SIMULATION OF SILICON THERMAL OXIDATION AND STRESS ANALYSIS IN FLASH MEMORY TECHNOLOGY

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Silicon oxidation is still one of the outstanding problems in microelectronic industry and in fundamental research, that The Electrochemical Society dedicates regularly a biannual conference on the physics and chemistry of the Si/SiO_2 interface. The formation of oxide on bare silicon surface is indeed a key technology process in the elaboration of MOS devices in ULSI technology and particularly for the new "flash memory" technology. The oxidation problem has also a research valence because the challenge in the understanding of the basic oxidation mechanisms for the prediction of the kinetic and structural properties of very thin oxide films.

From a modeling point of view the Deal and Grove model has been widely used to describe oxide growth in wet or dry ambient since 1965, but recently it became less adequate when the devices industry needs to address the growth of very thin films. Thus, later studies were dedicated to the "anomalous high" (Figure 2) oxidation rate with respect that predicted by the shrinking core approach of the Deal and Grove model. Fundamental studies about oxygen diffusion and silicon oxidation were performed both experimentally and theoretically. Despite the importance of the subject, the prevailing modeling approach was based on the derivation of "enhancing factors" to be used to correct the Deal and Grove predictions.

To be completely described from a fundamental point of view, the oxidation process needs that all the following aspect should be considered together:

- the diffusion of the "oxidizing species", i.e. molecular or radical oxygen;
- the reaction at interface to convert the silicon lattice in oxide lattice;
- the expansion of the solid volume due to the composition change (the molar volume of silicon oxide is 120% larger than those of crystalline silicon);
- the induced stress status due to the volume expansion that alters the reaction-diffusion parameters.

Moreover, from the industrial point of view, also the trench shape have to be considered in order to minimize the stress insisting in the underneath silicon matrix (Figure 3 and 4). This aspect is of paramount importance to improve reliability of devices because the formation of dislocations and point defects. To be fully complete the model should finally estimates the dielectric properties of the oxide by the evaluations of the oxide defects density (porosity and tunnels, micro-cracks, ….).

Our aim is to obtain a simple chemical engineering like model addressing all the aspects above with exception of the estimation of the properties of the dielectric film. The transient diffusion-reaction equations followed by the stress equations in pseudo-steady state approach were numerically solved first in 1D (figure 1) framework and then in 2D geometry to consider trench shape effects. To validate the model literature data were compared with model prediction. Particularly the examined process is inherent to the early stage of the thermal oxide growth induced by the exposition to dry oxygen in a multiwafer low-pressure horizontal furnace .

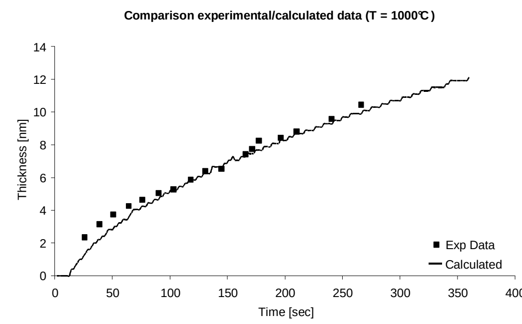

Figure 1: Comparison between calculated and experimental film thickness vs. oxidation time, at 1000°C with C_{O2}^{bulk} = 3.8*10^{-6} (mol/cm^3)

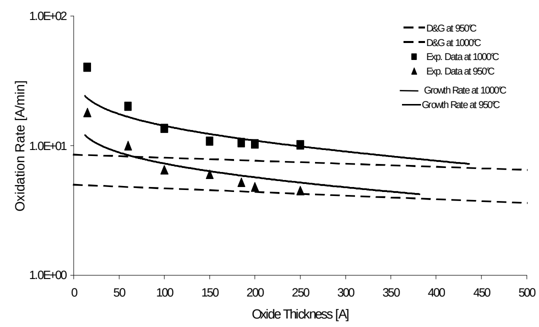

Figure 2: Comparison between the diffusion-reaction and Deal and Grove model.

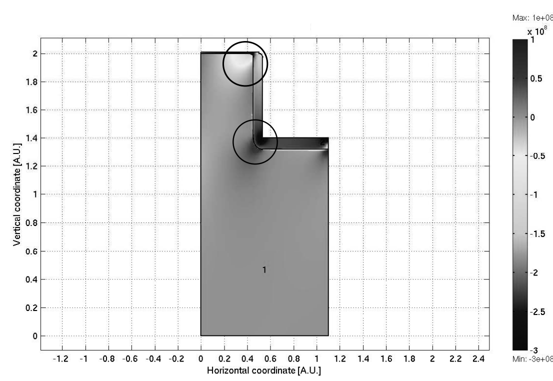

Figure 3: Lateral Stress [Pa] calculated with a 90° trench corner and 40 nm wall oxide

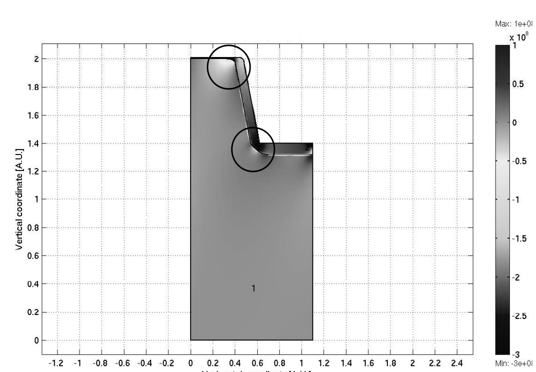

Figure 4: Lateral Stress [Pa] calculated with a 75° trench corner and 40 nm wall oxide