SIMULATION OF SEMICONDUCTOR DEVICES AND PROCESSES Vol. 6
Edited by H. Ryssel, P. Pichler - September 1995

Multidimensional Nonlinear Viscoelastic Oxidation Modeling

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Abstract

This paper describes the oxidation module for the process simulator FLOOPS. Simulation results for silicon oxidation in two and three dimensions are demonstrated.

Introduction

The accurate simulation of LOCOS and advanced LOCOS processes for submicron processes is very important. As device dimensions have decreased, the need for three dimensional simulation has become critical. Since FLOOPS is an object oriented simulator, it is easy to include and test different models. We have used two dimensional models to choose the most accurate and efficient methods. Some of these models have been implemented and tested in three dimensions.

Two Dimensional Models

The most advanced two dimensional model is a stress dependent nonlinear viscoelastic model with velocity as the unknown. It is similar to those proposed by Peng[1] and Senez[2]. Element rotation effects are taken into account in the residual stresses as they are updated at each time step. The stress dependencies on oxidant diffusion and reaction rates are from Kao[3] and Sutardja[4]. Eyring plasticity is used to model nonlinear viscosity[4] for oxide, nitride and polysilicon. The simulator uses both velocity pressure and velocity

formulations. The velocity pressure technique results in smoother stress contours and better nonlinear convergence when oxide is modeled as incompressible as Peng[1] did. Senez[2] does not enforce incompressibility and gets good results. Due to the fact that this greatly eases the nonlinear convergence while giving accurate results, this is currently the recommended oxidation model in FLOOPS.

The nonlinear iterations are solved with the numerical relaxation technique[5,6]. Including the elastic effect is beneficial for this technique, in fact trying to use this on a viscous incompressible problem is extremely time consuming. Grid quality is critical for this nonlinear iteration scheme, the most important points are to avoid high aspect ratio and unevenly sized triangles. The grid in FLOOPS is not remeshed between time steps as done by Collard[6] and Senez[2]. Grid quality is maintained by splitting edges in the middle when new grid needs to be added. This helps prevent high aspect ratio triangles from forming. A second technique for helping convergence is to make each oxide grid points' position the average of it's neighbors. In brief tests this technique has greatly improved performance without loss of accuracy. For example the nonlinear stress dependent viscoelastic simulation shown in figure 1a without grid averaging took 14% more CPU time than the simulation shown in figure 1b which was run with grid averaging. When the plots of the simulations are overlaid there is no difference between the simulations with and without grid averaging. This is surprising because by changing the position of the nodes some error in the stress terms should be introduced. This error is probably no worse that interpolation error introduced by regriding and not taking into account rotation of the stresses as done by Senez[2].

Three Dimensional Models

As device dimensions decrease, modeling of LOCOS and modified LOCOS processes will have to be performed in three dimensions. The reasons for this is that three dimensional effects dominate at small dimensions. There are several numerical problems associated with three dimensional simulation of oxidation. The main problem is associated with handling the grid. At the present time linear hexahedra are supported for linear viscous and nonlinear viscoelastic simulations. This is accomplished by using velocity relaxation in the silicon and oxide to retain the grid quality and prevent nodes overrunning one another while moving the boundaries. This has allowed us to begin to investigate three dimensional LOCOS structures while a tetrahedral based moving boundary code is developed. Figure 2 shows linear viscous simulations of two LOCOS examples. The

simulations are of 4um by 2um and 4um by 1um nitride lines. The oxidant contours encroach further under the narrower nitride. This causes an increased birds beak length.

Nonlinear viscoelastic simulations have been run using velocity relaxation in the oxide until the grid becomes distorted and or not fine enough. Velocity relaxation introduces some error into the residual stresses but when three dimensional cross sections of longer lines are compared to two dimensional simulations the differences are minor. Figures 3 a & b show a 1000° C LOCOS simulation after stripping the nitride. The nitride line was 0.6um by 2um and 1000 A thick. The final field oxide thickness is ~3500A. The birds beak length parallel to the narrow edge of the nitride is ~0.35um and along the longer edge is ~0.2um. Figure 3a demonstrates that the oxidant concentration encroaches further around the corner causing more growth under the tip of the line. Figure 3b shows the pressure contours. The higher tensile regions (white) are further under the tip indicating the increased growth and lifting of the nitride.

Conclusion

A stress dependent nonlinear viscoelastic oxidation simulator has been described. The program can simulate both two and three dimensional isolation structures.

References

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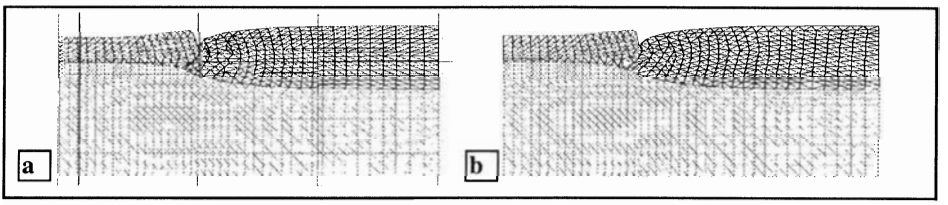

Figure 1. Comparison of 1100 C 40 min LOCOS simulation results a: without and b: with grid averaging between time steps.

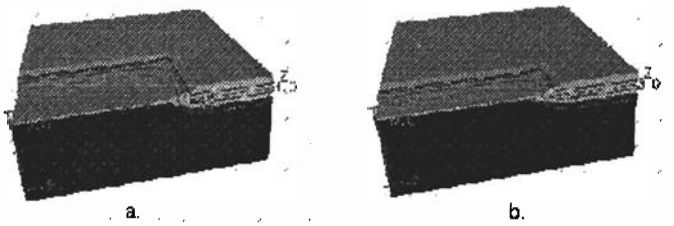

Figure 2. Linear viscous simulations of a: 4umx2.0um nitride line and b: 4umx1.0um nitride line. Oxidant contour lines are from $2.5*10^{19}$ (dark) to $5*10^{18}$ (light) cm^{-3}.

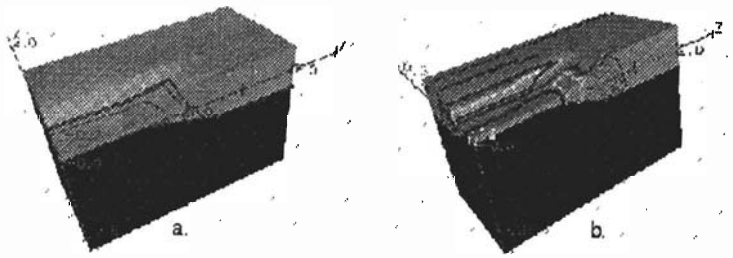

Figure 3. Nonlinear stress dependent LOCOS simulations: a: Oxidant contours (contours as above) b: Pressure contour lines from $-1*10^{10}$ (white) to $-1*10^{9}$ (black) dynes/cm^2.