A NEW FINITE ELEMENT APPROACH TO THE LOCAL OXIDATION OF SILICON

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Abstract

A new finite element approach to the local oxidation of silicon is presented, which is based on the definition of a smooth transition zone between silicon and silicon dioxide. By a suitable parameter identification, this regularization is equivalent to the standard sharp interface model based on the fundamental work of Deal and Grove. The oxide body is defined implicitly by a silicon distribution function which couples the oxidant diffusion to the mechanical displacement due to the volume expansion of the chemical reaction. The main advantage is that the finite element mesh remains topologically invariant and that no remeshing is necessary during the progress of oxidation. It is shown in numerical examples that this approach offers the possibility to treat problems which impose severe difficulties to other methods.

1 Introduction

During the past 10 years several numerical approaches to the simulation of local oxidation of silicon have been published. They model a process step which is most important for defining the geometric structure of highly integrated semiconductor devices. A part of the wafer is masked by silicon nitride, which resists an oxidant diffusion; exposed parts are penetrated by the oxidant (oxygen or steam) which reacts at the interface of already existing dioxide and silicon to new dioxide. This chemical reaction has two consequences: Firstly, silicon is consumed, so the interface moves during oxidation; secondly, the produced dioxide has more than twice the volume of the original silicon - the oxide layer is lifted up.

In a physical model the oxidation of silicon is described as a transient coupled system of equations for oxidant diffusion, chemical reaction and mechanical displacement. The moving interface between oxide and silicon renders the whole system a free boundary problem.

All published numerical approaches are based on the fundamental work of Deal and Grove [1] who described the oxidation of silicon in one dimension. Two-dimensional oxidation simulators can be classified into three groups. The first approach [2] maps the silicon dioxide domain in each time step onto a simple numerical domain. It is thus restricted to relatively simple oxide geometries like bird’s beak structures. The second approach uses the boundary element method for oxidant diffusion and mechanical displacement. It suffers from the restriction of the boundary element method to essentially linear problems and can thus hardly take into account modern physical oxidation models like stress dependant oxidant diffusion or reaction coefficients.

The most general third approach uses the finite element method to compute in every time step the oxidant concentration along the Si-SiO₂-interface. From this concentration the displacement of boundary nodes according to the newly created oxide volume is computed and thus boundary displacements for the mechanical part of the problem are defined. After the structural computation (usually by elastic or viscous models) the
silicon dioxide domain is updated and, at least after each few steps, a (costly) remeshing of the structure has to be performed.

Although many problems can be solved successfully with these methods there remain a few important questions which are hard to be answered with these 'standard' approaches. Among others these are:

- **Structures without pad oxide below the nitride mask.** The Si-SiO₂-interface meets the lower boundary of the nitride domain in a right angle. So an algorithm which displaces interface-nodes has to observe the shape of the nitride layer as a side condition. As this is algorithmically rather involved, most programs are limited to initial structures with pad oxides; the resulting oxide shape then has to be corrected in some heuristic procedures.

- **Structures which do not only change geometry but also the topology during oxidation.** An example is a 'sandwich' structure of initial bulk silicon, an oxide layer, polysilicon and a nitride mask on top. First, the polysilicon is oxidized up to a point where the growing oxide meets the oxide layer below the polysilicon. For every interface-tracking algorithm this situation is extremely difficult. It can only 'survive' the partial collapse of polysilicon by continuously monitoring the distance of every interface node to the buried oxide and by redefining the domain of computation at the moment of contact.

- **Complex constitutive laws for the structural problem.** Some authors (e.g. [10]) suggest oxidation models which explain stresses along the Si-SiO₂-interface assuming plastic behaviour of silicon and dioxide in the close vicinity of the interface. Others suggest history-dependant (e.g. viscoelastic) models of oxide motion. Yet a numerical simulation of these material laws depends on the knowledge of stress and strain-states at (physical) points in oxide as they move during oxidation time. If a remeshing of the oxide range is necessary, these domain informations have to be interpolated in a costly procedure from one domain to another.

- **General three-dimensional oxidation simulation.** Three-dimensional problems on arbitrary domains can hardly be modelled by other methods than a finite element approximation. Yet mesh construction in 3D is very costly and remeshing after each time step is no realistic possibility.

This paper presents a new approach to the simulation of oxidation of silicon which

- has by construction no difficulty to simulate problems of the first two classes,
- offers the possibility to incorporate general mechanical models in a natural way,
- can in principle be transformed to three-dimensional problems without imposing the necessity to remesh the domain during simulation.

The new approach uses the idea of a smooth transition zone from silicon to dioxide which has been presented in [11] [12] and [13]. It will be shown that by a suitable parameter identification and a simple extraction procedure an equivalent sharp interface line results which is identical to that of the standard model. The transition zone between silicon and dioxide can therefore either be interpreted as a mean to model the roughness of the interface (for the physical evidence of this roughness see for example [14]) or simply as a mathematical tool to regularize the free boundary problem.

In the next section the new model will be presented. Section 3 describes some algorithmic aspects and in section 4 numerical examples show the effectiveness of the algorithm. This paper is restricted to a simple physical model (stress independant oxidant diffusion and reaction, elastic mechanical displacement). Yet more general models can easily be implemented on the basis of the same principles.
2 The model

For the definition of the model problem consider figure 1. The domain of computation $\Omega$ is composed of the pure-silicon dioxide range $\Omega_1$, the interface range $\Omega_2$ with a mixture of silicon and dioxide, the pure silicon range $\Omega_3$ and the nitride mask $\Omega_4$. Define now on $\Omega_1 \cup \Omega_2 \cup \Omega_3$ a normalized silicon concentration $\eta$ as

$$\eta(x,t) = \frac{C_{Si}(x,t)}{C_{Si0}} ,$$

where $x$ is the spatial coordinate, $t$ the time, $C_{Si}(x,t)$ the silicon concentration at time $t$ and point $x$ and $C_{Si0}$ the concentration of silicon atoms in pure crystal. $\eta$ is 1 in $\Omega_3$, 0 in $\Omega_1$ and between 0 and 1 in the interface $\Omega_2$. (The oxidant diffusion in nitride, i.e. $\Omega_4$ can be neglected, therefore $\Omega_4$ will only be considered for the structural displacement.)

The oxidant diffusion in $\Omega_1 \cup \Omega_2 \cup \Omega_3$ shall be described by

$$\nabla(D(\eta(t))\nabla C(x,t)) = k(\eta(t))C(x,t) \quad \text{on} \quad \Omega_1 \cup \Omega_2 \cup \Omega_3$$

for every fixed time $t$ ,

with the boundary conditions

$$C = C^* \quad \text{on} \quad \Gamma_2$$

and

$$\frac{\partial C}{\partial n} = 0 \quad \text{on} \quad \Gamma_3 \cup \Gamma_4 .$$

$k$ is, unlike in the standard model, the strength of a spatial sink and not a surface reaction coefficient at the sharp interface.

Obviously, the chemical reaction in the interface range $\Omega_2$ changes the relative silicon concentration $\eta$, i.e. in a time interval $t, t + \Delta t$ and a test volume $\Delta V$ (where we assume the oxidant concentration $C$ to be constant), $k(\eta(t))C(x,t)\Delta V\Delta t$ particles of oxygen react with $k(\eta(t))C(x,t)\Delta V\Delta t/(N_1 \lambda)$ unit volumes of silicon to form
\[ V_{\text{SiO}_2}^{\text{new}} = k(\eta(t))C(x,t)\Delta V \Delta t / N_1 \]  

unit volumes of silicon dioxide.

Here \( N_1 [\text{part./nm}^3] \) is the number of oxidant molecules incorporated into one unit volume of silicon dioxide, \( \lambda \) is the volume expansion factor \((\approx 2.2)\) for the reaction from silicon to dioxide. Letting \( \Delta t \to 0 \) and noting that \( \eta \) is the relative density of silicon it follows that

\[ \frac{\partial \eta}{\partial t} = -\frac{1}{\lambda} k(\eta(t))C(x,t)/N_1 . \]  

The additional volume per unit volume silicon after oxidation is given by

\[ V^{\text{new}} = \frac{\lambda - 1}{\lambda \Delta t} \Delta V k(x, \eta(t))C(x,t)/N_1 , \]  

which produces strains in the control volume and thus loads the coupled displacement problem.

Let us assume now that the Si-SiO\(_2\)-Si\(_3\)N\(_4\)-body deforms elastically and let \( \theta(x,y) = (u(x,y), v(x,y))^T \) be the displacement field in \( \Omega \).

In the theory of linear elasticity with small displacements and strains (which can be assumed in every time step) the strain tensor is defined as

\[ \epsilon := \begin{pmatrix} \epsilon_x \\ \epsilon_y \\ \gamma_{xy} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial y} \\ 0 & 0 \end{pmatrix} (u, v)^T =: L_E \theta . \]  

Assuming a linear material law the stress tensor is given by

\[ \sigma = M(\epsilon - \epsilon_0) . \]  

\( \epsilon_0 \) are prestrains due to the volumetric expansion resulting from the chemical reaction.

We will assume that there are no distributed body forces except those resulting from prestrains. Then the system of differential equations for the elastic body is given by

\[ A(\theta) = L_E^T M (L_E \theta - \epsilon_0) = 0 \]  

Together with appropriate traction and displacement boundary conditions, (10) defines the mechanical displacement in every time step.

Now the question arises, how the volume expansion \( V^{\text{new}} \) in (7) is related to prestrains \( \epsilon_0 \) for the deformation problem. From the plain strain condition it follows that

\[ V^{\text{new}} = \epsilon_{0x} + \epsilon_{0y} \]  

The choice of a second condition for \( \epsilon_0 \) controls stresses due to the volume expansion along the interface (see equ. (9)). If we assume stress-free growth along a planar interface (a condition which is implicitly assumed by displacing interface-nodes, too), we have to ensure that \( \epsilon = \epsilon_0 \) in a planar reactive range.

In our algorithm we use the following approximation. Let \( \epsilon_t^{\Delta t}, \epsilon_t^{\Delta t}, \sigma_t^{\Delta t} \) be principle strains and the principle direction of the strains at time \( t - \Delta t \). We assume that the ratio of the strain components and
the principle direction at a point of reaction does not change much until time $t$. So $\epsilon_0$ is imposed into the same principle direction with the same ratio of the principle components, i.e.

$$
\epsilon_{0I}^I = c\epsilon_I^{t-\Delta t}, \quad \epsilon_{0II}^I = c\epsilon_{II}^{t-\Delta t}, \quad \alpha_0^I = \alpha^{t-\Delta t}
$$

(12)

with a constant $c$ to be chosen such that (11) is satisfied.

Obviously there is large ambiguity in the choice of (12). Yet it has turned out numerically that the shape of the oxide body is rather unsensitive to the special choice of $\epsilon_0$. On the other hand more sophisticated stress generation and relaxation mechanisms (e.g. [10]) could provide more realistic stress results in the viscosity of the interface.

Another crucial point in the definition of an oxidation model based on an extended reactive layer is the identification of parameters $D$ and $k$ in (2) as functions of the silicon distribution function $\eta$. In ([13]) the question is investigated, how $D$ and $k$ can be chosen so that the oxide growth is equivalent to the sharp-interface model. We will give a short summary of these results. First it has to be defined what is meant by this equivalence. Having in mind a process simulation system consisting of an oxidation simulator coupled to an impurity diffusion simulator, a sharp interface line has to be extracted from the silicon distribution function. A natural choice is to define the line where $\eta = .5$ as equivalent sharp interface, a line which can easily be extracted from $\eta$ by a standard contour line algorithm for postprocessing finite element results. For the parameter identification we will now consider in a one-dimensional analogon the following two problems:

The first one,

$$
D_{ox}C'' = 0 \quad \text{on} \quad -x_0 < x < 0, \quad C(-x_0) = C_0, \quad D_{ox}C'(0) = -k_sC(0)
$$

(13)

is the standard one-dimensional Deal-Grove model. $D_{ox}$ is the diffusion coefficient of the oxidant in SiO$_2$, $k_s$ the (surface) reaction rate.

The second one,
\[(D(z)C')' = k(z)C , \quad C(-x_0) = C_0 , \quad C(\infty) = 0 \quad (14)\]

is the one-dimensional analogon to the diffusion part of the smoothed problem. In figure 2 the two solutions together with the equivalent sharp interface \(x_I\) are sketched.

We will call parameter functions \(k(z)\) and \(D(z)\) equivalent with respect to the sharp interface \(x_I\) to \(k_s\) and \(D_{ox}\), if

\[\int_{-x_0}^{\infty} k(t)C_{\text{smooth}}(t)dt = D_{ox}C_{\text{Deal-Grove}}' \quad (15)\]

and if the solution \(C_{\text{Deal-Grove}}\) of (13) and \(C_{\text{smooth}}\) of (14) coincide in an interval \([-x_0, \zeta_0]\) of pure dioxide. Via the reaction volume condition (15) guarantees the same growth of the oxide bodies for the two models.

Obviously, \(k\) has to be equal to 0 and \(D\) has to be equal to \(D_{ox}\) in pure dioxide. In ([11]) several models for \(k\) in the reactive layer and in silicon have been investigated. The most simple one, which works satisfactorily in numerical examples, assumes a linear increase of the reaction coefficient with the silicon density, i.e.

\[k(\eta) = \eta(x)k_{max} \quad (16)\]

\(k_{max}\) controls the thickness of the interface layer \(\Omega_2\). The bigger \(k_{max}\), the steeper the concentration decay and the thinner the reaction layer.

By a second condition to \(k\) and \(D\) the equivalence of the two models can be achieved. In [13] it has been shown that (15) holds if

\[k(z)D(z) = k_a^2 = \text{const.} \quad \text{for} \quad x > \zeta_0 , \quad k(z) = 0 \quad , \quad D(z) = D_{ox} \quad \text{for} \quad -x_0 \leq x \leq \zeta_0 \quad (17)\]

where \(k_a\) can easily be derived from \(k_s\). More details and the proof can be found in [13].

3 The algorithm

The coupling variable for the diffusion and displacement problem is, via the chemical reaction, the volume expansion and the related pre-strain tensor. In a finite element approximation prestrains are discretized by a projection of the strain operator (8) onto the space spanned by the shape functions and by integration of the elements [15]. If a numerical integration is used, pre-strains are only evaluated at integration points of elements within the reactive layer \(\Omega_2\). So the differential equations (2), (6) and (10) are coupled at the integration points. We can now define the basic algorithm for the oxidation simulation.

**Algorithm:**

1. Define an initial domain \(\Omega\) and a silicon distribution \(\eta\), thus introducing the dioxide, silicon and interface range. (The discretization of nitride is straightforward and needs not be described explicitly.)

2. Define a finite element mesh, initialize time \(t = 0\) and a direction of initial growth.

3. Initialize material coefficients \(D\) and \(k\) and the mechanical material constants at all integration points.

4. Solve the quasistationary diffusion problem (2) to (4).

5. Compute the reacting quantity of oxidant and silicon at each integration point from (5).
6. Update the silicon distribution function $\eta$ at all integration points according to (6).

7. Compute prestrains at all integration points from the reacting volume according to the local growth direction.

8. Solve the displacement problem (10).

9. Update nodal coordinates.


11. Set $t = t + \Delta t$ and goto 3.

The finite element mesh remains topologically invariant during the time of simulation, only nodes are displaced according to the results of the mechanical problem. As the dioxide body is defined only implicitly via the silicon distribution function, a change of topology does not impose additional difficulties. Moreover, as integration points move with the growth of the oxide, physical models like plasticity or viscoelasticity can be implemented without the necessity to interpolate data from one mesh to another.

Several improvements to this basic algorithm have been incorporated into our simulation system. One obvious possibility to save computation time in each displacement step follows from the high rigidity of silicon compared to dioxide or nitride. It can be assumed a priori that pure silicon elements will not deform. So the corresponding elements matrices need not be assembled into the whole system matrix and can be replaced by boundary conditions. Another possibility, which is easier to implement, is to fix pure silicon nodes and to eliminate the corresponding equations from the total system.

4 Numerical examples

In a first one-dimensional example the equivalence of the smoothed formulation with the Deal-Grove model will be verified. The following parameters were chosen for the computation:

$C^* = 0.003[part./nm^3], D_{ox} = 80000[mm^2/s]$ in pure silicon dioxide, $k_s = 500[mm/s]$.

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 36 nm was assumed and a total of 29 elements was used. Figures 3 shows and the relative error for $k_{max} = 33.33, 41.66$ and 50nm/s as dashed, dotted and dash-dotted lines compared to the Deal-Grove model. For all three sets of parameters the relative error is (except in the first 3 steps) nowhere bigger than 1.8 %.

The second example shows the advantages of the new method in a two-dimensional model problem. A 'sandwich' structure as shown in figure 4 to 8 is oxidized. The initial structure (figure 4) is composed of a layer of oxide between bulk silicon and polycrystalline above, partially masked by a nitride layer. First, a bird's beak in poly forms out (figure 5), showing the capability of the approach to track the interface passing through the interior of elements. Figure 6 shows the structure shortly before, figure 7 immediately after the two oxide ranges meet. The final figure 8 shows the oxidation proceeding into the bulk silicon.

This example shows that our algorithm can easily treat problems of the first two problem classes mentioned in the introduction, which lead to severe difficulties for algorithms based on a sharp interface formulation. It can readily be seen that the interface meets the nitride layer vertically, a fact which results simply from the natural (flux free) boundary condition of the diffusion problem in each time step.

The change of topology of the oxide body does not impose any difficulty to the computation. In a standard approach, much effort would have to be spent to be able to observe the partial collapse of the poly-layer.
Figure 3: Relative error for displacement of upper boundary

Figure 4: Domain before oxidation
Figure 5: Domain shortly after begin of oxidation

Figure 6: Domain before collapse of poly-layer
Figure 7: Domain at moment of collapse of poly-layer

Figure 8: Domain after end of oxidation
All computations have been performed on an Apollo-DN 570, an average time step for a mesh with 564 nodes being less than 36 CPU-seconds.

5 Conclusions

A new approach for simulation of local oxidation of silicon has been presented, considering the interface between silicon and dioxide not as a sharp line but as a smooth transition layer. According to theoretical investigations it could be shown that by a suitable parameter definition identical results to the standard Deal-Grove model can be obtained. The main advantage is that no remeshing is necessary during oxidation. Moreover the approach offers the chance to be transformed to three-dimensional problems, where the possibility to save remeshing is even more attractive than in two dimensions.

References


