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Chemical Processes for Micro- and Nanofabrication
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Lecture 11
Thermal Oxidation, part 2

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Reading:
Chapter 4, *Fabrication Engineering at the Micro- and Nanoscale*, 4th edition, Campbell

Deal-Grove Model

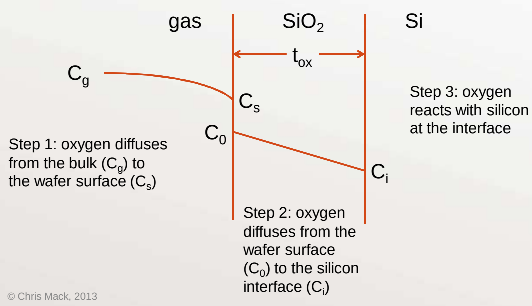
- Silicon Dioxide is grown in a furnace by supplying a source of oxygen to the silicon surface and reacting at a high temperature
- Bruce Deal and Andy Grove (of Fairchild Semiconductor) developed a simple kinetic mechanism/model for oxide growth

B. E. Deal and A. S. Grove, "General Relationship for the Thermal Oxidation of Silicon", *Journal of Applied Physics*, **36**(12), 3770–3778 (Dec, 1965).

Deal-Grove Mechanism

- Three-step mechanism:
  - Oxygen diffuses through the gas to the top of the wafer
  - Oxygen diffuses through the oxide that has formed on the wafer to the Si interface
  - Oxygen reacts with silicon to form SiO_2
- Limitations of the model
  - 1D model (planar substrates)
  - Not accurate for heavily doped silicon
  - Not accurate for thin oxides, < 20 - 25 nm

Deal-Grove Mechanism



Step 1: Oxygen Diffuses through Gas

- Approximate Fick's first law as a linear equation

$$J_1 = D\frac{dC}{dx} \approx \frac{D_g}{\delta}\left(C_g - C_s\right) = h_g\left(C_g - C_s\right)$$

J_1 = flux of reactant (O) to wafer surface
D_g = diffusivity of reactant in gas
C_g = bulk reactant concentration = $\frac{n}{V} = \frac{P_g}{kT}$
C_s = surface gas concentration
δ = boundary layer thickness
$h_g = D_g/\delta$ = mass transfer coefficient

Henry's Law

- Concentration adsorbed on the surface is proportional to its partial pressure in gas

$$C_0 = HP_s = HC_s kT$$

H = Henry's gas law constant
C_0 = reactant concentration adsorbed on the surface
C_s = gas reactant concentration at surface
k = Boltzmann's constant
T = absolute temperature

Step 2: Oxygen Diffuses through SiO_2

- Approximate Fick's first law as a linear equation

$$J_2 = D\frac{dC}{dx} \approx \frac{D}{t_{ox}}(C_0 - C_i)$$

J_2 = flux of reactant through oxide
D = diffusivity of reactant in SiO_2
C_0 = reactant concentration at top of SiO_2
C_i = reactant concentration at Si interface
t_{ox} = SiO_2 thickness

Step 3: Oxygen Reacts with Silicon

- Assume first-order reaction at the Si interface

$$J_3 = k_s C_i$$

J_3 = flux of reactant as it reacts
k_s = reaction rate constant
C_i = reactant concentration at Si interface

Note: as silicon is consumed, its concentration stays constant since the SiO_2/Si interface moves down

Steady State

- Assume that the Si interface reaction is the rate-limiting step
- Steady state is reached where all fluxes are equal

$$J_1 = J_2 = J_3 = J_{SS}$$

- Solve for the two unknown concentrations (C_0 and C_i) and eliminate them from equation

Steady State Solution

- The result:

$$J_{SS} = \frac{Hk_sP_g}{1 + \frac{k_s}{h} + \frac{k_s t_{ox}}{D}} \qquad where\ \ h = \frac{h_g}{HkT}$$

- We can convert flux of oxygen to rate of oxide growth using the density of oxygen atoms in SiO_2 ($N_1 = 2.2 \times 10^{22}$ cm^{-3})

$$\frac{dt_{ox}}{dt} = \frac{J_{SS}}{N_1}$$

Integrating

$$\frac{dt_{ox}}{dt} = \frac{Hk_sP_g}{N_1\left(1 + \frac{k_s}{h} + \frac{k_s t_{ox}}{D}\right)}$$

$$\left(1 + \frac{k_s}{h} + \frac{k_s t_{ox}}{D}\right)dt_{ox} = \frac{Hk_sP_g}{N_1}dt$$

$$\int_{t_0}^{t_{ox}}\left(1 + \frac{k_s}{h} + \frac{k_s t_{ox}}{D}\right)dt_{ox} = \int_0^t \frac{Hk_sP_g}{N_1}dt$$

Result: the Deal-Grove Model

$$t_{ox}^2 + At_{ox} = B(t + \tau)$$

$$A = 2D\left(\frac{1}{h} + \frac{1}{k_s}\right)$$

$$B = \frac{2DHP_g}{N_1}$$

$$\tau = \frac{t_o^2 + At_o}{B}$$

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WHAT STARTS HERE CHANGES THE WORLD

Lecture 11: What have we learned?

- What are the three sequential steps in the Deal-Grove mechanism?
- What are the limitations of the Deal-Grove model?
- Explain the steady-state assumption used in the derivation
- Be familiar with the derivation of the Deal-Grove model

 13