NUMERICAL MODELING OF MOS-DEVICES: METHODS AND PROBLEMS

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ABSTRACT - Methods and problems in the field of modern MOS-modeling are reviewed. Models for surface scattering and impact ionization, physical parameters which are of particular relevance for MOS-Transistor simulation programs, are explained. The various conceptional approaches for the numerical solution of the classical semiconductor equations are compared. An example of application of a simulation program on the analysis of problems which are important at present is sketched.

1. INTRODUCTION

Numerical MOS-modeling has become a basic requirement for the development of prototype devices, although the first modeling attempts were made relatively recently. A two dimensional solution of Poisson's equation with application to a MOS structure was probably first published by Loeb et al. /45/ and Schroeder and Muller /64/ in 1968. Since then much work has been contributed dealing with simulation of MOS devices due to their intrinsically two dimensional nature, e.g.: in 1971 /87/, in 1972 /88/, in 1973 /39/, /48/, in 1976 /36/, in 1977 /31/, in 1978 /54/, /83/, in 1979 /40/, /65/, in 1980 /18/, /55/, /66/, /84/, in 1981 /41/, /60/, /93/, in 1982 /58/, /61/, /62/, /90/ and in 1983 /42/, /51/. Two dimensional transient simulations of MOSFET's have been carried out in, e.g.:/49/, /53/ and /95/. Three dimensional static modeling has been published in, e.g.:/14/, /37/, /74/.

In the following chapters particular emphasis will be laid on two phenomena of major importance for MOS-Transistor modeling: these are the influence of surface scattering on carrier mobility and the contribution of impact ionization to carrier generation. The established concepts for device modeling in general are assumed to be familiar to the reader. As basic literature for the newcomer one can suggest the monographs /44/, /50/ and /69/ or the various conference proceedings, e.g.:/3/, /10/, /11/, /12/, /24/, /47/ and /85/ or the review papers /8/, /26/, /29/ and /52/.

2. SURFACE SCATTERING

Out of the many scattering effects which the carrier mobility is determined by only surface scattering will be treated here as it is the essential effect in MOSFET's. In theory surface scattering consists of a lot of different mechanisms such as surface roughness scattering, scattering by interface charges, scattering by surface phonons and various quantum effects. Unfortunately, the problems associated with conduction at surfaces have not been investigated as deeply as one would expect. Many physics oriented investigations are carried out at low temperatures because the results can be interpreted much more easily. Therefore, all models which are presently used have been constructed on a fully empirical basis with a scope to reflect the main experimental findings as well as possible.

It was Yamaguchi who suggested one of the earliest models /92/. He has used the formula of Scharfetter and Gummel /63/ for lattice scattering, impurity scattering and mobility reduction due to velocity saturation ($\mu_{n,p}^{LIE}$) and an additional factor to reduce the mobility in the presence of an electric field component perpendicular to the current flow direction.

$$\mu_{n,p}^{LIES} = \mu_{n,p}^{LIE} \cdot \frac{1}{\sqrt{1 + \frac{|\vec{E} \times \vec{J}_{n,p}|}{E_{n,p}^{crit} \cdot |\vec{J}_{n,p}|}}} \qquad (2.1)$$

This model has been used and recommended by many others, too, e.g. /23/, /26/, /27/, /53/, because it has been claimed that excellent agreement with experimental results is obtained. However, Thornber /82/ has strongly criticized Yamaguchi's treatment using theoretical arguments. The saturation velocity $v_{n,p}^{sat}$ associated with $\mu_{n,p}^{LIE}$ is scaled with the same factor, obviously, as the mobility. Sabnis and Clemens /59/ have experimentally proved that surface scattering is almost independent of the doping concentration. Cooper and Nelson /19/, /20/ have shown with elaborate measurements that the influence of surface fields on the saturation velocity is relatively small, which is in contradiction to former opinions (cf. /38/) but which is quite believable considering their experiments. Very careful measurements on that subject have been published in /77/, too. Thornber's suggestion /82/ to use a relation of the form (2.2) for the total effective mobility μ^{LIES} is well accepted today.

$$\mu^{LIES} = \mu^{LIES}(\mu^{LIS}(\mu^{LI}, E_{\perp}), E_{||}, v^{sat}(E_{\perp})) \qquad (2.2)$$

The function μ^{LIS} combines the mobility due to lattice and ionized impurity scattering with the influence of surface scattering ($E_\perp$ denotes the field component responsible for surface scattering) to a cold carrier mobility, which is then combined with the driving force denoted by $E_\parallel$ (usually the field component parallel to the current flow direction or the gradient of the carrier quasi-Fermilevel) and the saturation velocity which might be a function of $E_\perp$ to the total effective mobility μ^{LIES}. μ^{LIS} may have the functional form of (2.1) as long as good agreement between simulated and measured results is obtained. Yamaguchi, as a matter of fact, has revised his model in a later paper /94/ by exactly following the suggestions of Thornber.

I have suggested the following expression for the influence of surface scattering /67/, /68/.

$$\mu^{LIS}_{n,p} = \mu^{LI}_{n,p} \cdot \frac{x + x^{ref}_{n,p}}{x + b_{n,p} \cdot x^{ref}_{n,p}} \tag{2.3}$$

x denotes the distance perpendicular to the interface. Directly at the interface (x=0) the mobility is reduced by a factor 1/b; at a distance $x=x^{ref}$ it is reduced by the factor 2/(1+b); and at greater distance from the surface it naturally follows that the reduction factor approaches unity. x^{ref} represents a characteristic length which describes the range of influence of the surface.

$$x^{ref}_{n,p} = \frac{x^{o}_{n,p}}{1 + \frac{E_{n,p}}{E^{crit}_{n,p}}} \tag{2.4}$$

This range is modeled as a function of the carrier driving force (field component parallel to current flow or magnitude of the gradient of the corresponding quasi-Fermi potential). The formulation of x^{ref} produces a reduction in the range of influence of surface scattering for greater driving forces, thereby velocity saturation appears. Carriers already traveling with the saturation velocity can be considered not to experience the influence of the surface as much as cold carriers /46/. The parameter "b" in (2.3) describes the strength of the influence of surface scattering.

$$b_{n,p} = 2 + \frac{E_\perp}{E^{crit}_{\perp n,p}} \tag{2.5}$$

It is modeled as a function of $E_\perp$ which can be the electric field

component perpendicular to current flow, or the electric field component perpendicular to the interface, or, what I suggest, the projection of the electric field component perpendicular to the current flow direction onto the direction perpendicular to the surface. The formulation of b is based on the fact that the charge carriers are pressed against the surface by an electric field, which results in a greater scattering, in such a way that a greater mobility reduction occurs. Without any electric field one also observes a mobility reduction due to surface roughness scattering (b=2). However, it is to note that (2.3) is a fully phenomenological expression neither of which the structure nor the associated parameters may be claimed to be correct in a theoretical sense. It simply represents my experience which has been confirmed over several years by many users of our simulation tools that an expression with such a structure nicely reflects the experimental observations.

There are plenty more suggestions on how to treat surface scattering phenomenologically. The interested reader could have a look at, e.g., /2/, /4/, /17/, /28/, /77/, /89/.

3. IMPACT IONIZATION

The physical mechanism of major importance for particularly miniaturized MOSFET's in the context of generation/recombination modeling is impact ionization. Two partial processes have to be considered.

a) electron emission: an electron from the valence band moves to the conduction band by consuming the energy of a high energetic electron in the conduction band and leaving a hole in the valence band.
b) hole emission: an electron from the valence band moves to the conduction band consuming the energy of a high energetic hole in the valence band. A hole is left at the valence band edge.

These partial rates can be written:

$$G_n^{II} = \alpha_n \cdot \frac{|\vec{J}_n|}{q} \tag{3.1}$$

$$G_p^{II} = \alpha_p \cdot \frac{|\vec{J}_p|}{q} \tag{3.2}$$

The total rate is simply the sum of the partial rates.

$$R^{II} = -G_n^{II} - G_p^{II} \tag{3.3}$$

α_n and α_p are the ionization rates for electrons and holes defined as generated electron-hole pairs per unit length of travel and per electron and hole, respectively. For instance, an electron generates over a distance $1/\alpha_n$ one electron-hole pair on average. The energy which is consumed from the ionizing carrier is termed ionization energy or threshold energy for ionization E_i. This quantity has been a subject to a lot of discussions lately with results differing widely. Similarly, the theoretical results for the ionization rates α_n, α_p are not unique. However, both theoretical and experimental investigations indicate a good approximation to be an exponential dependence of the ionization rates upon the electric field component E in direction of current flow.

$$\alpha_n = \alpha_n^{\infty} \cdot \exp\left(-\left(\frac{E_n^{crit}}{E}\right)^{\gamma_n}\right) \tag{3.4}$$

$$\alpha_p = \alpha_p^{\infty} \cdot \exp\left(-\left(\frac{E_p^{crit}}{E}\right)^{\gamma_p}\right) \tag{3.5}$$

The exponents γ_n, γ_p are found in the range [1,2]. As a matter of fact fairly early theoretical considerations by Shockley /75/ predict the exponents to be one, which has been also the very old experimental finding by Chynoweth /16/. A different treatment by Wolff /91/ predicts the exponents to be two. A menu of numerical values for the coefficients of (3.4) and (3.5) compiled from literature data is given in /69/. Temperature dependent ionization coefficients which are claimed to perfectly fit measurements have been given in /25/, /57/.

Baraff /9/ has claimed these theories to be two limiting cases of a more rigorous model. For low fields Shockley's model is more suitable, whereas for high fields Wolff's model is asymptotically correct. Unluckily, Baraff's results cannot be given in closed form; they have been obtained by a numerical solution of the Boltzmann transport equation, however, restricted to the assumption of an unrealistic band structure. However, a universal plot for both electrons and holes has been presented, which shows

$$\alpha \cdot \lambda = f\left(\frac{E_r}{E_i}, \frac{E_i}{q \cdot \lambda \cdot E}\right) \tag{3.6}$$

λ is the mean free path between collisions with high energetic phonons; E_r is the average loss of energy defined per such collision; and E_i denotes the ionization energy, as already defined.

There is still the pending question whether these theoretically obtained results agree with experimental results. The answer to this question is not a trivial one. Provided that one takes the numerical values for λ, E_r and E_i from /22/, the measured results of Lee et al. agree satisfactorily with Baraff's results. The experimental results of, e.g. Van Overstraeten et al. /86/ and Grant /32/, would require totally unrealistic values for λ, E_r and E_i to agree with Baraff's results. On the other hand, in, e.g. /61/, /76/, /81/ the ionization rates of Van Overstraeten et al. have been used, whereby good agreement between experimental and simulation results on device breakdown phenomena has been obtained. The influence of the models for the ionization coefficients upon simulated device performance can be indeed very pronounced /1/.

Chwang et al./15/ have rigorously obtained the same results as Baraff with a completely different approach for the calculation, however, with essentially the same assumptions.

More recently it has been tried to calculate the impact ionization coefficients by Monte Carlo methods taking into account a realistic band structure /72/, /73/, /80/. This interesting work, however, is subject to considerable controversy /13/, /35/.

In the context of impact ionization in very small devices and for low bias applications one problem, the dark space phenomenon, has to be faced. In regions of a device with a large gradient of the electric field component parallel to current flow all models of impact ionization which we have discussed can be expected to overestimate the ionization rates. The carriers first have to gain an energy on their path through the device which is larger than the threshold energy for ionization before impact ionization can take place. The ionization rate at a specific place, thus, will depend, qualitatively spoken, not only on the local field, but also upon the field distribution in that vicinity. Therefore, the dark space phenomenon is frequently termed a non-local effect, e.g. /56/. A rigorous treatment of this and related phenomena /71/ with models consisting of pure differential equations is impossible; it is also inconsistent with the usually assumed current relations because for their derivation moderate gradients for the electric field have been assumed (cf. /70/). In a very recent paper /43/ an approach to tackle this problem has been proposed, which is basically an extension of Shockley's "Lucky Electron" model. However, in order to understand the many detailed effects of impact

ionization many more experimental and theoretical investigations have to be undertaken.

4. NUMERICAL APPROACHES

Numerical models for the simulation of semiconductor devices are primarily based on the solution of the so-called basic semiconductor equations. These well known equations consist of Poisson's equation (4.1), the continuity equation for electrons (4.2) and the continuity equation for holes (4.3) together with suitable constitutive relations for the current densities $\vec{J}_{n,p}$ and models for the various physical parameters.

$$\text{div grad } \Psi = \frac{q}{\varepsilon} \cdot (n - p - C) \tag{4.1}$$

$$\text{div } \vec{J}_n - q \cdot \frac{\partial n}{\partial t} = q \cdot R \tag{4.2}$$

$$\text{div } \vec{J}_p + q \cdot \frac{\partial p}{\partial t} = -q \cdot R \tag{4.3}$$

The selfconsistent solution of this set of equations is a fairly expensive task in view of computational resources. Therefore several approaches towards a simplification of the basic equations have been developed by physically reasoning in order to reduce simulation costs. However, it is obvious that simplifications introduce systematic errors. The user of a device simulation program must therefore allways bear carefully in mind which restrictions his particular model is based on. In the following the various simplified approaches which have proven to be specifically usefull for the simulation of MOS-Devices will be sketched.

Approach 1: Poisson's equations is solved in two space dimensions with sophisticated assumptions on the quasi-Fermilevel of the minority carriers (electrons for an n-channel FET). The quasi-Fermilevel of the majority carriers (holes for an n-channel FET) is assumed to be constant which implies that no majority carrier current flow takes place. This method is only applicable for device operating conditions in the subthreshold regime. One program based on this approach is, e.g., GEMINI /33/.

Approach 2: Poisson's equation is solved in two space dimensions together with a one-dimensional continuity equation for the minority carriers. Majority carrier current flow is neglected. This model is

usefull in the subthreshold regime and close to threshold. Simulation programs which allow this mode of simplification are, e.g., GALENE /26/ and MINIMOS /66/.

Approach 3: Poisson's equation and the minority carrier continuity equation are solved consistently. Hole current flow is neglected. Simulations with this model allow a sufficiently accurate analysis of MOS-Transistors, if impact ionization is negligible. This approach is supported by all established MOS simulation codes, e.g., CADDET /48/, DEVICE /30/, GALENE /26/, MINIMOS /66/.

Approach 4: All three basic semiconductor equations (4.1), (4.2) and (4.3) are solved selfconsistently (possible with, e.g. GALENE /26/, MINIMOS /62/). This allows to account for impact ionization within the computations which enables the analysis of avalanche breakdown and substrate currents. However, it is to note that the basic semiconductor equations themselves have been derived under many non-trivial assumptions (cf. /69/). There arise conditions in practice for which their applicability is at least in doubt, if it exists at all, e.g.: quantuum effects, strong degenerate material, non-local effects. One certainly has to take trade-offs between accuracy and complexity to have an effortable tool, since the more elaborate results in semiconductor physics are too complex to constitute a generally applicable and still sufficiently simple model for device simulation. Physically motivated on should proceed for an actual simulation starting with the lowest approach and using the results succesively for the next higher approach. This strategy is frequently termed STEPSOLVING /26/.

Considering any of the approaches 2-4 the non-trivial question which linearization method to pick for the coupled nonlinear equations has to be dealt with. The classical method, Newton's method, leads to indeed a fairly complex implementation task and also to some difficulties in detail. One such problem is frequently termed overshoot. The initial guess is usually so far off the final solution that the Newton correction vector is overestimated in length. Therefore, a damp procedure has to be introduced to adjust appropriately the length of the correction vector. Besides many heuristic approaches the probably best suitable methods for the semiconductor equations have been presented in /6/ and /7/. To overcome the laborious work with Newton's method and it's associated problems a block-nonlinear iterative scheme has already been

introduced in the early days of modeling /34/. This scheme which is commonly termed Gummel iteration has been given preference by most authors of simulation programs because of the relatively simple implementation. However, the convergence properties can become fairly poor when the coupling between the respective equations is strong (cf. /21/).

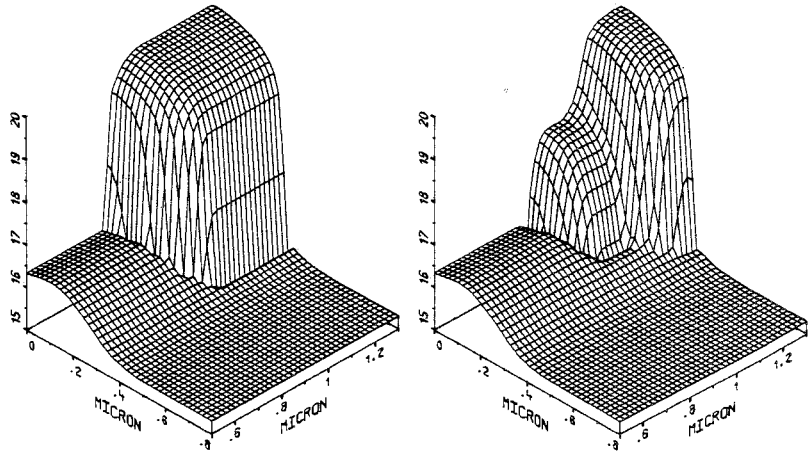
5. AN EXAMPLE: IMPACT IONIZATION IN LDD MOSFET'S

New concerns about degradation of transistor characteristics due to impact ionization are introduced by the scaling of feature sizes in VLSI devices. Therefore, many process modifications have been suggested to either reduce the peak electric field in the drain region or to shift the region of the peak electric field from underneath the gate electrode more down into the bulk, e.g., /78/, /79/. One such concept is based on having lightly doped drains (LDD). It is intuitively expected that MOSFET's with LDD are less sensitive to impact ionization than conventional devices. However, only little data has been published on the real performance bargain obtained by the LDD concept /5/.

To outline the influence of the LDD on the peak electric field and the impact ionization rate two transistors each with 1µm channel length have been simulated with the MINIMOS program /62/, /66/. The doping profile of these transistors is shown in Fig. 1. To give a better visibility only one half of the transistors, starting from the middle of the channel up to the heavily doped drain area, has been drawn.

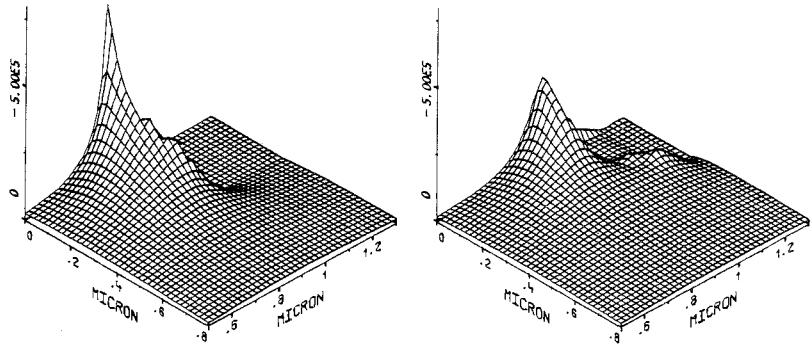
In Fig. 2 the lateral component of the electric field, i.e. the component parallel to the interface is shown. The windows of the drawings are the same as for the doping profiles. The peak electric field is reduced from $6.4 \cdot 10^{-5}$V/cm in the conventional structure to $3.3 \cdot 10^{-5}$V/cm in the device with the LDD at the bias conditions (UGS=1V, UDS=5V). The success of the LDD on reducing the peak electric field is clearly demonstrated thereby.

Fig. 3 shows the impact ionization rates for the two transistors. The maximum ionization rate is reduced from $4.2 \cdot 10^{28}$ pairs per cubic centimeter and second to about $1.3 \cdot 10^{27} cm^{-3} s^{-1}$. Furthermore the area covered by impact ionization is also smaller in the LDD device and the behavior close to the maximum is much smoother. Therefore, a non-neglible reduction of the substrate current (about 75%) can be observed.



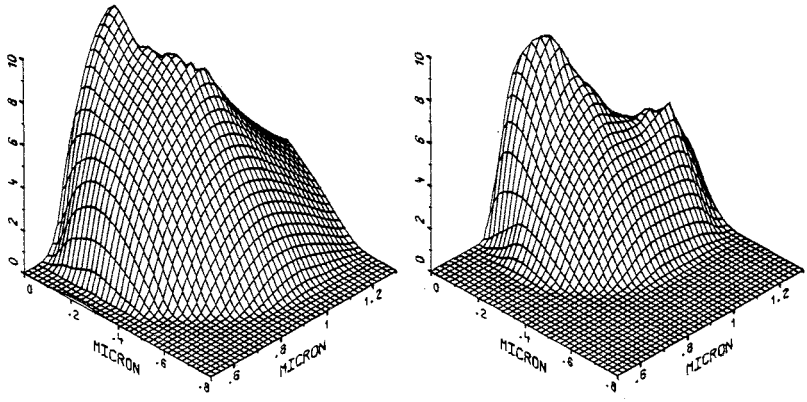
without LDD with LDD

Fig. 1: Doping profile, log.scale, [cm^{-3}]



without LDD with LDD

Fig. 2: lateral component of electric field, lin.scale, [V/cm]



without LDD with LDD

Fig. 3: Impact ionization rate
scale: $-\mathrm{sign}(R)\cdot\log(1+|R|/10^{18}\mathrm{cm}^{-3}\mathrm{s}^{-1})$, [ ]

6. CONCLUSION

Some aspects of modern MOSFET modeling have been reviewed. It should be explicitly stated that progress in this field can only be expected if progress in the understanding of the basic physical phenomena of carrier transport in MOSFET's is achieved. The mathematical prerequisites to model MOS-Transistors are sufficiently developed to carry out simulations for research purpose with a considerable, but acceptable amount of computer resources. However, as simulation programs improve in scope, reliability and accuracy, it can be expected that their use to aid device development will still significantly increase.

ACKNOWLEDGEMENT

I am in dept to Prof.H.Pötzl for many stimulating discussions and critically reading my manuscript. Considerable support has been granted by Siemens AG, Munich and by the "Fonds zur Förderung der wissenschaftlichen Forschung" (Project Nr.S43/10). I thank all of my colleages who have contributed to much of the material presented herein. Excellent computer access has been provided by Dipl.Ing.D.Schornböck with assistence of the whole staff of the computer center.

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