Numerical Techniques on Enhancing Robustness for Stress-Dependent Oxidation Simulation Using Finite Element Method in SUPREM-IV

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One of the major problems in simulating stress-dependent oxidation is slow convergence behavior or nonconvergence because of high nonlinearities, especially in the first few time steps, even in a simple initial structure for LOCOS. In this paper we present useful strategies to get stable convergence in a fully stress-dependent finite element oxidation simulator like SUPREM-IV [1].

The strategies are

First, in the stress-dependent oxidation simulation, we have to solve the coupled nonlinear equations of incompressible oxide flow and oxidant diffusion. There are two standard ways to treat the incompressible flow problem [2]. One is the mixed formulation (unknown variables are velocity and pressure), and the other is the penalty function formulation (unknown variable is velocity only). SUPREM-IV (version 8912) uses the second approach. By using a penalty function method, pressure variable is eliminated from the system of equations which reduces the computational cost and eliminate the zero diagonal entries in the matrix. In the penalty function method, the pressure is calculated from

$$p = -\lambda \nabla \cdot \boldsymbol{v}$$

where λ is the bulk modulus and is taken to be much larger than the viscosity μ ($\lambda/\mu \sim 10^{7\sim9}$) to approximate the incompressibility of oxide. It is important to select a good integration method for the incompressible term in the equations to achieve stability. In the finite element formulation, element stiffness matrix for flow problem is expressed by [2]

$$\boldsymbol{k}_{ab} = \int_{\Omega^e} \boldsymbol{B}_a^T \boldsymbol{D} \boldsymbol{B}_b \, d\Omega = \int_{\Omega^e} \boldsymbol{B}_a^T \overline{\boldsymbol{D}} \boldsymbol{B}_b \, d\Omega + \int_{\Omega^e} \boldsymbol{B}_a^T \overline{\overline{\boldsymbol{D}}} \boldsymbol{B}_b \, d\Omega = \overline{\boldsymbol{k}}_{ab} + \overline{\overline{\boldsymbol{k}}}_{ab}.$$

For the plane strain state, the material property matrix $\boldsymbol{D}$ can be written as

$$\boldsymbol{D} = \begin{pmatrix} \lambda+2\mu & \lambda & 0 \\ \lambda & \lambda+2\mu & 0 \\ 0 & 0 & \mu \end{pmatrix} = \overline{\boldsymbol{D}} + \overline{\overline{\boldsymbol{D}}}$$

where $\overline{\boldsymbol{D}}$ is the μ-part of $\boldsymbol{D}$, and the remainder is the λ-part. Due to the fact that $\lambda/\mu \gg 1$ and $\overline{\overline{\boldsymbol{k}}}_{ab}$ is proportional to λ, the numerical values of terms in $\overline{\overline{\boldsymbol{k}}}_{ab}$ tend to be very large compared with those in $\overline{\boldsymbol{k}}_{ab}$. The $\overline{\overline{\boldsymbol{k}}}_{ab}$-term is the part of the stiffness that attempts to maintain the volumetrically stiff behavior. Because typical finite elements tend to lock (i.e., there are proportionally too many incompressibility-type conditions), special treatment of $\overline{\overline{\boldsymbol{k}}}_{ab}$ is required to alleviate this tendency. One simple solution is to reduce the order of numerical quadrature employed to evaluate the integration of incompressible term $\overline{\overline{\boldsymbol{k}}}_{ab}$ below that used for the μ-part. This method is the reduced integration method [2]. Fig. 1 shows the difference of the integration points between SUPREM-IV [3] and this work.

The second strategy uses averaging of the mid-side node velocities at the Si/SiO_2 interface. If the velocity at the mid-side node is forced to set the mean value of the neighboring corner-node velocities, the convergence becomes stabilized significantly. This approach also been used in a 2D oxidation simulator CREEP [4]. The reason of this behavior is not known yet, but it can be speculated that the coupling of the reduced integration method and the diffusion problem requires an additional constraint in the velocity calculations.

The final strategy is a different choice of the element node number for oxidant diffusion. We use the 3-node element for the diffusion problem and the 6-node element for the flow problem. As was mentioned above, if the averaged value at the mid-side node on the interface is used, the concentration value at the mid-side node is no longer required. A simple way to treat this is to impose a constraint that forces a

linear change of concentration along the edges on the interface. But, this treatment alone is not sufficient for stability. We guess this is strongly related to the requirement of the velocity average procedure at the interface. Fig. 2 shows the difference between the finite element node used by SUPREM-IV [3] and by this work.

By using the above strategies, most of the cases tested achieve convergence over a wide range of initial structures and stress-dependent parameters. In some cases, however, poor convergence behavior is still observed during the oxidation. In these cases, the shape of the triangles appear to be quite distorted, because SUPREM-IV does not try to regrid during the oxidation. This issue remains to be studied.

Summary

In summary, major improvements in achieving stable convergence are realized by introducing the reduced integration formulation and an averaging procedure for the mid-side node velocities at the Si/SiO_2 interface. The 3-node element is introduced to discretize the oxidation diffusion equation as a remedy in reducing the instabilities that occur for stress dependent oxidation. These strategies are generally applicable for an oxidation simulator using the finite element method.

Acknowledgements

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References

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Figures

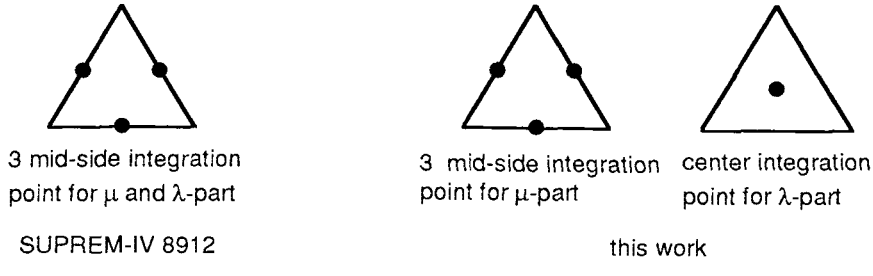

Fig. 1 Difference of integration point between SUPREM-VI 8912 and this work.

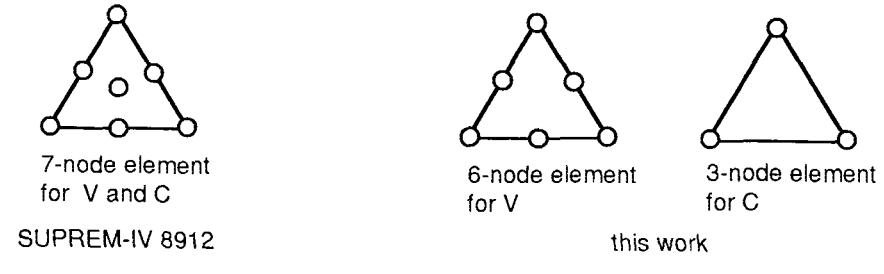

Fig. 2 Difference between finite element node used by SUPREM-VI 8912 and by this work based on CREEP[4].