Computational Microelectronics L13

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Oxidation

Oxidation

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

$$Si + 2H_2O \rightarrow SiO_2 + 2H_2$$ "Wet"

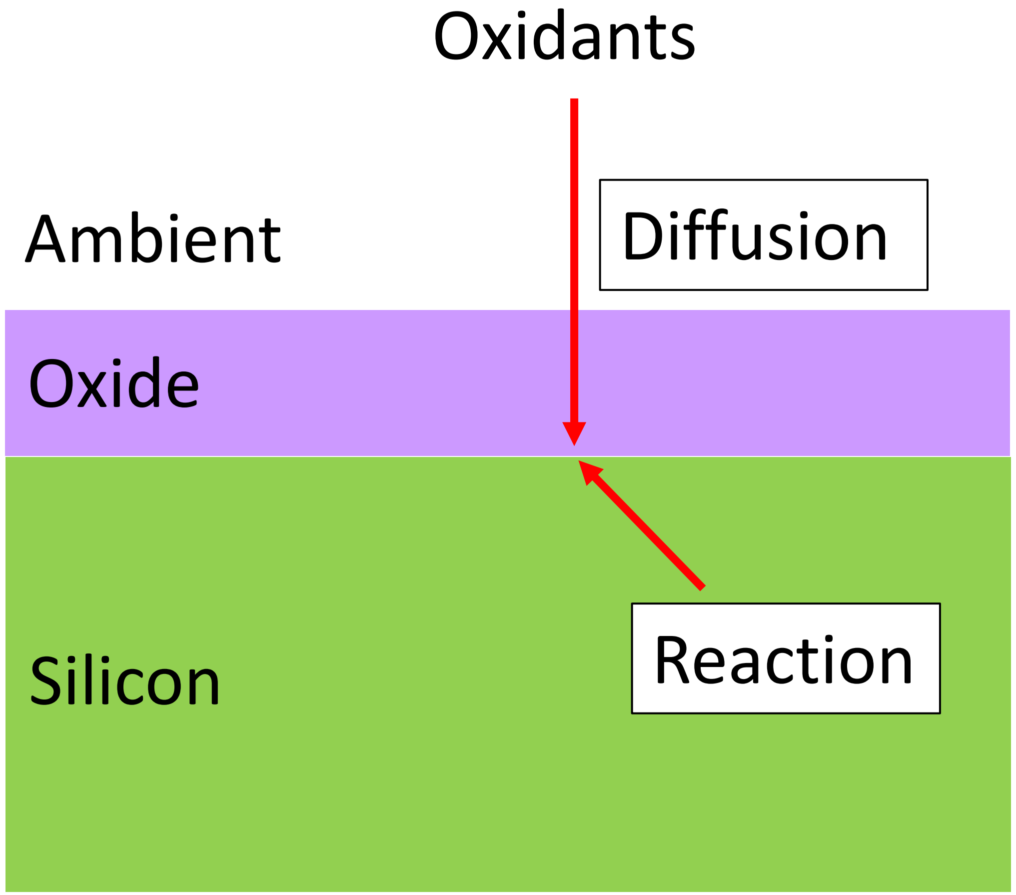
$$Si + O_2 \rightarrow SiO_2$$ "Dry"

  - Amorphous SiO_2 (Weight density, 2.27 g/cm^3 or 2.18 g/cm^3)
  - Cf.) Crystalline SiO_2 (Quartz, 2.65 g/cm^3)

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/cm^3
  - Si: 5×10^{22} atoms/cm^3



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 gate 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)

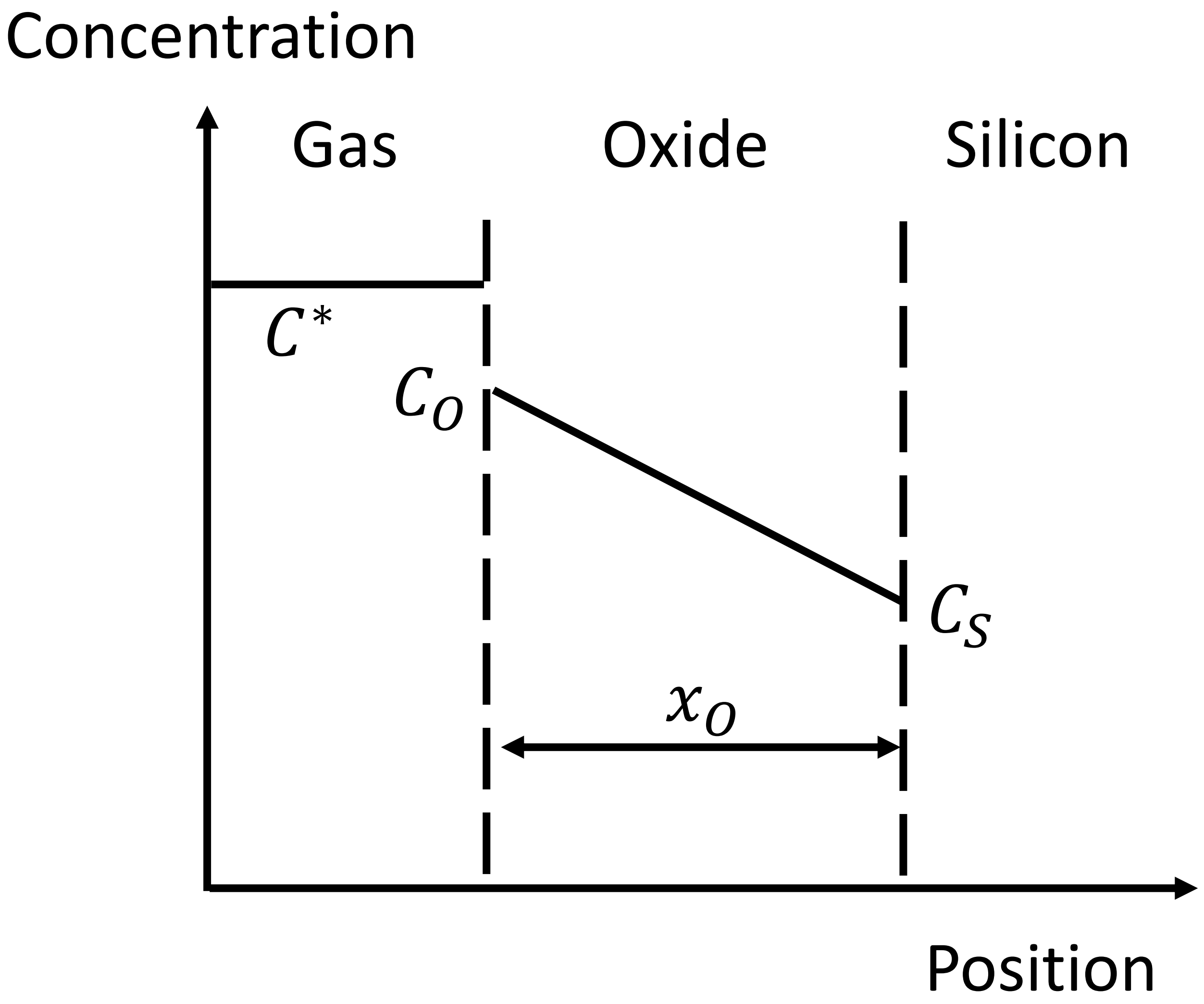
Derivation (1)

- 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 = 2.3X10^{22} /cm^3 for dry oxidation
N = 4.6X10^{22} /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)

- 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.

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

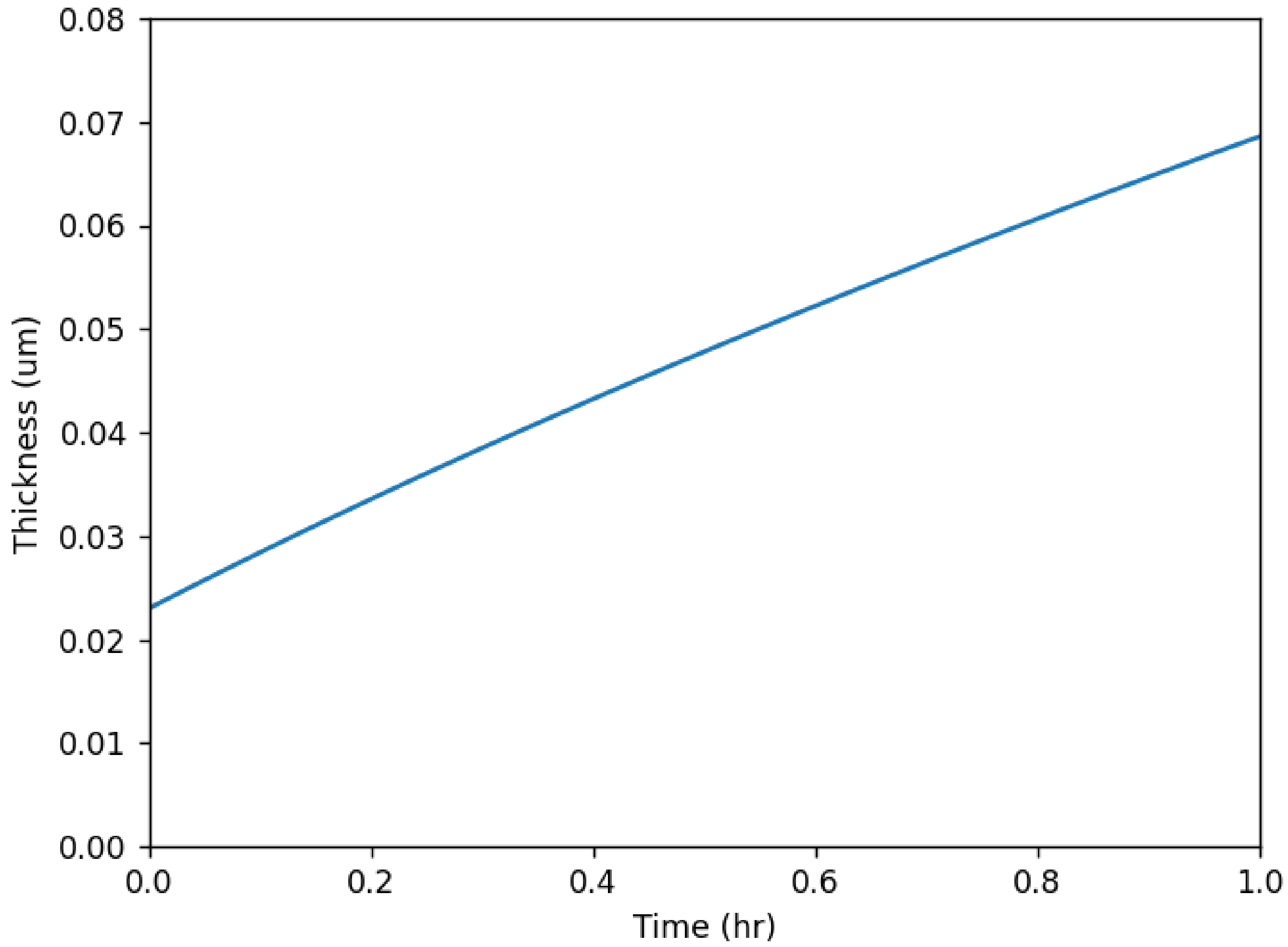
  - The time constant is given as

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

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

Result

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



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

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

Forward Euler

Forward Euler

- 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.

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Backward Euler

- 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

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

Thank you for your attention!