Lecture 11
Thermal Oxidation, part 2

Chris A. Mack
Adjunct Associate Professor

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

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

Henry’s Law

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

\[ C_g = H P_g = H C_p k T \]

\( H \) = Henry’s gas law constant
\( C_g \) = reactant concentration adsorbed on the surface
\( C_p \) = gas reactant concentration at surface
\( k \) = Boltzmann’s constant
\( T \) = absolute temperature
Step 2: Oxygen Diffuses through SiO₂

- Approximate Fick's first law as a linear equation

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

- \( J_2 \) = flux of reactant through oxide
- \( D \) = diffusivity of reactant in SiO₂
- \( C_0 \) = reactant concentration at top of SiO₂
- \( C_i \) = reactant concentration at Si interface
- \( t_{ox} \) = SiO₂ thickness

Step 3: Oxygen Reacts with Silicon

- Assume first-order reaction at the Si interface

\[ J_3 = k_r C_i \]

- \( J_3 \) = flux of reactant as it reacts
- \( k_r \) = reaction rate constant
- \( C_i \) = reactant concentration at Si interface

Note: as silicon is consumed, its concentration stays constant since the SiO₂/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

Integrating

\[
\begin{align*}
\frac{dt_{ox}}{dt} &= \frac{Hk_r P_g}{N_1 \left( 1 + \frac{k_s}{n} + \frac{k_r t_{ox}}{D} \right)} \\
\left( 1 + \frac{k_s}{n} + \frac{k_r t_{ox}}{D} \right) dt_{ox} &= \frac{Hk_r P_g}{N_1} dt \\
\int_{t_0}^{t_{ox}} \left( 1 + \frac{k_s}{n} + \frac{k_r t_{ox}}{D} \right) dt_{ox} &= \int_{t_0}^{t_{ox}} \frac{Hk_r P_g}{N_1} dt \\
\end{align*}
\]

Result: the Deal-Grove Model

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

- \( A = 2D \left( \frac{1}{h} + \frac{1}{k_s} \right) \)
- \( B = \frac{2DHk_r P_g}{N_1} \)
- \( \tau = \frac{t_{ox}^2 + At_{ox}}{B} \)
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