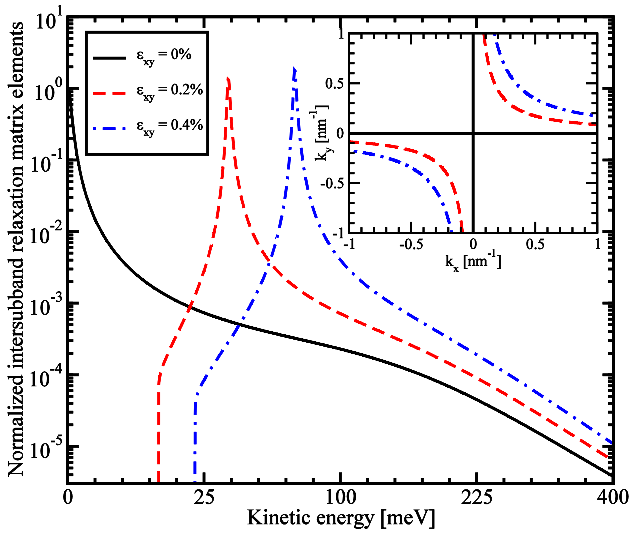

Fig. 5. Normalized intersubband relaxation matrix elements as a function of the conduction electrons kinetic energy in [110] direction. The inset shows the positions of the hot spots for different values of shear strain.

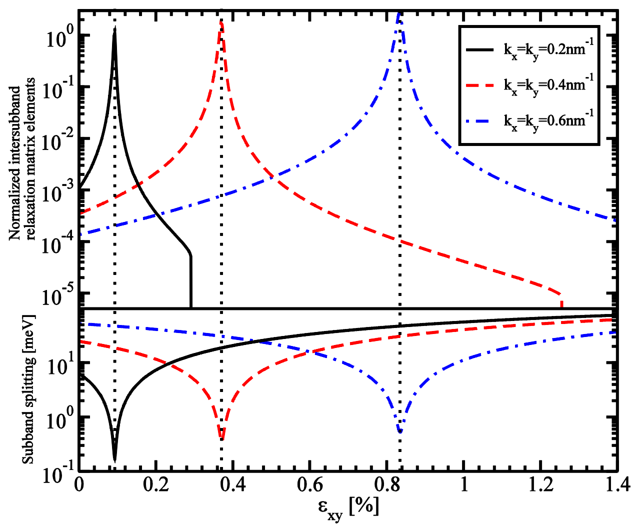

Fig. 3. Normalized intersubband relaxation matrix elements and subband splitting as a function of shear strain for different values of the wave vectors.

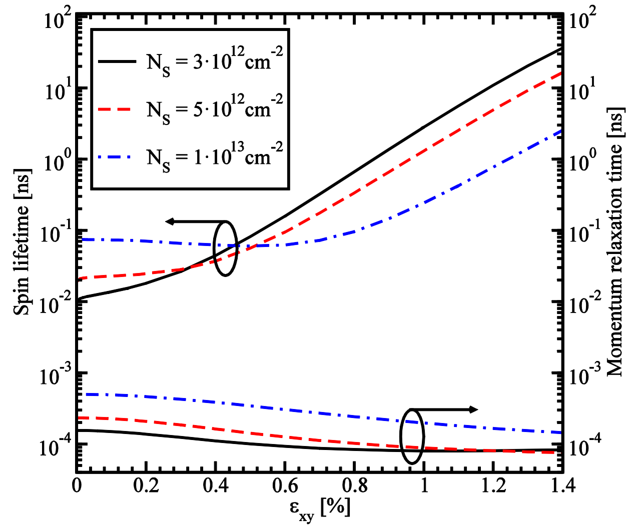

Fig. 6. Spin lifetime and momentum relaxation time as a function of shear strain for different values of electron concentration at room temperature.