THREE–DIMENSIONAL MODELING OF THERMAL OXIDATION OF SILICON BY MEANS OF THE FINITE ELEMENT METHOD

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ABSTRACT. A numerical model which is suitable to describe three-dimensional thermal oxidation of silicon is proposed. By oxidation the three material components silicon, silicon dioxide and oxidant molecules are involved. The model takes into account that the diffusion of oxidants, the chemical reaction, and the volume increase occur simultaneously in a so-called reactive layer. This reactive layer has a spatial finite width, in contrast to the sharp interface between silicon and dioxide in the convential formulation. The oxidation process is numerically described with a coupled system of equations for reaction, diffusion, and displacement. In order to solve the numerical formulation of the oxidation process the finite element scheme is applied.

INTRODUCTION

Thermal oxidation of silicon is one of the most important steps in fabrication of highly integrated electronic circuits, being mainly used for efficient isolation of adjacent devices from each other.
If a surface of a silicon body has contact with an oxiding atmosphere, the chemical reaction of the oxidant (oxygen or steam) with silicon results in silicon dioxide. This reaction consumes silicon and the newly formed silicon dioxide has more than twice the volume of the original silicon. If a silicon dioxide domain is already existing, the oxidants diffuse through the oxide domain and react at the interface of oxide and silicon to form new oxide so that the dioxide domain is penetrated.
Thermal oxidation is a complex process where the three subprocesses oxidant diffusion, chemical reaction, and volume increase occur simultaneously. The volume increase is the main source of mechanical stress and strain, and these cause displacement (Zelenka 2000).
From the mathematical point of view the problem can be described by a coupled system of partial differential equations, one for the diffusion of the oxidant through the oxide, the second for the conversion of silicon into silicon dioxide at the interface, and a third for the mechanical problem of the Si–SiO_2–body, which can be modeled as an elastic, viscoelastic, or viscous body.
All published approaches can be classified essentially into three groups. The first type of method (Lorenz et al. 1985) maps the silicon dioxide domain in each time step onto a a simple numerical domain. The second approach uses the boundary element method for diffusion and displacement (Matsumota and Fukuma 1985). The third one (Rank and Weinert 1990) models the domain of computation by finite elements.
For a realistic and accurate oxidation simulation the three subproblems should be coupled, however, most oxidation models decouple them into a sequence of quasi-stationary steps. In our model all subprocesses are coupled simultaneously and the oxidation process can be simulated in three dimensions.
We will restrict the following explanation to the most simple physical model of linear oxidant diffusion and linear elastic displacement of the Si–SiO_2–body.

MODEL

We define a normalized silicon concentration

$$\eta(\vec{x},t) = \frac{C_{Si}(\vec{x},t)}{C_{0Si}} \tag{1}$$

where $C_{Si}(\vec{x},t)$ is the silicon concentration at time t and point $\vec{x}$ (x, y, z) and C_{0Si} is the concentration in pure silicon. So η is 1 in pure silicon and 0 in pure silicon dioxide.
The oxidant diffusion is described by

$$D\Delta C(\vec{x},t) = k(\eta)C(\vec{x},t)\,. \tag{2}$$

Here D is the diffusion coefficient and $k(\eta)$ is the strength of a spatial sink and not just a reaction coefficient at a sharp interface like in the standard model (Deal and Grove 1965). $k(\eta)C(\vec{x},t)$ defines how many particles of oxygen per unit volume react in a unit time interval to silicon dioxide.
The change of η is described by

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

where λ is the volume expansion factor (=2.25) for the reaction from silicon to silicon dioxide, and N_1 is the number of oxidant molecules incorporated into one unit volume of silicon dioxide.
Furthermore, we define in (4) that $k(\eta)$ is linear proportional to η.

$$k = \eta(\vec{x},t)k_{max} \tag{4}$$

The chemical reaction of silicon and oxygen causes a volume increase. The additional volume in a reference volume silicon ΔV, where we assume that the oxidant concentration C is constant, is given by

$$V^{add} = \frac{\lambda - 1}{\lambda} \Delta t \Delta V k(\eta) C(\vec{x}, t) / N_1 \, . \tag{5}$$

We define the normalized additional volume V_{rel}^{add} as

$$V_{rel}^{add} = \frac{V^{add}}{\Delta V} \, . \tag{6}$$

For our model we assume, that the Si–SiO_2–body deforms elastically. In the theory of linear elasticity with small displacements $\vec{\theta}(x, y, z) = \{u(x, y, z)\, v(x, y, z)\, w(x, y, z)\}$ and strains ε_{ij} (i, j stands for x, y or z), the strain tensor $\tilde{\varepsilon}$ is defined as

$$\tilde{\varepsilon} = L_D \vec{\theta} \tag{7}$$

where $\vec{\theta}$ is the displacement vector and L_D is a differential operator, so that for example $\varepsilon_{xx} = \frac{\partial u}{\partial x}$ and $\varepsilon_{xy} = \frac{1}{2}(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})$.
Assuming a linear material, the stress tensor $\tilde{\sigma}$ is given by

$$\tilde{\sigma} = \mathbf{D} \tilde{\varepsilon} \tag{8}$$

where $\mathbf{D}$ is a (6x6) material matrix of elastic constants. The elastic constants are linear functions of Young's Modulus E and Poisson's ratio μ of the materials.
The force vector $\vec{f}(x, y, z) = \{f_x, f_y, f_z\}$ is the gradient of the stress tensor $\tilde{\sigma}$.

$$\vec{f} = \nabla \tilde{\sigma} \tag{9}$$

The most important part is that the volume expansion causes displacement. The normalized additional volume from (6) can be written as

$$V_{rel}^{add} = \varepsilon_x + \varepsilon_y + \varepsilon_z \, . \tag{10}$$

For an isotropic material the strain components are equal so that

$$\varepsilon_x = \varepsilon_y = \varepsilon_z = \frac{1}{3} V_{rel}^{add} \, . \tag{11}$$

With (7) and (11) the relationship between the volume expansion and the displacement is fully determined.

DISCRETIZATION

Weak Formulation

Before we start with the discretization we apply the weak formulation on (2) and (3).
So we apply the Galerkin method with linear test functions $N_k(\vec{x})$ on the diffusion equation from (2) and apply Green's theorem to remove the Laplace operator Δ as follows

$$\begin{aligned} k_{max} \int_V \eta\, C\, N_k\, dV &= D \int_V \Delta C\, N_k\, dV = \\ D \int_\Gamma \frac{\partial C}{\partial \vec{n}} N_k\, d\Gamma &- D \int_V \nabla C\, \nabla N_k\, dV \end{aligned} \tag{12}$$

where $\frac{\partial C}{\partial \vec{n}} = 0$ and so the term $\int_\Gamma \frac{\partial C}{\partial \vec{n}} N_k\, d\Gamma$ is also zero, and so (12) is simplified to

$$k_{max} \int_V \eta\, C\, N_k\, dV = -D \int_V \nabla C\, \nabla N_k\, dV \, . \tag{13}$$

The application of the Galerkin method with the same linear test functions $N_k(\vec{x})$ to the distribution function from (3) leads to

$$\int_V \frac{\partial \eta}{\partial t} N_k\, dV = k_{max} \int_V \eta\, C\, N_k\, dV \, . \tag{14}$$

Oxidant Diffusion

In order to solve (2) and (3) on a three-dimensional domain with the volume V_{global}, we split the domain up into tetrahedral elements with the volume V and perform a finite element discretization. The spatial discretization for $C(\vec{x})$ on a single tetrahedral element is

$$C(\vec{x}, t = t_n) = \sum_{i=1}^{4} c_i^{(t_n)} N_i(\vec{x}) \tag{15}$$

where $c_i^{(t_n)}$ is the oxidant concentration at node i and discrete time t_n. $N_i(\vec{x})$ is the form function on node i.
The spatial discretization for $\eta(\vec{x})$ on a single tetrahedral element is

$$\eta(\vec{x}, t = t_n) = \sum_{i=1}^{4} \eta_i^{(t_n)} N_i(\vec{x}) \tag{16}$$

where $\eta_i^{(t_n)}$ is the normalized silicon concentration at node i and discrete time t_n. $N_i(\vec{x})$ is the linear form function on a node i.
If we replace $C(\vec{x}, t)$ and $\eta(\vec{x}, t)$ in (13) with (15) and (16) we obtain

$$\begin{aligned} -D \int_V \Big(\sum_{i=1}^{4} c_i^{(t_n)} \nabla N_i\, \nabla N_k \Big) dV &= \\ k_{max} \int_V \Big((\sum_{i=1}^{4} \eta_i^{(t_n)} N_i \sum_{i=1}^{4} c_i^{(t_n)} N_i)\, N_k \Big) dV &= \\ k_{max} \int_V \Big((\sum_{i=1}^{4} \eta_i^{(t_n)}\, c_i^{(t_n)}\, N_i)\, N_k \Big) dV &. \end{aligned} \tag{17}$$

With the following substitution

$$M_{ki} = \int_V N_k(\vec{x})\, N_i(\vec{x}) dV \tag{18}$$

$$K_{ki} = \int_V \nabla N_k(\vec{x})\, \nabla N_i(\vec{x}) dV \tag{19}$$

(17) is simplified to

$$\sum_{i=1}^{4} \big(D\, K_{ki}\, c_i^{(t_n)} + k_{max}\, M_{ki}\, c_i^{(t_n)}\, \eta_i^{(t_n)} \big) = 0 \tag{20}$$

which is a non-linear equation system (k is the equation index) with the constants D, K_{ki}, k_{max} and M_{ki} and with the unknown variables $c_i^{(t_n)}$ and $\eta_i^{(t_n)}$ for one finite element.

Change of η

The spatial discretization for $C(\vec{x})$ and $\eta(\vec{x})$ is the same like in the last subsection and is already described by (15) and (16). Because of the time dependence of (3) an additional time discretization of the partial differential term $\frac{\partial \eta(\vec{x},t)}{\partial t}$ is necessary. The time discretization is performed with the simple Backward-Euler method as

$$\frac{\partial \eta(\vec{x}, t = t_n)}{\partial t} = \frac{\eta(\vec{x}, t_n) - \eta(\vec{x}, t_{n-1})}{\Delta t} \tag{21}$$

where t_n and t_{n-1} are two successive discrete times. If we replace $C(\vec{x}, t)$, $\eta(\vec{x}, t)$ and $\frac{\partial \eta(\vec{x},t)}{\partial t}$ in (14) with the discrete expressions (15), (16) and (21), we obtain

$$\begin{aligned} \frac{1}{\Delta t} \int_V \Big(\sum_{i=1}^{4} (\eta_i^{(t_n)} - \eta_i^{(t_{n-1})}) N_i\, N_k \Big) dV = \\ k_{max} \int_V \Big((\sum_{i=1}^{4} (\eta_i^{(t_n)}\, c_i^{(t_n)}) N_i\, N_k \Big) dV. \end{aligned} \tag{22}$$

With the substitution (18) the last equation is simplified to a non-linear equations system (k is the equation index)

$$\sum_{i=1}^{4} \Big(M_{ki} \, (\eta_i^{(t_n)} - \eta_i^{(t_{n-1})} - k_{max}\, c_i^{(t_n)}\, \eta_i^{(t_n)}) \frac{1}{\Delta t} \Big) = 0 \tag{23}$$

with the unknown variables $c_i^{(t_n)}$ and $\eta_i^{(t_n)}$ and with the constants M_{ki}, k_{max} and $\frac{1}{\Delta t}$ for one finite element. The values for $\eta_i^{(t_{n-1})}$ are already determined at the previous time step.

If we combine the two equation systems (20) and (23), we obtain a non-linear equations system for one finite element (with eight equations and the eight unknows $c_{1..4}^{(t_n)}$ and $\eta_{1..4}^{(t_n)}$). Now we are able to solve the system (for example with the Newton method) at each time point t_n and the values for $c_i^{(t_n)}$ and $\eta_i^{(t_n)}$ can be determined.

Mechanics

The finite element discretization for a mechnical system has been already often described, for example by (Zienkiewicz 1987). Because of this fact we will restrict this subsection only to some steps which are important for the oxidation simulation.
After discretization of the continuum, the relationship between strain and displacement (7) can be written as

$$\tilde{\varepsilon}^e = \mathbf{B}\, \vec{d^e} = [\mathbf{B_i}, \mathbf{B_j}, \mathbf{B_m}, \mathbf{B_p}] \tag{24}$$

in which $\tilde{\varepsilon}^e$ is the strain tensor, $\vec{d^e}$ is the displacement vector and i, j, m and p are the four nodes on a single thetrahedron.
The element displacement is defined by the 12 displacement components of the nodes as

$$\vec{d^e} = \left\{ \begin{array}{c} \vec{d_i} \\ \vec{d_j} \\ \vec{d_m} \\ \vec{d_p} \end{array} \right\} \quad \text{with} \quad \vec{d_i} = \left\{ \begin{array}{c} u_i \\ v_i \\ w_i \end{array} \right\} \quad \text{etc.} \tag{25}$$

The submatrix $\mathbf{B_i}$ for the node i is

$$\mathbf{B_i} = \begin{bmatrix} \frac{\partial N_i}{\partial x}, & 0, & 0 \\ 0, & \frac{\partial N_i}{\partial y}, & 0 \\ 0, & 0, & \frac{\partial N_i}{\partial z} \\ \frac{\partial N_i}{\partial y}, & \frac{\partial N_i}{\partial x}, & 0 \\ 0, & \frac{\partial N_i}{\partial z}, & \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z}, & 0, & \frac{\partial N_i}{\partial x} \end{bmatrix} = \begin{bmatrix} b_i, & 0, & 0 \\ 0, & c_i, & 0 \\ 0, & 0, & d_i \\ c_i, & b_i, & 0 \\ 0, & d_i, & c_i \\ d_i, & 0, & b_i \end{bmatrix} \tag{26}$$

with the linear form function $N_i(\vec{x})$ defined as

$$N_i(\vec{x}) = a_i + b_i\, x + c_i\, y + d_i\, z \tag{27}$$

in which a_i, b_i, c_i and d_i are constant geometrical coefficients for the finite element. For example b_i is

$$b_i = -\det \begin{vmatrix} 1, & y_j, & z_j \\ 1, & y_m, & z_m \\ 1, & y_p, & z_p \end{vmatrix} . \tag{28}$$

The entire inner virtual work on a finite element is

$$W_{inner} = \int_V \{\tilde{\varepsilon}^e\}^T \, \sigma^e dV \tag{29}$$

in which the transposed strain tensor is

$$\{\tilde{\varepsilon}^e\}^T = \vec{d^e}^T\, \mathbf{B^T} \tag{30}$$

and the stress tensor (8) can be written as

$$\sigma^e = \mathbf{D}\, \tilde{\varepsilon}^e = \mathbf{D}\, \mathbf{B}\, \vec{d^e} . \tag{31}$$

That leads us to the following equation for W_{inner}.

$$W_{inner} = \vec{d^e}^T \int_V \mathbf{B^T D B}\, \vec{d^e}\, dV \tag{32}$$

The outer virtual work on a finite element, caused by the node forces is

$$W_{outer} = \vec{d^e}^T\, \vec{f^e} . \tag{33}$$

On a element the inner work must be equal with the outer work.

$$W_{inner} = \vec{d^e}^T \int_V \mathbf{B^T D B}\, \vec{d^e}\, dV = \vec{d^e}^T \vec{f^e} = W_{outer} \tag{34}$$

With the substituation

$$\mathbf{K^e} = \int_V \mathbf{B^T D B} dV \tag{35}$$

where $\mathbf{K^e}$ is the so-called stiffnes matrix, we obtain a linear equation system for the mechanical problem.

$$\mathbf{K^e}\,\vec{d^e} = \vec{f^e} \tag{36}$$

The most important part is, how the volume increase (5), caused by the chemical reaction of silicon to silicon dioxide, loads the displacement problem.
Due to (11) we obtain the components ε_x^e, ε_y^e and ε_y^e for the strain tensor $\tilde{\varepsilon}^e$ and with

$$\vec{f_i^e} = -\mathbf{B_i^T D} \tilde{\varepsilon}^e \, V^e \tag{37}$$

the relationship between the volume expansion and the node forces is given, and with (36) and (37) the displacements on the nodes is fully determined.

By coupling (20), (23) and (36), a local equation system for one finite element is given, which is a complete numerical formulation of the oxidation process with its oxidant diffusion, chemical reaction and volume increase at any time.

SIMULATION PROCEDURE

In the first step of the simulation procedure, we perform a finite element discretization. With this aim in view we split up the Si–SiO_2–body into tetrahedral elements and that results in a tetrahedral grid on the domain. The size of the tetrahedrons and, as a result of that, the number of the finite elements can be influenced by the meshing module.
In the next step we set the initial values for the oxidant concentration C and the normalized silicon concentration η on the grid nodes. For example η must be 1 in a pure silicon domain.
Since the oxidation process is time dependent, the actual simulation time must be reset at the beginning of the simulation.
As shown in Fig. 1, we iterate over all finite elements and build the local equation system for one element for every actual discrete time. The local system describes the oxidation process numerically for one element with the coupled system for diffusion, chemical reaction and the displacement problem. Note, that it would be wrong to solve the relative simple local equation system for one element. The finite element method includes the superpostition principle but not in the way to add up locally calculated results in order to determine the global results. In our case "global" has a spatial meaning and stands for the whole discretized domain.
In order to describe the global oxidation process we need a global coupled equation system. The components of the global equation system are assembled from the local equation system by using the superpostition principle.

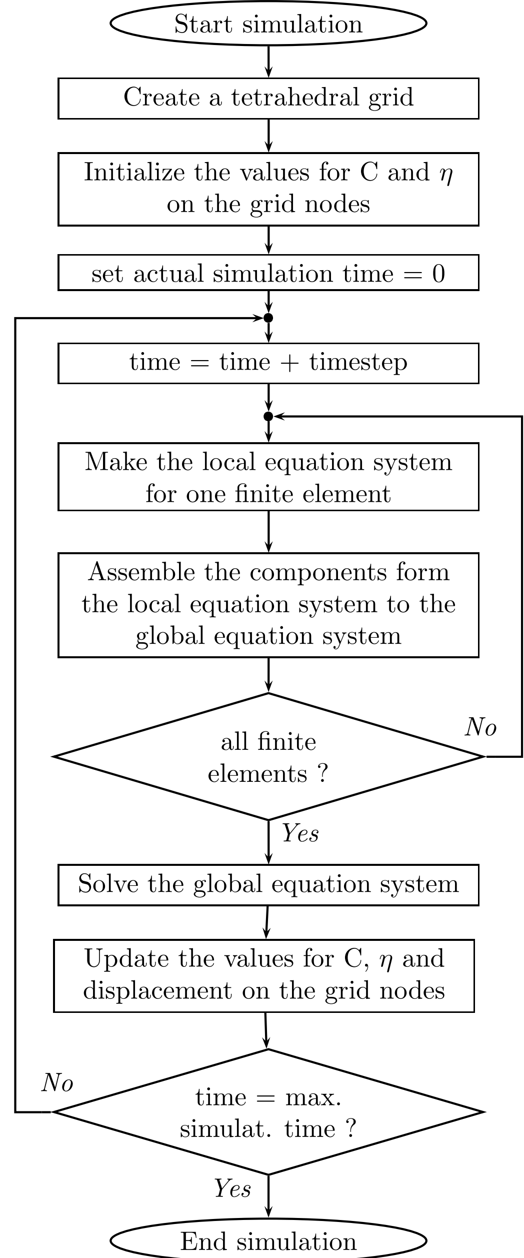

Figure 1: Simulation procedure

After the iteration over all elements is finished, the global assembled equation system is also finished. Now the global non-linear equation system can be solved and we obtain the results for the C, η and displacement values for the global discretized oxdidation process for the actual time step.
With these results we update the values for C, η and displacement on the grid nodes by adding up the new results to the already existing values on the grid nodes and so the values for C, η and displacement always keep pace with the actual simulation time.
If the above described procedure is finished, we increase the actual simulation time and start with the assembling loop again as long as the actual time is equal to the maximum simulation time.

A DEMONSTRATIVE EXAMPLE

As example a silicon body with the initial dimension (0.5 x 0.4 x 0.5) μm as shown in Fig. 2 is oxidized. For the simulation the following parameters were chosen:

$C^* = 3 \cdot 10^7\,[\frac{\text{part.}}{\mu\text{m}^3}]$, $D = 0.08\,[\frac{\mu\text{m}^2}{\text{s}}]$, $k_{\text{max}} = 40\,[\frac{1}{\text{s}}]$.

Here C^* is the surface oxidant concentration.
In this example only the upper surface of the body has contact with the oxiding atmosphere. As shown in Figs. 2 − 4 the bottom surface is fixed and on the rest of the surfaces there are free mechanical boundary conditions applied.
In the Figs. 2 − 4 the angel of view is always the same and the proportions of the body geometry are also true, so that the displacement effects caused by the volume increase can be watched correct.
The colour in the figures shows the value of the normalized silicon concentration. This means that blue is pure silicon dioxide and red is pure silicon and the other colours are the reaction layer.

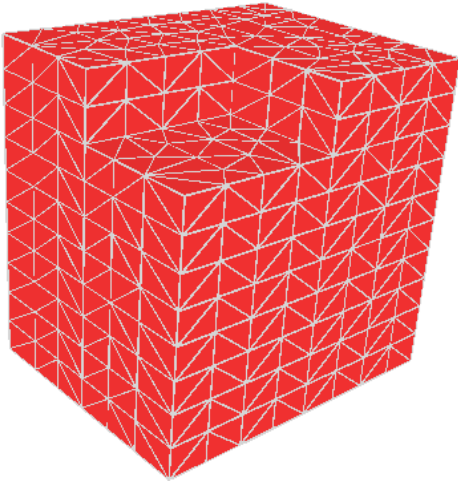

Figure 2: Initial silicon body before oxidation.

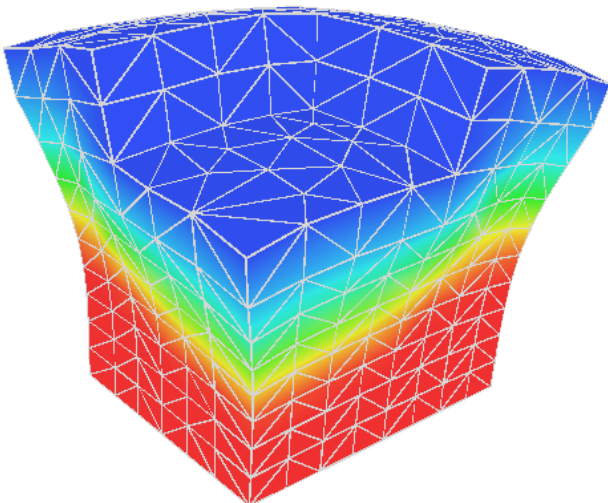

Figure 3: Deformation and silicon dioxide distribution (blue region) at some time t_1.

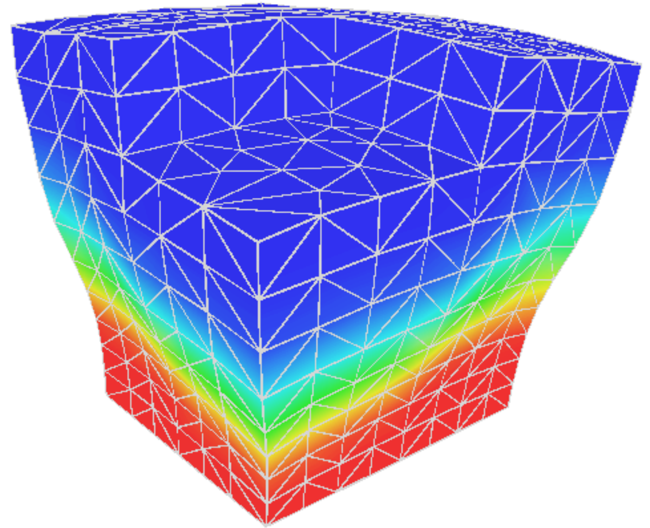

Figure 4: Deformation and silicon dioxide distribution (blue region) at time $2 * t_1$.

CONCLUSIONS

A three-dimensional oxidation model which is based on the finite element technique has been proposed. In this model it is assumed that the interface beween the silicon and oxide is a reaction layer with finite width instead of a sharp interface. In this layer there is a mixture of the three components silicon, oxidants, and oxide.
One of the advantages of this model is that the numerical formulation, consisting of a coupled differential equation system, describes the complete physical oxidation process in a very realistic way.
As demonstrated on a numerical example, this model is a powerful tool to simulate the whole oxidation process on three-dimensional semiconductor structures.

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