ON-STATE MODELLING OF SEMICONDUCTOR FLOATING REGIONS USING GUMMEL'S ALGORITHM

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SUMMARY

It is generally accepted that Gummel's decoupled algorithm, for the solution of the three semiconductor equations, fails to converge when the problem includes PN junction isolated non-contacted, i.e. floating regions.

This failure to converge can manifest itself in the form of non-physical negative carrier concentrations that show no tendency to disappear as the iteration cycle is successively repeated.

In this paper a corrective procedure is presented that, when applied to every mesh point at which a negative carrier concentration occurs, results in decaying negative concentrations and ultimate convergence. In addition it is demonstrated that the choice of boundary conditions can affect convergence for floating region problems.

Two examples are given to demonstrate the convergence properties of the modified algorithm for both forward and reverse bias conditions.

1. INTRODUCTION

There are two main iterative approaches to solving the three semiconductor equations:-

$$\mathrm{Div}(\mathrm{Grad}(V)) = -q/\varepsilon\ (p-n+N) \qquad (1)$$

$$\mathrm{Div}(\underline{J}_n) = -R \qquad (2)$$

$$\mathrm{Div}(\underline{J}_p) = +R \qquad (3)$$

where $\underline{J}_n = -q\,\mu_n n\,\mathrm{Grad}(V) + D_n \mathrm{Grad}(n)$ (4)

and $\underline{J}_p = -q\,\mu_p p\,\mathrm{Grad}(V) - D_p \mathrm{Grad}(p)$ (5)

The simplest approach is that due to Gummel [1,2] i.e. the decoupled method, which proceeds as follows:-

(a) Equation (1) is solved for the potential (V) with an assumed initial distribution of electrons and holes (n and p respectively). It is also assumed during the iterative solution for V that the electron and hole quasi-Fermi levels (V_n and V_p respectively) do not change so that n and p are related to the varying potential via:

$$n = n_i \exp[q(V-V_n)/kT] \quad (6)$$

$$p = n_i \exp[q(V_p-V)/kT] \quad (7)$$

(b) Equation (2) is then solved for n with the new potential and hole distributions resulting from step (a).

(c) Equation (3) is solved for p with the new potential and electron distributions.

(d) If certain convergence criteria are not met the procedure is repeated from step (a) with the new initial distributions.

The second approach, called the coupled approach, seeks to solve all three equations simultaneously [2]. When discretised the three equations are assembled into one large matrix (3Nx3N, where N is the number of nodes) and solved via Newton linearisation.

Gummel's algorithm is relatively easy to implement, converges well from a poor starting guess of the potential and carrier distributions, and requires significantly less memory than the coupled approach. However it has generally been reported that the method fails to converge when the problem contains PN junction isolated non-contacted i.e. floating, regions. The coupled approach is believed to be superior in this respect though convergence is difficult to obtain as a good starting guess is essential for any problem solved using this method.

At our laboratory a general 2D on-state model named HECTOR [3], has been written based on the Gummel algorithm. In this paper the effect of boundary conditions on convergence will be discussed, also a simple modification to Gummel's basic algorithm will be presented that results in the convergence of the program HECTOR for floating region problems from a poor initial guess of the potential and carrier

distributions. Two examples are given to illustrate the convergence properties, the first is a reverse bias floating ring edge termination problem for which a comparison can be made with our off-state program TRIPOS [4,5]. The other is a forward bias problem concerning a breakover diode which is essentially a four layer structure with no contact to the substrate.

2. 2D ON-STATE MODEL HECTOR

HECTOR is a general 2D on-state finite difference program based on Gummel's algorithm, however before proceeding further it is important to note the method used for solving the carrier continuity equations. Because of the need for highly accurate computation of the carrier densities (small inaccuracies result in large potential inaccuracies) a direct solver is used that performs a complete LU matrix decomposition.

A problem is considered converged if the maximum potential change at a mesh point, on solution of (1), is less than a fraction (typically 0.01) of a thermal volt.

At an early stage of development, the program employed first order reflecting boundary conditions. In the following section a demonstration of the effect of such boundary conditions on the convergence of floating region problems will be given. In its current form HECTOR employs second order boundary conditions at reflecting boundaries.

3. BOUNDARY CONDITIONS

Experience gained from the development of the program TRIPOS suggested that first order reflecting boundary conditions invariably lead to computational problems.

A simple example clearly demonstrated that the use of first order boundary conditions, within HECTOR, was the cause of convergence failure for some problems involving floating regions and that normal convergence could be obtained if second order boundary conditions were used.

Figure 1 shows a rectangular region of n-type silicon completely surrounding a p-type floating region, the structure being symmetric about axis CD. Contacts were applied along AE and BF with a potential difference of 1 volt. When first order boundary conditions were employed convergence could be obtained with the problem area defined by AEFB. However the equivalent, smaller, problem area ACDB would not converge, i.e. the residuals would not decay to the required accuracy. Applying second order boundary conditions in the two cases resulted in convergence to the same solution.

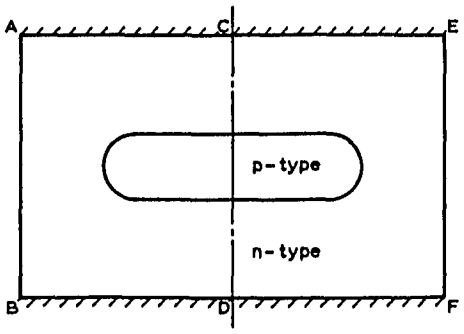

Figure 1: Device structure for demonstrating the effect of boundary conditions

Whilst convergence could be obtained, in this case, by a proper choice of boundary condition, it was found that if a PN junction was formed, by diffusion into the semiconductor along boundary AE (of Fig. 1), then negative carrier concentrations appeared during the iteration process and convergence could not be obtained for either forward or reverse bias conditions irrespective of the choice of boundary condition. To obtain convergence it was necessary to develop a procedure for dealing with the negative carrier concentrations.

4. CORRECTION PROCEDURE FOR NEGATIVE CARRIER CONCENTRATIONS

Negative carrier concentrations arise, in HECTOR, because for a non-converged solution, of the three equations, the potential and other carrier distribution are incompatible with a positive concentration. This can be deduced as we solve for the carrier concentrations using a direct solver.

The reasoning behind the corrective procedure is to modify the potential distribution so that it becomes consistent with a positive carrier concentration wherever negative concentrations occur. To this end the carrier concentration is restored to its equilibrium value and a voltage, determined by the magnitude of the negative carrier concentration at the mesh point, is added to the potential of that mesh point according to the inverse relations of equations (6) and (7) i.e.

$$v = -kT/q \ln(-n/n_i) \quad \text{for electrons} \qquad (8)$$

$$v = +kT/q \ln(-p/n_i) \quad \text{for holes} \qquad (9)$$

Applying this corrective procedure on successive iterations results in a damping out of any negative concentrations that may occur and ultimately to convergence.

As an illustration of HECTOR's ability to converge floating region problems the next two sections contain examples of its use under both forward and reverse bias conditions.

5. ANALYSIS OF A FLOATING RING SYSTEM

Figure 2 shows the device structure to be used in this example. A potential difference of 100 volts was applied between the substrate and main junction, which was held at 0 volts. The two rings are floating and as a starting guess the ring potentials were set equal to the main junction voltage and all carrier concentrations set to their equilibrium values. Figure 3 shows the surface potential after 30 iterations, it can be seen that a positive potential is being developed on each ring by the modified algorithm. Figure 4 shows the fully converged surface potential after 153 iterations the last occurrence of a negative concentration being at iteration 81.

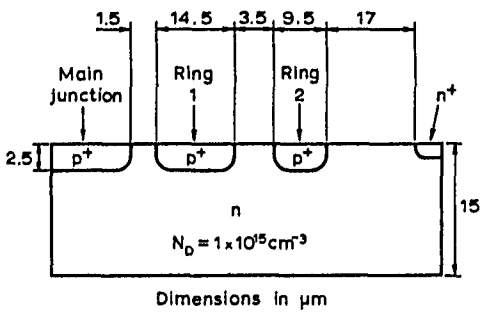

Figure 2: Device structure for testing reverse bias floating region convergence

This reverse bias example was deliberately chosen as a severe test for the algorithm to demonstrate its robustness. The large number of iterations required for convergence is a consequence of the large voltage applied. For on-state problems the speed of convergence, for floating region problems, of the modified algorithm compares well with the time taken for problems in which all semi-conductor regions are contacted.

For comparison with our off-state model, Figure 5 shows a TRIPOS analysis of the same structure under identical bias conditions, agreement is to within approximately 0.5 volts for the ring potentials.

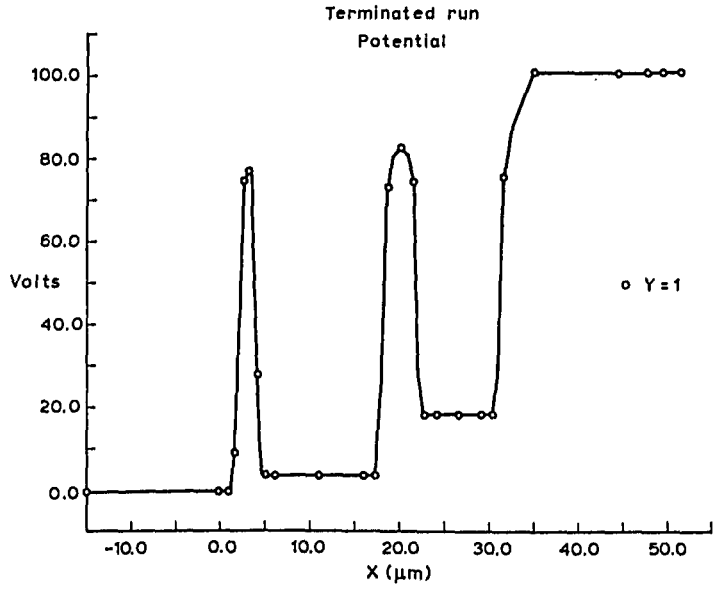

Figure 3: Calculated surface potential for reverse bias floating region problem after 30 iterations

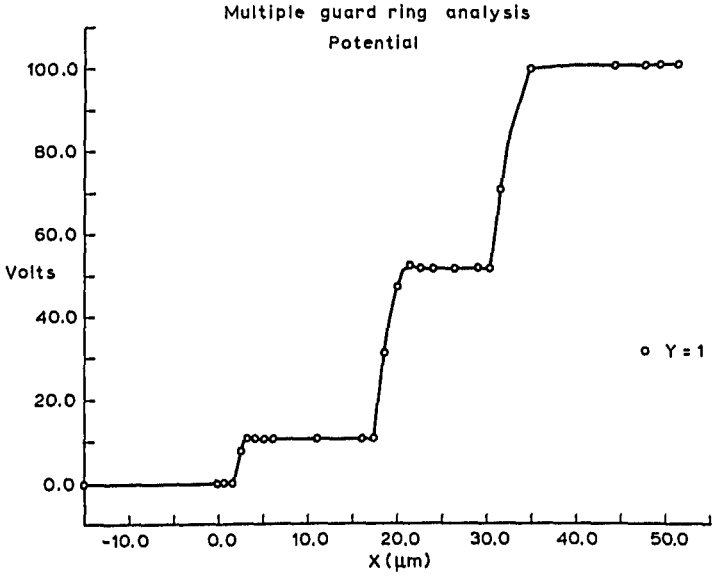

Figure 4: Converged surface potential for reverse bias floating region problem after 153 iterations

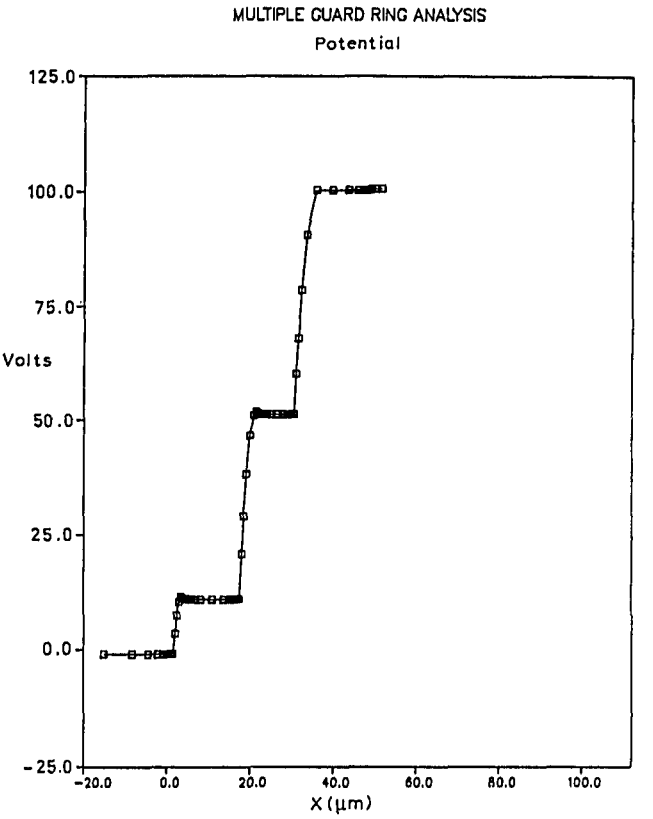

Figure 5: TRIPOS (off-state model) converged surface potential for reverse bias floating region problem

6. ANALYSIS OF A BREAK OVER DIODE

Thyristor and break-over diode (BOD) problems have also been tackled successfully. To illustrate this, Figure 6 shows the structure of a BOD, which is essentially two thyristors (one inverted) placed side by side.

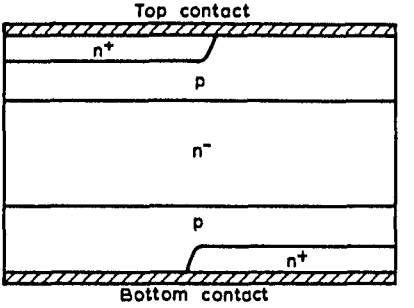

Figure 6: BOD device structure

As each thyristor in the BOD structure has two possible states, the starting condition for an on-state solution is obtained by splitting one of the contacts so that its associated N^+P junction can be forward biased to initially fill the device with carriers. This initial condition need not be calculated to full convergence, indeed only a few iterations are needed to introduce sufficient carriers. For this example an N^+P junction was forward biased at 1 volt and allowed to run for 4 iterations to obtain the starting condition.

Restoring the structure to that shown in Figure 6 and continuing the iteration procedure, for 1 volt applied across the device, resulted in convergence after 68 iterations. Figure 7 shows a vector plot of the converged total current flow for this example.

7. CONCLUSIONS

A somewhat heuristic, but effective, procedure has been presented that results in convergence of the Gummel alogorithm when solving the three semiconductor equations for a problem containing PN junction isolated non-contacted regions. Further the importance of employing the correct i.e. second order, boundary conditions at reflecting boundaries has been emphasised.

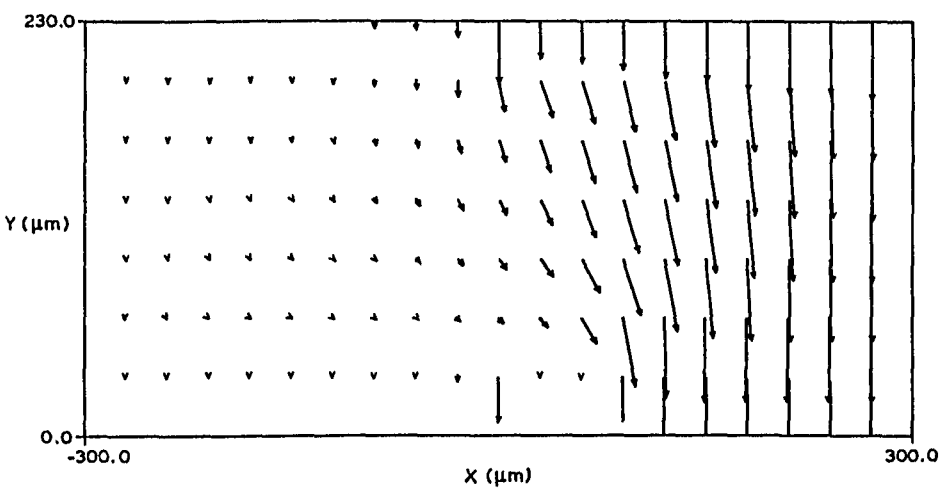

Figure 7: Converged, on-state, total current vector plot for BOD with 1 volt applied

8. REFERENCES

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