Electron Subband Structure and Controlled Valley Splitting in Silicon Thin Body SOI FETs: Two-Band k·p Theory and Beyond

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1. Introduction

For analytical subband structure calculations in silicon (Si) it is commonly assumed that the energy dispersion of the conduction band valleys is well described by a parabolic approximation with the transversal mass m_t and the longitudinal mass m_l. However, in presence of shear strain a more general description based on the two-band **k·p** Hamiltonian is necessary [1-3]. Within the two-band **k·p** model the subband structure for an infinite square well potential can be found analytically. Due to the valley degeneracy, the unprimed subbands remain two-times degenerate within the **k·p** approach. Recently, a valley splitting larger than the spin splitting was reported [4]. Lifting degeneracy reduces scattering and improves the coherence time in spin qubits, which makes silicon-based quantum devises promising for future applications in quantum computing. In this work we propose an alternative mechanism to create and control the valley splitting by applying shear strain.

2. Method and Results

Within the two-band **k·p** model the dispersion relation of a [001] valley is of the form [1-3]

$$E = k_z^2 + \left(k_x^2 + k_y^2\right) m_l / m_t - 2\sqrt{k_z^2 + \delta^2}\,, \qquad (1)$$

where all the wave vectors are normalized by $k_0 = 0.15 \times 2\pi / a$, the position of the minimum relative to the X point. Energies are in units of $\hbar^2 k_0^2 / (2m_l)$, $\delta^2 = (\eta - m_l k_x k_y / M)^2$, $\eta = m_l D\varepsilon_{xy} / k_0^2$ is dimension-less shear strain, $M^{-1} \approx m_t^{-1} - m_0^{-1}$, ε_{xy} denotes the shear strain component, and D=14 eV is the shear strain deformation potential [1,4]. Excellent agreement between the two-band **k·p** model (1) and the results of empirical pseudo-potential (EPM) band structure calculations with the parameters from [2,5] is demonstrated in Fig.1. Tensile stress in [110] and compressive stress in [-110] direction is assumed. For this setup only shear strain component ε_{xy} is nonzero. The shear strain ε_{xy} substantially modifies the energy dispersion in the [001] valleys. The k_z dispersion is shown in Fig.2 for several values of shear strain. The valley minimum moves both in energy and position, approaching the X-point of the Brillouin zone for larger strain $\eta \to 1$.

The subband energies can be found analytically for an infinite square well potential, which is a good model for an ultra-thin Si film. The dispersion of the unprimed subbands in a [001] thin Si film of thickness t is

$$E_n = p_n^2 + \left(k_x^2 + k_y^2\right) m_l / m_t - 1 - \delta^2 / (1 - p_n^2)\,, \qquad (2)$$

where $p_n = (\pi n)/(tk_0)$. For zero strain $\eta = 0$. The denominator of the last term in (2) describes the dependence of the non-parabolicity parameter on the film thickness [5] for the unprimed subbands as shown in Fig.3. This increase of the non-parabolicity parameter with t leads to a decrease of low-field mobility as compared to the mobility computed with the bulk value α =0.5 eV^{-1}. The relative correction is about 7% for t= 3 nm and 15% for t=2.5 nm (Fig.4).

The **k·p** theory predicts the same dispersion (2) for both [001] valleys and cannot describe the valley splitting. To go beyond the **k·p** theory, we introduce an auxiliary tight-binding model defined on a lattice of sites each containing two localized orbitals $\alpha(\mathbf{r})$ and $\beta(\mathbf{r})$ in such a way that it mimics the two-band bulk k_z dispersion [6]. In a finite array of $2N$ sites the two Bloch functions are:

$$\begin{aligned}\psi_\pm(\mathbf{r}, E) = \sum_{i=1,2}\sum_{n=-N}^{N} C_i \exp(ik_i na/2)(a(k_i)\alpha(\mathbf{r} - na/2) \\ + ib(k_i)\beta(\mathbf{r} - na/2)) \pm C.C.,\end{aligned} \qquad (3)$$

where k_i are defined by $E_n(k_i)$=E, a is the Si lattice constant, $a(k_i)$, $b(k_i)$ are the coefficients in the linear combination of two basis functions and are determined from the two-band **k·p** model, and $C.C.$ is complex conjugate. Proceeding as in [6], the following equation for p_n is readily obtained:

$$\sin(p_n^\pm k_0 t) = \pm \frac{\delta p_n^\pm \sin\left(\dfrac{1 - \delta^2 - p_n^{\pm 2}}{1 - p_n^{\pm 2}} k_0 t\right)}{\sqrt{(1 - p_n^{\pm 2})(1 - \delta^2 - p_n^{\pm 2})}}. \qquad (4)$$

It follows from (4) that for $\delta = 0$, when the dispersion is purely parabolic, the valley splitting is exactly zero. Since δ depends strongly on shear strain, applying uniaxial [110] stress to [001] ultra-thin Si film generates valley splitting proportional to strain. Uniaxial stress is currently used to enhance performance of modern MOSFETs, where it is introduced in a controllable way. For small δ (4) gives

$$\Delta E_v = 2\frac{k_0^2}{m_l}\left(\frac{\pi n}{k_0 t}\right)^2 \frac{\delta}{k_0 t}\sin(k_o t) \qquad (5)$$

for the valley splitting, so that the splitting is engineered by adjusting strain and t.

3. Conclusion

In conclusion, an alternative way to induce controllable valley splitting in ultra-thin Si films by applying uniaxial stress is proposed. For small stress values the splitting is shown to depend linearly on shear strain. Valley splitting rapidly increases with decreasing Si thickness and can be larger than the spin splitting.

The work is supported by the Austrian Science Fund FWF, Project P19997-N14, and by the EUROSOI+ Thematic Network on SOI Technology, Devices and Circuits.

References

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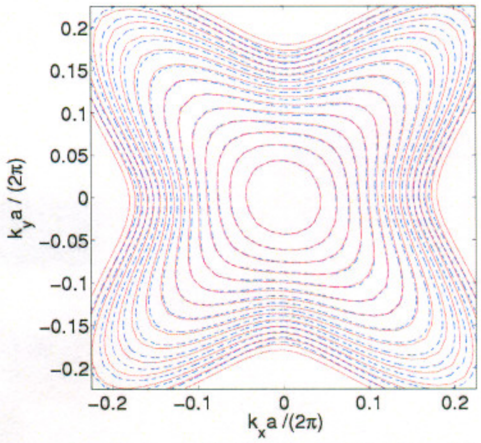

Fig.1: *Comparison between Eq.(1) (dashed lines) and the results of EPM calculations (solid lines). The contour lines are spaced at 50 meV. Tensile stress along [110] and compressive stress along [-110] of 150 MPa in each direction is applied.*

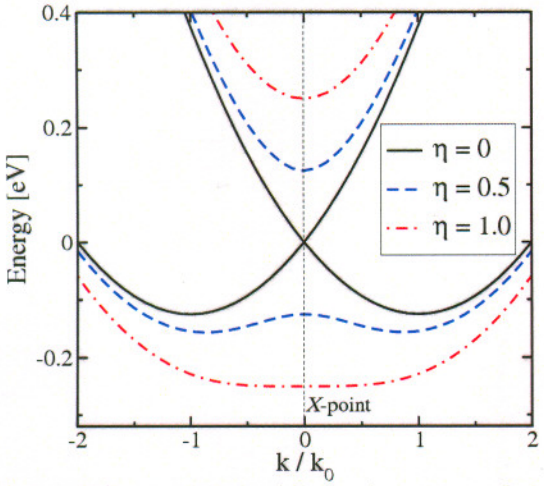

Fig.2: *Conduction band (1) for different shear strain values.*

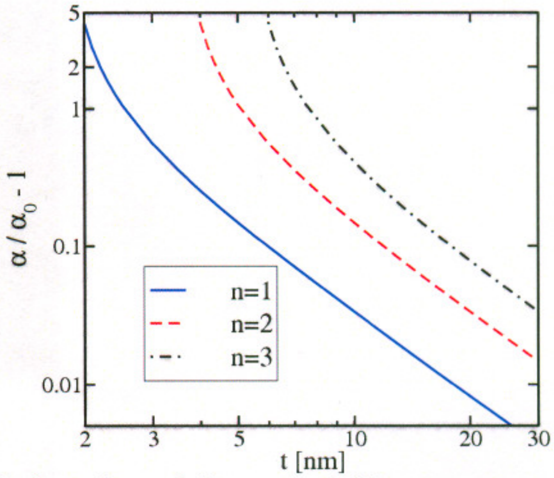

Fig.3: *Dependence of the non-parabolicity parameter on film thickness t.*

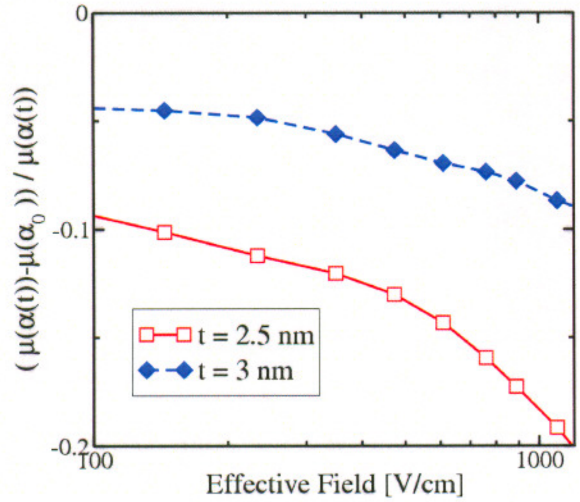

Fig.4: *Relative mobility correction due to thickness dependence of the non-parabolicity parameter as a function of effective field, for two Si film thicknesses. The correction is negative and reaches 20% for t=2.4 nm.*

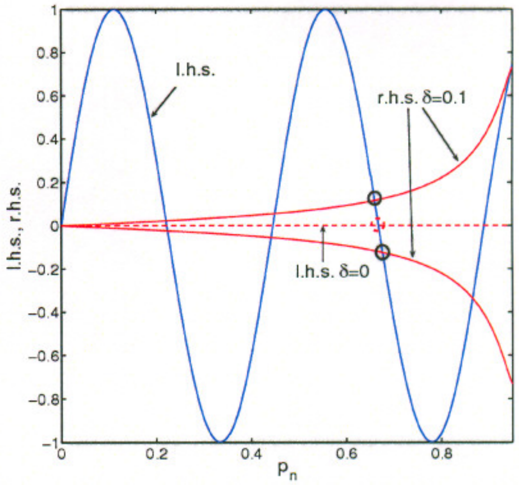

Fig.5: *The left-hand side (l.h.s) and the right-hand side (r.h.s) of (4) as function of p_n, without shear strain (dotted line) and for a nonzero shear strain. Intersections of l.h.s and r.h.s. reflect graphical solutions of (4). Splitting between roots $p_n^{\pm}$ results in valley splitting controlled by shear strain.*