Electron Subband Structure and Valley Splitting in Silicon Ultra-Thin Body SOI Structures from the Two-Band k·p Model

Viktor Sverdlov, Thomas Windbacher, Oskar Baumgartner, and Siegfried Selberherr

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

1. Introduction

Multi-gate FinFETs and ultra-thin silicon body SOI FETs are considered as perfect candidates for the 22 nm technology node and beyond. Strong quantization leads to a formation of quasi-two dimensional subbands in carrier systems within thin silicon films. For analytical hole subband structure calculations we employ a six-band **k·p** Hamiltonian. The electron subband structure consists of six equivalent minima located close to the *X*-points in the Brillouin zone. Close to the minimum the dispersion is usually described by a parabolic approximation with the transversal masses m_t and the longitudinal mass m_l. Isotropic non-parabolicity takes into account deviations in the density of states at higher energies. A more general description is however needed in ultra-thin silicon films [1], especially in the presence of shear strain. The two-band **k·p** Hamiltonian accurately describes the bulk structure up to energies of 0.5 - 0.8 eV [2]. It includes the shear strain component neglected in the parabolic approximation [2-4]. Shear strain is responsible for an effective mass modification and is therefore an important source of the electron mobility enhancement in ultra-thin silicon films [5,6].

2. Method and Results

The two-band **k·p** Hamiltonian of a [001] valley in the vicinity of the *X* point of the Brillouin zone in Si must be in the form [6]:

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

where $\sigma_{y,z}$ are the Pauli matrices, I is the 2×2 unity matrix, $k_0=0.15\times 2\pi/a$ is the position of the valley minimum relative to the X point in unstrained Si, ε_{xy} denotes the shear strain component, $M^{-1}\approx m_t^{-1}-m_0^{-1}$, and D=14 eV is the shear strain deformation potential [2-6]. The confining potential $U(z)$ along the <001> direction modulates profiles of the conduction bands. A good approximation for the confining potential in an ultra-thin silicon film is a square well potential with infinite walls (Fig.1). It allows to use the zero boundary conditions for the wave functions at the interfaces, which simplifies the analysis of the subband structure.

For each energy E there are four solutions for the wave vectors k_i (i=1,..,4) (Fig.2). For energies within the gap the two wave vectors are imaginary. The wave function is then a superposition of the solutions with the four eigenvectors. In the two-bands model the wave function is a spinor with two components. The subband quantization energies are obtained by equating *both* components of the spinor at both interfaces to zero. It results in a system of four linear homogeneous equations for the coefficients in the linear combination. Non-zero solutions exist when the following equations are satisfied:

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

Interestingly, the equations (2) coincide with the ones obtained from an auxiliary tight-binding consideration [7]. The ratio in the right hand side depends on the energy E, wave vector k_1, and strain $\eta=m_l D\varepsilon_{xy}/(\hbar k_0)^2$. For zero stress the ratio is equal to one, and the standard quantization condition $(k_1-k_2)t/2=\pi n$ is recovered. This condition is obtained from either of the two equations, therefore, the subbands are two-fold degenerate. Shear strain opens the gap between the two conduction bands at the *X*-point making dispersions non-parabolic. Shear strain makes the equations (2) non-equivalent removing the subband degeneracy and introducing a valley splitting. The valley split is linear in strain for small shear strain values and depends strongly on the film thickness [7]:

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

For higher strain values (2) must be solved numerically.

The value $k_2=\sqrt{k_1^2+4-4\sqrt{k_1^2+\eta^2}}$ becomes imaginary at high strain values. In this case the trigonometric functions in (2) are replaced by the hyperbolic ones. Special care must be taken to choose a correct branch of $\sqrt{k_2^2+\eta^2}$ in (2). The sign of $\sqrt{k_2^2+\eta^2}$ must be alternated, when the argument becomes zero as displayed in Fig.3. Results of the numerical solutions of (2) for valley splitting are shown in Fig.4 and Fig.5 for two different film thicknesses. For high strain values the dispersion of the lowest conduction bands becomes parabolic again. The quantization levels in a square well potential are therefore recovered in this limit.

Acknowledgement. This work was supported in part by the Austrian Science Fund FWF, project P19997-N14, and by the EUROSOI+ Thematic Network on SOI Technology, Devices and Circuits.

References

[1] K. Uchida *et al.*, IEDM 2006, p.1019.
[2] V. Sverdlov *et al.*, ESSDERC 2007, p.386.
[3] J.C. Hensel *et al.*, *Phys.Rev.*, **138**, p.A225, 1965.
[4] G.L. Bir and G.E. Pikus, Symmetry and Strain Induced Effects in Semiconductors. J.Willey & Sons, NY, 1974.
[5] E. Ungersboeck *et al.*, *IEEE T ED*, **54**, 2183, 2007.
[6] K.Uchida *et al.*, IEDM 2005 p.135.
[7] V. Sverdlov *et al.*, *Solid State Electron.*, accepted, 2008.

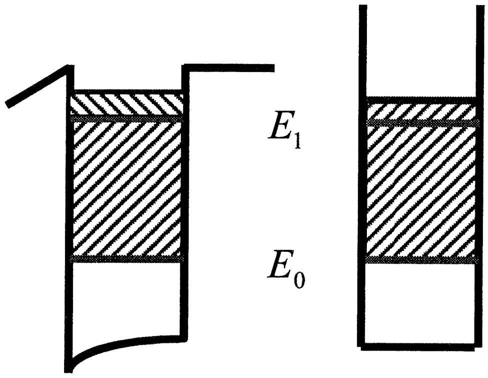

Fig.1: *Potential in an ultra thin SOI film of a single gate MOSFET (left) and a corresponding model square well potential with infinite walls.*

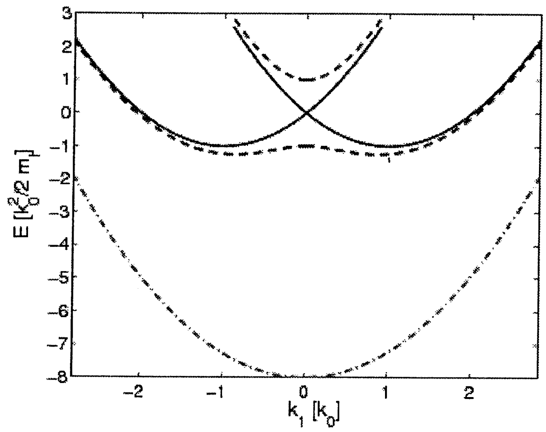

Fig.2: *Conduction band profile close to the X point for* $\eta = 0$ *(solid lines),* $\eta = 0.5$ *(dashed lines), and* $\eta = 4$ *(dashed dotted line).*

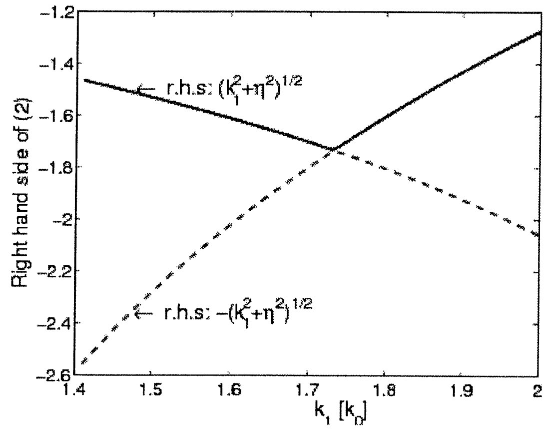

Fig.3: *The right hand side of equation (2) plotted close to the point* $\sqrt{k_2^2 + \eta^2} = 0$. *It is clearly seen that the sign of the square root must be alternated at this point.*

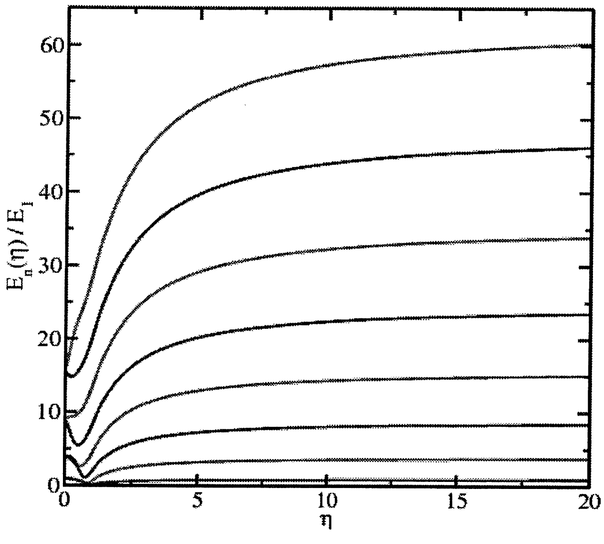

Fig.4: *Subband quantization energies* E_n *from (2) (normalized to the ground subband energy) for a film thickness of 6.5 nm. The valley splitting appears for non zero shear strain* η.

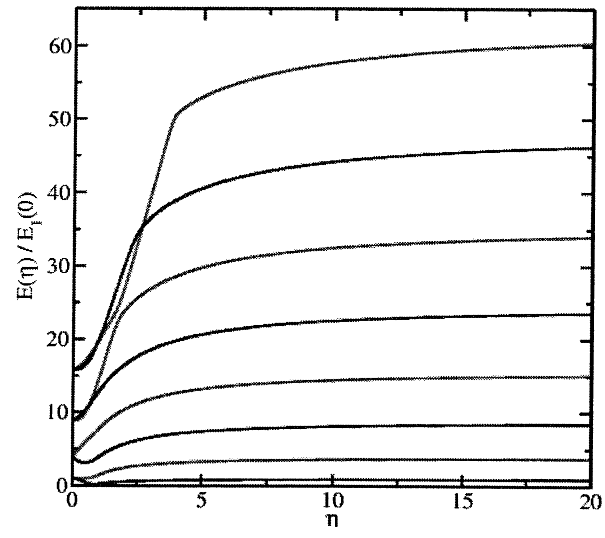

Fig.5: *The same as in Fig.4, for a film thickness of 3.3 nm. The valley splitting depends strongly on the film thickness. The valley splitting is maximal at high strain values.*