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Electron subband dispersions in ultra-thin silicon films from a two-band k·p theory

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Abstract The electron subband structure in a thin (100) silicon film is analyzed based on a two-band **k·p** theory. For unprimed subbands the dependence of the nonparabolicity parameter on film thickness is obtained. The two-band **k·p** theory gives a thickness dependence of the effective masses for primed subbands. Limitations of the model are discussed. The importance of the nonparabolicity parameter dependence on the film thickness for transport is demonstrated.

Keywords **k·p** method · Device simulation · Subband structure · Quantum transport · Monte Carlo method

1 Introduction

The **k·p** theory is a well established method to describe the band structure analytically. The conduction band in Si is usually approximated by six equivalent minima located close to the X points of the Brillouin zone. Usually the electron dispersion is described by the parabolic effective mass approximation, with two transversal masses m_t and the longitudinal mass m_l. The constant nonparabolicity parameter α_0 is introduced to describe deviations in the density of states from the purely parabolic dispersion. It was recently indicated [1] that the isotropic α_0 may not be sufficient to explain the mobility behavior at high carrier concentrations in a FET with (110) ultra-thin body (UTB) orientation, and direction-dependent nonparabolicity has to be introduced. Therefore, a more refined description of the subband structure beyond the usual nonparabolic approximation is needed.

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2 Two-band k·p theory: bulk

In this work we report the subband structure in [001] UTB FETs obtained within an efficient two-band **k·p** model [2]. The model predicts nonparabolicity effects due to the coupling between the two lowest conduction bands [3, 4]. Let us consider the particular valley along the [001] direction (z-axis). The band closest to the first conduction band Δ_1 ($i = 1$) is the second conduction band $\Delta_{2'}$ ($i = 2$). The two bands become degenerate exactly at the X point along the [001] direction in the Brillouin zone. The minimum of the conduction band is only $k_0 = 0.15(2\pi)/a$ away from the X point. Including only these two bands and treating their coupling as a perturbation, the dispersion relation around the minimum is well described by degenerate perturbation theory. We start with the construction of the Hamiltonian in the vicinity of the X point.

Diagonal elements of the **k·p** Hamiltonian H_{ii} corresponding to the two independent bands $i = 1, 2$ are:

$$H^0_{ii}(k) = (-1)^{i-1}\frac{\hbar}{m_0}k_z p + \frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2 k_x^2}{2m_t} + \frac{\hbar^2 k_y^2}{2m_t}, \qquad (1)$$

where m_0 is the free electron mass, m_t is the transversal, and m_l is the longitudinal effective mass. The values of k_z

are counted from the X point. The coupling between the two bands is described by the off-diagonal terms [2]:

$$H_{12}^{0}(k) = \frac{\hbar^2 k_x k_y}{M}. \tag{2}$$

The parameter M can be obtained within the $\mathbf{k}\cdot\mathbf{p}$ perturbation theory:

$$\frac{1}{M} = \frac{2}{m_0^2}\left|\sum_{l\neq i,j}\frac{(p_y)_{1l}(p_z)_{l2}}{E_l(X) - E_{\Delta_1}(X)}\right|.$$

The value of M computed by the empirical pseudo-potential method (EPM) is close (but not equal) to $M' = m_0/(1 - m_t/m_0)$ reported in [2]. Using degenerate perturbation theory, one obtains the following bulk dispersion relation:

$$E(\mathbf{k}) = \frac{\hbar^2 k_z^2}{2m_l} + \frac{\hbar^2(k_x^2 + k_y^2)}{2m_t} - \sqrt{\left(\frac{\hbar}{m_0}k_z p\right)^2 + \left(\frac{\hbar^2 k_x k_y}{M}\right)^2}. \tag{3}$$

The parameter p is related to the position of the band minimum k_0 through $p = \hbar k_0 m_0/m_l$. Introducing dimensionless wave numbers $\tilde{k}_x = k_x/k_0$, $\tilde{k}_y = k_y/k_0$, $\tilde{k}_z = k_z/k_0$, the energy $\tilde{E}(\tilde{\mathbf{k}}) = E(\tilde{\mathbf{k}})/E_0$ with $E_0 = \hbar^2 k_0^2/2m_l$, and defining $\Delta = \tilde{k}_x\tilde{k}_y m_l/M$, we rewrite (3) as

$$\tilde{E}(\tilde{\mathbf{k}}) = \tilde{k}_z^2 + \frac{m_l}{m_t}(\tilde{k}_x^2 + \tilde{k}_y^2) - 2\sqrt{\tilde{k}_z^2 + \Delta^2}. \tag{4}$$

Expanding (4) for small Δ and averaging the angular dependence [3], one obtains the following expression for the nonparabolicity parameter α_0:

$$\alpha_0 = \frac{1}{8E_0}\left(\frac{m_t}{M}\right)^2. \tag{5}$$

Substituting Si parameter values into (5), we estimate $\alpha_0 = 0.6\ \mathrm{eV}^{-1}$, which is close to the phenomenological value $\alpha_0 = 0.5\ \mathrm{eV}^{-1}$. In the next section the subband structure in UTB Si films obtained from the two-band $\mathbf{k}\cdot\mathbf{p}$ theory is considered.

3 Subband structure in (100) UTB films

In an UTB film the band bending inside the film can be neglected as compared to subband energies. Let us consider a [001] UTB flat band film. Due to size quantization there will be ladders of subbands formed. An unprimed two-fold degenerate ladder occurs from the two [001] oriented valleys, while the remaining four valleys yield the four-fold degenerate primed subband ladder.

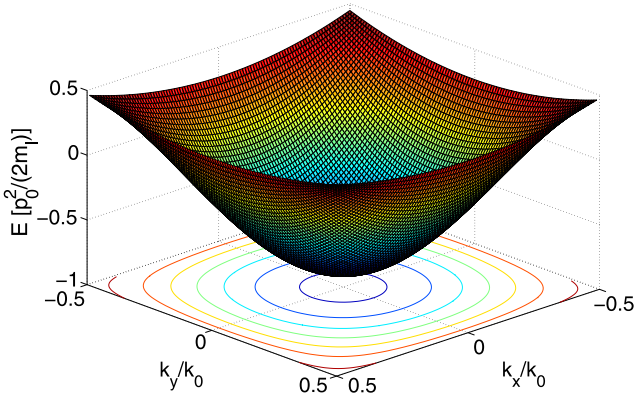

Fig. 1 Dispersion relation (4) for the first unprimed subband ($p_0 = \hbar k_0$), for (001) Si film with thickness $t = 5$ nm

We begin the analysis with the unprimed ladder. In order to find the dispersion, we first solve (4) with respect to $\tilde{k}_z$:

$$\tilde{k}_z = \left[\left(1 \pm \sqrt{1 + \tilde{E} - \tilde{\epsilon} + \Delta^2}\right)^2 - \Delta^2\right]^{1/2}, \tag{6}$$

where $\tilde{\epsilon} = m_l(\tilde{k}_x^2 + \tilde{k}_y^2)/m_t$. For $\Delta = 0$ (6) results in $\tilde{k}_z = 1 \pm q_z$, with

$$q_z = \sqrt{1 + \tilde{E} - \tilde{\epsilon}}. \tag{7}$$

Due to size quantization in a film of thickness t, q_z takes the values $q_z = \pi n/(tk_0)$, where n is a non-zero integer. Substituting these q_z values into (7) results in the well-known subband dispersion for parabolic bands:

$$E_n^{(0)}(\mathbf{k}) = \frac{\hbar^2\pi^2 n^2}{2m_l t^2} + \frac{\hbar^2}{2m_t}(k_x^2 + k_y^2) - \frac{\hbar^2 k_0^2}{2m_l}, \tag{8}$$

The last term describes the energy of the conduction band minimum relative to the energy at the X point.

For $\Delta \neq 0$ we look for a solution of (6) in the form $\tilde{k}_z = x \pm q_z$. Substitution of $\tilde{k}_z$ into (6) results in the following system of equations for x and q_z:

$$\begin{aligned} x^2 + q_z^2 &= 2 + \tilde{E} - \tilde{\epsilon}, \\ xq_z &= \sqrt{1 + \tilde{E} - \tilde{\epsilon} + \Delta^2}. \end{aligned} \tag{9}$$

The quantization condition for an ideal quantum well is $q_z = \pi n/(tk_0)$. The value x, which determines the overall phase factor of the wave function, depends on Δ and the film thickness t:

$$x = \sqrt{1 - \frac{\Delta^2}{1 - \frac{\pi^2 n^2}{t^2 k_0^2}}}.$$

The dispersion relation is then obtained as

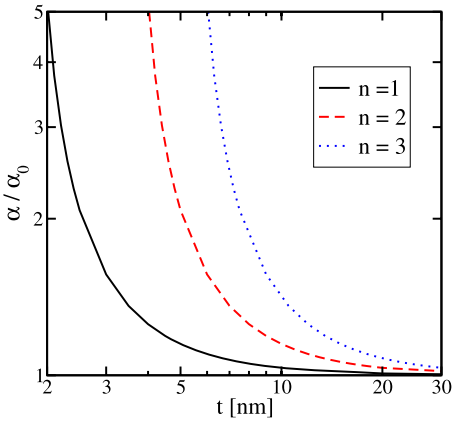

Fig. 2 Dependence of the nonparabolicity parameter on (100) Si film thickness t for three lowest unprimed subbands

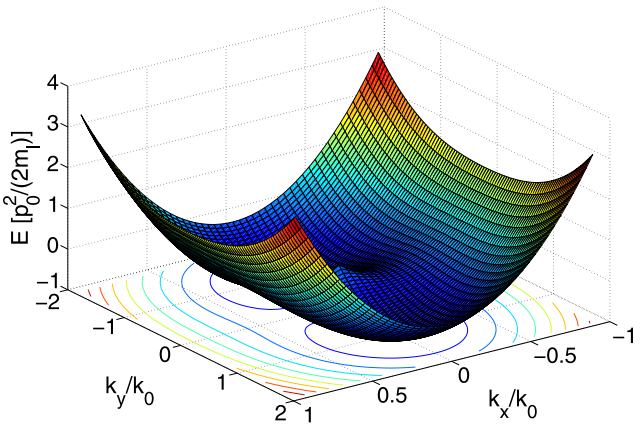

Fig. 3 Dispersion relation for the first primed subband for (100) Si film with thickness $t = 5$ nm

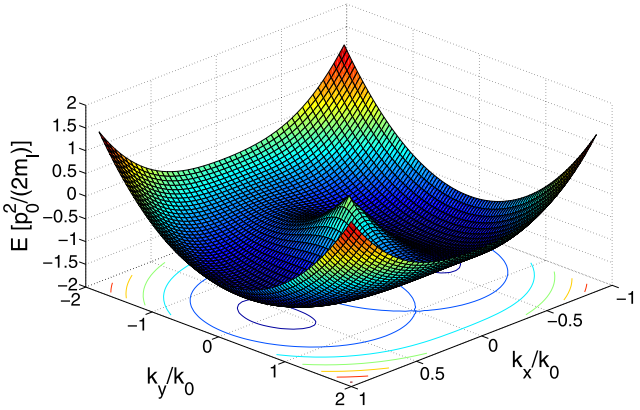

Fig. 4 Dispersion relation for the first primed subband for (100) Si film with thickness $t = 2.5$ nm

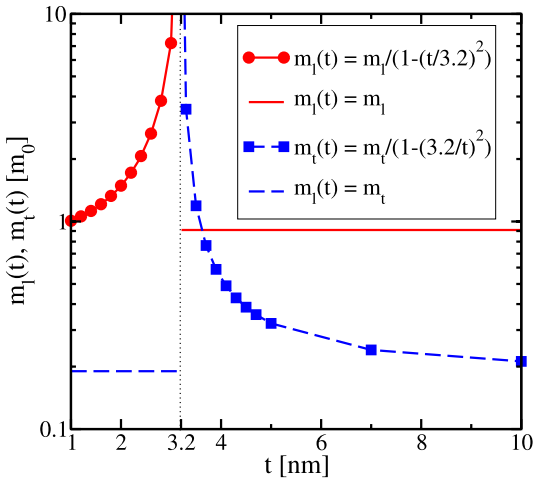

Fig. 5 Dependence of the effective masses on the Si film thickness t at the minimum of the first primed subband.

$$E_n(\mathbf{k}) = E_n^{(0)}(\mathbf{k}) - \frac{\hbar^2 k_x^2 k_y^2 m_l}{2M^2 k_0^2} \frac{1}{1 - \frac{\pi^2 n^2}{t^2 k_0^2}}. \tag{10}$$

The dispersion relation (10) is shown in Fig. 1, for $n = 1$ and $t = 5$ nm. The last term in (10) describes deviations of the dispersion relation from the purely parabolic one and gives the correction to the constant density of states of a purely parabolic dispersion. By analogy to the bulk case the subband nonparabolicity parameter α is introduced in such a way that the approximate isotropic nonparabolic dispersion relation

$$\varepsilon_n(1 + \alpha_n \varepsilon_n) = \frac{\hbar^2(k_x^2 + k_y^2)}{2m_t}$$

reproduces the density of states close to the subband minimum obtained with the exact dispersion relation (10). This leads to the thickness dependent subband nonparabolicity parameter α_n:

$$\alpha_n = \alpha_0 \left[1 - \frac{\pi^2 n^2}{t^2 k_0^2}\right]^{-1}. \tag{11}$$

The thickness-dependence is illustrated in Fig. 2 for the first three subbands. We note that α_n may change its sign for $t \leq 1$ nm, which is a range, however, in which the **k**·**p** approximation becomes questionable.

For the primed subbands we use (4) with k_x and k_z interchanged. We quantize k_z as $k_z = \pi n/tk_0$. The dispersion for $t = 5$ nm is shown in Fig. 3 and displays the minima at $\tilde{k}_z = \pm 1$ and $k_y = 0$. It is interesting that for $t^2 \leq (\pi n/k_0)^2 m_l m_t/M^2$ the minimum of (4) moves to $k_z = 0$, $\tilde{k}_y = \pm(\pi n/tk_0)(m_t/M)$. The corresponding dispersion is shown in Fig. 4 for $t = 2.5$ nm. We note that the minima are positioned outside of the first two-dimensional Brillouin zone centered at the Γ point, which is an indication that the simple two-band **k**·**p** theory may not be accurate enough,

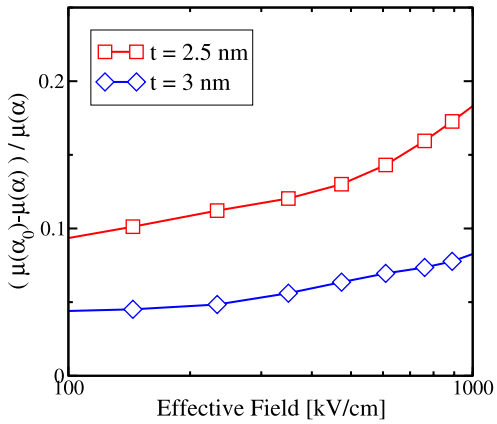

Fig. 6 Relative correction to the channel mobility due to the thickness-dependence of the nonparabolicity parameter in the unprimed subbands.

and a more refined study is needed which takes the Bloch amplitude structure into consideration. Assuming that (4) with quantized k_x is valid, this results in an interesting effective mass dependence at the subband minimum shown in Fig. 5. We note that recent first-principle calculations of the subband parameters in Si films [5] indicated an increase of the m_l effective mass in primed subbands, in qualitative agreement with predictions from the two-band $\mathbf{k}\cdot\mathbf{p}$ theory for $t^2 \geq (\pi n/k_0)^2(m_l m_t)/M^2$. It was pointed out in [5] that the minimum position and the m_l behavior depends on the method of dangling bonds passivation, or the boundary conditions at the Si film-oxide interfaces. It was also shown in [5] that the effective mass of the unprimed subbands does not depend on the Si film thickness, in agreement with predictions of the $\mathbf{k}\cdot\mathbf{p}$ theory.

Finally, the low-field mobility with the nonparabolicity parameter dependent on film thickness is compared with the mobility computed with constant α_0 in Fig. 6. Electron-phonon interaction and surface roughness scattering are taken into account. The relative correction to the mobility is about 5–10% for $t = 3$ nm and 10–20% for $t = 2.5$ nm.

4 Conclusions

In conclusion, the subband dispersion in (100) UTB Si films is analyzed using a two-band $\mathbf{k}\cdot\mathbf{p}$ model. The importance of the dependence of the nonparabolicity parameter on the film thickness for transport is demonstrated.

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