TWO DIMENSIONAL PROCESS SIMULATION USING A QUADRATIC FINITE ELEMENT DISCRETISATION. THE CONNECTION WITH DEVICE SIMULATION

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ABSTRACT

A two dimensional process simulator -MO.BI.DI.C- has been developed. The program can simulate ion implantation through arbitrary masks as well as the interaction between impurity diffusions under inert or oxidizing ambients. For boron and arsenic, the diffusion model incorporates electric field, charged vacancies and clustering effects. The phosphorus diffusion is based upon Fair's model. MO.BI.DI.C can handle various boundary conditions that allow the simulation of predeposition, evaporation and segregation. The two dimensional oxide growth is given by an analytical formula, and the diffusion equations are solved in the evolutive physical domain. Finite element method, with quadratic 6-noded triangles gives the spatial discretisation while an incomplete implicite scheme iterates the temporel problem. The process simulation results can be introduced in the device analyzer MINIMOS. This paper presents the process simulator, namely the basic models and the numerical approach, as well as the process device connection in the case of a standard n-MOS polysilicon gate technology.

1. INTRODUCTION

Interest in two dimensional process simulation becomes significant as dimensions of integrated structures decrease whereas microfabrication cost and complexity increase. The aim of such simulations is to calculate the lateral range of impurity diffusion during high temperature process steps under various ambients, so providing device simulators with realistic topological description of components, doping profiles and

surface shapes.

Most of process simulators are based upon the finite difference method [1-4] , this choice being highly motivated by the implementation facilities of this method in simulation package. In another way, finite element approach is under investigation [5, 8] in order to get free with spatial limitations. This method permits a good description of surface shapes and allows to consider two dimensional multi-layer simulations. More, locally refined meshes can be used [8] to obtain accurate description of solutions without prohibitive C.P.U. times.

The topic of this paper is, first, to present some numerical results obtained with the recently developed process simulator -MOBIDIC- using quadratic finite element discretisation In a second way, a standard n-MOS polysilicon gate technology is simulated and the 2-D computed doping profiles which are in good agreement with experimental data, are introduced in the M.O.S. analyser MINIMOS 2.2 . The first electrical results are given.

After a short presentation of the process models that have been included in MOBIDIC -Section 2- the algorithmic procedures are discussed -section 3-. In section 4, the n.MOS process is described as well as simulation results and experimental validation. The last point -section 5- presents the connection with MINIMOS program. The notations are defined in the annex.

2. PROCESS MODELS

2.1 Ion implantation

Two dimensional implanted profiles are obtained with Runge's method [9] , in which the vertical and lateral distributions are assumed to be Gaussian. In the case of multi-layer mask, each layer is taken as an equivalent thickness of silicon this transformation being performed according to the stopping power of the mask material [1]. Data for range and deviations are taken from Gibbons' tables [10].

2.2 Impurity diffusion model

2.2.a Boron and Arsenic

Boron and Arsenic redistribution is governed by the following diffusion equation [1]:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}(D\,\frac{\partial N}{\partial x}) + \frac{\partial}{\partial y}(D\,\frac{\partial N}{\partial y}) \pm \frac{\partial}{\partial x}(D.N.\frac{\partial \Psi}{\partial x}) + \frac{\partial}{\partial y}(D.N.\frac{\partial \Psi}{\partial y}) \qquad (1)$$

in which the conduction term includes the self induced electric field effect, the sign depending upon the charged state of the impurity (+For As, -For B). The reduced potential, Ψ, is calcu-

lated with :

$$\Psi = \mathrm{Log}\ \frac{n}{ni} \qquad (2)$$

The equation (1) is written in the hypothesis that only the electrically active atoms can diffuse. The diffusion enhancement due to the charges vacancies effect [11] is taken into account by the expression of the effective diffusivity :

$$D = D_i\ \frac{1 + \beta F}{1 + \beta} \qquad (3)$$

with $F = \frac{n}{n_i}$, $\beta = 100$ for As

$F = \frac{n_i}{n}$, $\beta = 19$ for B

When Arsenic is present in high concentration,cluster formation occurs. The equilibrum ratio between atomic and active arsenic concentration is taken from [12] :

$$C_{As} = N_{As}\left[1 + \frac{cl}{r}\ \frac{(N_{As}/N_{max})^{cl}}{1 - (N_{As}/N_{max})^{cl}}\right] \qquad (4)$$

The electron concentration, n, is calculated,in the hypothesis of local neutrality, from the concentration of the different species : boron, active and atomic arsenic and charged clusters.

2.2.b Phosphorus

The phosphorus diffusion model developed by Fair and Tsai [13] has been implanted in MOBIDIC. This concentration dependent model includes the diffusion retardation due to high doping level [14] . The overall diffusivity is calculated with the instantaneous values of the atomic and active peak concentrations.

2.2 Oxidation

An analytical method is implanted to calculate the two-dimensional oxide growth. For a field oxide, the thickness oxide variation versus the lateral dimension, x, is given by [14]

$$dox(x,t) = d_i + (dox_{1D}(t) - d_i)\ .\ \frac{1}{2}[1 + \mathrm{erf}(\frac{\sqrt{2}}{\delta}\ .\ \frac{x}{dox_{1D}(t) - d_i})] \qquad (5)$$

The one dimensional oxide growth , $dox_{1D}(t)$,is calculated with the well known linear parabolic model [15] . The shape factor δ, is deduced from process conditions.

During the oxidation, the impurity redistribution at the Si/SiO_2 interface is governed by a segregation mechanism. The segregation kinetics is considered faster than the oxidation one and the resulted impurity concentration discontinuity :

$$\frac{C_{si}}{C_{siO_2}} = m \tag{6}$$

is imposed in the calculation.

For phosphorus and boron, the diffusion coefficient under oxidizing ambient is modified to simulate the OED (oxidation enhanced diffusion) effect. The diffusivity is expressed as the sum of vacancy and intersticiel contributions according to [16].

All the default values of process models are taken from SUPREM program [17].

3. NUMERICAL ASPECTS

As a variational formulation is not available in the case of non-linear diffusivity, the finite element formulation is based upon a weighted residual approach, the time integration being led by a step by step calculation [18].

3.1 Problem formulation

The two dimensional silicon domain is divided into 6-noded triangles using quadratic form function. The classical Galerkin procedure [18] is applied to the diffusion equations. Assuming a Green transformation,the numerical treatment leads to the following matrix system :

$$[K(C)]\ \underset{\sim}{C} + [M]\ \dot{\underset{\sim}{C}} = 0 \tag{7}$$

where $\underset{\sim}{C}$ and $\dot{\underset{\sim}{C}}$ are the computed nodal vectors of the concentration values and their derivatives. A simple first order time discretisation is implemented to increment the matrix system (7). The temporal scheme is given by an incomplete implicit formula :

$$[M]\ \frac{\underset{\sim}{C}_{k+1} - \underset{\sim}{C}_k}{\Delta T} + [K(\underset{\sim}{C}_k)]\ \underset{\sim}{C}_{k+1} = 0 \tag{8}$$

where the concentration dependent matrix K is updated for each time step.

Frontal method and Gaussian elimination are used to solve the system (8) in core, the storage requirement being reduced by an optimal node ordering given by the Cuthill Mc Kee algorithm. In the case of multi-impurity problem, the system (8) is solved alternatively for each diffusion equation.

3.2 Simulation criteria

The temporal resolution simplicity have required a systematic study of the time step influence. The time step is preserved constant and the number of temporal loops is automatically selected versus the non linear degree of the diffusion equation [8,19]. The overall problem formulation allows the exploitation of locally refined meshes [19]. Optimal idealisations are generated from a triangle pattern library by assembling of blocks with automatic redundant nodes elimination. The local refinement position is parametrised by the input process data. An automatic mesh optimization is currently developed. Figure 1 presents a source/drain typical mesh, when the high density triangle area coincides with the final junction front location.

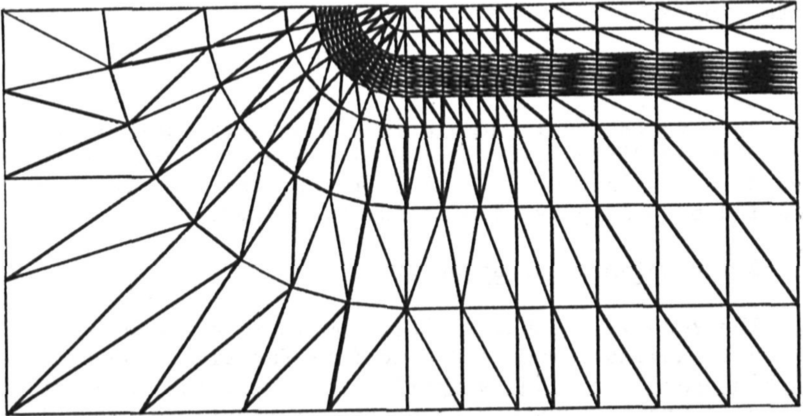


Figure 1 : Source/Drain typical mesh

3.3 Oxidation simulation

As the finite element method allows arbitrary displacement of the discretisation points the diffusion under oxide growth is performed in the physical domain. The numerical procedure consists in introducing a re-meshing algorithm after each diffusion step. The oxidized boundary motion, equation (5), is distributed in the mesh and the node translation preserve the triangle topology allowing an immediate grid to grid interpolation. The diffusion equations are solved only in the silicon. The oxide growth and segregation effects are contained in a Newman condition on the oxidized surface :

$$D.\ \underset{\sim}{\nabla C}.\ \underset{\sim}{n} = -V_{ox}\ C_{si}\left(\frac{1}{m} - \alpha\right)$$

where V_{ox} is the local normal oxidation rate.

3.4 Typical simulation results

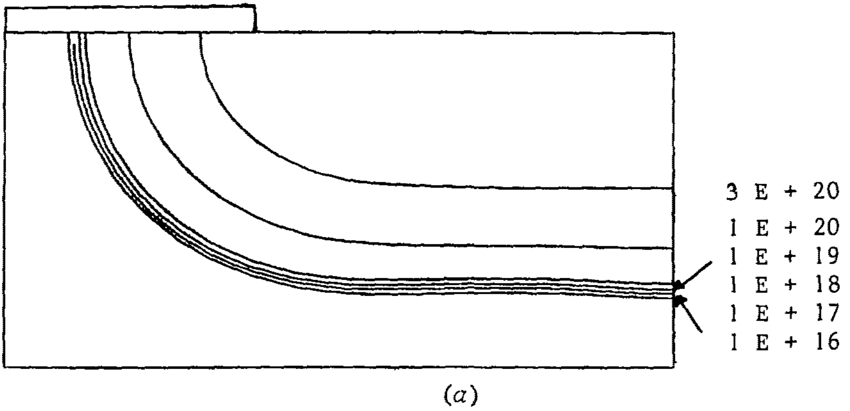
To illustrate the program efficiency and the previous remarks, three simulation results are presented. The first one is an inert annealing of a high dose arsenic implant. The simulation results, figure 2a and 2b, illustrate the arsenic clustering model and attest the algorithm validity in an extremely non linear diffusion case. The second exemple is a two dimensional phosphorus predeposition simulation. The computed doping profiles, figure 3a and 3b are in good agreement with published data [14], and obviously show the two-dimensional formation of the "plateau", kink and tail regions [13]. The third simulation consists in a boron-arsenic simultaneous diffusion in oxidizing ambiant. This example summaries the major numerical difficulties induced by the process models, namely, high concentration boron and arsenic diffusion, interaction between impurity, segregation and evolutive domain. The isoconcentrations for boron and arsenic, figure 4a, exhibit pronounced coupling effects and determine the lateral extension of each doped layer. Figure 4b presents the two dimensional junction on the final mesh.

4. TWO DIMENSIONAL SIMULATION OF A STANDARD n-MOS POLYSILICON GATE TECHNOLOGY

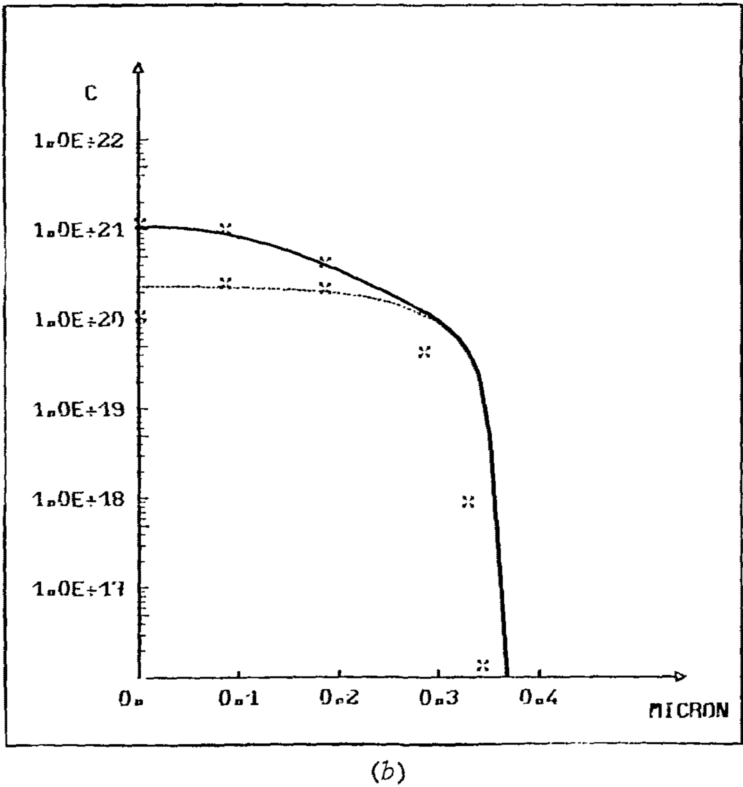
The simulation of a standard n-MOS process has been performed using the models and the algorithms described in section 2 and 3. We have studied the particular region between the MOS channel and the source or drain region. The purpose of this study was to use the MOBIDIC program in a real technological environment. This was done in order to acquire a better physical understanding of the fabricated devices and to provide an evaluation of the simulator performance. This device characterization allows us to verify the adequacy of two-dimensional models in the particular case of this technology.

4.1 Process description

The technology used here is a 6-micron nMOS polysilicon gate process. The isolation is achieved with a classical LOCOS technique for 1 micron field oxide. A 950 Å gate oxide is formed at 1100°C on the <100> p-substrate ($1.10^{15} cm^{-3}$). The threshold voltage adjustement of the enhancement mode transistor is realised by boron ion implantation through the gate oxide (E = 60 KeV, $N_{\alpha} = 3.10^{11} cm^{-2}$). LPCVD polysilicon (4500 Å) is then deposited as gate material and doped by phosphorus predeposition (950°C, 65 min.). The etching of the polysilicon is performed in a planar SF6 plasma reactor. The following steps have been considered for the simulation : source and drain are formed by phosphorus implantation through the polysilicon mask and the remaining 950 Å oxide (E + 120 KeV, $N_{\alpha} = 5.10^{15} cm^{-2}$) followed by a reoxidation step at 1000°C (5 min dry, 15 min.wet 5 min. dry and 10 min.N_2),a passivation CVD oxide deposited on the circuit is finally annealed at 1000°C for 15 minutes prior

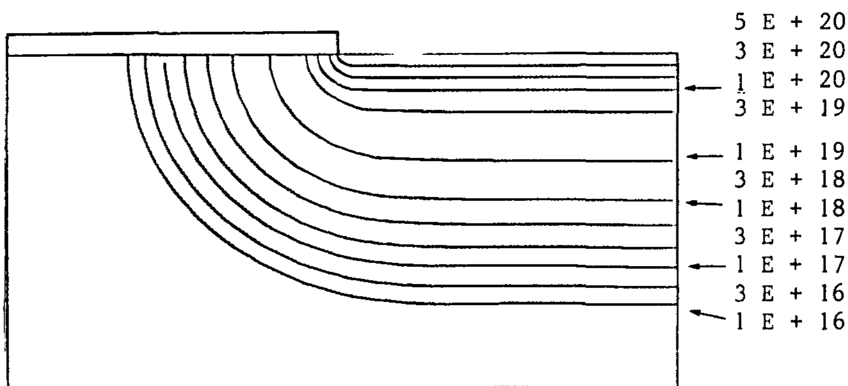


(a)

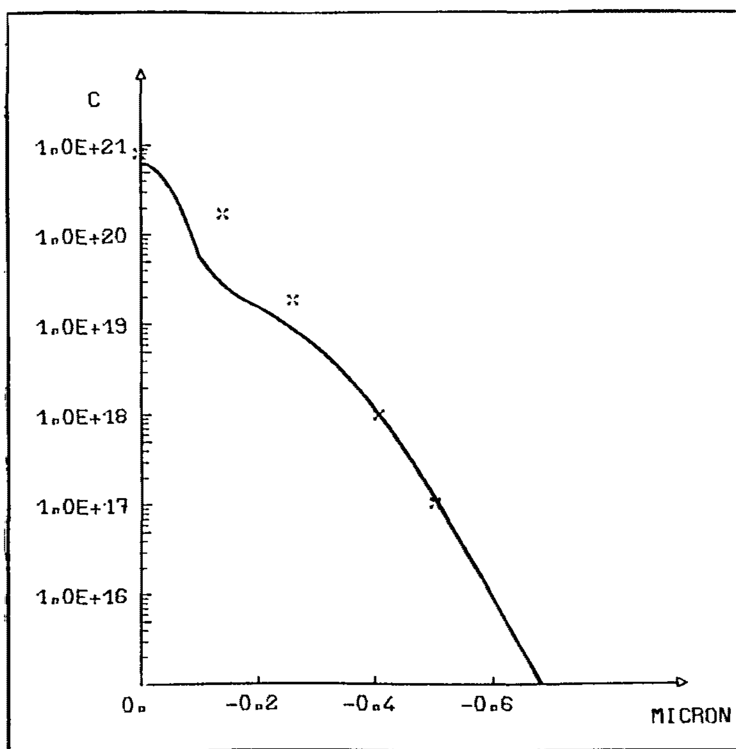


(b)

Figure 2 : *Inert annealing (1000°C) of arsenic implantation (140.keV, $2.10^{16} cm^{-2}$)*
(a) Isovalues
(b) Cross section view
Full lines : atomic concentration
Dashed lines : active concentration.
⁑ experimental data from [20]

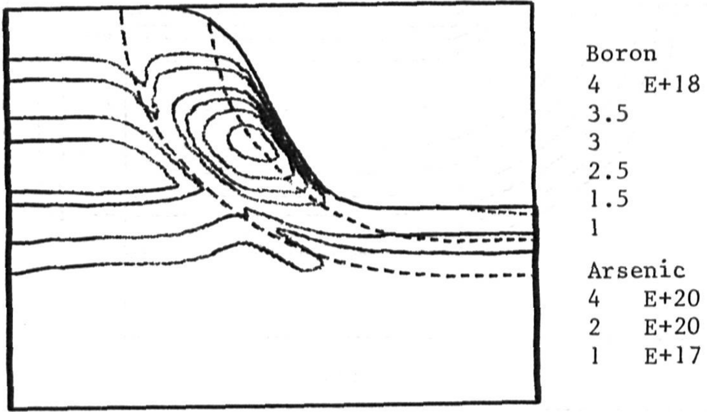


(a)

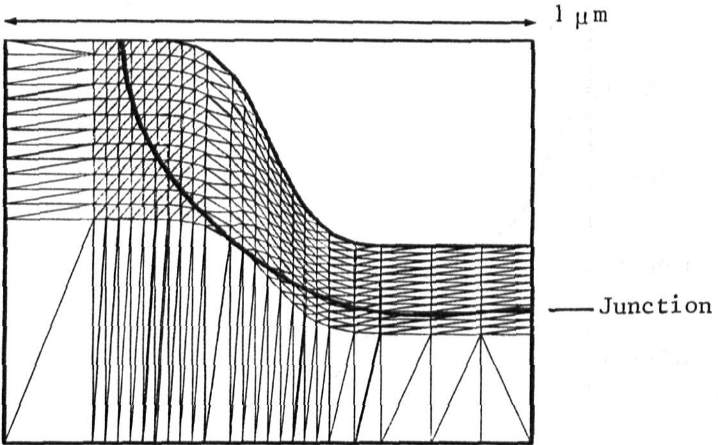


(b)

Figure 3 : *Phosphorus predeposition*
$C_S = 7.10^{20}$ cm^{-3} 30 mn 900°C
(a) Isovalues
(b) Cross section view
⁑ experimental data from [14]



(a)



(b)

Figure 4 : Arsenic-boron diffusion in oxidizing ambient

. homogenous arsenic implant $E = 100$ KeV
$N_a = 10^{14} cm^{-2}$

. local arsenic implant $E = 80$ KeV
$N_a = 5.10^{15} cm^{-2}$

(a) full lines : boron
dashed lines : arsenic

(b) junction and final mesh

to the metalisation. We can summarize the different steps to be simulated in three principal phases :

Phase 1 : Phosphorus ion implantation through oxide (120 KeV, $N_{\square} = 5.10^{15}\ cm^{-2}$)

Phase 2 : Redistribution in oxidizing ambient (1000°C, 25 min.)

Phase 3 : Redistribution in neutral ambient (1000°C, 25 min.)

4.2 Process simulation

Some starting characterizations have been carried out to use the real technological input data for the simulation. The etch profile after plasma treatment has been analysed by the SEM technique. This was done to obtain the correct mask function needed in Runge's formulation [9]. This profile is approximated by the two lines described in figure 5. The silicon-silicon dioxide

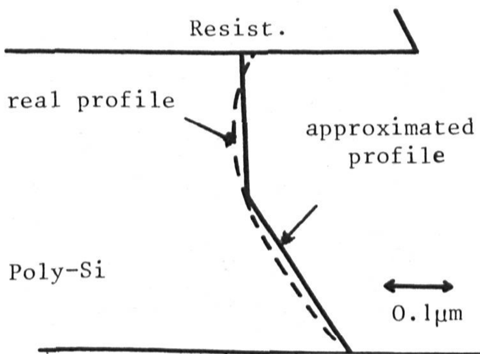


Figure 5 : Poly-silicon profile

interface after oxidation was also characterized by the SEM method to identify the parameter of the analytical formulation used for the mesh deformation, equation (5). A δ value of 1.7 has been estimated for the 950 Å starting oxide and the 2450 Å final thickness. The complete process has been simulated in three phases as described before.

Figure 6(a) shows the two dimensional profile after phosphorus implantation through the real polysilicon mask profile and the remaining gate oxide on source and drain area. Figures 6(b) exibits the doping profile after the oxidation steps. The simulation involves the determination of SiO_2-Si interface according to the measured profile. The segregation at this interface as well as the oxidation enhanced diffusion effect have been taken into account considering a constant oxidation rate. Finally, figure 6(c) shows the impurity profile after the neutral ambient treatments at the end of the process.

An experimental verification is presented on the SEM micrograph of figure 7. This picture was obtained by coloration

technique at the end of the 6-micron process. The deleneated region is expected to define an isoconcentration curve, the value of which can be determined by 1D analytical tools. This concentration was measured by the spreading resistance method and a value of 1 E 19 cm^{-3} was found. The comparison between the simulated curve of figure 6(c) for the same value and the micrograph of figure 7 give an excellent agreement.

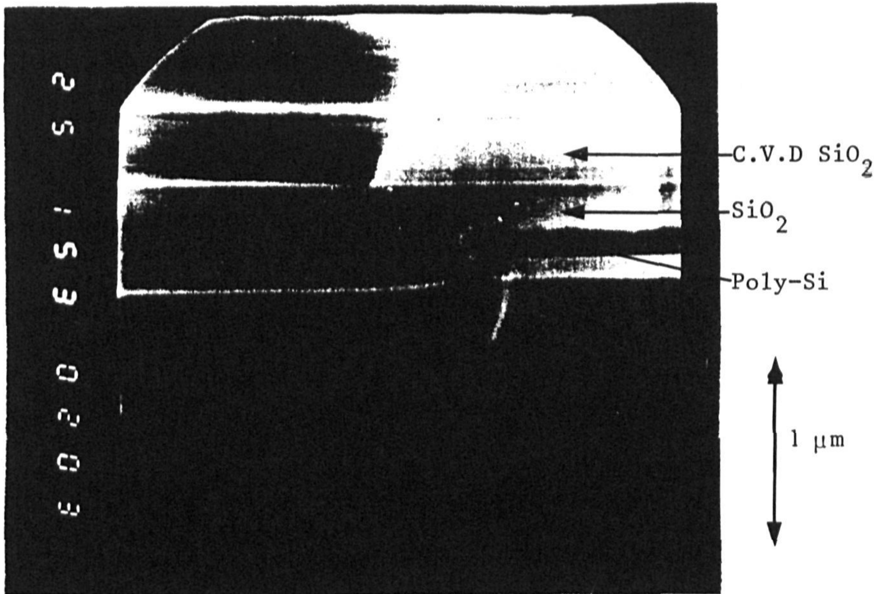
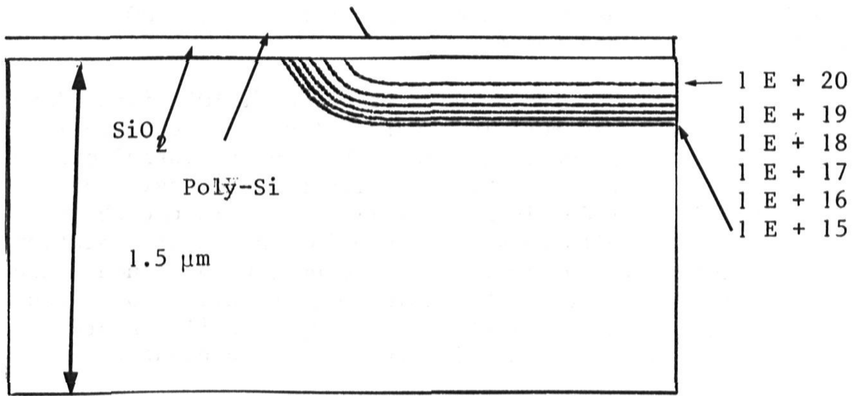


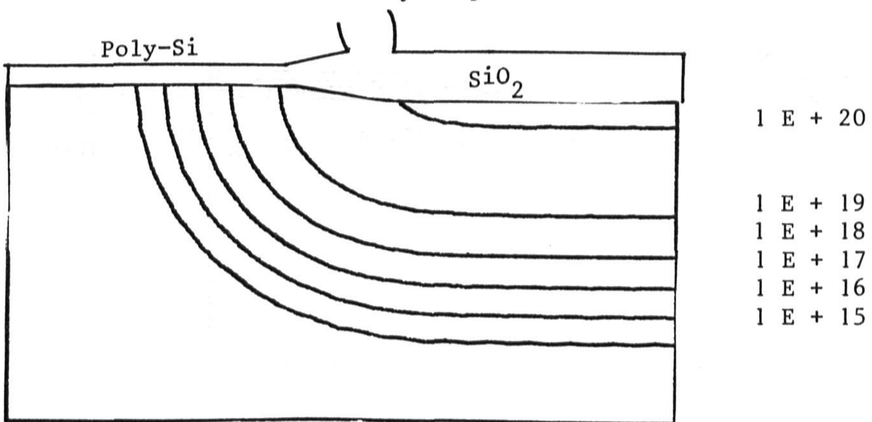
Figure 7 : SEM micrograph of a n-MOS transitor at the end of the process-cross section view-

5. CONNECTION WITH DEVICE SIMULATORS

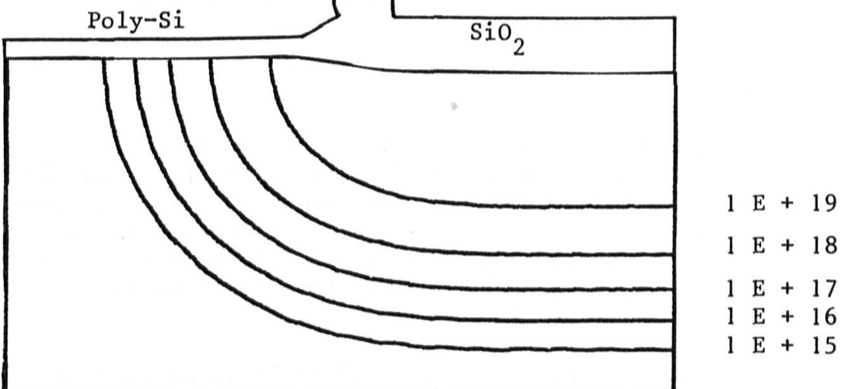
The connection between two dimensional process and device simulators proves to be a powerful tool for integrated circuit design and process development [2]. Numerically, it allows the optimum process steps choice, facing certain limitations in scaling down structures. More, an evident manufacturing interest lays on the obtention of the electrical behaviour sensibility of integrated structures via the process parameters shifts. Such a tool is, here, in development. An interface has been developed between MOBIDIC and MINIMOS 2.2 [21] programs. The complete physical description of component is obtained by grid to grid interpolation, the translation and symetry operations are automatically carried out in regard on the final polysilicon gate length. Only the source/drain doping profiles are computed with MOBIDIC, the one-dimensional channel implant being given by SUPREM II [17] . Figure 8 presents the whole doping profile



(a) after phase 1



(b) after phase 2



(c) after phase 3

Figure 6 : Simulated doping profile of the n-MOS process

of an enhancement-type transistor simulated in the n-MOS technology described in section 4.

The device simulation needs a standard MINIMOS input data in which the SUPREM and MOBIDIC binary files names are mentioned. For example, figures 9a and 9b exhibit the potential distribution and the lateral current density for the device of figure 8. The further developments will consist in the obtention of compared results between simulation and experimentation about the electrical behaviours of component, with standard and modified processing step as threshold voltage variation versus gate length and channel implant. This study is still in progress, and does not allow quantitative results presentation.

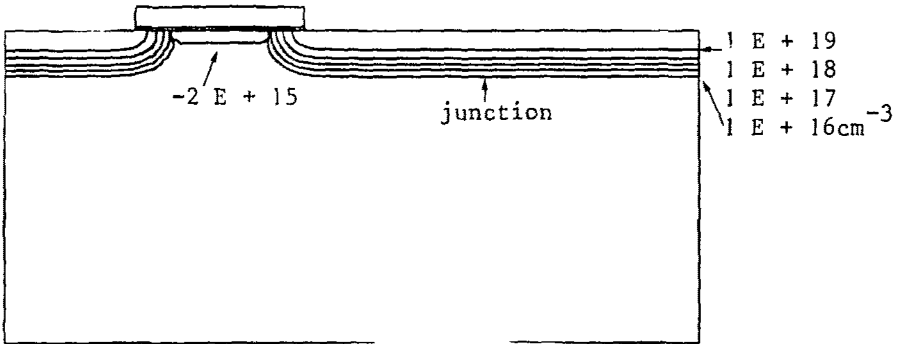
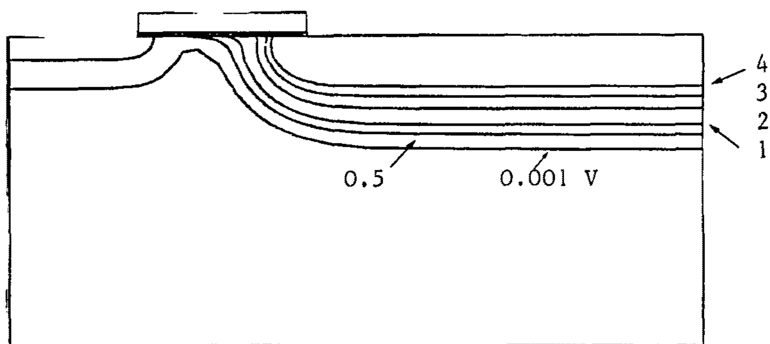


Figure 8 : Doping profile of a 5 μm gate length n-MOS transistor

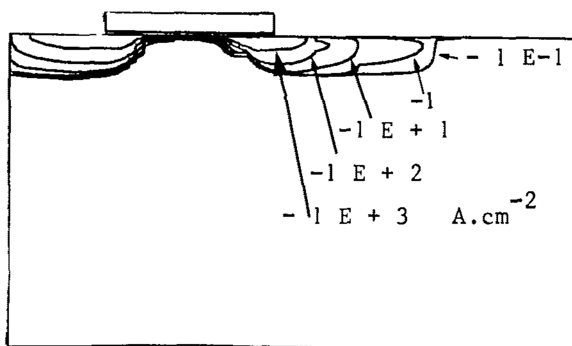
6. CONCLUSION

Finite element method using quadratic form function is used to perform process simulation. This spatial discretisation associated with an incomplete implicite temporal scheme is proved to accurately solve the major numerical problems induced by the process models. Moreover prohibitive C.P.U. time is avoided by the exploitation of the finite element versatility like mesh optimization and node translation.

The resulted process simulator -MOBIDIC- is applied to a standard n-MOS technology. The comparison between experimentation and simulation attests the program validity and its ability to handle multiple process steps. An interface with device analyzer MINIMOS is completed and a systematic study will be carried out to estimate the agreement level between all simulated results and measurements.



(a)



(b)

Figure 9 : *Device simulation results on transistor of figure 8*
Bulk voltage : 0V
Source voltage : 0V
Gate voltage : 2V
Drain voltage : 5V

(a) Electrical potential
(b) Lateral current density

NOTATIONS

- C : Atomic concentration
- N : Active concentration
- D : Effective diffusion coefficient
- n : Free electron concentration
- n_i : Intrinsic concentration
- D_i : Intrinsic diffusion coefficient
- C_{As} : Arsenic atomic concentration
- N_{As} : Arsenic active concentration
- Cl : Atom number by cluster
- r : Cluster electric charge
- N_{max} : Arsenic electrical solubility
- d_i : Uniform initial oxide thickness
- C_{si} : Dopant concentration in the silicon near the si/siO_2 interface
- C_{Ox} : Dopant concentration in the oxide near the si/siO_2 interface
- m : Segregation coefficient
- $[K(C)]$: Equivalent stiffness matrix
- $[M]$: Equivalent mass matrix
- ΔT : Time step increment
- k : Temporal loop number
- $\underset{\sim}{n}$: Normal vector to the boundary
- C_s : Imposed surface concentration for predeposition

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