Perspectives of Silicon for Future Spintronic Applications from the Peculiarities of the Subband Structure in Ultra-Thin Films

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1. Introduction

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. 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. 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 a coherent spin transport through an undoped silicon wafer of 350 μm length was demonstrated [1]. 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. This degeneracy must be removed and become larger than the spin Zeeman splitting. Experiments provide a controversial insight on this issue. Conductivity measurements on an electron system composed of thin silicon films in Si-SiGe heterostructures in magnetic field reveal that the valley splitting is small [2]. At the same time, recent experiments on the conductance through a point contact created by additionally confining a quasi-two-dimensional electron system in lateral direction with the help of additional gates demonstrate a splitting between equivalent valleys larger than the spin splitting [2]. In this work we try to explain the controversy by considering a two-band **k·p** model for the conduction band. We demonstrate that a large splitting between the two unprimed subbands with the same number can be induced by a shear strain component.

2. Method

We use the two-band **k·p** Hamiltonian to describe the conduction band in presence of shear strain ε_{xy} [3,4]. In case of unprimed subbands of a (001) film with thickness t the model provides the following equation for y_n [5]:

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

Here $k_0 = 0.15(2\pi)/a$ is the position of the valley minimum with respect to the X–point, and $\eta = m_l \,|\, D\varepsilon_{xy} - \hbar^2 k_x k_y / M \,|\, / \hbar^2 k_0^2$ [6]. For $\eta = 0$ the quantized momentum is $y_{0n} = \pi n/(k_0 t)$ for both subbands.

3. Results

We solve (1) numerically. The subband quantization energies are shown in Fig.1 as function of η for a film of the thickness t=5.43nm. 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. Fig.3 shows the effective masses of the two ground subbands. Surprisingly, 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 results in the dispersion relation:

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

It demonstrates that without strain ($\varepsilon_{xy} = 0$) the two ground subbands have different masses in [110] direction. The difference in masses results in the splitting between the subbands linear with the magnetic field and in the enhanced splitting between the two different subbands in a [110] point contact. The strain-induced subband splitting is rapidly increasing with decreased film thickness (Fig.6).

4. Conclusions

We have shown that the two-fold degeneracy of the unprimed subbands is lifted 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, the valley splitting can be controlled and made larger than the Zeeman splitting by shear strain. This makes silicon very attractive for spintronic applications.

This work was supported by the Austrian FWF project P19997-N14.

References

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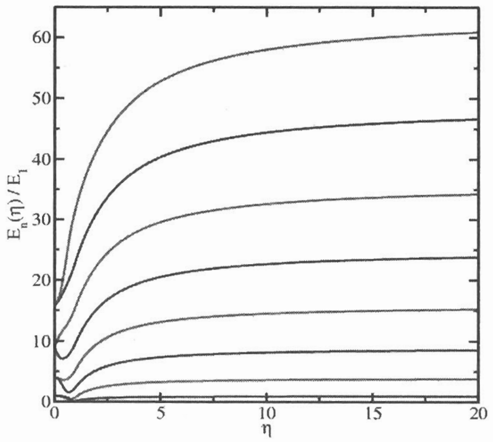

Fig.1: *Normalized positions of the subband minima with respect to the strain-dependent conduction band minimum as function of dimensionless shear strain for a film of thickness t=5.43nm.*

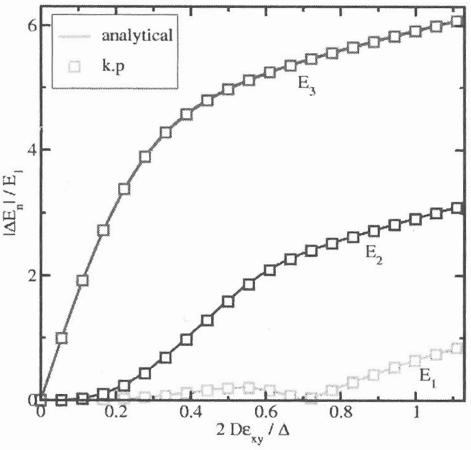

Fig.2: *Strain-dependent splitting between the minima of the unprimed subbands with the same n.*

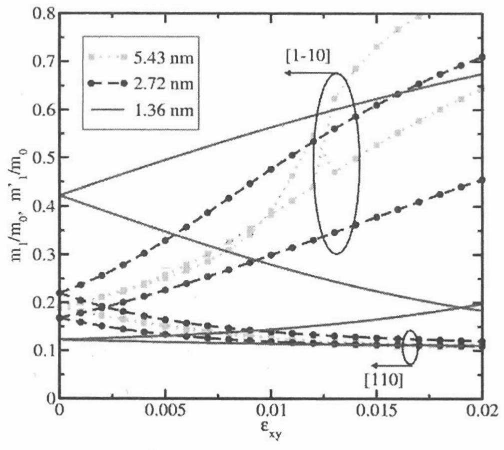

Fig.3: *Effective masses of the two ground subbands. In ultra-thin films the effective masses of the two ground subbands are different even without stress.*

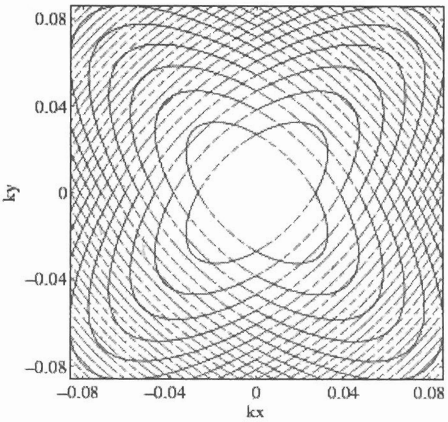

Fig.4: *Dispersions of the two ground subbands for a film thickness of 1.36nm. The lower subband dispersion is described by the unification of the two ellipses with different masses, while the second subband is described by their intersection.*

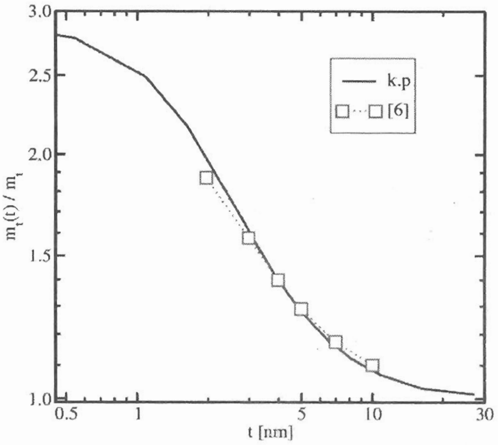

Fig.5: *The thickness dependence of the effective mass of the lowest primed subbands computed with the two-band* ***k·p*** *model (solid line) is in excellent agreement with the full-band calculations [6] (filled symbols).*

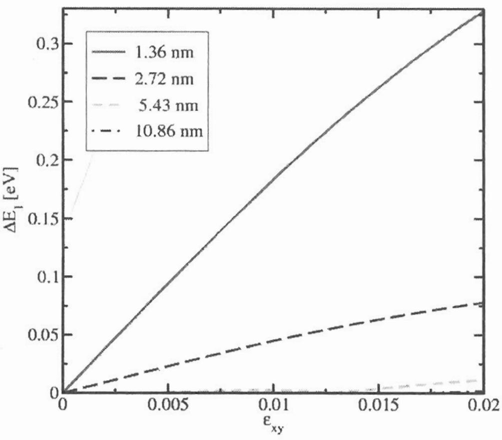

Fig.6: *Shear strain induced splitting of the ground subbands, for several film thicknesses. In ultra-thin films the splitting is larger than kT already for moderate stress.*