Modeling Stress Effects on Thin Oxide Growth Kinetics

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Abstract--This paper describes the development of a thin oxide growth model, which includes stress dependencies and, hence, allows the modeling of non-planar structures with thin oxides.

In trench isolation structures, the trench surface is normally lined with an oxide film before any trench filling to assure a good electrical interface and insulating properties. Traditionally this is achieved by thermal oxidation. However, this process can be a major source for generating stresses. It may be easy to visualize that oxidation occurring in a confined corner in which the volume expansion is more difficult, will show strong stress-dependences. The stresses not only induce defect formation and increased leakage currents but also retard the oxidation at trench corners. This forms sharp corners which can result in undesired "humps" in the subthreshold I-V characteristics or even failure of the dielectric if it is substantially thinner than on the trench sidewalls. Therefore, a large number of process parameters must be considered in order to achieve defect-free oxidized trench structures. As a consequence, oxidation temperature, oxidation thickness and oxidation ambient have been studied to achieve less stress and smoother corners in a trench structure.

Experimental results show that oxidation at higher temperatures can achieve rounded corners even when the liner oxide is scaled down to 30 nm. Fig. 1 shows a trench structure immediately after a liner oxide was grown. The liner thermal oxide for this isolation structure was grown at a temperature of 950°C. One can see sharp corners in this trench

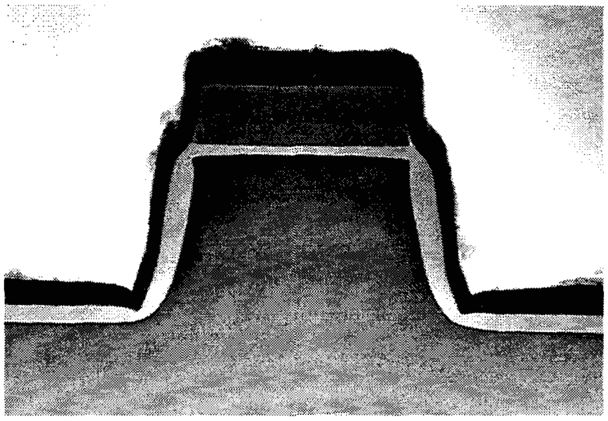

Fig. 1 Trench structure with a liner oxide grown at 950°C before trench filling. A sharp corner is shown in this trench structure, while a rounded corner is obtained for the same thickness of oxide grown at a higher temperature. (Photo courtesy M. Tavassoli, HP Lab.)

structure, while a perfectly rounded corner is obtained when the same thickness of oxide is grown at a higher temperature. As the corner of trench structures plays a governing role in the performance and reliability of these advanced device structures, it is important to develop simulation tools that can predict accurate stress levels and 2D oxidation rates for these strongly stress-dependent areas.

Many studies have been done dealing with stress-dependent oxidation kinetics for thick oxides. Although there is general agreement that the oxide growth rate can be modeled by the Deal-Grove model and SiO_2 viscous flow [1], [2], [3], opinions diverge as to the mechanisms governing the initial stages of oxide growth. Because the growth of thin oxide films during the thermal oxidation of silicon is still not well-understood even in planar oxides, the simulation of nonplanar thin oxides is very difficult. This paper will describe the

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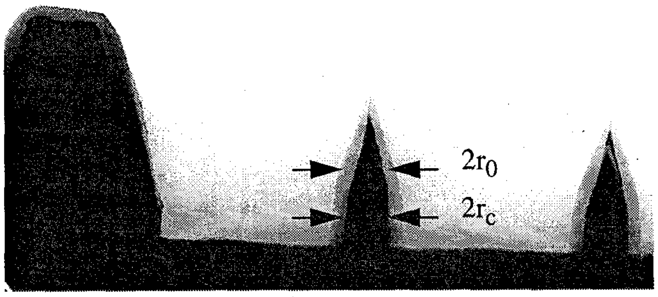

Fig. 2 The shape of the entire oxidized silicon pillar. r_c is the radius of the silicon core, and r_0 is the final outside radius of the oxide.

development of a phenomenological thin oxide growth model that includes stress dependencies and, hence allows modeling of trench isolation structures with thin oxides.

To study the oxidation mechanism on those strongly stress-dependent areas, experiments were performed as follows. First, the mask for silicon cylinders was patterned by electron beam lithography, and then the masking patterns were transferred into the silicon substrate by anisotropic reactive ion etching. The fabrication process can achieve 10 nm to 200 nm radii silicon nano-pillars. Fig. 2 shows a silicon pillar structure after oxidation. The oxidation data show that the grown oxide thickness is strongly dependent on the initial radii of the silicon nano-pillars. The oxide thickness decreases when the pillar radius decreases, due to higher stress.

The fact that the stress-dependent Deal-Grove model can predict non-planar oxidation kinetics in the thick oxide regime suggests that a more general oxide model of the same type might be suitable in the stress dependent, thin oxide regime. One possible oxide model is the Han and Helms [4] parallel oxidation model where we introduce additional stress dependent oxidation rates and oxide viscosity [2], [3]. In the parallel oxidation model, the enhanced growth in the thin regime has been accounted for by using two parallel streams of oxidation, as in (1).

$$\frac{dX_{ox}}{dt} = \frac{B_1}{(2X_{ox} + A_1)} + \frac{B_2}{(2X_{ox} + A_2)} \quad (1)$$

These two parallel oxidation processes, one at the interface and the other at the surface of the oxide, occur at the same time. Their work, using an ^{18}O tracer, showed that new oxide grows primarily at the SiO_2-Si interface, but ^{18}O reacts noticeably at the oxide surface too. In addition, in the limit of thick oxides, the parallel oxidation model approaches a parabolic growth law similar to the Deal-Grove model. Han and Helms fit rate constants to several sets of planar oxidation data over a wide range of thicknesses and temperatures. Since the B_1/A_1 term is known to fit thick oxide stress dependent kinetics and since the addition of the B_2/A_2 term fits thin oxide planar oxidation kinetics, we have chosen to add a stress dependence to the B_2 and A_2 terms to thus allow a complete 2D stress dependent modeling capability over the full range thickness.

Using initial values for the stress-free rate constants from Han and Helms and a viscosity in unstressed SiO_2 (η_0) from data on thin film relaxation [3], the model is matched to oxidation data for nano-pillars with different radii to extract the stress dependent coefficients such as the activation volume of viscous flow V_c, the activation volume for diffusivity V_d, and the activation volume for the oxidation rate dependence V_r for both oxidation streams as shown in (2), (3), (4), (5), (6).

$$\eta = \eta_0 \frac{(\tau V_c / (2kT))}{\sinh(\tau V_c / (2kT))} \quad (2)$$

$$\frac{B_1}{A_1} = \left(\frac{B_1}{A_1}\right)_0 exp((\sigma_{rr} V_r) / (kT)) \quad (3)$$

$$B_1 = (B_1)_0 exp(-(PV_d)/(kT)) \quad (4)$$

$$\frac{B_2}{A_2} = \left(\frac{B_2}{A_2}\right)_0 exp((\sigma_{rr} V'_r)/(kT)) \quad (5)$$

$$B_2 = (B_2)_0 exp(-(PV'_d)/(kT)) \quad (6)$$

A semi-analytic procedure was carried out. The stress was calculated using the expressions in an analytic solution for plastic flow on an isotropic cylindrical geometry[3], [5]. Then a new growth rate was computed using the parallel oxidation equation. Based on the new growth rate, the stress can be recomputed in the analytic solution. After several iterations, the reaction rates and stresses reach self-consistent values. Table 1 shows the low-stress viscosity and the extracted activation volume of viscous flow V_c for different temperatures. The low-stress viscosities are reasonably close to Rafferty's thin film's values. The activation volumes for flow are of the same order of magnitude as Rafferty's wet oxide experimental data and the temperature dependence is similar.

This model has been used to predict the oxidation of thin planar surfaces as well as narrow pillars of radii from 10 to 200 nm as shown in Fig. 3 and Fig. 4. Agreement of the model to the experiments over a wide temperature range of 800°C-1000°C, time and pillar dimensions is within 5 percent. The extreme case of self-limiting oxidation [6] is properly characterized by this model as shown in Fig. 5.

In summary, we have proposed a stress-dependent oxidation model with two parallel streams and stress-dependent oxidation parameters which can predict stress dependent thin oxide growth kinetics, including the extreme case of self-limiting oxidation on silicon nano-pillars.

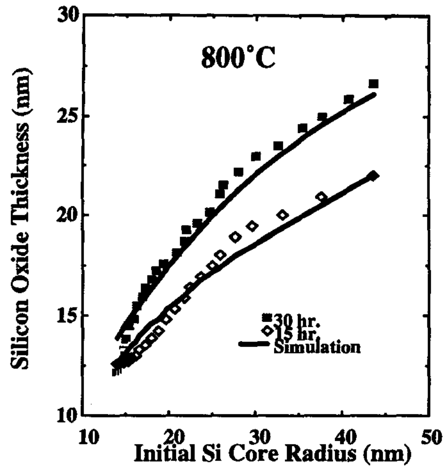

Fig. 3 Applying stress dependent coefficients with the parallel oxidation model, we obtain good fits for the oxide growth characteristics as a function of the nano-pillar radius at different oxidation times.

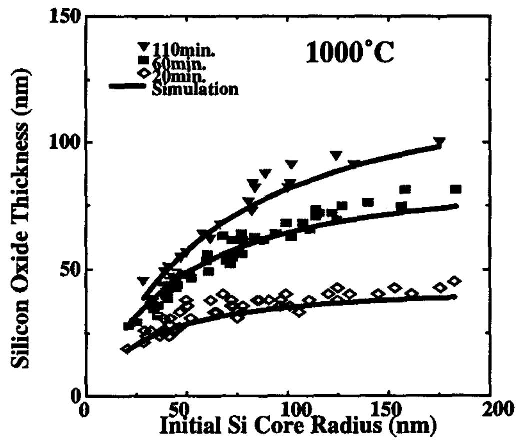

Fig. 4 With the stress dependent coefficients, the parallel oxidation model also accounts for oxidation data at 1000°C, and at different oxidation times.

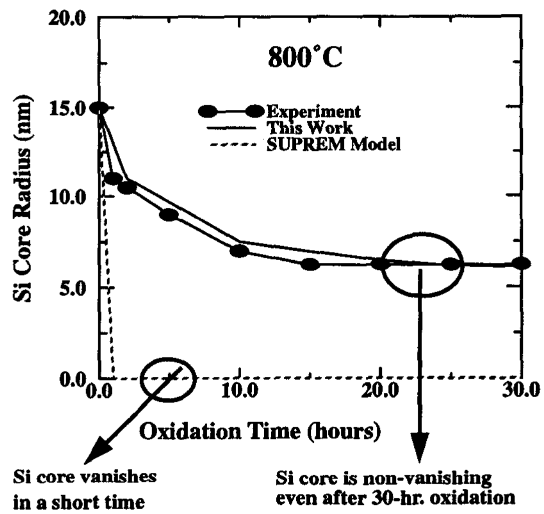

Fig. 5 A comparison of the parallel oxidation model and SUPREM model. The dots represent experimental data from Liu [6]. SUPREM predicts that the Si core vanishes in a short time while our simulation obtains a good fit to the self-limiting oxidation data of silicon nano-pillars at temperatures of 800°C.

Table 1: Extracted values of activation volume of viscous flow V_c for various temperatures.

Temp	800°C	850°C	950°C	1000°C
Viscosity η_0 (poise)	1.3×10^{23}	3.7×10^{20}	5×10^{18}	4.8×10^{16}
V_c ($Å^3$)	399	492	600	1200

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