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Subband structure in ultra-thin silicon films

V. A. Sverdlov[1,2], O. Baumgartner[1], S. Tyaginov[3,4], Th. Windbacher[1] and S. Selberherr[1]

[1] Institute for Microelectronics, TU Wien, Gußhausstraße 27-29, A-1040 Wien, Austria
[2] V. A. Fock Institute of Physics, Universitu of St Petersburg, Ulyanovskaya 1, 198904 Petrodvorets, St Petersburg, Russia
[3] Christian Doppler Laboratory for TCAD at the Institute for Microelectronics,TU Wien, Gußhausstraße 27-29, A-1040 Wien, Austria
[4] Ioffe Physical-Technical Institute, St Petersburg, Russia

Introduction

Silicon is composed of nuclei with predominantly zero spin and is characterized by a negligible spin-orbit interaction. Silicon is therefore attractive for spintronic applications. Coherent spin transport through a silicon wafer of 350 μm length was demonstrated in a recent ground-breaking experiment [1]. However, since the conduction band consists of six equivalent valleys, the valley degeneracy is a potential source of increased decoherence and must be removed. Biaxial stress lifts the degeneracy by moving two of the valleys down. Various experiments provide a controversial insight on the splitting between the two remaining valleys. Conductivity measurements on an electron system composed of thin silicon films in Si-SiGe heterostructures in magnetic field reveal a small valley splitting [2]. From the other side, recent experiments on the conductance through a point contact created by additionally confining a quasi-two-dimensional electron system in lateral direction demonstrate a splitting between equivalent valleys larger than the spin splitting [2]. In this work we address the controversy based on a two-band $\mathbf{k} \times \mathbf{p}$ model for the conduction band. We also demonstrate that a large splitting between the two unprimed subbands with the same number can be induced by a shear strain component.

1. Method

The two-band $\mathbf{k} \times \mathbf{p}$ Hamiltonian is employed to describe the conduction band in presence of shear strain ε_{xy} [3,4]. For the unprimed subbands of a [001] silicon film the following equation for y_n is obtained [5]:

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

with t being the layer thickness, $k_0 = 0.15(2\pi/a)$ is the position of the valley minimum with respect to the X point, and $\eta = m_l|D\varepsilon_{xy} - \hbar^2 k_x k_y/M|/k_0^2$ [5]. Note, that for $\eta = 0$ the quantized momentum $y_{0n} = \pi n/(k_0 t)$ is for both subbands.

2. Results

The dependencies of the subband quantization energy vs. η of for a film of the thickness $t = 5.43$ nm obtained solving (1) numerically are shown in Fig. 1. Degeneracy between the subbands is removed resulting in a splitting which becomes large at high strain values. Fig. 2 shows that the dependence of the splitting is not necessarily monotonous. The effective masses of the two ground subbands are depicted in Fig. 3. It was revealed that in ultra-thin films without strain the masses of the two ground subbands are not equal. The contour plots of the dispersions of the subbands are shown in Fig. 4. The two-band model provides the dependence on the film thickness of the effective mass in the first primed subband shown in Fig. 5 in comparison to first-principle results [6]. In order to demonstrate the unusual behavior we solve (1) by perturbation, which

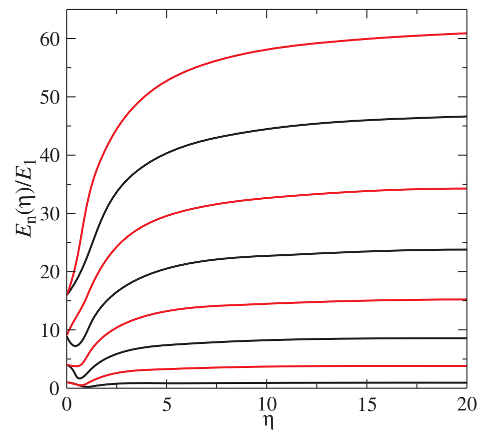

Fig. 1. Normalized positions of the subband minima with respect to the strain-dependent conduction band minimum as function of dimensionless shear strain for a film of thickness $t = 5.43$ nm.

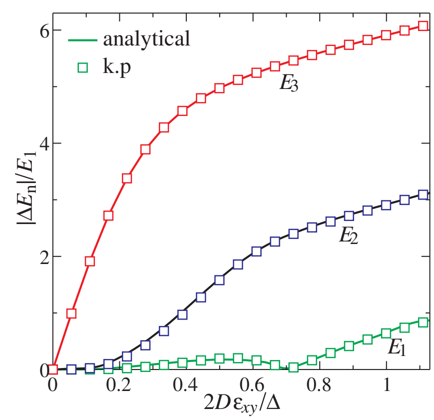

Fig. 2. Strain-dependent splitting between the minima of the unprimed subbands with the same n.

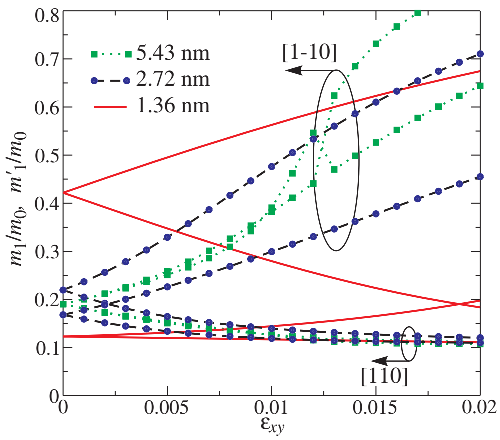

Fig. 3. Effective masses of the two ground subbands. In ultra-thin films the effective masses of the two ground subbands are different even without stress.

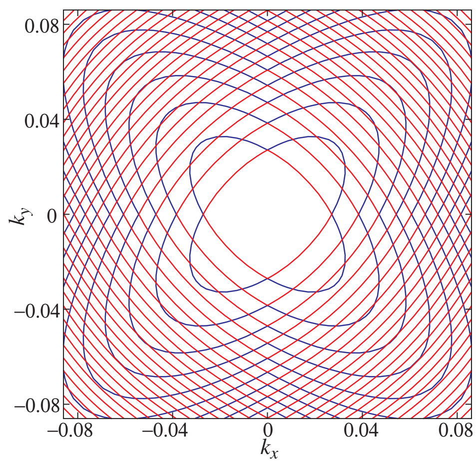

Fig. 4. Dispersions of the two ground subbands for a film thickness of 1.36 nm. The lower subband dispersion is described by the unification of the two ellipses with different masses, while the second subband is described by their intersection.

results in the dispersion relation:

$$E_n^{\pm} = \frac{\hbar^2 k_0^2 y_{0n}^2}{2m_l} + \frac{\hbar^2\left(k_x^2+k_y^2\right)}{2m_t} \pm \frac{y_{0n}^2\left|D\varepsilon_{xy} - \frac{\hbar^2 k_x k_y}{M}\right|}{\left|1-y_{0n}^2\right|}\sin(k_0 t), \tag{2}$$

providing that without strain ($\varepsilon_{xy} = 0$) the two ground subbands is characterized by different masses in [110] direction. Such a difference results in the splitting between the subbands linear vs. the magnetic field and in the enhanced splitting between the two different subbands for the case of a [110] point contact. The strain-induced subband splitting increases rapidly with decreased film thickness (Fig. 6).

3. Conclusions

We have shown that the two-fold degeneracy of the unprimed subbands is eliminated in thin films. This results in a subband splitting 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, one controls and makes the valley splitting

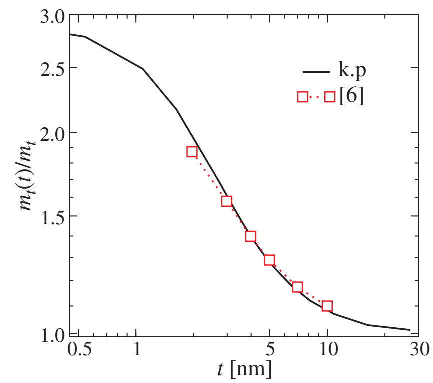

Fig. 5. The thickness dependence of the effective mass of the lowest primed subbands computed with the two-band $\mathbf{k}\times\mathbf{p}$ model (solid line) is in excellent agreement with the full-band calculations [6] (symbols).

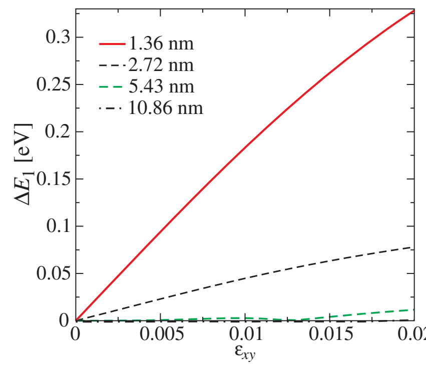

Fig. 6. Shear strain induced splitting of the ground subbands, for several film thicknesses. In ultra-thin films the splitting is larger than kT already for moderate stress.

larger than the Zeeman splitting with shear strain. Therefore silicon appears to be very attractive for spintronic applications.

Acknowledgements

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