Thermal Oxidation of Si

- General Properties of SiO_2
- Applications of thermal SiO_2
- Deal-Grove Model of Oxidation

Thermal SiO_2 is amorphous.
Weight Density = 2.2 gm/cm^3
Molecular Density = 2.3E22 molecules / cm^3

Crystalline SiO_2 [Quartz] = 2.65 gm/cm^3

Thermal SiO_2 Properties

(1) Excellent Electrical Insulator

Resistivity > 1E20 ohm-cm

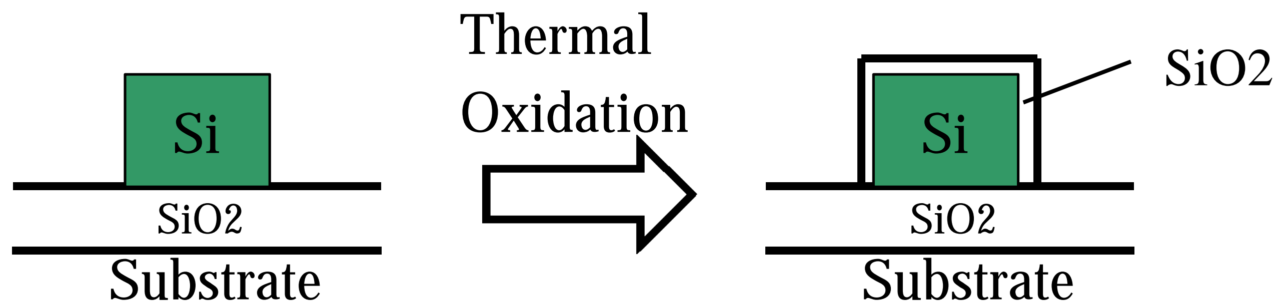
Energy Gap ~ 9 eV

(2) High Breakdown Electric Field

> 10MV/cm

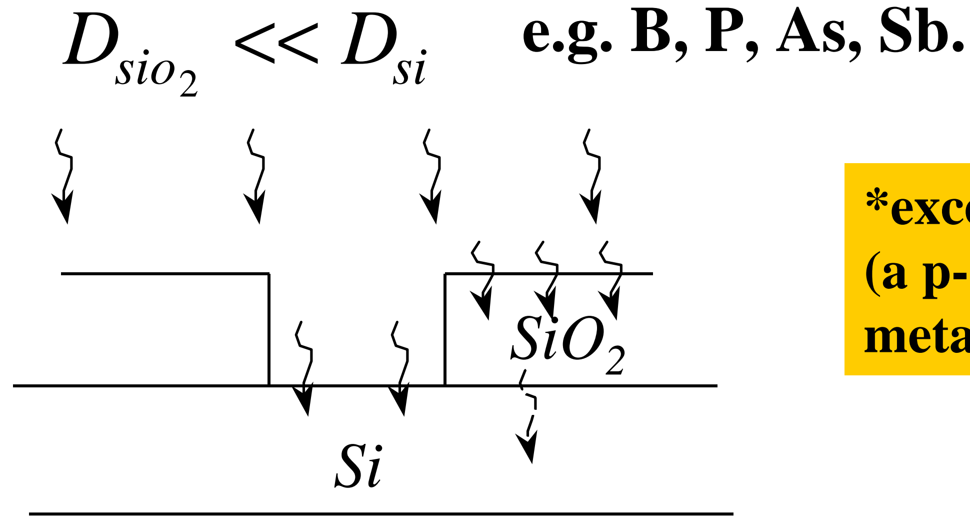
(3) Stable and Reproducible Si/SiO_2 Interface

(4) Conformal oxide growth on exposed Si surface



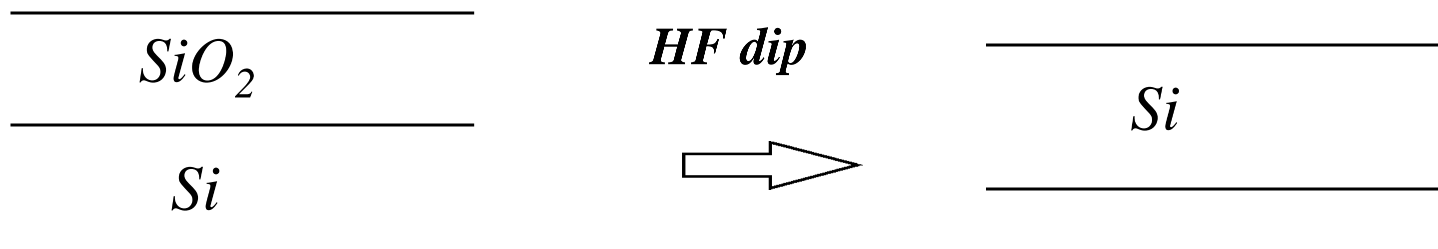
(5) SiO_2 is a good diffusion mask for common dopants

$D_{sio_2} << D_{si}$ **e.g. B, P, As, Sb.**

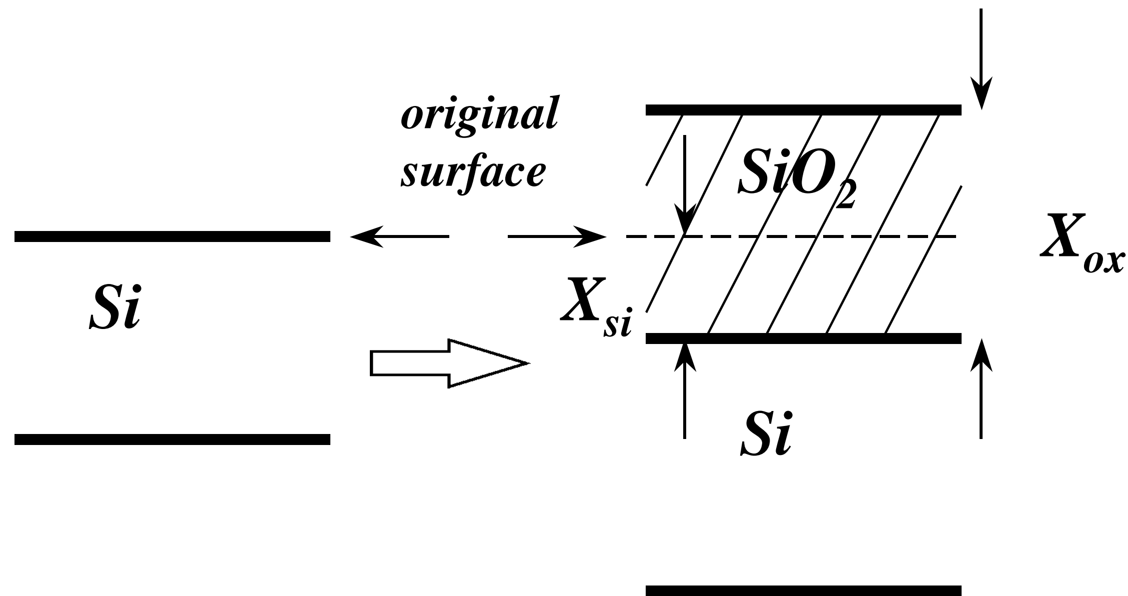


***exceptions are Ga (a p-type dopant) and some metals, e.g. Cu, Au**

(6) Very good etching selectivity between Si and SiO_2.



Thickness of Si consumed during oxidation



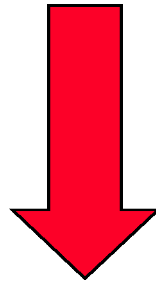
$$X_{si} = X_{ox} \bullet \frac{N_{ox}}{N_{si}}$$

molecular density of SiO2

atomic density of Si

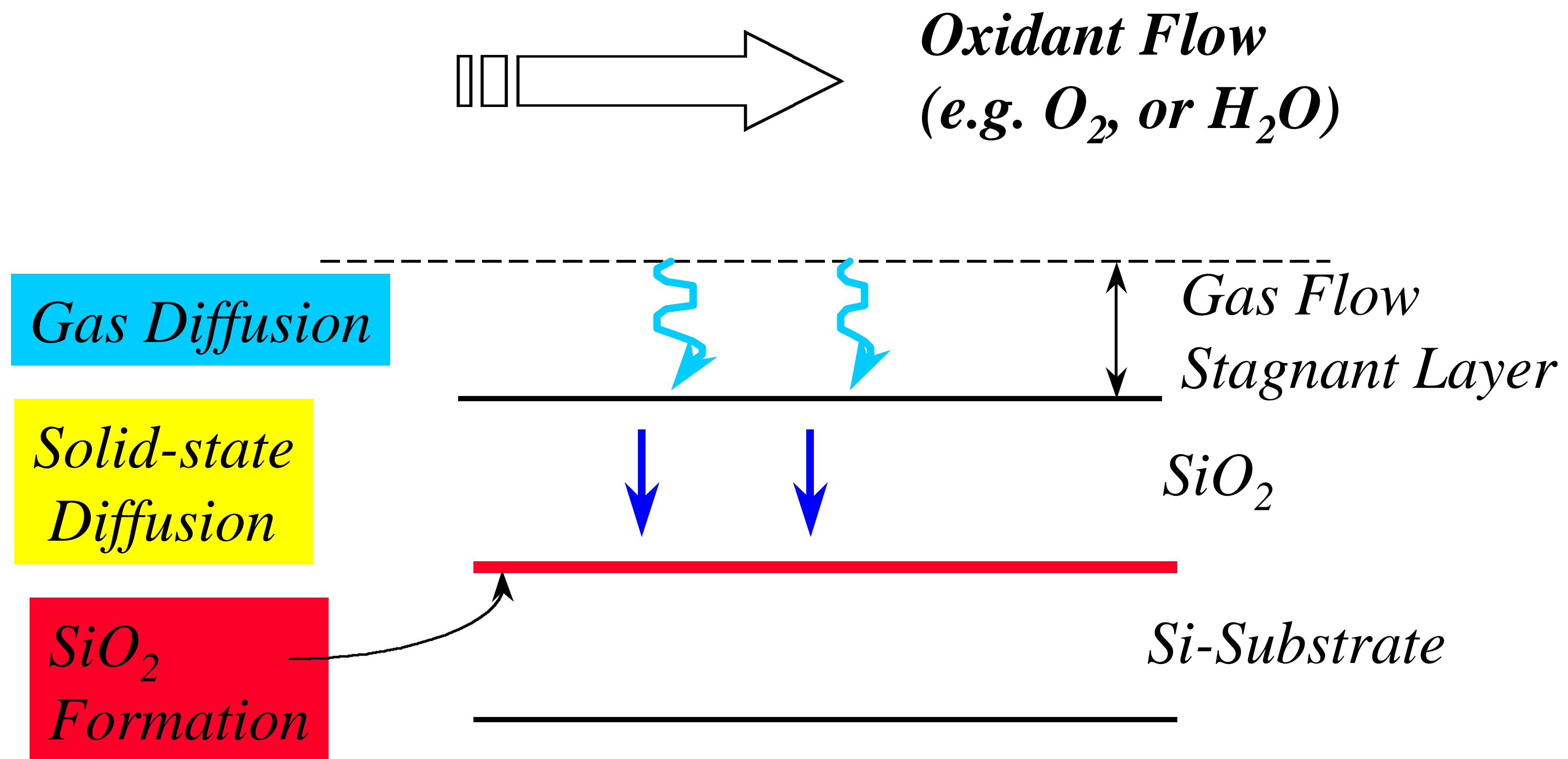
$$= X_{ox} \bullet \frac{2.3 \times 10^{22} \, molecules / cm^3}{5 \times 10^{22} \, atoms / cm^3} = 0.46 X_{ox}$$

1μm Si oxidized

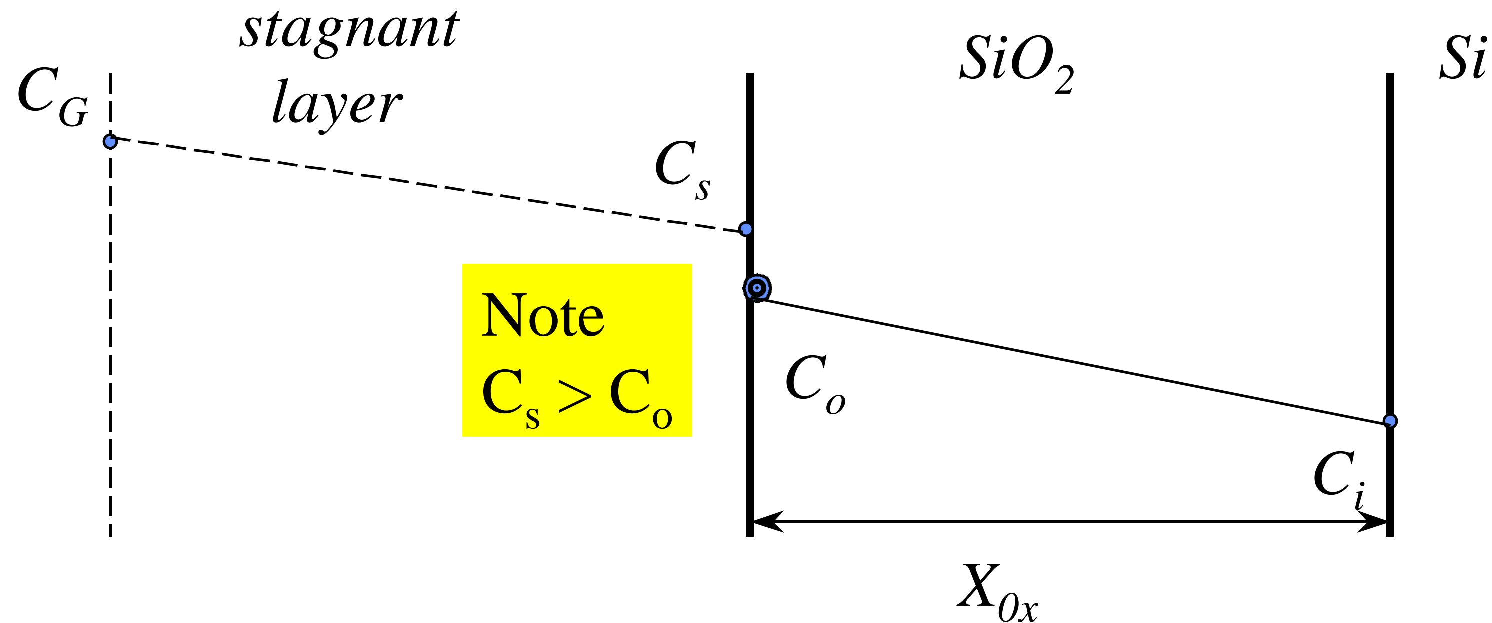


2.17 μm SiO_2

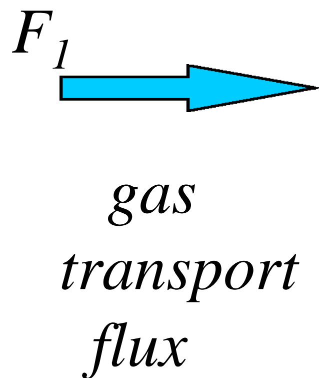
Kinetics of SiO_2 Growth

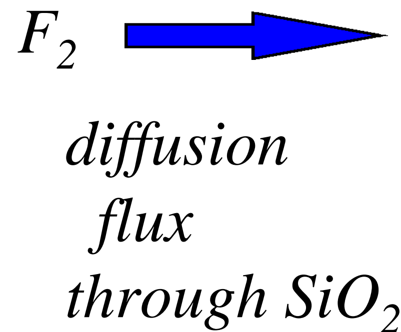


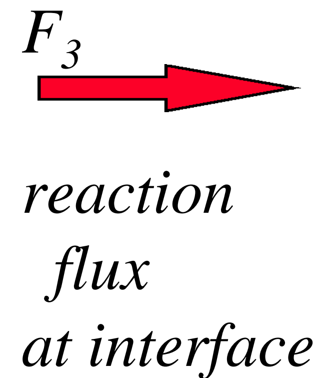
Deal-Grove Model



F_1 F_2 F_3







$$F_1 = h_G(C_G - C_S)$$

$$F_2 = -D\frac{\partial C}{\partial x}$$

Fick's Law of Solid-state Diffusion.

$$\cong D \cdot \left(\frac{C_o - C_i}{X_{ox}} \right)$$

$$F_3 = k_s \cdot C_i$$

We use ***Henry's Law*** to relate C_o and C_s

$$C_o = H \cdot P_s$$

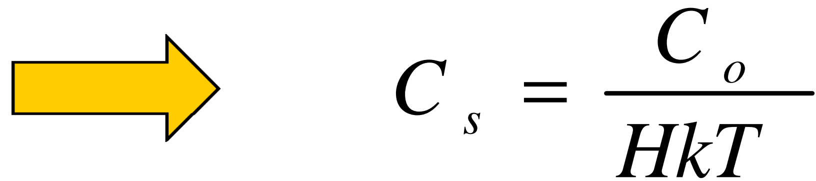
Henry's constant

partial pressure of oxidant at surface [in gaseous form].

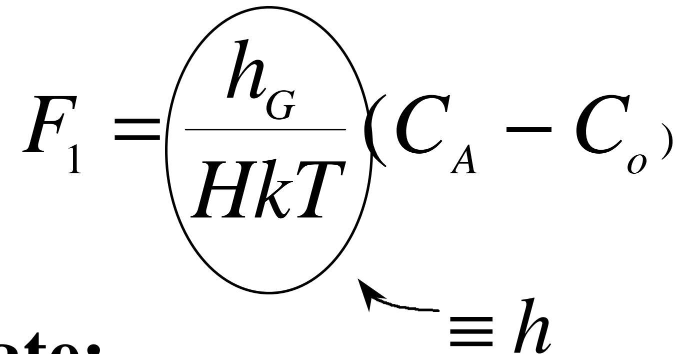
$$= H \cdot (kT \cdot C_s)$$

use $C_s = \frac{N}{V}$

$PV = NkT$



Define $C_A \equiv (HkT \cdot C_G)$



At steady-state:

$$F_1 = F_2 = F_3$$

① ②

2 equations:
2 unknown: C_o & C_i

$$C_i = \frac{C_A}{1 + \frac{k_s}{h} + \frac{k_s X_{ox}}{D}}$$

$$C_o = C_i \cdot \left(1 + \frac{k_s X_{ox}}{D} \right)$$

$$F \left(= F_1 = F_2 = F_3 \right) = k_s \cdot C_i = \frac{k_s C_A}{1 + \frac{k_s}{h} + \frac{k_s X_{ox}}{D}}$$

Now, to convert F into Oxide Thickness Growth Rate

$$F = N_1 \cdot \left(\frac{dX_{ox}}{dt} \right)$$

N_1: *oxidant molecules/unit volume required to form a unit volume of SiO_2.*

ΔX_{ox}

SiO_2 | Si

F →

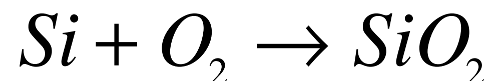
$\{\Delta t\}$

$$\frac{dX_{ox}}{dt} = \frac{F}{N_1}, \quad F = \frac{k_s C_A}{1 + \frac{k_s}{h} + \frac{k_s X_{ox}}{D}}$$

$$N_1 \bullet \frac{dX_{ox}}{dt} = \left[\frac{k_s C_A}{1 + \frac{k_s}{h} + \frac{k_s X_{ox}}{D}} \right]$$

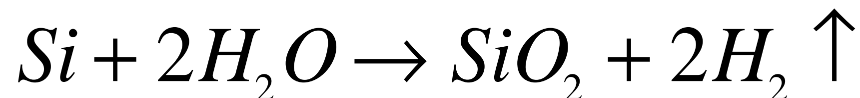
[Comment]

$N_1 = 2.3 \times 10^{22} / cm^3$ *for O_2 as oxidant*



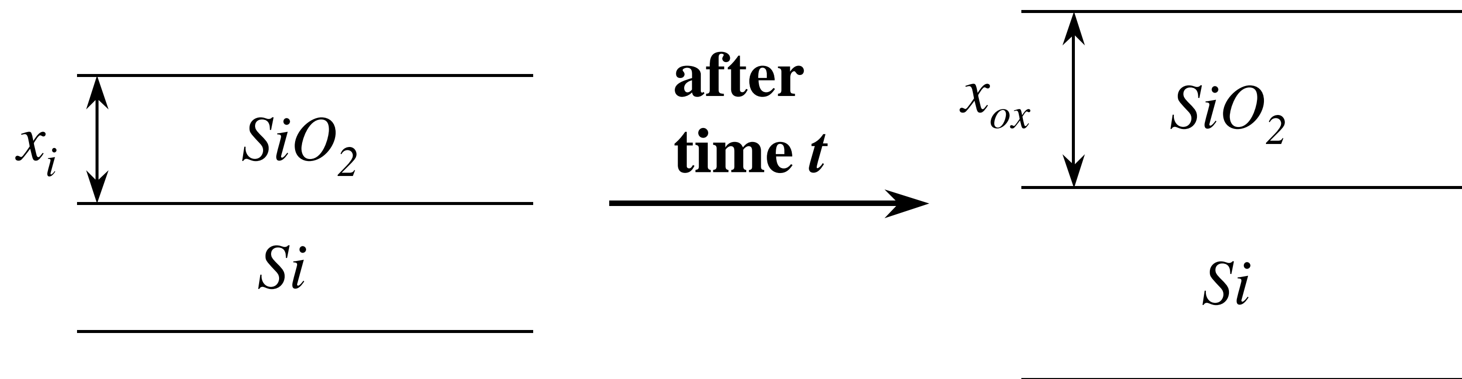
$$Si + O_2 \rightarrow SiO_2$$

$N_1 = 4.6 \times 10^{22} / cm^3$ *for H_2O as oxidant*



$$Si + 2H_2O \rightarrow SiO_2 + 2H_2 \uparrow$$

Boundary Condition: At $t = 0$, $X_{ox} = X_i$



Solution

$$X_{ox}^{2} + AX_{ox} = B(t + \tau)$$

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

$$B \equiv \frac{2DC_A}{N_1}$$

$$\tau = \frac{X_i^{2} + AX_i}{B}$$

$$X_{ox} = \frac{A}{2}\left\{\sqrt{1+\left(\frac{t+\boldsymbol{t}}{A^2/4B}\right)}-1\right\}$$

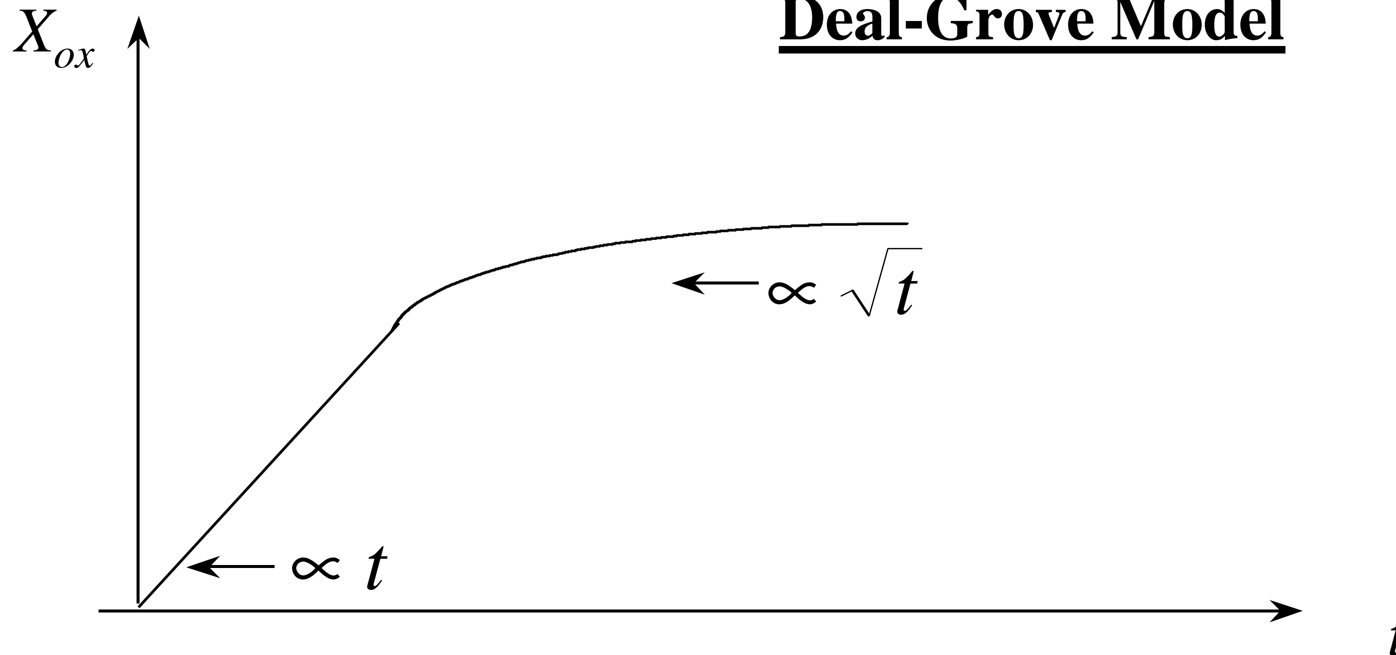
(Case 1) Large t [large X_{ox}]

$$\boldsymbol{X_{ox} \rightarrow \sqrt{Bt}}$$

(Case 2) Small t [Small X_{ox}]

$$\boldsymbol{X_{ox} \rightarrow \frac{B}{A}t}$$

Deal-Grove Model



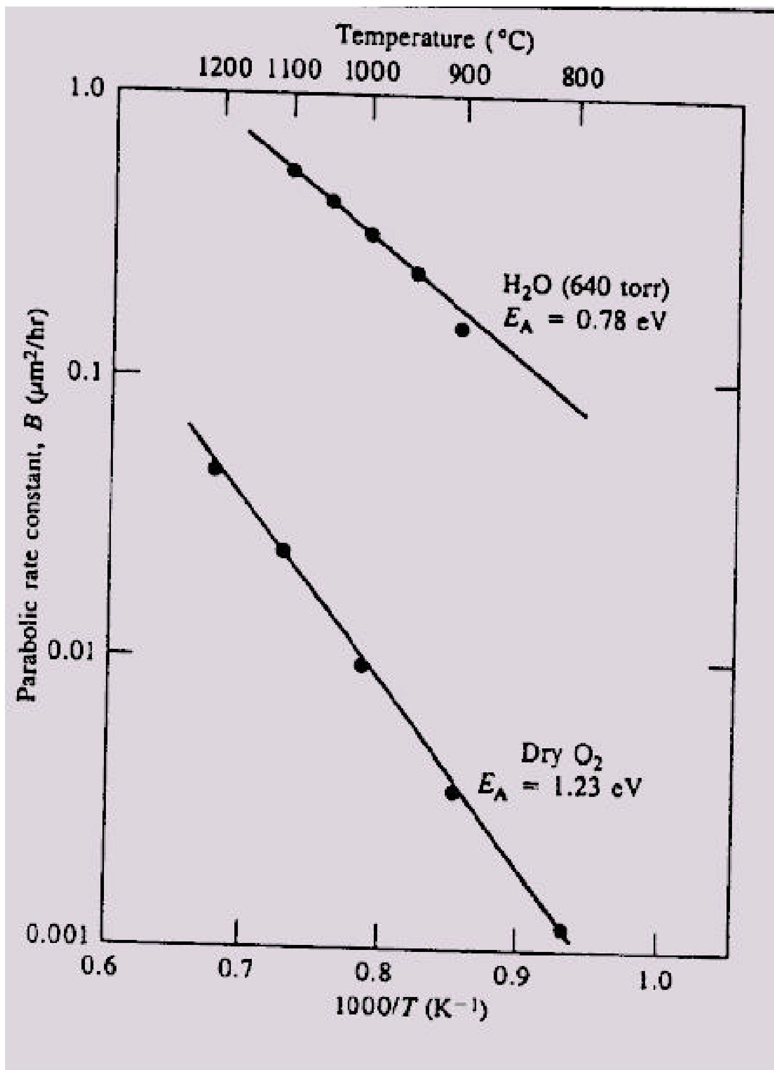
$$X_{ox}^{2} + AX_{0x} = B(t + t)$$

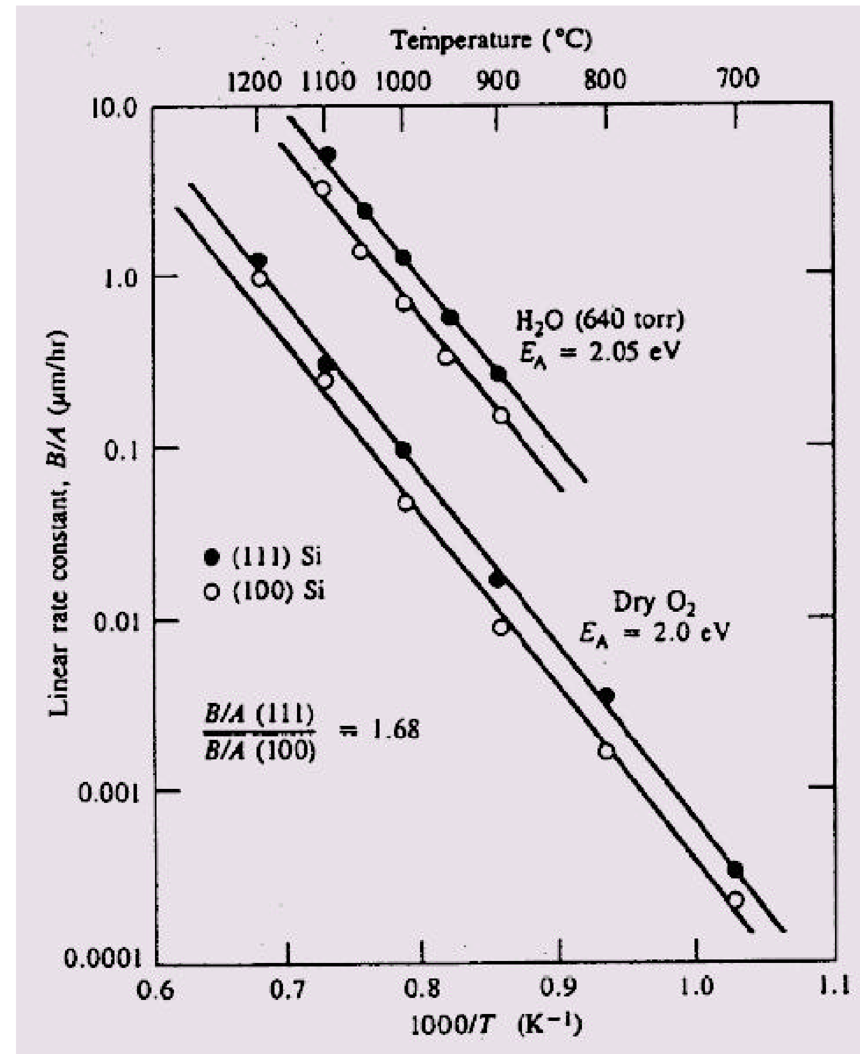
$$2X_{ox}\frac{dx_{ox}}{dt} + A\frac{dx_{ox}}{dt} = B$$

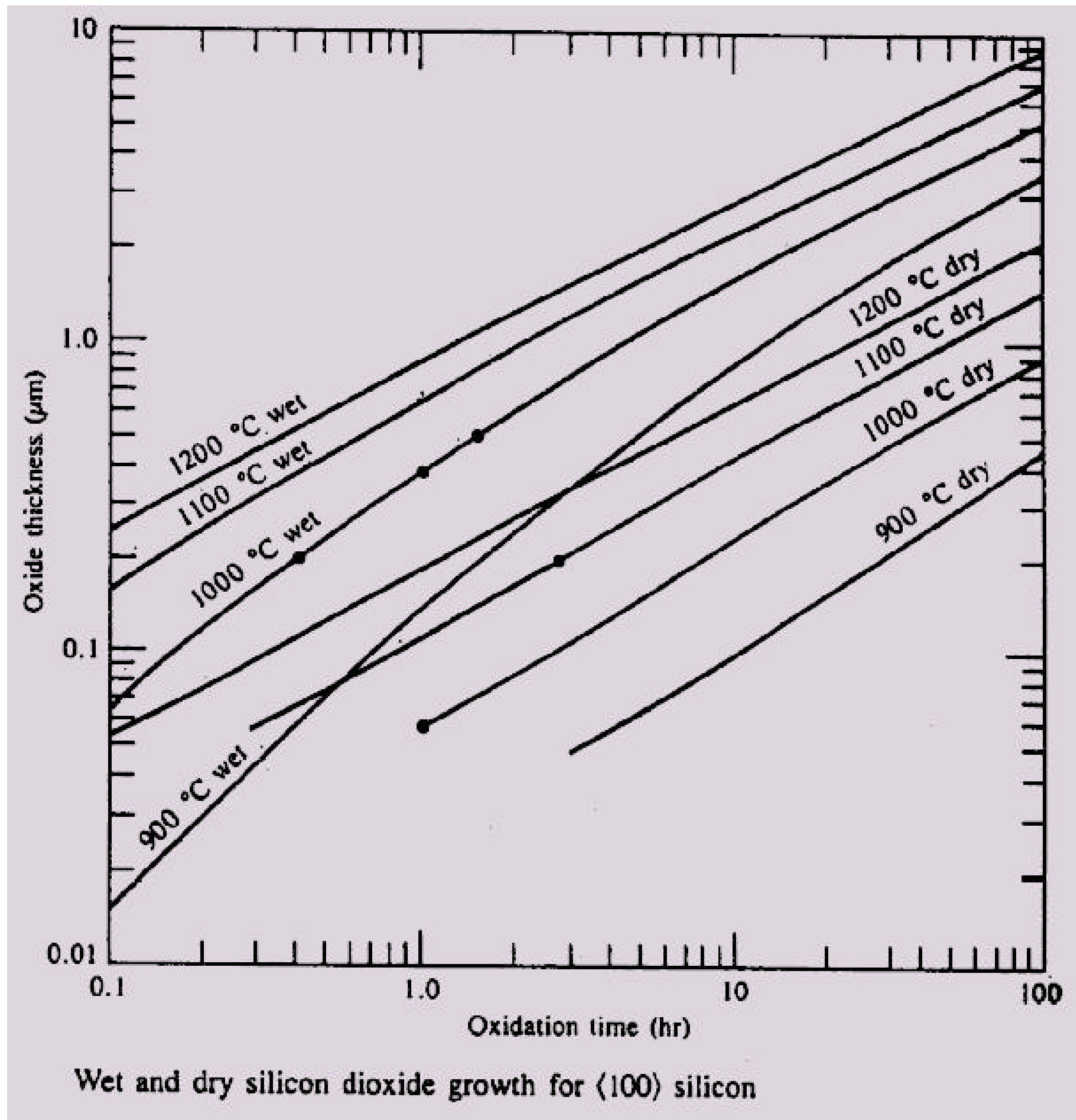
$$\therefore \frac{dx_{ox}}{dt} = \frac{B}{A + 2X_{ox}}$$

Oxide Growth Rate slows down with increase oxide thickness

B = Parabolic Constant
B/A = Linear Constant







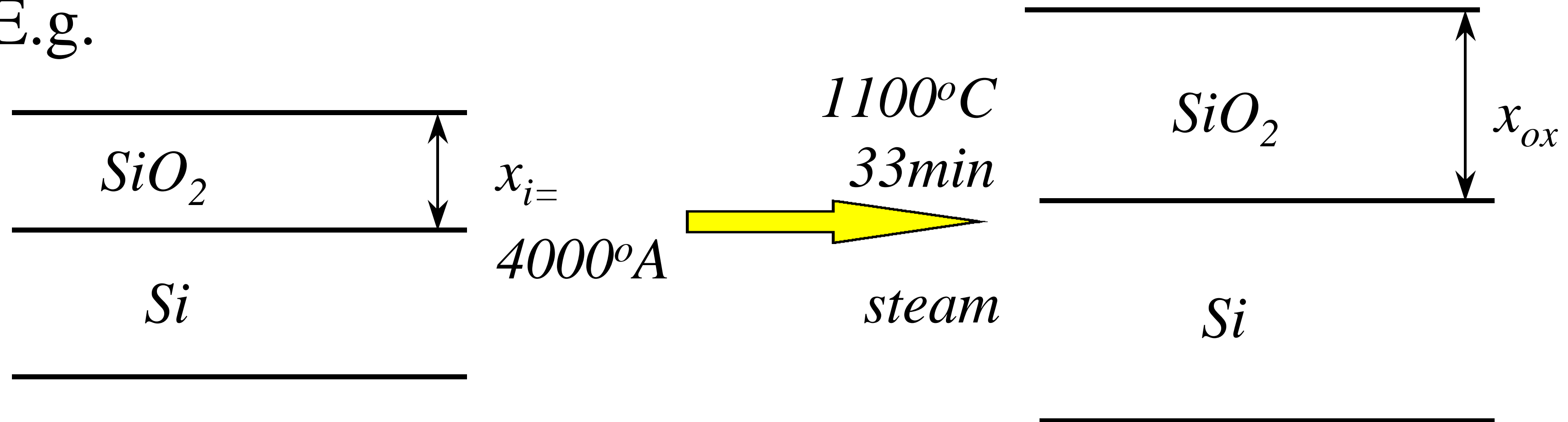
Oxidation Charts

The charts are based on

$X_i = 0$!

Two Ways to Calculate Oxide Thickness Grown by Thermal Oxidation

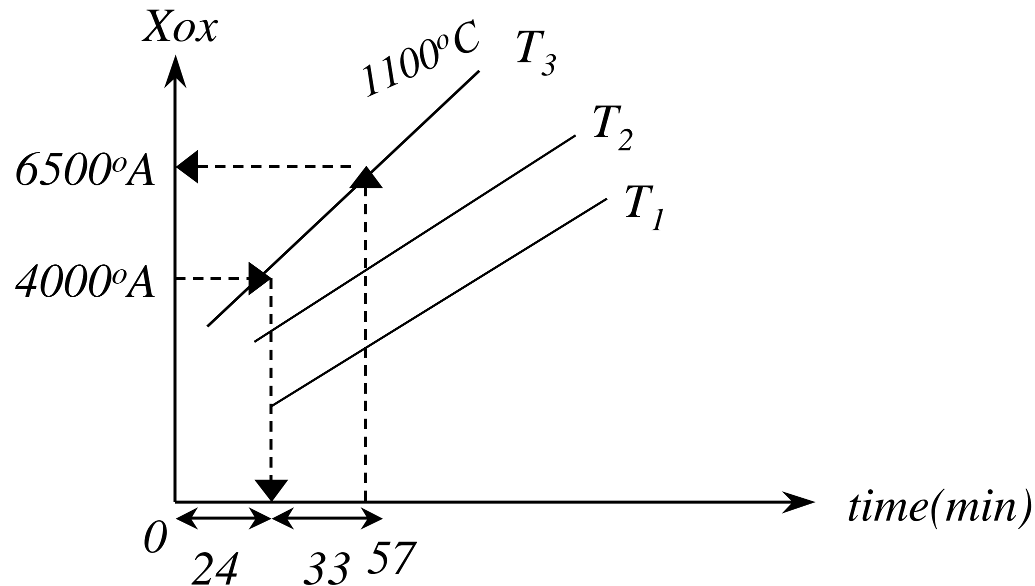
E.g.



Method 1: Find B & B/A from Charts

Solve $$X_{ox}^{2} + AX_{ox} = B(t + \boldsymbol{t})$$

Method 2: Use Oxidation Charts



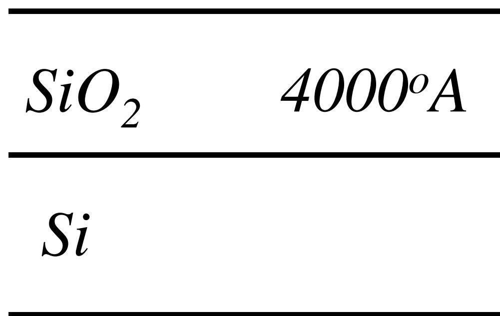
The charts are based on $X_i = 0$!

$$X_i = 4000\ A \Rightarrow t = 24 \text{ min}$$ *at 1100°C from chart*

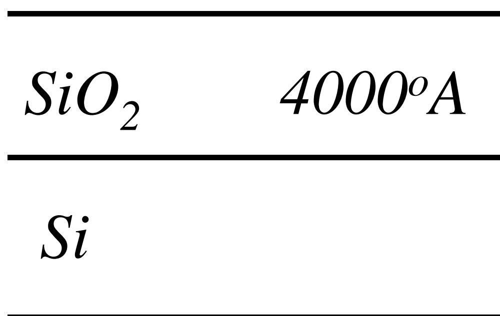
∴ Total effective oxidation time

$$(24 + 33) \text{ min} = 57 \text{ min}$$ *if start with* $X_i = 0$

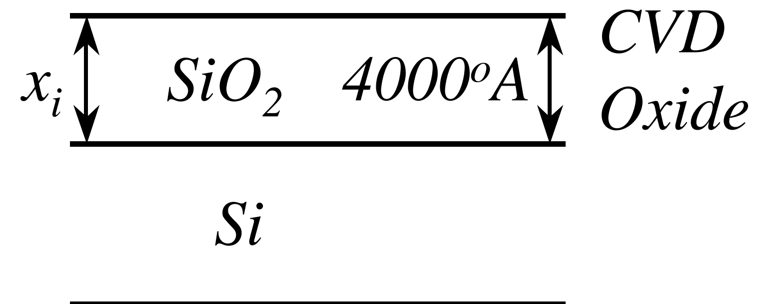
(1) Grown at 1000°C, *t=5hrs*



(2) Grown at 1100°C, *24min*



(3) CVD Oxide



τ is the same for all three cases shown here

Effect of X_i on Wafer Topography