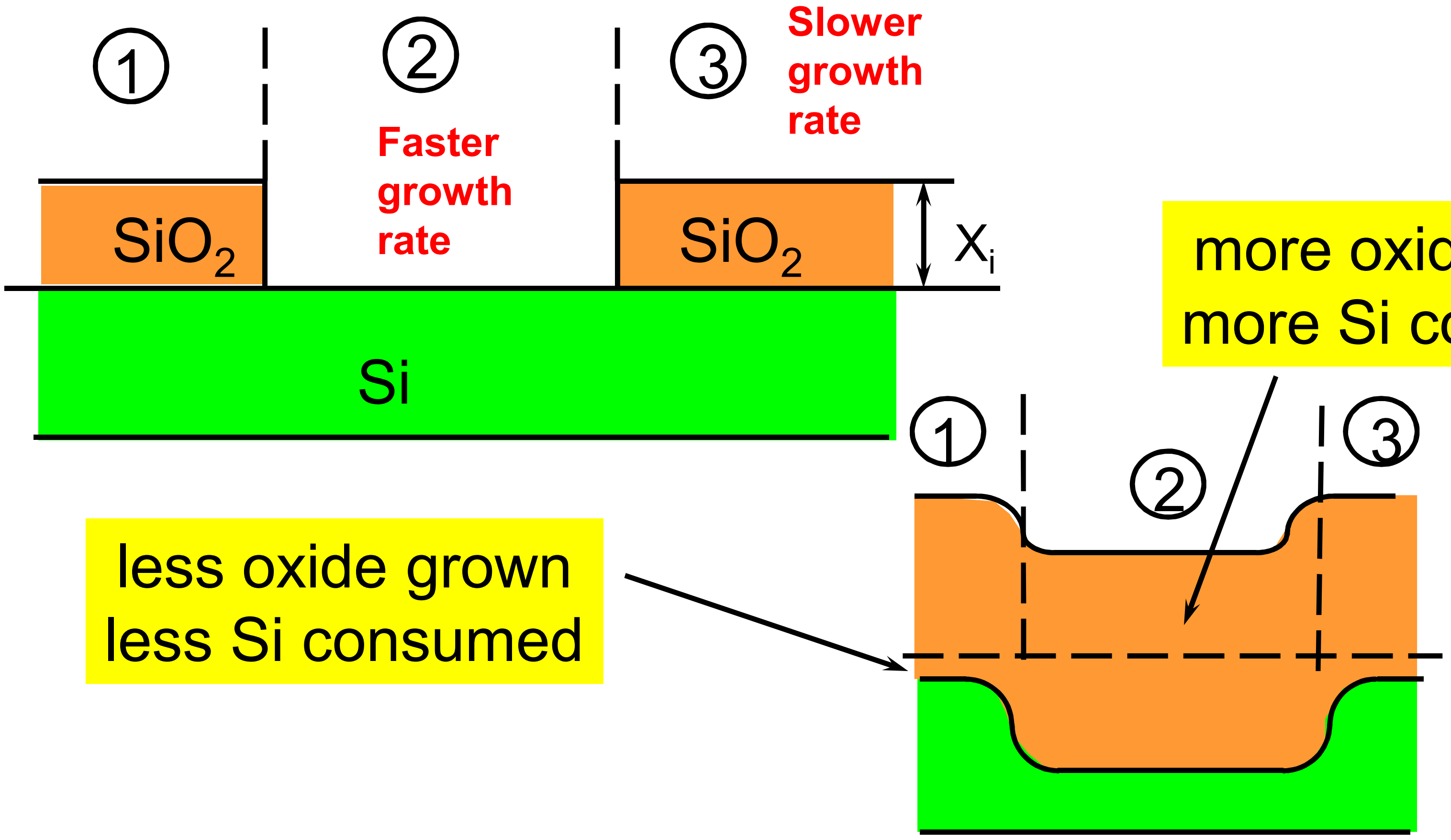
Effect of X_i on Wafer Topography



more oxide grown
more Si consumed

less oxide grown
less Si consumed

Factors Influencing Thermal Oxidation

- Oxidation Temperature
- Ambient Type (Dry O_2, Steam, HCl)
- Ambient Pressure
- Substrate Crystallographic Orientation
- Substrate Doping

High Pressure Oxidation

$$B/A = C_A / [N_1(1/k_s+1/h)] \propto C_A \propto P_G$$

$$B = 2DC_A / N_1 \propto C_A \propto P_G$$

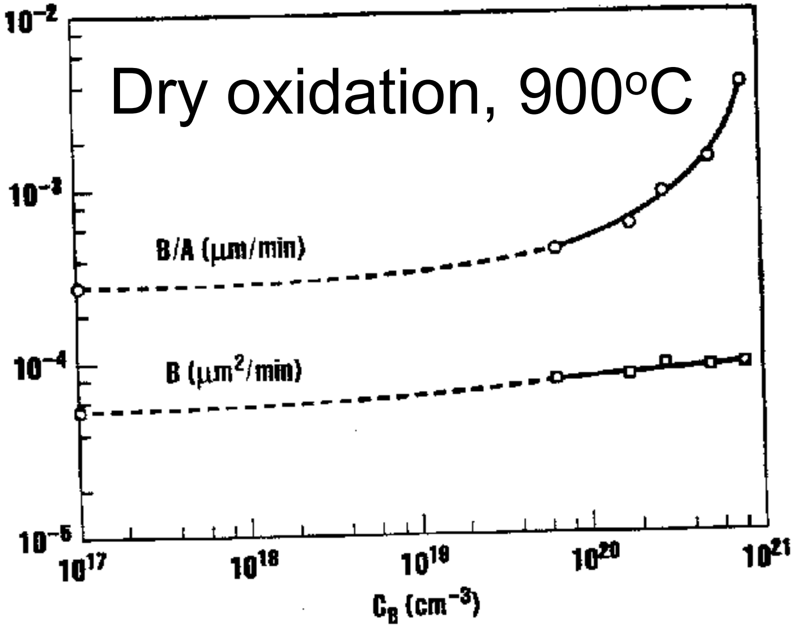
When P_G increases, both B and B/A will increase.
Therefore oxidation rate increases.

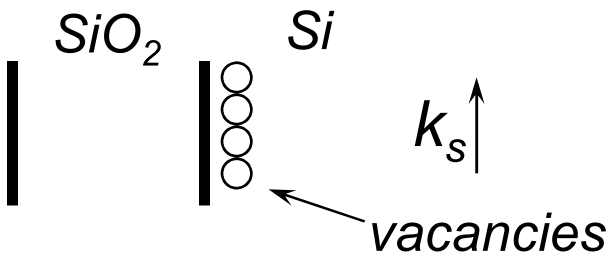
1) The oxidation temperature can be reduced if the pressure is increased, to achieve a given oxidation rate

2) To grow a given oxide thickness at same temperature, time can be reduced

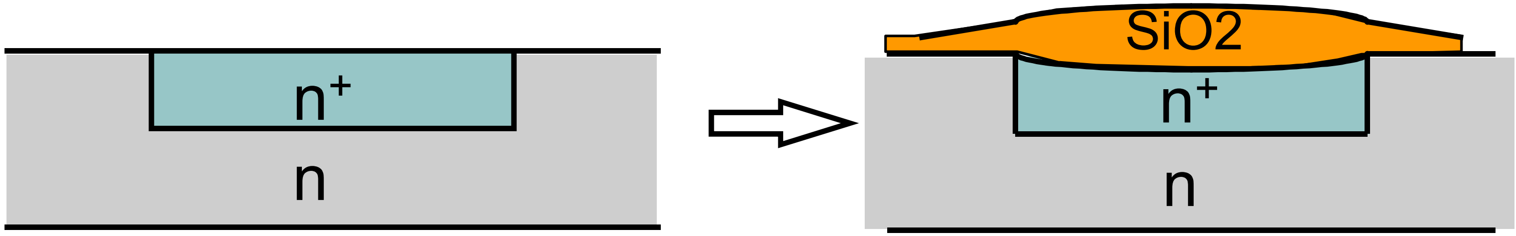
High Doping Concentration Effect

Coefficients for dry oxidation at 900°C
as function of surface Phosphorus concentration

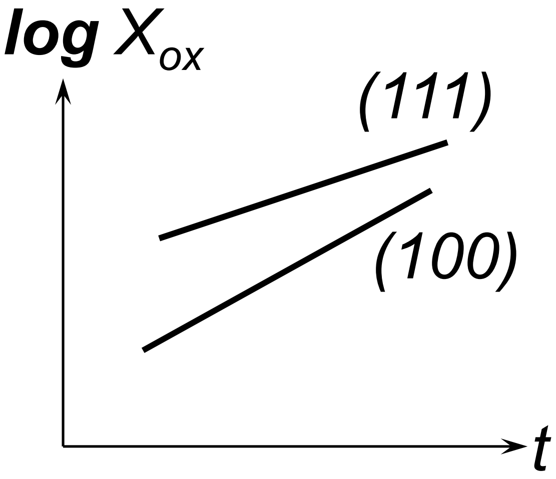


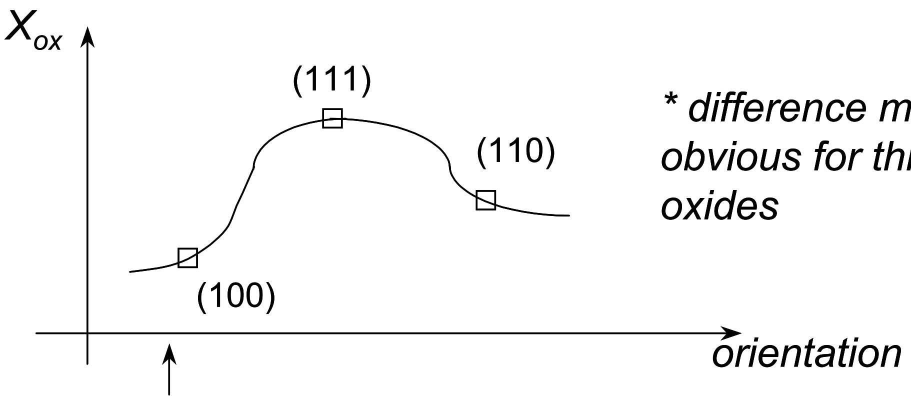


* highly doped Si has more vacancies



Substrate Orientation Effect

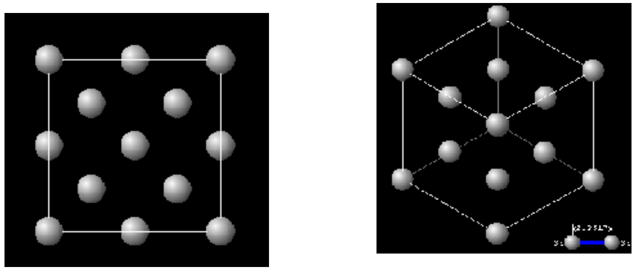


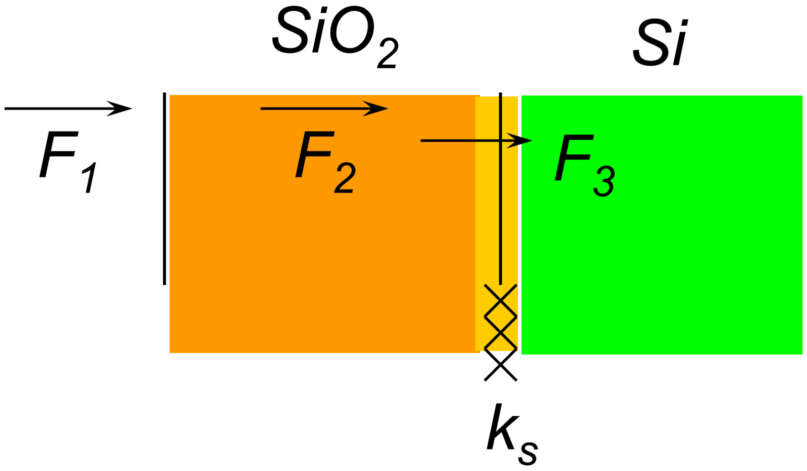


** difference more obvious for thin oxides*

most IC's made with (100) Si

Reason:
(111) surface has more Si bonds than (100) Surface

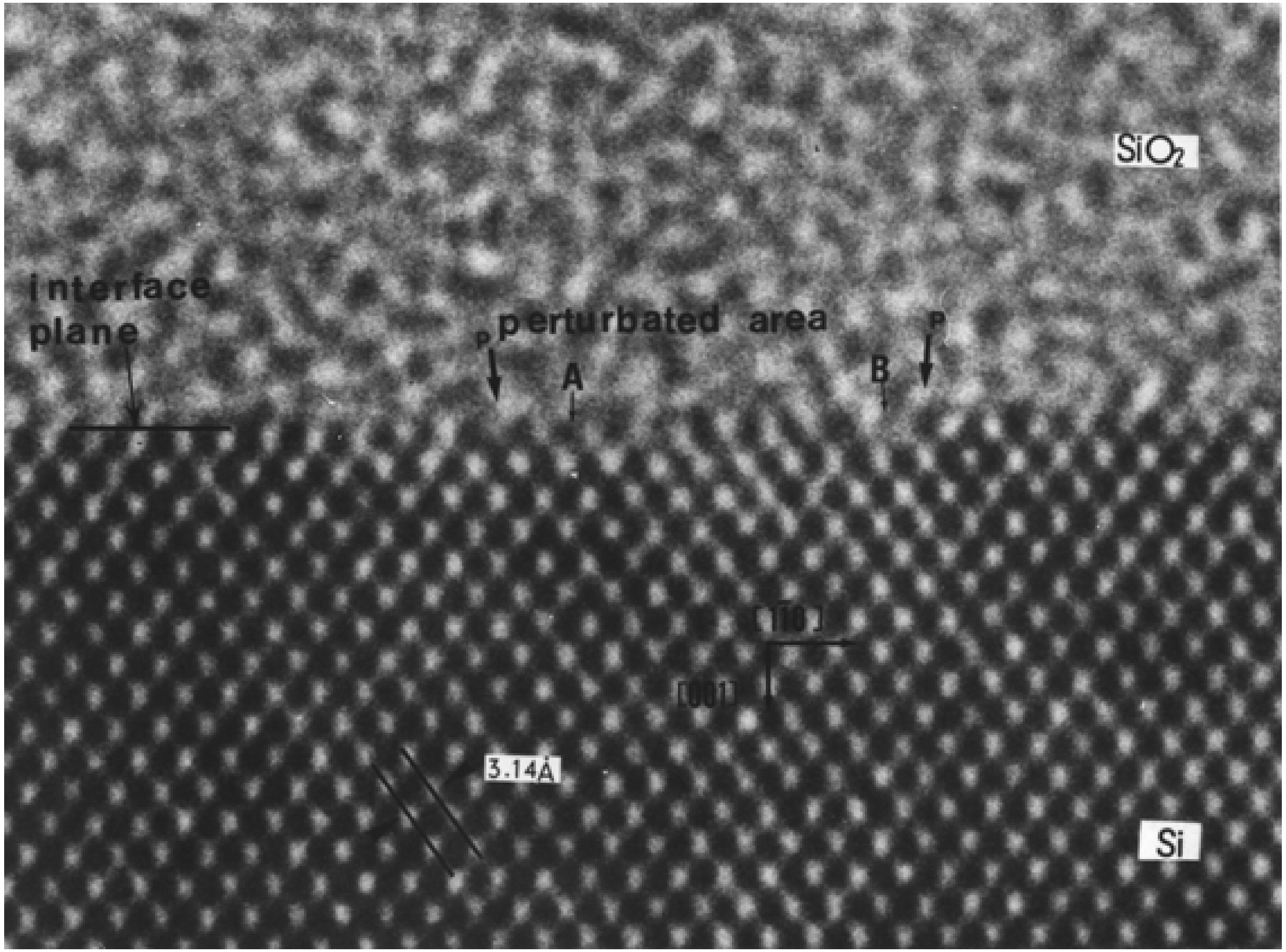




k_s(111) > (k_s(100)

Transmission Electron Micrograph of Si/SiO2 Interface

Amorphous
SiO2



Crystalline
Si

Oxide Charges

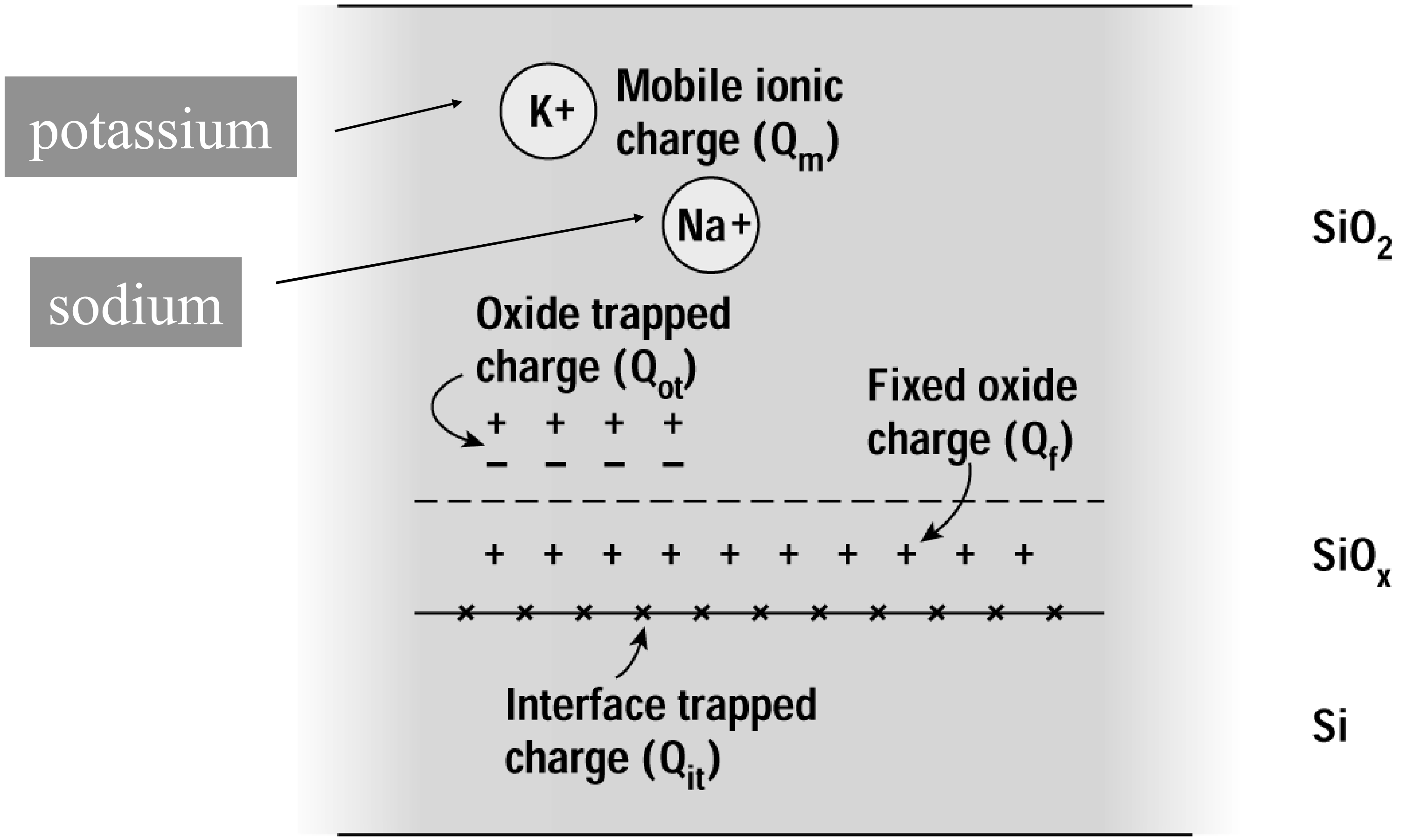


Figure 4.14 Silicon–silicon dioxide structure with mobile, fixed charge, and interface states *(© 1980, IEEE, after Deal).*

To minimize Interface Charges Q_f and Q_{it}

- Use inert gas ambient (Ar or N2) when cooling down at end of oxidation step

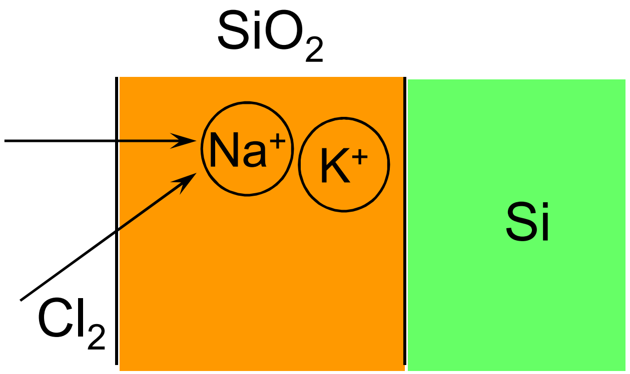
- A final annealing step at 400-450^{o}C is performed with 10%H_2+90%N_2 ambient ("***forming gas***") after the IC metallization step.

Oxidation with Chlorine-containing Gas

- Introduction of halogen species during oxidation
  e.g. add ~*1- 5%* HCl or TCE (trichloroethylene) to O_2

→ Immobilize alkaline(e.g. Na^+,K^+) ions in oxide

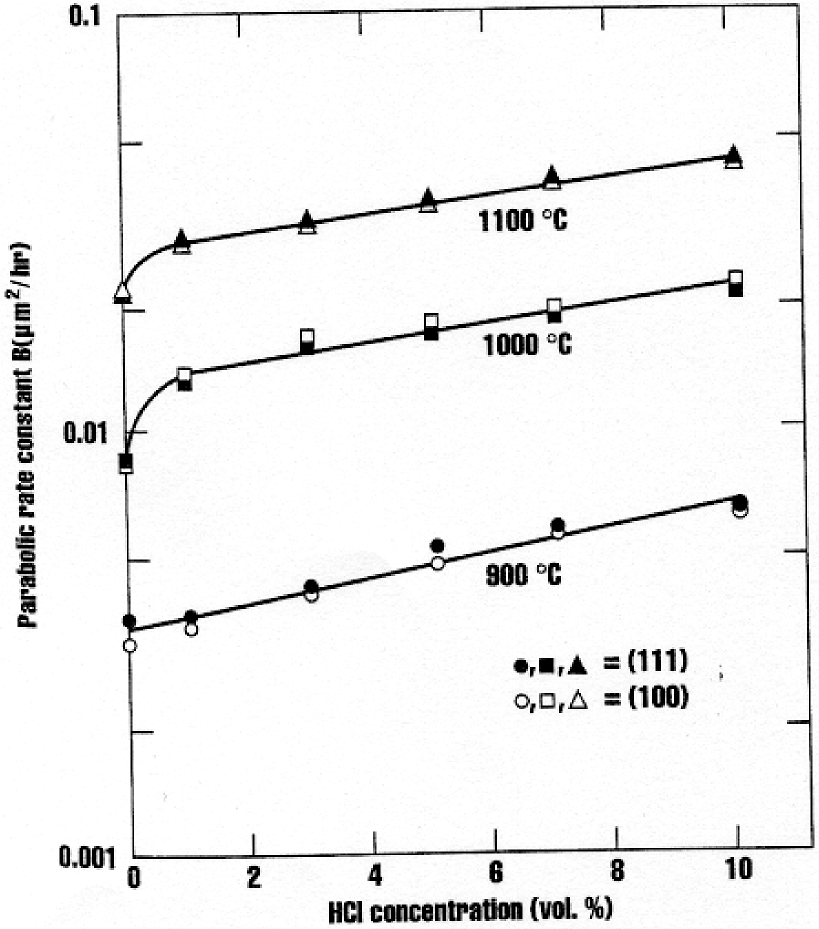
→ improved SiO_2/Si interface properties

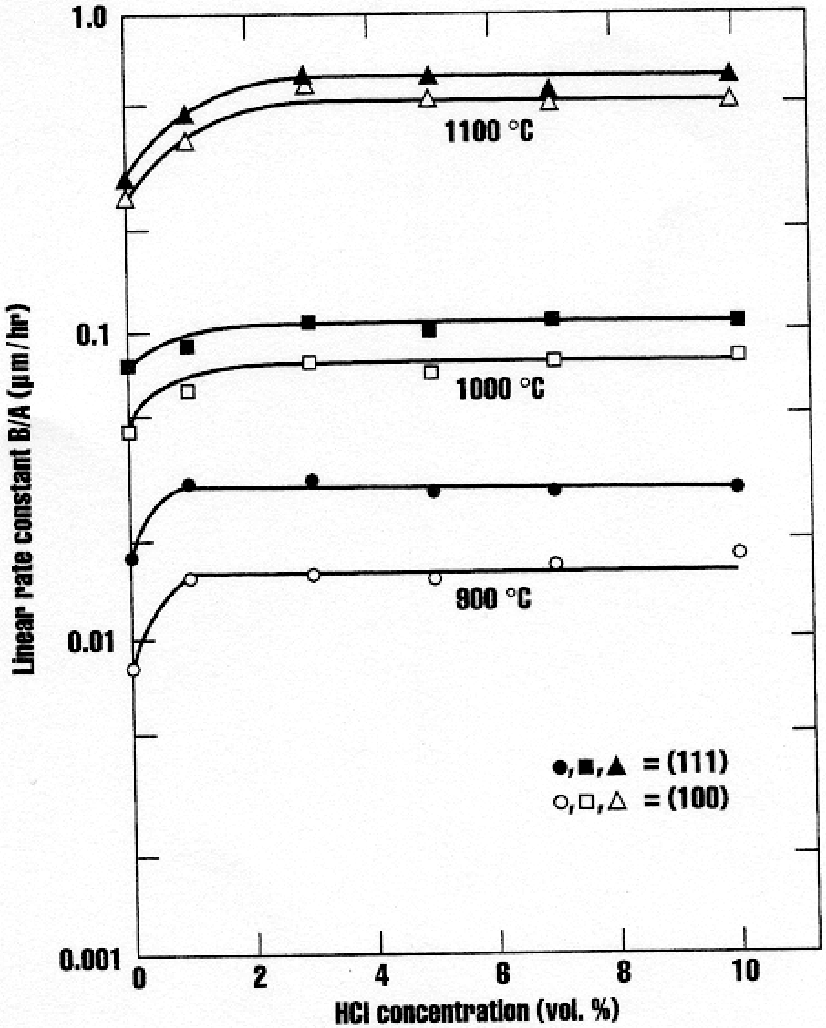


$$M + Cl \rightarrow MCl$$

Effect of HCl on Oxidation Rate

$$HCl + O_2 \rightarrow H_2O + Cl_2$$





SUMMARY of Deal Grove Model

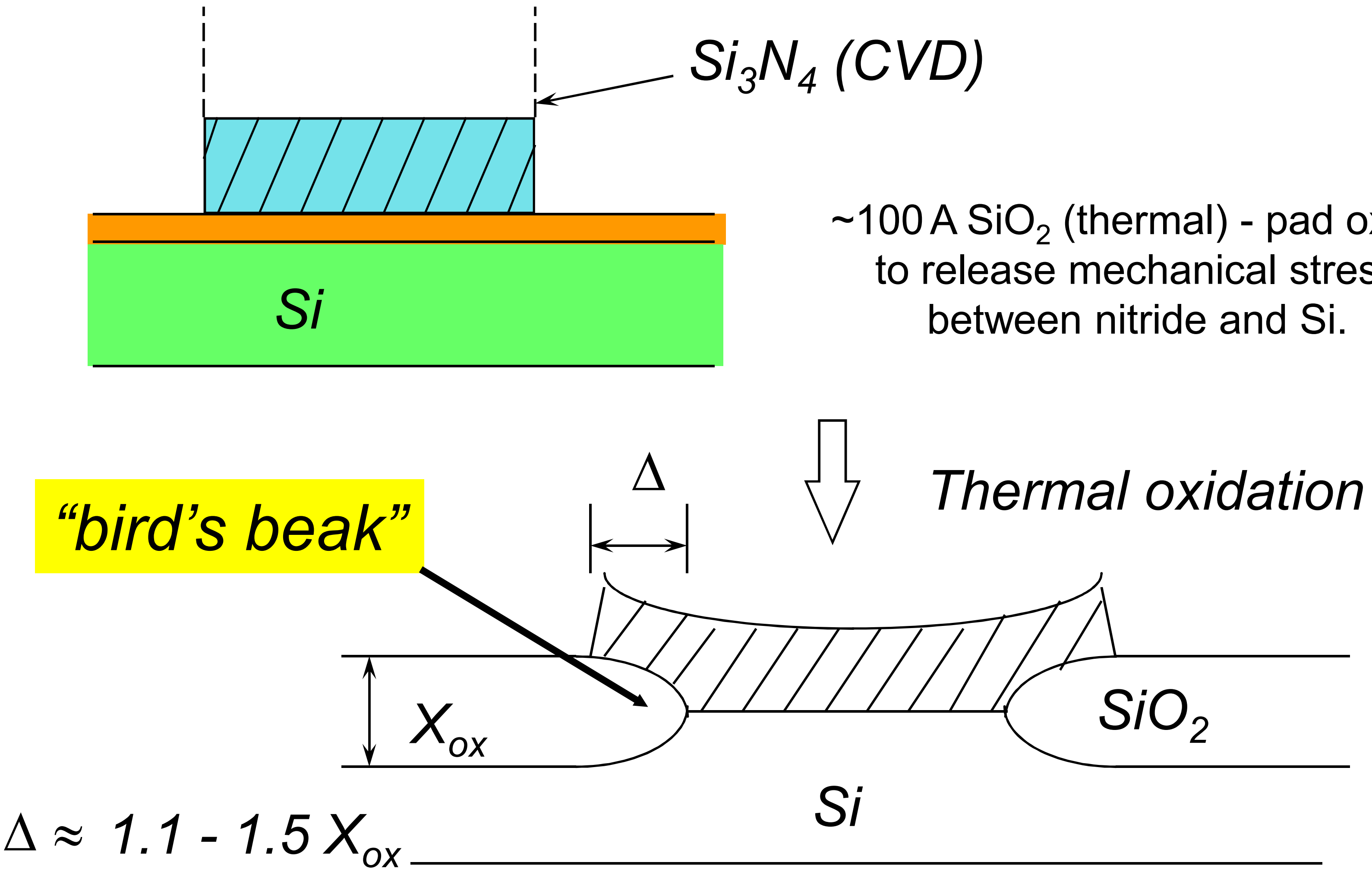
$$X_{ox}^2(t) + A\,X_{ox}(t) = B\,(t+\tau)$$

The growth rate $\frac{dX_{ox}}{dt} = \frac{B}{A+2X_{ox}}$ slows down as X_{ox} increases

Dependence of B/A and B on Processing Parameters

	Linear Constant B/A	**Parabolic Constant B**
Oxidation Pressure	linear with oxygen pressure (actually $\propto P^{0.8}$)	linear with oxygen pressure
Steam versus O_2	larger for steam oxidation	larger for steam oxidation
Si crystal orientation	B/A(111):B/A(100) = 1.68:1	independent of orientation
Dopant type and concentration in Si	increases with dopant concentration	insensitive
Addition of Cl-containing gas in oxidation ambient	insensitive	increases

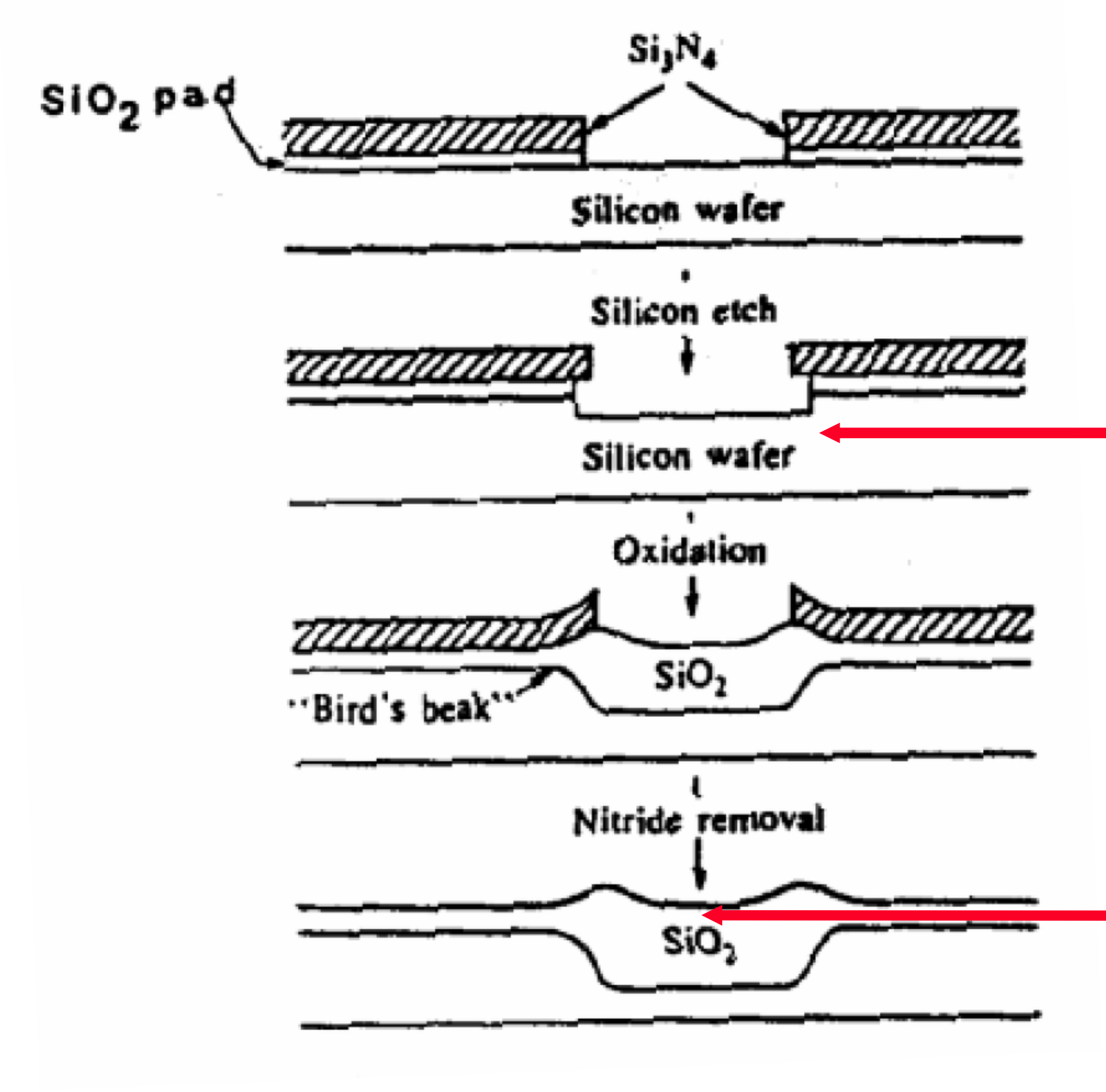
Local Oxidation of Si [LOCOS]



~100 A SiO_2 (thermal) - pad oxide
to release mechanical stress
between nitride and Si.

$$\Delta \approx 1.1 - 1.5\ X_{ox}$$

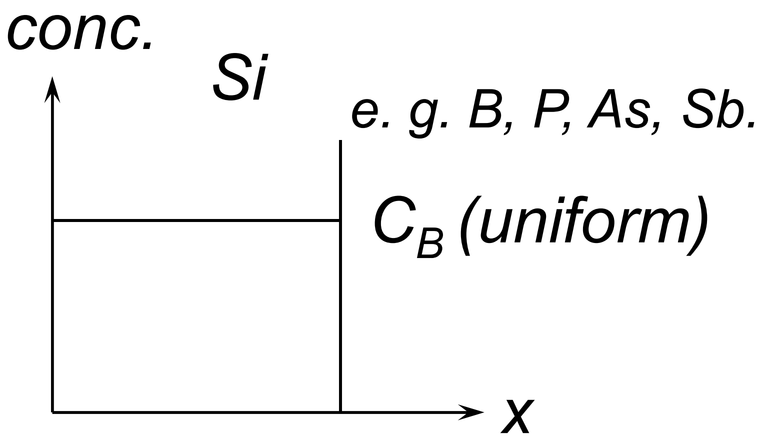
Fully Recessed LOCOS

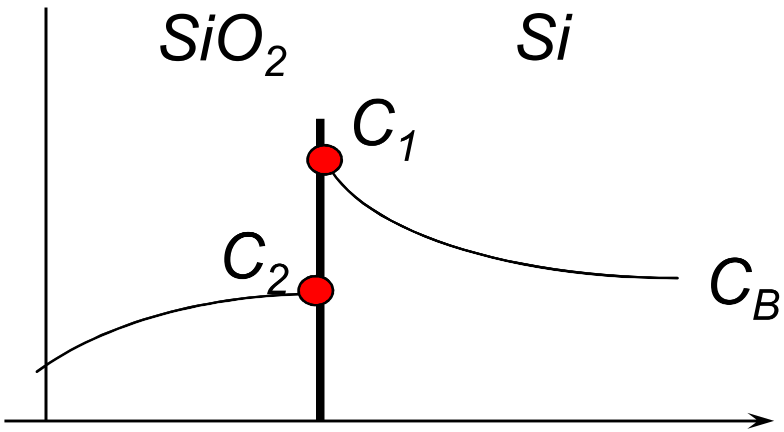


Si substrate is etched to a depth of ~1/2 the intended grown oxide thickness

Grown oxide surface is approximately planar with substrate surface

Dopant Redistribution during Thermal Oxidation





Segregation Coefficient at interface

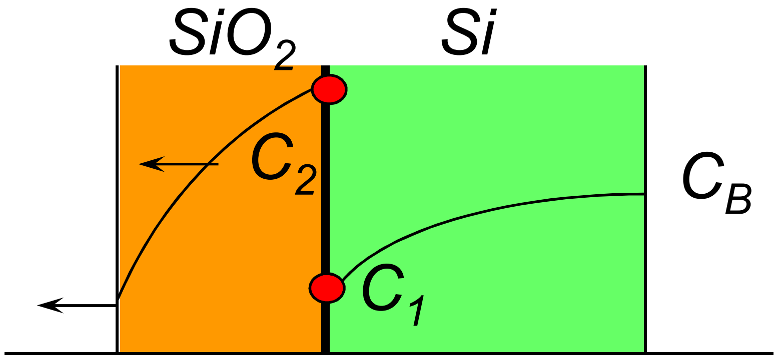
Fixed ratio

$$m \equiv \frac{\text{equilibrium dopant conc. in Si}}{\text{equilibrium dopant conc. in SiO}_2}$$

$$= \frac{C_1}{C_2} \qquad \text{(can be>1 or <1)}$$

Four Cases of Interest

(A) m < 1 and dopant ***diffuses slowly*** in SiO_2

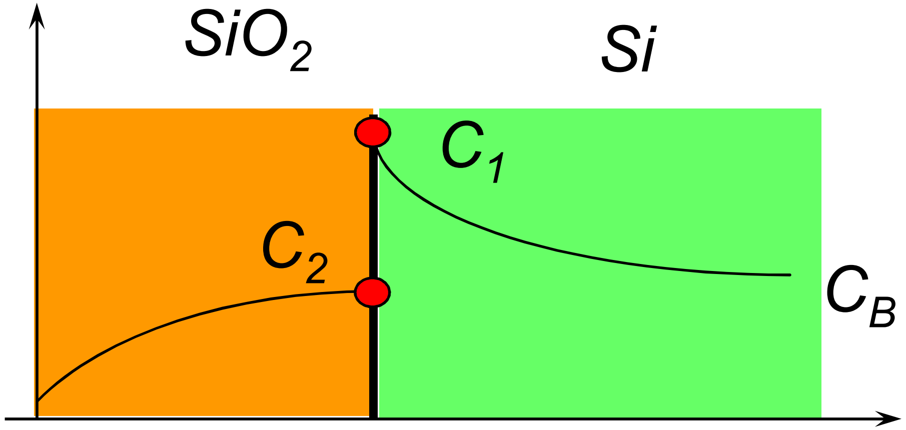


e. g. B (m = 0.3)

Flux loss through SiO_2 surface not considered here.

$\Rightarrow$ B will be depleted near Si interface.

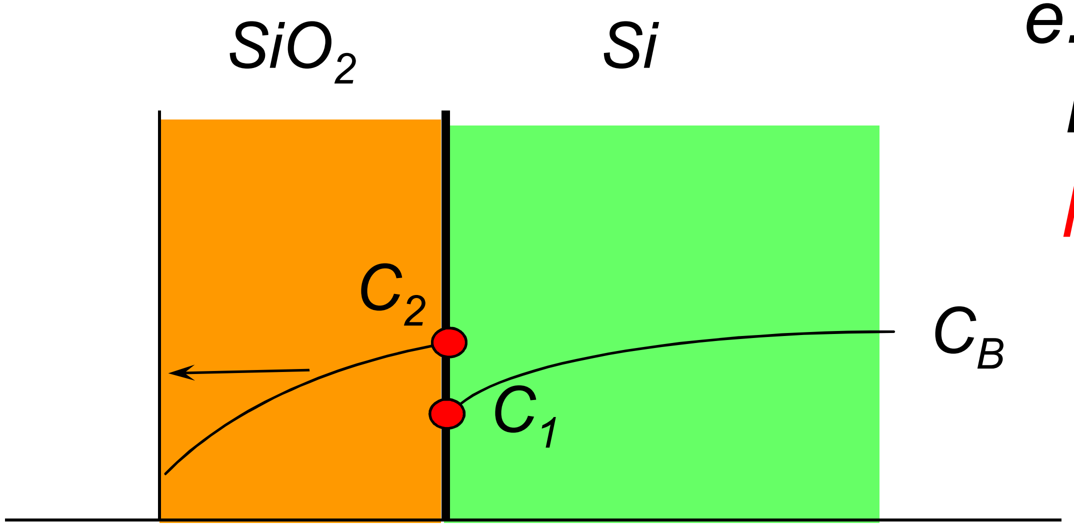
(B) m > 1, dopant ***diffuses slowly*** in SiO_2.



e.g. P, As, Sb

⇒ dopant piling up near Si interface for P, As & Sb

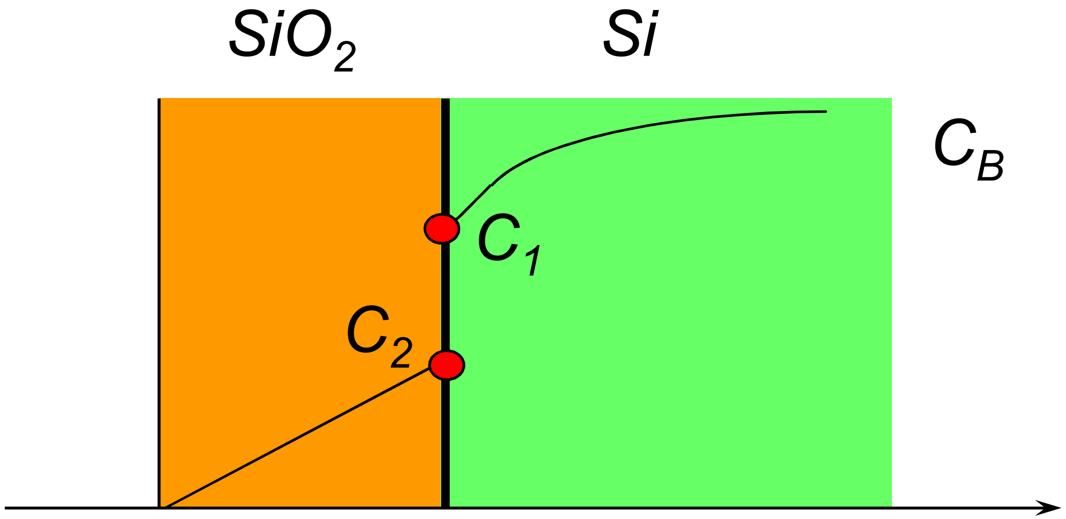
(C) m < 1, dopant ***diffuses fast*** in SiO_2



e. g.

B, oxidize with presence of H_2

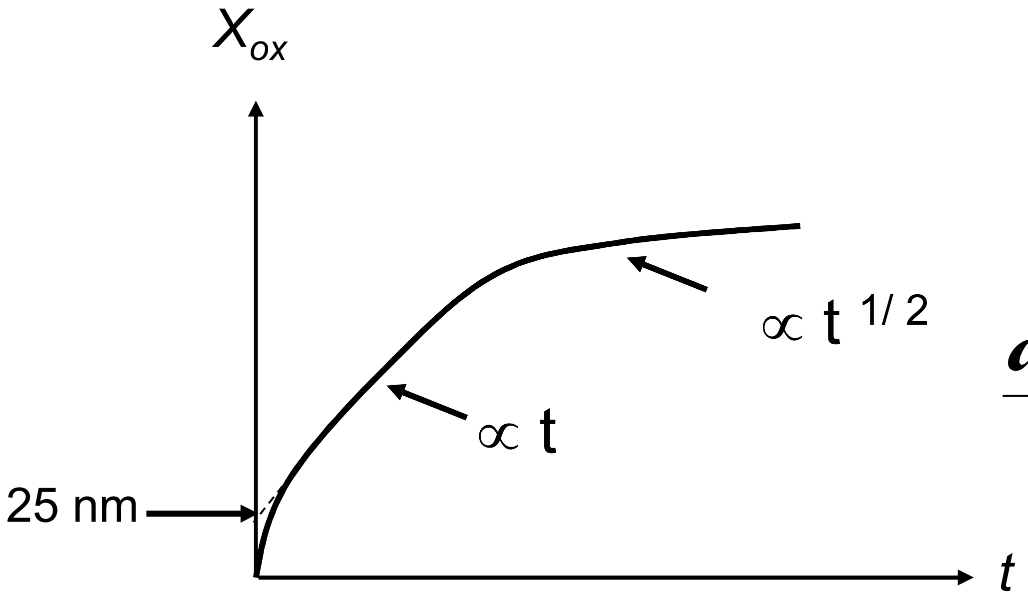
(D) m > 1, dopant ***diffuses fast*** in SiO_2



e. g. Ga (m=20)

Thin Oxide Growth

The Deal-Grove model provides excellent agreement with experimental data except for thin (<20 nm) SiO_2 grown in O_2



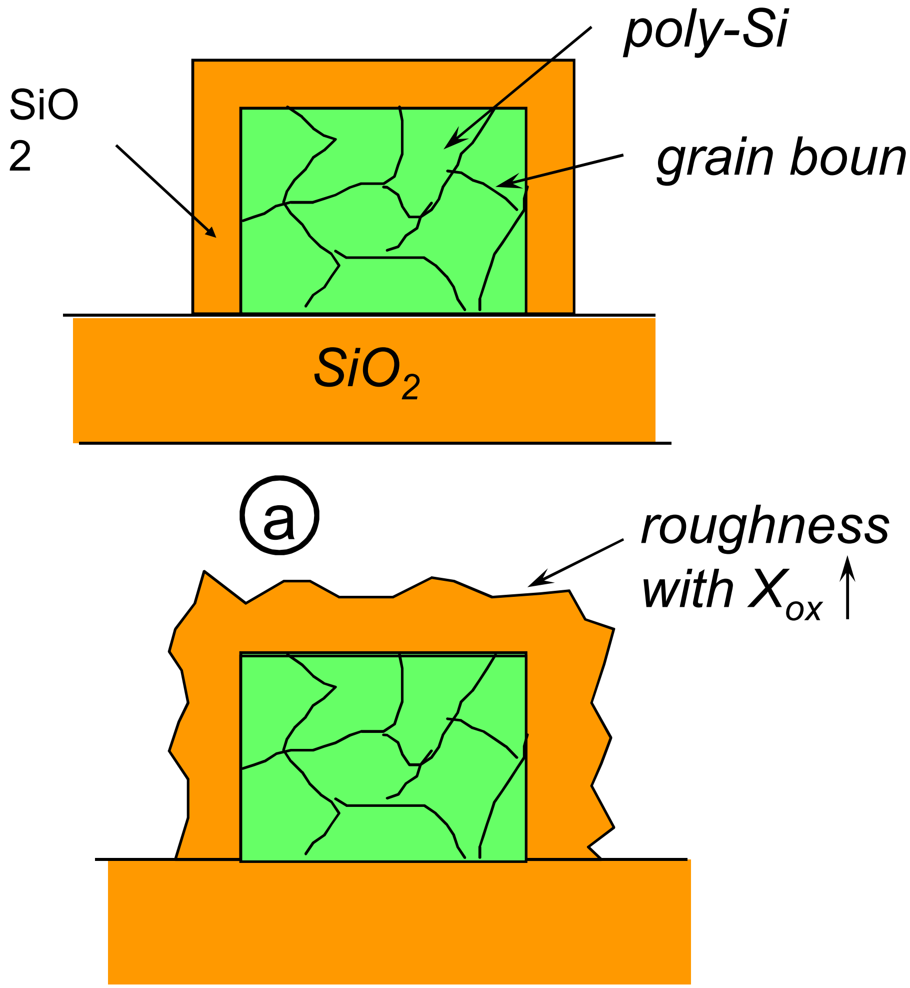
When X_{ox} becomes large, additional term becomes zero

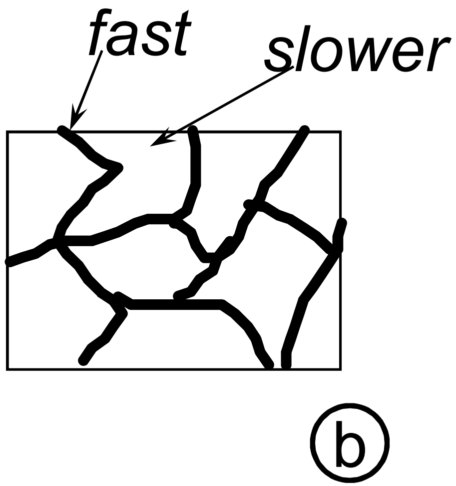
$$\frac{dX_{ox}}{dt} = \frac{B}{A+2X_{ox}} + Ce^{-X_{ox}/L}$$

$L \sim 7nm$

=> For thick oxides grown in O_2 on bare Si, assume X_i =25 nm when using the Deal-Grove equations

Polycrystalline Si Oxidation

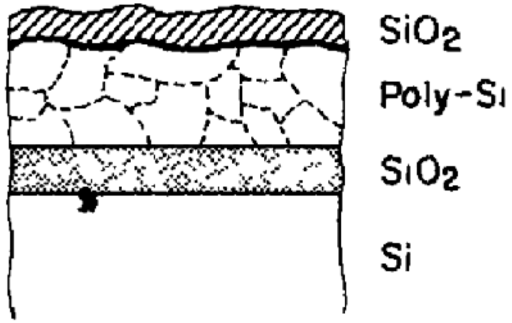




Overall growth rate is higher than single-crystal Si

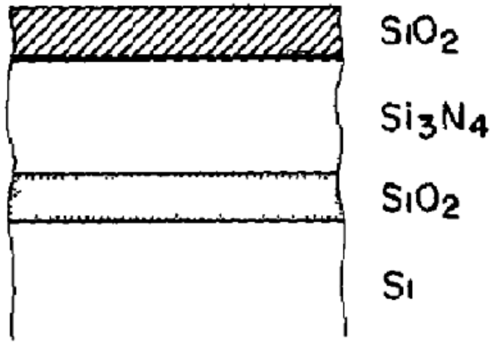
Thermal Oxidation of Si-containing Thin Films

* SiO2 is the final reaction product



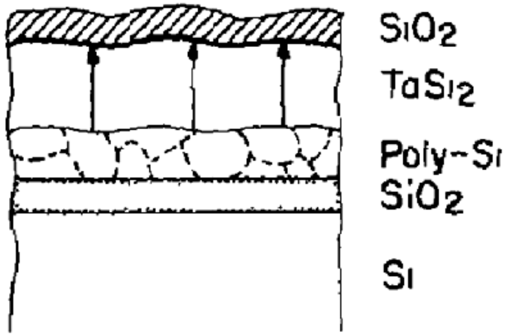
POLYCRYSTALLINE SILICON

$Si + O_2 \rightarrow SiO_2$



SILICON NITRIDE

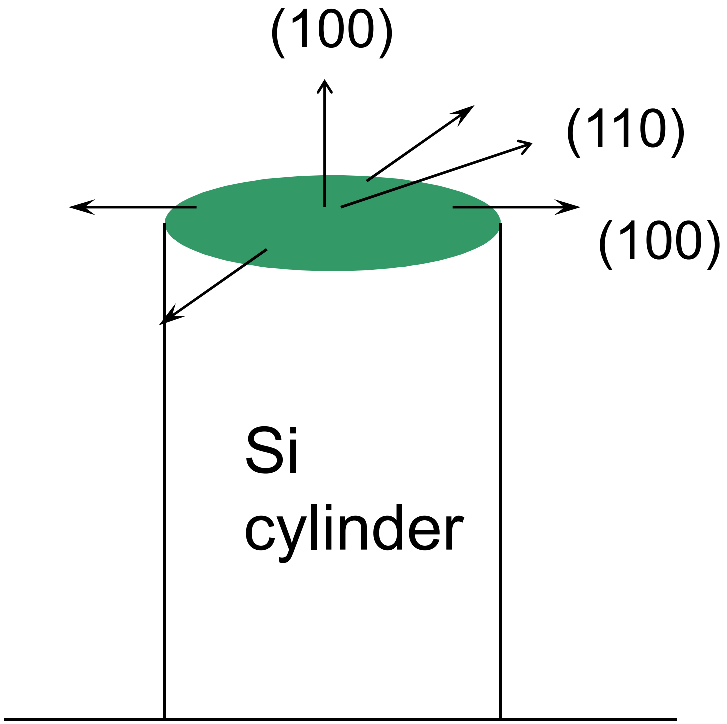
$Si_3N_4 + 3\ O_2 \rightarrow 3\ SiO_2 + 2\ N_2$

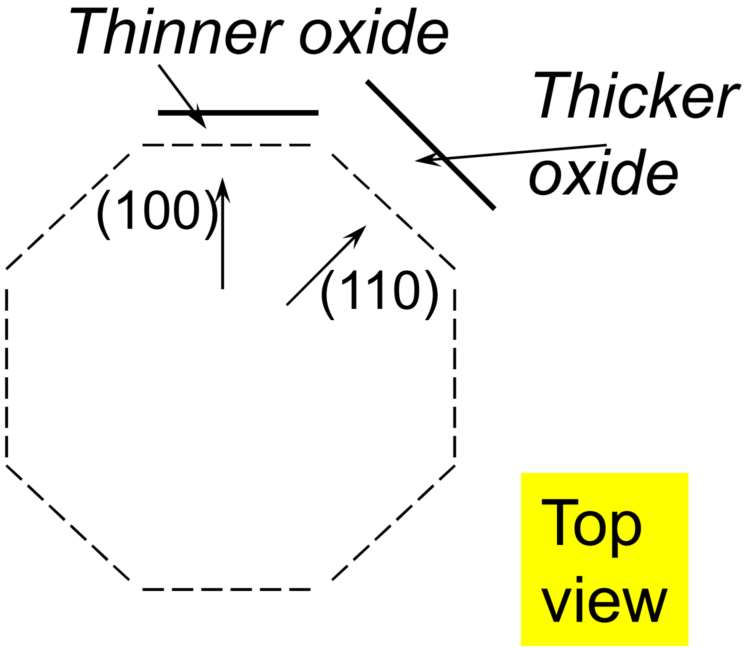


TANTALUM SILICIDE

$TaSi_2 + Si + O_2 \rightarrow SiO_2 + TaSi_2$

2-Dimensional Oxidation Effects





Mechanical stress created by SiO_2 volume expansion also affects oxide growth rate (if interested, see Kao et al, International Electron Devices Meeting Digest, 1985, p.388)

Summary of Thermal Oxidation Module

- Volume change with thermal oxidation.
- Deal-Grove Oxidation Model : Linear (B/A) and Parabolic (B) Constants.
- Calculate oxide grown using: (i) Oxidation charts , and (ii) D-G Model.
- Factors influencing oxidation: Temp, Ambients, Doping Conc, Pressure, Substrate Orientation.
- Oxide Charges.
- LOCOS.
- Qualitative understanding of : dopant redistribution during oxidation, Thin Oxide Growth, Oxidation of Poly-Si and Si-containing films.