Valley Splitting and Spin Lifetime Enhancement in Ultra-Scaled MOSFETs

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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. However, large spin relaxation in gated silicon structures was experimentally observed. Understanding the details of spin propagation in ultra-scaled MOSFETs is urgently needed.

We investigate the conduction electron spin relaxation due to surface roughness and electron-phonon scattering in (001) silicon films. The [001] equivalent valley coupling through the Γ-point results in a subband splitting in confined electron structures [1]. The values of the valley splitting obtained from a 30-band $\mathbf{k}\cdot\mathbf{p}$ model [2], an atomistic tight-binding model [3], and our $sp^3d^5s^*$ code are shown in Fig.1. Although looking irregular, the results follow a certain law. Fig.2 demonstrates a good agreement of the results of the tight-binding calculations with the analytical expression for the subband splitting [4]

$$\Lambda_\Gamma = \frac{2\pi^2\,\Delta_\Gamma}{(k_0 t)^3}\sin(k_{0\Gamma} t), \qquad (1)$$

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.

Additional subband splitting can be introduced through the strain-induced valley coupling through the X-point. To accurately describe the band structure in strained silicon including the spin degree of freedom we generalize the perturbative two-band $\mathbf{k}\cdot\mathbf{p}$ approach [5,6] developed at the X-point by accounting for the intrinsic spin-orbit interaction. The partly diagonalized Hamiltonian in the vicinity of the X-point along the k_z axis [1-3] is conveniently written as

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

where $H_{1,2} = \left[\frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2(k_x^2+k_y^2)}{2m_t} + (-1)^j\delta + U(z)\right] I$, and $H_3 = \left[\frac{\hbar^2 k_0 k_z}{m_l}\right] I$. Here I is the identity 2x2 matrix, $\delta = \sqrt{\left(D\varepsilon_{xy} - \frac{\hbar^2 k_x k_y}{M}\right)^2 + \Delta_{SO}^2\left(k_x^2+k_y^2\right) + \Lambda_\Gamma^2}$, m_t and m_l are the transversal and the longitudinal silicon effective masses, $M^{-1} \approx m_t^{-1} - m_0^{-1}$, $k_0 = 0.15\times 2\pi/a$ is the position of the valley minimum relative to the X-point in unstrained silicon, ε_{xy} denotes the shear strain component, the value Δ_{SO} = 1.27meVnm, D = 14eV is the shear strain deformation potential, and $U(z)$ is the confinement potential. The splitting through the Γ-point is accounted for through Λ_Γ.

Fig.3 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 values.

The surface roughness scattering matrix elements are taken to be proportional to the square of the product of the subband wave function derivatives at the interface [7]. The electron-phonon scattering is taken in the deformation potential approximation [8].

The surface roughness intersubband spin relaxation matrix elements with and without the Λ_Γ term are shown in Fig.4. The difference in the matrix elements' values calculated with and without the Λ_Γ term (inset Fig.4) can reach two orders of magnitude. Hence, the valley coupling through the Γ-point must be taken into account for the accurate spin lifetime calculations.

The peaks on the matrix elements' dependences (Fig.4) are correlated with the unprimed subband splitting minima (Fig.5). For higher strain values the peaks corresponding to strong spin relaxation hot spots are pushed towards unoccupied states at higher energies (Fig.5). This leads to the strong increase of the spin lifetime demonstrated in Fig. 6. The increase is less pronounced, if the Λ_Γ 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.

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References

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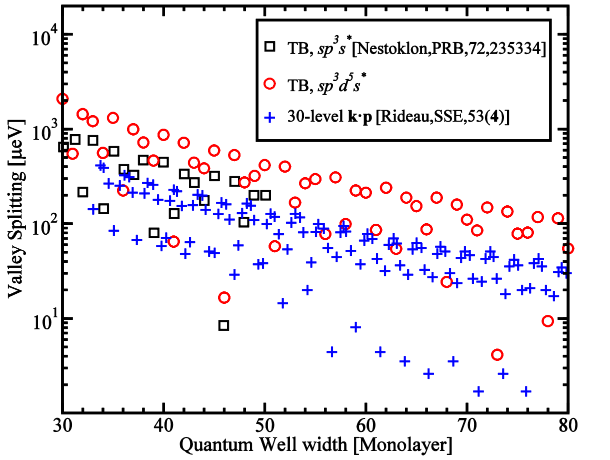

Fig. 1. Valley splitting in a Si quantum well at zero strain as a function of the quantum well width including results from literature [4,5].

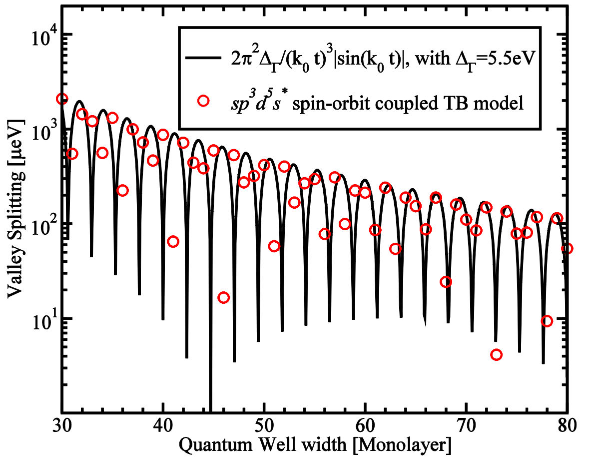

Fig. 2. Dependence of the valley splitting on the quantum well width from the tight binding (TB) model and the analytical expression with Δ_Γ=5.5eV.

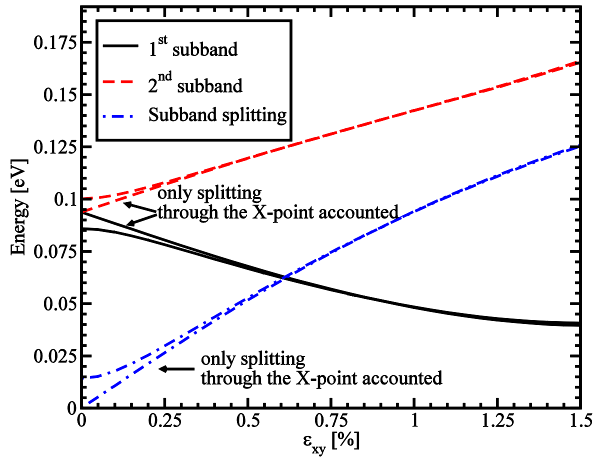

Fig. 3. Dependence of energy of the 1st and the 2nd subbands together with the subband splitting on shear strain for film thickness 2.1nm.

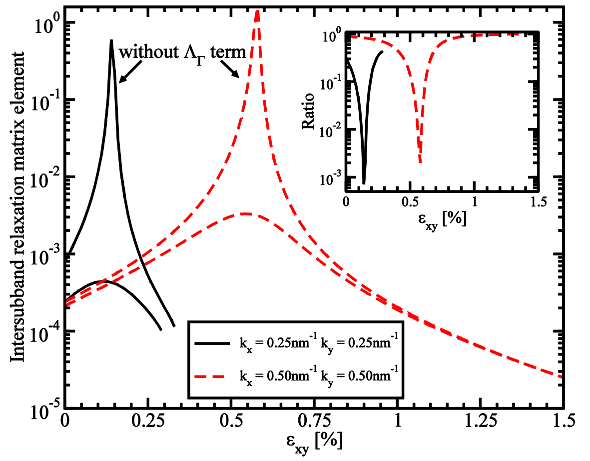

Fig. 4. Dependence of the normalized intersubband relaxation matrix elements on shear strain for the film thickness 2.1nm. The inset shows ratio of the matrix elements with the Λ_Γ term to the matrix elements without the Λ_Γ term.

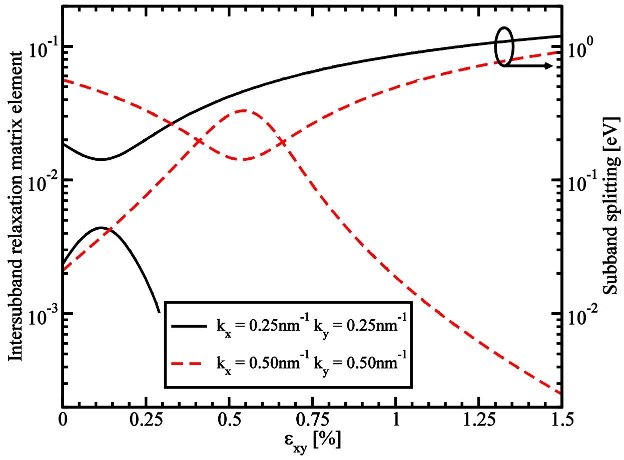

Fig. 5. Intersubband relaxation matrix elements normalized to the intrasubband scattering matrix elements at zero strain as a function of shear strain for the film thickness 2.1nm.

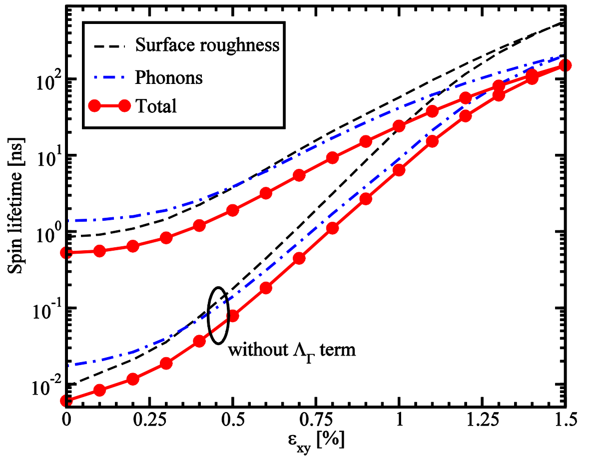

Fig. 6. Dependence of spin lifetime on shear strain for T=300K and film thickness 2.1nm.