Electron Subband Dispersions in Ultra-Thin Silicon Films from a Two-Band **k·p** Theory

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The **k·p** theory is a well established method to describe the band structure analytically. The conduction band in Si is usually approximated by three pairs of equivalent minima located close to the X-points of the Brillouin zone. It is commonly assumed that close to the minima the electron dispersion is well described by the effective mass approximation, with the two transversal masses m_t and the longitudinal mass m_l. The constant nonparabolicity parameter $\alpha = 0.5\ \text{eV}^{-1}$ is introduced to describe deviations in the density of states from the purely parabolic dispersion. It was recently indicated [1] that direction-dependent nonparabolicity has to be introduced to explain the mobility behavior at high carrier concentrations in a FET with (110) ultra-thin body (UTB) orientation. Therefore, a more refined description of the subband structure beyond the usual nonparabolic approximation is needed.

In this work we report the subband structure in [001] UTB FETs obtained within an efficient two-band **k·p** theory proposed recently [2]. The theory naturally includes the nonparabolicity effects [2] due to the interaction between the two lowest conduction bands.

Within this theory the dispersion in a [001] valley is in the form

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

where all the wave vectors are normalized by the position $k_0 = 0.15 \times 2\pi / a$ of the minimum along the [001] direction measured from the X point. Energies are measured in units of $\hbar^2 k_0^2 / (2m_l)$, and $\Delta^2 = (m_l k_x k_y / M)^2$, $M^{-1} \approx m_t^{-1} - m_0^{-1}$. In (1) k_z is measured from the X point. k_z is found in the form

$$k_z^{\pm} = p_0(\Delta^2) \pm \frac{\pi n}{t k_0},\ n = ...-2, -1, 1, 2,... \qquad (2)$$

for quantization in UTB film with thickness t. The location p_0 of the subband minimum is obtained from the condition that both values $k_z^{\pm}$ give the same energy. This results in p_0 dependence on Δ and n and leads to the dispersion

$$E = \left(\frac{\pi n}{t k_0}\right)^2 + \frac{m_l}{m_t}\left(k_x^2 + k_y^2\right) - 1 - \frac{\Delta^2}{1 - (\pi n / t k_0)^2}\ ,$$

shown in Fig.1. The denominator in the last term describes the dependence of the nonparabolicity parameter on the film thickness for unprimed subbands, which is shown in Fig.2.

For primed subbands we use (1) with k_z and k_x interchanged, and $\Delta \to m_l(\pi n / t k_0) k_y / M$. The dispersion shown in Fig.3 displays the minimum at $k_x = \pm 1$ and $k_y = 0$. For $t^2 < (\pi n / k_0)^2 (m_l m_t / M^2)$ the minimum is at $k_x = 0$, $k_y = \pm(\pi n / t k_0)(m_t / M)$, as shown in Fig.4. This results in interesting effective mass dependences close to the subband minimum as shown in Fig.5. Finally, the low-field mobility with the dependence of the nonparabolicity parameter on film thickness taken into account is compared with the mobility computed with $\alpha = 0.5\ \text{eV}^{-1}$ in Fig.6. Relative corrections are about 5-10% for t= 3nm and 10-20% for t=2.5 nm.

In conclusion, the subband dispersion in (100) UTB Si films within the two-band **k·p** theory is analyzed for the first time. The importance of the nonparabolicity dependence on the film thickness for transport is demonstrated.

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[1] K. Uchida *et al.*, IEDM 2005, p.135.
[2] V.Sverdlov *et al.*, SISPAD 2007, in print.

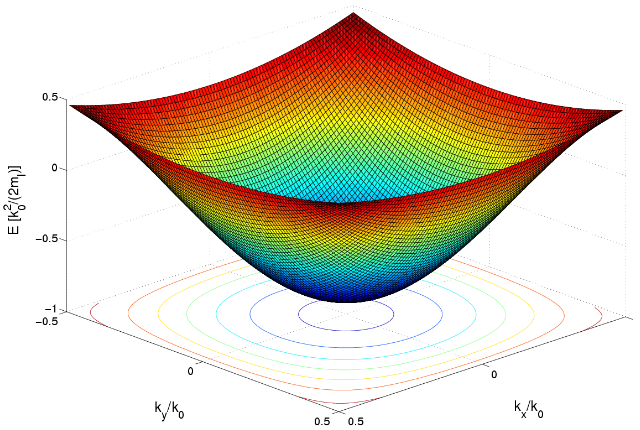

Fig. 1. Dispersion relation (3) for the first unprimed subband, for (001) silicon film with thickness *t* = 5 nm.

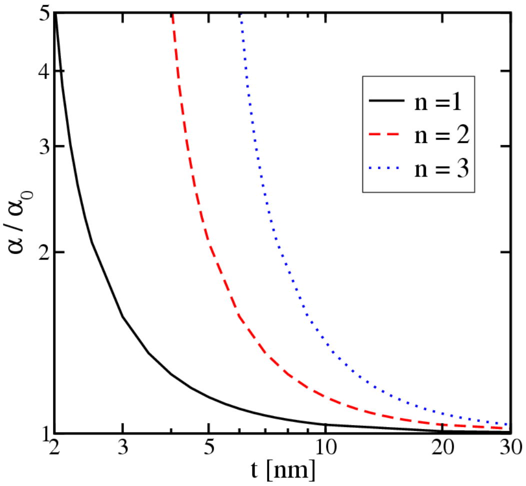

Fig. 2. Dependence of the nonparabolicity parameter on (100) Si film thickness *t* for three lowest unprimed subbands.

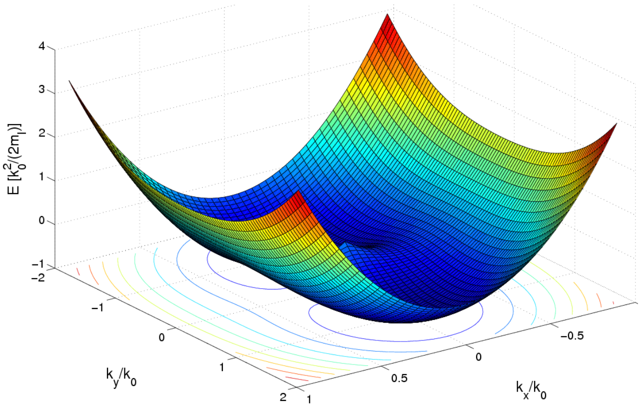

Fig. 3. Dispersion relation for the first primed subband for (100) Si film with thickness *t* = 5 nm.

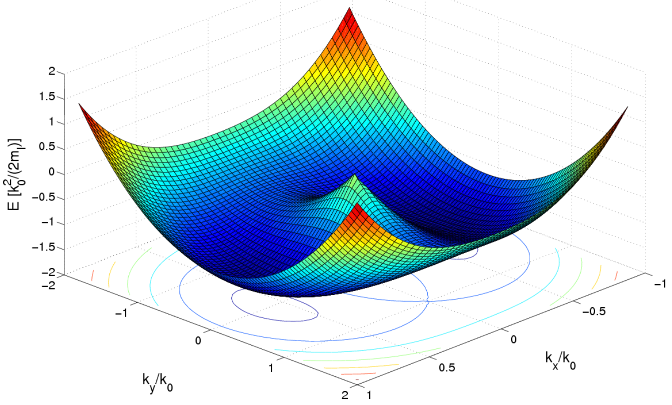

Fig. 4. Dispersion relation for the first primed subband for (100) Si film with thickness *t* = 2.5 nm.

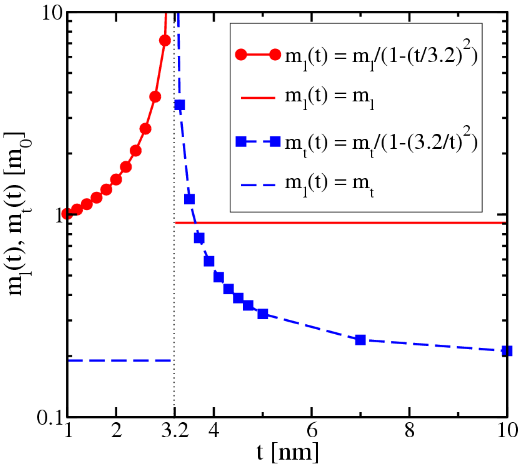

Fig. 5. Effective masses dependences on Si film thickness *t* at the minimum of the first primed subband.

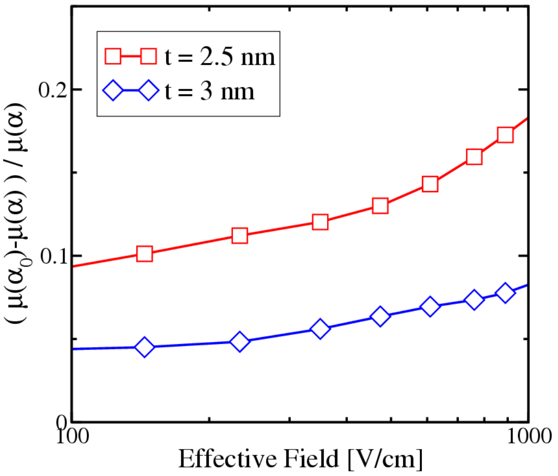

Fig.6. Relative correction to the mobility due to dependence of the nonparabolicity parameter in unprimed subbands and dispersion (1) in primed subbands.