Three-Dimensional Simulation of Thermal Oxidation and the Influence of Stress

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In our oxidation model [1] we use a normalized silicon concentration $\eta(\mathbf{x},t)$ so that the value of η is 1 in pure silicon (Si) and 0 in pure silicon dioxide (SiO_2). Advantageously our model takes into account that the diffusion of oxidants, the chemical reaction and the volume increase occur simultaneously in a so-called reaction layer. In contrast to the sharp interface between Si and SiO_2 like in the standard model [2], this reaction layer has a spatial finite width (see Fig. 1) where the value of η lies between 0 and 1. Also thin film oxidation [3] as well as the coupling to the diffusion of dopants is properly treated by our model.

During the oxidation process the chemical reaction consumes Si and the newly formed SiO_2 has more than twice the volume of the original Si. This significant volume increase is the main source of stress and strain in the materials. The oxidation process is described by a coupled system of partial differential equations, one for the oxidant diffusion, the second for the conversion of Si into SiO_2, and a third for the mechanical problem. For the mechanics an elastic or a viscoelastic model [4] can be applied. The whole numerical formulation is solved by applying the finite element method.

As representative example a $(1.2 \times 0.3 \times 0.4)$ µm Si block with a 0.2 µm thick silicon nitride (Si_3Ni_4) mask is oxidized. The result of this oxidation process after a time t_1 is shown in Fig. 1. For a more physical interpretation with a sharp interface between Si and SiO_2 the two regions can be extracted from the η-distribution by determining that $\eta \leq 0.5$ is SiO_2 and $\eta > 0.5$ is Si as shown in Fig. 2.

Since the oxidant diffusion and the chemical reaction are exponentially reduced with the pressure in the material, the oxidation process itself is highly stress dependent. As shown in Fig. 4 the highest pressure in SiO_2 is under the edge of the Si_3Ni_4 mask, because in this area the stiffness of the mask prevents the desired volume expansion of the newly formed SiO_2. Due to the mentioned stress dependence the oxidation process in these areas is considerably reduced.

If the stress dependence is not included in the simulation of the oxidation process, the simulation results will not agree with the real physic behavior, because the oxidant diffusion and the chemical reaction also occur under the Si_3Ni_4 mask without restriction. Because of this phenomenon the SiO_2 region at the same oxidation conditions is much more expanded than with the stress dependence as shown in Fig. 3. In addition, the larger forces under the Si_3Ni_4 mask cause larger displacements of this mask.

References

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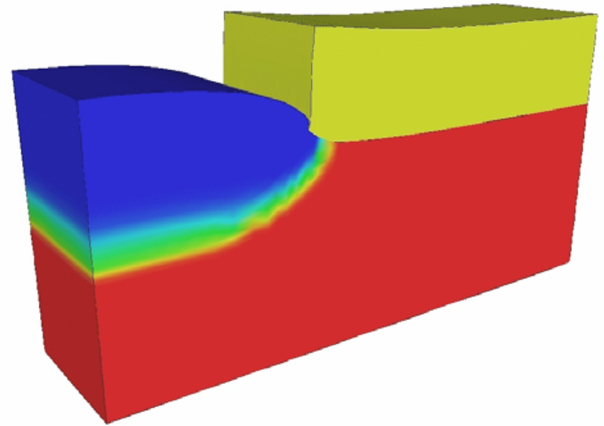

Figure 1: η-distribution and reaction layer with stress dependent oxidation at time t_1.

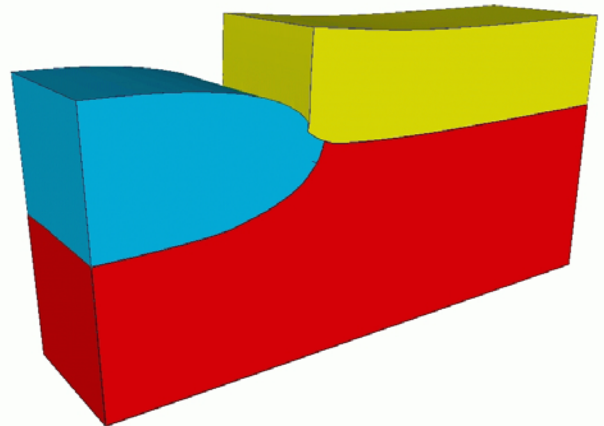

Figure 2: SiO_2 region (sharp interface) with stress dependent oxidation at time t_1.

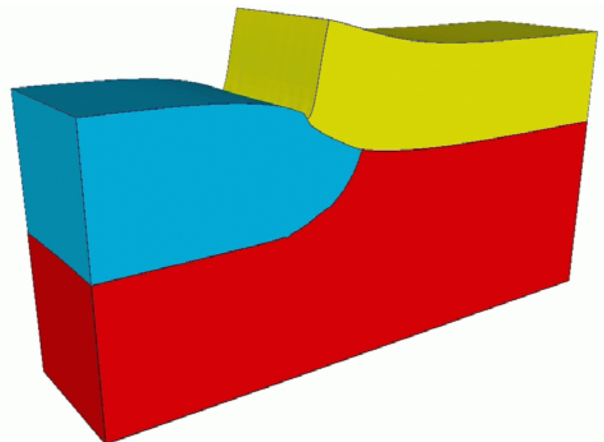

Figure 3: SiO_2 region (sharp interface) without stress dependent oxidation at time t_1.

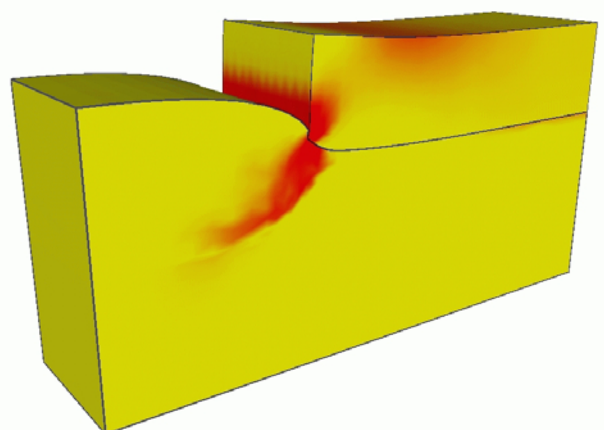

Figure 4: Pressure distribution with stress dependent oxidation at time t_1.