

## **PROCESS LAB: OXIDATION**

### **Contributors:**

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### **At a glance:**

Simulates 1-D oxidation of silicon using Deal-Grove and Massoud models.

### **Description:**

Thermal oxidation of silicon is key process in integrated circuit fabrication. For example it is used in the formation of gate dielectrics, pad and field oxides. This tool implements the classic Deal-Grove linear parabolic model as well as the Massoud additional term to model the rapid initial oxidation regime. Users may select the models, the oxidation ambient (dry or wet oxidation), oxidation time (in min), initial oxide thickness (in  $\mu\text{m}$ ), temperature (in  $^{\circ}\text{C}$ , K, or F), pressure (in Atm) and crystal orientation ( $\langle 100 \rangle$  or  $\langle 111 \rangle$ ) in their simulations. Oxidation thickness versus time and rate of change of oxide thickness versus time may be plotted after the simulation.

### **Notes:**

#### Models

$$\frac{dx_o}{dt} = \frac{B}{2x_o + A} + C \exp\left(-\frac{x_o}{L}\right)$$

Linear/Parabolic Deal-Grove	Massoud Rapid Initial Oxidation Term
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The Deal-Grove model would show the general behavior of an initially linear growth rate that becomes parabolic as the oxide grows. The Deal-Grove model alone, however, does not model initial rapid oxidation of the silicon. Therefore, if the Deal-Grove model is used without the Massoud correction term, an initial oxide of about 15 nm should be used to mimic the rapid initial growth, and give more reasonable answers for oxidation thicknesses.

There is a 2.2X volume expansion during thermal oxidation, so growing 1 unit of oxide consumes 0.45 units of silicon. The stress associated with this volume expansion is not accounted for in these models.

#### Oxidation Ambient

There are two possible ambients in this tool: Dry  $\text{O}_2$  and Wet  $\text{O}_2$ , which is mostly  $\text{H}_2\text{O}$  but contains some  $\text{O}_2$ .  $\text{SiO}_2$  grows much faster in the Wet  $\text{O}_2$  ambient than it does in dry  $\text{O}_2$ . The principal reason for this is that the oxidant solubility in  $\text{SiO}_2$  is much higher for  $\text{H}_2\text{O}$  than for  $\text{O}_2$ .

## Temperature

Both B (parabolic) and B/A (linear) terms of the Deal-Grove model are described by Arrhenius expressions of the form:

$$B = C_1 \exp\left(-\frac{E_1}{kT}\right)$$
$$\frac{B}{A} = C_2 \exp\left(-\frac{E_2}{kT}\right)$$

where  $E_1$  and  $E_2$  are the activation energies, and  $C_1$  and  $C_2$  are the preexponential constants.  $C$  in the Massoud correction can also be described by an Arrhenius expression.

## Pressure

As there is no widely accepted first principles model to explain the pressure dependence of  $O_2$  growth kinetics, the Deal-Grove model is used with these corrections:

$$\frac{B}{A} = \left(\frac{B}{A}\right)^i P, \quad B = (B)^i P \text{ for } H_2O$$
$$\frac{B}{A} = \left(\frac{B}{A}\right)^i P^{0.8}, \quad B = (B)^i P \text{ for } O_2$$

The  $i$  superscripts refer to the respective values at 1 Atm.

## Crystal Orientation

Oxidation growth rates are faster on the (111) surfaces than they are on (100) surfaces, as there is a higher density of atoms and thus more reaction sites on (111) surfaces. Only the reaction at the Si/SiO<sub>2</sub> interface and not the diffusion of the oxidants should be affected by the crystal orientation. Therefore, in the context of the Deal-Grove model, only the B/A linear term is affected. Orientation effects are incorporated as follows:

$$\left(\frac{B}{A}\right)_{111} = 1.68 \left(\frac{B}{A}\right)_{100}$$

## Simulation Plots

Oxide thickness versus time or rate of change of oxide thickness versus time may be plotted after each simulation. Users may compare the plots of all previous simulations with different parameters. Some of the graphical features include the ability to zoom in

on the plots, obtain values of the individual plot points, and change the axes scales. Users may also show all simulations in the current session on the same plot.

### Reference

James Plummer, Michael Deal, Peter Griffin, *Silicon VLSI Technology, Fundamentals, Practice and Modeling*, Prentice Hall, 2000.