Two Dimensional Stress Analysis during Thermal Oxidation

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Abstract

With the trend towards high integration of LSIs, it has become increasingly important to control or minimize local mechanical stresses which develop in silicon substrates and cause substrate failure during LSI fabrication. In particular, during thermal oxidation, a large stress is induced at the interface between silicon and silicon dioxide. This is because of the volume expansion in the newly grown silicon dioxide, and the mismatch in the thermal expansion coefficients. This stress is large and sometimes causes dislocation to form in the silicon substrate. Therefore, stress control during thermal oxidation is very important for improving product reliability.

This paper presents a two-dimensional oxidation process simulation program, OXSIM2D, [1] which analyzes silicon dioxide growth on silicon surfaces and the change in stress in the total structure. The numerical model used is shown in Fig. 1. There are three main stages, which are repeated until oxidation finishes. The first stage analyzes oxidizing species diffusing through the existing silicon dioxide layer, assuming a quasi-static state. This analysis is made by the finite element method with 4-node quadrilateral elements. Two new ideas are incorporated into this analysis: stress-dependent diffusion which was originally proposed by Kao et al., [2] and anisotropic diffusion caused by the thin film effect. The second stage models the movement of the silicon/silicon dioxide boundary and the chemical reaction is there. The existence of the "White Ribbon", a thin nitride layer which forms at the interface under the silicon nitride mask, is analyzed as an oxidation barrier. The rate constant of the chemical reaction at the interface is reduced in the area under the nitride mask. After the boundary movement, finite element meshes are refined by the boundary-fitted coordinate transformation technique. The last stage analyzes visco-elastic stress using the finite element method. Isotropic initial strain tensors corresponding to the body expansion are applied to the transition region, which is defined as the area in which silicon changes to silicon dioxide in the time increment. Intrinsic stress in nitride masks and thermal stress generated before and after oxidation are also taken into account. Viscosity is used to represent the stress relaxation which occurs at high temperatures.

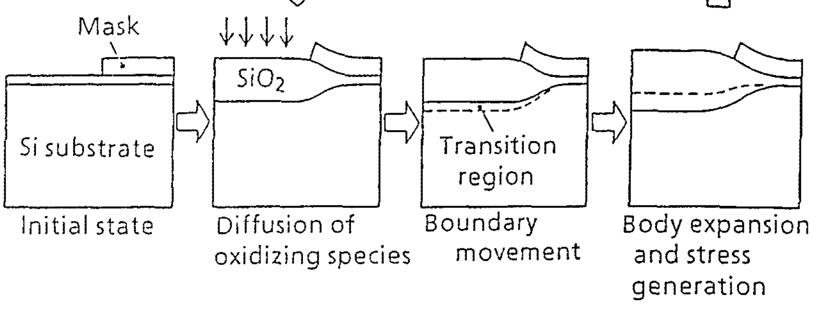

Fig.1 Numerical Model in OXSIM2D

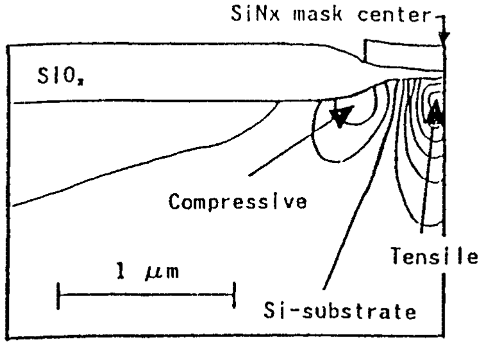

Fig.2 Normal Stress Distribution in LOCOS structure (Mask Width 1 μm)

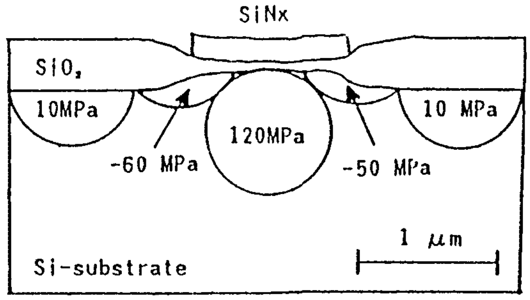

Fig. 4 Normal Stress Distribution measured using Raman Spectroscopy

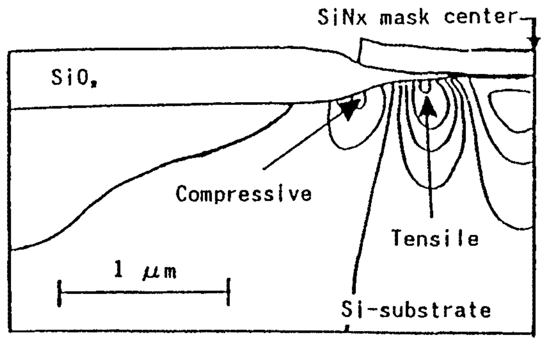

Fig.3 Normal Stress Distribution in LOCOS structure (Mask Width 2 μm)

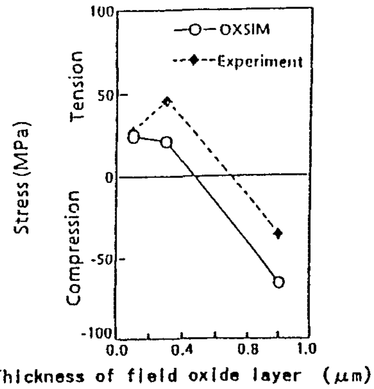

Fig.5 Average Stress Change in Si-substrate under Nitride Mask

An example of simulated normal stress distribution in a LOCOS structure is shown in Fig. 2. Thickness of the nitride mask is 150 nm and width is 1.0 μm, and the oxidation was performed under pyrogenic conditions. Stress concentration occurs at two areas in the substrate under the nitride mask. Tensile stress is concentrated near the silicon surface under the center of the nitride mask. On the other hand, compressive stress develops at the LOCOS edge. This compressive stress is caused by the volume expansion of the newly grown silicon dioxide. Since the silicon dioxide wants to expand, the side walls of the LOCOS structure push the silicon substrate under the nitride mask. The reason for the tensile stress concentration near the silicon surface under the center of the nitride mask is the deflection of the nitride mask caused by the growth of the "Bird's Beak". Since the Young's modulus of the nitride mask is higher than that of silicon, and the nitride mask is distorted into a concave shape, tensile stress develops at the silicon surface. This tensile stress does not always develop near the silicon surface under the center of the nitride mask. The position of the stress concentration depends on the length of the "Bird's Beak". When the Bird's Beak does not grow much, the tensile stress concentration occurs near the mask edge, as shown in Fig. 3.

The normal stress distribution measured using microscopic Raman spectroscopy[3] is shown in Fig. 4. The spatial resolution is 1 μm. It shows the existence of both the compressive stress at the LOCOS edge and the tensile stress at the center of silicon surface. The simulated stress is compared with the measured stress in Fig. 5. It was found that the predicted stress agrees well with the measured stress.

References

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[2] D. B. Kao, et al., IEEE Trans. Electron Devices, ED-35(1988), 25.
[3] T. Englert, et al., Solid State Electronics, 23(1980), 31.