Verification of the Viscoelastic Oxidation Model Using Simple Test Structures

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1. Introduction

There have been several publications on the numerical solution of viscoelastic oxidation. However, most of the results were examined only from the aspect of oxide shape; there was little discussion of calculated stress and retardation of oxidation due to compressive stress.

In this work, oxidation of a flat plate substrate and a cylindrical substrate was simulated, because experimental data are available for these simple structures. We can use the data as a model reference. After the verification of the basic properties, we will apply the 2D-oxidation simulator to practical device structures.

2. Physical model and solution method

We developed a standard 2D-oxidation simulator based on the viscoelastic oxidation model. In this program, the oxide was treated as elastic solid for compression and Maxwell body for shear. A step-by-step solution was used to obtain the viscoelastic stress[1].

Oxidant concentration was obtained by solving the two-dimensional diffusion equation in a steady state. Stress effects on the surface reaction constant and the oxidant diffusivity were incorporated in some calculations. Self-consistent solutions were obtained by the numerical relaxation technique[2].

It is not known at present how to assign the oxidation strain. In this work, two different assignments were assumed; uniaxial strain normal to the interface and dilational strain[3].

3. Results for test structures

(1) Flat plate

EerNisse measured the stresses that develop in planar oxidation[4]. Because his measurement was performed at oxidation temperature, the result does not contain the stress induced by thermal mismatch.

Fig.1 shows the calculated stress in a SiO_2 film during flat plate oxidation. Dilational oxidation strain was assumed. The average stress over the film is plotted in Fig.(2) as a function of oxidation temperature. The stresses calculated using constant (i.e. stress-independent) viscosity are two orders higher than the stresses obtained from the measurement of the wafer curvature[4]. If we use shear-stress-dependent viscosity[5], the value of the stresses drops to a reasonable level. However, extremely small viscosity occurred in such calculations. More consideration on the lateral component of the oxidation strain is necessary.

(2) Convex cylinder

Oxidation of a cylindrical substrate was simulated using the stress-dependent oxidation parameters extracted by Sutardja ($V_k = 12.5Å^3$, $V_d = 75Å^3$, $V_0 = 180\text{-}800Å^3$). Uniaxial oxidation was assumed. The results are displayed in Fig.3 and Fig.4. Fig.4 shows that the larger the curvature of the substrate, the thinner the oxide, and the retardation of oxidation is pronounced at low temperatures. These results agree with Kao's experiments[6]. However, the value of $V_k = 12.5Å^3$ obtained by the viscous flow model is slightly small for the viscoelastic oxidation model. Additional fit to the experimental data is required.

4. Application example

As a practical example, LOCOS structure was simulated. In this calculation, constant viscosity was used, and stress dependence of the oxidation parameters was ignored because numerical instability arises in stress-dependent calculation. The result of LOCOS structure is displayed in Fig.5. Fig.5(a) is the result of uniaxial oxidation, and Fig.5(b) is the result of dilational oxidation. These results demonstrate the influence of the oxidation strain tensor on the stress distribution and oxide shape. The actual shape is similar to the shape of Fig.5(a). The stress created in uniaxial oxidation is smaller than that in dilational oxidation. However, the stresses are one order higher than the stresses measured in flat plate oxidation. Shear-stress-dependent viscosity should be used.

References

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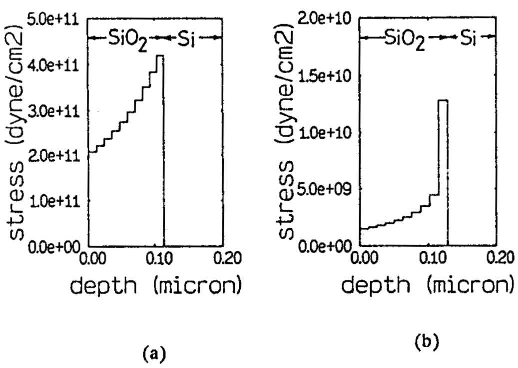

Fig.1. Plots of the stresses induced by planar oxidation. (a)constant viscosity; (b)shear-stress-dependent viscosity.

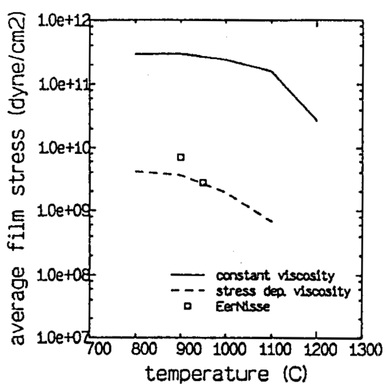

Fig.2 Average film stress as a function of oxidation temperature.

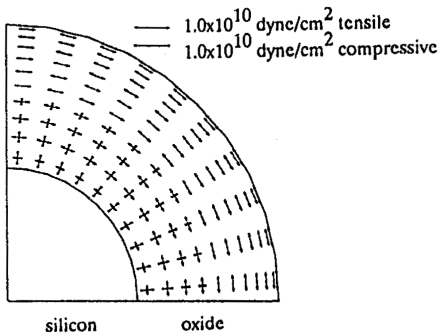

Fig.3 Principal stress in the oxide formed on a cylindrical substrate.

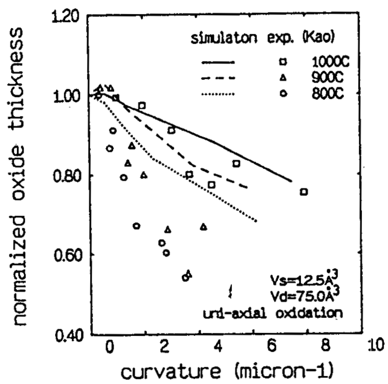

Fig.4 Normalized oxide thickness as a function of curvature.

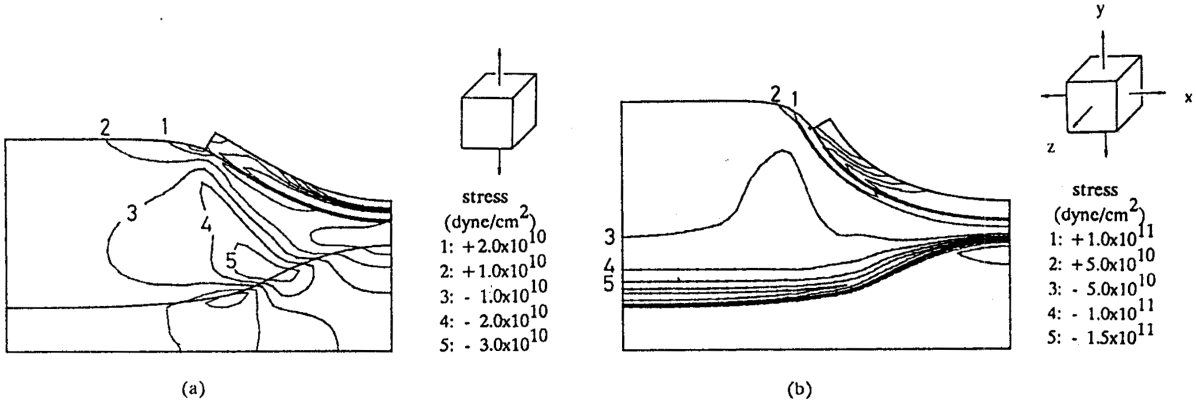

Fig.5 x-component of the stress in LOCOS structure (950C° wet).
(a) uniaxial oxidation; (b) dilational oxidation.