Two-Band k·p Model for the Conduction Band in Silicon: Impact of Strain and Confinement on Band Structure and Mobility

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For analytical calculations the conduction band of Si is usually approximated by three pairs of equivalent valleys located near the *X*-points of the Brillouin zone. It is commonly assumed that the valley dispersion is well approximated by a non-parabolic dispersion with the transversal mass m_t and the longitudinal mass m_l. A constant non-parabolicity parameter α is introduced to describe deviations in the density of states from the purely parabolic dispersion. There are experimental indications that the effective masses depend on shear strain [1] and the silicon film thickness [2]. The parabolic band structure ignores these effects completely.

In this work we demonstrate that the recently proposed [3] two-band **k·p** model describes accurately dependences of the valley shifts and the effective masses on the shear strain component. The theory includes non-parabolicity effects due to the interaction between the two lowest conduction bands and provides an analytical expression for the dependence of the effective masses on shear strain.

Within the two-band **k·p** model the dispersion relation in a [001] valley is of the form [3,4]

$$E = k_z^2 + \left(k_x^2 + k_y^2\right) m_l / m_t - 2\sqrt{k_z^2 + \delta^2}\,, \qquad (1)$$

where all the wave vectors are normalized by $k_0 = 0.15\times 2\pi / a$, the position of the minimum relative to the X point. Energies are in units of $\hbar^2 k_0^2/(2m_l)$, and $\delta^2 = (\eta - m_l k_x k_y / M)^2, \eta = 2m_t D\varepsilon_{xy} / k_0^2, M^{-1} \approx m_t^{-1} - m_0^{-1}$, ε_{xy} denotes the shear strain component, and D=14 eV is the shear strain deformation potential [3,4]. Excellent agreement between the two-band **k·p** model (1) and the results of empirical pseudopotential (EPM) band structure calculations is demonstrated in Fig.1

In [001] ultra-thin Si films with thickness *t* the dispersion of the unprimed subbands found from the two-band **k·p** model is

$$E_n = p_n^2 + \left(k_x^2 + k_y^2\right) m_l / m_t - 1 - \delta^2 / (1 - p_n^2)\,, \qquad (2)$$

where $p_n = (\pi n)/(tk_0)$. Examples of quantization for $\eta = 0$ and 0.3 are shown in Fig.2. For strain $\eta = 0$ the model (2) describes a non-parabolic subband dispersion (Fig.3). The denominator in the last term describes the dependence of the non-parabolicity parameter on the film thickness (Fig.4) for the unprimed subbands. Finally, the low-field mobility with the dependence of the non-parabolicity parameter on the film thickness taken into account is compared with the mobility computed with α=0.5 eV^{-1} in Fig.5. Relative corrections are about 7% for *t*= 3nm and 15% for *t*=2.5 nm.

In conclusion, the two-band **k·p** model for the conduction band in Si is shown to describe the dependences of the band parameters on shear strain and UTB thickness, which have a profound impact on the mobility.

The work was partly supported by the Austrian Science Fund FWF, Project P19997-N14.

References

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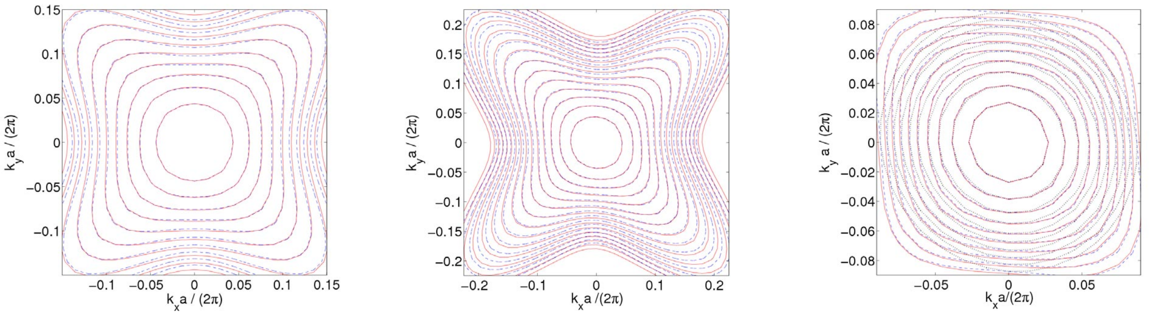
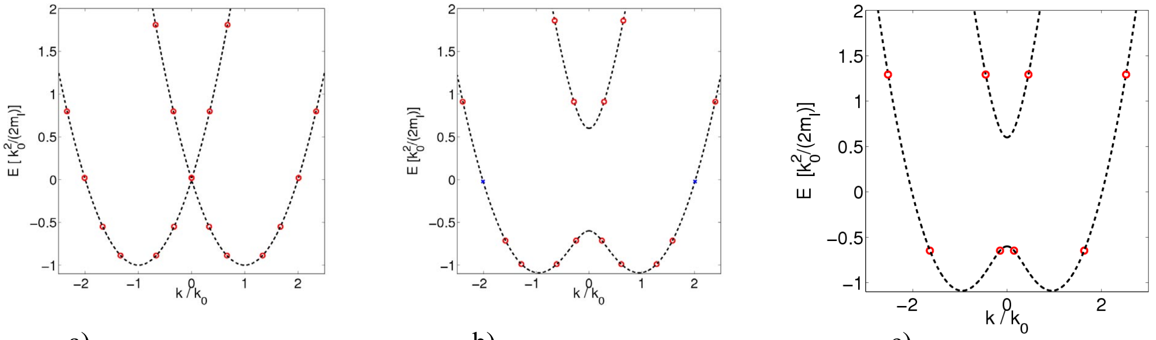


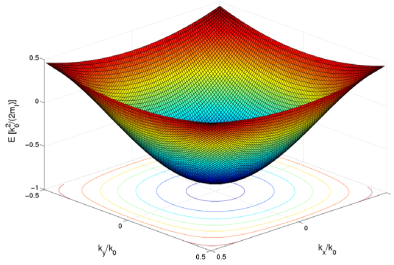
a). b). c).

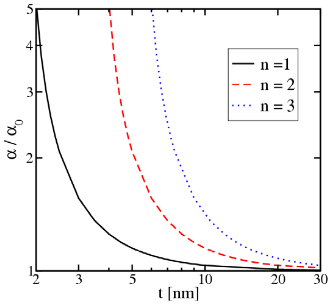
Fig.1: Comparison between Eq.(1) (dashed lines) and the results of EPM calculations (solid lines). The contour lines are spaced at 50 meV (panels a and b) and 20 meV for the panel c. No stress is applied at panel a), while tensile stress along [110] and compressive stress along [-110] of 150 Mpa in each direction is applied at the panels b and c, respectively. The parabolic approximation with strain-dependent effective masses is also shown in panel c (dotted contour lines).



a). b). c).

Fig.2: Dispersion relation (2) for the first unprimed subband for a (001) silicon film of thickness *t* = 5.4 nm (panels a and b) and *t* = 2.5 nm (panel c). No strain is applied at panel a, while normalized shear strain η =0.3 at the panels b and c, respectively.





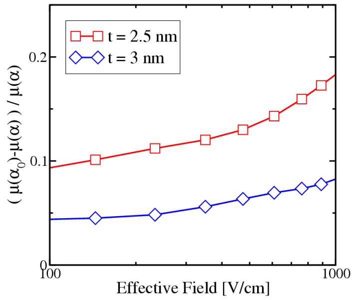


Fig.3: Dispersion relation (2) for the first unprimed subband, for a (001) silicon film of thickness *t* = 5 nm.

Fig.4: Dependence of the non-parabolicity parameter on (100) Si film thickness *t* for three lowest unprimed subbands.

Fig.5: Relative mobility difference due to the dependence of the non-parabolicity parameter on UTB thickness in the unprimed subbands.