Modeling corner oxidation

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ABSTRACT

This paper will present some of the numerical and algorithmic details of SiO_2 modeling in SUPREM-IV. Grid manipulation in both the SiO_2 and the substrate is described, and the material modeling of the SiO_2 is discussed. A trench sidewall oxidation example is presented. Cusps are found to form at the trench corners even in the absence of stress-retarded growth coefficients.

Moving grid programming is a difficult and messy job; this part of the program has gone through three complete rewrites, and the present version of the code has an expected lifetime of about six months.

Two questions arise when the Si-SiO_2 interface moves: what happens to silicon nodes as the interface approaches them, and what happens to SiO_2 nodes as their volume expands? Almost all two-dimensional process modeling codes have the same answer to the first question: silicon nodes retreat into the substrate. This was the first approach taken in but it was soon recognized that as the grid retreated into the substrate, it was difficult to prevent dopants and defects from being carried along. To avoid this form of unphysical numerical diffusion, all subsequent work in SUPREM-IV has maintained a fixed grid in the substrate. The moving boundary is now handled on the silicon side by stripping out silicon interior nodes when the moving interface threatens to overtake them. Figure 1 illustrates a pad oxidation at two subsequent time steps. It should be apparent how nodes under the moving boundary are removed, while bulk nodes are unchanged.

The second question is not addressed by most other codes, since they neglect the oxide bulk. The exceptions are oxidation-only simulators[1,2], which completely regenerate the grid at each time step. That approach is presumably ideal, provided a good enough grid generator is available, and it may even be required in some cases. However we have chosen a cheaper scheme, which involves only minor updates to the grid at each time step. The basis of the algorithm is to examine the layer of SiO_2 triangles just behind the moving interface. When that layer becomes overstretched, a new layer is inserted a very short distance behind the interface. Subsequent SiO_2 growth then lifts this layer away from the interface. The principal attractions of this scheme are that it is simple, computationally cheap, grid points flow exactly as does the physical SiO_2, and because successive grids are so closely related, no interpolation is needed. Figure 2 illustrates the process. In the time between the two grid snapshots, a new layer has been inserted behind the moving interface.

The thin sidewall oxide was analyzed by modeling oxidation as a three-step process: oxidant diffusion, interface reaction, and elastic deformation. The first two steps were proposed by Deal and Grove[3]. The last step is required to predict the shape of two-dimensional oxides. Viscous flow of oxide has been proposed for wet oxides grown at high temperatures[2]. The elastic model is better suited to low temperature or dry oxidation, as it is known that there is considerable stress in oxides grown under these conditions[4]. Experiments are under way to determine when to apply these and other oxide models.

An important consideration in designing processes for trench capacitors is the integrity and uniformity of the oxide grown on the sidewall. It is known[5] that oxides on shaped sidewalls can be quite nonuniform, with significantly reduced oxide thickness at both convex and concave corners. This reduction has been attributed to stress-retarded growth coefficients. The elastic simulation shows that part of the reduction is also purely geometrical. A SiO_2 cusp was found to form using stress-independent coefficients. Figure 3 shows the evolution of the cusp grown on a trench with 80° sidewalls. The flat oxide is 0.1μ thick and grown at 950°C for 240 minutes.

References

1. A. Poncet, "Finite Element Simulation of Local Oxidation of Silicon," *Summer Course on VLSI process and Device Modeling*, Heverlee, Belgium, June 7-10, 1983.
2. D. Chin, "Two-Dimensional Oxidation," PhD dissertation, Department of Electrical Engineering, Stanford University, June 1983.
3. B.E. Deal and A.S. Grove, "General Relationship for the Thermal Oxidation of Silicon," *J. Appl. Phys.*, vol. 36(12), pp. 3370-3378, 1965.
4. E.A. Taft, "The Optical Constants of Silicon and Dry Oxygen Oxides of Silicon at 5461A," *J. Electrochem. Soc.*, vol. 125, p. 968, 1978.
5. R.B. Marcus and T.T. Cheng, "The Oxidation of Shaped Silicon Surfaces," *J. Electrochm. Soc.*, vol. 129(6), 1982.

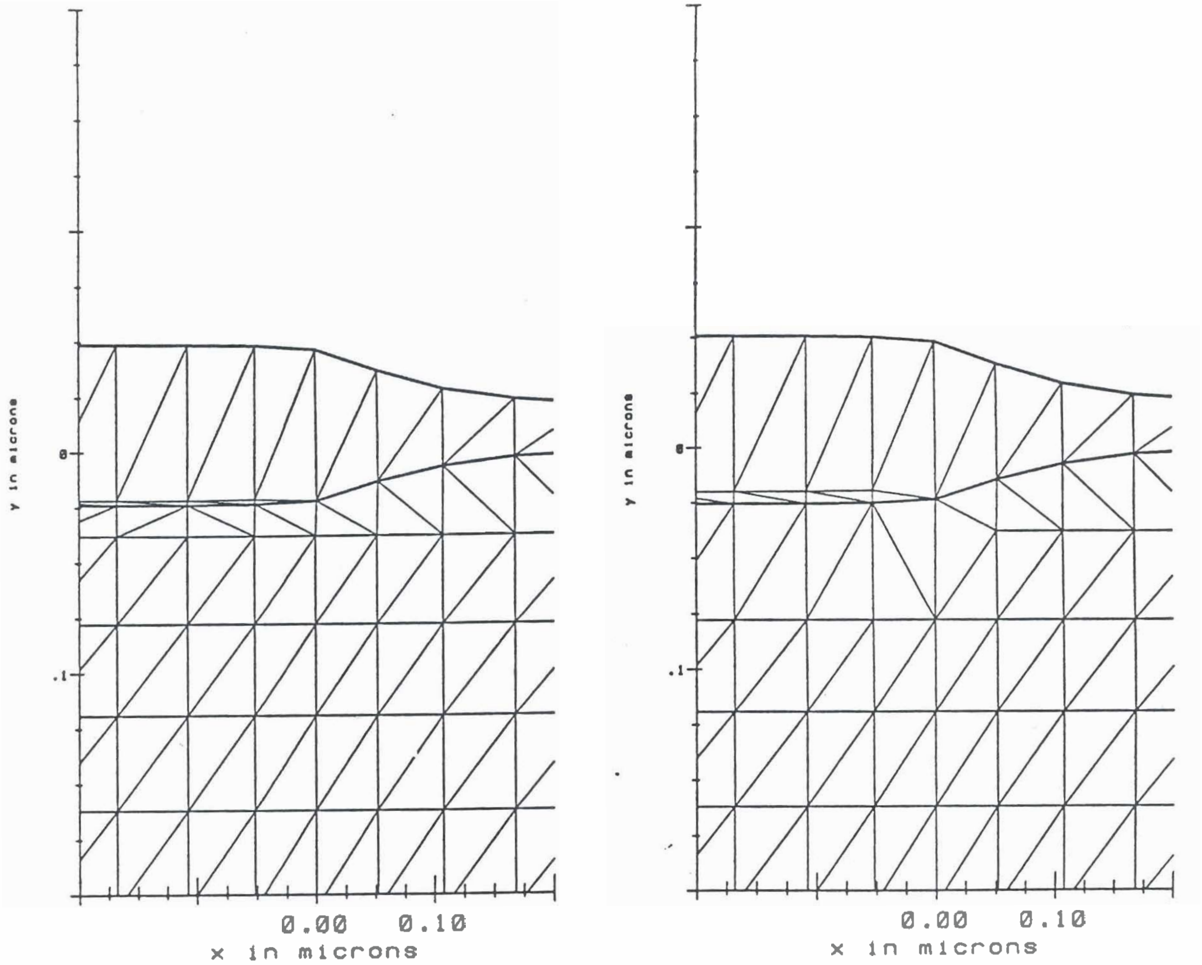

Figure 1. Silicon grid removal during oxidation

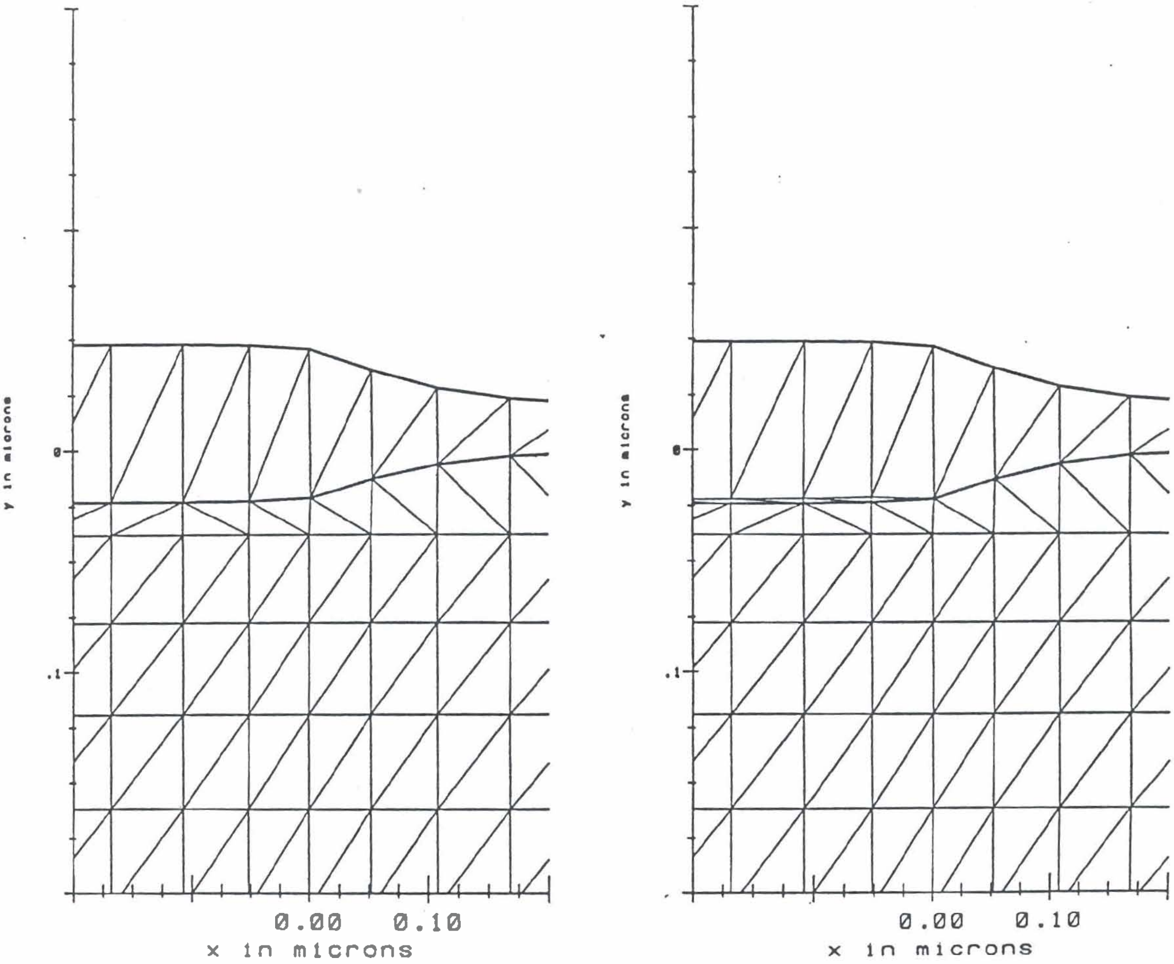

Figure 2. Oxide grid addition during oxidation

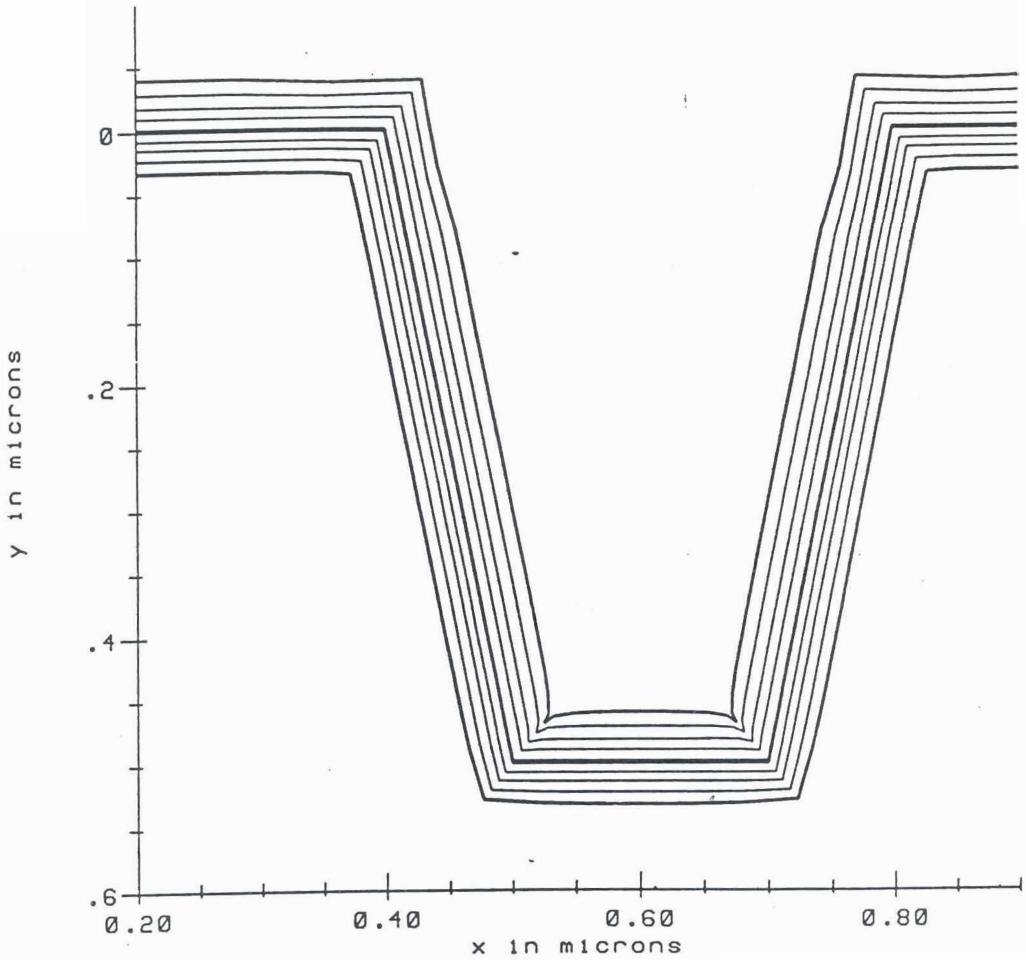

Figure 3. Development of oxide cusp at trench corner (dry 240'' @ 950$_{eC}$)