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OSIRIS II, A TWO-DIMENSIONAL PROCESS SIMULATOR FOR SIMOX STRUCTURES USING BOTH ANALYTICAL AND NUMERICAL RESOLUTION TECHNIQUES

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SUMMARY

In this paper we present a numerical strategy to solve the diffusion equation in the case of SIMOX device with a LOCOS isolation. In such a two-dimensional structure, the silicon domain is variable with time, particulary during the field oxide growth. To avoid numerical problems, a "mixed" solution (both numerical and analytical) is used. This simulation of the impurity redistribution is included in a process simulator for SOI structures, SIMOX II.

INTRODUCTION

During the past years effort has been devoted to the developement of two-dimensional (2D) process simulators. Consequently several 2D process simulators for bulk silicon do actually exist. However, they are unable to simulate the redistribution of impurities on other structures - e.g. SIMOX (Separation by IMplanted OXygen) which has potential advantages compared to bulk silicon for advanced CMOS devices (Partridge, 1986).

To separate between devices on the SIMOX structure, two isolation techniques are generaly used (Auberton-Hervé, 1986). The first one is the isolation by a mesa technique (isolation between devices is obtained by etching moats around each device), and the second one is the LOCOS (LOcal Oxidation of Silicon) isolation which is the most used for CMOS devices either on bulk silicon or on SIMOX structures (fig. 1).

We have developed a 2D process simulator for SIMOX structures, "OSIRIS II" (Sweid, 1988), which allows the simulation of the following steps:

- resist, nitride and oxide deposition and etching,
- ion implantation of Boron, BF2, Arsenic, Phosphorus, and Antimony,

- growth of oxides in dry or steam ambient, with the formation of the field oxide in the case of LOCOS technology,
- redistribution of impurities in an inert or oxidizing ambient.

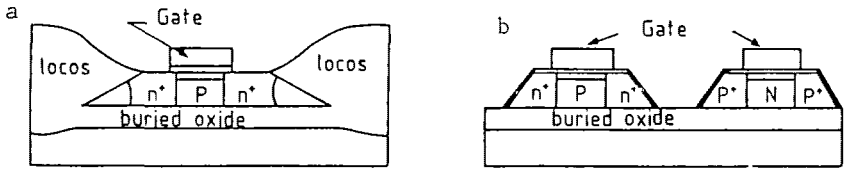

Fig. 1. The two isolation techniques on SIMOX structures a) LOCOS isolation. b) Mesa technique

We present our numerical strategy for solving the diffusion equation in the case of SIMOX devices with a LOCOS oxidation as the main goal of this paper.

On a SIMOX structure, the silicon domain Ω is variable with time, particulary during the field oxide growth (it is restangular at first and becomes triangular at the end of process, fig. 2).

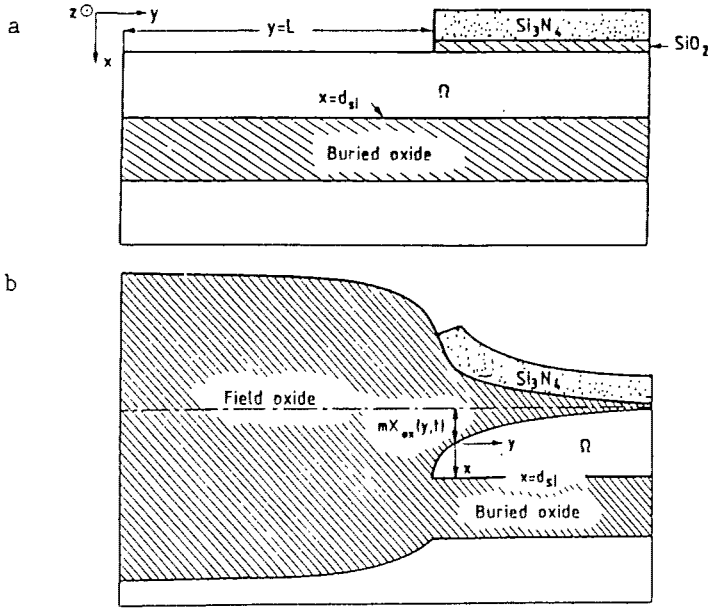

Fig. 2. Geometries of the silicon domain Ω during the field oxide formation: a) During ion implantation. b) At the end of the oxide formation

To avoid numerical problems (the numerical resolution based on the finite difference method does not converge as the thickness of the silicon domain vanishes in the isolation region), a mixed solution in then used to solve the diffusion equation in SIMOX structures. An analytical model is developed for the simulation of impurity redistribution in the whole of the silicon domain until the isolation is formed; the analytical solution is then limited to the region I, where the concentrations are low, while in region II (active zones) the diffusion equation is solved numerically (fig. 3).

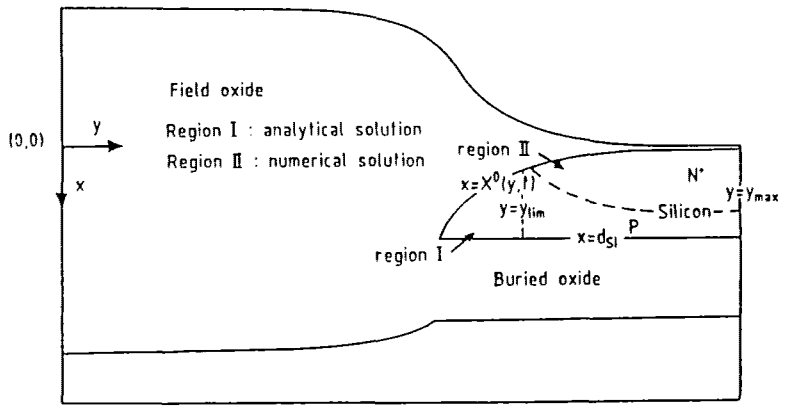

Fig. 3. Geometries of the silicon domain Ω when a mixed solution is used to solve the diffusion equation.

Analytical resolution of the diffusion equation

As we mentioned earlier, an analytical solution is used until the field oxide is formed, as only low doses are used to implant impurities in the isolation region ($\leq 10^{13}cm^{-2}$), concentrations are still inferior to intrinsec concentration ($n_i \# 10^{18}\ cm^{-3}$). The diffusion coefficient is then independent of the concentration

$$(1) \qquad \mathcal{D}[T(t),\ C_a] = \mathcal{D}[T(t)]$$

Where $C_a = C_a(x,y,t)$ is the concentration density of impurity atoms, t is the drive-in time, and T is the annealing temperature. The redistribution of impurities is obtained by solving the low-concentration diffusion equation

$$(2) \qquad \frac{\partial C_a}{\partial t}(x,y,t) = \mathcal{D}\left[\frac{\partial^2 C_a}{\partial x^2}(x,y,t) + \frac{\partial^2 C_a}{\partial y^2}(x,y,t)\right]$$

in the silicon domain Ω.

In an inert ambient, the diffusion of impurities is obtained by solving (1) in the silicon domain Ω (fig. 4) with the boundary conditions as indicated on fig. 4 and the following initial condition (Sweid, 1988)

$$C_a(x,y,t = 0) = I(x,y) \tag{3}$$

Where $I(x,y)$ is the implantation profile of all implanted ions with a vertical mask localized at $y = L$, and d_{si} is the thickness of silicon layer.

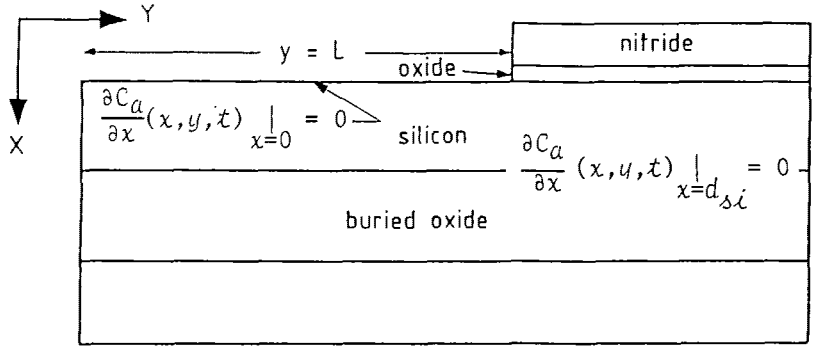

Fig. 4. Geometry of the silicon domain Ω in the isolation region at the begining of the process with the indicated boundary conditions.

We note $C_1(x,y,t)$ the solution of the diffusion equation with the boundary conditions and a unit-impulse source as initial condition

$$C_a(x,y,t = 0) = \delta(x',y') = \delta(x-x')\ \delta(y-y') \tag{4}$$

Where δ denotes the Dirac delta function.

For an initial condition given by (3), the solution of the system is given by the relation

$$\begin{aligned} C_a(x,y,t) &= \int_{-\infty}^{+\infty} dy' \int_{0}^{d_{si}} C_1(x,y,t) I(x',y')\ dx' \\ &= C_x(x,t)\ C_y(y,t) \end{aligned} \tag{5}$$

with

$$C_x(x,t) = \left(\frac{I_{max}}{2d_{si}}\right)\left[I_2 + 2\sum_{n=1}^{n=+\infty} \cos\left(\frac{n\pi x}{d_{si}}\right) I_3(n) \exp\left(-\frac{Dn^2\pi^2 t}{d^2_{si}}\right)\right] \tag{5a}$$

and

$$(5b) \qquad C_y(y,t) = erfc\left(\frac{y - L}{\sqrt{4Dt + 2d^2_{rpy}}}\right)$$

Where $erfc(t)$ is the complementary error function, I_{max} is the peak concentration of the implanted profile, and I_2 *and* $I_3(n)$ are two integrals (a complete development of the solution is presented in (Sweid, 1988)).

The growth of the oxide is performed in an oxidizing ambient which modifies the diffusion profiles (Sheid, 1986).

To solve the diffusion equation during this technological step, we used the model proposed by Huang and Welliver (1970). The impurity profile can then be divided into two parts accordingly (Lee, 1981)

$$(6) \qquad C_a(x,y,t) = C_i(x,y,t) + C_c(x,y,t)$$

Where $C_i(x,y,t)$ is the same as Eq. (5) (but applying the diffusion coefficient for oxidation), and $C_c(x,y,t)$ is a correction factor which takes into account oxidation effects as boundary movement and segregation at the silicon/oxide interface.

Furthermore, the oxidation causes a change of the x coordonate. (The origin of x is always located at the silicon/oxide interface (fig. 5)). We take into account of this change by using the following transformation

$$(7) \qquad X_{eff}(t) = \frac{d_{si} - X^o(y,t)}{d_{si}}\, x + X^o(y,t)$$

Where $X^o(y,t)$ is the equation for the position of the silicon/oxide interface.

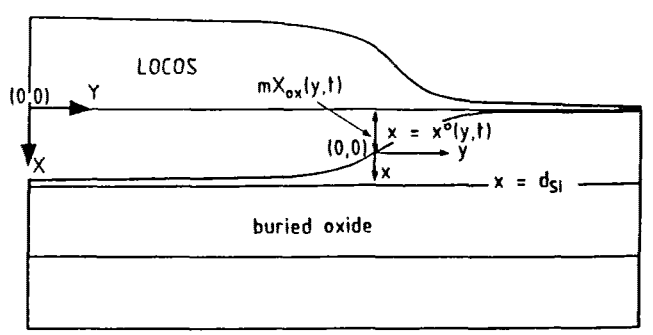

Fig. 5. Geometries of the silicon domain Ω in the isolation region during the isolation region formation.

To obtain $C_C(x,y,t)$, we use the flux relationship at the silicon/oxide interface. The rate of flow is (Lee, 1981)

$$(8) \qquad \mathcal{D} \frac{\partial C_a}{\partial x}(x,y,t)\Big|_{x=0} = (k-m)C_a(0,y,t)\, V_{ox}(y,t)$$

where $V_{ox}(y,t)$ is the oxide growth velocity, k the segregation coefficient at the oxide/silicon interface, and m the ratio of the grown oxide to the silicon consumed.

For $C_C(x,y,t)$, we found

$$(9) \qquad C_C(x,y,t) = C_{2x}(x,t)C_y(y,t)$$

With

$$(9a) \qquad C_{2x}(x,t) = A\, erfc\left(\frac{X_{eff}(t)}{2\sqrt{\mathcal{D}t}}\right)$$

Where A is determined using (8). $C_y(y,t)$ is the same as Eq.(5b) The resultant 2D diffused profile is then

$$(10) \qquad C_a(x,y,t) = C_y(y,t)\,[C_{1x}(x,t) + C_{2x}(x,t)]$$

To allow a ramp-up (ramp-down) diffusion process during all the anneals we have developed an iterative method for calculating the 2D diffused profile. Thus (10) [or (5)] can be expressed as a first-order forward difference over time, while at $t = t_{(n+1)}$ we have

$$C_a(x,y,t)\Big|_{t=t_{n+1}} = C_a(x,y,t_n) + \Delta t \frac{\partial C_a}{\partial t}(x,y,t_n)$$

$$(11) \qquad \Delta t = t_{n+1} - t_n$$

Numerical resolution of the diffusion equation

In region II, which is the source and drain region (fig. 3). the diffusion equation is nonlinear, and must be treated numerically (diffusion coefficients are dependent on concentration). The system to be solved is (Guillemot, 1987)

$$\Delta[\mathcal{D}(C_n)\nabla C_n] = \frac{\partial C_n}{\partial t}(x,y,t) \qquad X^o(y,t) \leq x \leq d_{si}$$

$$y_{lim} \leq y \leq y_{max}$$

$$\left.\begin{aligned} &\frac{\partial C_n}{\partial y}(x,y,t)\Big|_{y=y_{max}} = 0 \\ &C_n(x,y,t)\Big|_{y=y_{lim}} = F\ C_a(x,y,t) \end{aligned}\right\} X^o(y,t) \leq x \leq d_{si}$$

(12)

$$\left.\begin{aligned} &\mathcal{D}(C_n)\,\vec{\mu}\,\nabla C_n\Big|_{x=0} = (k-m)V_o x(y,t)\,\vec{\mu}\,C_n\Big|_{x=0} \\ &\frac{\partial C_n}{\partial x}(x,y,t)\Big|_{x=d_{si}} = 0 \end{aligned}\right\} y_{lim} \leq y \leq y_{max}$$

"Natural" boundary conditions are applied between the analytical and the numerical region (the concentration obtained both analytically and numerically must be the same), where $\mathcal{D}(C_n)$ is the concentration dependent diffusion coefficient, C_a and C_n are the concentrations in region I and region II respectively, $\vec{\mu}$ is the unit normal vector to silicon/oxide interface, and $y = y_{lim}$ the separation interface between the two regions.

The physical domain in region II is mapped into a fixed-time and invariant rectangular domain by means of the following transformation

$$(12) \qquad \zeta = \frac{x - X^o(y,t)}{d_{si} - X^o(y,t)}\, d_{si}$$

Thus, the so-obtained differential equations are discretized with the classical method of finite-difference and a Crank-Nicolson sheme. The solution is obtained using the Gauss-Siedel method.

On fig. 6, the grid of finite difference and its deformation during oxidation is given with the location of the interface between the two regions.

Simulation of a MOS device on a SIMOX structure

As a conclusion, OSIRIS II is used to simulate the processing sequence for a MOS device in fig. 7. The process schedule is the following:

- Field implant with boron (100Kev, $10^{12}cm^{-2}$).
- Field oxidation (270 mn in steam ambient at 1000°C).
- Etching of 0.05 µm of oxide.
- Dry oxidation (100 mn, 950°C, dry, 3%HCL).
- Implantation of Boron ($10^{12}cm^{-2}$, 30 Kev) thus adjusting the threshold voltage.
- Implantation of source and drain with arsenic ($10^{15}cm^{-2}$, 120 Kev).
- Anneal process (950°C, 30 mn).

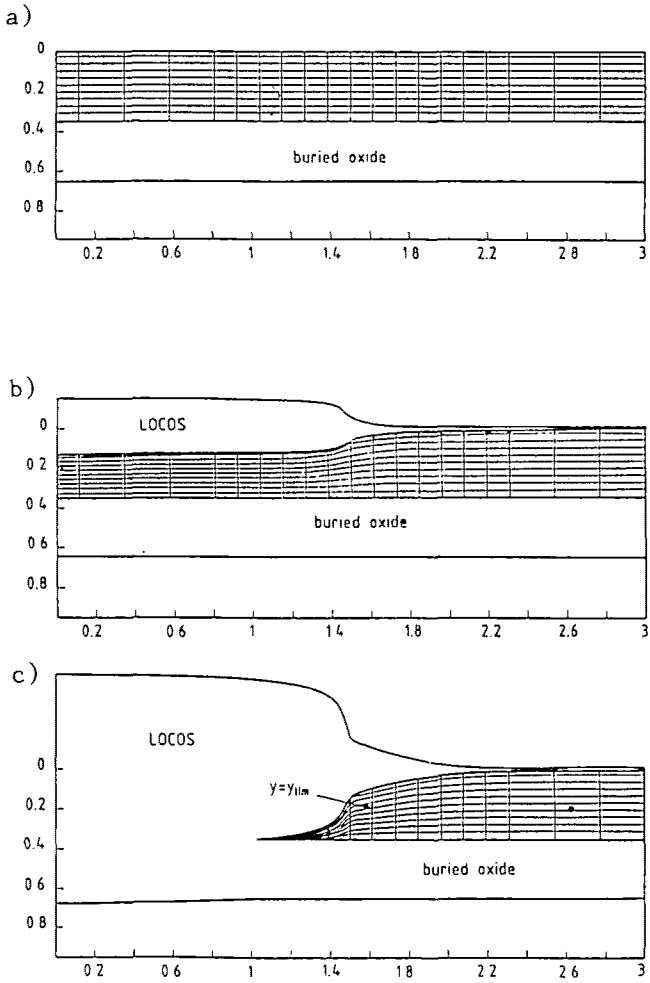

Fig. 6. a) At the begining of the process b) During oxidation. c) At the end of the field oxide formation.

CONCLUSION

In this paper the authors solved the diffusion equation for SIMOX structure using a mixed solution. This method is included in a 2D process simulator for SOI structures called OSIRIS II. As an example acomplete simulation of an n-channel MOS device on is presented.

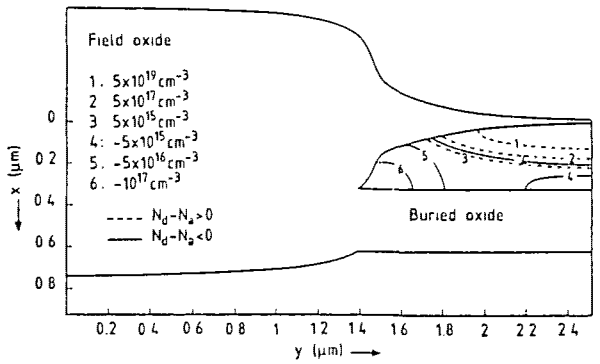

Fig. 7. Equidensity contours of the net consentration after activation annealing.

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