Numerical Modeling of Oxidation Coupled with Stress Effects

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Abstract

A numerical modeling of oxidation coupled with stress effects is described. This report deals with the solution method based on a finite difference approach using the coordinate transformation method and a relaxation technique for the inclusion of the stress effects. The model is applied to simulations of oxidation in both the LOCOS and trench structures.

PHYSICAL MODEL

The physical model of oxidation is based on a steady-state oxidant diffusion and a slow incompressible viscous flow of oxide [1]. The oxide growth in the nonplanar structure depends on the oxidation-induced stress and it is numerically modeled by three stress-dependent physical parameters of the surface reaction rate k, effective oxidant diffusivity D_{eff}, and viscosity μ [2].

SOLUTION METHOD

An efficient numerical apporach has been already developed for the 3-D nonplanar oxidation modeling and it has successfully applied for the analysis of LOCOS structure without considering the stress effect [3]. It is based on the finite difference approach using the coordinate transformation method in nonplanar structures. To realize numerical modeling of oxidation coupled with the stress effects, the following numerical handlings are investigated and applied [4].

(1) To obtain the self-consistent solution of oxidation kinetics equations with the stress effect, a relaxation technique is applied to the oxidant and velocity/pressure calculation procedure. This is because the stress-dependent parameters are greatly changed by the local stress, especially at the initial oxide growth. Fig.1 shows a flow chart of this calculation procedure. The normal stress σ_{nn} and pressure P are relaxed using a relaxation factor ω_s and ω_p, respectively. As a result, this method allows the simulations of the large stress effects.

(2) For acculate estimation of the local stress values, this work clarifies the role of the boundary condition at the free oxide surface. The following boundary condition with the normal stress balance is applied to the hydrodynamic equation with zero divergence,

$$P = P_a - \frac{\gamma}{R} + 2\mu \frac{\partial v_n}{\partial n} \qquad (1)$$

where P, P_a, γ, R, and v_n are the pressure in oxide, the ambient pressure, surface tension, local curvature and normal component of velocity. It is different from the original model with pressure balance used by Chin et al. [1]. Fig.2 shows that the normal stress balance is more adequate model of the boundary condition than the pressure balance.

APPLICATIONS

Fig.3 shows a simulation result of LOCOS with thick nitride film (0.18μm). In Fig.3, a large compressive stress induced by the thick nitride film bending reduces the oxide growth rate at the Si/SiO_2 interface in the bird's beak region. Fig.4 shows a simulation result of oxide shapes in trench structure. The result shows the difference of the oxide growth behavior between at the concave and convex corners. The retardation of oxide growth is much enhanced at the concave corner than at the convex corner in the case of the trench stucture with sloped sidewalls (50°).

CONCLUSION

Oxidation kinetics equations including the stress-dependent physical parameters have been successfully solved by the finite difference approach with the coordinate transformation method. The relaxation method has been introduced to include the stress effect. It has been found that this method allows the accurate evaluation of the local stress and the retardation of oxide growth in the LOCOS and trench structures.

REFERENCES

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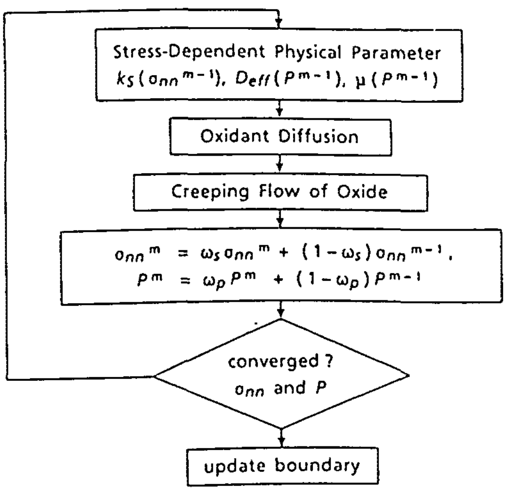

Fig.1. Flow chart of the relaxation technique for solving oxidation kinetic equations coupled with stress effects.

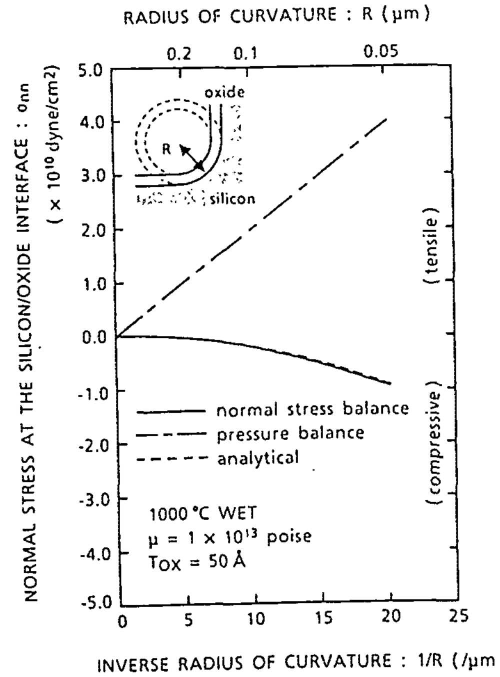

Fig.2. The comparison of the normal stress value with boundary conditions in a concave corner of trench.

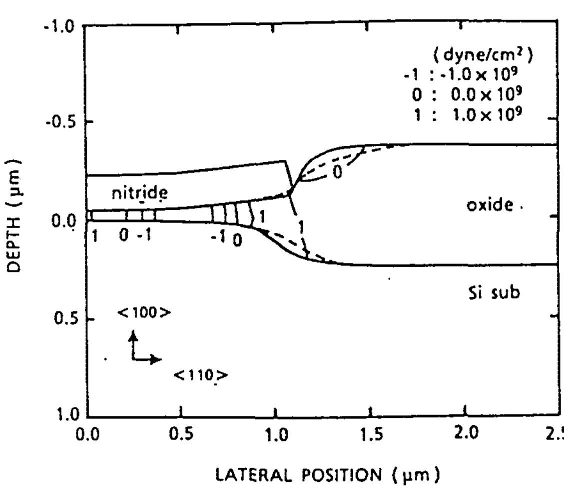

Fig.3. Cross-sectional oxide shapes of LOCOS obtained by simulations with stress effects. Broken lines show the oxide shape obtained from the experimental data.

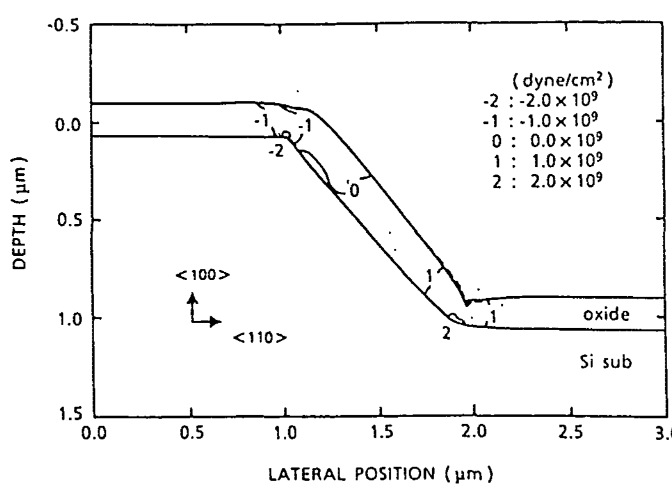

Fig.4. Cross-sectional oxide shapes of trench structure obtained by simulations with stress effects. Broken lines show the oxide shape obtained from the experimental data.