

TWO-DIMENSIONAL COUPLED DIFFUSION MODELING

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The recent advances in device miniaturization - in particular for VLSI - necessitate a better understanding of the various physical processes and their interplay to keep pace with the technological requirements for device and circuit fabrication. To contribute reaching this goal we investigate two-dimensional coupled diffusion phenomena. For that purpose we have developed a general purpose diffusion simulation program which is capable to treat an arbitrary number of physical quantities involved in diffusion processes (acceptors, donors, vacancies, interstitials, electrostatic potential, ...). Thereby many of the assumptions which are usually made for the simulation of diffusion can be waved (field enhancement factor, charge neutral approximation, static cluster relation, ...).

To illustrate the capabilities of our code we present as an easy example the coupled diffusion of boron and arsenic with field enhancement. Neglecting cluster and precipitation effects for the sake of transparency we use the following three equations in this example:

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

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

$$\text{div grad } \psi = \frac{q}{\epsilon} \cdot (2 \cdot n_i \cdot \sinh(\frac{\psi}{U_t}) + C_B - C_{As}) \quad (3)$$

(1) and (2) are the continuity equations for boron and arsenic, respectively; (3) represents Poisson's equation. We assume in this example the validity of Boltzmann statistics which is indeed given for the usual processing conditions as confirmed by experimental findings. However, Fermi statistics, if necessary, would just change the space charge term to a more complicated form. The diffusion coefficients are modeled with superimposed Arrhenius expressions for particles diffusing with neutral (boron and arsenic), negatively charged (arsenic) and positively charged vacancies (boron). Formulae (4) and (5) are used for boron and arsenic, respectively, the coefficients of which have been taken from established literature data.

$$D_B = 0.037 \frac{\text{cm}^2}{\text{s}} \cdot \exp\left(\frac{-3.46\text{eV}}{kT}\right) + 0.72 \frac{\text{cm}^2}{\text{s}} \cdot \exp\left(\frac{-3.46\text{eV} - q \cdot \psi}{kT}\right) \quad (4)$$

$$D_{As} = 0.066 \frac{\text{cm}^2}{\text{s}} \cdot \exp\left(\frac{-3.44\text{eV}}{kT}\right) + 12.0 \frac{\text{cm}^2}{\text{s}} \cdot \exp\left(\frac{-4.05\text{eV} + q \cdot \psi}{kT}\right) \quad (5)$$

We simulate an inert annealing step at 1000C temperature. The intrinsic concentration at this temperature is taken as $6.35 \cdot 10^{18} \text{cm}^{-3}$. A homogeneously doped boron substrate (10^{15}cm^{-3}) implanted with arsenic (10^{15}cm^{-2} , 130keV, LSS, Gaussian) through a mask (35nm) with an infinitely steep edge to field oxide (at the origin of the coordinate axis in the following figures).

The main concern of this small example is the influence of the diffusing arsenic profile on the boron profile via the coupling by the field term in the continuity equations. The diffusion of the arsenic profile is here of minor interest so that we concentrate on the discussion of the electrostatic potential and the boron profile.

The field term in the continuity equation for boron causes a current of doping atoms in the direction of positive gradients of the potential. That means that at the start of the diffusion due to the gradients of the potential at the surface and in the bulk the boron profile is made to form a U-shaped maximum of increased concentration. At the flank of this ring the boron profile is depleted and forms a dent (Fig. 1). The maximum near to the surface is smaller than the maximum in the bulk. This is caused by the less pronounced gradient of the electrostatic potential at the surface. Since the ambient condition at the surface inhibits a flux of boron perpendicular to the surface the concentration of boron is relatively strong depleted in this region. The minima of the boron profile are caused by the gradients of the potential in lateral and vertical direction at the origin of the coordinate system.

The potential profile spreads with increasing diffusion time corresponding to the spreading arsenic profile. The maximum of the boron profile close to the surface is, therefore, reduced (Fig. 2) and vanishes finally (Fig. 3&4), whereas the maximum in the bulk increases and spreads. The dents of the boron profile at the sides of the maxima behave like the maxima themselves; they vanish or increase in depth and magnitude with increasing time vice versa. Nevertheless it should be mentioned that the minimum of the boron profile remains at the surface next to the mask edge (origin of the coordinate system) because of the process described earlier. Effected by the field in vertical and lateral direction the boron profile forms a distinct peak value with increasing diffusion time. After 1500s diffusion time no significant change in the qualitative behaviour of diffusion will take place.

An experimental verification of this fairly simple example is, most unfortunately, not possible, since the resolution of even the most modern, e.g., SIMS equipment is too rough for that purpose. However, we have certainly verified the numerical accuracy of our program with pathological problems whose solution is known. To obtain the required reliability of our code a fairly high level of numerical sophistication had to be reached; for instance, the mesh used in our program is fully adaptive (automatically) in space and time to ensure that the discretization error is acceptably small (cf. Fig.1-Fig.4). "Perfect" agreement between simulation results and measurements cannot be expected for any process simulation program so far, because most of the physical models in use today are too simplistic to fit a broad spectrum of conditions without changing parameters.

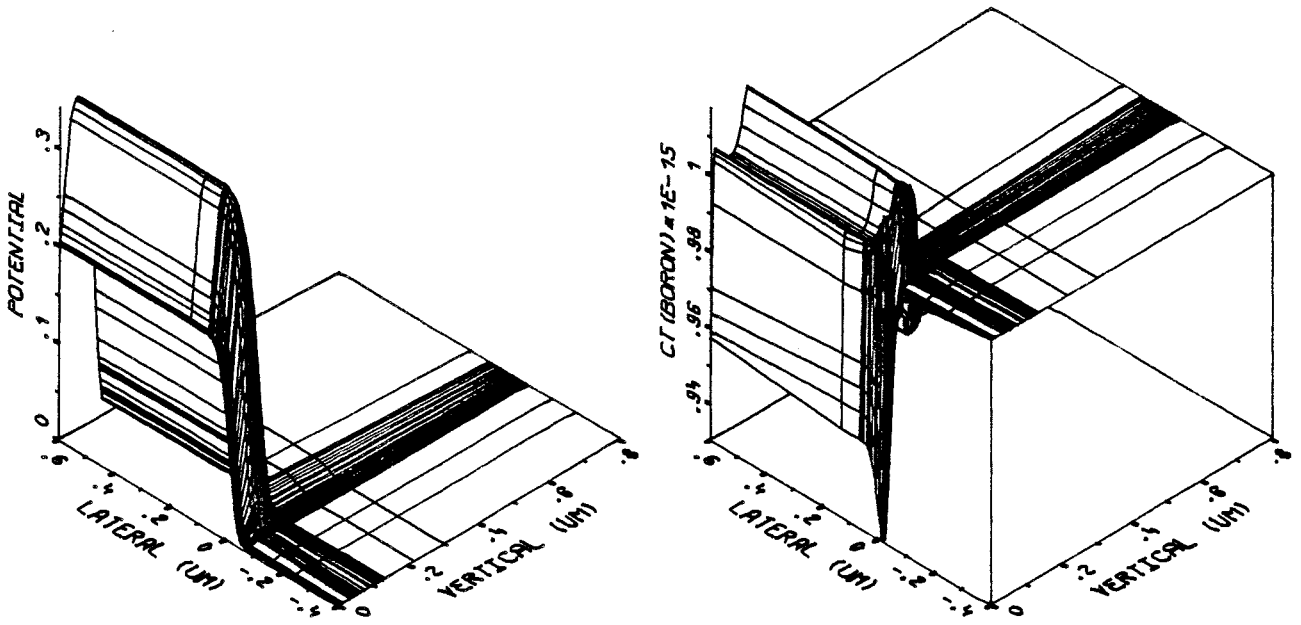


Fig.1 electrostatic potential - $t=10s$ - boron concentration

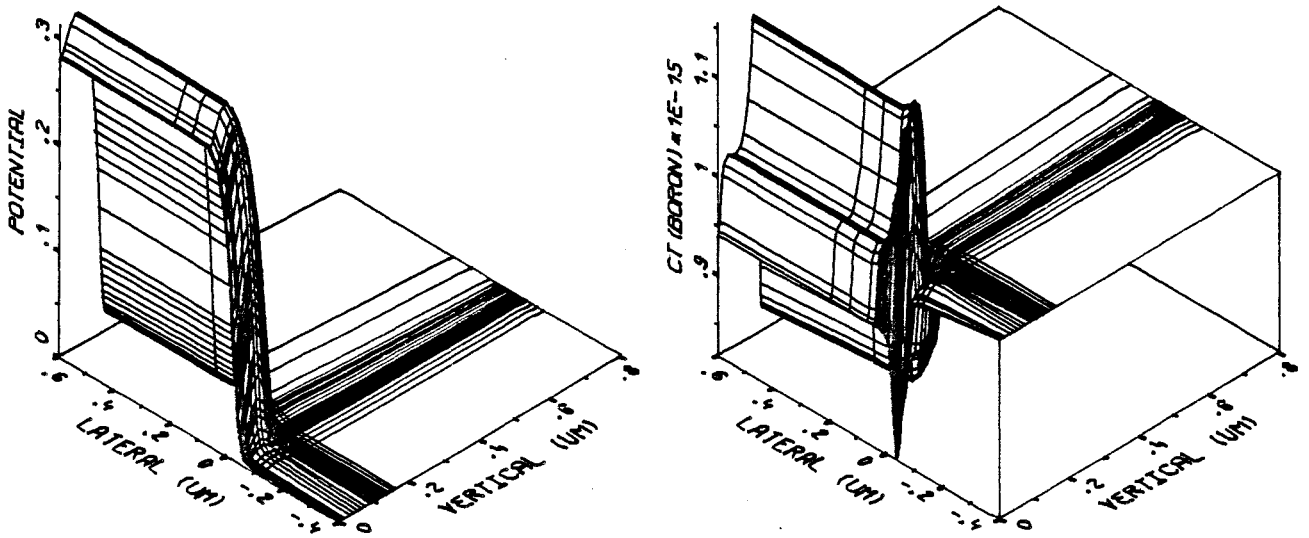


Fig.2 electrostatic potential - $t=100s$ - boron concentration

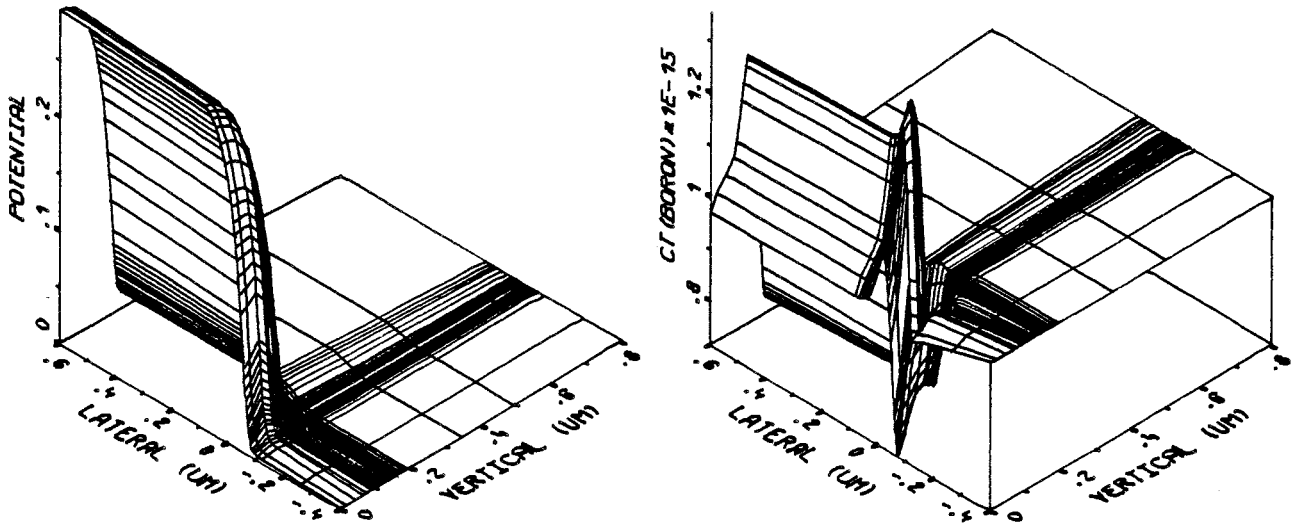


Fig.3 electrostatic potential - t=500s - boron concentration

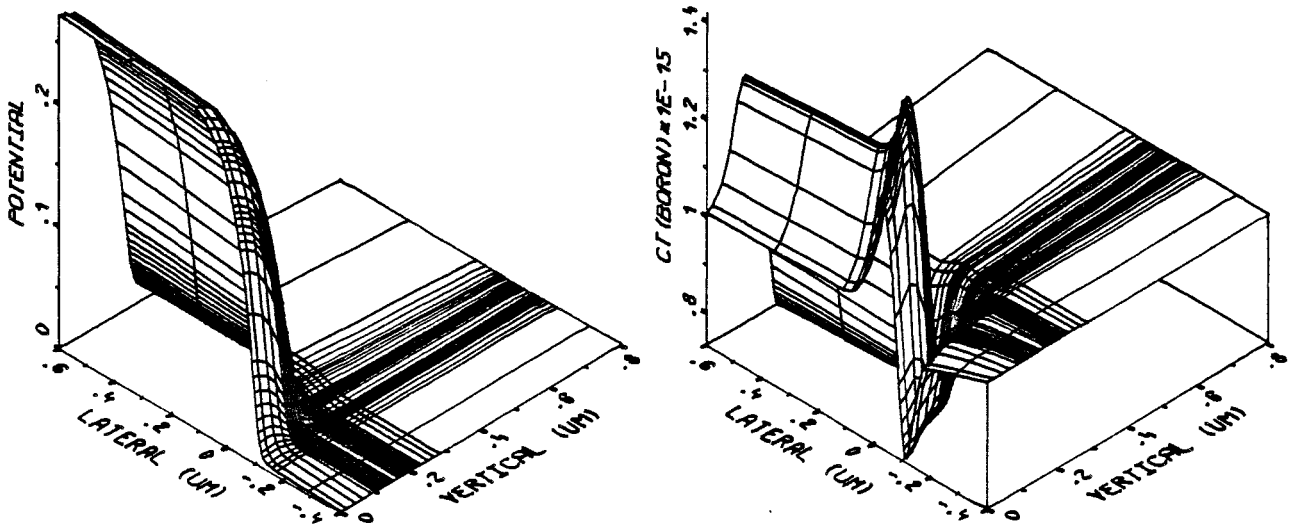


Fig.4 electrostatic potential - t=1500s - boron concentration