Full Band and Approximated Solutions of the Schrödinger Equation in Silicon Inversion layers.

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Abstract

In this paper, we investigated the quantization in the MOSFET inversion layer by solving the Schrödinger EQuation (SEQ) in the momentum space according to the 3D Full Band (FB) structure of silicon. For the first time, we explain the dependence of the eigenvalues on the momentum **k** in the plane of transport and discuss its periodicity. Furthermore, we discuss the solution of the SEQ around the energy minima, compare the Non-Parabolic model with the FB results, and propose a new efficient procedure to achieve an accurate energy dispersion in the subbands.

1 Introduction

It has been recently recognized that even decananometric MOSFETs are not ballistic [1], and that the scattering along the channel and close to the drain can significantly degrade the on-current [1, 2]. With a supply voltage still around $1V$ for high-performance devices [**?**], a realistic modeling of nano-MOSFETs demands the energy dispersion of the 2D electron gas well above the subband minimum, where the accuracy of the conventional non-parabolic models cannot be given for granted. This paper analyzes the possible of effects of subband quantization beyond the conventional parabolic or non-parabolic models.

2 Full Band Solution

We denote with z the direction of the 1D confining potential $U(z)$ and with $\mathbf{K}$=$(\mathbf{k}, k_z)$ the total electron wavevector. If we now expand the *unknown* eigenfunction in terms of Bloch functions with coefficients $A_\mu^{(n)}(\mathbf{k}, k_z)$ [3], we find that the SEQ can be written, for each **k** vector in the transport plane, as the eigenvalue problem:

$$E_{FB}^{(n)}(\mathbf{k}, k_z)A_\mu^{(n)}(\mathbf{k}, k_z) + \frac{2\pi}{L}\sum_{n',k_z'} U_T(k_z - k_z')A_\mu^{(n')}(\mathbf{k}, k_z')f_{k_z,k_z'}^{(n,n')}(\mathbf{k}) =$$

$$\epsilon_\mu(\mathbf{k})A_\mu^{(n)}(\mathbf{k}, k_z), \qquad f_{k_z,k_z'}^{(n,n')}(\mathbf{k}) =< u_{n,\mathbf{k},k_z}|u_{n',\mathbf{k},k_z'} > \tag{1}$$

where $U_T(q_z)$ is the Fourier Transform of the $U(z)$, L is a normalization length in the quantization direction and $\epsilon_\mu(\mathbf{k})$ is the eigenvalue. $E_{FB}^{(n)}(\mathbf{k}, k_z)$ and $f_{k_z,k_z'}^{(n,n')}(\mathbf{k})$ denote the energy in the n-th band of the 3D FB structure and the *overlap integrals* of the periodic parts $u_{n,\mathbf{k},k_z}$ of the Bloch functions, respectively. Both of them were obtained according the well-established Non-Local-Pseudopotential method [4]. In the derivation of Eq.1 it is assumed that $U_T(q_z + g_z) \ll U_T(q_z)$i, where g_z is the z component of a vector in the reciprocal lattice space.

Throughout this paper we discuss different approaches to solve the SEQ. For a fair comparison, all the methods will be used with the same $U(z)$ obtained from a conventional Schrödinger-Poisson solver with parabolic bands. As it can be seen, Eq. 1 is an eigenvalue equation for each **k** value, and, furthermore, the calculation of $\epsilon_\mu(\mathbf{k})$ involves different bands of the 3D FB dispersion. As a result, the solution of Eq. 1 is computationally prohibitive when it is to be coupled to the Poisson and transport problems, hence most of the paper concerned with transport have discussed Eq. 1 only around the energy minima, and understandably moved to approximated solutions [5, 6].
Fig.1 illustrates the lowest eigenvalue $\epsilon_0(\mathbf{k})$ versus **k** obtained from Eq. 1 by including the two lowest bands of the 3D FB structure. The 2D bands $\epsilon_\mu(\mathbf{k})$ are found to be periodical in the **k** plane within the marked square. In fact we note that, assuming a $<100>$ orientation for the interface, the Wigner-Seitz cell in the real space of the 2D system is a square with a 45 degrees orientation, and with a lateral dimension of $a_0/\sqrt{2}$. Consequently, the first Brillouin Zone (BZ) in the reciprocal space is also a square, with a 45 degrees orientation, and with a lateral dimension of $2\pi\sqrt{2}/a_0$, which finally explains the periodicity domain indicated in Fig.1.
It is worth pointing out that, in order to obtain the periodicity of Fig.1, it is necessary to solve Eq. 1 for k_z values ranging in more BZs of the 3D FB structure.

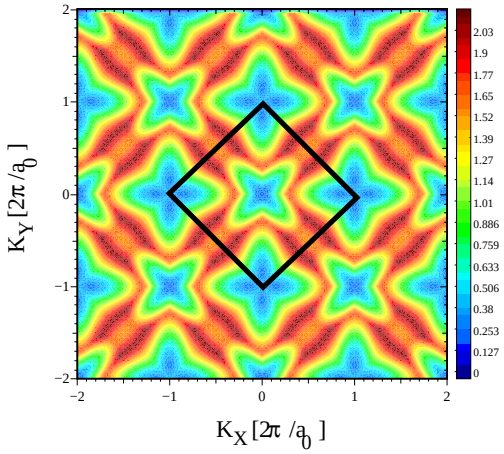

Figure 1: Contour plot of the lowest eigenvalue versus the momentum **k=(**k_x**,**k_y**)** in the transport plane. The square indicates the first Brillouin Zone of the 2D system. SOI MOSFET, silicon thickness $T_{SI} = 9.4$nm and channel doping $N_A = 10^{15}cm^{-3}$. The inversion density is $N_{INV}\approx 10^{13}cm^{-2}$.

3 Effective Mass Approximation

A significant simplification of Eq. 1 is obtained by rewriting the equation around the υ-th minimum of the 3D FB structure, thus leading to the Effective Mass Approximation (EMA) [3, 5]. However, even in the EMA approach, the solution of the SEQ for each **k** is computationally prohibitive for transport applications, so that an approximated expression is necessary to describe the dependence of the eigenvalue on **k** (where **k** and k_z are now to be referred to the minimum ($\mathbf{k}_m^{(\upsilon)}$,$k_{zm}^{(\upsilon)}$). To this purpose, $E_{FB}^{(\upsilon)}$ around the minimum has been universally simplified with Non-Parabolic (NP) expressions [5, 7]. However, this does not eliminate the need for solving the SEQ for each **k**, because, in

order to achieve that, the key point is to decouple the **k** from the k_z dependence in the E_{FB}. Following [7], we can account for the NP factor *only in the parallel energy*:

$$\epsilon_{\mu}^{(\upsilon)}(\mathbf{k}) \approx \epsilon_{\mu 0}^{(\upsilon)} + (2\alpha)^{-1}[-1 + \sqrt{1 + 2\alpha\hbar^2(k_x^2/m_x + k_y^2/m_y)}], \tag{2}$$

where $\epsilon_{\mu 0}^{(\upsilon)}$ is the eigenvalue calculated for $\mathbf{k}$=0 assuming a parabolic dependence of E_{FB} on k_z. Following a similar reasoning, we propose an approximated solution for Eq. 1 around the minimum obtained by keeping only the lowest band of the 3D FB dispersion (n=0) and then by expanding the $E_{FB}^{(0)}$ with respect to k_z to get $E_{FB}^{(0,\upsilon)}(\mathbf{k}, k_z) \approx (\hbar^2/2m_z^{(\upsilon)}k_z^2) + E_{FB}^{(0,\upsilon)}(\mathbf{k}, k_z{=}0)$, i.e. assuming that the $E_{FB}^{(0,\upsilon)}$ is parabolic in k_z with the same mass as in the minimum. The corresponding $\epsilon_{\mu}^{(\upsilon)}(\mathbf{k})$, hereafter denoted as the **kz2** model, is given by:

$$\epsilon_{\mu}^{(\upsilon)}(\mathbf{k}) \approx \epsilon_{\mu 0}^{(\upsilon)} + E_{FB}^{(0,\upsilon)}(\mathbf{k}, 0) \tag{3}$$

By definition, the $\epsilon_{\mu 0}^{(\upsilon)}$ is the same in both NP and **kz2** models, as well as in the conventional parabolic model. We have verified (not shown), that the $\epsilon_{\mu 0}^{(\upsilon)}$ tracks very well the FB results for both Bulk and SOI MOSFETs, because the parabolic expansion in k_z for the $E_{FB}^{(0,\upsilon)}$ is a good approximation for the **k** at the minimum.

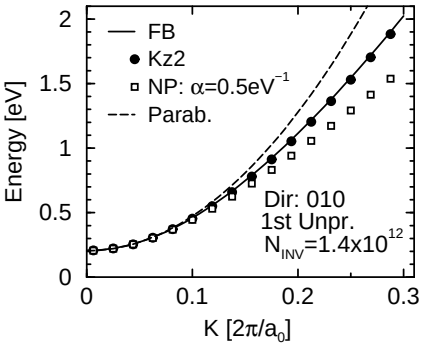

Figure 2: Energy dispersion within the first *unprimed* subband in the <010> direction. The Full Band (FB) solution is compared to the approximated **kz2**, non-parabolic (NP) and parabolic solutions. The **kz2** approximation is in close agreement with the FB case. Bulk MOSFET, $N_A{=}3{\times}10^{18}cm^{-3}$ and inversion density $N_{INV}{=}1.4{\times}10^{12}cm^{-2}$.

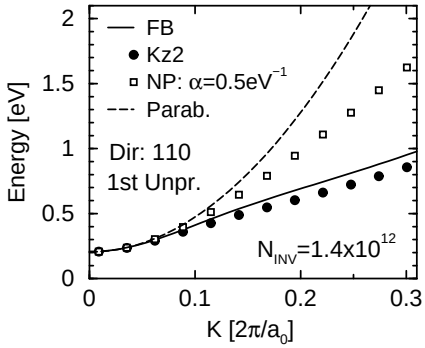

Figure 3: Same as Fig.2 for first *unprimed* subband in the <110> direction. The **kz2** approximation is in close agreement with the FB case, whereas the NP and parabolic approximations are vastly wrong.Same device as in Fig.2.

Figs.2 and 3 show the energy dispersion within the lowest *unprimed* subband in the <010> and <110> direction, respectively. The **kz2** model reproduces the FB results very closely. The NP models, instead, are reasonably accurate for the <010> direction (and the equivalent <100>), whereas they vastly overestimate the energy along the <110> direction.

For the *primed* minimum, we found that the results are similar to Fig.2 in the <100> direction (not shown), whereas all the approximated methods deviate from the FB results in the <010> direction (Fig.4). The reason is that (see Fig.5), if we consider different (k_x,k_y) along the <110 > direction, the FB energy changes drastically its dependence

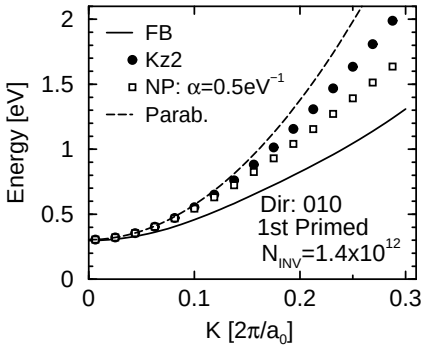

Figure 4: Same as Fig.4 for first Primed subband in the <010> direction. All the approximated solutions differ appreciably from the FB solution. Same device as in Fig.2.

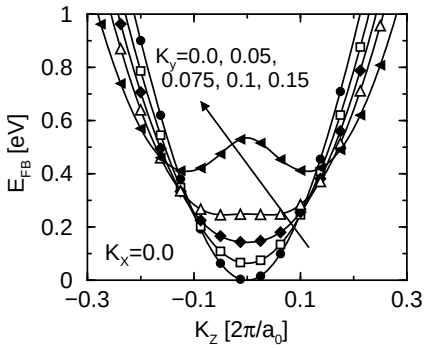

Figure 5: Bulk silicon FB energy E_{FB} versus k_z for different **k**=(k_x,k_y) values along the <010> direction around a *primed* minimum. Note that (k_x,k_y) are referred to the minimum, so that k_x=0 means k_x is exactly at the minimum. When k_y moves from the minimum the E_{FB} is a strongly non-parabolic function of k_z. Same device as in Fig.2.

on k_z, and the parabolic dependence on k_z assumed by all the approximated methods becomes incorrect.
More results pointing out interesting differences between the FB and the approximated solutions of the SEQ will be presented at the conference together with a comparison of the calculation of the Density of States.

4 Conclusions

In conclusion, we have presented a methodology to solve the quantization problem in the MOSFET according to the 3D Full Band (FB) structure, that can be used to benchmark simplified models. Furthermore, we have proposed an approach to efficiently and accurately model the energy dispersion within the subbands, that can be used to develop transport models for the 2D electron gas beyond the non-parabolic band approximation.

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