

# Simulation of Advanced-LOCOS Capability for Sub-0.25 Micron CMOS Isolation

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**Abstract**—The visco-elastic oxidation model has been calibrated on 0.35 and 0.25 $\mu\text{m}$  CMOS LOCOS-type isolation structures. Simulation is used to assess the capability of advanced LOCOS options for sub-0.25 micron CMOS. At reduced active area pitch the active-area lifting phenomenon restricts the thickness of field oxide which may be grown. Predictions of the maximum field oxide and active area encroachment are made for an active area pitch of 0.6 $\mu\text{m}$ .

## I. INTRODUCTION

Advanced LOCOS remains an attractive option for sub-0.25 micron CMOS isolation because of its relative process simplicity and low cost as compared to shallow trench isolation (STI). However, fundamental physical limitations of the oxidation process may prevent LOCOS based isolation from meeting design specifications. In this paper calibrated 2D process simulation is used to assess these limitations and to predict field oxide growth in a 0.6 $\mu\text{m}$  pitch active area (AA) line/space structure for a range of standard and modified LOCOS schemes. Process model calibration has been extended to cover high temperature and high pressure in an  $\text{O}_2$  ambient. Mechanical stress effects on field oxide thinning and active area lifting are assessed and figures of merit for the active area encroachment and the maximum field oxide thickness which can be grown before incurring active area lifting are predicted for each LOCOS scheme.

## II MODEL CALIBRATION

The stress-dependent viscous and visco-elastic oxidation models in TSUPREM-4 [1] have been calibrated against cross-sectional TEM measurements of the field oxide shape at the active area edge for a range of advanced-LOCOS options at isolation pitches down to 0.8 $\mu\text{m}$  for CMOS generations 0.5, 0.35 and 0.25 $\mu\text{m}$ . LOCOS technologies considered include: standard and optimised, Poly-Buffered (PB-), Poly-

Encapsulated (PE-) [2] and High Pressure (HP-) LOCOS. Model parameters have been calibrated for the effects of layer thicknesses, oxidation temperature, ambient and pressure, with attention to their influence on field oxide thinning in a narrow active area space, and pad oxide thickness increase (active area lifting) under a narrow line. Design of Experiment methods have been used to assess the sensitivity of the isolation shape to the model parameters and to optimise the coefficient values.

Figure 1 shows a comparison of TEM measurement and calibrated simulation for PE-LOCOS for a 0.7 $\mu\text{m}$  nitride linewidth. The processing sequence starts with patterning of the nitride/pad oxide layer stack. A controlled HF etch is then used to undercut the nitride and create a small cavity in the pad oxide. After re-oxidation of the exposed surfaces a thin polysilicon layer is deposited to fill the cavity and encapsulate the nitride. The silicon-filled cavity is of paramount importance for the control of bird's beak growth. During field oxidation the cavity silicon slowly oxidises creating a large local compressive stress due to material volume change in a confined space. This stress reduces both the cavity oxidation rate and the oxidant diffusion in the pad oxide, so preventing the bird's beak from growing. Residual silicon in the cavity can be seen in figures 1 in both the TEM and simulation. The visco-elastic model parameters (stress-dependent activation volumes for oxidation, diffusion and viscosity, oxide and nitride viscosity) used here were calibrated from standard LOCOS isolation at the same temperature, the polysilicon viscosity was set to a value between that of oxide and nitride. These give good agreement to the PE-LOCOS measurement.

Figure 2 shows the simulation results for an optimised standard LOCOS variant in which the oxidation ambient is

dry O<sub>2</sub> and field oxidation is performed at a high temperature (1150°C). This has two advantages: (a) the oxidation kinetics are dominated by the parabolic regime (due to reduced value of the Deal-Grove A parameter) giving less oxidation under the nitride mask; and (b) the low oxide viscosity and long oxidation time gives a reduced stress. The Deal-Grove coefficients have been extracted from planar oxide growth measurements for the temperature range 1000-1150°C and for oxide thickness 0.05-0.5µm in 1 atmos. O<sub>2</sub> with fitted values  $B/A_{100} = 1.2 \times 10^7 \exp(-2.53\text{eV}/kT) \mu\text{m}/\text{min}$  and  $B = 54.84 \exp(-1.41\text{eV}/kT) \mu\text{m}^2/\text{min}$ . Oxidation of the nitride is a significant effect in these conditions and has been included in the model. A consequence of low oxide viscosity is that the oxide thickness in a narrow field region is *greater* than that in wide regions, since oxide grown under the nitride can flow out into the neighbouring field oxide and add proportionally more thickness to the narrower field regions [3].

To decrease the large thermal budget associated with oxidation in O<sub>2</sub>, a high pressure ambient can be used. The model for high temperature O<sub>2</sub> oxidation at atmospheric pressure can be extended with reasonable accuracy to LOCOS at 1100°C and 25 atmospheres by just scaling the Deal-Grove parameters ( $B/A \sim p^{0.75}$  and  $B \sim p^{1.0}$ ) and with no change to the viscosities. The reduced thermal budget decreases the active area encroachment since stresses have less time to relax and so retard the oxidant diffusion under the active area.

### III PREDICTIVE SIMULATION

The calibrated process models have been used to predict isolation performance at the smaller pitch of 0.6µm to evaluate and compare the capabilities of different LOCOS schemes. In all cases the main limitation is active area lifting which occurs when bird's beaks link-up underneath the narrow nitride line. This can be reduced by: (a) designing LOCOS stacks which retard oxidation under the nitride by stress (thick nitride layer or silicon filled cavity) or by reducing the oxidant flux (by introducing a spacer, or reducing the pad oxide thickness); or (b) optimising the oxidation kinetics (high temperature; high pressure; and/or O<sub>2</sub> ambient). For each isolation scheme, the oxide growth in the field region and active area has been monitored as a function of oxidation time. In each scheme, there is a process-specific maximum field oxide thickness, above which the minimum width active area is completely lost.

Fig. 3 shows the case of standard LOCOS with a "stiff" thick nitride/thin pad oxide layer stack. The active area oxide starts thickening after 30 minutes at 1000°C for 0.6µm pitch. The lifting curve is rather steep and is parallel with the field oxide growth curve, so that there can be no further gain in field oxide thickness by allowing AA lifting to occur and then etching back. The lifting is sensitive to the shape of the nitride edge profile: a vertical edge gives a better isolation due

to the more abrupt stress. PB-LOCOS does not give any significant advantage over standard LOCOS: the AA oxide lifting curve is steepened due to polysilicon oxidation under the nitride and the buried depth of the field oxide is reduced. Fig. 4 shows the case of PE-LOCOS in a steam ambient at 975°C. AA lifting is delayed until 90 mins due to the silicon cavity induced stress. However, this stress also reduces the oxidation rate in the narrow field region and causes severe field oxide thinning. Fig. 5 shows high temperature standard LOCOS. The onset of AA lifting is softer and the absence of field oxide thinning allows a thicker field oxide to be used.

### IV DISCUSSION

The simulation predicted values for the maximum field oxide thickness at polysilicon gate and AA encroachment are shown in figures 6 and 7 for a set of isolation schemes each with optimised nitride and pad oxide thickness. The field oxide thickness under the gate takes account of post-LOCOS oxide etch steps. Depending on the scheme, the effective field oxide thickness is in the range 180-300 nm and the active area encroachment 20-60 nm per edge. For very high temperature and O<sub>2</sub> oxidation ambient, mechanical stress is minimised by low viscosity oxide flow resulting in negligible or inverse field oxide thinning, but at the expense of increased active area encroachment. Simulation has shown that the slope of the lifting curve is also sensitive to process conditions, allowing a greater toleration of AA lifting in certain cases and hence decreased sensitivity to line-width variation. The reduced field oxide thickness (<300nm) can be sufficient for lateral isolation at reduced supply voltage (1.8V).

### V CONCLUSIONS

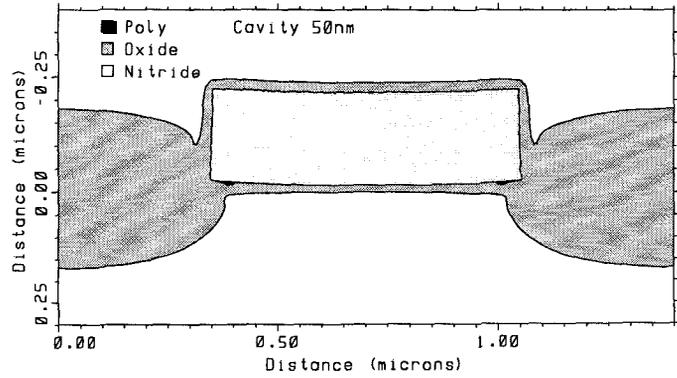
The visco-elastic oxidation model has been calibrated for a range of isolation structures and oxidation conditions. Simulation has been applied to the optimisation of advanced-LOCOS schemes with a 0.6 micron active area pitch. The field oxide thickness is limited by active area lifting to a maximum of 300nm. High temperature conditions give increased oxide thickness, but at the cost of increased active area encroachment. Combining high temperature dry O<sub>2</sub> with very high ambient pressure decreases this encroachment but introduces greater mechanical stress.

### ACKNOWLEDGEMENTS

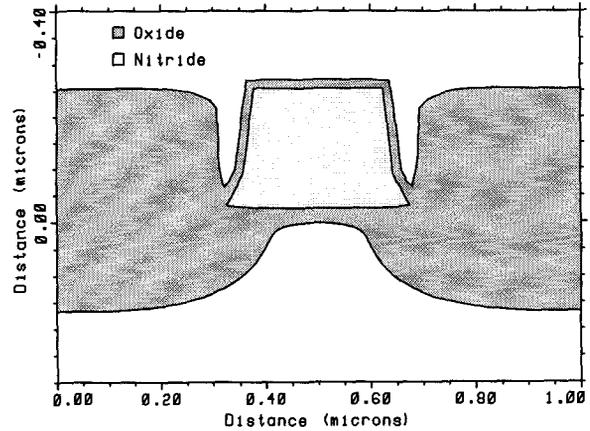
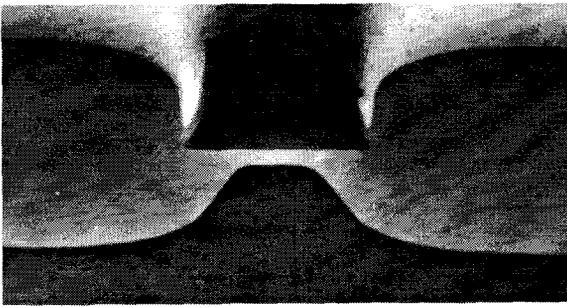
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### REFERENCES

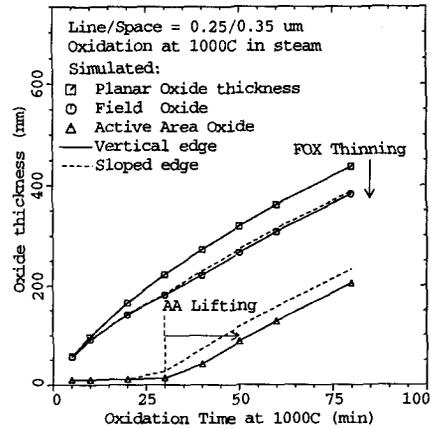
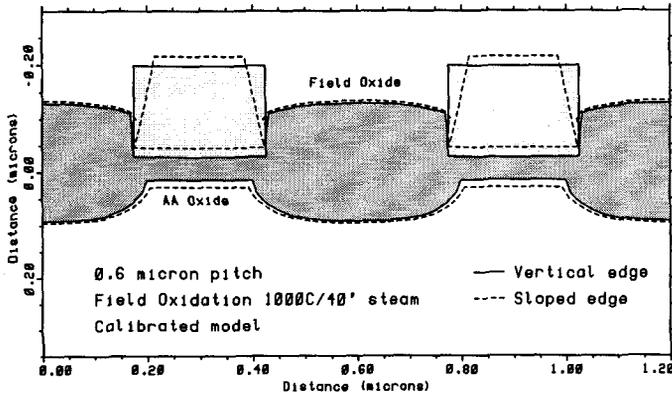
- [1] TMA TSUPREM-4, Two-Dimensional Process Simulation Program, v6.4 (1996)
- [2] G Badenes et al "Optimisation of polysilicon encapsulated LOCOS for 0.25 micron CMOS: correlation between cavity dimensions, mechanical stress and gate oxide integrity" Proc. Symp. ULSI-97 (eds H Z Massoud, H Iwai, C Claeys, RB Fair) ECS vol 97-3, p467.
- [3] P Bellutti et al, Semicond. Sci. Technology **10** 1700 (1995)



**Figure 1:** TEM cross-sectional micrograph for a PE-LOCOS with  $0.7\mu\text{m}$  nitride line/space and comparison with calibrated simulation. Layer thicknesses: pad oxide 15nm; nitride 200 nm; and 20 nm a-Si. Field oxidation performed at  $975^\circ\text{C}$ .



**Figure 2:** TEM cross-sectional micrograph for a High Temperature LOCOS with  $0.37\mu\text{m}$  nitride linewidth and comparison with calibrated simulation. Layer thicknesses: pad oxide 12 nm; nitride 230 nm. Oxidation at  $1150^\circ\text{C}$  in  $\text{O}_2$ .



**Figure 3:** Performance of standard LOCOS with oxidation in steam at  $1000^\circ\text{C}$  for  $0.6\mu\text{m}$  pitch active area. The oxide thickness at the centre of the field and active area regions is plotted as a function of oxidation time. The effect of a non-vertical nitride edge profile is also shown.

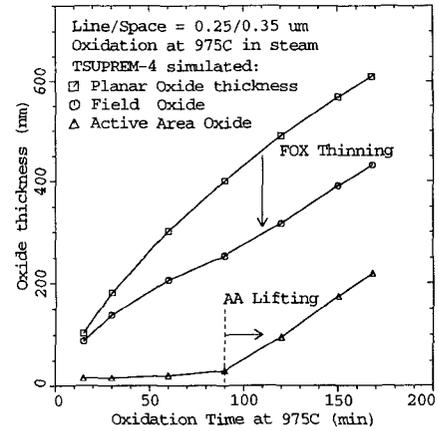
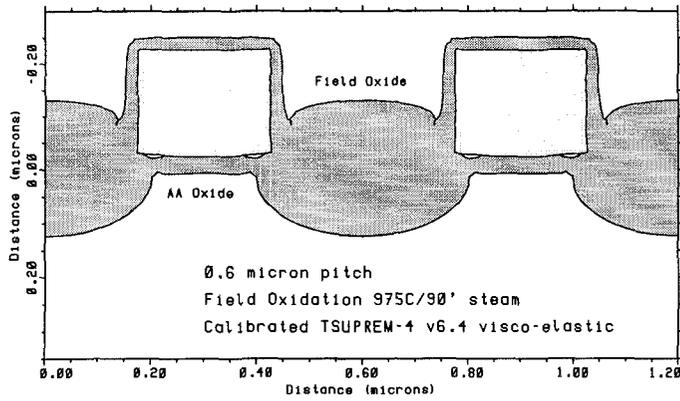


Figure 4: Simulated performance of PE-LOCOS with oxidation in steam at 975°C at 0.6 $\mu$ m pitch.

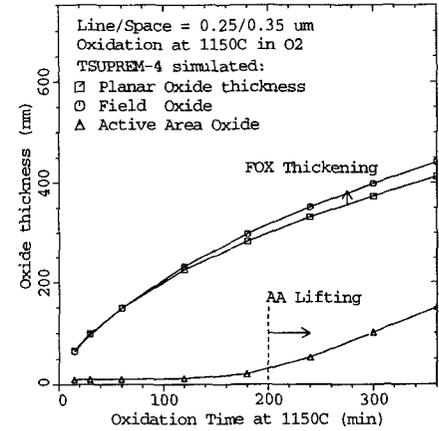
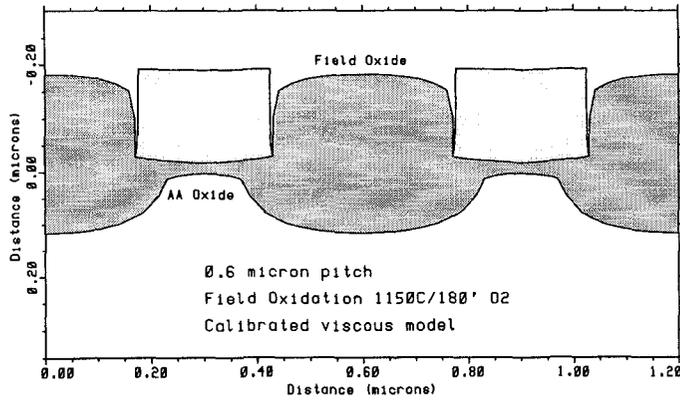


Figure 5: Simulated performance of high temperature dry O<sub>2</sub> LOCOS at 1150°C at 0.6 $\mu$ m pitch.

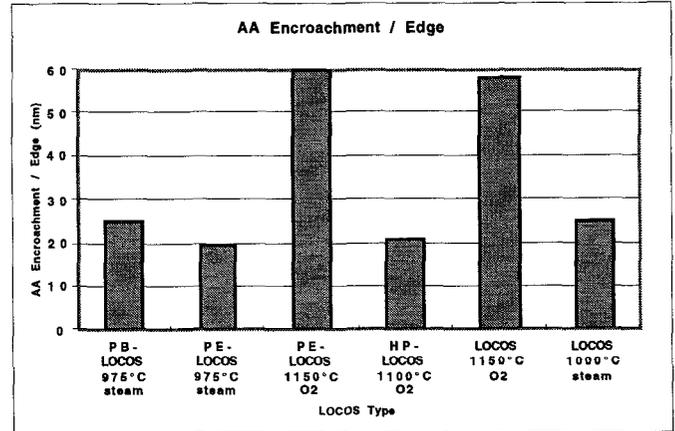
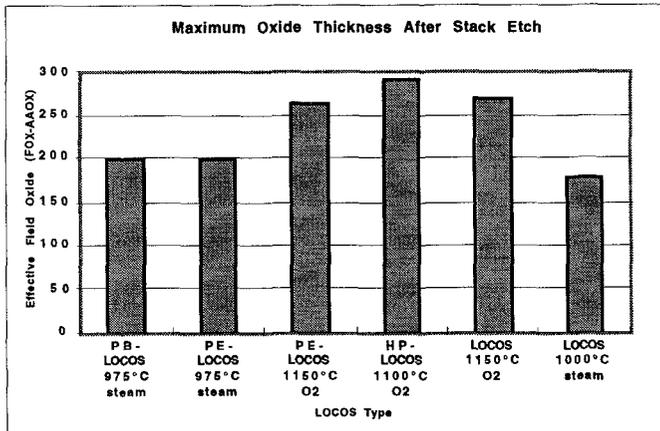


Figure 6: Simulated maximum field oxide thickness under the poly gate for PB-, PE- and standard LOCOS for steam, O<sub>2</sub> high temperature and high pressure (HP) ambient conditions.

Figure 7: Simulated active area encroachment for the various LOCOS options shown in figure 6.