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Recent developments of the two-dimensional technological process simulator OSIRIS

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Résumé. — La simulation numérique des processus technologiques est très importante pour la fabrication des circuits intégrés. Dans cet article, les auteurs présentent une version plus complète du simulateur bidimensionnel OSIRIS, prenant en compte la diffusion simultanée de deux impuretés. Les modèles utilisés pour l'implantation ionique et la redistribution des dopants sont brièvement rappelés. Un nouveau modèle a été développé pour la croissance de l'oxyde de champ : il permet une très bonne simulation du « bec d'oiseau » obtenu par le procédé SEMIROX. Comme exemple, la réalisation d'un dispositif N-MOS complet est simulée par le programme, qui donne le profil des impuretés et la forme de l'oxyde à la fin du processus.

Abstract. — The numerical simulation of technological processes is very important for the fabrication of integrated circuits. In this paper, the authors present a more complete version of the two-dimensional simulator OSIRIS, taking into account the simultaneous diffusion of two impurities. The models used for ion-implantation and redistribution of dopants in silicon are briefly recalled. A new analytical model for oxide growth has been developed which gives very good simulation of the « bird's beak » of SEMIROX structures. Finally, a complete simulation of a N-Channel MOS device is presented, with the redistributed impurity profiles and the oxide layer shape at the end of the process.

1. Introduction.

The numerical simulation of the technological processes become very important for the fabrication of integrated circuits. Especially for MOS circuits several two-dimensional simulators [1-3] have been proposed in order to take into account the inhomogeneity of the field oxide thickness and the lateral diffusion effects. Similar to the simulators given in [1, 2], the authors have developed the program OSIRIS [4, 5]. It allows the simulation of a complete device fabrication process including the following steps :

- resist deposition and removing
- oxide or nitride deposition and etching
- ion-implantation or predeposition of boron, arsenic, phosphorus and antimony
- redistribution of one or two impurities in an inert or oxidizing ambient
- growth of the gate or field oxide.

In our program the solution of the diffusion equation is performed numerically using a finite

difference method. An original and accurate simulation of the « bird's beak » formation in the case of a semi-recessed oxide (SEMIROX process) is presented in this paper. Section 2 briefly describes the modelling of ion-implantation and the resolution of the diffusion equation. The detailed simulation of the field oxide growth is presented in section 3. In the last section, the simulation of a complete N-Channel MOS circuit fabrication process is given.

2. Ion-implantation and redistribution of impurities.

In this section the models for ion-implantation and diffusion of impurities are briefly recalled.

2.1 ION-IMPLANTATION. — Ion-implantation and chemical predeposition are the two selective doping techniques used to create localized junctions in a semiconductor : silicon dioxide, polysilicon or resist act as a mask for impurities in silicon. Predeposition can be treated as an impurity diffusion. Therefore, only models used for ion-implantation of boron,

arsenic, phosphorus and antimony are developed here. The silicon wafer geometry is presented in figure 1.

Fig. 1. — Silicon wafer geometry for modelling ion-implantation.

We assumed that an ion entering the target at a point y will come to rest at a point (x_0, y_0) with the probability density $P_x(x_0)P_y(y - y_0)$. P_x is the probability density in the x -direction (vertical direction parallel to the direction of ion-beam) and P_y is the probability density in the y -direction (lateral direction). According to Furukawa [6], the distribution P_y of implanted ions is supposed to be a Gaussian function with a lateral deviation ΔR_y . To simulate the vertical direction of the final resting points of ions, the simple Gaussian approximation is no longer valid: experiments have shown that profiles are skewed and possess tails. Three measured and tabulated lengths [7] characterized these profiles: the average projected range R_p , the standard deviation ΔR_x and the skewness γ . From these three parameters, two distributions are widely used: two joint half-Gaussian for arsenic, phosphorus and antimony [8] and a modified Pearson IV function for boron [9].

In the case of a vertical and infinitely high mask edge (resist for example), the impurity concentration is given by an analytical expression [10]. In a more general case of an arbitrarily shaped mask edge, it is assumed that the stopping power of the mask nearly equals the stopping power of silicon [11]. The mask is then considered as a silicon layer and the two-dimensional profile is obtained numerically. The application presented in section IV gives a first example of boron implantation with a photoresist mask considered as a vertical mask edge, and a second one concerning arsenic implantation through a field oxide.

2.2 REDISTRIBUTION OF IMPURITIES. — The process of thermal diffusion of dopant impurities is an essential part of all semiconductor device fabrication. This effect is described by the well known diffusion equation [12, 13]:

$$\frac{\partial N_k}{\partial t}(x, y, t) = \text{div} \left[D_k (\text{grad } N_k - Z_k \frac{N_k}{2n_i} \text{grad } M) \right] \quad (2.1)$$

where

N_k is the concentration of the k -th impurity, D_k is the effective diffusion coefficient of the k -th impurity, $Z_k = 1$ for acceptor-like impurities, $= -1$ for donor-like impurities, n_i is the intrinsic carrier concentration in the semiconductor, and

$$M = \sum_k Z_k N_k.$$

This relation is based on the assumption of a complete impurities ionization. The effective diffusion coefficient for boron, arsenic and antimony can be written as [9]:

$$D_k = D_k^0 \cdot \frac{1 + \beta_k f_k}{1 + \beta_k} \quad (2.2)$$

where D_k^0 is the intrinsic diffusion coefficient of the k -th impurity, β_k is a phenomenological coefficient equal to 19 for boron, 100 for arsenic and 1 for antimony; $f_k = p/n_i$ or n/n_i for acceptor-like or donor-like impurities, respectively, or phosphorus, the well known model of Fair and Tsai [14] is used.

The non-linear diffusion equation must be solved

Fig. 2. — Physical domain Ω used to solve the diffusion equation.

for the silicon wafer geometry shown in figure 2. The physical domain Ω is described by :

$$\begin{cases} X^0(y, t) \leq x \leq L_0 \\ 0 \leq y \leq Y_M \end{cases}$$

where L_0 is the useful silicon layer thickness and $X^0(y, t)$ is the equation for the position of the silicon/oxide interface. In the case of redistribution in an oxidizing ambient the domain Ω varies with time. It is assumed to be symmetric, or large enough in the y -direction. So the boundary conditions are given as follows :

— *Conditions of symmetry :*

$$\left. \begin{aligned} \frac{\partial N_k}{\partial y} \Big|_{y=0} &= 0 \\ \frac{\partial N_k}{\partial y} \Big|_{y=Y_M} &= 0 \end{aligned} \right\} X^0(y, t) \leq x \leq L_0.$$

— *Assumption of sufficiently deep domain :*

$$\frac{\partial N_k}{\partial x} \Big|_{x=L_0} = 0 \quad 0 \leq y \leq Y_M.$$

The boundary condition at oxide/silicon interface is written by assuming that there is no diffusion into the oxide and that, at all times, the segregation corresponds to equilibrium ; so that :

$$\begin{aligned} (k_s - m) N_k v_{\text{SiO}_2} \cdot \mathbf{n} = \\ = D_k \left(\frac{\partial N_k}{\partial n} - Z_k \frac{\frac{N_k}{2 n_i}}{\sqrt{\frac{M^2}{4 n_i^2} + 1}} \frac{\partial M}{\partial n} \right) \end{aligned} \quad (2.3)$$

where

k_s is the segregation coefficient of the k impurity at the oxide/silicon interface,

m is the fractional total oxide growth due to the consumption of silicon,

v_{SiO_2} is the oxide growth rate,

$\mathbf{n}$ is the unit normal vector to the SiO_2/Si interface.

Then, the physical domain Ω is mapped into a fixed-time invariant rectangular domain by means of a coordinate transformation [1].

Next, the classical method of finite differences [15] and a Crank-Nicolson scheme [16] are used to discretize the so obtained partial differential equations. The numerical solution is performed using the Gauss-Seidel method. The strong non-linearity of the problem does not allow a method of overrelaxation to be used.

Using all these methods we have developed the program OSIRIS of reduced size and reasonable CPU time [10].

3. Simulation of the field oxide growth.

Selective oxidation provides a simple way of isolation of integrated circuits on silicon. In the LOCOS process, a nitride layer deposited on a pad-oxide is used as an oxidation mask : this process is known to give rise to a « bird's beak », due to lateral oxidation under the mask [17].

An accurate simulation of this effect is necessary in order to ensure a better control of the technological oxidation process. Solving the complete set of physical differential equations governing the oxide growth and the simultaneous viscous flow, one can obtain quite good results but it is difficult and computer-time consuming [18-20]. Therefore, in this section, we present semirecessed oxide shapes obtained by using simple parametric relationship based on the analysis of experimental data [17, 21, 22].

First, as is shown in figure 3, two shapes of the « bird's beak » can be experimentally observed, depending on the stress exerted by the mask. In the

Fig. 3. — Classification of the bird's beak shapes observed experimentally ● shape 1, ○ shape 2, △ unclassified shape.

case of the shape 1 (Fig. 4a), the nitride layer and the pad-oxide thickness, e_n and e_{ox} respectively, are thin, resulting in a low mask stress. In the case of shape 2 (Fig. 4b), the nitride layer is thick, resulting in a large mask stress.

Two analytical functions Z_1 and Z_2 are thus needed to fit the contours at the oxide/silicon interface and at the oxide/ambient or nitride interface. Two complementary-error functions are used for shape 1 :

$$Z_1(y) = a_1 \operatorname{erfc}(b_1 y + c_1) + d_1 \quad (3.1)$$

$$Z_2(y) = a_2 \operatorname{erfc}(b_2 y + c_2) + d_2. \quad (3.2)$$

For shape 2, because of the strong mask stress, a pinch of the oxide appears under the nitride edge, for the upper interface, and shifted back a length δ ,

Shape 2 :

$$Z_1(y) = a'_1 \operatorname{erfc} [b'_1(y - \delta)] \quad \text{for } y \geq \delta$$

where

$$a'_1 = H_1$$

$$b'_1 = \frac{\sqrt{E}}{L_{bb}}$$

$$Z_1(y) = e'_1 \frac{d'_1 - y}{d'_1 - y + q} \quad \text{for } y \leq \delta$$

where

$$d'_1 = \delta - \frac{H_1 q}{H_1 - e'_1}$$

$$e'_1 = mE_{0x}$$

$$Z_2(y) = a'_2 \operatorname{erfc} (b'_2 y) + c'_2 \quad \text{for } y \geq 0$$

where

$$a'_2 = -H$$

$$b'_2 = \frac{\sqrt{E}}{L_{bb}}$$

$$c'_2 = -e_{0x}$$

$$Z_2(y) = e'_2 \frac{d'_2 - y}{d'_2 - y + q} \quad \text{for } y \leq 0$$

where

$$d'_2 = \frac{-H_2 q}{H_2 + e'_2}$$

$$e'_2 = (m - 1) e_{0x}$$

E_{0x} is given by Deal and Grove's model [23], L_{bb} and H are plotted in figures 5-9 and can be described by :

$$L_{bb} = K_L [(-T_{0x} + 1580.3) E_{0x}^{0.67} \times \exp \left[-\frac{(e_n - 0.08)^2}{0.06} \right] e_{0x}^{0.3}] \quad (3.7)$$

$$H = K_H \left((-1.75 e_n + 0.445) E_{0x} \exp \left(-\frac{T_{0x}}{200} \right) \right) \quad (3.8)$$

where T_{0x} is the absolute temperature, $K_L = 8.25 \times 10^{-3}$, $K_H = 402.00$, and E_{0x} , e_{0x} and e_n are measured in μm .

Within the range of interest :

$$0.1 \mu\text{m} \leq E_{0x} \leq 1.5 \mu\text{m} ,$$

$$850^\circ\text{C} \leq T_{0x} \leq 1100^\circ\text{C} ,$$

$$0.05 \mu\text{m} \leq e_n \leq 0.2 \mu\text{m} ,$$

$$\text{native oxide} \leq e_{0x} \leq 0.05 \mu\text{m} ,$$

$$\langle 100 \rangle \text{ substrate} .$$

Hereafter, we compare the shape of the « bird's beak » obtained by Secondary Electron Microscopy

Fig. 5. — Length L_{bb} of lateral oxidation under the mask for the bird's beak versus field oxide thickness E_{0x} .

Fig. 6. — Length L_{bb} of lateral oxidation under the mask versus pad-oxide thickness e_{0x} .

Fig. 7. — Length L_{bb} of lateral oxidation under the mask versus processing temperature T_{0x} .

Fig. 8. — Lifting H of the mask during oxidation for the bird's beak versus oxide thickness E_{ox} .

Fig. 9. — H/E_{ox} versus nitride thickness e_n .

(SEM) with simulated profiles. A good agreement between experimental data and analytical results can be observed in figure 10.

4. Simulation of a N-Channel MOS device.

As an example, OSIRIS is used to simulate the entire processing sequence for the N-Channel MOS device in figure 11. The process schedule is the following :

- Field implant with boron (120 keV , 10^{13} cm^{-2}).
- Field oxidation ($950 \text{ }^\circ\text{C}$, 300 min).
- Gate oxidation up to $0.05 \text{ } \mu\text{m}$.
- Depletion implant with arsenic (180 keV , $2 \times 10^{11} \text{ cm}^{-2}$).
- Enhancement implant with boron (40 keV , $2 \times 10^{11} \text{ cm}^{-2}$).
- Dry argon anneal ($900 \text{ }^\circ\text{C}$, 30 min).
- Source-drain implant with arsenic (120 keV , 10^{15} cm^{-2}).
- Reflow process ($850 \text{ }^\circ\text{C}$, 30 min).
- Contacts.

The process employs six different mask operations and uses a local oxidation of silicon (LOCOS) scheme for isolation. For simulation, the device is divided into 5 main parts. The surface topographies and corresponding equi-density contours for impurity concentrations, at the end of the process, are given in figure 12.

5. Conclusion.

We have developed a complete two-dimensional simulator of technological processes OSIRIS. The most important process steps for MOS devices such as predeposition, ion-implantation, oxide growth and thermal redistribution of doping impurities can be simulated.

The modelling of ion-implantation is performed using a Gaussian function for the lateral distribution while two empirical functions are used for the vertical ion-distribution : a joint half-Gaussian function for arsenic, phosphorus and antimony and a modified Person IV function for boron. Concerning the field oxide growth, a new analytical model has been developed, allowing a very good simulation of the « bird's beak » which appears in the LOCOS process. The diffusion for one or two impurities is described by solving the non-linear system of diffusion equations. OSIRIS uses the finite differences method with a Crank-Nicolson scheme. The system so-obtained is solved using a modified Gauss-Seidel method. The redistribution of impurities can be simulated in an inert or oxidizing ambient : the physical domain of the device is always mapped into a fixed-time invariant rectangular domain by means of a coordinate transformation.

Finally, OSIRIS is used to simulate a complete N-Channel MOS device. The redistributed impurity profiles for this latter application are presented along with the corresponding oxide layer shapes at the end of the process.

Fig. 10. — Comparison between experimental and simulated field oxide shapes.

Fig. 11. — Cross sectional view of an N-Channel MOS device. The parts A-E of the circuit are simulated in figure 12.

Fig. 12. — Results of OSIRIS simulations showing the equidensity contours and corresponding oxide shape at the end of the process : a) part A of the MOS device, b) part B, c) part C, d) part D, e) part E.

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