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Electron mobility and spin lifetime enhancement in strained ultra-thin silicon films

Dmitri Osintsev *, Viktor Sverdlov, Siegfried Selberherr

Institute for Microelectronics, TU Wien, Gußhausstraße 27-29, A-1040 Wien, Austria

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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. Understanding the details of the spin propagation in silicon structures is a key for building novel spin-based nanoelectronic devices. We investigate the surface roughness- and phonon-limited electron mobility and spin relaxation in ultra-thin silicon films. We show that the spin relaxation rate due to surface roughness and phonon scattering is efficiently suppressed by an order of magnitude by applying tensile stress. We also demonstrate an almost twofold mobility increase in ultra-thin (001) SOI films under tensile [110] stress, which is due to the usually neglected strain dependence of the scattering matrix elements.

1. Introduction

Ongoing miniaturization of microelectronic devices pushes research to develop models which can accurately describe transport processes taking place in ultra-thin body SOI MOSFETs. Mobility enhancement in such structures is an important issue. Stress is routinely used to enhance the carrier mobility. However, it is expected that in ultra-thin SOI structures stress becomes less efficient for this purpose [1].

Spintronics is the rapidly developing and promising technology exploiting spin properties of electrons. A number of potential spintronic devices has been proposed [2,3]. Silicon, the main element of microelectronics, is also promising for spin-driven applications [4], because it is composed of nuclei with predominantly zero spin and is characterized by small spin-orbit coupling. Both factors favour to reduce the spin relaxation. However, the experimentally observed enhancement of spin relaxation in electrically gated lateral-channel silicon structures [5] could compromise the reliability and become an obstacle in realizing spin-driven devices. Deeper understanding of scattering and spin relaxation mechanisms in thin silicon films is therefore needed.

We investigate the surface roughness and electron–phonon limited electron mobility and spin relaxation in silicon films under shear strain. We show that due to the usually neglected dependence of the surface roughness scattering matrix elements on strain the electron mobility in such structures shows a two times increase with strain. Shear strain also results in a degeneracy lifting between the unprimed subbands resulting in a spin lifetime increase by at least an order of magnitude.

2. Model

In order to find the corresponding scattering matrix elements, the subband structure and the wave functions in silicon films must be calculated. For this purpose the effective **k** · **p** Hamiltonian describing the electron states in the conduction band of the two relevant [001] valleys in presence of shear strain ε_{xy}, spin–orbit interaction, and confinement potential $U(z)$ is written in the vicinity of the X-point along the k_z-axis in the Brillouin zone as [6,7]

$$H = \begin{bmatrix} H_1 & H_3 \\ H_3^\dagger & H_2 \end{bmatrix}, \tag{1}$$

where H_1, H_2, and H_3 are written as

$$H_1 = \begin{bmatrix} \frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2(k_x^2+k_y^2)}{2m_t} - \frac{\hbar^2 k_0 k_z}{m_l} + U(z) & 0 \\ 0 & \frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2(k_x^2+k_y^2)}{2m_t} - \frac{\hbar^2 k_0 k_z}{m_l} + U(z) \end{bmatrix}, \tag{2}$$

$$H_2 = \begin{bmatrix} \frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2(k_x^2+k_y^2)}{2m_t} + \frac{\hbar^2 k_0 k_z}{m_l} + U(z) & 0 \\ 0 & \frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2(k_x^2+k_y^2)}{2m_t} + \frac{\hbar^2 k_0 k_z}{m_l} + U(z) \end{bmatrix}, \tag{3}$$

$$H_3 = \begin{bmatrix} D\varepsilon_{xy} - \frac{\hbar^2 k_x k_y}{M} & (k_y - k_x \mathrm{i})\Delta_{so} \\ (-k_y - k_x \mathrm{i})\Delta_{so} & D\varepsilon_{xy} - \frac{\hbar^2 k_x k_y}{M} \end{bmatrix}. \tag{4}$$

* Corresponding author.
E-mail address: osintsev@iue.tuwien.ac.at (D. Osintsev).

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Here $M^{-1} \approx m_t^{-1} - m_0^{-1}$, $D = 14$ eV is the shear strain deformation potential, $\Delta_{so} = 1.27$ meV nm, 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. The unprimed subband energies and the four component wave functions are used to evaluate the scattering matrix elements and rates. The primed subbands can be described in a similar fashion [1].

We are considering the surface roughness (SR) and electron–phonon scattering mechanisms contributing to the spin and momentum relaxation.

The spin and momentum relaxation times are calculated by thermal averaging of the corresponding subbands in-plane momentum $\mathbf{K}_i$ dependent scattering rates $\tau_i(\mathbf{K}_i)$ [6,8,9] as

$$\frac{1}{\tau} = \frac{\sum_i \int \frac{1}{\tau_i(\mathbf{K}_i)} f(E_i)(1 - f(E_i)) d\mathbf{K}_i}{\sum_i \int f(E_i) d\mathbf{K}_i}, \tag{5}$$

$$\int d\mathbf{K}_i = \int_0^{2\pi} \int_{E_i^{(0)}}^{\infty} \frac{\mathbf{K}_i}{\left|\frac{\partial E_i}{\partial \mathbf{K}_i}\right|} d\varphi dE, \tag{6}$$

Here $f(E) = [1 + \exp((E - E_F)/k_B T)]^{-1}$, where k_B is the Boltzmann constant, T is the temperature, E_F is the Fermi energy, $E = E_i^{(0)} + E_i(\mathbf{K}_i)$, $E_i^{(0)} = E_i(\mathbf{K}_i = 0)$ is the energy of the bottom of the subband i, and

$$\left|\frac{\partial E_i}{\partial \mathbf{K}_i}\right| = \left|\frac{\partial E(\mathbf{K}_i)}{\partial \mathbf{K}_i}\right|_{\varphi, E}, \tag{7}$$

is the derivative of the subband dispersion along $\mathbf{K}_i$ at the angle φ defining the $\mathbf{K}_i$ direction. The surface roughness momentum (spin) relaxation rate in the subband i is calculated in the following way [7,9]

$$\begin{aligned} \frac{1}{\tau_i^{SR}(\mathbf{K}_i)} = &\frac{2(4)\pi}{\hbar(2\pi)^2} \sum_j \int_0^{2\pi} \pi\Delta^2 L^2 \frac{1}{\epsilon_{ij}^2(\mathbf{K}_i - \mathbf{K}_j)} \frac{\hbar^4}{4m_l^2} \frac{|\mathbf{K}_j|}{\left|\frac{\partial E(\mathbf{K}_j)}{\partial \mathbf{K}_j}\right|} \\ &\cdot \left[\left(\frac{d\Psi_{i\mathbf{K}_i\sigma(-\sigma)}}{dz}\right)^* \left(\frac{d\Psi_{j\mathbf{K}_j\sigma}}{dz}\right)\right]^2_{z=\pm\frac{t}{2}} \\ &\times \exp\left(\frac{-(\mathbf{K}_j - \mathbf{K}_i)L^2}{4}\right) d\varphi. \end{aligned} \tag{8}$$

$\mathbf{K}_i$, $\mathbf{K}_j$ are the in-plane wave vectors before and after scattering, φ is the angle between $\mathbf{K}_i$ and $\mathbf{K}_j$, ϵ is the dielectric permittivity, L is the autocorrelation length, Δ is the mean square value of the surface roughness fluctuations, $\Psi_{i\mathbf{K}_i}$ and $\Psi_{j\mathbf{K}_j}$ are the wave functions, and $\sigma = \pm 1$ is the spin projection to the [001] axis.

The intervalley spin relaxation rate contains the Elliott and Yafet contributions [8], which are calculated in the following way

$$\begin{aligned} \frac{1}{\tau_i^{LA}(\mathbf{K}_i)} = &\frac{4\pi k_B T}{\hbar\rho\upsilon_{LA}^2} \sum_j \int_0^{2\pi} \frac{1}{2\pi} \frac{|\mathbf{K}_j|}{\left|\frac{\partial E(\mathbf{K}_j)}{\partial \mathbf{K}_j}\right|} \left[1 - \frac{\left|\frac{\partial E(\mathbf{K}_j)}{\partial \mathbf{K}_j}\right| f(E(\mathbf{K}_j))}{\left|\frac{\partial E(\mathbf{K}_i)}{\partial \mathbf{K}_i}\right| f(E(\mathbf{K}_i))}\right] \frac{1}{2} \\ &\cdot \int_0^t \left[\Psi_{j\mathbf{K}_j-\sigma}^\dagger(z) M' \Psi_{i\mathbf{K}_i\sigma}(z)\right]^* \left[\Psi_{j\mathbf{K}_j-\sigma}^\dagger(z') M' \Psi_{i\mathbf{K}_i\sigma}(z')\right] dz d\varphi. \end{aligned} \tag{9}$$

Here the matrix M' is written as

$$M' = \begin{bmatrix} M_{ZZ} & M_{SO} \\ M_{SO}^\dagger & M_{ZZ} \end{bmatrix}, \tag{10}$$

$$M_{ZZ} = \begin{bmatrix} \Xi & 0 \\ 0 & \Xi \end{bmatrix}, \tag{11}$$

$$M_{SO} = \begin{bmatrix} 0 & D_{SO}(r_y - ir_x) \\ D_{SO}(-r_y - ir_x) & 0 \end{bmatrix}, \tag{12}$$

where $\Xi = 12$ eV is the acoustic deformation potential, $(r_y, r_x) = \mathbf{K}_i + \mathbf{K}_j$, and $D_{SO} = 15$ meV$/k_0$ [8] with $k_0 = 0.15 \cdot 2\pi/a$ defined as the position of the valley minimum relative to the X-point in unstrained silicon. In contrast to mobility calculations, when the main contribution to (8) and (9) is due to intrasubband scattering, the spin relaxation is mostly determined by intersubband transitions.

Intrasubband transitions are important for the contributions determined by the shear deformation potential. The spin relaxation rate due to the transversal acoustic phonons is calculated as [10]

$$\begin{aligned} \frac{1}{\tau_i^{TA}(\mathbf{K}_i)} = &\frac{4\pi k_B T}{\hbar\rho\upsilon_{TA}^2} \sum_j \int_0^{2\pi} \frac{1}{2\pi} \frac{|\mathbf{K}_j|}{\left|\frac{\partial E(\mathbf{K}_j)}{\partial \mathbf{K}_j}\right|} \left[1 - \frac{\left|\frac{\partial E(\mathbf{K}_j)}{\partial \mathbf{K}_j}\right| f(E(\mathbf{K}_j))}{\left|\frac{\partial E(\mathbf{K}_i)}{\partial \mathbf{K}_i}\right| f(E(\mathbf{K}_i))}\right] \frac{1}{2} \\ &\cdot \int_0^t \int_0^t \exp\left(-\sqrt{q_x^2 + q_y^2}|z - z'|\right) \\ &\cdot \left[\Psi_{j\mathbf{K}_j-\sigma}^\dagger(z) M \Psi_{i\mathbf{K}_i\sigma}(z)\right]^* \left[\Psi_{j\mathbf{K}_j-\sigma}^\dagger(z') M \Psi_{i\mathbf{K}_i\sigma}(z')\right] \\ &\cdot \left[\sqrt{q_x^2 + q_y^2} - \frac{8q_x^2 q_y^2 - (q_x^2 + q_y^2)^2}{q_x^2 + q_y^2}|z - z'|\right] dz dz' d\varphi, \end{aligned} \tag{13}$$

where $\rho = 2329 \frac{\text{kg}}{\text{m}^3}$ is the silicon density, $\upsilon_{TA} = 5300 \frac{m}{s}$ is the transversal phonons' velocity, $(q_x, q_y) = \mathbf{K}_i - \mathbf{K}_j$, and M is the 4×4 matrix written in the basis for the spin relaxation rate.

$$M = \begin{bmatrix} 0 & 0 & D/2 & 0 \\ 0 & 0 & 0 & D/2 \\ D/2 & 0 & 0 & 0 \\ 0 & D/2 & 0 & 0 \end{bmatrix}. \tag{14}$$

Here $D = 14$ eV is the shear deformation potential.

The intravalley spin relaxation rate due to longitudinal acoustic phonons is calculated as [10]

$$\begin{aligned} \frac{1}{\tau_i^{LA}(\mathbf{K}_i)} = &\frac{4\pi k_B T}{\hbar\rho\upsilon_{LA}^2} \sum_j \int_0^{2\pi} \frac{1}{2\pi} \frac{|\mathbf{K}_j|}{\left|\frac{\partial E(\mathbf{K}_j)}{\partial \mathbf{K}_j}\right|} \left[1 - \frac{\left|\frac{\partial E(\mathbf{K}_j)}{\partial \mathbf{K}_j}\right| f(E(\mathbf{K}_j))}{\left|\frac{\partial E(\mathbf{K}_i)}{\partial \mathbf{K}_i}\right| f(E(\mathbf{K}_i))}\right] \frac{1}{2} \\ &\cdot \int_0^t \int_0^t \exp\left(-\sqrt{q_x^2 + q_y^2}|z - z'|\right) \\ &\cdot \left[\Psi_{j\mathbf{K}_j-\sigma}^\dagger(z) M \Psi_{i\mathbf{K}_i\sigma}(z)\right]^* \left[\Psi_{j\mathbf{K}_j-\sigma}^\dagger(z') M \Psi_{i\mathbf{K}_i\sigma}(z')\right] \\ &\cdot \frac{4q_x^2 q_y^2}{\left(\sqrt{q_x^2 + q_y^2}\right)^3} \left[\sqrt{q_x^2 + q_y^2}|z - z'| + 1\right] dz dz' d\varphi. \end{aligned} \tag{15}$$

Here $\upsilon_{LA} = 8700 \frac{m}{s}$ is the speed of the longitudinal phonons and the matrix is defined with (14).

The momentum relaxation time is evaluated in the standard way [9]. The electron mobility in inversion layers in [110] direction is calculated as [9]

$$\begin{aligned} \mu_{110} = &\frac{e}{4\pi^2\hbar^2 k_B T n_s} \sum_i \int_0^{2\pi} d\phi \int_{E_i^{(0)}}^{\infty} dE \frac{|\mathbf{K}_i|}{\left|\frac{\partial E(\mathbf{K}_i)}{\partial \mathbf{K}_i}\right|} \\ &\cdot \left(\frac{\partial E(\mathbf{K}_i)}{\partial \mathbf{K}_i}\right)^2_{\varphi=\pi/4, E} \tau_{110}^{(i)} f(E)(1 - f(E)), \end{aligned} \tag{16}$$

where $n_s = \sum_i n_i$, n_i is the population of subband i, and $\tau_{110}^{(i)}$ is the momentum relaxation time in subband i for [110] direction.