TWO-DIMENSIONAL COUPLED DIFFUSION MODELING

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To satisfy the need for a better understanding of process models, their interactions and mathematical consequences we have developed general purpose simulators with automatic grid generation in space and time. These codes can handle physical models given by partial differential equations without the necessity for simplifications so that decisive limitations (field enhancement factor, charge neutrality approximation...) can be dropped. To investigate the influence of the field effect on diffusion we have simulated one- and two-dimensional B-As-diffusion coupled by the Poisson equation. As conclusive result the validity of the quasi-neutral approximation is shown to hold for engineering problems.

1. INTRODUCTION

The design of new generations of small devices requires a better understanding of the physical processes involved and their inter-action. Usually the existing simulation programs handle only specific physical quantities so that an implementation of advanced models often exceeds the capabilities of these programs.

To overcome these difficulties we have developed general purpose solvers which are capable to treat an arbitrary number of coupled differential equations for physical quantities such as acceptors, donors, vacancies, interstitials, electrostatic potential, etc. The computation errors are minimized by using sophisticated formalisms which have been adapted from well established device modeling programs[3,9]. Automatic mesh generation in space and time relieves the user from non-physical problems[10].

2. COUPLED DIFFUSION WITH FIELD ENHANCEMENT

To demonstrate the capabilities of our codes we investigate the influence of the field enhancement and the charge neutrality approximation in multi-dopant systems. Especially near p-n junctions the electric field affects strongly the redistribution of the dopants. This effect leads to displacements of p-n junctions and to mutual influences of the dopants. The mathematical formulation of a boron and arsenic diffusion, taking the field effect into consideration, is given by (1), (2) and (3).

$$\text{div grad } \Psi = \frac{q}{\varepsilon} \cdot (2 \cdot n_i \cdot \sinh(\frac{\Psi}{U_t}) + C_B - C_{As}) \quad (1)$$

$$\frac{\partial C_B}{\partial t} = \text{div } (D_B (\text{grad } C_B - \frac{C_B}{U_t} \cdot \text{grad } \Psi)) \quad (2)$$

$$\frac{\partial C_{As}}{\partial t} = \text{div } (D_{As}(\text{grad } C_{As} + \frac{C_{As}}{U_t} \cdot \text{grad } \Psi)) \quad (3)$$

Neglecting clustering and precipitation effects these formulae are valid under the assumption of Boltzmann statistics which is an acceptable assumption in practice[6]. Since this set of equations can be easily expanded to more dopants we can concentrate our investigations without loss of universality on this reduced system. In existing simulation programs the Poisson equation is for the sake of simplicity replaced by the quasi-neutral assumption[2,4,7,8,12] (eq.4).

$$\Psi = U_t \cdot \text{arsinh}(\frac{C_{As}-C_B}{2 \cdot n_i}) \quad (4)$$

This simplification leads to a reduction of the number of equations to be treated and is therefore commonly used to diminish computer resources. Former investigations on the accuracy of this assumption did not lead to conclusive results so that the question whether the quasineutral assumption gives sufficiently accurate results is still pending[1,5,11].

Since the difference between the models is caused by space charge we concentrate our investigations on boron and arsenic p-n junctions with fairly high concentrations.

3. TWO-DIMENSIONAL RESULTS

The two-dimensional example represents a worst case situation. We have simulated an inert annealing step at 1000°C. The initial doping concentration has been obtained by ion implantations of boron ($4 \cdot 10^{15}$ cm^{-2}, 80 keV, Pearson IV distribution) without mask and of arsenic ($4 \cdot 10^{15}$ cm^{-2}, 90 keV, Joined-Half-Gaussian-distribution) through an infinitely steep field oxide mask at the origin of the coordinate system. These implantations have been chosen to exceed the intrinsic number. Clustering and precipitation effects have been neglected in order to yield the desired worst case estimations. The diffusion coefficients have been modeled with superimposed Arrhenius expressions according to well established formulae[10].

Fig.1 shows the boron profile, Fig.2 the electrostatic potential after 10 seconds diffusion time. At this point of time the boron profile is slightly enhanced in the regions of strong gradients of the arsenic profile. The arsenic on the other hand is, caused by the smaller diffusion coefficient, nearly unaffected. Fig.3 and Fig.4 are pointing out the situation at 150 seconds diffusion time. At this moment the boron profile shows a region of considerably increased concentration.
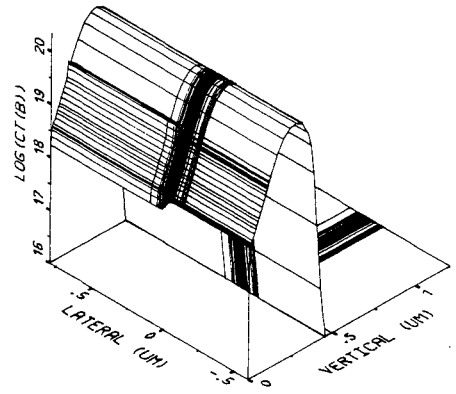

FIGURE 1
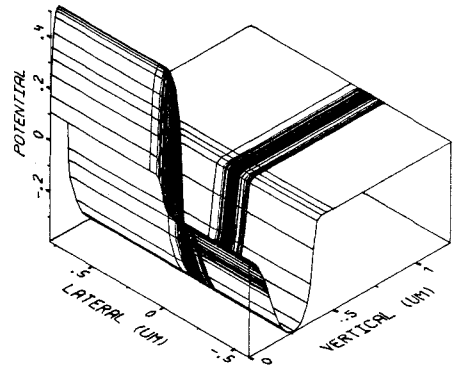Boron Concentration at 10 sec.

FIGURE 2
Electric Potential at 10 sec.

This maximum has been forced by the divergence of the electric field in the vicinity of the p-n junction. Analogously, the arsenic profile forms a maximum at the same position as the maximum of the boron profile. This means that the p-n junction becomes steeper and steeper in this period.

As one can see in Fig.2 the vertical component of the electric field at the surface is negative in regions with high arsenic concentration and positive elsewhere. This causes the boron in these regions to migrate from the surface to the bulk. Due to the spreading arsenic profile the electrical field

at the surface decreases. In the following the diffusion current exceeds the dopant migration caused by the electrical field. Therefore the flux of boron enhances the concentration at the surface but is still strongly retarded. In regions sufficiently far off the arsenic accumulation the boron profile spreads uninfluenced.

For diffusion times exceeding 500 seconds, represented by Fig.5 and Fig.6, the maxima of concentration of the boron and arsenic profiles are spreading ambipolar so that the steepness of the p-n junction will be reduced.
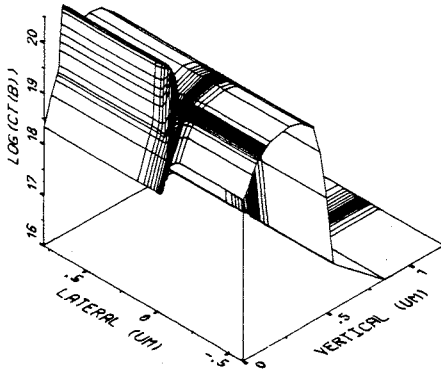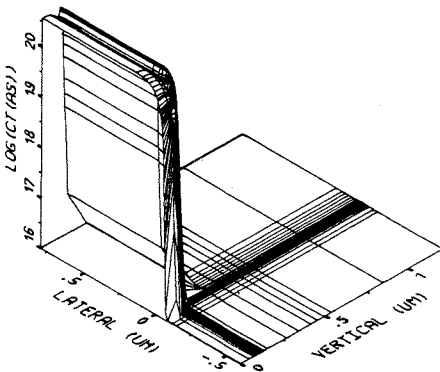
FIGURE 5
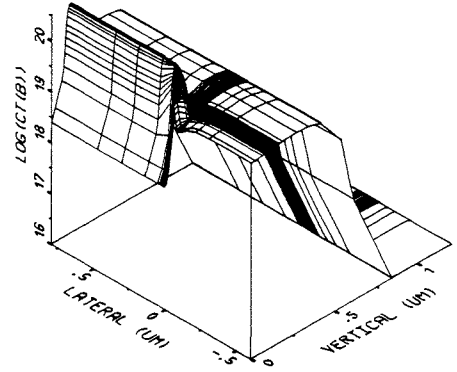Boron Concentration at 500 sec.

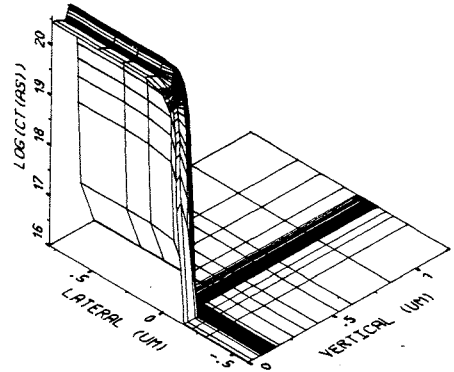FIGURE 3
Boron Concentration at 150 sec.

FIGURE 6
Arsenic Concentration at 500 sec.

However, significant differences between Poisson equation and charge neutral approximation could not be observed in the final results of the simulation. In order to verify these results we simulated similar problems in one dimension with much higher computational accuracy.

4. ONE-DIMENSIONAL INVESTIGATIONS

To answer the still pending question of the admissibility of the charge neutral equation we used our one-dimensional code to investigate the migration of dopants near p-n junctions. As an example we present an inert diffusion

FIGURE 4
Arsenic Concentration at 150 sec.

step at 800°C for 300 min. The implantation
data for this example have been the same as
those of the two-dimensional example with the
exception of the distributions which are now
assumed to be Gaussian. Under the
consideration of the same limitations we
expected larger differences in the results due
to the decreasing intrinsic number. To
compensate the reduced diffusion coefficient we
had to choose significantly longer diffusion
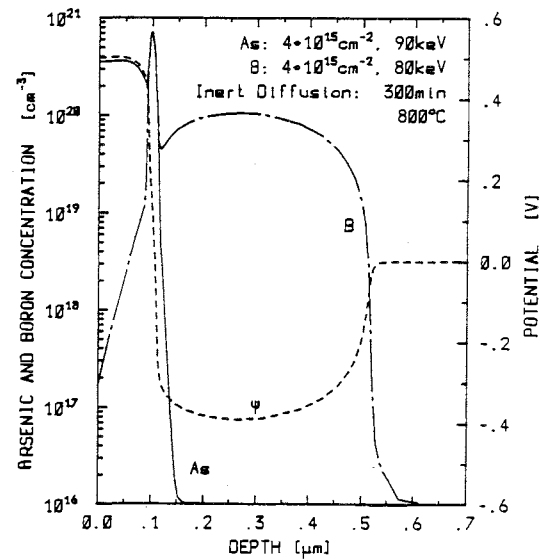times. The results of the simulation are
displayed in Fig.7.

FIGURE 7
Concentrations and Potential after 300 min.

As observed in the two-dimensional analysis
both, the boron and the arsenic profile show
very distinct maxima of the same shape and
value in the vicinity of the p-n junction
whereas elsewhere the profiles are very flat.
These maxima cause a very rapid change of the
potential and therefore a considerable electric
field. Since differences could be expected
mainly near to the p-n junction Fig.8 shows the
interesting details at 300 seconds diffusion
time. The main effect is given by a slight

displacement of the p-n junction. As one can
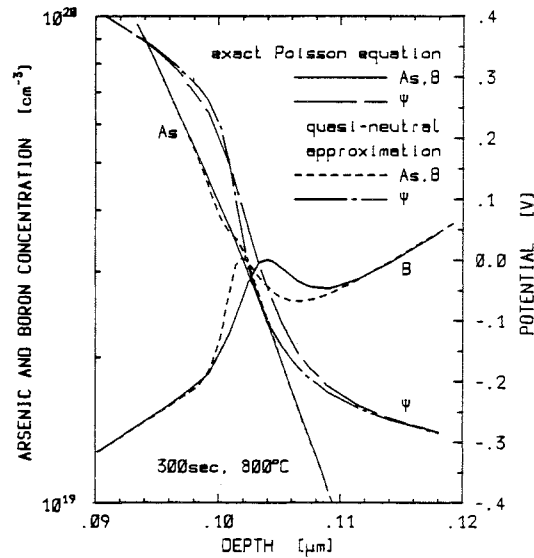see, the qualitative behaviour is unaffected.

FIGURE 8
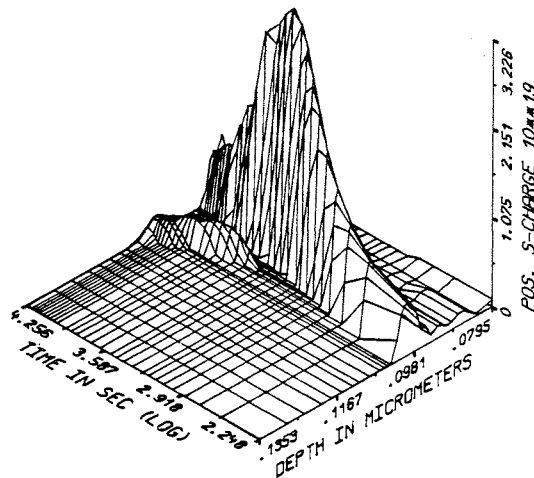Concentrations and Potential after 300 sec.

FIGURE 9
Positive Space Charge

Our simulations indicate the existence of two diffusion periods. In the first period the diffusion is strongly field controled. This means that the local increase of dopants in the vicinity of the p-n junction leads to an increase of the electric field and therefore to a stronger migration of dopants. This self-enhancing procedure is opposed by the ambipolar spreading of the profiles. A good impression of the transient behaviour can be gained by regarding the positive space charge over time in Fig.9. This picture shows a maximum of space charge after approximately 4000 sec. diffusion time. The maximum indicates the transition from field controled to ambipolar diffusion in the region of the p-n junction. Therefore we do not expect the differences between the models to increase after this point of time.

5. CONCLUSION

All our investigations have shown that the quasi-neutral approximation is a good approach to simplify the simulation when the diffusion time exceeds the field controled period. Even if the diffusion time is of the same order as the field controled period, the agreement between the two models is qualitatively good in the vicinity of the p-n junction and excellent elsewhere in the simulated domain. We can therefore recommend the use of the quasi-neutral assumption in engineering programs where fast performance and small memory requirements are powerful arguments.

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