IMPLEMENTATION OF NITRIDE OXIDATION IN THE 2D PROCESS SIMULATOR IMPACT-4.

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To shrink the dimension of devices, new isolation technologies, with respect to classical LOCOS, have to be evaluated. This paper deals with the study of one of these possible alternatives: the LOCOS/ Recessed-LOCOS NCLAD structure. In this process a thin nitride layer encapsulates the oxide-nitride stack to prevent the formation of long bird's beak [1]. The efficiency of this technique is dependent on the nitride oxidation. In order to study this process, via simulation, it is therefore necessary to model nitride oxidation: a "modified Deal and Grove" model has been implemented and calibrated in the 2D Process simulator IMPACT-4 [2]. The implementation problems and relative solutions are described.

The equation governing wet oxidation of nitride is given by [3-4]:
$Si_3N_4 + 6\ H_2O \longrightarrow 3SiO_2 + 4\ NH_3$.   (1).
The Deal and Grove model [5] has been applied to describe the reaction (1). From experimental results published by Enomoto [6] and Rebora [7], the values of the linear (B/A) and parabolic (B) parameters have been calibrated for a range of temperature between [$920°C$ - $1100°C$]: $B = 1.96 \times 10^{+5} \times exp^{\frac{-2.68eV}{kT}}$ (μ^2/min) (2)
$A = 3.7 \times 10^{-1} \times exp^{\frac{-0.287eV}{kT}}$ (μ) (3). B and B/A determine respectively the diffusivity D and the reaction rate k. The pressure dependence of B has been deduced from [7]. It appears that, for pressures lower than 1atm, the parabolic coefficient B is given by: $B = 1.96 \times 10^{+5} \times exp^{\frac{-2.68eV}{kT}} \times P^{0.8}$ (μ^2/min).
The model has been implemented in the 2D process simulator IMPACT-4 [2].

The main problem in the implementation is caused by the very different diffusion and reaction rate coefficients for nitride and silicon [5] respectively. For this reason, the implementation of nitride oxidation in IMPACT-4 required to differenciate the oxide growing on nitride (oxynitride) from the one on silicon (silicon oxide), without defining a new material, in order to attribute to the elements of each kind of oxide its proper coefficients. In 1D simulations, as oxidation occures either on silicon or on nitride, the parameters of oxidation can be attributed easily. In 2D simulations, silicon and nitride simultaneously oxidize. The reaction rate coefficient k is attributed according to the surface on which oxidation is performed. Concerning diffusion coefficient, a test has been introduced on mesh elements. This test is made in order to permit nitride oxidation ($D(nit) \neq 0$) only on air contacted oxynitride and to cancel nitride oxidation under nitride masks, because of stress effects: ($D(nit) = 0$). In order to distinguish between oxide and oxynitride, for each oxide mesh element (triangle) all its neighbors are evaluated; if they contact both air and nitride, this element is oxynitride ($D = D(nit)$), otherwise it is silicon dioxide ($D = D(si)$), as explained on figure 1. The limit of this method in 2D is for oxynitride thickness larger than two divisions of the mesh (about 1000Å, for IMPACT meshes). The cases which have been studied are within this mesh limit.

The difference of diffusion coefficient between oxynitride and silicon oxide can be chemically explained by the gradient of oxygen concentration experimentally observed in oxynitride layer [8]. To reproduce this effect, a gradient of diffusion is numerically introduced for oxynitride (figure 2).
Numerical simulation has been performed in case of 1D examples to check-out the validity of our calibration. Figures 3 and 4 compare the numerical results to experimental data for temperatures equal to $950°C$ and $1100°C$. Furthemore, the analytical results given by the model of Kamins [9] have been added to the figures. One can conclude that our calibration shows an excellent accuracy for the range of temperature and pressure which has been studied.

NCLAD LOCOS and Recessed-LOCOS have been processed at 1050°C, 1atm, in wet ambient to grow 5500Åof field oxide. Their corresponding classical structures have also been processed for comparision. 2D simulations of these isolation structures have been performed with IMPACT-4. The results are reported on figures 5 to 8, where it can be noticed that the simulations are in good agreement with SEM photos. NCLAD present a reduced bird's beak. If nitride oxidation is not taken into account, one can observe that it has rather no influence on the bird's beak shape in case of classical LOCOS or Recessed-LOCOS, while it underestimates the bird's beak thickness for NCLAD versions.

A Deal and Grove model for silicon nitride oxidation has been implemented in the process simulator IMPACT-4, using an appropriate test on mesh oxides elements to differenciate oxynitride from silicon oxide, and defining a diffusion coefficient gradient in oxynitride layer. This tool can be used to study NCLAD structures, and other advanced isolation structures affected by nitride oxidation.

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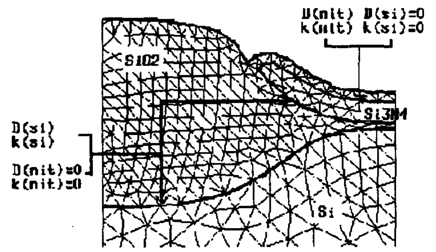

Figure 1: Definition of diffusivity and reaction rate, of nitride (D(nit), k(nit)) and silicon oxide (D(si), k(si)) according to position in growing oxide.

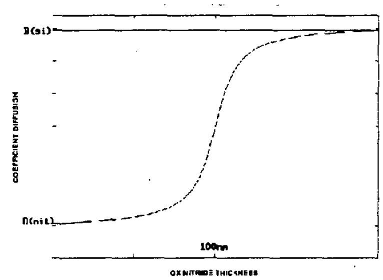

Figure 2: Gradient of diffusion coefficient in oxynitride growing on nitride: D(nit)=Diffusion coefficient in oxynitride; D(si)=Diffusion coefficient in silicon oxide.

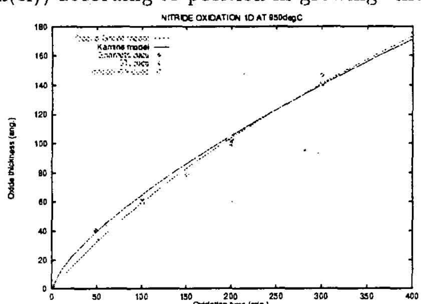

Figure 3: Nitride oxidation 1D at 9 50°C.

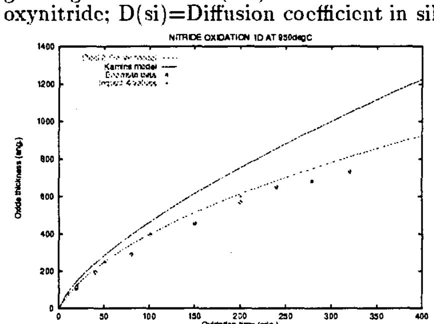

Figure 4: Nitride oxidation 1D at 1100°C.

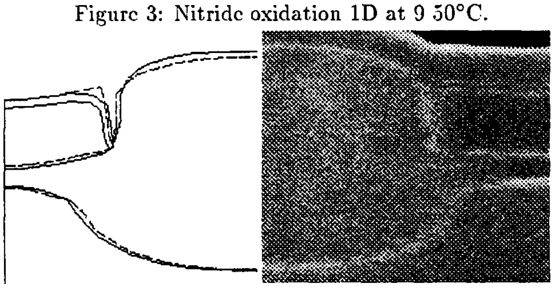

Figure 5: Simulation and SEM photo of a LOCOS structure oxidized at 1050°C. Plain line: simulation with nitride oxidation model; dashed line: without nitride oxidation.

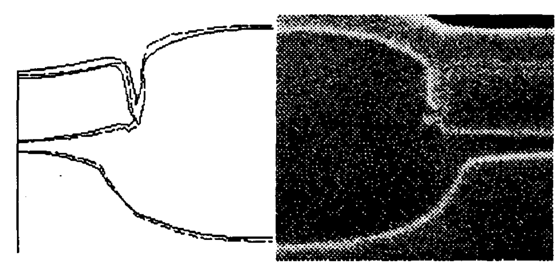

Figure 6: Simulation and SEM photo of NCLAD structure oxidized at 1050°C, with a second nitride layer of 300Å. Plain line: simulation with nitride oxidation model; dashed line: without nitride oxidation.

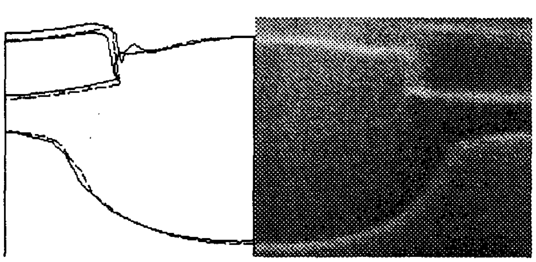

Figure 7: Simulation and SEM photo of Recessed LOCOS oxidized at 1050°C. Plain line: simulation with nitride oxidation model; dashed line: without nitride oxidation.

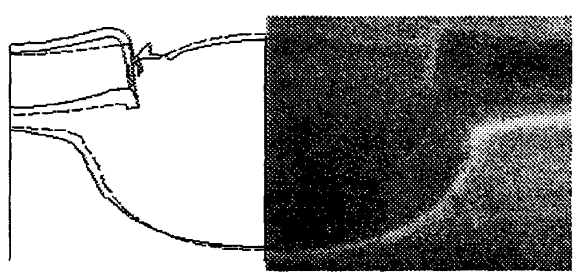

Figure 8: Simulatiyon and SEM photo of NCLAD Recessed-LOCOS oxidized at 1050°C, with a second nitride layer of 300Å. Plain line: simulation with nitride oxidation model; dashed line: without nitride oxidation.