

Computational Microelectronics

Lecture 2 Oxidation

Sung-Min Hong (smhong@gist.ac.kr)

Semiconductor Device Simulation Laboratory
School of Electrical Engineering and Computer Science
Gwangju Institute of Science and Technology

Oxidation

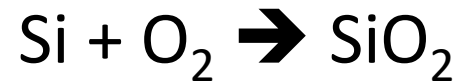
Oxidation

- Producing a thin layer of silicon dioxide on the surface of a wafer

- Reactions



“Wet”

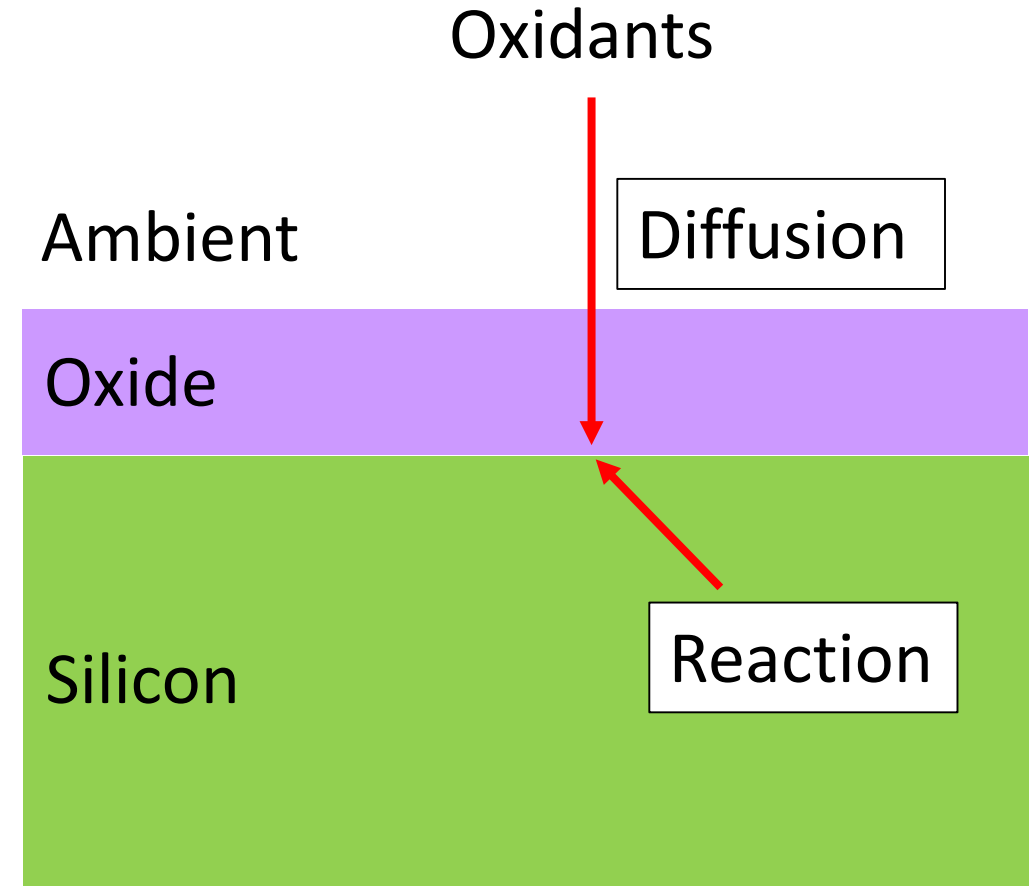


“Dry”

- Amorphous SiO_2 (Weight density, 2.27 g/cm³ or 2.18 g/cm³)
 - Cf.) Crystalline SiO_2 (Quartz, 2.65 g/cm³)

Kinetics

- Basic process for the oxidation of silicon
 - Diffusion of oxidants
 - Reaction at the interface
- 125 % volume expansion
 - SiO_2 : 2.3×10^{22} molecules/cm³
 - Si: 5×10^{22} atoms/cm³



Oxidation parameters

- Oxidant species
 - Dry: Low oxidation rate. Best material characteristics and quality
 - Wet: Much faster than dry oxidation, due to the oxidant solubility limit
- Temperature
 - Oxidation rate increases significantly with the furnace temperature.
- Pressure
 - Oxidation rate increases with the hydrostatic pressure in the furnace.
- Crystal orientation
 - Faster oxide growth on (111)-surfaces than on (100)-surfaces

Deal-Grove model

- Well established model for thermal oxide growth

General Relationship for the Thermal Oxidation of Silicon

Journal of Applied Physics **36**, 3770 (1965); <https://doi.org/10.1063/1.1713945>

B. E. Deal *and* A. S. Grove

- (1) Transported from the bulk of the oxidizing gas to the outer surface of oxide (Adsorption)
- (2) Transported across the oxide film towards silicon (Diffusion)
- (3) Reacts at the interface with silicon and forms a new layer of SiO_2 (Reaction)

Derivation (1)

- Flux equations

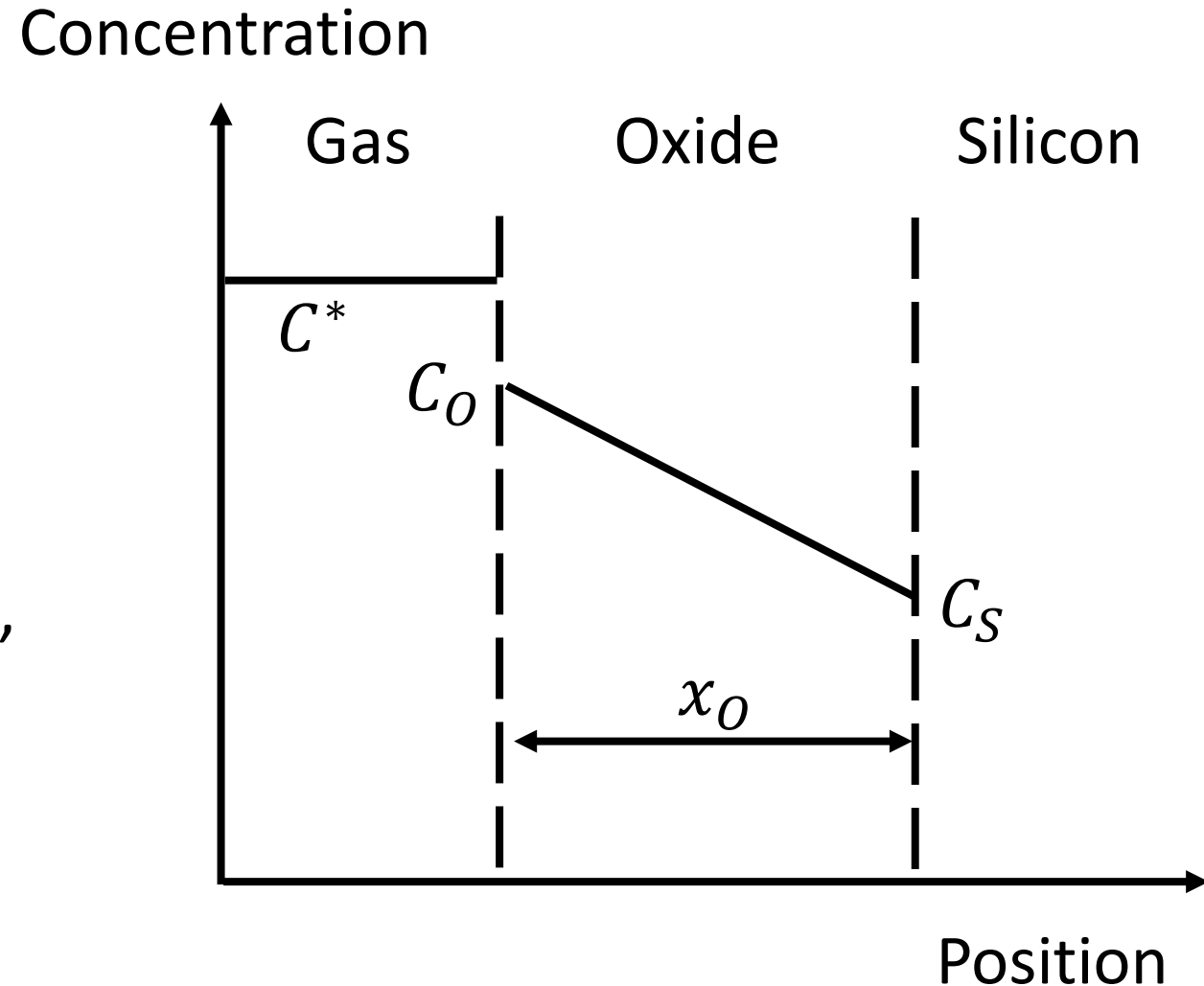
- (1) $F_1 = h(C^* - C_O)$

- (2) $F_2 = D \frac{\partial C}{\partial x} = D \frac{C_O - C_S}{x_O}$

- (3) $F_3 = k_s C_S$

- When $F_1 = F_2 = F_3 = F$,
we can show:

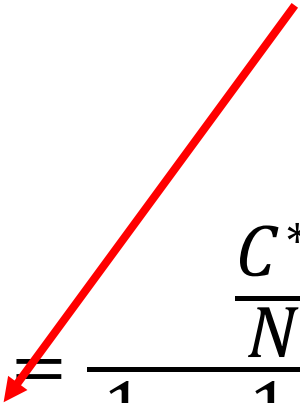
$$F = \frac{C^*}{\frac{1}{k_s} + \frac{1}{h} + \frac{x_O}{D}}$$



Derivation (2)

$N = 2.3 \times 10^{22} \text{ /cm}^3$ for dry etching
 $N = 4.6 \times 10^{22} \text{ /cm}^3$ for wet etching

- Oxide growth rate

$$\frac{dx_o}{dt} = \frac{F}{N} = \frac{\frac{C^*}{N}}{\frac{1}{k_s} + \frac{1}{h} + \frac{x_o}{D}}$$


– In a simplified form,

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

(Then, what are A and B ?)

– Now we have

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

Derivation (3)

- Integration from $t = 0$ to $t = t$

- After integration,

$$x_O^2 + Ax_O = B(t + \tau)$$

- Of course, τ is related with the initial thickness, x_i .

$$x_i^2 + Ax_i = B\tau$$

- Now, the thickness can be expressed as a function of time:

$$x_O = \frac{A}{2} \left(\sqrt{1 + \frac{4B}{A^2} (t + \tau)} - 1 \right)$$

Two limiting cases

- Long oxidation

- In this case, $\frac{4B}{A^2}(t + \tau)$ becomes dominant.

$$x_O \cong \sqrt{Bt}$$

- Short oxidation

- In this case, $\sqrt{1 + \frac{4B}{A^2}(t + \tau)} \cong 1 + \frac{2B}{A^2}(t + \tau)$.

$$x_O \cong \frac{B}{A}(t + \tau)$$

- Two Deal-Grove parameters, B and $\frac{B}{A}$

Example) Dry oxidation at 1000 °C

- Assume the following Deal-Grove parameters.

$$B = 0.0117 \mu\text{m}^2/\text{hr}$$
$$\frac{B}{A} = 0.0709 \mu\text{m}/\text{hr}$$

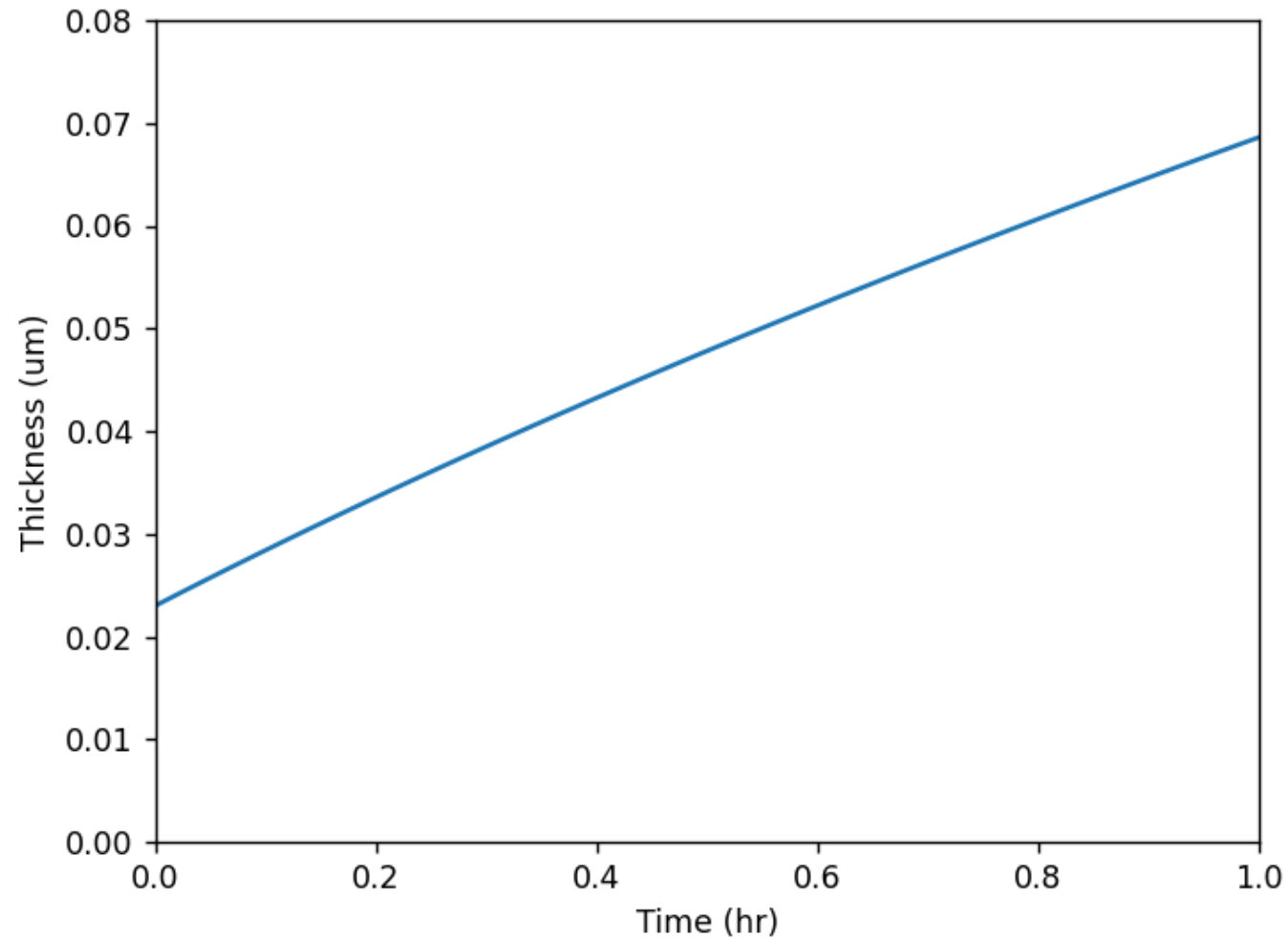
- The time constant is given as

$$\tau = 0.37 \text{ hr}$$

- (It means that the initial thickness, x_i , is 23 nm.)

Result

- How long does it take to have a 40-nm-thick film?



HW#2

- Due: AM08:00, August 30
- Problem#1
 - Draw your own graph for the previous example, by using $x_0 = \frac{A}{2} \left(\sqrt{1 + \frac{4B}{A^2} (t + \tau)} - 1 \right)$. Attach your code.

Time integration

Revisiting the same problem

- Oxide growth rate

- We must solve the following differential equation:

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

- Let us solve the above equation numerically.

- Consider two time instances, t_k and t_{k+1} , which are quite close to each other. Then, the time derivative at t_k is approximated as

$$\left. \frac{dx_o}{dt} \right|_{t_k} \approx \frac{x_o(t_{k+1}) - x_o(t_k)}{t_{k+1} - t_k}$$

Revisiting the same problem

- Equation at t_k

- Under an approximate form,

$$\frac{x_O(t_{k+1}) - x_O(t_k)}{t_{k+1} - t_k} = \frac{B}{A + 2x_O(t_k)}$$

- Now, we can find

$$x_O(t_{k+1}) = x_O(t_k) + (t_{k+1} - t_k) \frac{B}{A + 2x_O(t_k)}$$

- From $x_O(t_k)$, we can calculate $x_O(t_{k+1})$.

- Starting from $t_0 = 0$, we can repeat the above calculation.

HW#2

- Problem#2

– Repeat Problem#1. However, in this case, do not use $x_O = \frac{A}{2} \left(\sqrt{1 + \frac{4B}{A^2} (t + \tau)} - 1 \right)$. Instead, use $x_O(t_{k+1}) = x_O(t_k) + (t_{k+1} - t_k) \frac{B}{A + 2x_O(t_k)}$. Try various values for $t_{k+1} - t_k$. Compare the results obtained from two methods. Attach your code.

Thank you!