Strain-Controlled Valley Splitting in Si-SiGe Heterostructures

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A splitting between equivalent valleys larger than the spin splitting was recently reported in a gate confined electron system in thin Si films grown on SiGe substrate [1]. This degeneracy lifting reduces scattering and improves the coherence time. The valley splitting larger than the spin splitting opens a way to build spin qubits, which makes silicon-based quantum devices promising for future applications in quantum computing. In this work we propose an alternative mechanism to create and control the valley splitting in Si-SiGe heterostructures by applying shear strain. Uniaxial stress is already used for performance enhancement of modern MOSFETs, and its application to control the valley splitting is technologically possible.

We have adopted the two-band **k·p** model for analytical calculations [2-4]. In contrast to the usually assumed parabolic energy dispersion for the conduction band valleys with the transversal mass m_t and the longitudinal mass m_l, the two-band **k·p** model is able to describe the conduction band structure in the presence of shear strain. A good agreement of the analytical two-band **k·p** model with the results of numerical pseudo-potential band structure calculations (EPM) with parameters from [5] is shown in Fig.1. Within the two-band **k·p** model the subband structure for an infinite square well potential can be found analytically. The dispersion in the first unprimed subband is compared against the parabolic approximation with strain- and thickness-dependent transversal effective masses in Fig.2. The valley degeneracy, however, is not removed even when the dispersion is not parabolic (Fig.3, Fig.4), and the unprimed subbands remain two-fold degenerate within the two-band **k·p** approach.

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 in such a way that it mimics the dispersion obtained within the two-band **k·p** model [6]. Considering symmetric and asymmetric wave functions including the Bloch amplitudes for a finite array of $2N$ sites [6], one obtains two sets of equations determining the subband energies of the unprimed subband ladder (Fig.5). It then follows that for shear strain $\varepsilon_{xy} = 0$, when the bands are purely parabolic, the valley splitting is exactly zero. Applying uniaxial [110] stress to [001] ultra-thin Si films generates the valley splitting proportional to strain ε_{xy}. For small ε_{xy} the valley splitting is:

$$\Delta E_v = 2\left(\frac{\pi n}{k_0 t}\right)^2 \frac{D\varepsilon_{xy}}{k_0 t}\sin(k_o t) \ , \qquad (1)$$

where D=14 eV is the shear deformation potential, $k_o = 0.15(2\pi / a)$, a is the lattice constant in Si. The valley splitting is inversely proportional to the film thickness t in the third power, in agreement with [6]. The splitting can be well controlled by applying strain and adjusting the Si film thickness t.

As follows from the two-band **k·p** theory [2-4], the nonparabolicity depends on the combination $\eta = m_l(D\varepsilon_{xy} - k_x k_y / M)/k_0^2$, which is non-zero in laterally confined electron systems even without stress. In recent experiments [1] the additional confinement was introduced by lateral gates and by applying a magnetic field. Fig.6 demonstrates the valley splitting as function of gate voltage and magnetic field obtained within our approach, which is in agreement with [1]. This opens an alternative way to interpret experimental results using Eq.(1).

In summary, the proposed alternative way to induce controllable valley splitting in ultra-thin Si films by applying uniaxial strain opens new perspectives for spintronic applications. The valley splitting increases with increased shear strain and decreasing Si thickness and can be larger than the spin splitting.

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References

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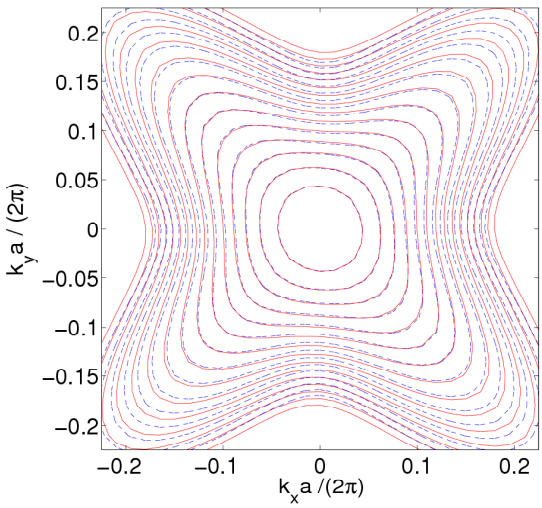

Fig.1: *Comparison between the the two-band **k·p** theory (dashed) and EPM calculations (solid lines). The contour lines are spaced at 50 meV. Tensile [110] and compressive [-110] stress of 150 MPa is applied.*

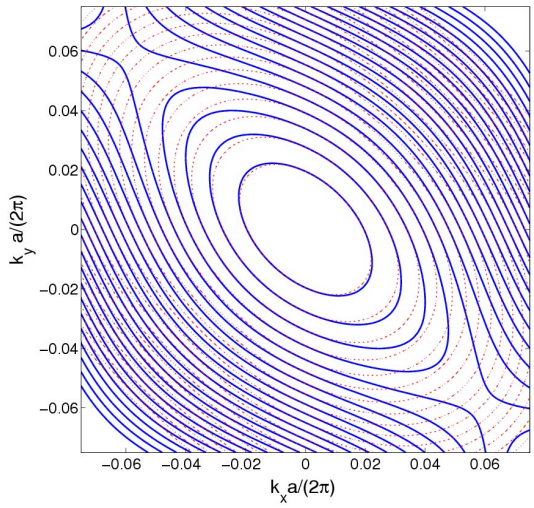

Fig.2: *Subband dispersion (solid lines) and parabolic approximation for unprimed subbands. t=5.4 nm,* $\varepsilon_{xy} = 0.9\%$ *The contour lines are spaced at 10 meV.*

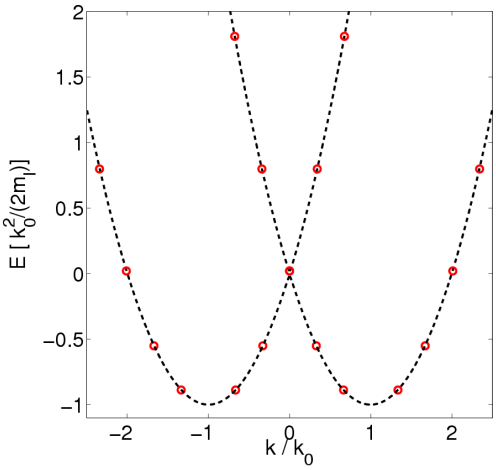

Fig.3: *Subband energies in unstrained Si film from the two-band **k·p** theory.*

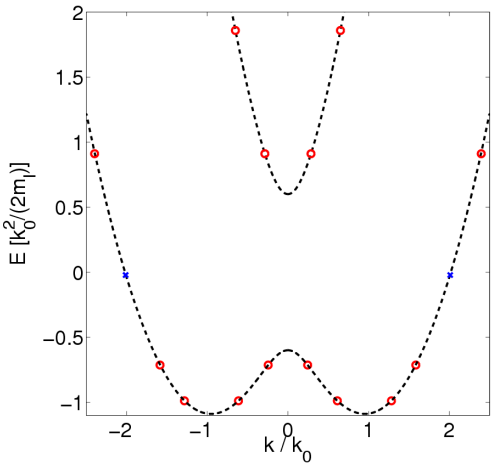

Fig.4: *Same as in Fig.3 in a stressed Si film. The gap at the X-point leads to nonparabolic dispersion*

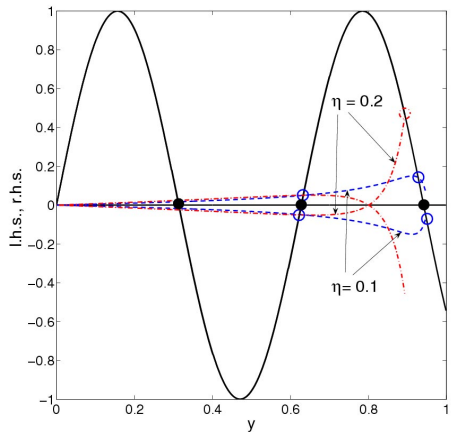

Fig.5: *The valleys are two-fold degenerate (filled circles) without strain. For non-zero shear strain the degeneracy is lifted.*

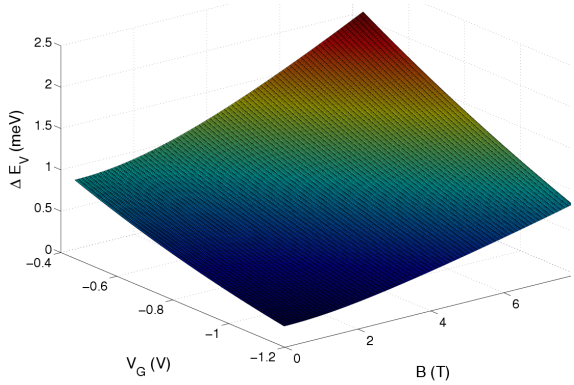

Fig.6: *Valley splitting in a laterally confined electron system in an external magnetic field.*