Calculation of Contact Currents in Device Simulation

Gerd Nanz, Peter Dickinger, and Siegfried Selberherr, *Senior Member, IEEE*

***Abstract*—We present an accurate new method for the calculation of the contact currents in a device simulation program which is applicable to arbitrarily shaped device geometries. The method is based on the evaluation of a volume integral of the calculated current densities over the whole device area with a suitably chosen weight function. Different types of weight functions are discussed and compared with the commonly used line integral along the contact. The results are illustrated by three examples: an I^2L memory cell, an MOS transistor, and a resistor with a reverse-biased diode.**

I. Introduction

TERMINAL current calculation is a difficult postprocessing step in device simulation because the results are very sensitive to small changes in the solution and the space grid. The conventional method of integrating the current densities along the contact or a closed line around the contact often gives wrong values because there are not enough grid points to guarantee an accurate calculation of the contact currents. Furthermore the singularities of the derivatives of the basic variables at the ends of the contact with the change of the boundary conditions can introduce significant cancellation errors [1]. The numerical conservation of terminal currents indicates the accuracy of the solution obtained from the simulation [2]. For some applications the leading digits of the results obtained by the evaluation of the line integral are more or less random and the results indicate only the order of magnitude of the currents. We have derived a new method, which is more accurate. The line integral has been transformed into a weighted volume integral, thus taking into account the current densities at all grid points. By this method the quality of the current conservation in the device is a measure for the accuracy of the solution over the whole device area.

In Section II our method will be explained for stationary simulations, and the reason why some types of weight functions will not work will be pointed out. The results are illustrated by an MOS transistor and a resistor with a reverse-biased diode. In Section III the weights for the displacement current are briefly discussed, showing the results for a transient simulation of a dynamic RAM cell.

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The authors are with the Institute for Microelectronics, Technical University Vienna, A-1040 Vienna, Austria.

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II. Calculation of Currents

In this Section various types of weight functions for our method are discussed: the line integral as a special case of our method; weight functions based on the solution of a set of Laplace equations; and weight functions based on the solution of a set of continuity-equation-like partial differential equations with different boundary conditions.

A. Method

The total current density, $\vec{J}_{\text{tot}}$, in a device consists of three parts:

$$\vec{J}_{\text{tot}} = \vec{J}_n + \vec{J}_p + \vec{J}_D.$$

Here $\vec{J}_n$ and $\vec{J}_p$ denote the particle current densities of electrons and holes, respectively, and

$$\vec{J}_D = -\epsilon \cdot \frac{\partial}{\partial t} \operatorname{grad} \psi$$

is the displacement current density (ψ being the electrostatic potential, ϵ the permittivity constant and t the time variable). The terminal current, I_i, at the ith contact is calculated by

$$I_i = \oint_{\partial\Omega} w_i \cdot \vec{J}_{\text{tot}}\, ds, \tag{1}$$

where $\partial\Omega$ denotes the outer boundary of the semiconductor area, Ω. This means that a line integral around the ith contact has to be evaluated with a suitably chosen weight function, w_i.

Transforming (1) from a line integral along $\partial\Omega$ into a volume integral over Ω and inserting the right-hand side of the continuity equations, we obtain, by using different weight functions for each type of current,

$$\begin{aligned} I_i &= \oint_{\partial\Omega} w_i \cdot \vec{J}_{\text{tot}}\, ds \\ &= \int_\Omega [(\operatorname{grad} w_{n_i}) \cdot \vec{J}_n + (\operatorname{grad} w_{p_i}) \cdot \vec{J}_p \\ &\quad + (\operatorname{grad} w_{D_i}) \cdot \vec{J}_D]\, dA \\ &\quad + \int_\Omega \left[q \cdot w_{n_i} \cdot \left(R + \frac{\partial n}{\partial t} \right) - q \cdot w_{p_i} \cdot \left(R + \frac{\partial p}{\partial t} \right) \right. \\ &\quad \left. - \epsilon \cdot w_{D_i} \cdot \operatorname{div} \left(\frac{\partial}{\partial t} \operatorname{grad} \psi \right) \right] dA. \end{aligned} \tag{2}$$

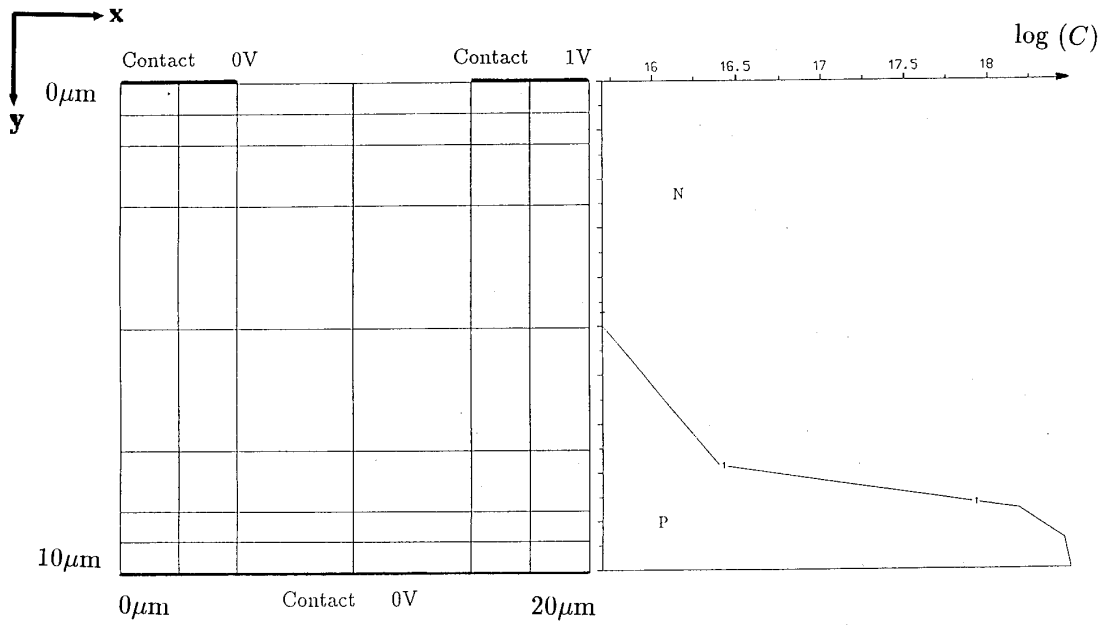


Fig. 1. Geometry and doping of resistor with diode.

Here R denotes the net generation/recombination and q the elementary charge. Note that in the stationary case (2) shrinks to the simple formula

$$I_i = \int_\Omega [(\text{grad } w_{ni}) \cdot \vec{J}_n + (\text{grad } w_{pi}) \cdot \vec{J}_p + q \cdot R \cdot (w_{ni} - w_{pi})]\, dA.$$

B. Choice of the Weight Functions

A problem arises in the choice of the smooth weight function, w_i, as required e.g., by Mock [2]. For the line integral the weight functions must only be specified on $\partial\Omega$. Usually w_i is assumed to be 1 at the ith contact, 0 at all other contacts, and arbitrary otherwise. This means that the line integral is only a special case of the volume integral with a special type of weight function.

The weight functions for the volume integral have to be chosen more subtly because the method must be applicable to arbitrarily shaped device geometries. First, it is straightforward to define the w_i independent of the solution (ψ, n, p). Then the w_i have to be calculated only once for each space grid, thus saving a significant amount of CPU time. Taking w_i as the solution of

$$\text{div grad } w_i = 0 \tag{3}$$

with the boundary conditions (cf. weight function for line integral)

$w_i = 1$ at the ith contact

$w_i = 0$ at all other contacts

$\frac{\partial w_i}{\partial \vec{n}} = 0$ otherwise (especially at interfaces)

shows that these weight functions do not provide satisfactory results ($\partial/\partial\vec{n}$ derivative with respect to the outer normal). The reason is shown by the following example of the 20 μm by 10 μm resistor with a reverse-biased diode, given in Fig. 1.

The line integral with an integration path parallel to the x axis should give the current of the reverse-biased diode independent of the y coordinate. But this is only true for the p-doped region with small current densities. In the other part of the device, the values of the line integral increase with the same order of magnitude as the carrier concentrations. Cross sections of the electron concentration and the current density in the y direction at $x = 10$ μm are given in Figs. 2 and 3, respectively. The values of the line integrals are given in Table I. This effect is based on the round-off errors and the cancellation error in the calculation of the current densities from the (majority) carrier concentrations, which usually vary over more than 15 orders of magnitude [3]. Therefore a different type of weight function has to be used for the calculation of terminal currents. This function must depend on the physical properties of the device.

Again w_i is the solution of a partial differential equation, because only by such a rigorous approach the applicability to arbitrary device structures is guaranteed. The partial differential equation is of the form

$$\text{div } (f(x, y) \text{ grad } w_i) = 0,$$

where $f(x, y)$ denotes a suitably chosen smooth function which depends on certain physical properties of the device. The boundary conditions are the same as for (3). It should be mentioned that formally (3) is a special case of this approach with $f(x, y) = 1$, but from the numerical

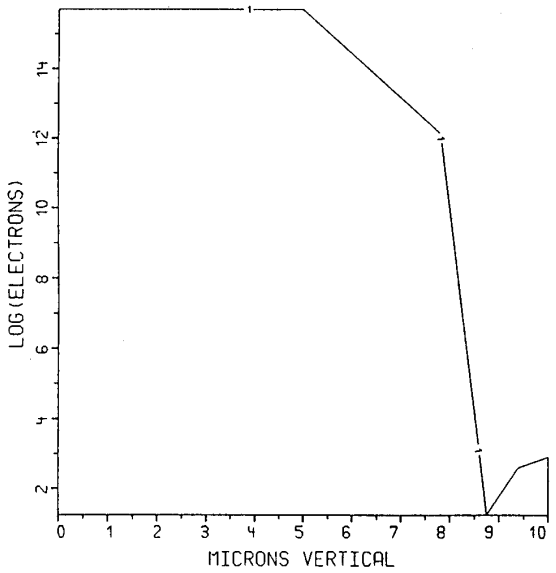


Fig. 2. Electron concentration in resistor with diode (x = 10 μm).

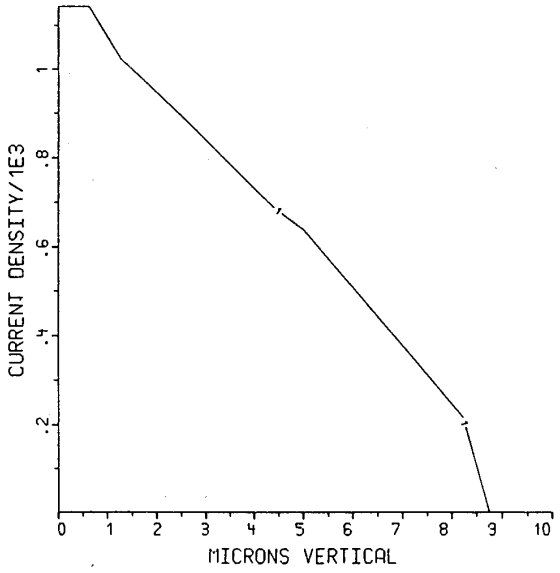


Fig. 3. Current density in resistor with diode (x = 10 μm).

TABLE I

y Coordinate [μm]	Electron Concentration [cm^{-3}]	Electron Current Density [A/cm^2]	Line Integral [A/cm]
0.0000	$8.0 \cdot 10^{2}$	$4.5 \cdot 10^{-11}$	
0.3125			$8.9 \cdot 10^{-14}$
0.6250	$4.0 \cdot 10^{2}$	$4.5 \cdot 10^{-11}$	
0.9375			$6.1 \cdot 10^{-14}$
1.2500	$1.7 \cdot 10^{1}$	$4.5 \cdot 10^{-11}$	
1.8750			$6.1 \cdot 10^{-14}$
2.5000	$4.6 \cdot 10^{16}$	$1.8 \cdot 10^{0}$	
3.7500			$9.8 \cdot 10^{-2}$
5.0000	$5.0 \cdot 10^{16}$	$7.7 \cdot 10^{-1}$	
6.2500			$3.0 \cdot 10^{-1}$
7.5000	$5.0 \cdot 10^{16}$	$1.3 \cdot 10^{-1}$	
8.1250			$4.0 \cdot 10^{-1}$
8.7500	$5.0 \cdot 10^{16}$	$7.7 \cdot 10^{-1}$	
9.0625			$5.0 \cdot 10^{-1}$
9.3750	$5.0 \cdot 10^{16}$		
9.6875			$-5.7 \cdot 10^{-5}$
10.0000	$5.0 \cdot 10^{16}$		

point of view the discretization schemes can be completely different.

First, $f(x, y) = C(x, y)/n_{intr}$ is chosen, which means the active doping concentration, $C(x, y)$, divided by the intrinsic carrier concentration, n_{intr}. This method fails because in cases of high current the current densities become almost independent of the doping profile. Especially for the simulation of breakdown phenomena this will result in wrong contact currents. For our reverse-biased diode the currents are overestimated by a factor of about 10^4.

The choice $f(x, y) = n_{cn}/n_{intr}$ for the electron current and $f(x, y) = p_{cn}/n_{intr}$ for the hole current, where n_{cn} and p_{cn} denote the carrier concentrations in the device under the assumption of space charge neutrality and thermal equilibrium, is nearly equivalent to the previous choice (doping profile). For our reverse-biased diode and currents are over estimated by a factor of about 10^3.

The advantage of these two weight functions would have been that they have to be calculated only once for each grid. Because of the reported reasons they are not applicable to a general device simulation program. Therefore the weight functions must really depend on the actually calculated solution.

For the first approach, $f(x, y) = (n + p)/n_{intr}$ has been chosen (n the electron concentration, p the hole concentration). The results again are not satisfactory because for very large gradients of $n + p$, leading to sharp valleys, the weight function has a "strange" shape. Furthermore

the substrate currents in an MOS transistor may be overestimated by a factor of about 10^3.

The analysis of the numerical effects shows that the weight function must have the following property: In regions with large carrier concentrations the gradient of the weight function should be small. This means that the electron current and the hole current have to be treated separately, in order to provide the best possible accuracy for arbitrary types of devices. We solve for the electron current:

$$\operatorname{div}\left(\frac{n}{n_{\text{intr}}}\operatorname{grad} w_{n_i}\right) = 0 \tag{4}$$

and for the hole current:

$$\operatorname{div}\left(\frac{p}{n_{\text{intr}}}\operatorname{grad} w_{p_i}\right) = 0. \tag{5}$$

For the sake of simplicity the intrinsic carrier concentration, n_{intr}, is assumed to be constant over the whole device area. The discretization of (4) and (5) can be done in an analogous way as for the continuity equations [4].

This approach to contact current calculation provides *a priori* numerical current conservation of the order of the discretization error for the solution of the *linear* partial differential equations (4) and (5), which in most cases is of the order of the machine accuracy.

In order to make the numerical current conservation a real criterion for the accuracy of the solution of the semiconductor equations we slightly change the boundary conditions of (4) and (5), e.g.

$$w_{n_i,p_i} = 1.1 \quad \text{at the } i\text{th contact}$$

$$w_{n_i,p_i} = -0.1 \quad \text{at all other contacts}$$

$$\frac{\partial w_{n_i,p_i}}{\partial \vec{n}} = 0.0 \quad \text{otherwise.}$$

The solution of this system has values between -0.1 and 1.1. Cutting the solution at 0 and 1, we obtain a function, $\tilde{w}$, which is steady but not differentiable, showing plateaus around each contact. Since (2) requires a differentiable weight function, we smooth $\tilde{w}$ by a function, g, with the following properties [5]:

$$g(0) = 0$$

$$g(1) = 1$$

$$g'(0) = 0$$

$$g'(1) = 0.$$

For this the polynomial of third order,

$$g(x) = -2 \cdot x^3 + 3 \cdot x^2,$$

provides very good results. A further advantage of these "smoothened" functions, $g(\tilde{w}(x, y))$, can be observed: Because of the plateaus around each contact, the gradients of the weight functions vanish close to contacts, thus avoiding evaluation of the current densities at the singular endpoints of the contacts.

The weights for the displacement current are discussed in Section III.

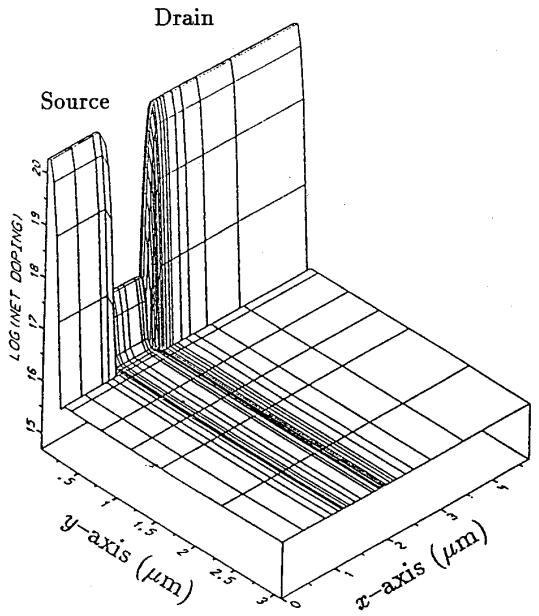


Fig. 4. Doping profile of MOS transistor.

C. Example: MOS Transistor

In order to illustrate the results of our investigation, we present the plots of the different weight functions for the contacts of a conventional MOS transistor in the ON condition ($V_{\text{Drain}} = 5$ V, $V_{\text{Substrate}} = 0$ V, $V_{\text{Source}} = 0$ V, $V_{\text{Gate}} = 1$ V, $V_{\text{Threshold}} \approx 0.4$ V). The simulations have been performed with our fully two-dimensional transient device simulator BAMBI, which solves the basic semiconductor equations on a finite-boxes grid in a totally self-consistent way.

In Fig. 4 the doping profile of our MOS transistor is given. Figs. 5, 6, and 7 present the electron concentration n, the hole concentration p, and the sum of electrons and holes, $n + p$, respectively.

The following plots present the different types of weight functions for the substrate contact of the MOS transistor. The weight of Fig. 8 calculated for $f(x, y) = 1$ shows high gradients. These gradients cause incorrect results of the substrate current by a factor of about 10^7 because the weight function does not account for the special operating condition and the related cancellation errors. Fig. 9 is a plot of the weight function for $f(x, y) = C(x, y)/n_{\text{intr}}$. Again the weight function cannot account for the special operation condition resulting in high gradients toward the substrate contact.

In Fig. 10 the weight for $f(x, y) = (n + p)/n_{\text{intr}}$ is given. The function w_i has a "strange" shape which is even grid-dependent, showing very sharp edges. Parts (a)

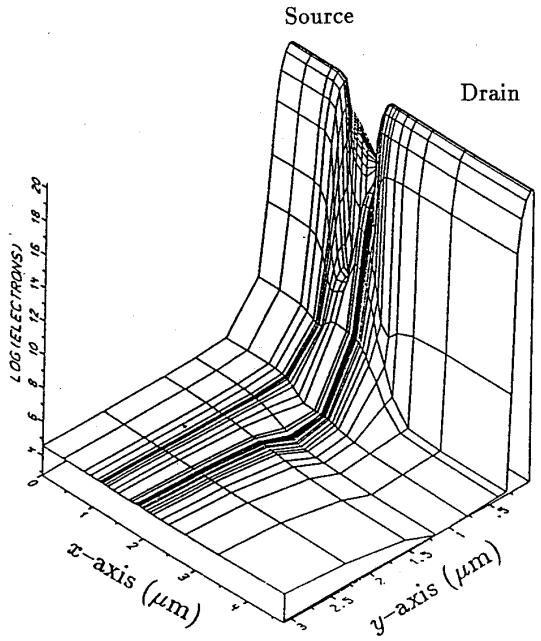


Fig. 5. Electron concentration of MOS transistor (V_{Drain} = 5 V, $V_{Substrate}$ = 0 V, V_{Source} = 0 V, V_{Gate} = 1 V).

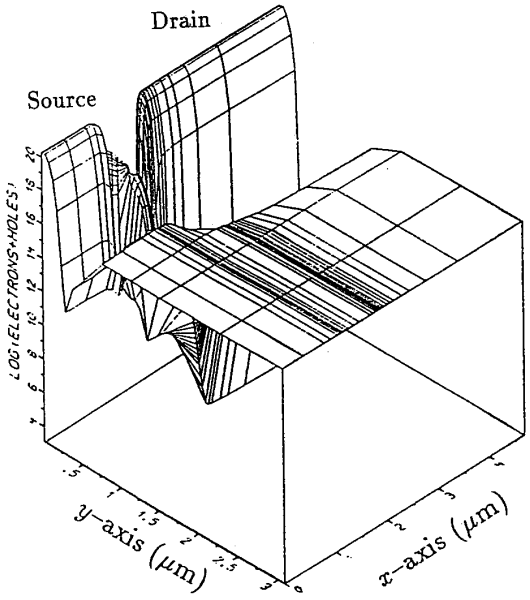


Fig. 7. Sum of electrons and holes of MOS transistor (V_{Drain} = 5 V, $V_{Substrate}$ = 0 V, V_{Source} = 0 V, V_{Gate} = 1 V).

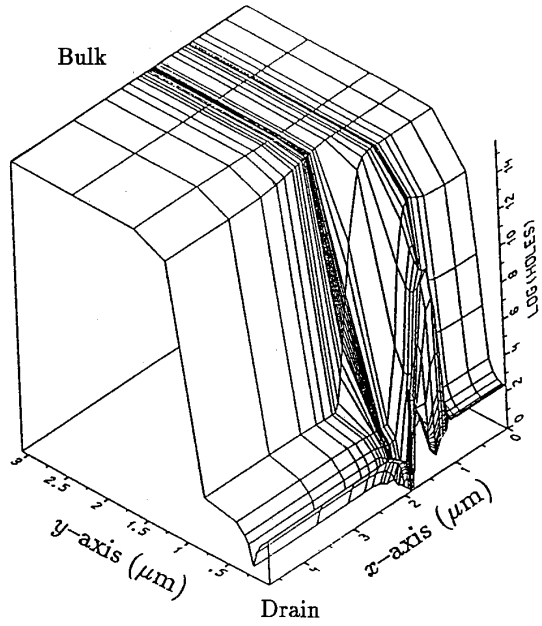


Fig. 6. Hole concentration of MOS transistor (V_{Drain} = 5 V, $V_{Substrate}$ = 0 V, V_{Source} = 0 V, V_{Gate} = 1 V).

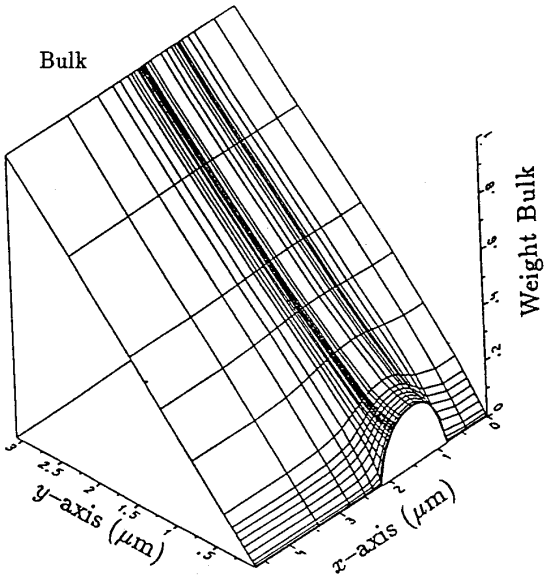


Fig. 8. Weight of substrate contact for $f(x, y) = 1$ (Laplace equation).

and (b) of Fig. 11 provide the weights calculated from (4) and (5) with the contact boundary conditions -0.1 and 1.1. The plateaus around the contacts can be clearly seen. By avoiding the evaluation of the current densities close to the singularities almost the same numerical conservation of currents can be achieved if the grid is sufficiently accurate. The results obtained by BAMBI agree with the results computed by MINIMOS, e.g. [6], where a heuristic approach is used to synthesize suitable weight functions for MOS devices.

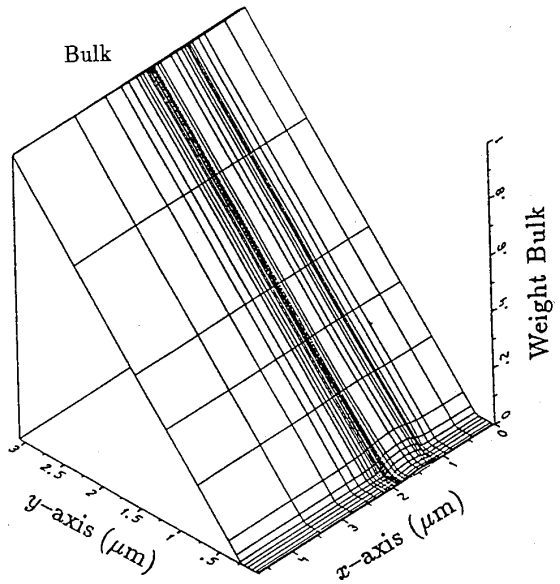


Fig. 9. Weight of substrate contact for $f(x, y) = C(x, y)/n_{intr}$ (doping profile).

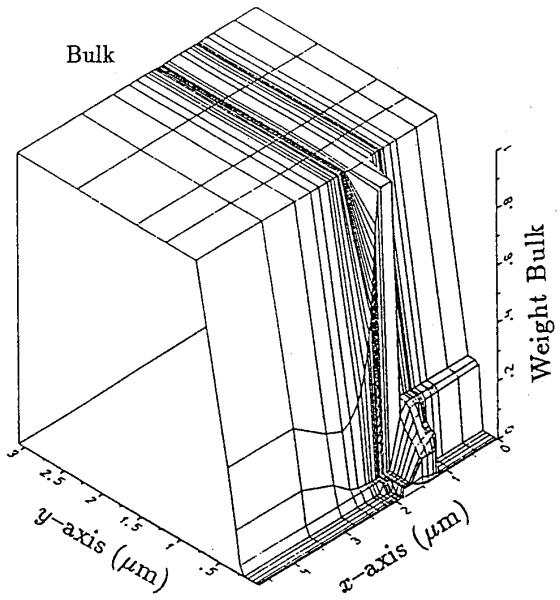


Fig. 10. Weight of substrate contact for $f(x, y) = (n + p)/n_{intr}$ (solution).

III. Transient Simulations

For time-dependent simulations, the displacement current must also be considered. Since this current depends only on the electrostatic potential, which is assumed to have a linear variation between two neighboring grid points, it is sufficient to use a weight function calculated from the Laplace equation (3). These weight functions must be computed only once for each space grid on the whole device area, including dielectric regions.

In order to illustrate the superiority of our method we have performed a comparison of (1) and (2) for the behavior of a dynamic I^2L memory cell [7]. In Fig. 12 the geometry of our dynamic RAM cell can be seen. The word line, W_p, is connected to the p-type injector; the row select line is the collector terminal of the npn transistor. The

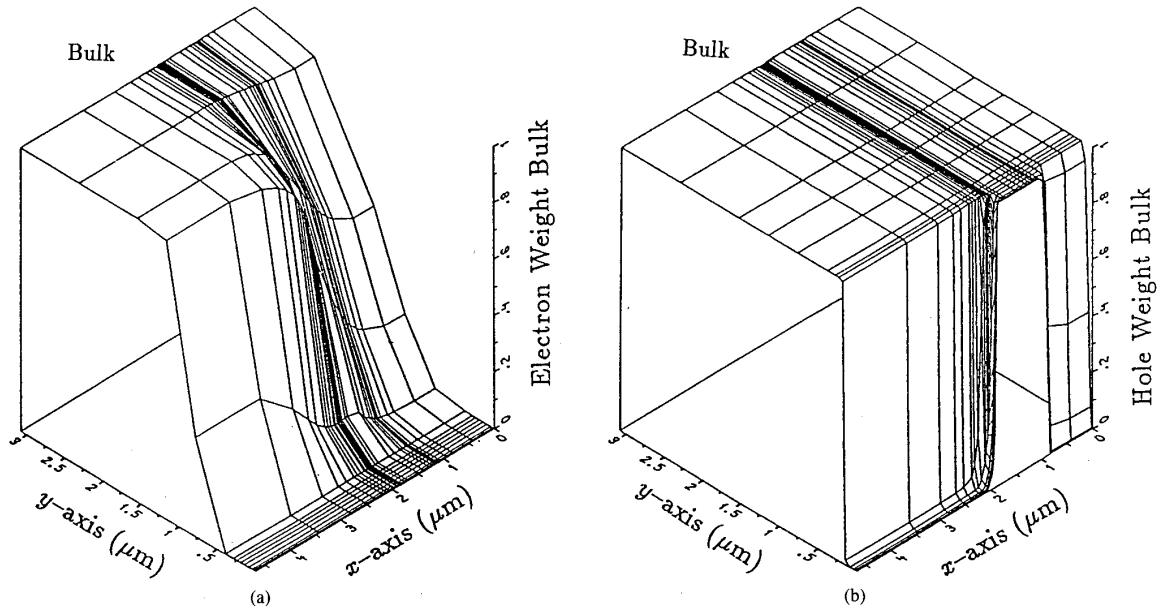


Fig. 11. (a) Weight for electron current of substrate contact for $f(x, y) = n/n_{intr}$ (solution, smooth). (b) Weight for hole current of substrate contact for $f(x, y) = p/n_{intr}$ (solution, smooth).

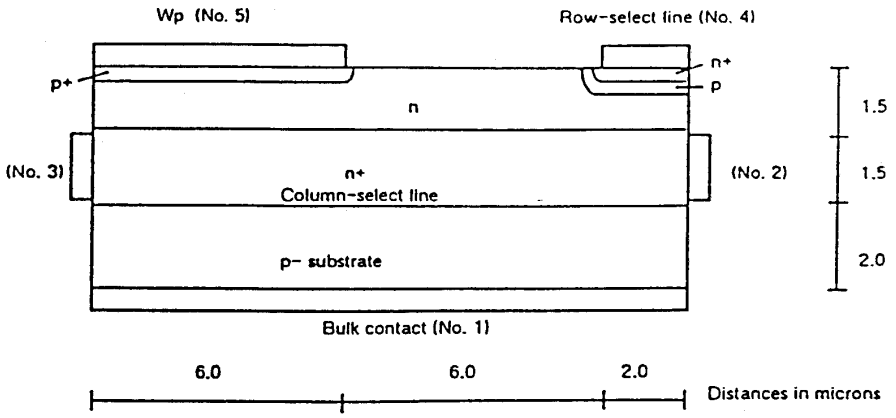


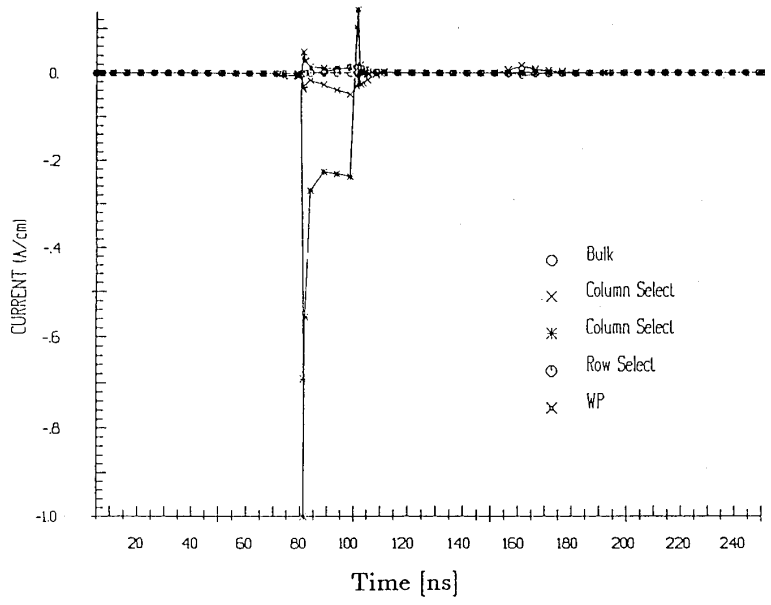
Fig. 12. Geometry and doping of I^2L memory cell.

heavily doped buried n^+ region represents the column select line. The logic is determined by the presence or absence of charge stored in the emitter junction depletion layer of the npn device. The following operations have been performed: write 1/read (0 ns–60 ns), write 0 (70 ns–120 ns), and read (140 ns–250 ns).

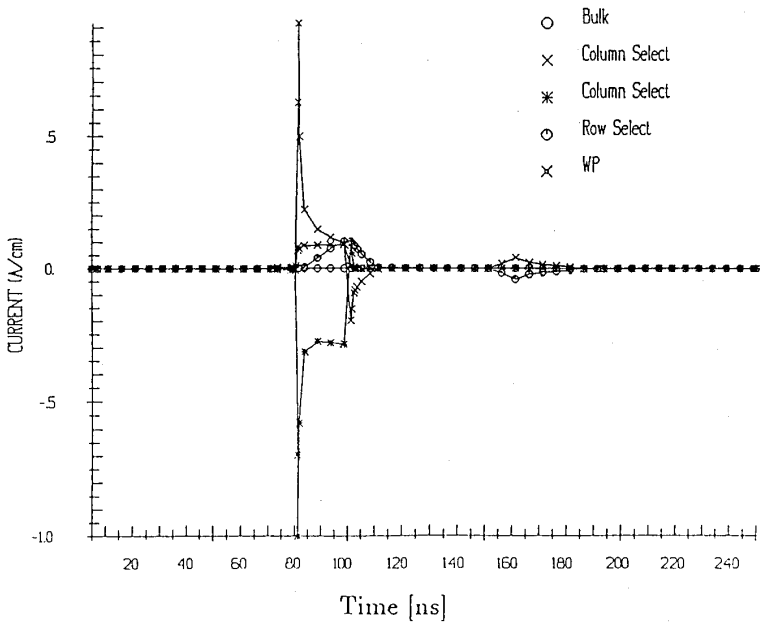
In Fig. 13 the transient contact currents computed according to formula (1) (Fig. 13(a)) and according to our new method with (4) and (5) (Fig. 13(b)), respectively, are shown. There is not only a quantitative difference after about 80 ns but also a qualitative. This results from an insufficient number of grid points near the bulk contact and the word line, W_p, for the evaluation of the line integral. Furthermore for formula (1) the numerical current conservation is very poor, giving an algebraic sum of all currents which is higher than the smallest contact current in the device.

IV. Conclusion

We have presented an accurate new method for calculating contact currents in a device simulation program. Owing to the special choice of boundary conditions for the weight function in the evaluation of a volume integral,



(a)



(b)

Fig. 13. (a) Time/current diagram evaluating line integral (1). (b) Time/current diagram evaluating volume integral (2) with weight functions calculated from (4), (5), and (3) (for displacement current)..

numerical trouble caused by singularities is avoided. Various types of weight functions have been discussed, showing the advantages and the disadvantages of each. With our new method, the current densities over the whole device area are taken into account, thus making the result independent of the definition of an integration path in the space grid. In this way, round-off errors are avoided as far as possible and the quality of the conservation of currents in the device becomes a real measure of the accuracy of the solution.

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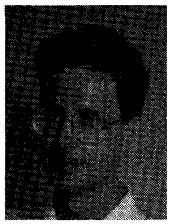
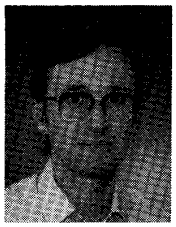
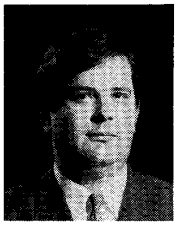


Gerd Nanz was born in Munich, Germany, on October 10, 1959. He received the Diplommathematiker degree from the Technical University of Munich in 1985.

From 1985 to 1986 he was an assistant teacher in the Department for Civil Engineering at the Technical University of Munich, where he was also involved in the development of self-adaptive finite element programs. In November 1986 he joined the Institut für Allgemeine Elektrotechnik und Elektronik of the Technical University of Vienna, Austria, and he completed his Ph.D. thesis, on numerical methods in device simulation, in 1989 at the Institut für Mikroelektronik. Since 1990 he has been working on device and process simulation at the Campusbased Engineering Center Vienna (Digital Equipment Corporation).



Peter Dickinger was born in Gmunden, Austria, in 1961. He received the Diplomingenieur degree in electrical engineering from the Technical University of Vienna in 1987. He joined Prof. Selberherr's simulation group in August 1987. In 1990 he completed his Ph.D. thesis, dealing with network and device simulation of high-voltage DMOS devices. Since 1990 he has been employed by the Austrian government.



Siegfried Selberherr (M'79–SM'84) was born in Klosterneuburg, Austria, on August 3, 1955. He received the Diplomingenieur degree in control theory and industrial electronics from the Technical University of Vienna in 1978.

Since that time he has been with the Institut für Allgemeine Elektrotechnik und Elektronik (previously called the Institut für Physikalische Elektronik) at the Technical University of Vienna as Professor. He completed his thesis, entitled "Two Dimensional MOS-Transistor Modeling," in 1981. Dr. Selberherr has been holding the 'venia docendi' on computer-aided design since 1984. He has been head of the Institut für Mikroelektronik since 1988. His current topics are modeling and simulation of problems for microelectronics engineering.

Dr. Selberherr has authored or coauthored more than 100 publications in journals and conference proceedings. Furthermore, he is the author of the book *Analysis and Simulation of Semiconductor Devices*. In 1983 he received the Dr. Ernst Fehrer award; in 1985 he received the award of the Nachrichtentechnische Gesellschaft; in 1986 he was honored with the Dr. Herta Firnberg Staatspreis; and in 1987 he received the Heinz Zemanek award. Dr. Selberherr is a member of the Association for Computing Machinery (1979), the Society of Industrial and Applied Mathematics (1980), and the Verband deutscher Elektrotechniker (1984). He is editor of *The Transactions of the Society for Computer Simulation*, of *Electrosoft*, of *Mikroelektronik*, and of the Springer-Verlag book series Computational Microelectronics.