2-Dimensional Diffusion with constant D
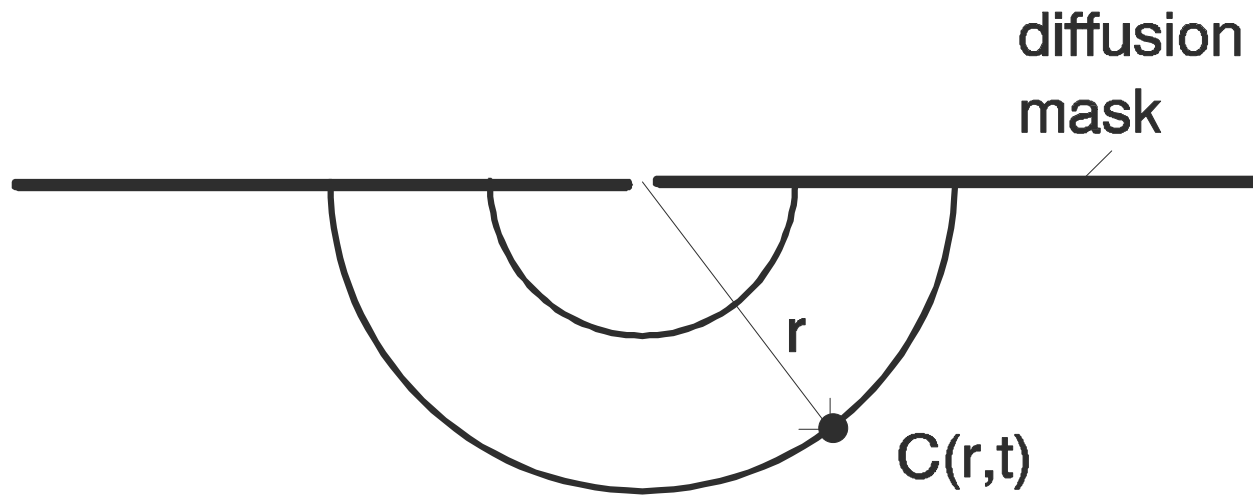
Example 1 Drive-in from line source with s atoms/cm

$$D\frac{\partial^2 C}{\partial r^2} + \frac{D}{r}\frac{\partial C}{\partial r} = \frac{\partial C}{\partial t}$$

Diffusion Equation in ***cylindrical coordinates***

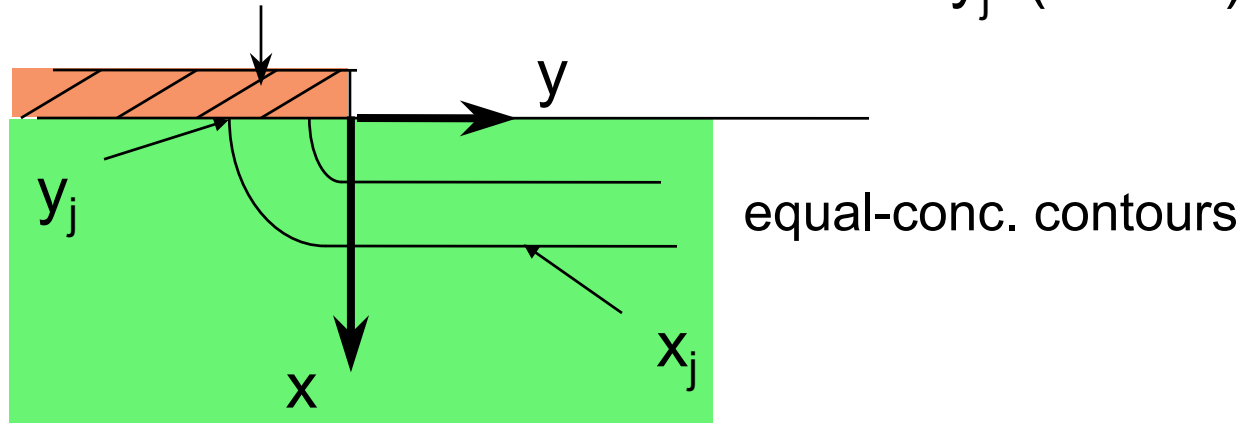$$\therefore \ C(r, t) = \frac{s}{2\pi Dt} \, e^{-r^2/4Dt}$$

Line source with s atoms/cm

diffusion
mask

r

C(r,t)

Two-Dimensional Drive-in Profile (cont.)

Example 2 : Semi-Infinite Plane Source

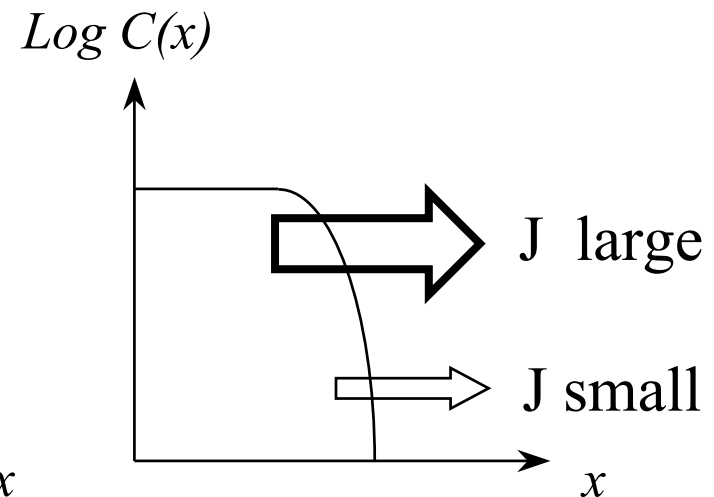Diffusion mask

y_j (at x=0) < x_j (at y $\rightarrow \infty$)

y_j

equal-conc. contours

x_j

x

$$C(x,y,t) = \frac{Q}{2\sqrt{\pi Dt}} \ e^{-x^2/4Dt} \ [\ 1 + \text{erf}\,(\frac{y}{2\sqrt{Dt}})\ ]$$

where Q = predep dose in #/cm^2

Rule of Thumb : y_j ~0.7-0.8 x_j

High Concentration Diffusion Effects

1) E-Field Enhanced Diffusion
2) Charged point defects enhanced diffusion

Log C(x)

**High conc. profile:
D gets larger
when C(x)
is large**

**Low conc profile:
Erfc or gaussian**

x

Log C(x)

J large

J small

x
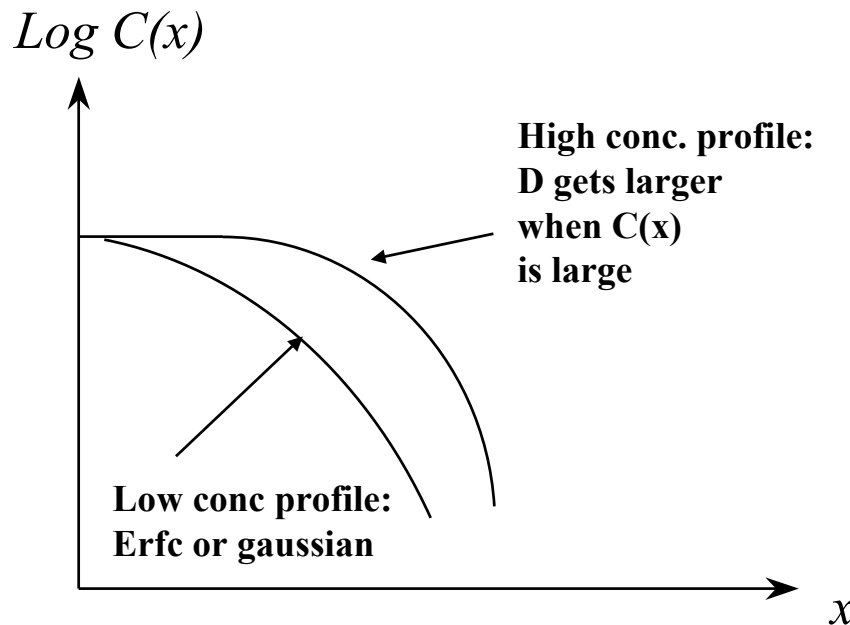
* C(x) looks "flatter"
at high conc. regions

(1) Electric-field Enhancement

Example: Acceptor Diffusion

$N_a(x)$

$N_a(x)=N_a^-(x)$

$p(x)$

hole gradient

Hole diffusion
tendency

$E_{build-in}$
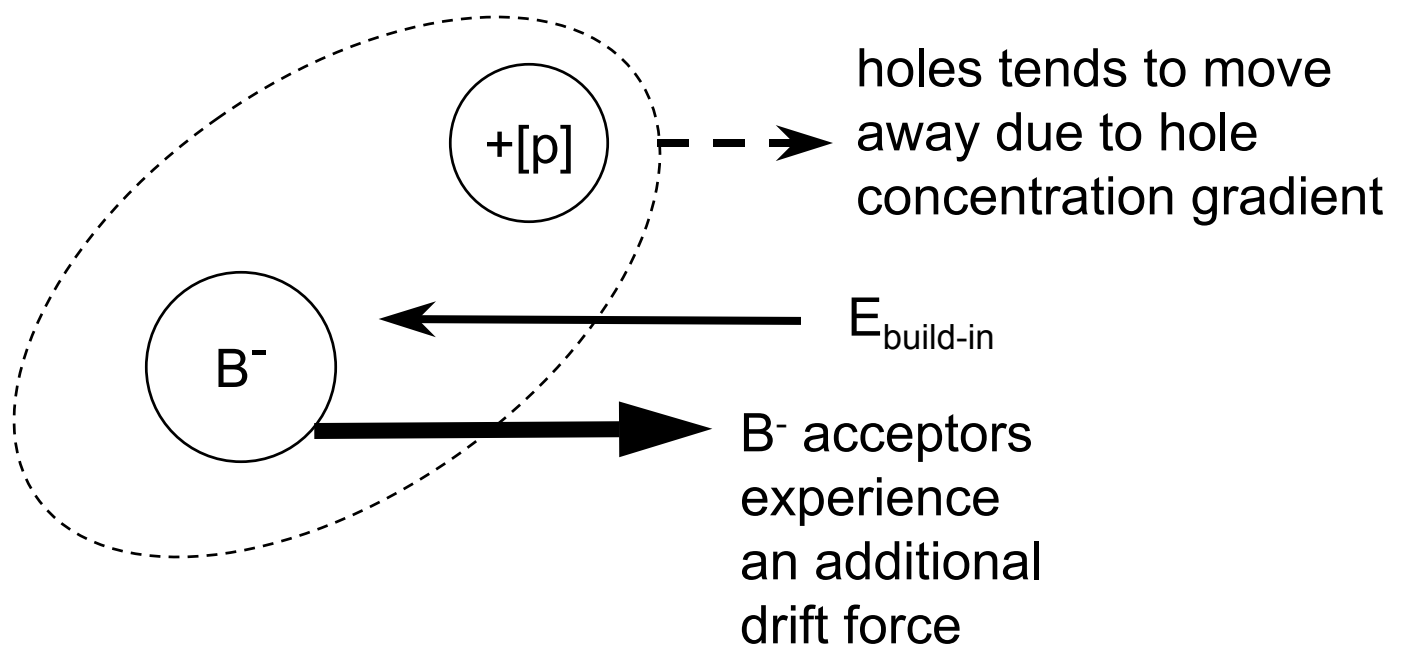
x
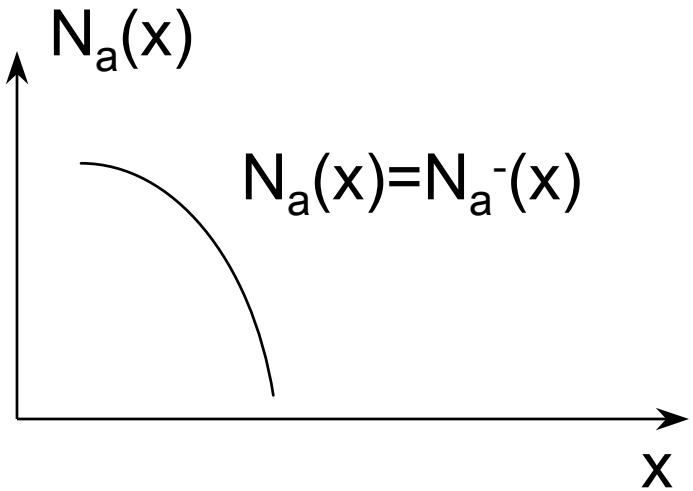
Complete acceptor
ionization at diffusion temperature
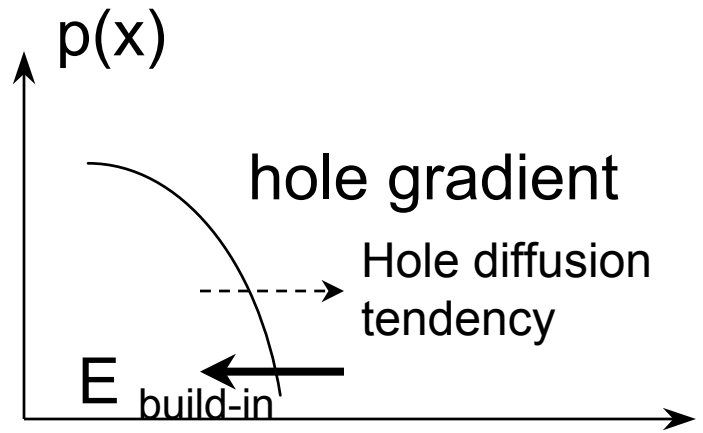
At thermal equilibrium, hole current =0
Hole gradient creates build-in
electric field to counteract the hole
diffusion tendency

holes tends to move
away due to hole
concentration gradient

$E_{build-in}$

B⁻ acceptors
experience
an additional
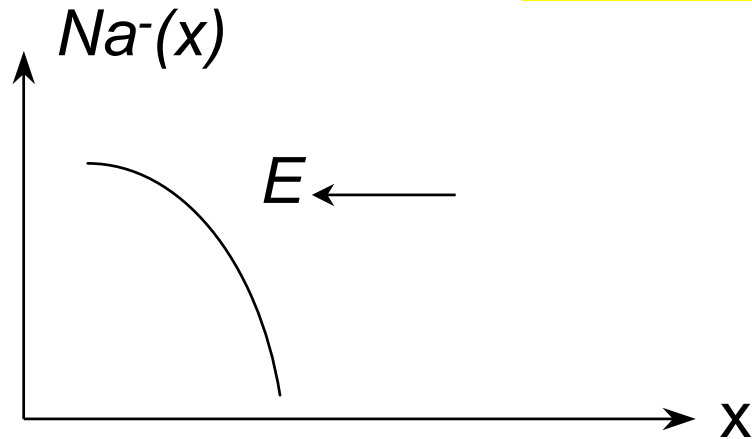drift force

Enhanced
Diffusion for B⁻ acceptor atoms

Calculation of build-in Electric Field E

$$J_p = q \cdot \mu_p \cdot p \cdot E - qD_p \cdot \frac{dp}{dx} = 0$$

at thermal equilibrium.

$$\Rightarrow E = \frac{kT}{q} \cdot \frac{1}{p} \cdot \frac{dp}{dx}$$

$$= \frac{kT}{q} \cdot \frac{d[\ln p]}{dx}$$

Calculation of total diffusion flux F

$Na^-(x)$

E

x

Total acceptor atom flux = (diffusion + drift) components

$$F = - D_A \, dN_A/dx \quad - \mu_A \cdot E \cdot N_A$$

Since $\mu_A = D_A/[kT/q]$ from Einstein's Relationship

7

$$F = -D_A \cdot \left[\frac{dN_A}{dx} + \frac{d[\ln p]}{dx} \cdot N_A \right]$$

$$From\ (1)\ p = n + N_A^{-}\ \ charge\ Neutrality$$

$$(2)\ pn = n_i^2\ \ Law\ of\ Mass\ Action$$

$$(1)\ \&\ (2) \therefore\ p = \frac{N_A + \sqrt{N_A^2 + 4n_i^2}}{2}$$

$$\therefore \frac{d[\ln p]}{dx} = \frac{dN_A}{dx} \cdot \frac{1}{\sqrt{N_A^2 + 4n_i^2}}$$

$$\therefore \quad F = -D_A \cdot \frac{dN_A}{dx} \cdot \underbrace{\left[1 + \frac{1}{\sqrt{1 + \frac{4n_i^2}{N_A^2}}} \right]}_{h-factor}$$

$$If \quad n_i >> N_A \quad h \rightarrow 1 \quad \text{low dopant conc.}$$

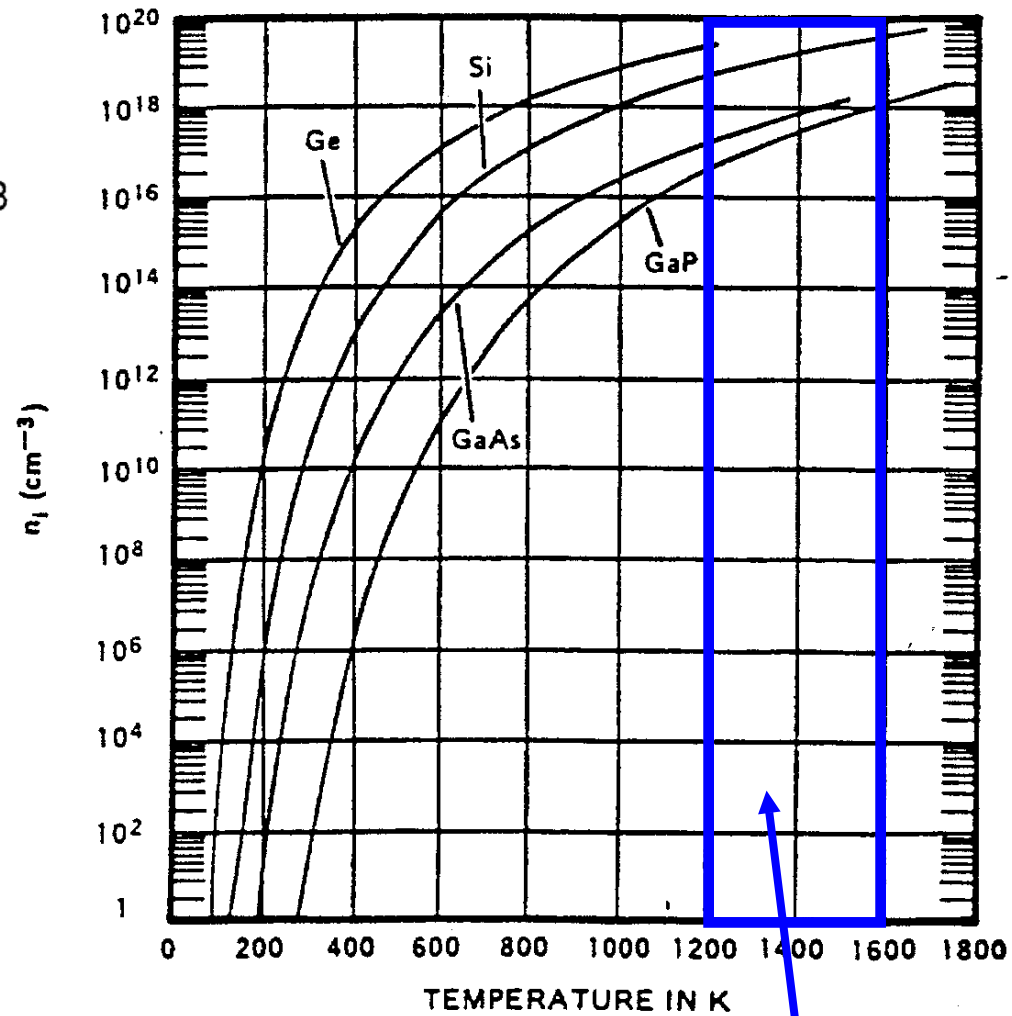$$n_i << N_A \quad h \rightarrow 2 \quad \text{high dopant conc.}$$

Value of h depends on concentration N_A

Intrinsic Carrier Concentration n_i

$\underline{\underline{Si}}$:

$$n_i = 3.9 \times 10^{16} T^{3/2} e^{-\frac{0.605eV}{kT}} /cm^3$$

If n or p > $n_i(T_{diffusion})$, we will expect to observe high concentration diffusion effects.
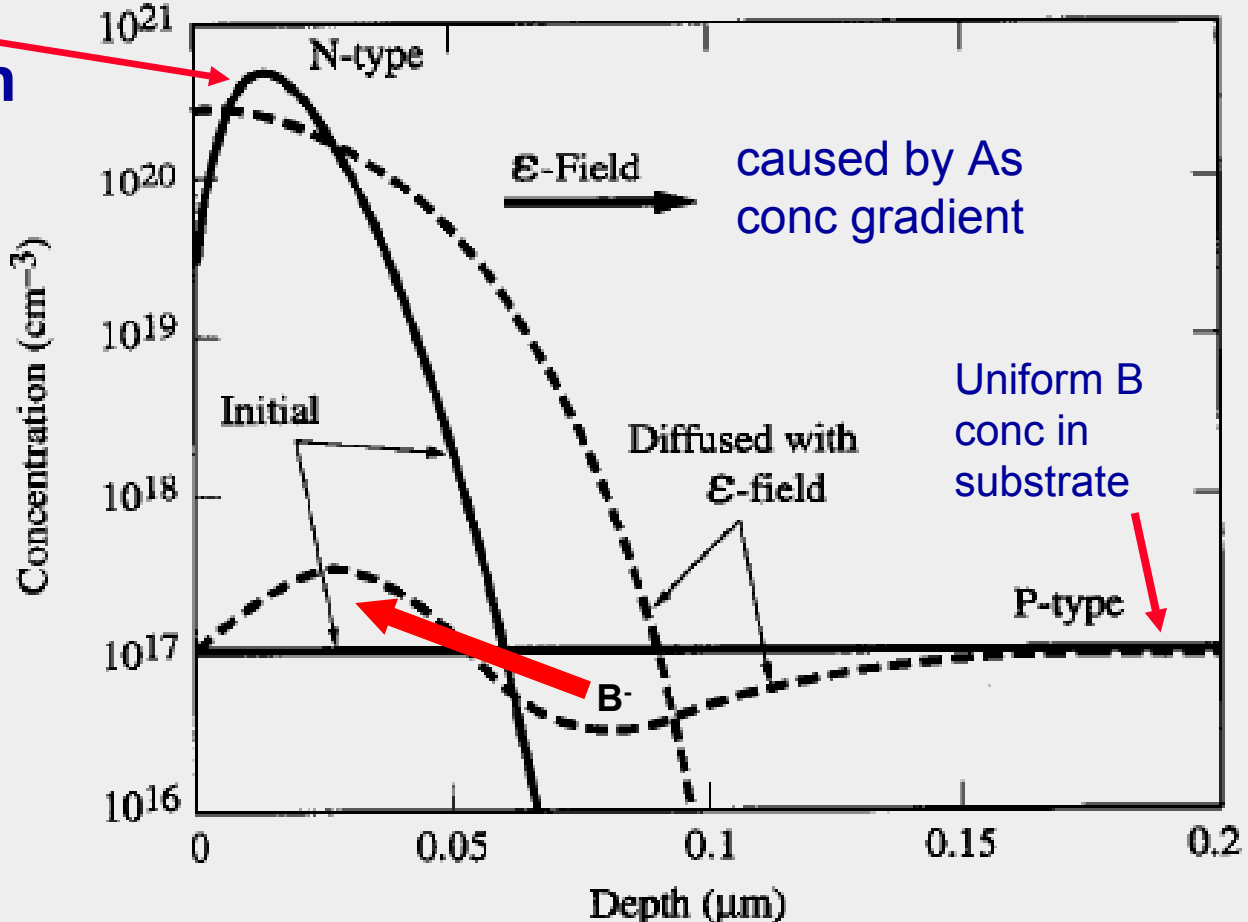

Temp range for dopant diffusion

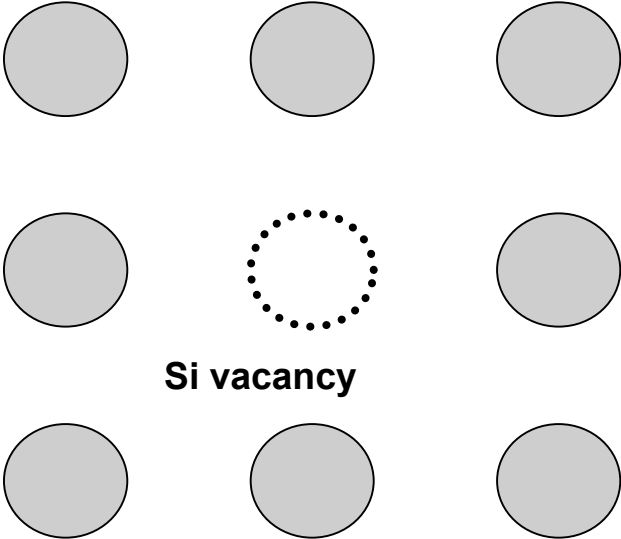# E-Field Effect Example

How the uniform substrate concentration is perturbed by E-field of diffusion specie

As diffusion

caused by As conc gradient

Uniform B conc in substrate

(2) Diffusion Enhanced by Charged Point Defects (e.g. Vacancies)

Si vacancy

V^o = neutral

V^+ = + vacancy

V^- = - vacancy

$V^=$ = - - vacancy

…..

Possible Point Defect Configurations

(a)

V^+ V^0 V^-

(b)

Tetrahedral Interstitial

Hexagonal Interstitial

(c)

$(Al)^0$, acceptor I^+

$(Al)^-$, acceptor I^0
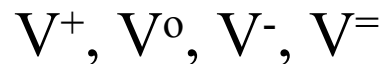
$(Al)^+$, donor

For reference only
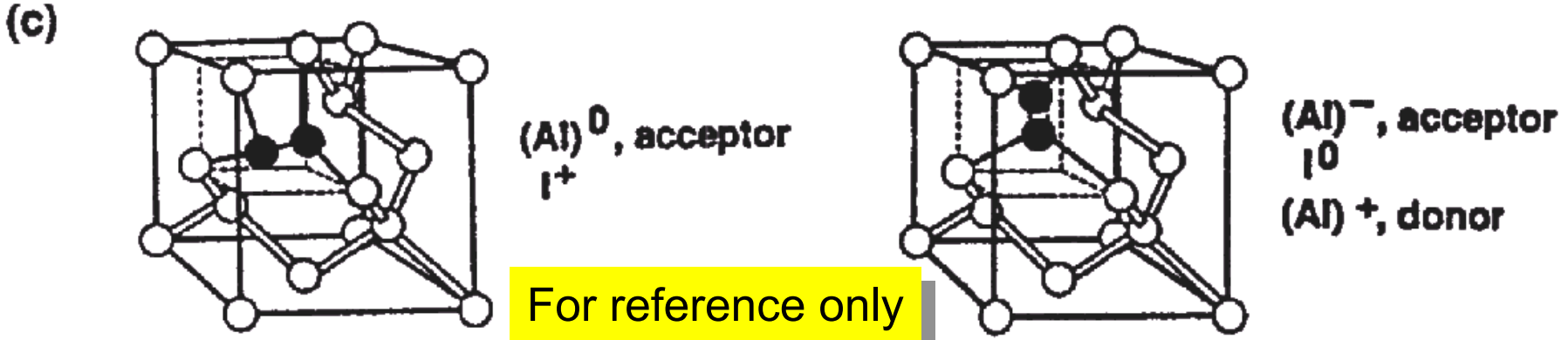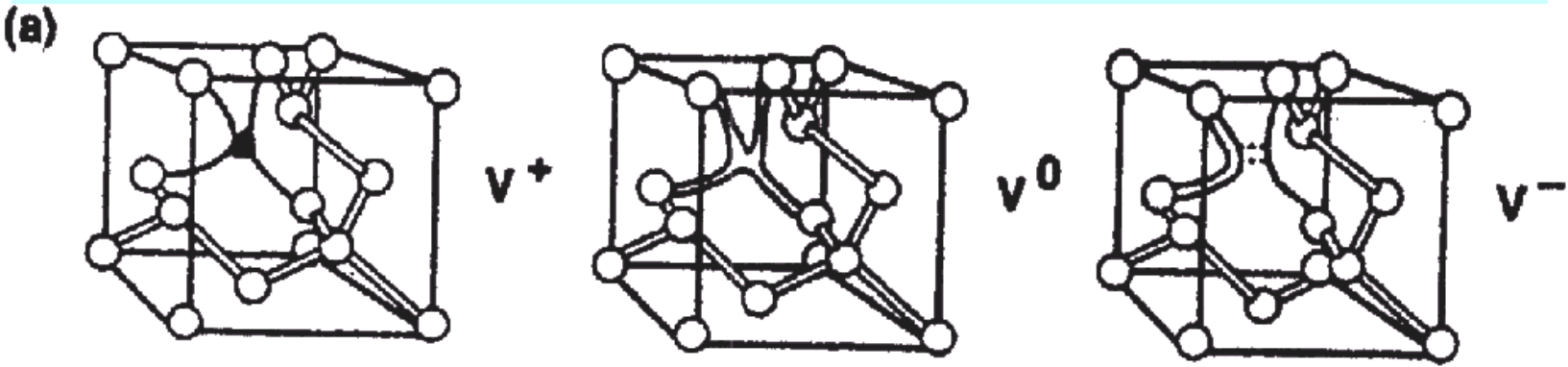
How processing steps affect point defect concentrations

- **Neutral** interstitial and vacancy point defects present at thermal equilibrium

$$\text{At } 1000^o\text{C}, \quad C_{Io}^* \sim 10^{12} \text{ /cm}^3$$
$$C_{Vo}^* \sim 10^{13} \text{ /cm}^3$$

- **Charged** Point Defects enhanced by heavy doping; total point defect concentrations enhanced by ~10x

$$I^+, I^o, I^-$$
$$V^+, V^o, V^-, V^=$$

- Point defects Injected by interfaces during oxidation (total point concentrations enhanced by ~10x)

- **Implantation collisions (total defect concentrations enhanced by ~ 1000x)**

Derivation of charged vacancy concentration

Law of Mass Action

For the reaction :
$$a \bullet A + b \bullet B \leftrightarrow c \bullet C$$

$$\frac{[A]^a [B]^b}{[C]^c} = K_c$$

[ ] denotes concentration

K_c = equilibrium Constant at Temp T

1) Negatively charged vacancies
$$V^o + r \bullet \text{electrons} \leftrightarrow V^{-r} \quad (r = 1,2,3\ldots)$$

$$K_c = \frac{[V^o]\, n^r}{[V^{-r}]} = \frac{[V^o]\, n_i^{\,r}}{[V_i^{-r}]}$$

same K_c for undoped Si

$$\frac{[V^{-r}]}{[V_i^{-r}]} = \left[\frac{n}{n_i}\right]^r$$

where n = electron concentration ,
[ ] denotes the concentrations ,
subscript i denotes condition for intrinsic Si

2) Positively charged vacancies
$$V^o + r \bullet \text{holes} \leftrightarrow V^{+r} \quad (r = 1,2,3\ldots)$$

$$\frac{[V^{+r}]}{[V_i^{+r}]} = \left[\frac{p}{n_i}\right]^r = \left[\frac{n_i}{n}\right]^r$$

p = hole concentration

Charged Vacancy Enhanced Diffusion

$$\mathrm{D_{total}} = D^o + D_i^+ \cdot \left(\frac{p}{n_i}\right) + D_i^- \cdot \left(\frac{n}{n_i}\right) + D_i^= \cdot \left(\frac{n}{n_i}\right)^2 + \ldots$$

Why each diffusivity written with n_i as normalization factor ?

Consider the +charge vacancy first , $D^+ \propto [V^+]$.
From Law of Mass Action: $[V+] \propto p$
Therefore , $D^+ \propto p$ and can be written as $D^+ = K \bullet p$
where K is a proportionality constant

Let us multiply K by n_i and call it D_i^+, then $D^+ = D_i^+ \bullet (p / n_i)$
The physical meaning of D_i^+ is diffusivity D^+ for undoped silicon
because $p = n_i$ for undoped silicon

Similarly, D_i^- and $D_i^=$ are diffusivity values for undoped Si
due to –charge and = charge vacancies

Charged Vacancy Enhanced Diffusion

$$D_v = D^o + D^+ + D^- + D^= + ...$$

$$= D^o + D_i^+ \cdot \left(\frac{p}{n_i}\right) + D_i^- \cdot \left(\frac{n}{n_i}\right) + D_i^= \cdot \left(\frac{n}{n_i}\right)^2 + ...$$

$D^o = D_{io} \exp(-E_{ia} / kT)$ <-- diffusion coefficient for diffusion via neutral vacancies

$D_i^+ = D_o^+ \exp(-E_a^+/kT)$ <-- diffusion coefficient for diffusion via singly positively charged vacancies

$D_i^- = D_o^- \exp(-E_a^-/kT)$ <-- diffusion coefficient for diffusion via singly negatively charged vacancies

$D_i^= = D_o^= \exp(-E_a^=/kT)$ <-- diffusion coefficient for diffusion via doubly negatively charged vacancies

Note that $p/n_i = n/n_i = 1$ for intrinsic (i.e. undoped) material!

Example : High Concentration Arsenic diffusion profile becomes "box-like"
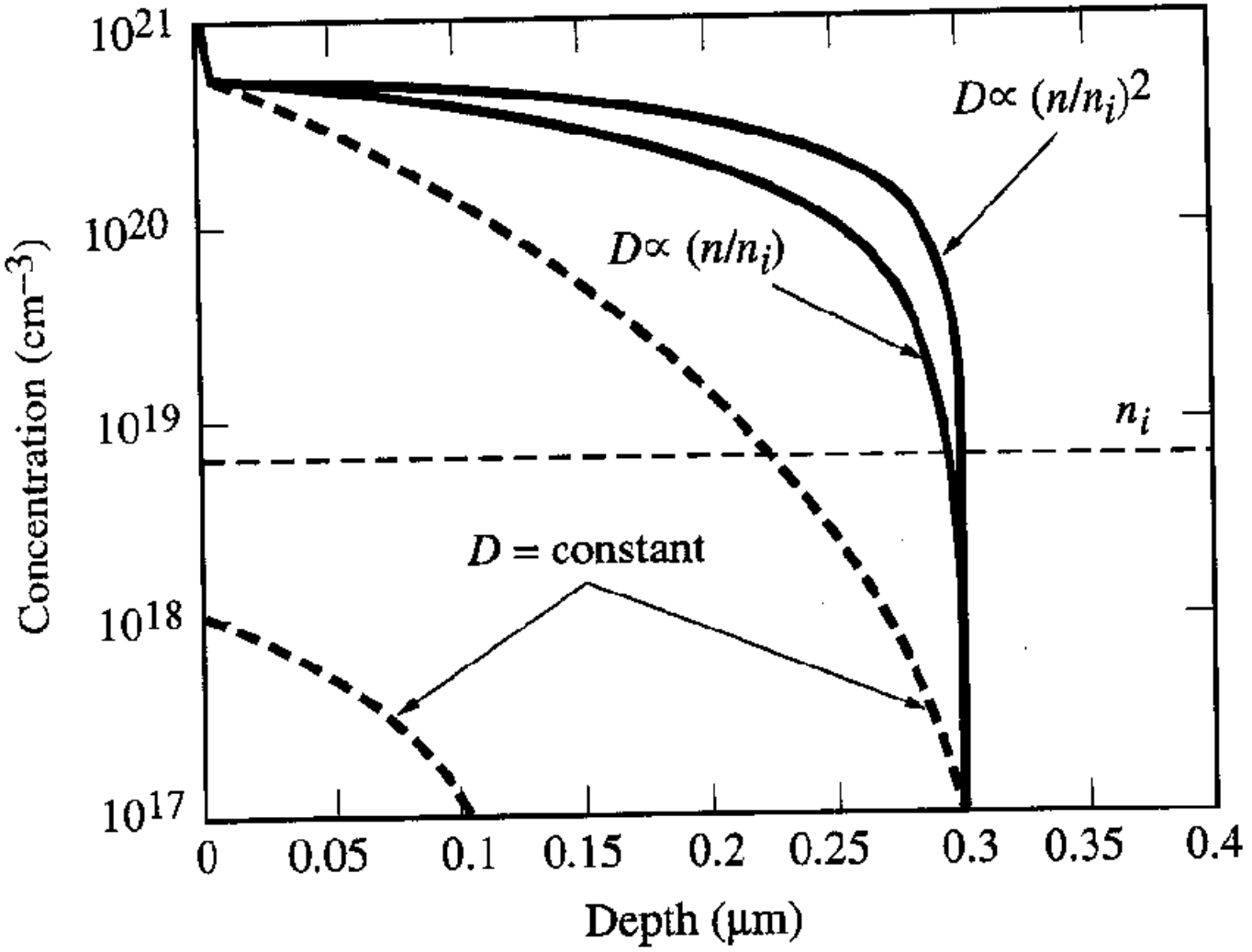
Summary of High-Concentration Diffusion

First, Check if doping concentration is $> n_i(T)$ or $< n_i(T)$

If doping conc $< n_i$:

$D = D^o$

Use constant diffusivity solutions
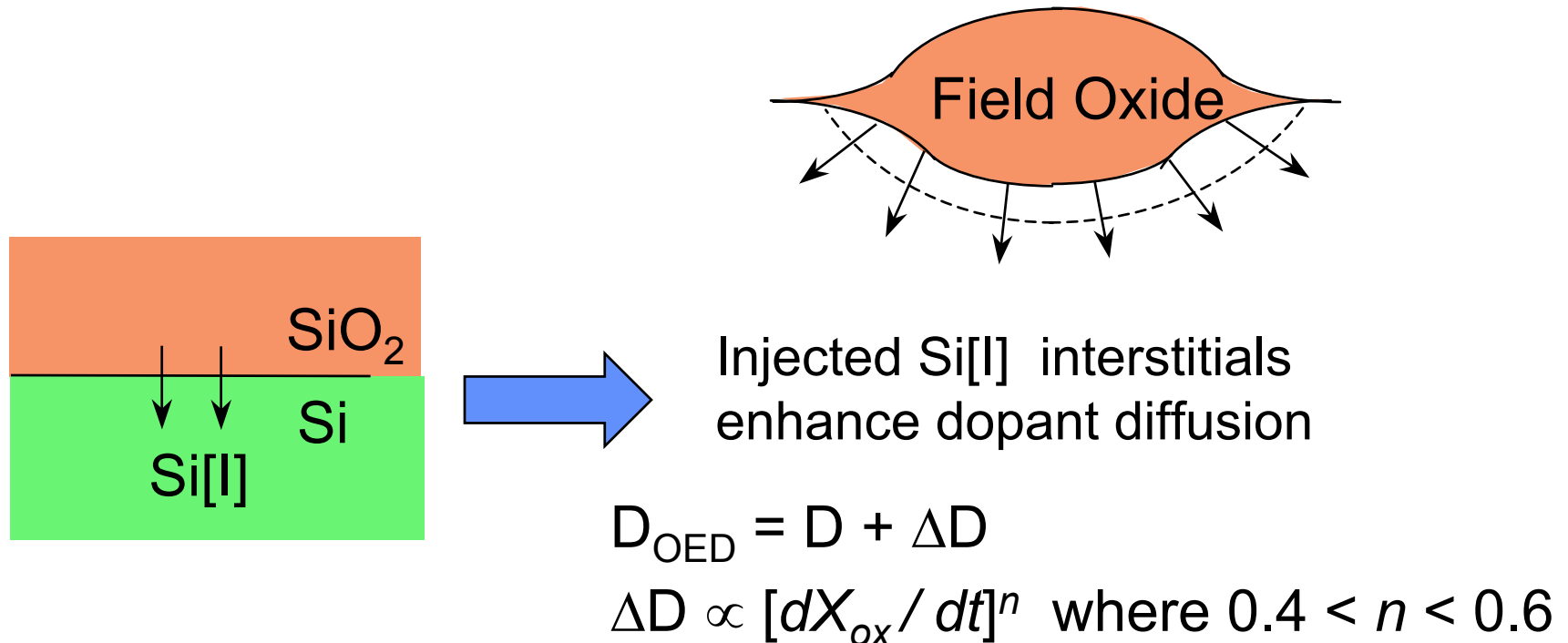(profile is erfc or half-gaussian)

If doping conc $> n_i$:

Use $D = D_v = h [D^o + D^+ + D^- + D^= + \ldots]$
(*Solution requires numerical techniques*)

Oxidation Enhanced Diffusion (OED)

Diffusivity is enhanced for B and P underneath a growing oxide

Example:

Channel-stop implant diffuses faster during field oxidation

Field Oxide

SiO$_2$

Si

Si[I]

Injected Si[I] interstitials enhance dopant diffusion

$D_{OED} = D + \Delta D$

$\Delta D \propto [dX_{ox} / dt]^n$ where $0.4 < n < 0.6$

Note: The dopant **Sb** shows retarded diffusivity during oxidation
=> it diffuses primarily via the vacancy mechanism

Transient Enhanced Diffusion (TED)

Dopant Implantation

Si
substrate

Implantation
induced point
defects
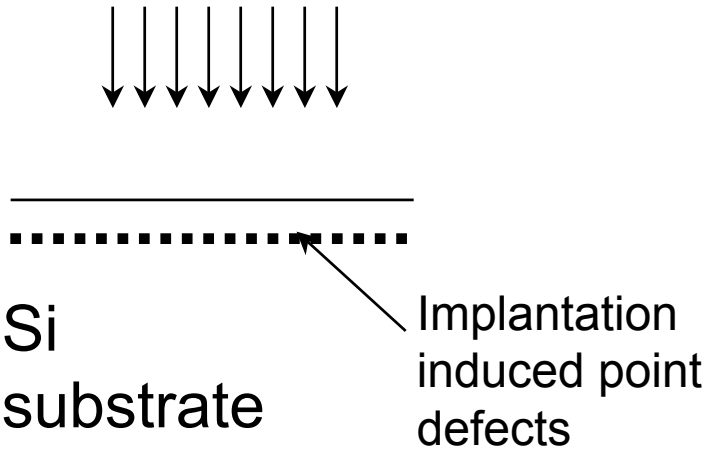
Implantation creates
large number of excess Si
interstitials and vacancies.
After several seconds of
annealing, the excess point
defects recombine.

C(x)

no annealing

900^oC, several minutes
(After excess point defects
recombine. slower diffusion)

x
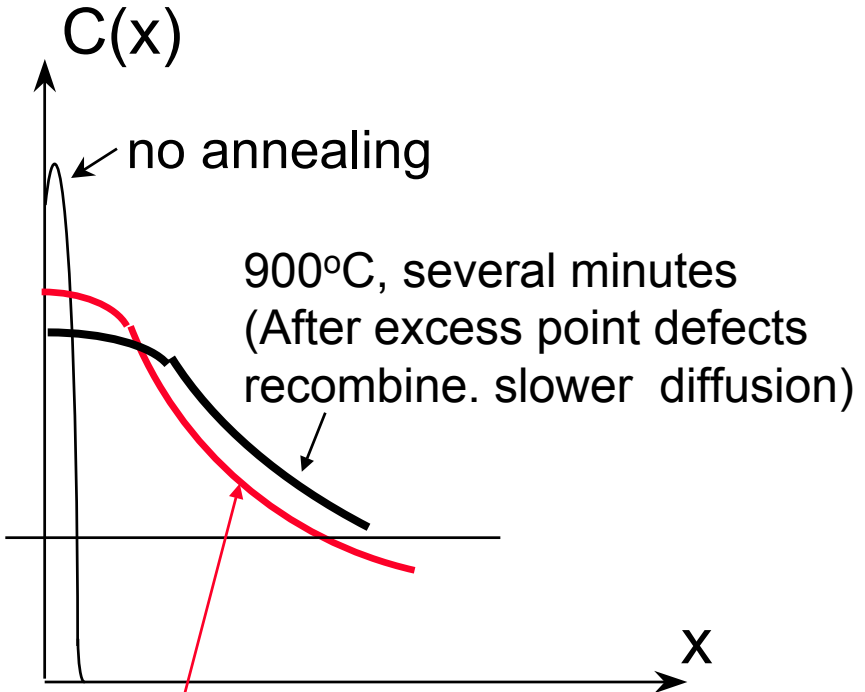
900^oC, several sec (TED)
Rapid diffusion due
to excess point defects

Junction Depth versus post-implantation annealing time

Junction Depth x_j

TED

Normal diffusion
(with high concentration effects)

Annealing time

seconds
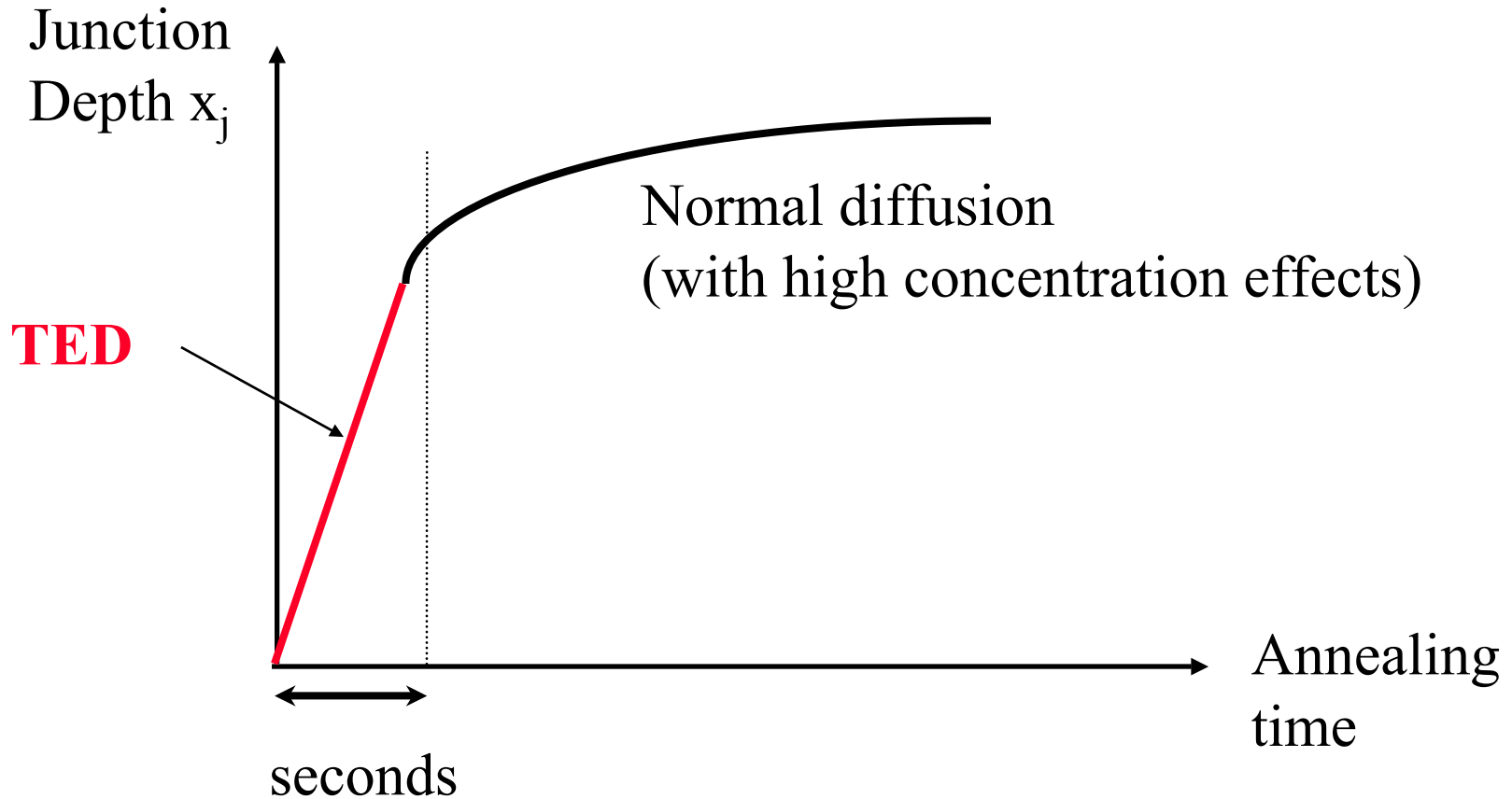
• Difficult to make ultra-shallow (< 0.1μm) junctions with implantation and annealing