

Local oxidation of silicon - a finite element approach

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Abstract. Local oxidation of silicon is an important step in processing highly integrated semiconductor devices. Oxygen diffuses through a layer of silicon dioxide to the interface with pure silicon below the dioxide. There the oxygen reacts with silicon to new dioxide which has more than twice the volume of the original silicon. Thus silicon is consumed and the dioxide layer is lifted up. In the standard finite element approach for simulation of this local oxidation the interface is modelled as a sharp line, making it necessary to remesh the dioxide-range. The new approach presented in this paper models the interface as a smooth transition zone and the dioxide is characterized as a density function over the domain of computation. Thus it is possible to solve on a topologically invariant finite element mesh in a time stepping procedure a coupled system of equations for the oxygen diffusion, the chemical reaction and the structural displacement. Numerical examples show the advantages of the new approach.

1. Introduction

Local oxidation of silicon (LOCOS) is a thermal step of semiconductor device processing, where oxygen diffuses through a layer of already existing silicon dioxide to the interface with pure silicon below. There silicon reacts with the oxygen to new dioxide, yielding strains due to the bigger volume of the dioxide. These strains cause a displacement of the structure, lifting up the old oxide-layer.

A numerical simulation of LOCOS has to deal with two main problems; the first one is how to couple the volumetric expansion at the interface in a consistent way to the displacement problem, the second one is the question how to track the moving interface line numerically over the time of the oxidation.

In the literature the interface is usually treated as a sharp line which defines the moving boundary for the differential equations of the diffusion and displacement problems. The strains arising from the chemical reaction are transformed to a displacement boundary condition, assuming a displacement perpendicular to the boundary. The problem of tracking the moving interface is usually treated by variable mesh algorithms. Finite difference approaches ¹ map the domain of computation in each time step to a rectangular domain, yielding immediate limitations to the generality of the domains of simulation. Boundary element methods ² need only model the boundary of the dioxide domain making it extremely easy to update the geometry after each time step. Yet the boundary element method suffers from its limitation to essentially linear problems, whereas a general computer code for simulation of local oxidation should be able to treat material nonlinearities like viscous flow of the dioxide and stress dependant diffusion coefficients or reaction rates.

Finite element methods for LOCOS simulation ^{3,4} update the mesh after every timestep. This often yields strongly distorted elements, or, if these are to be omitted, remeshing is necessary after each few steps.

All of the approaches mentioned above are even in two dimensions so complex that an application to threedimensional LOCOS simulation seems to be hardly possible. Strongly distorted elements in three dimensions are completely unacceptable and remeshing complex 3D-structures would be extremely time consuming.

In this paper an approach will be presented which is in a sense closer to physics, as it does not assume a sharp interface line but a narrow interface zone between silicon and oxide. The main advantage is, yet, that the approach can be transformed to three space dimensions much easier than the standard one. The basic idea goes back to methods which have been applied successfully to free surface seepage problems for more than a decade ^{5,6}.

2. Definition of the problem

2.1 Diffusion of oxygen

The timescale for the diffusion of oxygen through the oxide is much smaller than the timescale for the movement of the interface, so the problem of local

oxidation can be treated quasi-stationary, i.e. in each time step stationary problems for diffusion (and displacement) can be solved.

Let domains and boundaries be notated as in figure 1. Oxygen (or water in 'wet oxidation') diffuses through the SiO_2 -range Ω_1 . In the standard approach the differential equation is given by

$$\nabla \cdot (D_s \nabla C) = 0 \quad \text{on } \Omega_1$$

with the boundary conditions

$$\begin{aligned} \frac{\partial C}{\partial n} &= 0 && \text{on } \Gamma_3 \cup \Gamma_4 \\ C &= C^* && \text{on } \Gamma_2 \\ D_s \frac{\partial C}{\partial n} &= -k_s C && \text{on } \Gamma_1 \end{aligned} \tag{1}$$

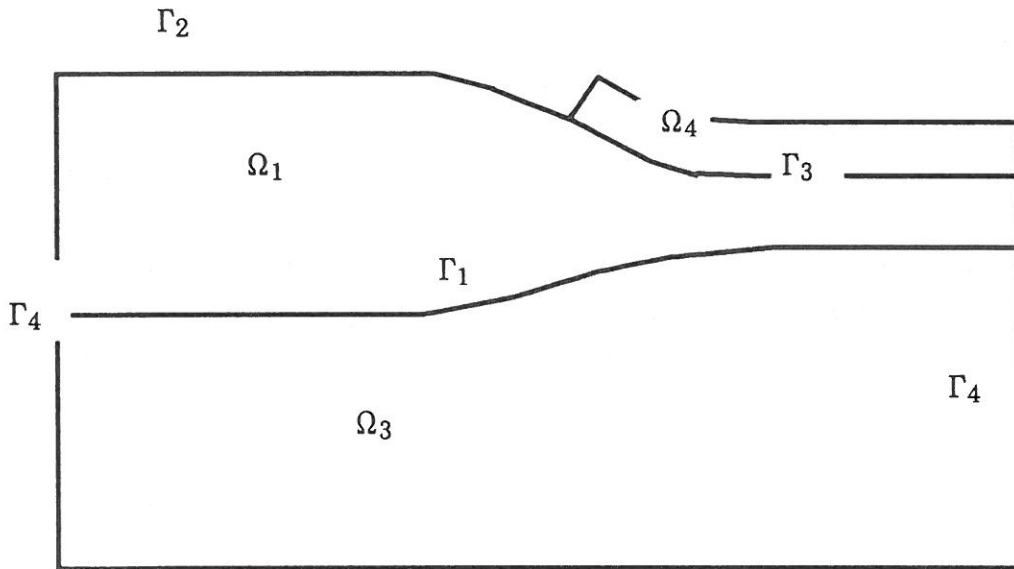


Figure 1 : domains and boundaries

D_s is the diffusion coefficient for oxygen in SiO_2 , C^* the ambient concentration and k_s the chemical reaction coefficient at the interface with Si. Ω_4 is a layer of

silicon-nitride masking the dioxide. As Si_3N_4 is nearly impertinent for oxygen, this layer can be neglected for the diffusion and has, due to its rigidity, only meaning for the structural displacement.

Formulation (1) assumes a sharp interface between Si and SiO_2 . From physical reasons and, as it will be shown, for numerical advantages this assumption shall be weakened and instead of a boundary condition on Γ_1 a 'sink' in a reaction range Ω_2 around the interface will be used (figure 2).

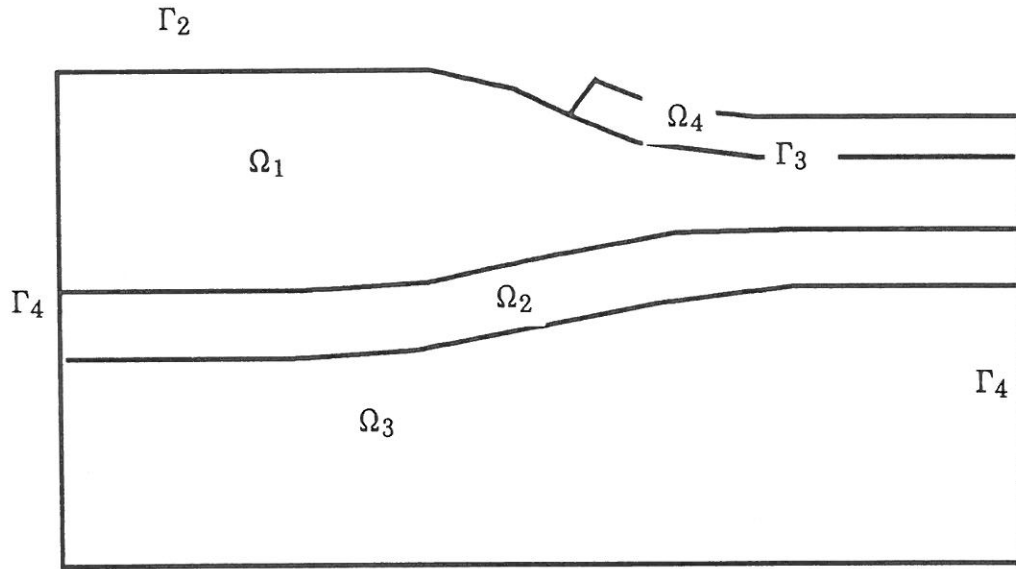


Figure 2 : domains and boundaries (new formulation)

The corresponding differential equation is :

$$\nabla \cdot (D_d(\mathbf{x}) \nabla C) = k_d(\mathbf{x}) C \quad \text{on } \Omega_1 \cup \Omega_2 \cup \Omega_3$$

with the boundary conditions

(2)

$$\frac{\partial C}{\partial n} = 0 \quad \text{on } \Gamma_3 \cup \Gamma_4, \quad C = C^* \quad \text{on } \Gamma_2$$

D_d is now a diffusion coefficient depending on the position \mathbf{x} , k_d is the strength of the sink, where

$$k_d(\mathbf{x}) = 0 \quad \text{for} \quad \mathbf{x} \in \Omega_1 \quad (3)$$

The physical meaning of k_d and D_d on Ω_2 and Ω_3 will be given later.

Equation (2) will now be transformed into its weak formulation.

Define the differential operator

$$L_D C = \left(\begin{array}{c} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{array} \right) C \quad (4)$$

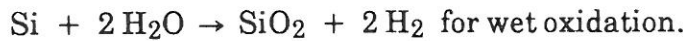
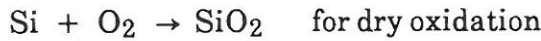
Let $\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3$ and define as test space $H_0^1(\Omega)$ and as trial space $H^1(\Omega)$.

Then a function $C(\mathbf{x}, y) \in H^1(\Omega)$ has to be found, which satisfies the Dirichlet boundary conditions so that for all $w \in H_0^1(\Omega)$:

$$\int_{\Omega} L_D w D_d L_D C d\Omega = \int_{\Omega} w k_d C d\Omega \quad (5)$$

2.2 The oxide growth

At the interface Γ_1 or, in the new formulation, in the interface range Ω_2 the following chemical reactions take place:



The chemical reaction results in a volumetric expansion

$$V_{\text{Si}} \rightarrow 2.2 V_{\text{Oxid}} \quad (6)$$

All approaches presented in the literature compute boundary displacements normal to the boundary Γ_1 from the volume expansion. This is surely unphysical in regions with strongly curved interface or where there is a strong variance of the oxygen concentration along the interface. These problems do not arise in the formulation with an interface zone Ω_2 . There, the 'disappearing' quantity of oxygen in a time step Δt is $Q = \Delta t k_d C(\mathbf{x}, y)$ and leads to a local volume expansion

$$\Delta V = 1.2 Q / N_1 \quad (7).$$

The factor 1.2 results from (6), N_1 is the number of unit volumes of oxygen reacting with one unit volume of silicon. The volume expansion then results in pre-strains in the formulation of the structural displacement model.

2.3 The structural problem

Let us assume for simplicity that the $\text{Si-SiO}_2\text{-Si}_3\text{N}_4$ -body deforms elastically what is justified for temperatures below 960° . For higher temperatures viscoelastic or viscous flow is observed. Yet this does not affect the principle ideas of this paper, so we will restrict to the elastic case. Let now $\theta(\mathbf{x}, \mathbf{y}) = (u(\mathbf{x}, \mathbf{y}), v(\mathbf{x}, \mathbf{y}))^T$ be the displacement field in Ω . For simplicity we assume a plane strain state which makes it possible to integrate analytically over the thickness of the domain.

In theory of linear elasticity with small displacements the strain tensor is defined as follows :

$$\varepsilon := \begin{pmatrix} \varepsilon_x & \gamma_{xy} \\ \varepsilon_y & \gamma_{xy} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial y} \end{pmatrix} (u, v)^T =: L_E \theta \quad (8)$$

Assuming a linear material law the stress tensor is given by

$$\sigma = M (\varepsilon - \varepsilon_0) \quad (9)$$

ε_0 are pre-strains due to increase of temperature, cristal growth or, as in our case, volumetric expansions from the chemical reaction. Assuming isotropic material, (9) reads as

$$\begin{pmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{pmatrix} = \frac{E}{1-\nu^2} \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1}{2}(1-\nu) \end{pmatrix} \begin{pmatrix} \varepsilon_x - \varepsilon_{x0} \\ \varepsilon_y - \varepsilon_{y0} \\ \gamma_{xy} - \gamma_{xy0} \end{pmatrix} \quad (9')$$

The external force on the body Ω shall be $p(\mathbf{x}, \mathbf{y}) = (p_x(\mathbf{x}, \mathbf{y}), p_y(\mathbf{x}, \mathbf{y}))$.

Then the system of differential equations for the elastic body is given by

$$\frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} = -p_x, \quad \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} = -p_y \quad (10)$$

Writing (10) as an operator equation yields

$$A(\theta) = L_E^T M (L_E \theta - \varepsilon_0) + p = 0 \quad (10')$$

Dirichlet boundary conditions are

$$u = u_0 \text{ and/or } v = v_0 \quad \text{on } \Gamma_D \quad (11)$$

Neumann boundary conditions are

$$\sigma_x n_x + \tau_{xy} n_y = t_x \text{ and/or } \tau_{xy} n_x + \sigma_y n_y = t_y \text{ on } \Gamma_N \quad (12)$$

where (n_x, n_y) is the outward normal on Γ and $(t_x, t_y) = t$ are boundary tractions.

For a weak formulation of (10) testfunctions $\psi = (w_u, w_v)^T$ are defined which vanish at the Dirichlet boundary Γ_D .

Multiplication of (10') with ψ , integration over Ω and a final partial integration yields the weak formulation.

Find θ , so that for all testfunctions ψ

$$\int_{\Omega} (L_E \psi)^T M L_E \theta d\Omega = \int_{\Omega} \psi^T (p + L^T M \varepsilon_0) d\Omega - \int_{\Gamma_N} \psi^T t d\Gamma \quad (13)$$

For our class of problems we can assume the boundary tractions t and the volume forces p to be 0 throughout the domain, simplifying the righthand side to a term only involving the prestrains ε_0 .

The local volume expansion ΔV is related to the prestrain tensor by

$$\Delta V = \varepsilon_{0y} + \varepsilon_{0x} \quad (14)$$

Assuming isotropy

$$\varepsilon_{0y} = \varepsilon_{0x} = 1/2 \Delta V \quad (15)$$

Obviously the assumption of small displacements in the definition (8) of the strain tensor is not satisfied in the problem of local oxidation with strains of up to 1.2. Yet, in our algorithm the time-stepping procedure will split the problem into a sequence of subproblems, each of which satisfies the assumption of small strains. After each time step the geometry of the structure is updated, a procedure corresponding to the 'updated Lagrange' formulation for problems with large displacements.

3. The finite element discretization

The Poisson equation (5) and the elasticity equations (13) will be discretized by finite elements. Concepts are the same for both equations, so we can restrict the discretization to the diffusion part.

The unknown function C shall be approximated by

$$C = \sum_{i=1}^m a_i N_i \quad (16)$$

with local shape functions N_i . If the same space for shape and testfunctions is used, the discretized weak formulation of (5) follows:

Find coefficients $a_i, i = 1, \dots, m$ such that for all testfunctions $N_j, j = 1, \dots, m$

$$\sum_{i=1}^m a_i \left(\int_{\Omega} L N_j D_d L N_i d\Omega - \int_{\Omega} k_d N_i N_j d\Omega \right) = 0 \quad (17)$$

Equation (17) corresponds to the following system of linear equations

$$(K_I - K_{II}) a = 0 \quad (18)$$

For the computation of the matrices K_I and K_{II} the domain Ω is split into elements Ω_I , every shape function N_I having support only on elements with the index subset I_I from $\{1, \dots, n\}$. Then (17) can be rewritten as

$$\sum_{l=1}^n \sum_{i \in I_l} a_i \left(\int_{\Omega_l} L N_j D_d L N_i d\Omega - \int_{\Omega_l} k_d N_i N_j d\Omega \right) = 0 \quad (19)$$

Because of their higher accuracy quadrilateral or higher order isoparametric elements are often preferred to the easiest triangular elements. Then integrals in (19) have to be approximated by numerical integration. Let \mathbf{x}_k , $k=1, \dots, g$ be Gaussian integration points in element l , w_k the corresponding weights and $|J_l(\mathbf{x}_k)|$ the Jacobian of the transformation from a standard element (where the integration points are originally defined) to element l at \mathbf{x}_k . Then the entries of matrices K_I and K_{II} have the following form:

$$k_{I,i,j} = \sum_{k=1}^g w_k L(N_j(\mathbf{x}_k)) D_d(\mathbf{x}_k) L(N_i(\mathbf{x}_k)) |J_l(\mathbf{x}_k)|$$

(20)

and

$$k_{II,i,j} = \sum_{k=1}^g w_k k_d(\mathbf{x}_k) N_j(\mathbf{x}_k) N_i(\mathbf{x}_k) |J_l(\mathbf{x}_k)|$$

Examining (20) it can readily be seen that material information, i.e. diffusion coefficient D_d and reaction coefficient k_d are evaluated only at the Gaussian points in each element. These will also be the points where the three subproblems (oxygen diffusion, chemical reaction and structural displacements) are coupled.

4. The algorithm

For the formulation of an algorithm to simulate the growth of oxide it is necessary to model the physical behaviour in the interface zone between silicon and dioxide, i.e. to identify the diffusion coefficient $D_d(\mathbf{x})$ and the reaction coefficient $k_d(\mathbf{x})$ in the interface and the silicon range. Although there is physical evidence for a distributed transition zone ⁷, it is difficult to identify parameters in this zone by experimental measurements. It is much easier to measure the sharp interface coefficient k_s , which can be interpreted as a balance coefficient for the distributed reaction governed by k_d and D_d . A detailed analysis of the relation of k_s , k_d , and D_d is given in ⁸. The result which will be used in the algorithm to be presented here is the following. Over the domain of computation a density function for silicon dioxide $\eta(\mathbf{x})$ can be defined as the relative volume of dioxide at a point \mathbf{x} . $\eta(\mathbf{x})$ is 1 in pure

dioxide and 0 in pure silicon. Obviously, $k_d(x)$ has to be equal to 0 if $\eta(x)$ is 1, i.e. in Ω_1 . If

$$k_s^2 = k_d(x) D_d(x) \quad \text{for all } x \in \Omega_2 \cup \Omega_3 \quad (21)$$

it can be proven in a onedimensional setting that the growth rate in the sharp formulation is exactly the same as that in the smoothed formulation. The quotient k_d/D_d can be shown to control the thickness of the interface layer. In ⁸ the following relation between $\eta(x)$ and $k_d(x)$ has been proposed:

$$k_d(x) = k_{d\max} (1 - \eta(x)) \quad (22).$$

With these definitions an algorithm can be formulated which couples the diffusion problem via the density function and eq. (22) to the displacement problem at the integration points in the elements. Oxygen 'disappears' in the integration points of the transition layers, producing new dioxide and thus modifying the density function and introducing prestrains at the same points for the displacement problem.

Algorithm :

1. Define an initial domain Ω and a density distribution $\eta(x)$ for silicon dioxide, thus introducing the dioxide, silicon and interface range. (The discretization of the nitride range is straightforward and needs not be described explicitly.)
2. Define a finite element mesh and initialize time $t = 0$.
3. Initialize material coefficients D_d , K_d , E and ν according to relations (21),(22) and the density distribution at all integration points.
4. Solve the quasistationary diffusion problem (2).
5. Compute the reacting quantity of oxygen and silicon at each integration point from (6) and (7).
6. Update the density function $\eta(x)$ at all integration points.
7. Compute the prestrains at all integration points from the reacting volume.
8. Solve the displacement problem (11).
9. Update nodal coordinates .
10. Set $t = t + \Delta t$ and go to step 3.

4. Numerical examples

In a first numerical example it will be shown in a onedimensional setting

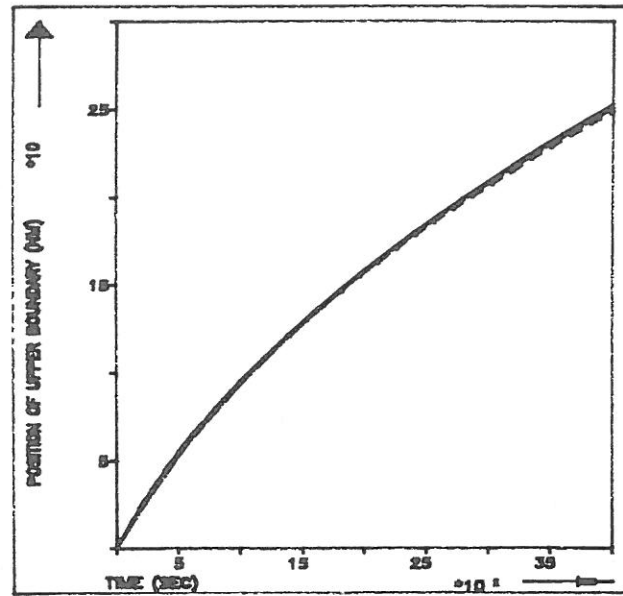


Figure 3 : Displacement of upper boundary of silicon-dioxide

that under conditions (21) and (22) the smoothed formulation yields , within the range of the approximation error, the same numerical results as the standard sharp interface formulation, for which an exact solution is available from the Deal-Grove-Model ⁹. Figure 3 shows the displacement of the upper end of silicon dioxide over the oxidation time. For the computation the following parameters were chosen, corresponding to wet oxidation at 1000 °C :

$$C^* = .003 \text{ part./nm}^3, D_d = 80000 \text{ nm}^2/\text{s} \text{ in pure silicon dioxide, } k_s = 500 \text{ nm/s}$$

Over an oxidation time of 4000 sec 20 time steps were performed. The uniform grid spacing for linear elements was 12 nm, an initial oxide thickness of 36nm was assumed and 29 elements were used. Figures 3 and 4 show the numerical results and the relative error for $k_{d\max} = 33.33, 41.66$ and 50 nm/s as dashed, dotted and dash-dotted lines compared to the analytical result of the Deal-Grove-model. For all

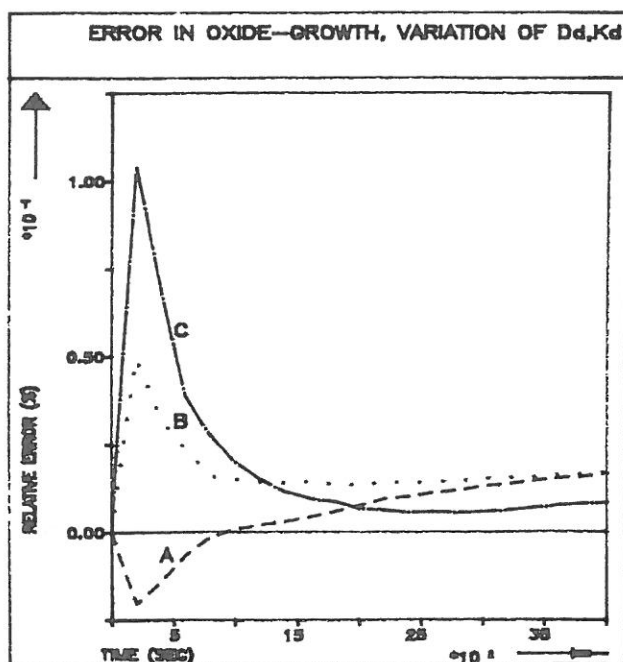


Figure 4 : Relative error for the displacement of the upper boundary

three sets of resulting parameters the error compared to the exact solution is (except in the first 3 timesteps) nowhere bigger than 1.8%. In figure 5 the concentration of oxygen for $k_{dmax} = 50$ is plotted for all time steps. The linear decay of the concentration corresponds to the dioxide range followed by the strongly decreasing concentration in the interface range and by a disappearing concentration in the silicon range. It can be seen that the finite element approximation is able to follow the relatively sharp decay of concentration in an interface with a width of about 30 nm.

In the second example a birds beak structure is simulated. Elastic and diffusion parameters are:

$E = 2.e-7 \text{ N/nm}^2$, $\nu = .3$ in silicon

$E = .66e-7 \text{ N/nm}^2$, $\nu = .17$ in dioxide

$E = 4.e-7 \text{ N/nm}^2$, $\nu = .3$ in nitride

$C^* = .003 \text{ part./nm}^3$, $D_d = 80000 \text{ nm}^2/\text{s}$ and $k_s = 790 \text{ nm/s}$.

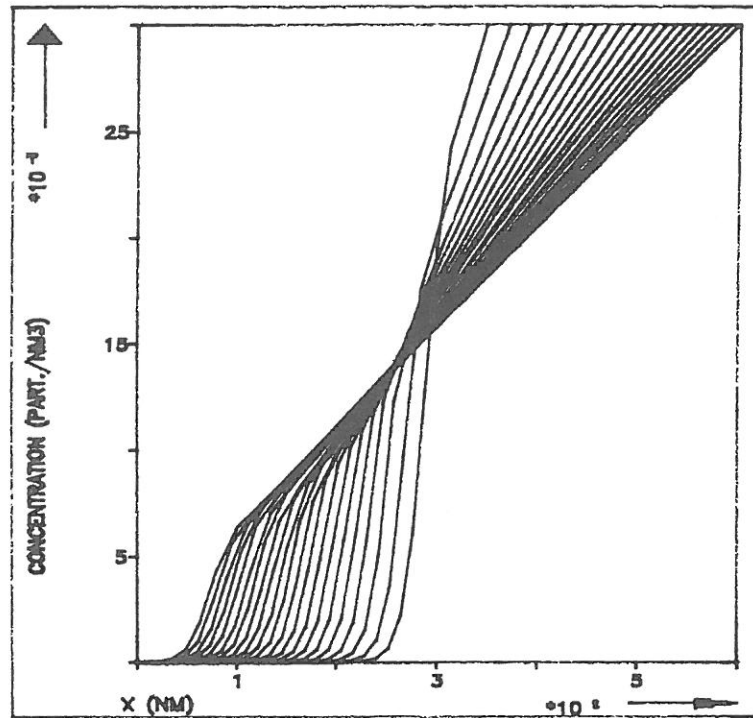


Figure 5: Oxygen concentration for 20 time steps

In the transition zone the elasticity modulus was interpolated between the silicon and dioxide values according to the density function η . Figure 6 a,b,c shows the structure before oxidation, after 2 timesteps and after 20 timesteps of 120 sec each. The main advantage of the new approach can be seen: the interface has no longer to be tracked by element edges but is given implicitly by the density function η . For the display, a density of .5 was used as an equivalent sharp interface between silicon and dioxide.

5. Conclusions

A new approach to simulation of local oxidation of silicon has been given which allows to treat the free boundary value problem on a topologically invariant finite element mesh. Unlike the standard approach only one finite element mesh has to be set up at the beginning of the simulation. The approach can readily be transformed to threedimensional LOCOS-simulation where it is nearly mandatory to use a fixed finite element mesh, as remeshing of 3D-structures after every few

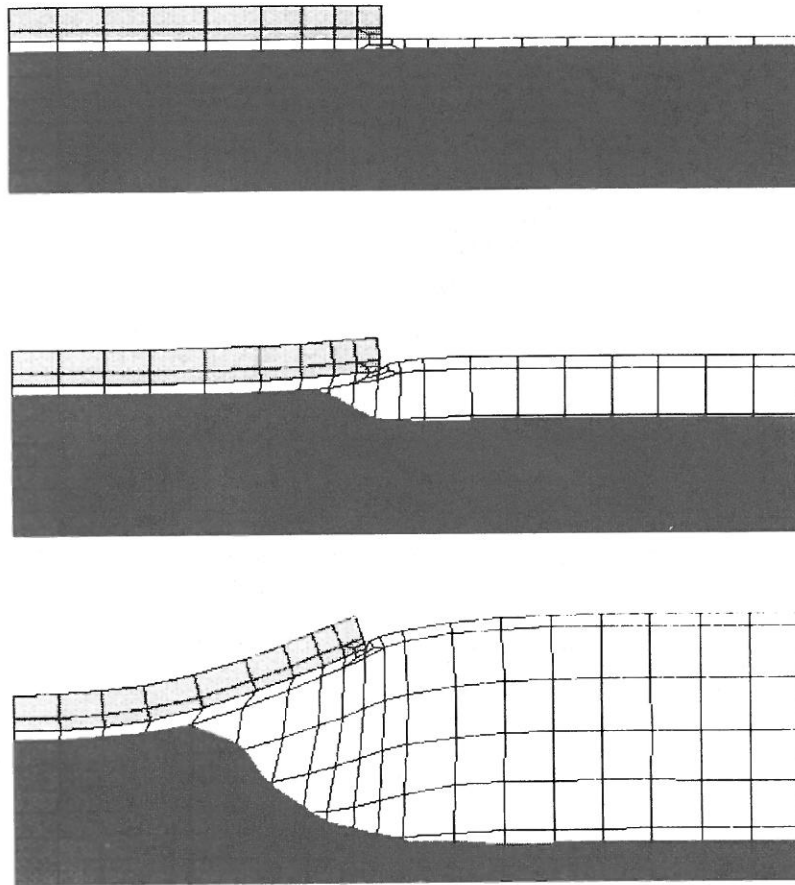


Figure 6 : Birds beak : Structure before oxidation, after 4 time steps and after the end of oxidation

time steps would be extremely costly. Moreover the new approach offers the possibility to investigate numerically physical phenomena like the roughness of the interface between silicon and dioxide which can be interpreted as a kind of transition zone. Finally it should be mentioned that this approach yields immediately stresses and strains not only in dioxide but also in silicon which could be used for controlling stress dependencies of dopand diffusion in silicon.

References

- /1/ Lorenz,J.; Pelka,J.; Ryssel,H.;Sachs,A.;Seidl,A.;Svoboda,M. ' COMPOSITE - A complete modeling program of silicon technology ', IEEE transactions on computer-aided design, Vol CAD-4, (1985)
- /2/ Needs,M.J.; Jovic,V.;Taylor,C.;Boad,K.;Cooke,M.J. 'A 2-D linear elastic model for the local oxidation of silicon using the boundary element method', Proc. of the Second Int. Conf. on Simulation of Semiconductor Devices and Processes, Swansea (1986)
- /3/ Pocet,A.'Finite-element simulation of local oxidation of silicon', IEEE transactions on computer-aided design, Vol CAD-4, No 1 (1985)
- /4/ Law,M.; Rafferty,C.; Dutton,R.W. 'SUPREM IV '. in : Process simulators for silicon VLSI and high speed GaAs Devices. Report. Integrated Circuits Laboratories. Stanford University. Stanford, Ca 94305 (1987)
- /5/ Katz,C.' Die Anwendung der Theorie der Methode der Finiten Elemente auf die ebene Sickerströmung mit freier Oberfläche', Diplomarbeit, Fakultät für Bauingenieur- und Vermessungswesen, Technische Universität München, Arcisstr. 21, D-8000 München 2 (1977)
- /6/ Rank , E. 'An adaptive finite element approach for the free surface seepage problem' Int.J. f. Num. Meth. Eng., Vol 23, p. 1217-1228 (1986)
- /7/ Sune,J.;Placencio,I.;Farres,E.;Barniol,N.;Aymerich,X.;' On the Si-SiO₂ interface roughness in VLSI-MOS structures. Phys. Stat. Sol. (a) 109, p 479-491 (1988)
- /8/ Weinert,U.; Rank,E. ' A simulation system for diffusive oxidation of silicon. I. One-dimensional analysis', submitted to J. Electrochem. Soc.
- /9/ Deal, B.E., Grove,A.S. ' General relationship for the thermal oxidation of silicon' J. Appl. Phys., Vol 36, No 12 (1965)

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