# Structural simulation in the process simulator MIMAS

Ernst Rank
*Numerische Methoden und Informationsverarbeitung, FB Bauwesen,*
*Universität Dortmund, Postfach 500 500, D-4600 Dortmund 50, West Germany*

Ulrich Weinert
*SIEMENS AG , Otto-Hahn-Ring 6 , 8000 München 83, West Germany*

## 1 Introduction

During the past two years the new process simulator MIMAS has been developed at SIEMENS which is able to handle completely general 2D structures and which integrates the most relevant process steps like etching, deposition, local oxidation, ion implantation and dopand diffusion in a transparent way to a process-CAD-system. In this paper the structural simulation part of MIMAS will be presented, general system aspects and the simulation capabilities for implantation and diffusion have been discussed in [1].

## 2 The structural simulation subsystem

The kernel of the structural simulation subsystem of MIMAS is a geometry database where the history of geometries for the simulated structure is stored. In this file-oriented database geometries *between* process steps (e.g. after etching, before oxidation) and also *during* process steps (e.g. for certain time steps during oxidation) are stored. The format of the database is derived from the SKEL/TRI datastructure of PLTMG [2] and stores as objects nodes, edges, regions and (optionally) triangles with their appropriate attributes. A database can be initialized or modified by an interactive graphical geometry editor or by the structural simulator SAMSON. This program has been developed on the basis of SAMPLE [3] and is able to handle arbitrary nonplanar multiregion domains. The meshgenerator used in our system is based on TRIGEN of PLTMG [2] and can refine the finite element mesh towards refinement zones (nodes or edges) which are identified either automatically (reentrant corners) or interactively. Special emphasis has been taken on the development of the geometry postprocessor BIBER, which is able to approximate zones of very fine geometry resolution (as they may be produces at material interfaces by the etch simulator or the oxidation simulator) by a consitent coarser geometry definition. This is necessary for a fully automatic finite element mesh contruction.

## 3 The oxidation simulator FELOX

Our oxidation simulator FELOX (**F**inite **E**lement simulator of **L**ocal **OX**idation) has been presented in [4],[5]. In its production version FELOX uses either an elastic or a viscous flow model for the mechanical displacement, can handle domains with up to four oxidizable species, can simulate complex oxidation processes (e.g. temperature ramping, change of ambient, pressure etc. during oxidation) and computes mechanical stresses in silicon , oxide and mask simultaneously. The basic idea of FELOX is the regularization of the free boundary value problem by the introduction of a smooth function $\eta$ for the relative silicon concentration at time t and a point x :

$$\eta(x,t) = \frac{C_{Si}(x,t)}{C_{Si0}} \quad . \tag{1}$$

$C_{Si}(x,t)$ is the silicon concentration at time $t$ and point $x$ and $C_{Si0}$ the concentration of silicon atoms in pure crystal.

The oxidant diffusion in a domain $\Omega$ (composed of silicon, oxide and a distributed interface layer) has the following form :

$$\nabla(D(\eta(t))\nabla C(x,t)) = k(\eta(t))C(x,t) \quad on \quad \Omega \tag{2}$$

for every fixed time $t$ , with appropriate Dirichlet boundary conditions at the exposed oxide surface.
For the relative silicon density $\eta$ the following ordinary differential equation can be derived:

$$\frac{\partial \eta}{\partial t} = -\frac{1}{\lambda} k(\eta(t))C(x,t)/N_1 \quad . \tag{3}$$

where $N_1[part./nm^3]$ is the number of oxidant molecules incorporated into one unit volume of silicon dioxide, and $\lambda$ is the volume expansion factor for the reaction from silicon to dioxide.
Due to the distributed chemical reaction zone prestrains are produced by the volume expansion. As change of local volume is related to the *trace* of the prestrain tensor $\epsilon_0$ and, as our problem is varying in time, it is appropriate to formulate an equation for the *rate of the trace of the prestrain* $\frac{\partial tr(\epsilon_0)}{\partial t}$ :

$$\frac{\partial tr(\epsilon_0)}{\partial t} = \frac{\lambda - 1}{\lambda} k(\eta(t))C(x,t)/N_1 \quad . \tag{4}$$

By an *a priori* assumption on the direction of the principal strains at the interface (4) can be used to compute prestrain rates at every point of the interface. These can then be used as load to either an elastic or a viscous flow displacement formulation. In (2) to (4) the dependence of $D$ and $k$ on the relative silicon density has still to be defined. In [5] it has been shown that these parameters can easily be computed from the linear and parabolic growth rates so that the *thickness* of the interface layer can be controlled and the motion of the line where the relative silicon density $\eta = .5$ is the same as the motion of the *sharp interface line* of the Deal-Grove model.
This new formulation allows us to contruct a finite element program which *does not have to trace the interface by element boundaries*, and thus does not impose the necessity to remesh the oxide domain as in other approaches. The interface is not used directly in the code, it is obtained by *postprocessing* the relative silicon density $\eta$ after every timestep.

## 4 A practical example

In the following a simulation of a test structure of the periphery in a 64MBit-DRAM is presented. The initial domain is shown in figure 1. Under the nitride a thin layer of poly as etch stopper was deposed above the oxide layer. From a previous etching step an undercut below the nitride layer has been formed. Objectives of the simulation were the following :

- When is the undercut completely filled during oxidation?
- How sensitive is the shape of the oxide body to the length and depth of the undercut?
- How long does the nitride mask have to be so that the poly-layer is not oxidized?
- Are stresses significant for the mechanical behaviour of the nitride mask?

The simulation showed some surprising results, mainly related to the undercut. Firstly, for the geometric properties used in our test structure, it cannot safely be decided *if the undercut closes at all* or if a thin slit remains open up to the end of oxidation. The reason is that the nitride layer is bent upwards with nearly the same speed as the oxide grows in that region. Figures 2 and 3 show two variants of our simulation. In figure 2 contact of the oxide layer with nitride was assumed after 53 minutes, when the distance of oxide and nitride was less than 2nm. In figure 3 no contact was assumed, until the end of oxidation after 300 minutes the overlap of oxide and nitride was nowhere more than 5 nm.
To simulate contact the geometry at contact time was edited by the interactive geometry editor, the new geometry was meshed and FELOX was restarted.

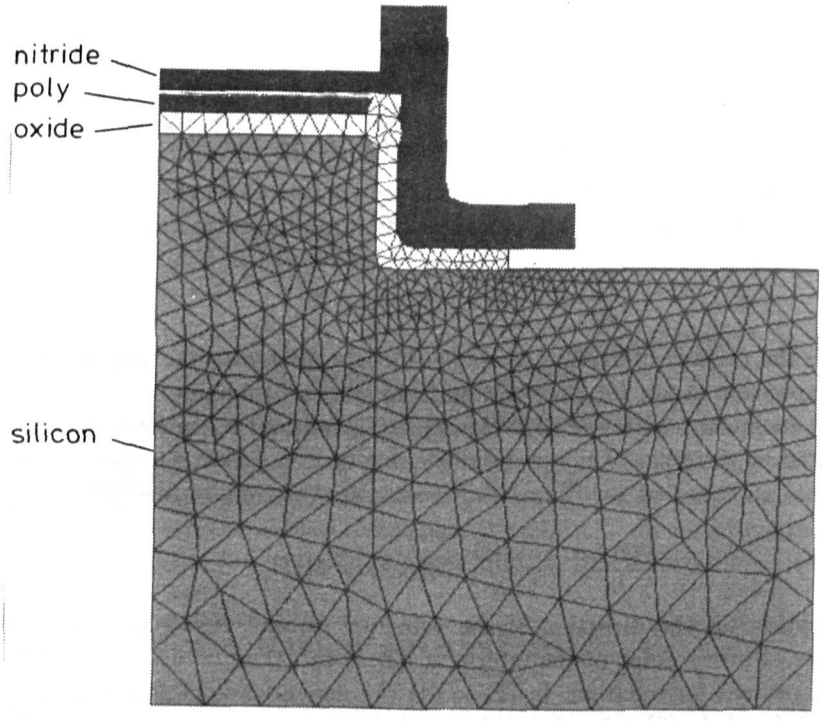


Figure 1: Domains before oxidation

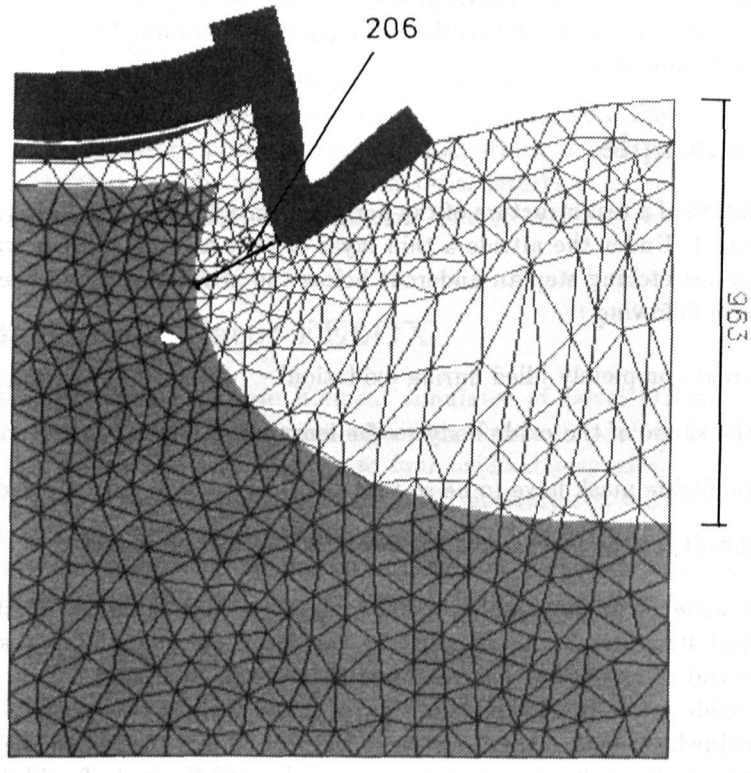


Figure 2: Domains after oxidation, contact assumed

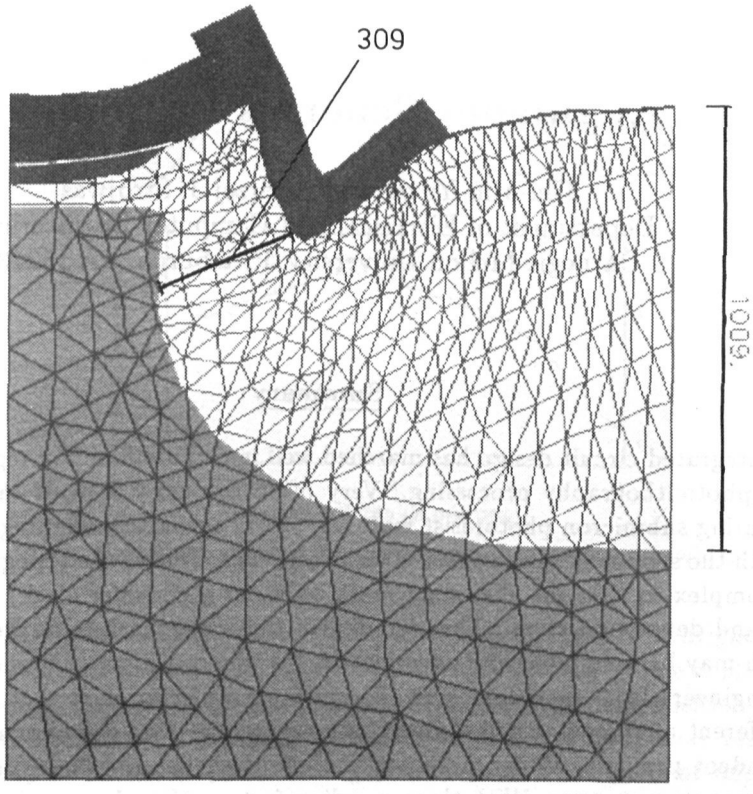


Figure 3: Domains after oxidation, no contact assumed

A typical width of the bird's beak is plotted for the two variants. Assuming contact this width is reduced from 309 nm to 206 nm, i.e. a completely different oxide structure is obtained. Moreover, a significant amount of poly is oxidized in the no-contact-case and the thin nitride layer on top of the poly is exposed to large bending moments which make cracks in that area probable.
The strong sensitivity of the overall structure on the behaviour in the undercut shows that serious problems in reproducibility will have to be expected for a structure as in figure 1. The immediate consequence of process engineers was therefore to modify the process so that this sensitivity was removed.
This example shows how *predictive* simulation can be used in practise. At an early stage of process development (i.e. before first silicon) sensitivities on, at a first glance second order phenomena can be found, corrections in the process sequence can easily be incorporated and expensive and time consuming erroneous test processes can be avoided.

## References

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