COMPARISON OF ADVANCED MODELS FOR COUPLED DIFFUSION

W.Jüngling, P.Pichler, S.Selberherr, E.Guerrero and H.Pötzl

Institut für Allgemeine Elektrotechnik und Elektronik
Abteilung für Physikalische Elektronik
Technische Universität Wien, Gußhausstraße 29, A-1040 WIEN, AUSTRIA

Abstract: We present one- and two-dimensional general purpose diffusion programs capable to treat an arbitrary number of physical quantities such as dopants and interstitials, vacancies, electrostatic potential, cluster, etc. We use our codes to evaluate existing models (e.g. coupled 2-dimensional diffusion) as well as to verify assumptions which are commonly used in simulation programs.

Introduction

The high level in device miniaturization necessitates a better understanding of the physical processes and their interplay to keep the computer simulation an efficient tool for process modeling. Our contribution to this goal has been the development of general purpose one- and two-dimensional simulation programs which include the possibility to treat an arbitrary number of physical quantities involved in diffusion processes (acceptors, donors, vacancies, interstitials, electrostatic potential, cluster, precipitates, ...). The program architecture permits in a simple way the evaluation of a physical model as well as the verification of assumptions which are usually made for the simulation of diffusion (field enhancement factor, space-charge-zero approximation, static cluster relation). The numerical accuracy of our programs has been verified with pathological problems the solutions of which are known. To obtain the requested reliability our codes had to reach a fairy high level of numerical sophistication (a fully (automatically) adaptive mesh in space and time and careful discretisation to minimize the local discretisation error). The conservation of the integral dose is a fundamental criterium for the reliability of a mesh in a one-dimensional inert diffusion. In all our computations it varies less than 0.1%.

Coupled Diffusion

Comparison between Poisson's equation and the space-charge-zero approximation

The first example represents a worst case estimation. Sufficiently high doses have been chosen for both arsenic and boron dopants to exceed the intrinsic number at the p-n junction. Clustering of arsenic has been neglected to obtain high electric fields and considerable space charge. The diffusion is described by Eq.(1) to Eq.(3). For the space-charge-zero approximation "grad div Ψ " is replaced by 0 in Eq.(3).

$$\frac{\partial C_B}{\partial t} = \mathrm{div}\left(D_B \left(\mathrm{grad}\, C_B - \frac{C_B}{U_t}\cdot \mathrm{grad}\, \Psi\right)\right) \quad (1)$$

$$\frac{\partial C_{As}}{\partial t} = \mathrm{div}\left(D_{As} \left(\mathrm{grad}\, C_{As} + \frac{C_{As}}{U_t}\cdot \mathrm{grad}\, \Psi\right)\right) \quad (2)$$

$$\mathrm{div}\,\mathrm{grad}\,\Psi = \frac{q}{\varepsilon}\cdot\left(2\cdot n_i\cdot \sinh\left(\frac{\Psi}{U_t}\right) + C_B - C_{As}\right) \quad (3)$$

The diffusivities are taken from established literature and include enhancement by charged point defects. Fig.1 shows the distribution after 30min. inert diffusion at 950C. In the first 100 seconds the dopant redistribution is field controlled and tries to minimize the electric field and to reduce the space charge (Fig.2). In the remaining time ambipolar diffusion dominates. The descending shapes in Fig.2 indicate the boundary between the two periods. The differences between the two models are small and reach remarkable values only near the p-n junction in the period between 10sec. and 100sec. as shown in Fig.3 (t=30sec. constant) and Fig.4 (x=0.099μm constant). After 100sec. the space charge ceases to a negligible value causing the main difference between the two models to disappear. The small differences are supplanted completely by ambipolar diffusion after 500sec. In the second example we use a lower boron concentration to obtain a more realistic p-n junction. Fig.5 reveals a "valley" in the boron profile which is caused by the electric field of the arsenic concentration. The small differences between the models are constrained to the p-n junction and disappear as soon as the junctions moves away from the depth under consideration. In further simulations we have extended our model by taking into account arsenic clustering. Although a strong interaction between the dopants takes place the space-charge-zero approximations proves to be a fairly good approach. Our calculations indicate that the space-charge-zero approximation can be used if a constraint of computer resources requires a simplification of a physical model.

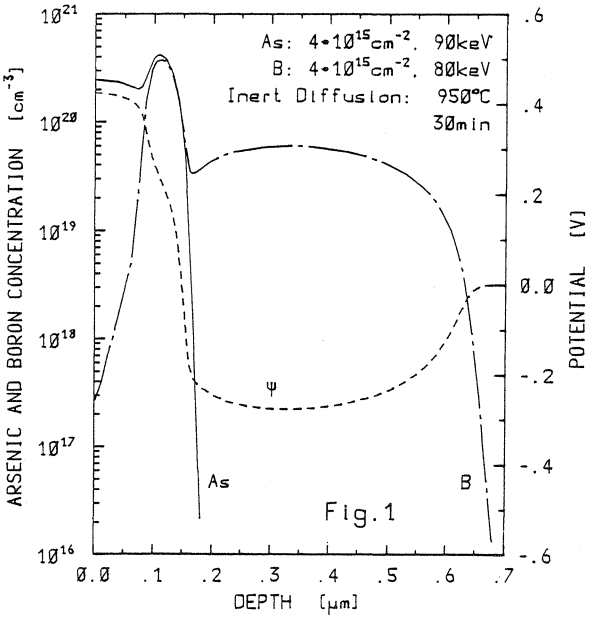
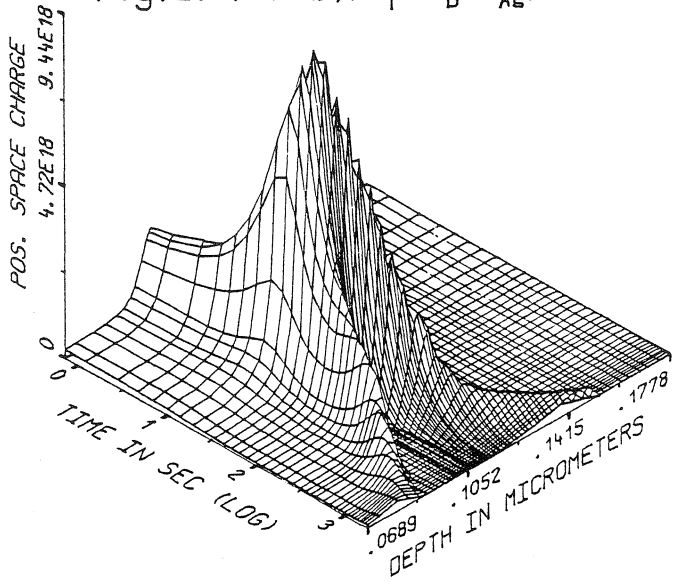
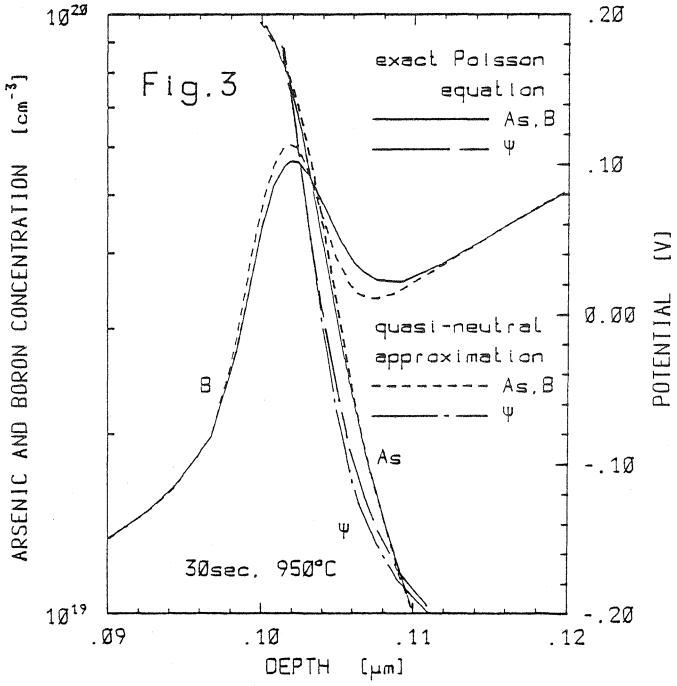
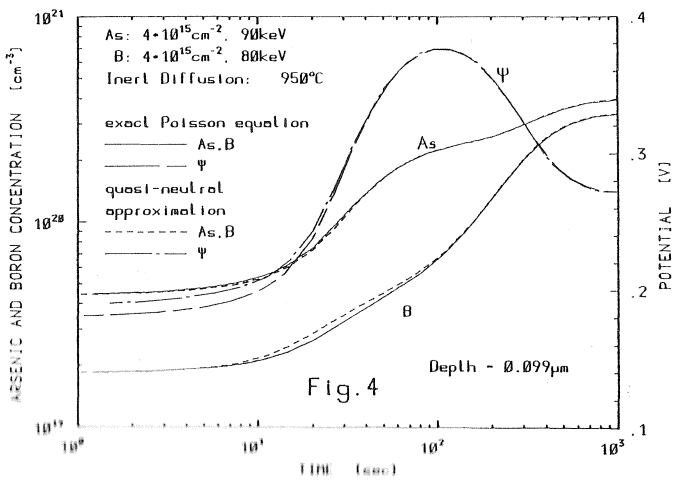


Fig.1

Fig.2: max(Ø,n-p+C_B-C_{As})







Ion Implantation: As: $4*10^{15}cm^{-2}$, 90keV
B: $7*10^{13}cm^{-2}$, 40keV
Inert Diffusion: 40min, 1000°C

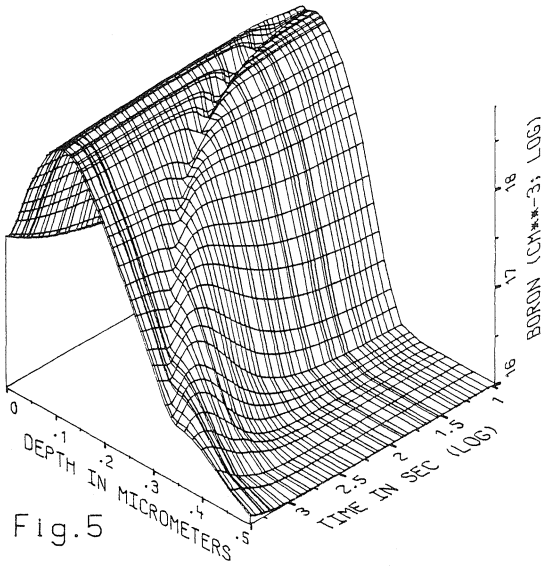
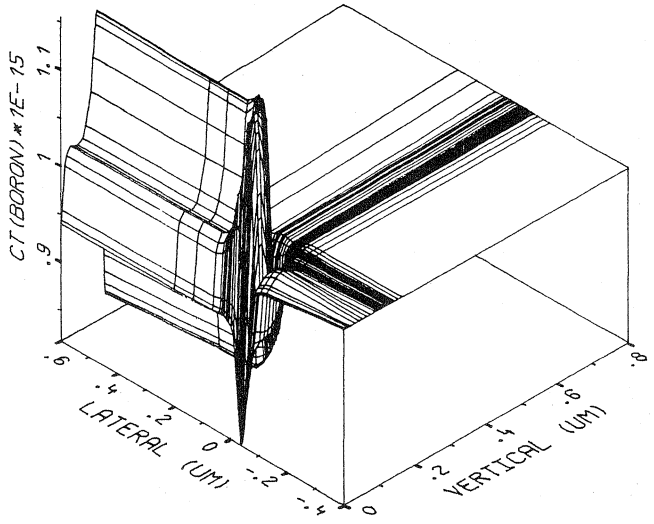


Fig.5

Two-dimensional coupled diffusion

As a simple example of the two dimensional program package we present an inert annealing step at 1000C. The physical model is given by Eq.(1) to Eq.(3). We assume a homogeneously doped boron substrate ($10^{15}cm^{-3}$) implanted with arsenic ($10^{15}cm^{-2}$, 130keV) through a mask (35nm) with an infinitely steep edge to field oxide at the origin of the coordinate system. Two dimensional effects are most clearly revealed by the boron profiles. Fig.6 and Fig.7 show the boron profiles after 100sec. and 1500sec. respectively. The boron motions are caused by a field controlled current trying to accumulate the boron atoms in regions of high arsenic concentrations. This leads to areas of accumulated and depleted boron. In the space domain where the arsenic profile bends, the area of depletion is larger than the area of accumulation causing the extreme accumulation of boron atoms.

Fig.6: Boron: 1000°C, 100sec



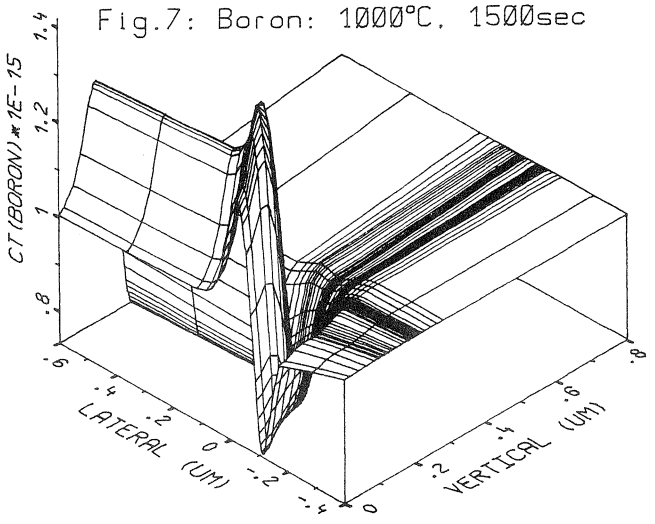


Fig.7: Boron: 1000°C, 1500sec

Dynamic Arsenic Clustering

Arsenic clustering has to be taken into account for the simulation of highly doped p-n junctions as well as for the accurate simulation of the resistivity of highly doped arsenic source and drain regions of MOS devices. Beyond its solubility concentration As forms clusters to achieve its thermodynamic equilibrium. The transformation from active into clustered arsenic is described by Eq.(4) to Eq.(6).

$$m \cdot As^{+} + k \cdot e^{-} \leftrightharpoons As_{Cl}^{(m-k)+} \qquad (m=3,k=1) \quad (4)$$

$$\frac{\partial C_{As}}{\partial t} = - \operatorname{div} J_{As} + k_D \cdot C_{Cl} - k_C \cdot C_{As}^{m} \cdot n^{k} \qquad (5)$$

$$m \cdot \frac{\partial C_{Cl}}{\partial t} = - k_D \cdot C_{Cl} + k_C \cdot C_{As}^{m} \cdot n^{k} \qquad (6)$$

At high temperatures (T>1000C) clustering is a very fast process. Fig.8 and Fig.9 show the typical time dependence of an annealing step after a high dose As implantation. At low temperatures (T=800C) the equilibrium between clustered and active arsenic is not obtained after 20min. Therefore a dynamic cluster model seems necessary for up-to-date process modeling. Since the physics of clustering is not yet fully understood we have used our codes to compare the measured values of [1] to simulations using the cluster model of [2]. To match the time dependence of laser annealing experiments, we had to choose m=7 and k=1 to obtain an optimal fit. Is seems remarkable that k_C, k_D can match the value and the time of the minimium in Fig.10, whereas the slope is only affected by m. These results indicate larger cluster sizes. Since the dynamics are mainly determined by the term $C_{As}^{m} \cdot n^{k}$ we believe that (m=6,k=2), (m=5,k=3) or (m=4,k=4) would lead to similar results.

References

[1] J.Goetzlich et. al.: CO_2 Laser Annealing of Ion-Implanted Si. Springer Series in Electrophysics, Vol.11, p.513-519, 1983

[2] M.Y.Tsai et. al.: Shallow Junctions by high-dose As implants in Si. J.Appl.Physics, Vol.51, No.6, June 1980

Ion Implantation:
As: $2 \cdot 10^{16} cm^{-2}$, 140keV, 25nm oxide coating
Annealing Step: 20min, 1000°C

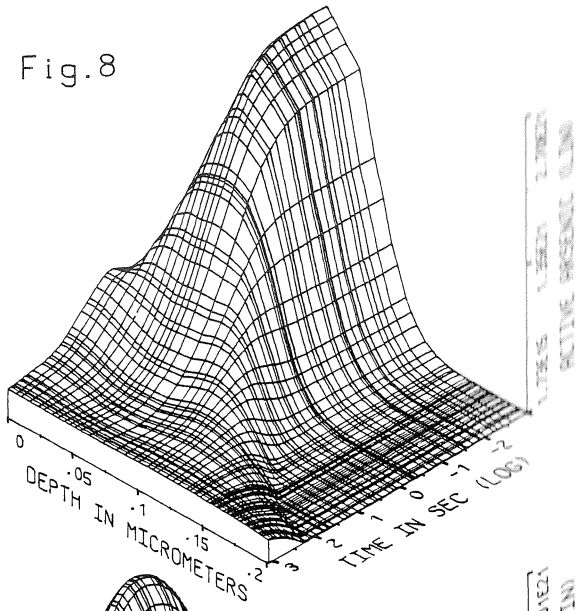


Fig.8

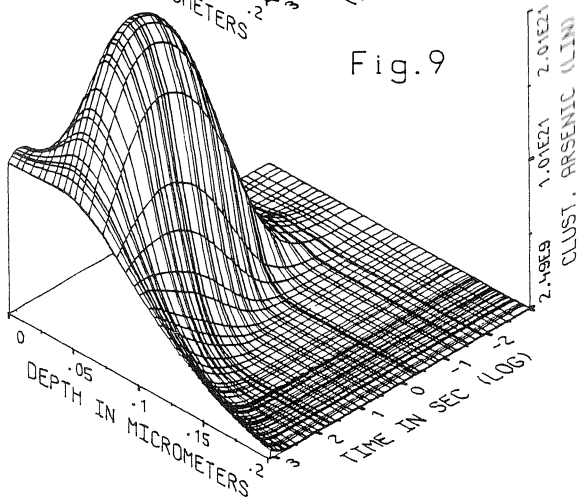


Fig.9

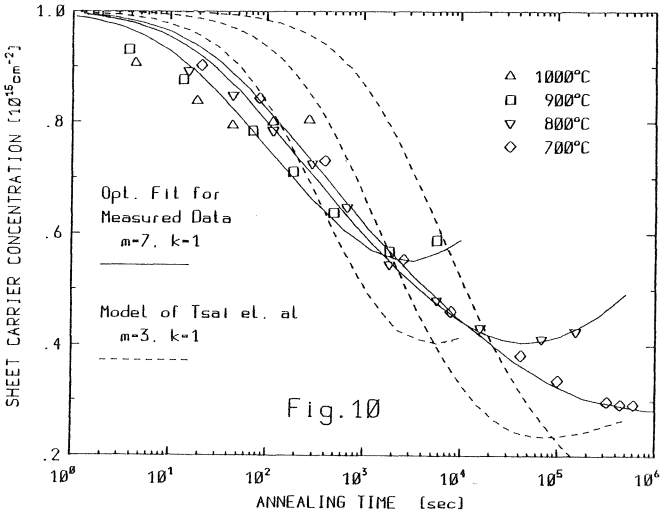


Fig.10

This work has been sponsored by the Siemens Research Laboratories, Munich, BRD and the Fond zur Förderung der wissenschaftlichen Forschung Project S43/10.