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A Comprehensive Modeling Study of Two-Dimensional Silicon Subbands Using a Full-Zone k.p Method

M. Szczap[1,2], N. Cavassilas[2], F. Michelini[2], F. Payet[1], F. Boeuf[1], and T. Skotnicki[1]
[1]STMicroelectronics, 850 rue Jean Monnet, 38920 Crolles Cedex, France
Phone: +33(0)4 38 92 36 88 E-mail: frederic.boeuf@st.com
[2]L2MP, CNRS, UMR 6137, Bât. IRPHE, Technopôle de Château-Gombert, 13384 Marseille Cedex 13

1. Introduction

So far, the continuous downscaling of MOSFETs dimensions has been a successful trend for keeping up with the ITRS requirements. Ultra-thin SOI transistors have revealed to be an interesting choice for applications below the 45 nm technology node because of their scalability [1]. In particular, the decrease of the silicon layer thickness (T_{Si}) has been proved to considerably reduce the short-channel effects [2], allowing the decrease of the substrate doping normally employed in bulk devices. In these conditions, it is reasonable to consider that carriers in the inversion layers are confined by a triangular quantum well whose slope is given by the effective field E_{eff}.

The well-known Airy analytical model has been widely used to obtain the electronic states in the inversion layer, which are necessary data for the calculation of transport properties such as mobility. But recent developments of quantum mechanical methods that include the full-band structure of Si [3, 4], e.g. the 30-band **k.p** method, allowed the investigation of the validity of such approximation in the case of thin and ultra-thin T_{Si}. To our knowledge, this has not been studied yet.

In this paper, we present results of two-dimensional (2D) (001)-Si subbands calculated with a 30-band **k.p** method [5] in the envelop function approximation [6], and compare them to Airy approximation. In particular, the E_{eff} and T_{Si} dependences of the electrons and holes energy levels are investigated. It is shown that for T_{Si} < 10 nm, the Airy approximation is no more valid for E_{eff} smaller than 0.8 MV/cm.

2. Computation of the 2D Silicon Subbands

We consider a triangular external electrical potential given by:

$$V = eE_{eff}z \tag{1}$$

where z is the direction of confinement, which corresponds to the crystal growth direction. The resolution of the Schrödinger equation gives rise to analytical solutions for the electrons wave functions and the energy levels:

$$\psi_i(z) = Ai\left(\left(\frac{2m_e eE_{eff}}{\hbar^2}\right)^{1/3}\left(z - \frac{E_i}{eE_{eff}}\right)\right) \tag{2}$$

$$E_i = \left(\frac{\hbar^2}{2m_e}\right)^{1/3}\left(\frac{3\pi eE_{eff}}{2}\left(i + \frac{3}{4}\right)\right)^{2/3} \tag{3}$$

The index i represents the level number, and m_e the electron effective mass. We thus obtain two sets of energy subbands: E_i with m_e=m_l, and E_i' with m_e=m_t. It must be noted that there is no T_{Si} dependence in equations 2 and 3.

We applied the same electrical potential V to our "full-zone" 30-level **k.p** model. The main advantage of this method is that both electrons and holes confined states, and their corresponding wave functions, can be calculated at any point of the 2D Brillouin zone (Figs. 1 to 3). Moreover, this method gives similar results to the tight-binding approach [7], another semi-empirical computational method that has been extensively used to investigate the confined states in bulk semiconductors.

3. Results and Discussion

First, we studied the influence of T_{Si} on the energy shifts of the six first subbands of the electrons in the 2-fold and 4-fold valleys, at various E_{eff} (0.05, 1 and 2 MV/cm). Although the majority of carriers occupy the three first subbands, at least six subbands are necessary for transport calculations [8]. Figs. 4 and 5 represent the difference between the energy levels obtained with the **k.p** method and those obtained with the Airy approximation vs. T_{Si}. Both figures show a universal behavior of this error when varying T_{Si}. For T_{Si} < 10 nm, the discrepancy between Airy approximation and the full-zone method becomes non negligible, even for high E_{eff}. Yet, it must be noted that the 2-fold error increases unexpectedly when T_{Si} increases, which may be due to a non sufficient optimization of the **k.p** coupling parameters. This can be greatly improved.

Then, we fixed T_{Si} to 10 nm and we studied the influence of E_{eff} on electrons and holes energy shifts (Fig. 6 and 7). Results show that for E_{eff} > 0.8 MV/cm, Airy approximation remains valid, whereas at small E_{eff}, the **k.p** method gives much higher results. Indeed, the latter correspond to the energy shifts obtained in the case of an infinite square well of size T_{Si}, which is easily understandable for very small E_{eff}. Airy approximation does not reproduce this result, since E_i tends to zero when E_{eff} tends to zero. We also demonstrate in Fig. 7 that it is possible to describe the holes energy levels with an Airy-like analytical expression, by inputting an appropriate set of effective masses.

Finally, device engineers might be interested in having access to charts giving energy shifts and effective masses for any E_{eff} and T_{Si}. As an example, we present in Fig. 8 charts giving the three first electron energy levels of the 2-fold valleys. Effective masses are to be studied in a future work.

4. Conclusions

A novel description of the 2D silicon subbands in a triangular quantum well has been presented using a full-zone 30-band **k.p** method. A comparison to Airy approximation revealed that for small to mean effective fields (up to 0.8 MV/cm), this model can not be applied to silicon layers of less than 10 nm. From a practical viewpoint, this full-zone method can provide charts of energy levels and effective masses. This should facilitate transport and compact modeling calculations. The energy shifts and effective masses calculated with this method can also be used as inputs in

the analytical model for phonon-limited electron mobility presented in [9].

Acknowledgements

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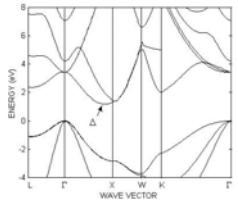

Figure 1: Band structure of bulk Si calculated with a 30-band k.p Hamiltonian. In bulk Si, electrons are mainly located in the 2-fold (Δ_2) and 4-fold (Δ_4) valleys designated by Δ.

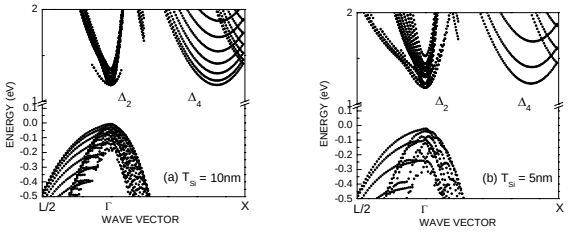

Figure 2: Subband structure of a (a) 10nm and (b) 5nm (001)-Si layer calculated using a 30-band **k.p** model under the envelop function approximation. Δ_2 electrons are in the center of the 2D Brillouin zone.

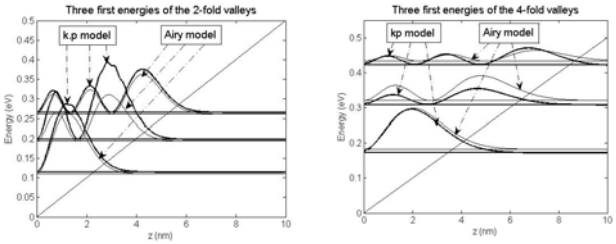

Figure 3: Representation of the two sets of energies (E_0, E_1, E_2) and (E_0', E_1', E_2') at E_{eff}= 0.5 MV/cm, and their associated wave functions. Thin lines, Airy solutions, bold lines, 30-band **kp** solutions.

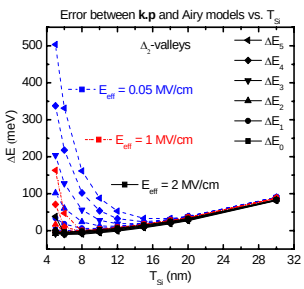

Figure 4: Calculated error between energy shifts of the 2-fold valleys obtained with the 30-band **k.p** and Airy models, in function of T_{Si} and for E_{eff}=0.05, 1 and 2 MV/cm.

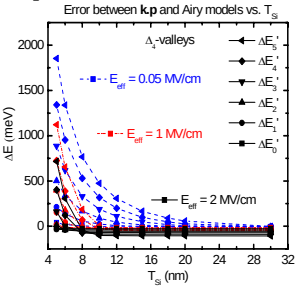

Figure 5: Idem as Fig. 4, but for the 4-fold valleys. Both figures present the same universal characteristics with T_{Si}.

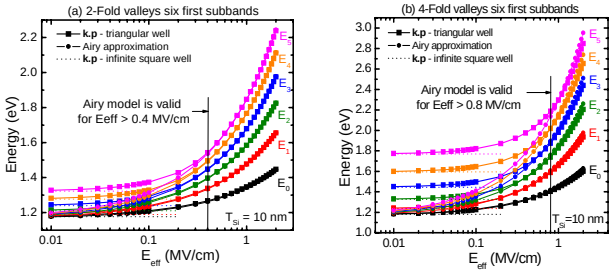

Figure 6: Calculated energy shifts of the six first electron subbands for (a) 2-fold valleys and (b) 4-fold valleys, in function of E_{eff}.

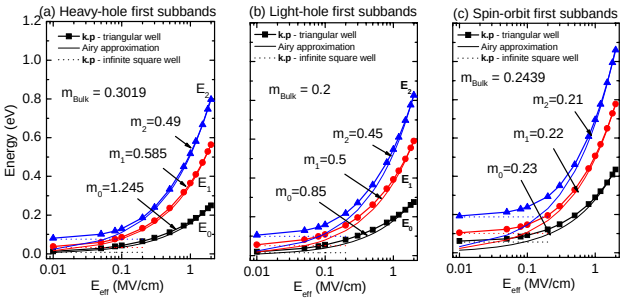

Figure 7: Calculated energy shifts of the three first hole subbands at T_{Si}=10nm for (a) heavy-hole, (b) light-hole and (c) spin-orbit bands, in function of E_{eff}.

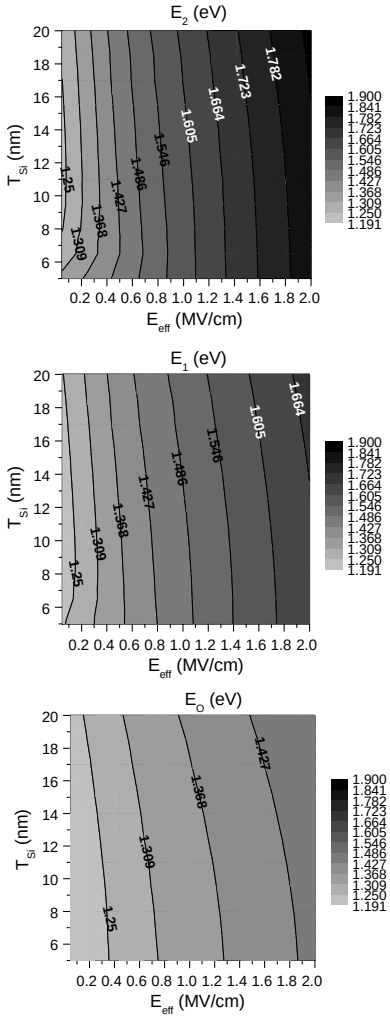

Figure 8: Color maps of the three first subbands of electrons in the 2-fold valleys in function of T_{Si} and E_{eff}.