THE STATUS OF MINIMOS

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ABSTRACT: MINIMOS, the Viennese two-dimensional MOS device simulation program, has been under development for almost seven years. The features of the most recent version of MINIMOS are described with particular regard to the implemented physical models. Some of the presently used numerical techniques are commented. An example demonstrates the capability of MINIMOS to tackle ULSI simulation problems.

1. HISTORY

The development of MINIMOS started in late 1978 with my Ph.D. project which was finished in 1981 [16]. In these days the first version of MINIMOS, MINIMOS 1.x, was made available to the public domain. This version was a fairly conventional one carrier model of the MOSFET in two space dimensions [15]. In late 1979 Schütz started within his Ph.D. project to implement majority carrier current flow and impact ionisation into MINIMOS. After completion of this project in 1982 [11]MINIMOS 2.x was released to the public domain. This simulation tool has been the very first which allows a selfconsistent treatment of avalanche [12], [13]. Impact ionisation has been taken into account by an additional inhomogeneity term, the avalanche generation rate, in the current continuity equations. Then a phase of little improvements took place for some time where a few of the various bugs — which one always has to face with a larger software project — could be eliminated and some improvement in tuning the physical models has been achieved [17], [18]. One development since then was the extension to account for a non-uniform lattice temperature by solving the heat flow equation [14]. However, the results one can obtain thereby are indeed no spectacular improvement. This version of MINIMOS has therefore not been released to the public domain.

The most recent and completed development of MINIMOS involves modifications to the transport model, i.e., the current relations, in order to account more appropriately for carrier heating. The underlying physical models have been derived by Hänsch [4], [5]. This version of MINIMOS is being released to the public domain as MINIMOS 3.x. Our present development concerns the extension of MINIMOS to allow simulations in three space dimensions. This work was started in late 1985.

Up to now MINIMOS has been licensed to about 300 institutions. It has been successfully implemented on about 120 different computers and 40 different operating systems.

2. THE BASIC EQUATIONS

The basic equations which are presently implemented in MINIMOS to describe current flow in silicon differ only slightly from the conventional equations. The Poisson equation (1) and the continuity equations for electrons (2) and holes (3) are "the" established basic equations which are in use in anybody's simulator. A derivation of these equations can be found in, e.g., [20].

$$\text{div grad } \psi = \frac{q}{\epsilon}\cdot(n - p - C) \tag{1}$$

$$\text{div } \vec{J}_n - q\cdot\frac{\partial n}{\partial t} = q\cdot R \tag{2}$$

$$\text{div } \vec{J}_p + q\cdot\frac{\partial p}{\partial t} = -q\cdot R \tag{3}$$

The current relations for electrons (4) and holes (5) are somehow different to the conventional drift/diffusion relations. They include the quantities Ut_n and Ut_p which are the electronic voltages for electrons and holes, respectively.

$$\vec{J}_n = -q\cdot\mu_n\cdot(n\cdot\text{grad } \psi - \text{grad } (Ut_n\cdot n)) \tag{4}$$

$$\vec{J}_p = -q\cdot\mu_p\cdot(p\cdot\text{grad } \psi + \text{grad } (Ut_p\cdot p)) \tag{5}$$

By setting the electronic voltages equal to the thermal voltage $Ut_o = \frac{k\cdot T_o}{q}$ and assuming the classical Einstein relations $D_n = \mu_n\cdot Ut_o$ and $D_p = \mu_p\cdot Ut_o$ one would obtain the conventional current relations. However,

the new current relations (4) and (5) together with appropriate models for the respective field dependent carrier mobilities and field dependent electronic voltages account properly for transport of hot carriers. A self-consistent derivation of (4) and (5) has been presented in [4]where also the superiority of the new relations is explained in some detail.

It is probably worthwhile to note that simply waiving the classical Einstein relations and modeling carrier mobilities and carrier diffusivities independently is not equivalent to using the current relations (4) and (5).

3. MOBILITY AND ELECTRONIC VOLTAGE

The current relations presented in the previous section constitute only an improvement for the description of current flow in semiconductors if consistent models for velocity saturation, which is reflected in the carrier mobilities, and electronic voltages are used. There is only one set of consistent models which has been derived by Hänsch based on a fairly tricky integration of the Boltzmann transport equation over the momentum space [5]. A review of the procedure of involved calculus and assumptions would have to go into quite a bit of detail, would be spatious and is therefore omitted. Only the final results will be presented and discussed here.

Velocity saturation is described by (6) which considering the structure of the equation appears to be within the range of conventional models. This actually has to be expected since the conventional models have proven their applicability for quite a variety of problems. The subscripts LISF stand for lattice-, impurity-, surface- and field-dependent-scattering as introduced in [19].

$$\mu_{LISF} = \frac{2 \cdot \mu_{LIS}}{1 + \sqrt[\beta]{1 + \left(\frac{2 \cdot \mu_{LIS} \cdot F}{v_{sat}}\right)^{\beta}}} \tag{6}$$

One of the key issues to obtain selfconsistent solutions with the new transport model is an appropriate choice for the respective driving force of electrons and holes. The conventional choices are either the inner products of electric field and respective current density, which was used in MINIMOS up to version 2.9, or the magnitudes of the gradients of the quasi-Fermilevels. The difference between these two choices, if used with the conventional equations, have been reported at several occasions to be marginal. However, none of these models is applicable in combination

with the new current relations. A quasi-Fermilevel does simply not exist for hot carriers; it is not possible to rewrite the current relations by using a substitution of variables into a form where the current densities are proportional to only one gradient of a scalar quantity, respectively. This fact can certainly be understood by physically reasoning, since quasi-Fermilevels do only exist close to equilibrium which definitely is not the case for hot carriers. The other formulation, the inner product of electric field and respective current density, does simply not work which seems not to be fully understood presently; if ignorantly implemented, the numerical model does either not converge or it converges to non-physical solutions if carrier heating is of significance. We have found (7) and (8) to serve conveniently as respective driving forces for electrons and holes.

$$F_{;n} = |\text{grad } \psi - \frac{1}{n} \cdot \text{grad } (Ut_n \cdot n)| \tag{7}$$

$$F_{;p} = |\text{grad } \psi + \frac{1}{p} \cdot \text{grad } (Ut_p \cdot p)| \tag{8}$$

The underlying idea is to interprete the magnitude of a particle current density as the product of particle concentration, mobility and magnitude of the driving force. Some evidence about the appropriateness of (7) and (8) is given by the fact that when carrier heating is neglected the expressions degenerate automatically into the magnitudes of the gradients of the respective quasi-Fermilevels. Furthermore, there is no evidence from any of the actual computations that something is wrong with these models, although it has to be stated that their success is not fully understood by only physically reasoning.

The exponent β in (6) is predicted to be exactly 2 by theory. This is also the optimal choice for electrons. The underlying physics with regard to velocity saturation is unfortunately much more complex for holes since there exist a heavy and a light hole band. β=1 is therefore used as an arbitrarily introduced fitting parameter to improve agreement between simulation and measurement. However, it can be speculated without any risk that (6) has to be structurally refined in order to obtain an analogously good description for the saturation of holes. As a practical consequence the simulation results for really small n-channel devices are usually in better agreement with experiment than the results for p-channel devices of the same size.

It is worthwhile to note that (6) was proposed fully independently by Jaggi already in 1969 [6], [7]; it has been sort of reinvented by Hänsch. The ideas which made Jaggi use this particular formulation have unfortunately not been published.

Our model for the electronic voltage has also been derived by Hänsch [4], [5]. It can be conveniently written as a function of mobility (9).

$$Ut = Ut_o + \tfrac{2}{3}\cdot\tau_\epsilon\cdot v_{sat}^2\cdot(\frac{1}{\mu_{LISF}} - \frac{1}{\mu_{LIS}}) \tag{9}$$

τ_ϵ denotes the energy relaxation time which is assumed to be a constant. This is no real restriction for silicon as confirmed by Monte-Carlo simulations [8]. One obtains the conventional transport model by assuming τ_ϵ=0 which can be proved by a simple calculus.

A new model for surface scattering is also implemented in MINIMOS 3. Experience over the last couple of years has indicated that the previous model implemented in MINIMOS 2.x (c.f.[19]) is pessimistic for modern technologies. It served well it's purpose for many applications, however, with modern technologies the Si/SiO_2 interface is significantly better than for older ones, which causes the mentioned pessimistic predictions. Presently we use:

$$\mu_{LIS} = \frac{\mu_{LI}}{1 + \dfrac{G(y)}{1+G(y)^2}\cdot(\dfrac{S}{v_{sat}})^2} \tag{10}$$

with:

$$G(y) = a\cdot exp((y/y_{ref})^2) \tag{11}$$

The x-coordinate is assumed to run parallel to the interface in channel length direction; the y-coordinate is perpendicular to the interface with positive direction pointing into the substrate; and the z-coordinate runs parallel to the interface in channel width direction.

The critical parameter in our new model is y_{ref} in (11), which describes the distance of influence of the interface. Numerical values for y_{ref} are in the order of a few tenth of a nanometer. However, a black-box value cannot be given and cannot be expected. For less experienced and/or older technologies y_{ref} is larger than for modern ones. The parameter a in (11) is much less sensitive; we recommend at present a value of 0.1.

For the zero-field bulk mobility μ_{LI} we use the expressions of Arora et al.[1].

The field components responsible for surface scattering are given with (12) and (13) for electrons and holes, respectively, in a conventional manner.

$$S_{;n} = \max\,(0,\ \frac{\partial \psi}{\partial y}) \tag{12}$$

$$S_{;p} = \max\,(0, -\frac{\partial \psi}{\partial y}) \tag{13}$$

(10) does not cause any mobility reduction for zero surface field. Thus surface roughness scattering is not accounted for with simply using (10). Our present feeling is that surface roughness scattering is of negligible importance for the current components parallel to the interface. It is only important for the current components perpendicular to the interface. Therefore an anisotropic effective mobility is implemented (14).

$$\mu = \mu_{LISF} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 - \dfrac{1}{1 + G(y) \cdot \dfrac{\mu_{LI}}{\mu_{LISF}}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{14}$$

The ideas which led to the above given model of surface mobility have been deduced from various quantuummechanical calculations and experimental observations. One fact which is not fully understood yet should probably been mentioned. The term $G(y)/(1+G(y)^2)$ in (10) exhibits a maximum at $y = y_{ref} \cdot \ln(1/a)$. This could give information on a possible relation between the two parameters, which will have to be subject of further investigations.

4. SOME NUMERICAL DETAILS

MINIMOS 3 is fully upward compatible to all previous versions of MINIMOS and will work with any input legal for a previous version. Some modifications of the format of the external files, however, have been performed to accomodate various enhancements.

The fully adaptive automatic mesh refinement algorithm has been considerably improved to equidistribute the discretisation errors of the partial differential equations. Essentially the criteria proposed in [21]are consequently obeyed. The semiconductor equations are scaled using the singular perturbation approach introduced by Markowich [9]. The discretisation is standard finite differences and precisely described in [19].

The three coupled nonlinear difference equations are solved with essentially Gummel's iterative method.

The solution of the linearized Poisson equation is performed with a block cyclic Jacobi conjugate gradient method (BCJCG), the background of which is given in [3]. The linearized continuity equations are solved by Gaussian elimination with checkerboard ordering of equations and unknowns [19]. Previous version of MINIMOS have used Stone's method for all three equations. In case of Poisson's equation the performance of BCJCG is just superior. Stone's method works principly for the continuity equations, however, under some not too well understood circumstances the convergence is extremely lousy. Actually, several dozens of different linear equation solvers have been tested including the various incomplete factorisation algorithms with conjugate gradient acceleration. The result of these (usually frustrating) investigations have led to the mentioned combination.

Last, but not least, a new schema for the computation of terminal currents has been implemented following ideas presented by Mock [10]in order to minimize the sensitivity with respect to mesh spacing.

5. AN EXAMPLE

In the following some results calculated with MINIMOS 3 for a realistic n-channel MOSFET with 0.5μm effective channel length are presented. With Fig.1 the geometrical specifications of the MOSFET are given for reference. The gateoxide thickness is 12.5nm; the substrate doping is $10^{17}cm^{-3}$ and a threshold tailoring implant is performed.

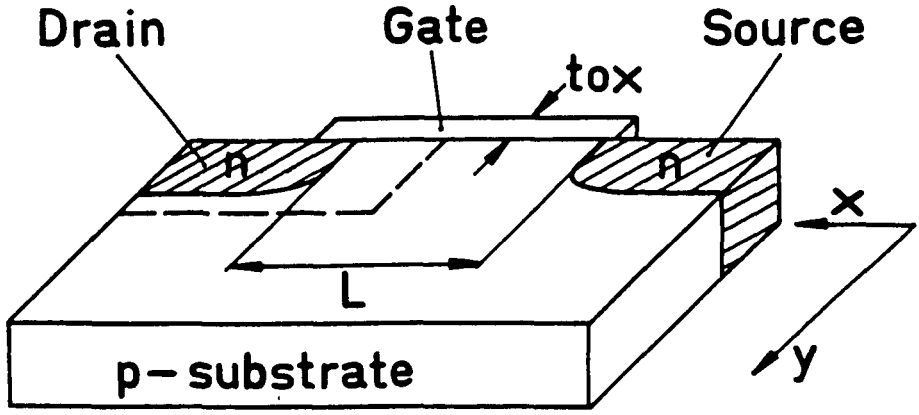

Fig.1 Structure of MOSFET

In Fig.2 and Fig.3 the electron concentration close to the drain (dashed area in Fig.1) is shown for a bias point leading to saturation (5V applied at the drain contact).

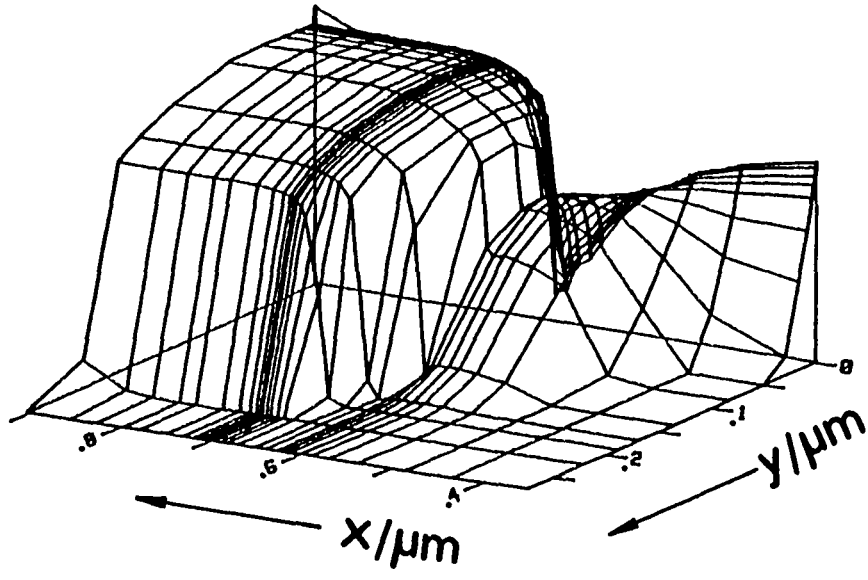

Fig.2 Electron Concentration τ_ϵ=0

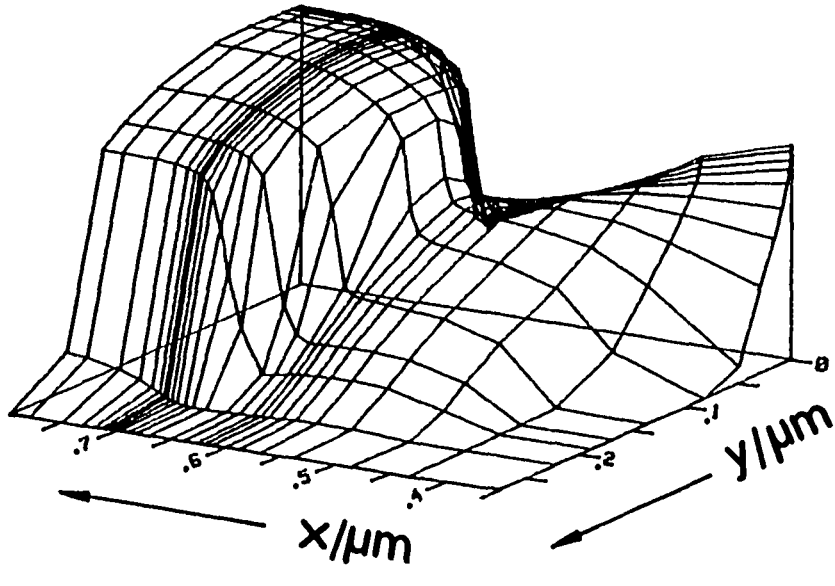

Fig.3 Electron Concentration τ_ϵ=0.1ps

The result in Fig.2 was calculated by assuming a vanishing energy relaxation time τ_ϵ which corresponds to the conventional semiconductor transport model. For the result in Fig.3 the energy relaxation time τ_ϵ=0.1ps has been taken. One can observe from these figures that the electron concentration becomes smoother due to carrier heating. Furthermore, the electrons are pushed into the substrate which increases the average distance of the carriers from the Si/SiO_2 interface. This modification will have to be taken into account for modeling injection of hot carriers into the gateoxide.

It could also be that models of impact ionisation in MOSFET's are effected thereby. However, we have found that the classical Chynoweth type formulation of impact ionisation seems to be indeed sufficiently accurate for substrate current calculation in combination with the outlined hot carrier transport model. In combination with a conventional transport model impact ionisation is usually overestimated which may be compensated somehow, pragmatically spoken, by adjusting the ionisation coefficients [13].

The distribution of the electrostatic potential is shown in Fig.4. It is essentially the same for both calculations, i.e., τ_ϵ=0 and τ_ϵ=0.1ps. The only difference is that large gradients of the electrostatic potential — which means large electric fields — are somehow smoothened. However, this does not appear as a dramatic change in the contourlines of the electrostatic potential.

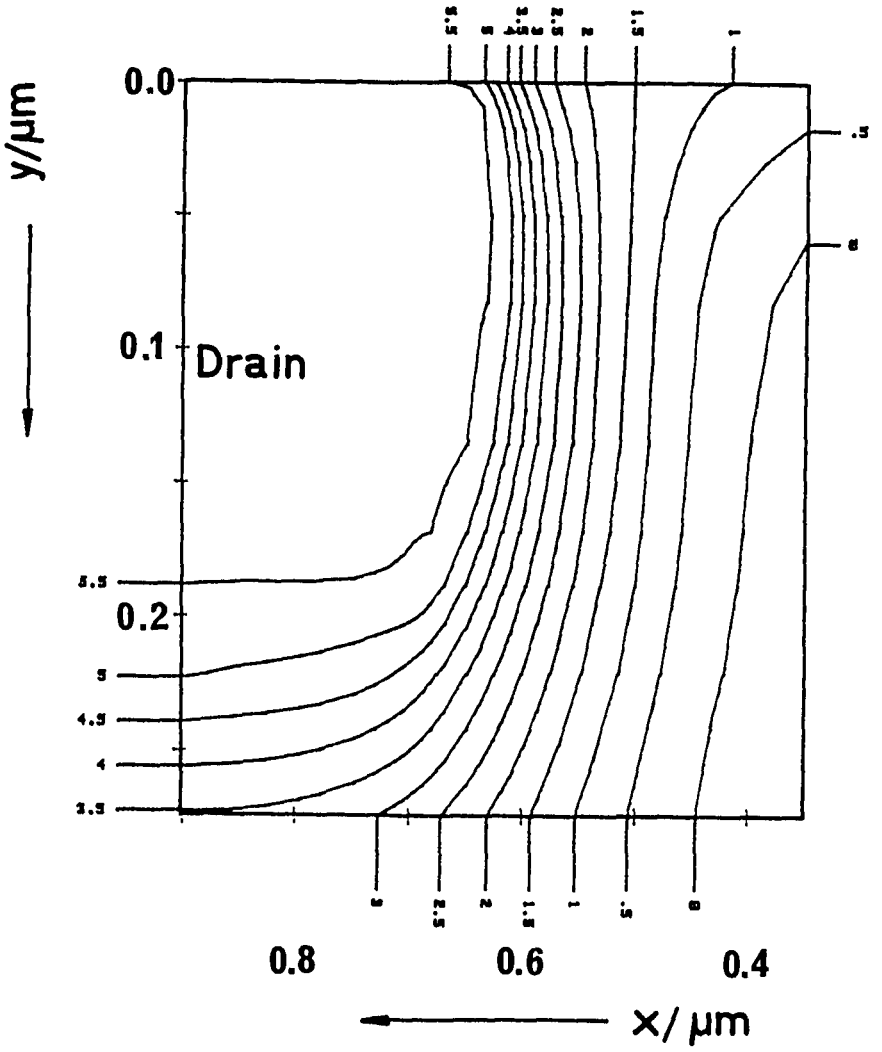

Fig.4 Electrostatic Potential

In Fig.5 the electronic temperature of the electrons is shown. The electronic temperature is proportional to the electronic voltage by q/k, i.e., elementary charge over Boltzmann's constant. The only reason why the electronic temperature is shown instead of the electronic voltage lies in the observation that a temperature can be judged more easily than a voltage because of the different units.

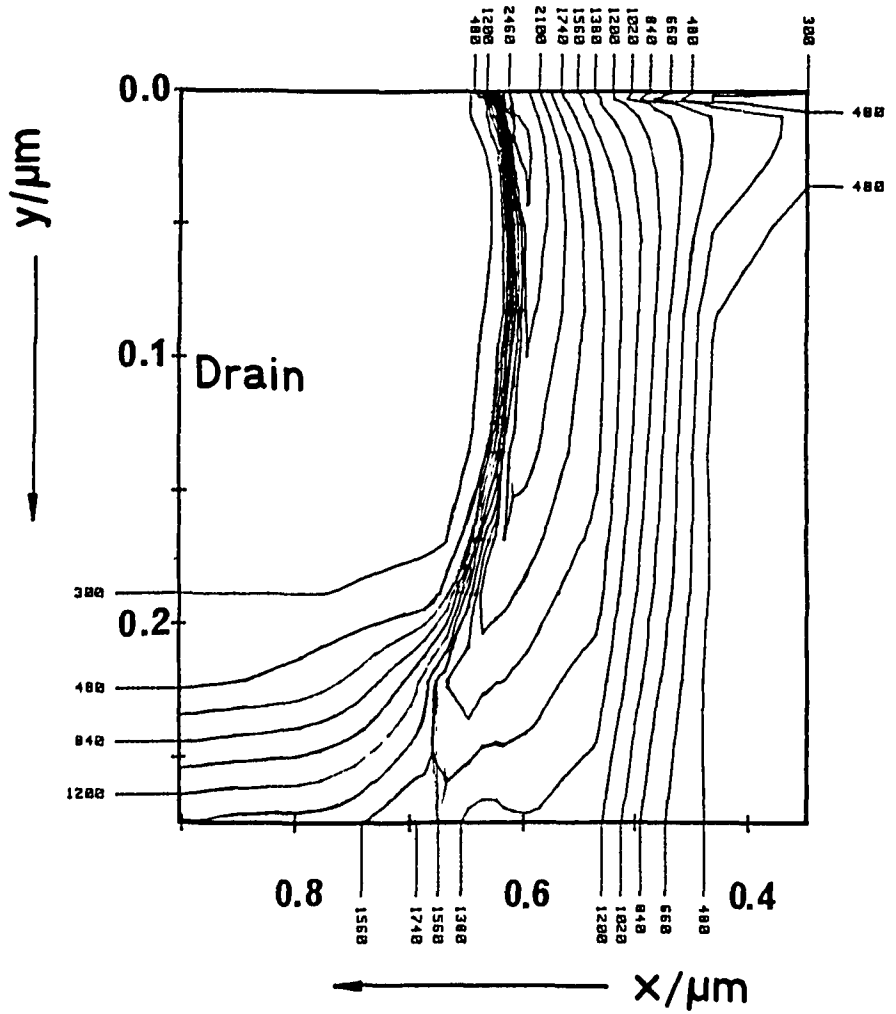

Fig.5 Electronic Temperature of Electrons

It should probably be noted, that the electronic temperature must not be mixed up with the lattice temperature which is kept constant at 300K for this example. Only for cold carriers the electronic temperature and the lattice temperature are equal. In our example the maximum of the electronic temperature is about eight times the equilibrium value. By comparison of Fig.3 and Fig.4 we see the expected correlation of the electronic temperature with the electric field.

6. CHARACTERISTICS

As a matter of observation any device simulator has been claimed so far to produce excellent agreement between calculated and measured characteristics. Having in mind the various fitting parameters and the uncertainty of the various device parameters it does not need much phantasy to believe in the possibility of tuning. Therefore, no figures showing perfect agreement between simulation and measurement will be given here. Instead a few qualitative remarks will be made.

With the new transport model substrate currents decrease and drain currents increase, if carrier heating is significant which means that the device under consideration must be sufficiently short. For a still usable short channel device with $1.25\mu m$ coded channel length the substrate current decrease can be up to a factor of 10. The drain current increase will proportionally be up to 40(not every small device is a short channel device!). We observe that agreement for one technology over a wide range of channel lengths including the smallest available devices can be achieved with only one set of parameters, whereas with the conventional model deviations occur for the short channel devices if the long channel devices fit. These deviations have been observed by many engineers, but they have usually been regarded to the uncertainty of various device parameters, like doping distribution?

7. CONCLUSION

A model of hot carrier transport in MOSFET's, which has been implemented in MINIMOS 3, has been presented. The underlying local approach should be a descent approximation for silicon devices because the only major effect being ignored is velocity overshoot which is negligibly small in silicon as confirmed by many Monte-Carlo investigations, e.g., [8]. It can be expected that our model will be able to reliably describe all MOSFET's for which ballistic transport can be ignored. This is for sure the case for all silicon devices with channel lengths larger than 0.4μm [2].

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