PROCESS LAB: OXIDATION FLUX

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At a glance:

Simulates oxidant concentration in oxide.

Description:

This tool gives users an understanding of the oxidant flux in the oxide during an oxidation process by showing the oxidant concentration in the oxide. Users may select the models (Deal-Grove or Deal-Grove with Massoud correction), the oxidation ambient (dry or wet oxidation), oxidation time (in min), initial oxide thickness (in μm), temperature (in ^{o}C, K, or F), pressure (in Atm) and crystal orientation (<100> or <111>) in their simulations. The simulation plot gives oxidant concentration versus oxide thickness.

Notes:

Models

There are three sequential steps that are necessary for oxidation:

1) Transport of oxidant in gas phase to oxide surface

$$F_1 = h(C^* - C_O),$$

where C^* is the oxidant concentration in the oxide that would be in equilibrium to gas pressure, and C_O is the oxidant concentration just inside the oxide surface.

2) Diffusion of the oxidant through the oxide to the Si/SiO_2 interface

$$F_2 = D(\frac{C_O - C_I}{x_o}),$$

where D is the oxidant diffusivity in oxide, and C_I is the concentration at the Si/SiO_2 interface.

3) Reaction at the Si/SiO_2 interface

$$F_3 = k_S C_I,$$

where k_S is the interface rate constant.

Under steady state conditions, $F_1=F_2=F_3$. From experimental observation, h is very large, thus F_1 is not the rate limiting step. Combining the above equations and knowing that h is very large leads to:

$$C_I \approx \frac{C^*}{1+\frac{k_S x_o}{D}},$$

$$\text{and } C_O \approx C^*.$$

There are two limiting cases for the above equations. When $\frac{k_S x_o}{D} << 1$, the oxidation is interface reaction rate controlled, which is generally the case for thin oxides. When $\frac{k_S x_o}{D} >> 1$, the overall growth rate is limited by the diffusion process, which is generally the case for thick oxides.

When we consider the rate of oxidation, combining these equations gives:

$$\frac{dx_o}{dt} = \frac{F}{N_1} \approx \frac{k_S C^*}{N_1\left[1+\frac{k_S x_o}{D}\right]},$$

where N_1 is the number of oxidant molecules incorporated per unit volume of oxide grown. $N_1 = 2.2e22\ cm^{-3}$ for O_2 oxidation and twice this value for H_2O oxidation.

Integrating the above equation leads to the equations describing oxide growth kinetics.

$$B = \frac{2DC^*}{N_1}$$

$$\frac{B}{A} \approx \frac{C^* k_S}{N_1}$$

Since we have the equations for B and B/A, an alternative expression for oxidation rate is:

$$\frac{dx_o}{dt} = \frac{B}{A+2x_o}$$

Oxidation Ambient

There are two possible ambients in this tool: Dry O_2 and Wet O_2. In this simulation we have assumed $C_O = 5e16\ cm^{-3}$ for dry O_2 and $C_O = 3e19\ cm^{-3}$ for wet 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.

Simulation Plots

Oxidant concentration versus thickness is plotted after each simulation. Note that 0 indicates the original silicon surface (or the middle of the initial oxide, if present), and the positive thickness is into the original silicon wafer while negative thickness indicates above the original silicon wafer. 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.

Reference

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