Mixed-hybrid finite element methods for coupled problems in silicon dioxide technology

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Abstract. In this work we deal with the numerical simulation of thermal oxidation in silicon device technology. This application is a complex coupled phenomen, involving the solution of a diffusion-reaction problem and of a fluid-structure interaction problem. Suitable iterative procedures are devised for handling nonlinearities and strong coupling between the sub-problems to be solved. In particular, we propose a unified dual-mixed hybrid formulation that allows for the simultaneous solution of the compressible/incompressible Navier equations in both solid and fluid domains. The accuracy and the flexibility of the proposed approach are demonstrated on benchmark test problems.

1 Introduction and motivation

Thermal oxidation of silicon is one of the several steps involved in the manufacturing of integrated circuits (IC). The silicon dioxide is the product of the following chemical reaction

$$\mathtt{Si} + \mathtt{O}_2 \rightarrow \mathtt{SiO}_2.$$

Silicon dioxide is thermally grown on the silicon wafer bulk to:

- electrically insulate basic devices like transistors and capacitors built on a single wafer
- act as gate oxide in Metal Oxide Semiconductor (MOS) structures or serve as a mask against dopant implantation.

Numerical simulation of the thermal oxidation process is aimed at predicting the oxide shape after oxidation in order to better assess the electrical performance of the device. Moreover, it is of relevant interest to analyze the stress history of the material in order to study its effect on the evolution of the oxidation process and to prevent mechanical failures. Realistic simulations of the process are achieved by taking into account different phenomena arising in a strongly heterogeneous assembling of materials. Fig.1 shows schematically the reduction from a 3D model to a 2D model of the local oxidation structure (LOCOS). The most widely adopted mathematical model of the oxidation process consists in solving two PDE systems, the first being a diffusion-reaction problem for the oxidant and the second a stress analysis in the oxide, nitride and silicon bulk. The two PDE systems are

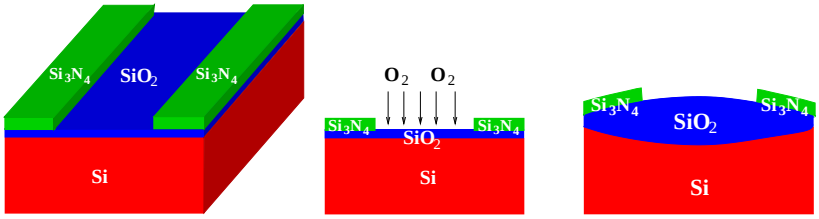

Fig. 1. Schematics of the thermal oxidation process in a local oxidation structure (LOCOS): 3D model (left), 2D reduction (center) at the beginning of the oxidation and 2D model (left) after process completion.

mutually dependent: the diffusion and kinetic reaction coefficients as well as the geometry of the deformed domain depend on the stress distribution; in turn, the chemical reaction forces the oxide-silicon interface to move, driving the mechanical problem. This first level of coupling is handled by using in the diffusion-reaction problem at the new time t^{n+1} the coefficients and the geometry computed from the stress field at time t^n. An incremental stress analysis is then performed on the structure subjected to the displacements due to the computed rate of silicon consumption and dioxide expansion (see Fig.2).

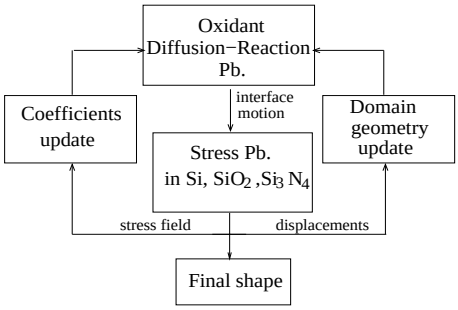

Fig. 2. Diagram flux for the full coupled problem.

This incremental stress analysis phase introduces a second nested level of coupling, since it requires solving a set of coupled mechanical problems, each one in a different material: the $\mathtt{Si_3N_4}$ mask and the $\mathtt{Si}$ bulk are indeed modeled as linear elastic materials, while a non-Newtonian incompressible fluid model with non-linear stress-dependent viscosity is used for the $\mathtt{SiO_2}$ [3]. Different strategies may be pursued to handle this second coupled problem. These will be object of discussion in Sect.3.1. The data exchanged between

the sub-blocks in both the coupled systems are fluxes and stress dependent quantities, so that the quality of their approximation clearly affects the accuracy of the overall computation. In a standard displacement finite element approach fluxes and stresses are typically post-processed quantities that suffer from a number of limitations. Examples of these limitations are the failure of the post-processed stresses at satisfying self-equilibrium and interelement traction reciprocity, the lack of continuity of the fluxes at the interelement interfaces and the possible onset of locking problems in the incompressible regime. The aim of this work is to investigate and demonstrate the use of alternative finite element formulations specifically tailored to overcome the above mentioned shortcomings. These formulations, known under the comprehensive name of mixed and hybrid finite element techniques and originally developed in the framework of structural analysis, approximate with the same accuracy and physical adherence both the primal fields (*e.g.* the displacements) and the dual fields (*e.g.* stresses and fluxes). A convenient implementation of the proposed methods, based on hybridization and static condensation, yields efficient numerical algorithms with computational effort comparable to standard displacement formulations.

The paper is organized as follows: in Sect.2 we discuss the finite element discretization of the diffusion-reaction problem and of the fluid-mechanical problem. Sect.3 deals with the decoupled algorithm used to iteratively solve the thermal oxidation problem, while Sect.4 demonstrates the performance of the numerical method on several benchmark test-cases. Finally, some concluding remarks are drawn in Sect.5.

2 Finite Element Discretization

In this section we discuss the finite element discretization of each subproblem in thermal oxidation.

2.1 Notation

In the following, we shall denote by Ω a bounded open set in $\mathbb{R}^2$ with Lipschitz continuous boundary $\Gamma = \Gamma_D \cup \Gamma_N \cup \Gamma_R$, where $\Gamma_D, \Gamma_N, \Gamma_R$ are the Dirichlet, Neumann and Robin portions of Γ, respectively, with $\Gamma_R = \emptyset$ in the fluid-mechanical problem. Let $\mathcal{T}_h$ be a regular partition $\mathcal{T}_h$ [2] of Ω into triangles K such that

$$\overline{\Omega} = \bigcup_{K \in \mathcal{T}_h} \overline{K}.$$

For each element $K \in \mathcal{T}_h$, we denote by ∂K the Lipschitz continuous boundary of K, by ∂K_{int} the portion of ∂K such that $\partial K \cap \Gamma = \emptyset$ and by n_K the unit outward normal vector along the boundary ∂K. Moreover, if v is any function defined in Ω, we denote by v^K its restriction to the element K and by $v_{\partial K}$ its restriction on the element boundary ∂K.

2.2 Diffusion-Reaction Problem

The diffusion-reaction problem is solved using the following primal-hybrid finite element nonconforming formulation:

find $C_h \in W^{NC}_{h,C^*}$ such that $\forall v_h \in W^{NC}_{h,0}$ we have

$$\sum_{K \in \mathcal{T}_h} \left(\int_K D \nabla C_h \cdot \nabla v_h \, dx + \int_{\partial K \cap \Gamma_R} D^{-1} k_s \, C_h \, v_h \, ds \right) = \int_K f \, v_h \, dx, \qquad (1)$$

where $W^{NC}_{h,g}$ is the set of affine functions that are:

- mid-point continuous on each edge of the triangulation
- equal to the average of g at the mid-point of each edge of Γ_D, for any function $g \in L^2(\Gamma_D)$.

In this formulation the primal variable C_h (approximate oxidant concentration) is sought to be a-priori discontinuous and the normal flux of the variable itself arises as a Lagrangian multiplier to enforce interelement continuity. The relaxation of interelement continuity for C_h has the advantage of providing an approximation p_h of the flux $p = -D\nabla C$ that satisfies element-by-element the self-equilibrium condition and that has continuous normal components across interelement edges between neighboring triangles. As a consequence, the normal component of the velocity of the interface is *directly* computed from the normal flux of the concentration as $V_n = -p_h \cdot n / C_h$, where n is the outward unit normal vector on the oxide-silicon interface (see [4] for the physical-mathematical derivation of the above relation). Notice that no post-processing on the computed approximate concentration field C_h is needed, unlike in standard displacement-based finite element methods. Moreover, optimal second order convergence in $L^2(\Omega)$ can be proved for C_h (see [6]).

2.3 Fluid-mechanical problem

For the solution of the fluid-mechanical problem, we adopt the novel dual mixed-hybrid finite element formulation introduced and analyzed in [1]. This method provides an accurate stress representation and at the same time handles under a unified formulation both the compressible and incompressible regimes by introducing a pressure function. This avoids resorting to the quasi-incompressible approximation, which is a common approach to deal with incompressible materials in this application field, or using separate computer codes, with a significant saving of software maintenance. The discrete formulation of the problem reads:

find $(\sigma_h, u_h, \lambda_h, p_h, \omega_h) \in (\Sigma_{h,g_N} \times U_h \times \Lambda_{h,g_D} \times Q_h \times W_h)$ such that

$$\begin{cases} \dfrac{1}{2\widehat{\mu}} \displaystyle\int_\Omega \sigma_h : \tau_h \, dx, + \sum_{K \in \mathcal{T}_h} \left(\int_K u_h \cdot \operatorname{div} \tau_h \, dx - \int_{\partial K_{int}} \lambda_h \cdot (\tau_h \, n) \, ds \right) \\ + \displaystyle\int_\Omega \frac{\rho_{\widehat{\lambda}}}{2} p_h \operatorname{tr} \tau_h \, dx + \int_\Omega \omega_h \operatorname{as} \tau_h \, dx = \sum_{K \in \mathcal{T}_h} \int_{\partial K \cap \Gamma_D} g_D \cdot (\tau_h \, n) \, ds \quad \forall \tau_h \in \Sigma_{h,0}, \\ \displaystyle\sum_{K \in \mathcal{T}_h} \int_K v_h \cdot \operatorname{div} \sigma_h \, dx = - \int_\Omega f \cdot v_h \qquad \forall v_h \in U_h, \\ \displaystyle\int_\Omega \rho_{\widehat{\lambda}} \left(\frac{1}{2} \operatorname{tr} \sigma_h + p_h \right) q_h \, dx = 0 \qquad \forall q_h \in Q_h, \\ \displaystyle\int_\Omega \theta_h \operatorname{as} \sigma_h \, dx = 0 \qquad \forall \theta_h \in W_h, \\ \displaystyle - \sum_{K \in \mathcal{T}_h} \int_{\partial K_{int}} \mu_h \cdot (\sigma_h n) \, ds = \sum_{K \in \mathcal{T}_h} \int_{\partial K \cap \Gamma_N} g_N \cdot \mu_h \qquad \forall \mu_h \in \Lambda_{h,0}, \end{cases} \tag{2}$$

where $\rho_{\widehat{\lambda}} = \dfrac{\widehat{\lambda}}{\widehat{\mu}(\widehat{\lambda} + \widehat{\mu})}$, $\widehat{\lambda}$ and $\widehat{\mu}$ being the Lamè coefficients of the material. Notice that for $\widehat{\lambda} = +\infty$ system (2) becomes the discrete approximation of the Stokes problem for incompressible fluids. As for the finite element spaces, for $k \geq 0$, we denote by $\mathbb{P}_k(K)$ the space of polynomials in two variables of total degree at most k on the element K and by $R_k(\partial K)$ the space of polynomials of total degree at most k on each edge of K. Notice that functions belonging to $R_k(\partial K)$ need not be continuous at the vertices of ∂K. Furthermore, we denote by $\mathbb{RT}_0(K)$ the lowest order Raviart-Thomas finite element space [5] on K and by $\mathcal{B}_K = \operatorname{curl}(b_K)$, where b_K is the cubic bubble function on K. The finite element spaces in (2) are defined as follows:

$$\begin{aligned} &\Sigma_{h,\xi} = \left\{ \tau^K \in (\mathbb{RT}_0(K) \oplus \mathcal{B}_K)^2, \, \tau^K n = \mathcal{P}\xi \text{ on } \Gamma_N \right\}, \; V_h = \left\{ v^K \in (\mathbb{P}_0(K))^2 \right\}, \\ &W_h = \left\{ \theta \in C^0(\overline{\Omega}) \mid \theta^K \in \mathbb{P}_1(K) \right\}, \qquad\qquad Q_h = \left\{ q^K \in \mathbb{P}_0(K) \right\}, \\ &\Lambda_{h,\eta} = \left\{ \lambda^K \in (R_0(\partial K))^2, \, \lambda = \mathcal{P}\eta \text{ on } \Gamma_D \right\}, \qquad\qquad \forall K \in \mathcal{T}_h, \end{aligned} \tag{3}$$

where $\mathcal{P}$ is the L^2 projection over the space of piecewise constant functions and ξ, η are given functions in $(L^2(\Gamma_N))^2$ and $(L^2(\Gamma_D))^2$, respectively. Notice that two kinds of Lagrangian multipliers have been introduced in formulation (2). The variable ω_h is a rotational parameter that avoids requesting the stress tensor to be sought *a priori* in a symmetric function space. The hybrid variable λ_h is instead the Lagrangian multiplier that enforces back the continuity of the normal component of the stress tensor across the interelement interfaces. The abstract analysis of the above formulation has been carried

out in [1], where in particular a superconvergence result has been shown for λ_h, as typical of mixed methods with hybridization.

3 Iterative algorithm for the coupled problem

The numerical solution of the full coupled problem is achieved by a sequence of successive steps. The computer code implements the following *staggered algorithm*:

For $n \geq 0$, given at the time level t^n the solution, the geometry and the diffusion and reaction coefficients, at the new time level t^{n+1} we have to:

1. solve the diffusion-reaction problem and compute the propagation velocity of the SiO_2-Si interface;
2. perform a mechanical stress-analysis in SiO_2, Si_3N_4 and Si domains;
3. determine the new geometry of the Si and SiO_2 and the maximum allowed time step Δt according to the present (deformed) configuration;
4. set $t^n = t^{n+1}$, $t^{n+1} = t^{n+1} + \Delta t$. Update the stress-dependent D and k_s coefficients;
5. update the nodal grid point configuration by relaxing the deformed mesh;
6. if $t^{n+1} < t^{max}$ goto 1, else end simulation.

This decoupled procedure has the advantage of splitting the solution of the full problem into several self-contained subproblems of smaller size. Particular attention must be paid to the solution of the stress problem at point 2. of the algorithm, topic that is addressed in the next section.

3.1 Fluid-mechanical coupled sub-problem

The stress analysis problem is a fluid-structure interaction problem. In its basic implementation, the Stokes problem in the SiO_2 domain is solved first and the computed normal stresses are used to load the elastic problem in the Si and Si_3N_4 domains. Eventually, no response from these latter materials is fed back to the SiO_2 domain. This strategy, usually referred to as Boundary Loading Method (BLM), is economical and widely adopted in the literature. However, real-life elastic materials do possess memory and as a consequence they tend to "squeeze out" the fluid while relaxing to their initial configuration. Accounting for this behavior by simply loading back the SiO_2 domain with the deformations computed from the Si and Si_3N_4 domains invariably leads to severe instabilities in the overall numerical procedure, as can be explained by the following argument. Assume that the fluid-mechanical system is modeled by a spring (elastic behavior) placed in series to a damper (fluid behavior). An elementary analysis reveals that solving iteratively the motion of the spring-damper system by a decoupled procedure leads to a conflicting request on the time step Δt: indeed, in order to ensure stability of the procedure, Δt should be small enough when the displacement of the spring is computed from the velocity imposed by the damper, while Δt should be large

enough when the velocity of the damper is computed from the displacement imposed by the spring. Based on the above considerations, we have adopted the following approach:

1. The interaction between the $\mathtt{Si}$ domain and the $\mathtt{SiO_2}$ -$\mathtt{Si_3N_4}$ domains is handled by the standard BLM, since it can be checked that the deformations produced by the $\mathtt{Si}$ domain on the $\mathtt{SiO_2}$ are negligible.
2. The interaction between the $\mathtt{SiO_2}$ and the $\mathtt{Si_3N_4}$ domains is handled by a coupled procedure, with an inner iterative map to solve for the nonlinear dependence of the oxide viscosity on the normal stresses. Notice that this coupling procedure is easily implemented due to the use of the unified compressible/incompressible formulation discussed in Sect.2, the only difference being in the numerical values of the Lamè parameters in the two subdomains.

4 Numerical results

As a first test case, we show the results for a simple fluid-elastic structure solved with the unified coupled procedure illustrated in the previous section. The domain Ω is the unit square, with the upper half behaving like a fluid, while the lower half behaving like an elastic solid (with a very low Young modulus). For a certain time interval a compressive load is applied on the top edge of the fluid domain. Then, the load is released and the elastic solid relaxes recovering its original shape and squeezing out the fluid, as shown in Fig.3 where some phases of the evolution of the phenomenon are displayed. The second benchmark problem that we have considered is the

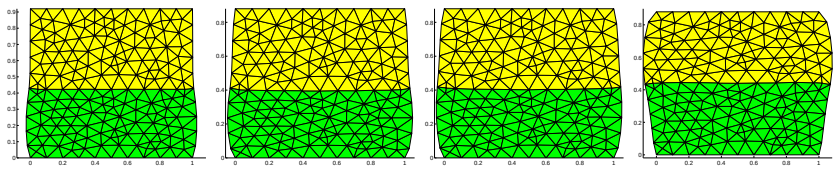

Fig. 3. Evolution of the coupled fluid-elastic solid system.

complete simulation of the thermal oxidation process in a LOCOS structure. The computational domain is one half of the domain shown in Fig.1. The geometry and the material properties have been chosen as in [4]. In Fig.4 the deformed configuration and the corresponding pressure field are shown at different time levels. The typical "bird's beak" shape of the final oxide configuration is clearly recognizable. Notice also how the largest stress arise on the junction line between the $\mathtt{SiO_2}$ and the $\mathtt{Si_3N_4}$ regions and in particular near the lateral edge of the $\mathtt{Si_3N_4}$ band.

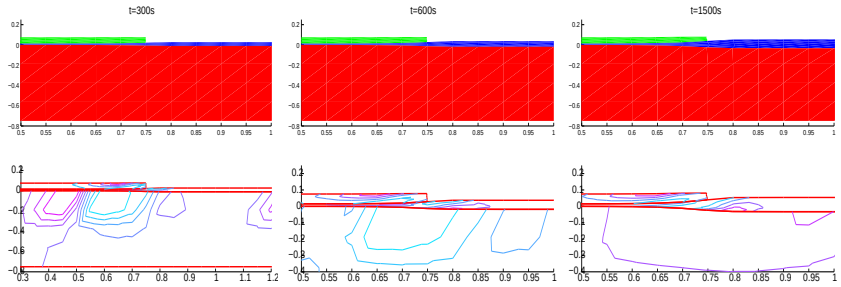

Fig. 4. Deformed configuration (top, zoom of the area) and pressure field (bottom) for $t = 300, 600, 1500$s.

5 Conclusions

Thermal oxidation in silicon device technology is a complex coupled phenomen, involving the solution of a diffusion-reaction problem and of a fluid-structure interaction problem. Special attention has been devoted in the present work to devising suitable iterative procedures for handling nonlinearities and strong coupling between the sub-problems to be solved. In particular, we have proposed a unified dual-mixed hybrid formulation that allows for the simultaneous solution of the compressible/incompressible Navier equations in both solid and fluid domains. Numerical results on benchmark test problems show the accuracy and the flexibility of the approach.

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