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# Computational Microelectronics

## L13

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# Oxidation

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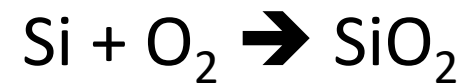
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- Producing a thin layer of silicon dioxide on the surface of a wafer

- Reactions



“Wet”

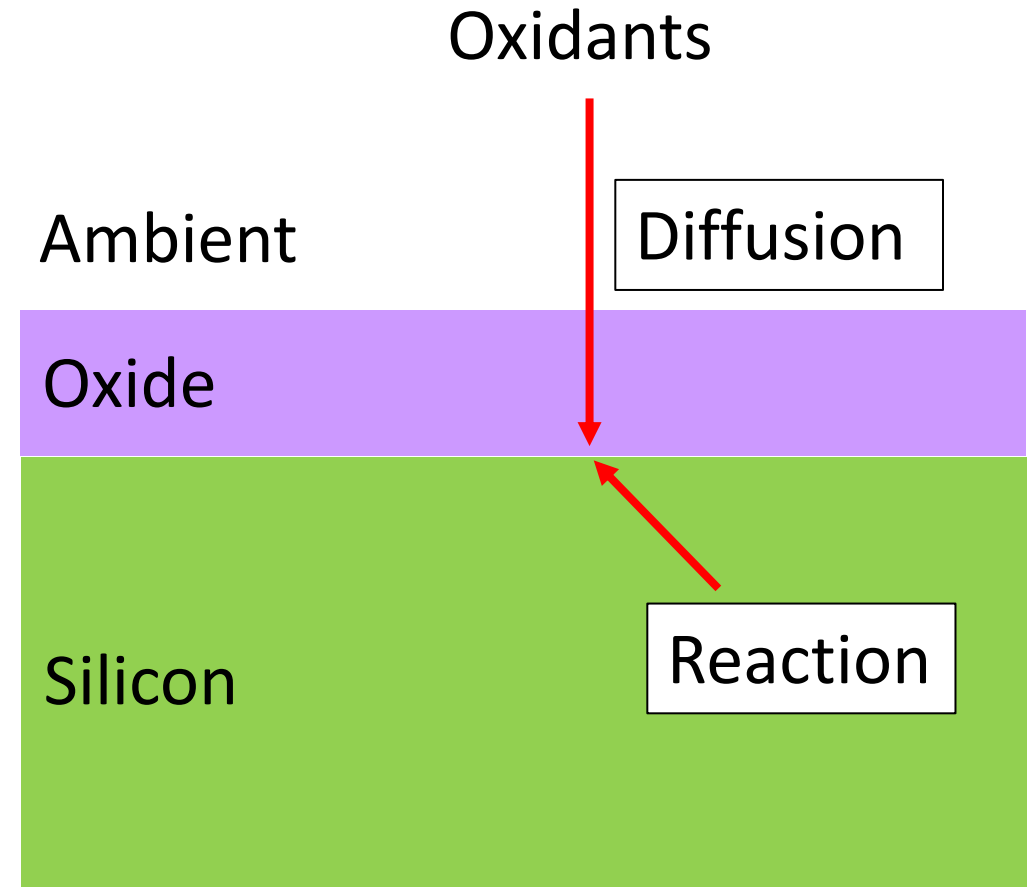


“Dry”

- Amorphous  $\text{SiO}_2$  (Weight density,  $2.27 \text{ g/cm}^3$  or  $2.18 \text{ g/cm}^3$ )
    - Cf.) Crystalline  $\text{SiO}_2$  (Quartz,  $2.65 \text{ g/cm}^3$ )

# Kinetics

- Basic process for the oxidation of silicon
  - Diffusion of oxidants
  - Reaction at the interface
- 125 % volume expansion
  - $\text{SiO}_2$ :  $2.3 \times 10^{22}$  molecules/cm<sup>3</sup>
  - Si:  $5 \times 10^{22}$  atoms/cm<sup>3</sup>



# Oxidation parameters

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- 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

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- 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  $\text{SiO}_2$  (Reaction)

# Derivation (1)

- Flux equations

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

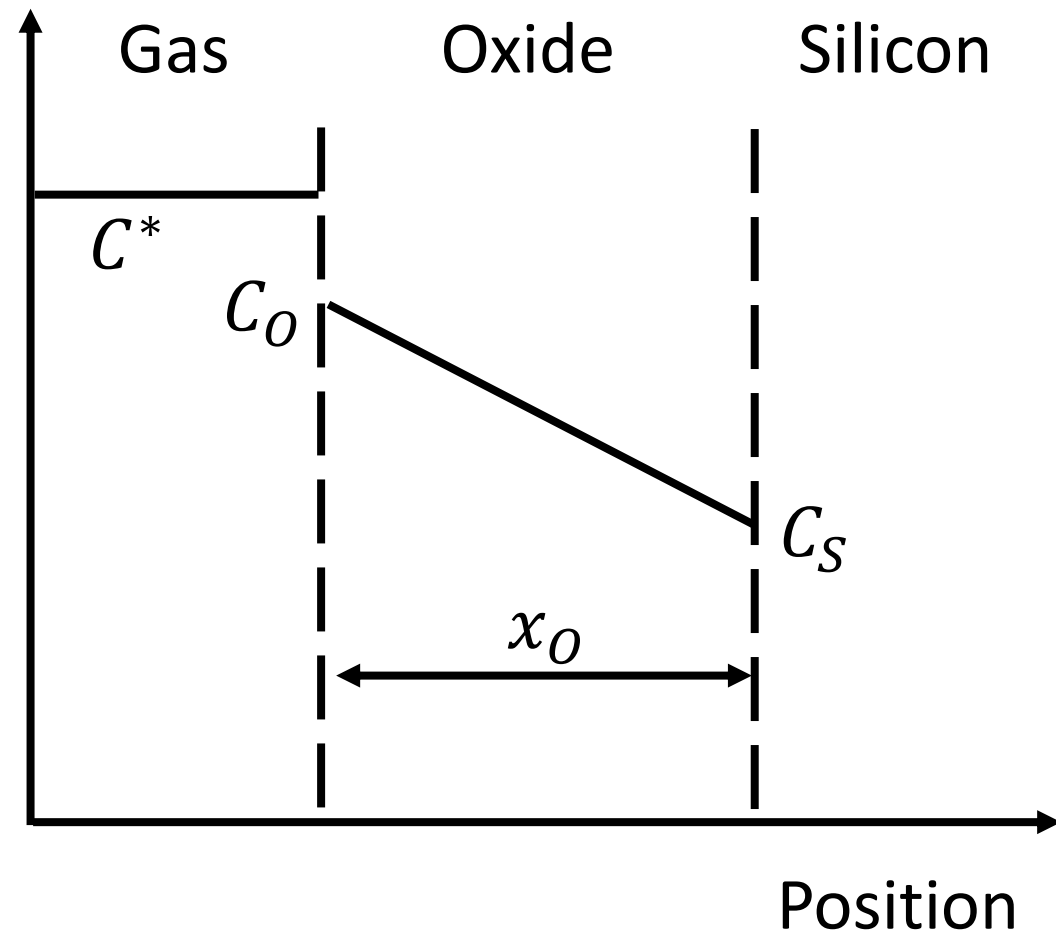
- (2)  $F_2 = D \frac{\partial C}{\partial x} = D \frac{C_O - C_S}{x_O}$

- (3)  $F_3 = k_S C_S$

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

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

Concentration



# Derivation (2)

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

- 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)

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

- After integration,

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

- Of course,  $\tau$  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

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- 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

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- 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

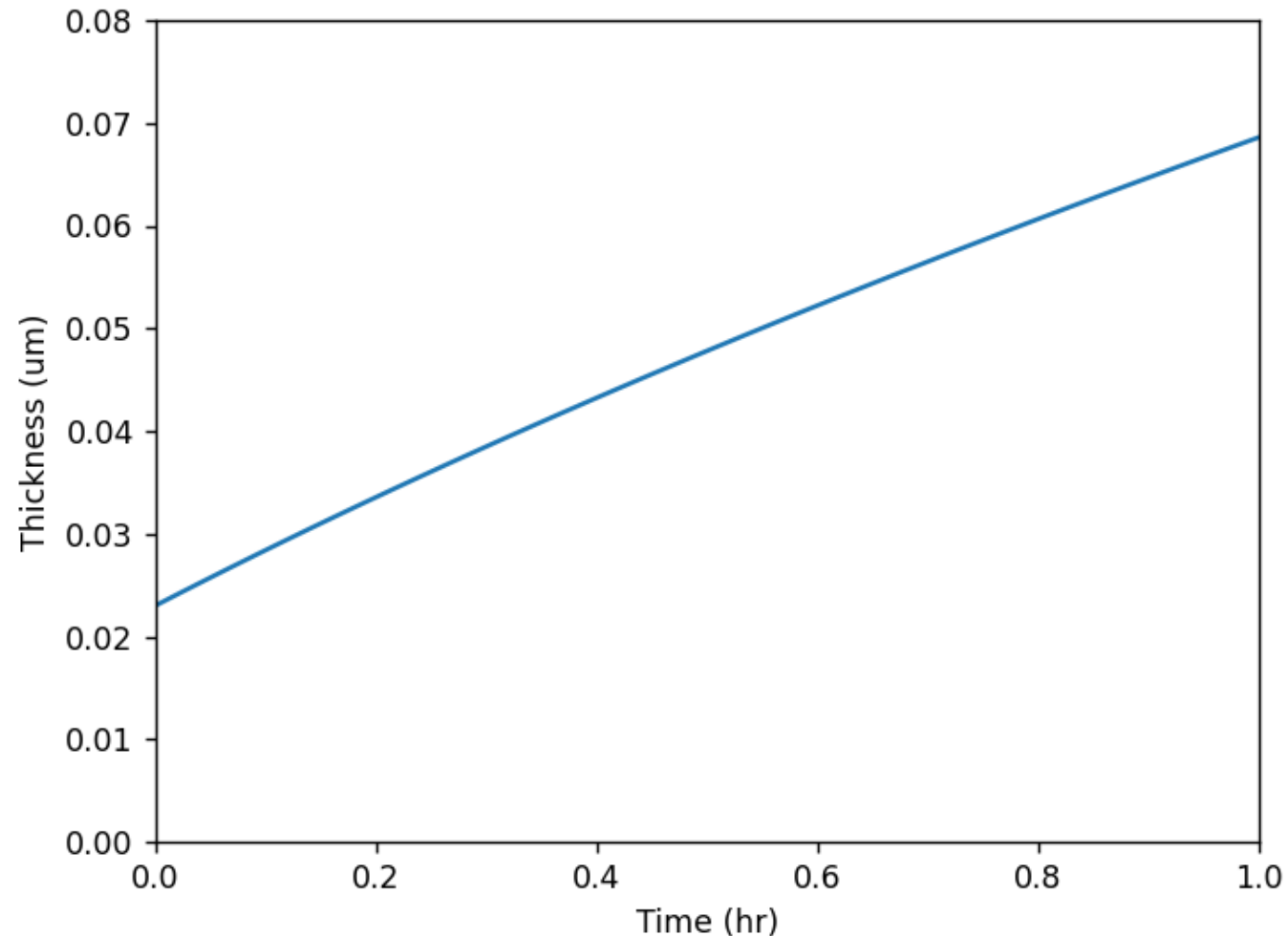
$$\tau = 0.37 \text{ hr}$$

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

# Result

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



# Revisiting the same problem

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- 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

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

Forward Euler

# Forward Euler

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- 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.

# Backward Euler

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- Equation at  $t_k$

- Under an approximate form,

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

- Now, we can find

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

- From  $x_O(t_{k-1})$ , we can calculate  $x_O(t_k)$ . **← Nonlinear**
  - Starting from  $t_1 = \Delta t$ , we can repeat the above calculation.

# Homework#13

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- Due: AM08:00, November 5
- Problem#1
  - Solve the example with the forward/backward Euler scheme.
  - Change  $\Delta t$  and observe the results.



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**Thank you for your attention!**