Modeling Stress Effects in Thermal Oxidation with the Boundary Element Method.

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In thermal oxidation of silicon, stress can play a crucial role in nonlinear system dynamics. The boundary element method is a simple technique for linear boundary value problems, especially with moving boundaries. This paper describes an adaptation of the boundary element method to include effects of stress on oxidation.

Given its reduced dimensionality, the boundary element method (BEM) is an attractive analysis tool for potential, elasticity and other linear boundary value problems. It can also be enhanced to handle nonlinear problems at some expense to efficiency and simplicity.

Subregion and internal cell are the two common procedures for dealing with nonuniformity in the domain. The former divides the domain into piecewise homogenous partitions; the latter treats the system as a single homogeneous entity and introduces domain solutions to account for the nonlinear effects. The internal cell approach is used for modeling nonlinear oxidant diffusion because it is a simple extension to our existing formulation. In steady-state diffusion, the divergence of flux ($F = -D\nabla C$) is zero:

$$\nabla \cdot \vec{F} = 0.$$

This expression can be rewritten as a Poisson equation:

$$\nabla^2 C = -\frac{1}{D}\nabla D \cdot \nabla C,$$

where the right hand side is conceptually a pseudo domain-source. As a perturbation term, internal cells are optional; their density and placement depends on the desired degree of accuracy in the solution. The creation of cells is straight forward and not too many of them are needed. We have thus achieve a good compromise between the simple mesh setup of the BEM and the need to model nonuniform domain behavior.

To model viscoplastic flow of oxide is a more difficult task. We have previously developed a generalized viscoelastic BEM that handles an extremely wide range of stress relaxation times [1]. To approximate nonlinear viscoplastic flow, we artificially change the time-relaxation behavior of stress at the boundary only. This approximation is supported by the following observations: (a) For a simple LOCOS structure, the oxide shapes obtained with elastic and slow viscous flow models are almost identical, although the stress distributions are different. Stress and strain behave almost like two seperate entities. (b) Plastic yield originates at the boundary and propagtes inwards.

Given that the force conservation law is independent of the material behavior, stress within the bulk should always assumes a smooth distribution and is dominated by boundary activities. If need arises, the pseudo-force procedure with internal cells, as used in some viscoplastic methods, can also be employed.

The stress parameters used in our simulations are obtained from Kao's model[2] with some modifications. First observed by Rafferty [3], Kao's model contains a positive feedback path that renders solutions non-existent in some cases. The switch from viscous flow to viscoelastic flow removes the anomality as stress can only reach an asymptotic value. However the new model still suffers from a sudden "solidification" misbehavior, therefore the dependency of viscosity on shear stress, as proposed by Sutardja [4], is also incoporated.

References

1 T.-L. Tung, J. Connor, and D. A. Dimitri, "A Boundary Element Method for Modeling Viscoelastic Flow," *IEEE Trans. Elec. Dev.*, Feb., 1988.

2 D. B. Kao, J. P. McVittie, W. D. Nix, and K. C. Saraswat, "Two-Dimensional Thermal Oxidation of Silicon - II. Modeling Stress Effects in Wet Oxides," *IEEE Trans. Elec. Dev.*, vol. ED-35, p. 25, 1988.

3 C. Rafferty and R. W. Dutton, "Two Dimensional Oxidation," SRC Top. Res. Conf. on Advance MOS Process and Device Models, April, 1987 (Private Commnunication).

4 P. Sutardja, W. G. Oldham, and D. B. Kao, "Modeling of Stress-Effects in Silicon Oxidation Including the Non-linear Viscosity of Oxide," 1987 IEDM Tech. Dig., p 264.