Reduction of Surface Roughness Induced Spin Relaxation in MOSFETs by Strain

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INTRODUCTION

Silicon, the main material of microelectronics, is predominantly composed of nuclei with zero spin and is characterised by weak spin-orbit interaction in the conduction band. This insures long distance spin propagation through the bulk, which in combination with a possibility of injecting spin at room temperature [2] makes fabrication of spin-based switching devices in the near future feasible. However, the experimentally observed enhancement in spin relaxation in electrically gated lateral-channel silicon structures [3] is an obstacle and a deeper understanding of fundamental spin relaxation mechanisms in silicon MOSFETs is urgently needed.

METHOD

We investigated numerically the dependences of the matrix elements responsible for surface roughness induced scattering and spin relaxation in silicon transistors as a function of shear strain and energy. To accurately describe the band structure in the presence of the intrinsic spin-orbit interaction the two-band **k·p** Hamiltonian [4] has been generalized to include the spin degree of freedom [5]. The Hamiltonian (1) (shown in Fig.1) is written in the vicinity of the X point along the k_z axis in the Brillouin zone. The basis is conveniently chosen as $[(X_1,\uparrow), (X_1,\downarrow), (X_{2'},\uparrow), (X_{2'},\downarrow)]$, where the up- and down-arrows indicate the spin projection at the quantization z axis. Here m_t and m_l are the transversal and the longitudinal 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, ε_{xy} denotes the shear strain component, $M^{-1} \approx m_t^{-1} - m_0^{-1}$, and D=14eV is the shear strain deformation potential. The term proportional to

$$\Delta_{SO} = 2\sum \frac{< X_1 \mid p_x \mid n >< n \mid \nabla V \times \mathbf{p} \mid_x X_{2'} >}{E_n - E_X} \qquad (2)$$

couples the states with the opposite spin projections from different valleys. The value Δ_{SO}=1.27meVnm computed by the empirical pseudopotential method (Fig.2) is close to the one used in [5]. In the presence of strain and confinement the four-fold degeneracy of the lowest subband is partly lifted. However, the degeneracy of the eigenstates with opposite spin projections, $\Uparrow>$ and $\Downarrow>$ is preserved. The degenerate states must be chosen to satisfy $<\Uparrow|\sigma_z|\Downarrow>=0$. The surface roughness scattering matrix elements are taken to be proportional to the square of the product of the subband function derivatives at the interface [6]. Fig.3 and Fig.4 show their dependences on strain and silicon film thickness for intra-subband and inter-subband scattering for the same spin projection. The inter-subband spin relaxation matrix element mixing and the up- and down-spin states from the two opposite valley is shown to decrease with strain rapidly (Fig.5). Thus, applying uniaxial stress along the [110] direction suppresses spin relaxation and can be used to boost both, mobility and spin lifetime.

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$$H=\begin{bmatrix} \frac{k_z^2}{2m_l}+\frac{k_0k_z}{m_l}+\frac{k_x^2+k_y^2}{2m_t}+U(z) & 0 & D\varepsilon_{xy}-\frac{k_xk_y}{M} & (k_y-k_xi)\Delta_{SO} \\ 0 & \frac{k_z^2}{2m_l}+\frac{k_0k_z}{m_l}+\frac{k_x^2+k_y^2}{2m_t}+U(z) & (-k_y-k_xi)\Delta_{SO} & D\varepsilon_{xy}-\frac{k_xk_y}{M} \\ D\varepsilon_{xy}-\frac{k_xk_y}{M} & (-k_y+k_xi)\Delta_{SO} & \frac{k_z^2}{2m_l}-\frac{k_0k_z}{m_l}+\frac{k_x^2+k_y^2}{2m_t}+U(z) & 0 \\ (k_y+k_xi)\Delta_{SO} & D\varepsilon_{xy}-\frac{k_xk_y}{M} & 0 & \frac{k_z^2}{2m_l}-\frac{k_0k_z}{m_l}+\frac{k_x^2+k_y^2}{2m_t}+U(z) \end{bmatrix} \quad (1)$$

Fig.1. Hamiltonian including strain and spin-orbit interaction. *U(z)* is the square well confinment of width *t* . The Hamiltonian was resolved numerically with respect to the eigenfunctions and eigenenergies by discretizing $k_z=\partial/\partial z$.

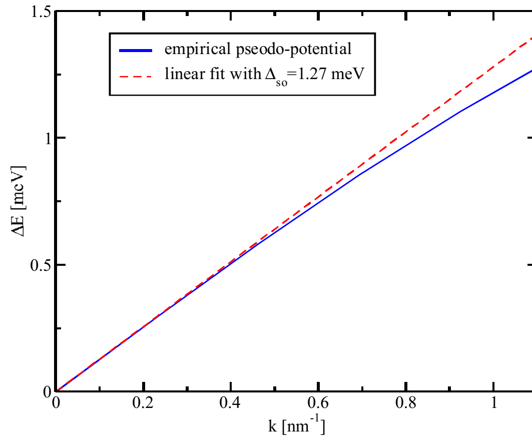

Fig. 2. Empirical pseudopotential calculations of the spin-orbit interaction strength by evaluating the gap opening at the X-point between X_1 and $X_{2'}$ for finite k_x.

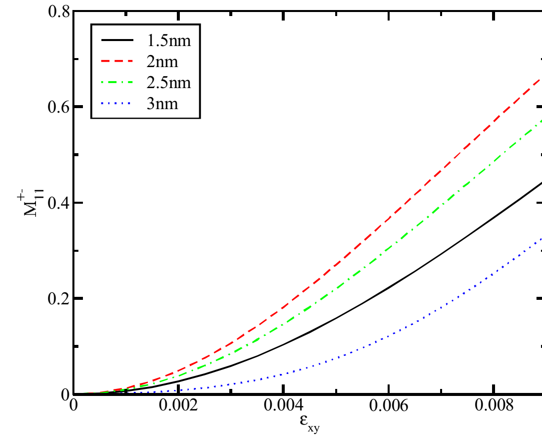

Fig. 4. Normalized intervalley scattering matrix elements as function of strain for different silicon film thicknesses. Being elastic, this scattering is zero in unstrained samples.

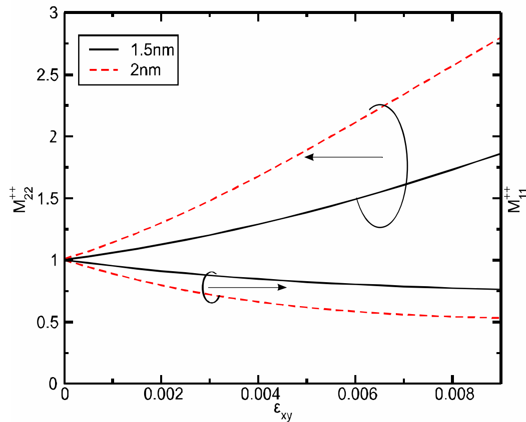

Fig. 3. Normalized intra-subband scattering matrix elements.

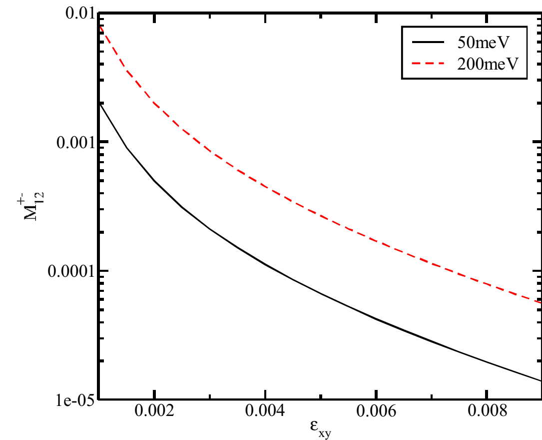

Fig. 5. Intervalley spin relaxation matrix elements reduction with strain for two values of energy.

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