Valley Splitting in Thin Silicon Films from a Two-Band k·p Model

V. Sverdlov, T. Windbacher, O. Baumgartner, F. Schanovsky, and S. Selberherr

Institute for Microelectronics, TU Wien, Gußhausstraße 27-29, A-1040 Wien, Austria
{sverdlov|windbacher|baumgartner|schanovsky|selberherr}@iue.tuwien.ac.at

1. Introduction

The rapid increase in computational power and speed of integrated circuits is supported by the continuing size reduction of semiconductor devices' feature size. Thanks to constantly introduced innovative changes in the technological processes the miniaturization of MOSFETs institutionalized by Moore's law successfully continues. The 45nm MOSFET process technology by Intel [1] and recently introduced 32nm technology [2] involve new high-k dielectric/metal gates and represents a major change in the technological process since the invention of MOSFETs. Although alternative channel materials with a mobility higher than in Si were already investigated [3], [4], it is believed that Si will still be the main channel material for MOSFETs beyond the 32nm technology node.

With scaling apparently approaching its fundamental limits, the semiconductor industry is facing critical challenges. New engineering solutions and innovative techniques are required to improve CMOS device performance. Strain-induced mobility enhancement is one of the most attractive solutions to increase the device speed. It will certainly maintain its key position among possible technological innovations for the future technology generations. In addition, new device architectures based on multi-gate structures with better electrostatic channel control and reduced short channel effects will be developed. A multi-gate MOSFET architecture is expected to be introduced for the 22nm technology node. Combined with a high-k dielectric/metal gate technology and strain engineering, a multi-gate MOSFET appears to be the ultimate device for high-speed operation with excellent channel control, reduced leakage currents, and low power budget. Confining carriers within a thin film reduces the channel dimension in transversal direction, which further improves gate channel control.

At the same time the search for post-CMOS device concepts has accelerated. Spin as a degree of freedom is promising for future nanoelectronic devices and applications. A concept of a racetrack memory recently proposed in [5] is based on the controlled domain wall movement by spin-polarized current in magnetic nanowires. Silicon, the main element of microelectronics, possesses several properties attractive for spintronic applications. Silicon is composed of nuclei with predominantly zero spin and is characterized by small spin-orbit coupling. In a recent ground-breaking experiment coherent spin transport through an undoped silicon wafer of 350 μm length was demonstrated [6]. The experiment was possible due to a unique injection and detection technique of polarized spins delivered through thin ferromagnetic films. Spin coherent propagation at such long distances makes the fabrication of spin-based switching devices likely already in the near future.

Spin-controlled qubits may be thought of as a basis for upcoming logic gates. However, the conduction band of silicon contains six equivalent valleys, which is a source of potentially increased decoherence. For successful applications the degeneracy between the valleys must be removed and become larger than the spin Zeeman splitting. Shubnikov-de-Haas measurements in an electron system composed of thin silicon films in Si-SiGe heterostructures reveal that the valley splitting is small [7]. At the same time, recent experiments on the conductivity measurements of point contacts created by confining a quasi-two-dimensional electron system in lateral direction with the help of additional gates deposited on the top of the silicon film demonstrate a splitting between equivalent valleys larger than the spin splitting [7].

In this work we demonstrate that a large valley splitting in the confined electron system can be induced by a shear strain component. Our analysis is based on the two-band **k·p** model for the conduction band in silicon. The parabolic band approximation usually employed for subband structure calculations of confined electrons in Si inversion layers is insufficient in ultra-thin Si films. The two-band **k·p** model includes strain and is shown to be accurate up to energies of 0.5eV. This model can therefore be used to describe the subband structure in thin silicon films, where the subband quantization energy may reach a hundred meV.

We first describe the subband structure in a thin unstrained silicon film. We demonstrate that the peculiarities of the subband dispersion obtained within the two-band **k·p** model result in a linear dependence of the valley splitting on the magnetic field. We show that a large valley splitting is observed in experiments on conduction quantization through a quantum point contact in [110] direction, but the

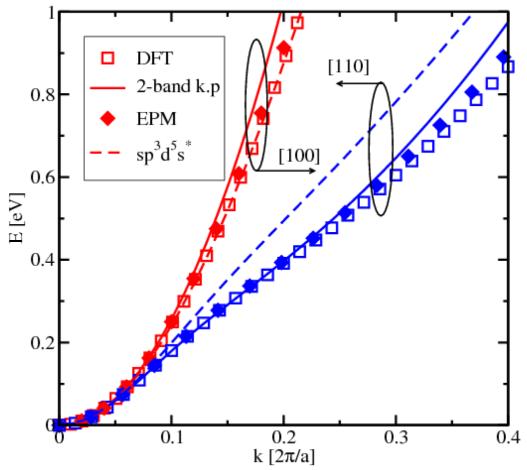

Fig.1: *Comparison of the conduction band of silicon computed with the density functional theory (DFT) [10], the empirical pseudo-potential method (EPM) [9], the sp^{3}d^{5}s* tight-binding method [11], and the two-band* ***k·p*** *model [8]. The two-band* ***k·p*** *model is accurate up to an energy of 0.5eV.*

splitting is suppressed in [100] point contacts. Finally, we demonstrate that the valley splitting is greatly enhanced in films strained in [110] direction.

2. Two-band k·p model

The closest band to the lowest conduction band Δ_1 near its minimum is the second conduction band Δ_2. These two bands are degenerate exactly at the X point. Since the minimum of the lowest conduction band in unstrained silicon is only $k_0 = 0.15(2\pi)/a$ away from the X point, where a is the lattice constant of unstrained silicon, the two bands must be included on equal footing in order to describe the dispersion around the minimum. More distant bands separated by larger gaps are included in the second order **k·p** perturbation theory [8], which results in the following two-band **k·p** Hamiltonian:

$$H = \left(\frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_t}\right) I + \left(D\varepsilon_{xy} - \frac{\hbar^2 k_x k_y}{M}\right)\sigma_x + \frac{\hbar^2 k_z k_0}{m_l}\sigma_z, \qquad (1)$$

where $\sigma_{x,z}$ are the Pauli matrixes, I is the 2×2 unity matrix, m_t and m_l are the transversal and the longitudinal effective masses, respectively, 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 [8]. This is the only form of the Hamiltonian in the vicinity of the X point allowed by symmetry considerations [8]. The two-band Hamiltonian (1) results in the following dispersion relations:

$$E = \frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_t} \pm \sqrt{\left(\frac{\hbar^2 k_z k_0}{m_l}\right)^2 + \delta^2}, \qquad (2)$$

where the negative sign corresponds to the lowest conduction band,

$$\delta^2 = (D\varepsilon_{xy} - \hbar^2 k_x k_y / M)^2 . \qquad (3)$$

The energy E and k_z are counted from the X-point. A comparison of (2) with the band structure of [001] valleys obtained numerically with the density functional theory (DFT) [10], empirical pseudo-potential method (EPM) [9], and with the tight-binding sp^{3}d^{5}s* model [11] in [100] and [110] direction is shown in Fig.1. The **k·p** model accurately describes the dispersion relation up to energies of about 0.5eV. Therefore, the **k·p** Hamiltonian (1) can be used to describe the subband structure in thin silicon films and inversion layers.

3. Subband dispersion in [001] thin silicon films

For [001] silicon films the confinement potential gives an additional contribution $U(z)I$ to the Hamiltonian (1). In the effective mass approximation described by (1) with the coefficient in front of σ_x set to zero, the confining potential $U(z)$ is known to quantize the six equivalent valleys of the conduction band of bulk silicon into the four-fold degenerate primed and the two-fold degenerate unprimed subband ladder. In ultra-thin films the unprimed ladder is predominantly occupied and must be considered. The term with σ_x in (1) couples the two lowest conduction bands and lifts the two-fold degeneracy of the unprimed subband ladder. The additional unprimed subband splitting, or the valley splitting, can be extracted from the Shubnikov-de-Haas oscillations and is typically in the order of a few tens μeV [7]. However, the valley splitting is greatly enhanced in a laterally confined two-dimensional electron gas [7]. The valley splitting is usually addressed by introducing a phenomenological intervalley coupling constant at the silicon interface [12]. Here we investigate the valley splitting based on the two-band **k·p** model (1) without introducing any additional parameters.

We approximate the confining potential of an ultra-thin silicon film by a square well potential with infinite potential walls. This is sufficient for the purpose to analyze the valley splitting in a quasi-two-dimensional gas due to interband coupling. Generalization to include a self-consistent potential is straightforward though numerically involved [13]. Because of the two-band Hamiltonian, the wave function Ψ is a spinor with the two components |0> and |1>. For a wave function with space dependence in a form $\exp(ik_z z)$ the coefficients A_0 and A_1 of the spinor components are related via the equation $H\Psi = E(k_z)\Psi$. For a particular energy E there exist four solutions k_i (i=1,…,4) for k_z of the dispersion relation (2), so the spatial dependence of a spinor component α is in the form $\sum_{i=1}^{4} A_\alpha^i \exp(ik_i z)$. The four coefficients are determined by the boundary conditions that both spinor components are zero at the two film interfaces. This leads to the following equations:

$$\tan\left(k_1 \frac{k_0 t}{2}\right) = \frac{k_2}{\sqrt{k_2^2+\eta^2} \pm \eta} \frac{\sqrt{k_1^2+\eta^2} \pm \eta}{k_1} \tan\left(k_2 \frac{k_0 t}{2}\right), \qquad (3)$$

where $\eta = m_l \,|\,\delta\,|/(\hbar k_0)^2$. The value of

$$k_2 = \sqrt{k_1^2 + 4 - 4\sqrt{k_1^2+\eta^2}} \qquad (4)$$

becomes imaginary at high η values. Then the trigonometric functions in (3) are replaced by the hyperbolic ones. Special care must be taken to choose a\the correct branch of $\sqrt{k_2^2+\eta^2}$ in (4): the sign of $\sqrt{k_2^2+\eta^2}$ must be alternated after the argument becomes zero. Introducing $y_n = (k_1 - k_2)/2$, (3) can be written in the form:

$$\sin(y_n k_0 t) = \pm \frac{\eta y_n \sin\left(\frac{1-\eta^2-y_n^2}{1-y_n^2} k_0 t\right)}{\sqrt{(1-y_n^2)(1-\eta^2-y_n^2)}} \qquad (5)$$

For small values of the parameter η we obtain from (5) the following dispersion relation for the unprimed subbands n:

$$E_n^{\pm} = \frac{\hbar^2}{2m_l}\left(\frac{\pi n}{t}\right)^2 + \hbar^2 \frac{k_x^2+k_y^2}{2m_t} \pm \left(\frac{\pi n}{k_0 t}\right)^2 \frac{\left|D\varepsilon_{xy} - \frac{\hbar^2 k_x k_y}{M}\right|}{k_0 t\,\left|1-(\pi n/k_0 t)^2\right|} \sin(k_o t) \qquad (6)$$

(6) demonstrates that the unprimed subbands are not necessarily degenerate and degeneracy is preserved only, when shear strain is zero and either k_x=0 or k_y=0.

4. Valley splitting in a magnetic field

For zero shear strain the Landau levels in an othogonal magnetic field B are determined from (6) using the Bohr-Sommerfeld quantization conditions:

$$E_m^{(1,2)} = \hbar\omega_c\left(m+\frac{1}{2}\right)\frac{\pi}{4\arctan\left(\sqrt{m_{(1,2)}/m_{(2,1)}}\right)}, \qquad (7)$$

where

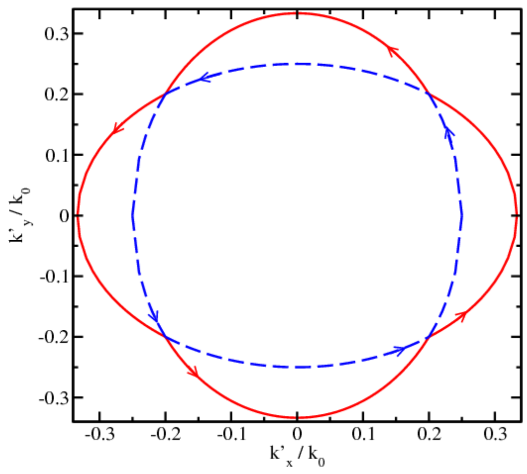

Fig.2: *Quasi-classical orbits of electron motion in a magnetic field corresponding to the subband dispersion (6). Kinematic moment components k'_x, k'_y are in <110> and <1-10> directions. The difference between the quasi-classical orbits causes the valley splitting (7) in a magnetic field perpendicular to the electron system.*

$$m_{(1,2)} = \left(\frac{1}{m_t} \pm \frac{1}{M}\left(\frac{\pi n}{k_0 t}\right)^2 \frac{\sin(k_o t)}{k_0 t\,\left|1-(\pi n/k_0 t)^2\right|}\right)^{-1}, \qquad (8)$$

and

$$\omega_c = \frac{eB}{\sqrt{m_1 m_2} c}$$

is the cyclotron frequency, e is the electron charge, and c is the speed of light. According to (7), the valley splitting $|E_m^1 - E_m^2|$ is linear regarding the magnetic field. In order to obtain the linear dependence, two conditions must be satisfied:

(i) no shear strain and
(ii) the cyclotron energy is smaller than the subband quantization energy.

Both conditions are satisfied in a biaxially stressed silicon film of 10nm thickness on SiGe used in [7] for magnetic fields as strong as 1T. It follows from (7) and (8) that the valley splitting can be several tens μeVs, which is consistent with the experiment [7].

5. Valley splitting in a point contact

We consider a point contact in [110] direction realized by confining an electron system of a thin silicon film laterally by depleting the area under additional gates. Without strain the low-energy effective Hamiltonian in the point contact can be written as:

$$H_{(1,2)} = \frac{\hbar^2 k_x'^2}{2m_{(2,1)}} + \frac{\hbar^2 k_y'^2}{2m_{(1,2)}} + \frac{1}{2}\kappa x'^2 + V_b, \qquad (9)$$

where the primed variables are along the [110] and [1-10] axes, the effective masses are determined by (8), κ is the spring constant of the point contact confinement potential $V(x')=\kappa x'^2/2$ in [1-10] direction, and V_b is a gate voltage dependent conduction band shift in the point contact [14]. The dispersion relation of propagating modes within the point contact is written as:

$$E_p^{(1,2)}=\frac{k^2 k_x'^2}{2m_{(2,1)}}+\hbar\omega_{(1,2)}\left(p+\frac{1}{2}\right)+V_b, \qquad (10)$$

where $\omega_{(1,2)}^2=\kappa/m_{(1,2)}$. Since the energy minima of the two propagating modes with the same p are

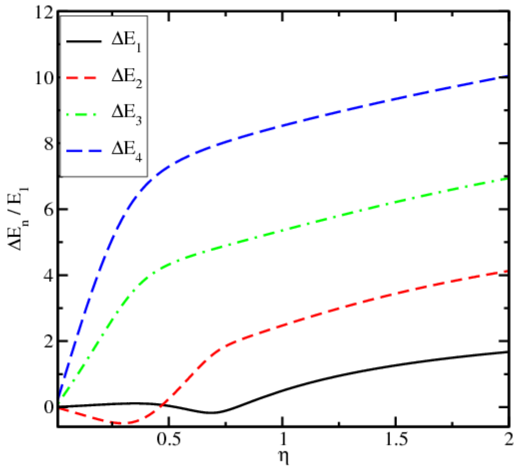

Fig.3: *Splitting between the unprimed subband energies, or the valley splitting, in a 6.5nm thick silicon film as a function of shear strain. The splitting values are normalized to the energy of the ground subband without strain. The value* $\eta=1$ *corresponds to the shear strain value* $\varepsilon_{xy}=0.016$. *The value of valley splitting may alternate its sign, in accordance to (6).*

separated, they are resolved in the conductance experiment through the point contact as two distinct steps. The valley splitting is $\Delta E_p=\hbar\,|\,\omega_1-\omega_2\,|$. The difference in the effective masses (8) and, correspondingly, the valley splitting can be greatly enhanced by reducing the effective thickness t of the quasi-two-dimensional electron gas which is usually the case in a gated electron system, when the inversion layer is formed.

In a [100] oriented point contact without strain the effective Hamiltonian is

$$H^{\pm}=\hbar^2\frac{k_x^2+k_y^2}{2m_t}\pm\left(\frac{\pi n}{k_0 t}\right)^2\frac{\left|\dfrac{\hbar^2 k_x k_y}{M}\right|\sin(k_o t)}{k_0 t\,|1-(\pi n/k_0 t)^2\,|}+\frac{\kappa}{2}x^2.$$

Due to symmetry with respect to k_y the subband minima in a point contact are always degenerate. For this reason the valley splitting in [100] oriented point contacts is greatly reduced.

6. Valley splitting by shear strain

It follows from (6) that shear strain induces a valley splitting linear in strain for small shear strain values and depends strongly on the film thickness [15]:

$$\Delta E_n=2\left(\frac{\pi n}{k_0 t}\right)^2\frac{D\varepsilon_{xy}}{k_0 t\,|1-(\pi n/k_0 t)^2\,|}\sin(k_0 t).$$

For higher strain values (3) must be solved numerically. Results shown in Fig.3 demonstrate that valley splitting can be effectively controlled by adjusting the shear strain and modifying the effective thickness t of the electron system. Uniaxial stress along [110] channel direction, which induces shear strain, is already used by industry to enhance the performance of MOSFETs. Therefore, its application to control valley splitting does not require expensive technological modifications.

7. Conclusion

The unprimed valley structure in (001) silicon thin films has been analyzed within the two-band **k·p** model. It is shown that the two-fold degeneracy of the unprimed subbands can be lifted leading to the so-called valley splitting which is proportional to the strength of the perpendicular magnetic field. The valley splitting can be enhanced in <110> oriented point contacts, while it is suppressed in a <100> point contact. Finally, the valley splitting can be controlled and made larger than the Zeeman splitting by shear strain.This makes silicon very attractive for spintronic applications.

8. Acknowledgment

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