Modeling of Macroscopic Transport Parameters in Inversion Layers

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Abstract

We present a parameter extraction technique for higher-order transport models for a 2D electron gas in ultra thin body SOI MOSFETs. To describe 2D carrier transport we have developed a self consistent Schrödinger-Poisson Subband Monte Carlo simulator. The method takes into account quantization effects and a non equilibrium distribution function of the carrier gas, which allows an accurate description of the parameter behavior for high electric fields. Finally the results are compared with the transport parameters of 3D bulk electrons and the influence of the channel thickness on the mobility is investigated.

1 Introduction

As the dimensions of modern semiconductor devices have reached the deca-nanometer regime, the drift-diffusion model, which is still the workhorse of today's TCAD tools, becomes more and more inaccurate [1]. Promising results have been obtained from higher-order transport models systematically derived from Boltzmann's equation [2] which can cover the important gate-length range down to about 25 nm [1]. An advantage of the drift-diffusion model is that it contains only one transport parameter, the carrier mobility which can be taken from measurement. For the energy-transport model and the six moments model additional parameters have to be supplied. However modeling of these transport parameters is highly critical. So far, these parameters have been determined using bulk Monte Carlo simulations and successfully used in table-based macroscopic transport models for nin-structures [2]. However, since the transport parameters are fundamentally affected by the surface properties and quantization in the inversion layer of ultra-thin body (UTB) SOI MOSFETs [3], the application of bulk parameters is questionable.
In Section 2, the transport equations of the six moments model are given incorporating the extracted transport parameters for a 2D electron gas obtained by the Schrödinger-Poisson Solver VSP [4] self consistently coupled with the Subband Monte-Carlo simulator VMC [5]. The according extraction technique is presented in Section 3 followed by a discussion of the results in Section 4.

2 Transport Model

Higher-order transport models are systematically derived from Boltzmann's equation applying the method of moments [6]. Modeling the scattering operator by a macro-

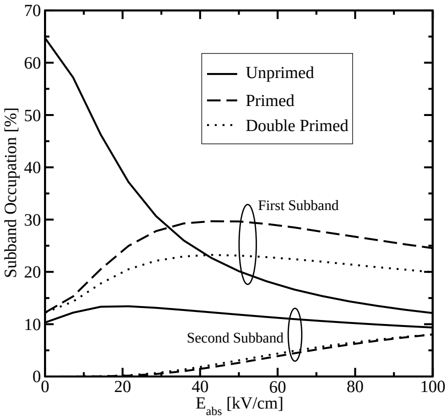

Figure 1: Populations of the first two subbands in the unprimed, primed, and double primed valleys versus the lateral field. Relative occupations are shifted to higher subbands in each valley for higher fields.

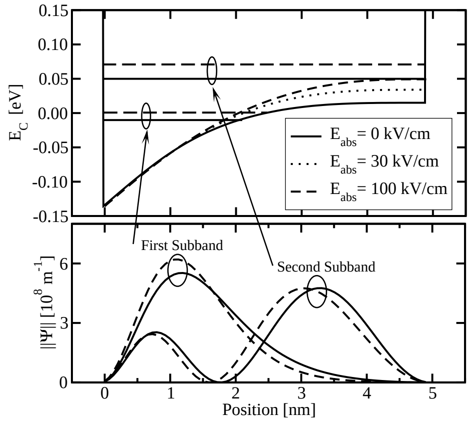

Figure 2: Conduction band and wavefunctions of a UTB SOI for different electric fields. Both the wavefunctions and subbands are shifted with increasing lateral fields.

scopic relaxation time approximation and multiplying with a proper set of weight functions, one obtains the drift-diffusion, the energy-transport and the six moments model [2]. The general moment equations read

$$\partial_t (nw_i) + \nabla \cdot (n\mathbf{V}_i) - i\mathbf{F} \cdot n\mathbf{V}_{i-1} = -n\frac{w_i - w_{i,0}}{\tau_i}\,, \tag{1}$$

$$n\mathbf{V}_i = -\frac{2\mu_i H_{i+1}}{3\mathrm{q}} \left(\nabla (nw_{i+1}) - n\mathbf{F}w_i \frac{3+2iH_i}{2H_{i+1}} \right). \tag{2}$$

In this hierachy, the even moments describe conservation equations while the odd ones are fluxes. w_{i+1} are related to the average energies of each moment while $\mathbf{V}_i$ is the average product of the velocity with the moment related energy. H_{i+1} are the non-parabolicity factors. Therefore the transport parameters arising in the six moment models are the carrier mobility μ_0, the energy-flux mobility μ_1, the energy relaxation time τ_1, the second-order energy-flux mobility μ_2, and the second-order energy relaxation time τ_2.

3 Parameter Extraction

In order to efficiently and rigorously extract the required parameter set, a self consistent Schrödinger-Poisson Subband Monte Carlo (SP-SMC) simulator [4, 5] has been developed. Based on the subband structure, MC calculations are performed taking phonon induced scattering and surface roughness scattering into account. The non-parabolicity of the band structure is treated by Kane's model. Parameters extracted at this step are valid within the low field regime. Once a driving field is applied in transport direction, the assumption of equilibrium carrier distribution is no longer valid: the carriers

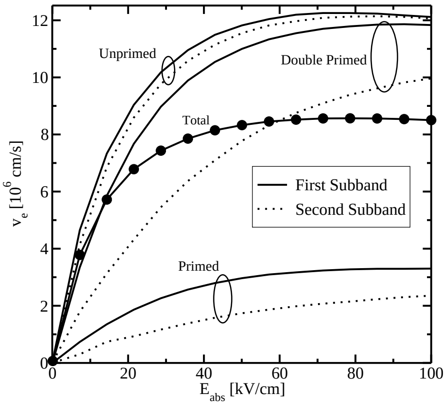

Figure 3: Velocities in the first and second subband of the unprimed, primed, and double primed valleys as well as the average total velocity versus the lateral field. An effective field of $450\,\mathrm{kV/cm}$ is applied.

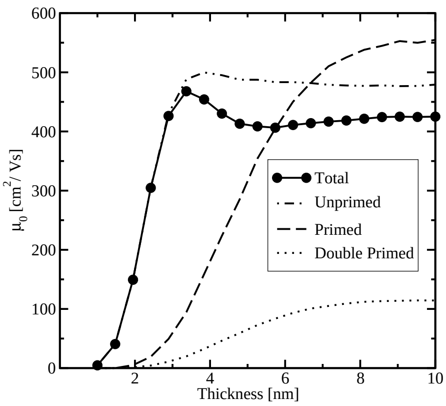

Figure 4: The mobilities of the unprimed, primed, and double primed valleys and the total average mobility as a function of the channel thickness at zero field condition.

gain kinetic energy resulting in a reoccupation of the subband ladders (Fig. 1) which itself shifts the wavefunctions within the inversion layer. Hence, the scattering rates are affected following from the change in the overlap integral of the scattering operator. Furthermore, the subband ladder reconfiguration leads to a variation of the spatial distribution function of the electrons which itself has an impact on the shape of the potential well that forms the inversion channel (Fig. 2).

4 Results

As an example, a UTB structure with a film thickness of 5 nm and an acceptor doping of $2 \times 10^{16}\,\mathrm{cm}^{-3}$ has been investigated. After convergence of the SP-SMC loop is achieved, the parameters are extracted from the SMC simulator. The resulting carrier velocities as a function of the lateral field are presented in Figure 3. Due to different conduction masses in transport direction of each valley as well as a strong occupation of the primed valley in the high field regime (see Fig. 1), the total velocity is lower than in the unprimed and the double primed valley. In Figure 4, we show the mobilities in each valley and the total average mobility as a function of the channel thickness. To first order the mobilities are indirectly proportional to the effective masses. Therefore the difference of the mobilities are due to different conduction masses in each valley. The hump in the total average mobility is due to a high occupation of the unprimed ladder (see Fig.1). Increasing channel thickness results in an occupation of the remaining subband ladders. Hence the total mobility increases until the occupation of the other ladders reaches the same value. This is the maximum point, the hump.
A comparison of the energy-flux mobility and the kurtosis-flux mobility as well as the corresponding relaxation times between a 2D and bulk electron gas is shown in Figures

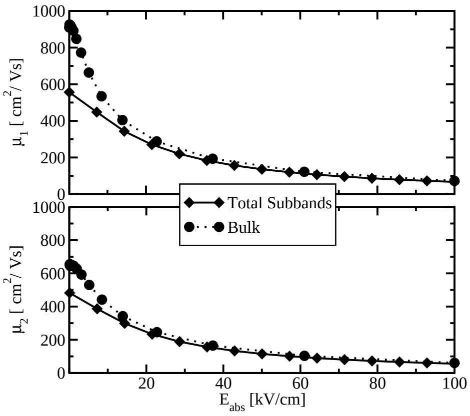

Figure 5: The energy-flux and the second-order energy flux mobility obtained by SP-SMC and bulk MC simulations. The mobilities behave analogously to the relaxation times.

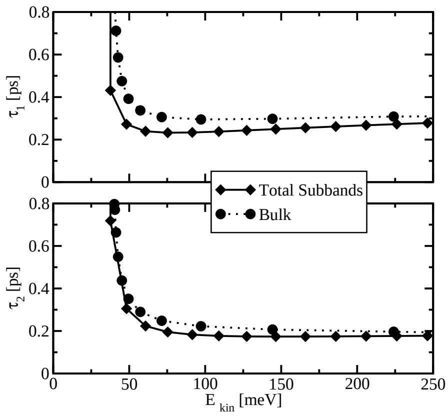

Figure 6: A comparison of the subband MC results with the bulk case for the energy relaxation time and the second-order energy relaxation time. The increased scattering rates in the SMC case lead to lower relaxation times compared to the bulk case.

5 and 6, respectively. We observed that the higher-order mobilities of the 2D electron gas is higher than in the bulk case which can be explained as follows: Due to Heisenberg's uncertainty principle, there is a wider distribution of momentum in the quantization aera, because of a higher localization of the particles than in the bulk. Hence there are more bulk phonons available that can assist the transition between electronic states. This will lead to an increase of the phonen rates and a decrease of the mobilities [7]. An increase of the phonon scattering rates will lead to a decrease of the relaxation times (see Fig. 6).

5 Conclusion

Advanced macroscopic transport models require an accurate set of transport parameters which are not directly accessible to measurements. With the presented approach it is possible to extract and tabulate a 2D parameter set for instance for the important case of ultra-thin body SOI MOSFETs.

References

[1] T. Grasser *et al.*, in *Proc. SISPAD* 1 (2004)
[2] T. Grasser *et al.*, J. Appl. Phys. **97**, 093710 (2005).
[3] H. Lucci *et al.*, in *Proc. ESSDERC* 321 (2004)
[4] M. Karner *et al.*, in *11th IWCE* 255 (2006)
[5] http://www.iue.tuwien.ac.at/software, *VMC 2.0 User's Guide*, Institut für Mikroelektronik, Technische Universität Wien, Austria, 2006.
[6] T. Grasser, PhysicaA **349**, 221 (2005).
[7] F. Gamiz *et al.*, J. Appl. Phys **89**, 5478 (2001).