AN EFFICIENT ALGORITHM FOR TRANSIENT AND STEADY-STATE NUMERICAL ANALYSES OF SEMICONDUCTOR DEVICES

B. M. Wilamowski and H. C. Howell

ABSTRACT

An efficient algorithm, requiring only the solution of a linear Poisson's equation, is used for the numerical analysis of semiconductor devices. Stable operation of this algorithm has been demonstrated even for very long time steps. Some examples, both steady-state and transient, are presented which demonstrate the power of this algorithm. Key words: Numerical analysis and semiconductor devices.

INTRODUCTION

In analyzing semiconductor devices, five basic equations must be solved simultaneously: two transport equations, two continuity equations, and Poisson's equation. The solutions of these equations yield the potential distribution, the electron and hole concentrations, and the electron and hole currents in the semiconductor. There are many approaches to solving these equations, but the most commonly used techniques are:

1. the implicit method using linearization and the Newton-Raphson algorithm [1] and

In both instances the semiconductor device is divided into small regions. Each region is then represented as a node in the model. The voltage, the electron and hole concentrations, and the recombination current must be found at each node. The electric field, along with the electron and hole currents, serves to connect the nodes.

To obtain a solution using the implicit method, a set of linearized equations for each node in the model must be solved simultaneously. In solving this large set of equations, round-off error often becomes a problem. Transient analysis using this technique requires that these equations be solved for each time step, so that the computation time becomes excessive and thus making this technique suitable only for main-frame computers. To reduce the computational effort, various modifications of the implicit method have been developed which use an iterative technique to generate an approximate solution; this is especially important if the two- or three-dimensional case is considered.

As opposed to the implicit method, Gummel's algorithms allow for the independent solution of the transport
equations and Poisson's equation in an iterative manner. However, Gummel's algorithms will not converge when high current effects or strong recombination phenomena are present, and are also of little use if high voltages are applied to the device.

**THE ALGORITHM**

The algorithm used herein was originally designed for the transient analysis of semiconductor devices [4]. If such transient analysis is carried on for a protracted period, then the steady-state solution will be obtained. The main advantage of this algorithm is, that for each time step, only Poisson's equation needs to be solved implicitly to obtain the potential distribution. Changes in the electron and hole concentrations at each node are explicitly calculated from the equations:

\[ \Delta n_j = \frac{\Delta t}{q v_j} (\Sigma_{nj} - I_{nj}) \]  
(1)

\[ \Delta p_j = \frac{\Delta t}{q v_j} (\Sigma_{pj} - I_{pj}) \]  
(2)

where \( v_j = \Delta x A \) is the volume of the region associated with node \( j \); \( I_{nj} = q v_j R \) is the recombination current at node \( j \); \( q \) is the electron charge; \( \Sigma_{nj} \) is the sum of the electron currents flowing into node \( j \); and \( \Sigma_{nj} \) is the sum of the hole currents flowing into node \( j \). In this fashion, all currents can be explicitly computed from the potential distribution and from the electron and hole concentrations obtained from Poisson's equation in the previous time step.

The main disadvantage of the algorithm given in [4] is, that in order to achieve convergence, very small time steps must be used (usually the time steps must be smaller than the dielectric relaxation time). This constraint requires that many time steps be used, resulting in a very large computational effort.

In order to use large time steps, when the time step is comparable or larger than the smallest time constant of the system, the classical approach requires the use of static, implicit solutions. In the approach presented herein, the values of \( \Delta t \) are artificially limited for critical nodes in order to obtain convergence. This approach can lead to significant errors in the transient analysis, but in itself causes no errors in the steady-state solution. The main difficulty in this approach is choosing the correct time step for each node so that a fast, stable solution is achieved. In the case of electrons, the time step \( \Delta t \) is calculated from

\[ \frac{1}{\Delta t_e} = \alpha \left( \frac{1}{\Delta t} + \frac{1}{\tau_e} + \frac{1}{\tau_r} \right) \]  
(3)

\[ \tau_r = \frac{\varepsilon \eta_0}{q \mu_e n} \]  
(4)

\[ \tau_r = \frac{\Delta x}{v} \frac{n}{J_n} \]  
(5)

where \( \Delta t \) is the initial time step; \( \tau_e \) is the electron life time; \( \tau_r \) is the electron relaxation time; \( \tau_r \) is the electron transient time for one section; \( v \) is the electron velocity in the vicinity of the node; and \( J_n \) is the electron
current. A set of equations similar to equations (3-5) is used for the holes. The parameter $\alpha$ controls the convergence of the solution and is chosen empirically with values that vary between 0.2 and 1.0. The smaller the value of $\alpha$ used, the slower the convergence of the solution, but the higher the stability of the solution.

The efficiency of this algorithm is very high. For the example given in this paper, five-to-six significant digits of accuracy were obtained for the potential, and also for the electron and hole concentrations, after about 50 iterations. To obtain a current balance, between 300 and 500 iterations are required. The number of iterations required in itself is not that impressive, but the computational effort during each iteration is relatively small, minimizing the overall computational effort.

It should also be noted that this algorithm will produce a reasonable transient analysis when the $\alpha$ chosen is small enough, but these small values of $\alpha$ require more time steps.

SAMPLE RESULTS

To illustrate the effectiveness of this algorithm, a silicon $nnp$ device is analyzed in the punch-through mode. This example was chosen for three reasons: firstly, high level injection exists, where the carrier concentration exceeds the impurity concentration; secondly, a large voltage occurs; and thirdly, the carrier transport is controlled by the space charge of the mobile carriers. Because of these phenomena, the common algorithms mentioned in the introduction are ineffective in dealing with this example. Both steady-state and transient analyses were run for this example and the results are shown in Figures 1 and 2, respectively. These computations were performed on an IBM/AT-type computer.

CONCLUSIONS

The algorithm given in [4], in which only Poisson's equation needs be solved implicitly, was modified. The stability of this modified algorithm was demonstrated even for very large time steps. In numerical analyses of semiconductor devices, the values of the carrier concentrations often vary by 20 orders of magnitude. These widely varying quantities force the use of extreme precision in computing the solutions using the common, implicit approaches. In these cases, the proposed modification can offer much higher accuracy, even without the use of extended precision. The efficiency of this modification is even more significant when extending this analysis into two or three dimensions.

REFERENCES

Fig. 1. Steady-state analysis for npn diode operating in the punch-through mode for external biasing from 1 to 10 V
Fig. 2. Transient analysis for an npn diode operating in the punchthrough mode during switching from 10 to 10 V in 10 ps increments.