# Experiment No. 8

**Aim:** Simulate 1D oxidation process with Deal-Grove model for different conditions (e.g. oxidation type, orientation, time, temperature, thickness etc.) and comment on the results obtained.

**Software Tool:** Technology Computer aided Design lab (TCAD) on nanohub.org

**Theory:**

**Oxidation Process 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 µm), temperature ( in ° C , K, or F), and crystal orientation (<100> or <111>) in their simulations. Oxidation thickness versus time and rate of change of oxide thickness versus time may be plotted after the simulation.

**Models**

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

Linear/Parabolic
Deal-Grove

Massoud Rapid
Initial Oxidation
Term

The Deal-Grove model would show the general behaviour 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.

**Oxidation Ambient**
There are two possible ambients in this tool: Dry $O_2$ and Wet $O_2$, which is mostly $H_2O$ but contains some $O_2$. $SiO_2$ grows much faster in the Wet $O_2$ ambient than it does in dry $O_2$. The principal reason for this is that the oxidant solubility in $SiO_2$ is much higher for $H_2O$ than for $O_2$.

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

$$B = C_1 \exp(-\frac{E_1}{kT})$$

$$\frac{B}{A} = C_2 \exp(-\frac{E_2}{kT})$$

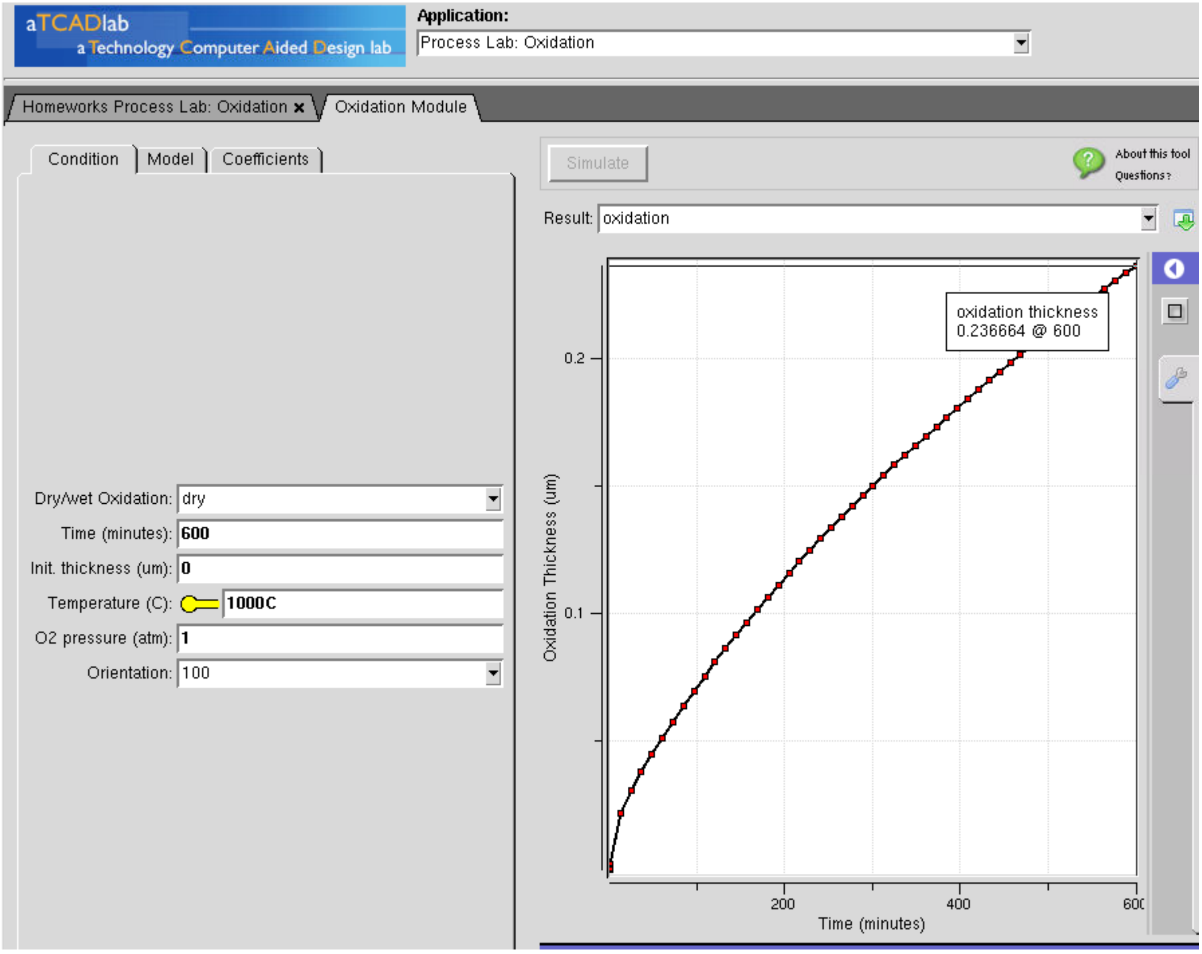
where $E_1$ and $E_2$ are the activation energies, and $C_1$ and $C_2$ are the pre-exponential constants. C in the Massoud correction can also be described by an Arrhenius expression.

## 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/$SiO_2$ 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:

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

## Oxidation GUI



Application: Process Lab: Oxidation

Dry/wet Oxidation: dry

Time (minutes): 600

Init. thickness (um): 0

Temperature (C): 1000C

O2 pressure (atm): 1

Orientation: 100

Result: oxidation

oxidation thickness
0.236664 @ 600

**Question1: Explain the effect of time on the thickness of the oxide layer ?**

**Question2 : Explain the effect of temperature on the thickness of the oxide layer ?**

**Question3 : Explain the effect of water vapor on the thickness of the oxide layer ?**

**Question4 : Explain the effect of Si orientation on the thickness of the oxide layer ?**

**Simulation Plots**

Oxide thickness versus time or rate of change of oxide thickness versus time , oxidation type, orientation, temperature may be plotted after each simulation.

## Conclusion: