Properties of Error Function erf(z) And Complementary Error Function erfc(z)

$$\mathbf{erf\ (z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-y^2}\, dy} \qquad \mathbf{erfc\ (z) \equiv 1 - erf\ (z)}$$

$$\mathrm{erf}\ (0) = 0 \qquad \mathrm{erf}(\infty) = 1 \qquad \mathrm{erf}(-\infty) = -1$$

$$\mathrm{erf}\ (z) \approx \frac{2}{\sqrt{\pi}} z \quad \text{for } z \ll 1 \qquad \mathrm{erfc}\ (z) \approx \frac{1}{\sqrt{\pi}} \frac{e^{-z^2}}{z} \quad \text{for } z \gg 1$$

$$\frac{d\ \mathrm{erf}(z)}{dz} = - \frac{d\ \mathrm{erfc}(z)}{dz} = \frac{2}{\sqrt{\pi}} e^{-z^2}$$

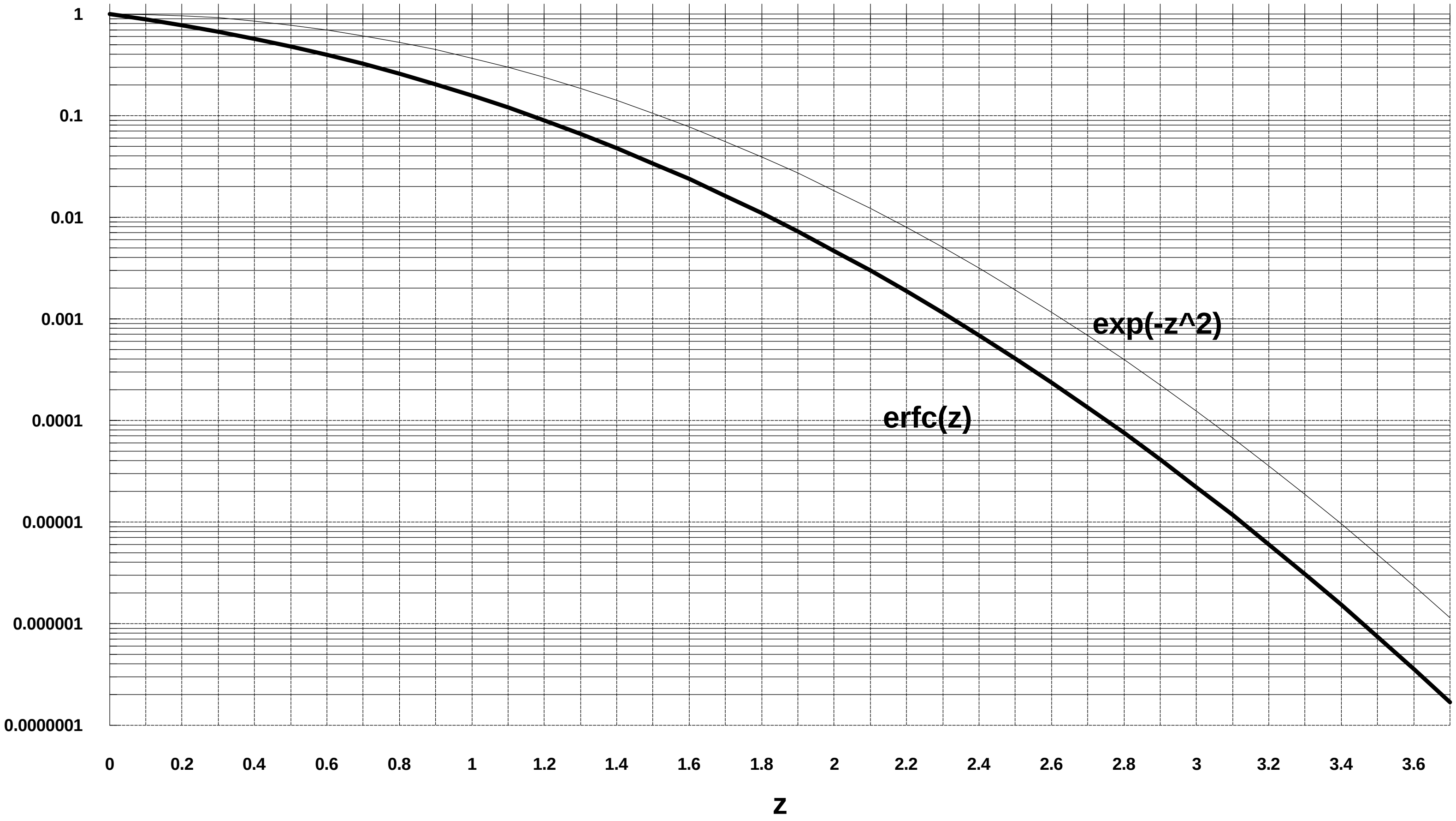
$$\frac{d^2\ \mathrm{erf}(z)}{dz^2} = - \frac{4}{\sqrt{\pi}} z\, e^{-z^2}$$

$$\int_0^z \mathrm{erfc}(y)dy = z\ \mathrm{erfc}(z) + \frac{1}{\sqrt{\pi}} (1-e^{-z^2}) \qquad \int_0^\infty \mathrm{erfc}(z)dz = \frac{1}{\sqrt{\pi}}$$

The value of erf(z) can be found in mathematical tables, as build-in functions in calculators and spread sheets. If you have a programmable calculator, you may find the following approximation useful (it is accurate to 1 part in 10^7): $\mathrm{erf}(z) = 1 - (a_1T + a_2T^2 + a_3T^3 + a_4T^4 + a_5T^5)\, e^{-z^2}$

where $T = \dfrac{1}{1+P\,z}$ and $P = 0.3275911$

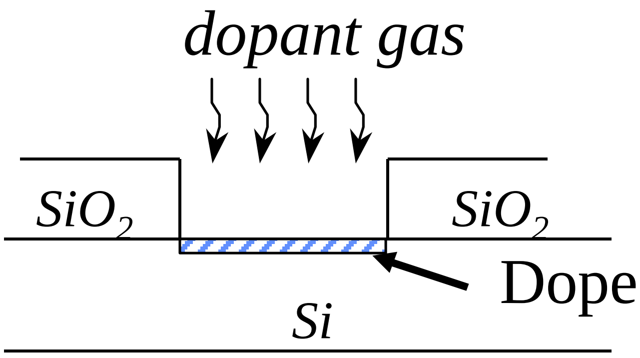
$a_1 = 0.254829592$ $a_2 = -0.284496736$ $a_3 = 1.421413741$ $a_4 = -1.453152027$ $a_5 = 1.061405429$



Dopant Diffusion

(1) Predeposition

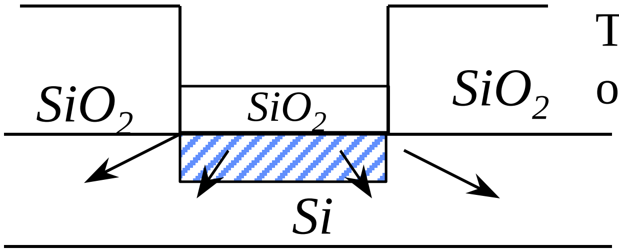
* dose control



Doped Si region

(2) Drive-in

* profile control
(junction depth;
concentration)



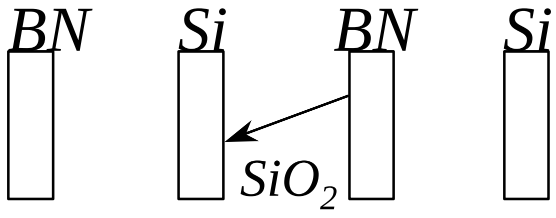
Turn off dopant gas
or seal surface with oxide

Note: Dopant predeposition by diffusion can also be replaced a shallow implantation step

Dopant Diffusion Sources

(a) Gas Source: AsH_3, PH_3, B_2H_6

(b) Solid Source



(c) Spin-on-glass

SiO_2+dopant oxide

(d) Liquid Source.

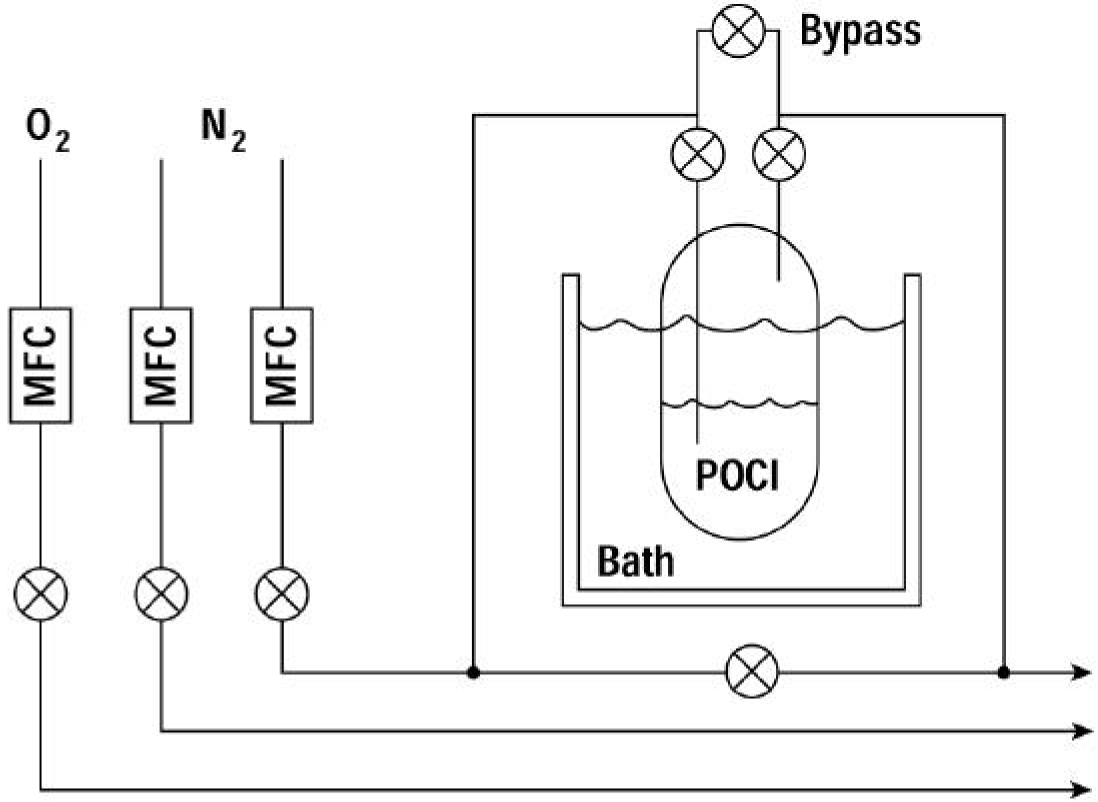
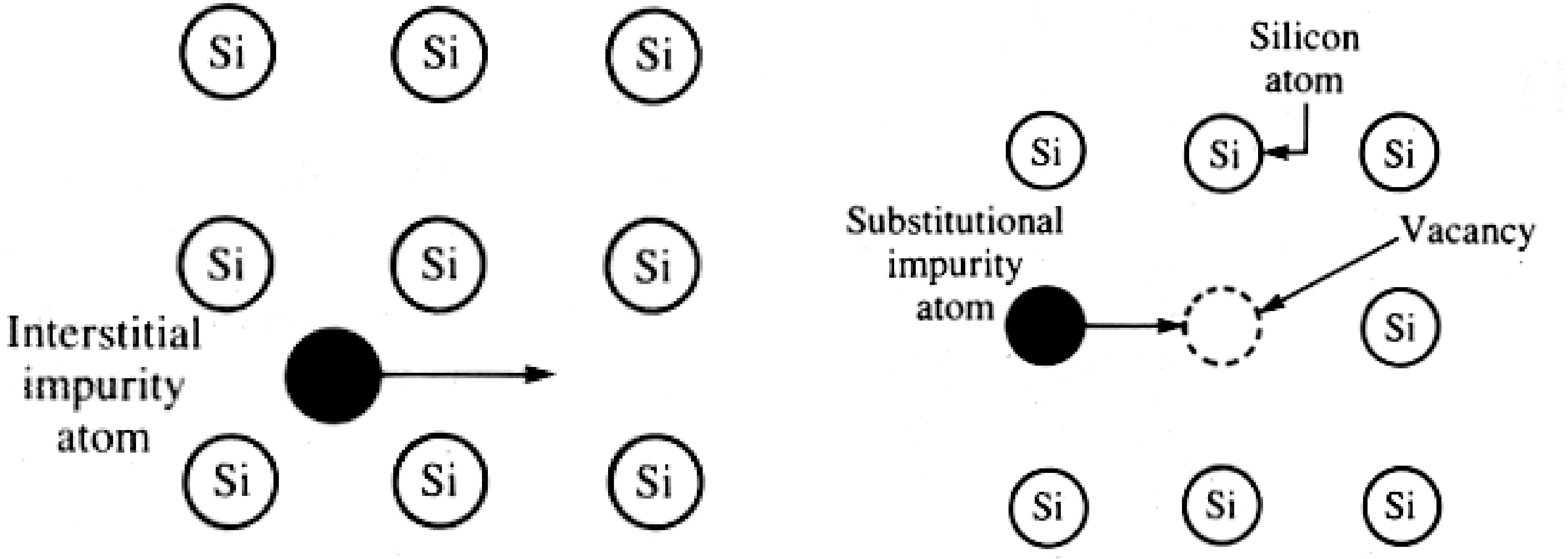


Figure 3.20 A typical bubbler arrangement for doping a silicon wafer using a POCl source. The gas flow is set using mass flow controllers (MFC).

Diffusion Mechanisms



(a) Interstitial

(b) Substitutional

Diffusion Mechanisms : (c) Interstitialcy

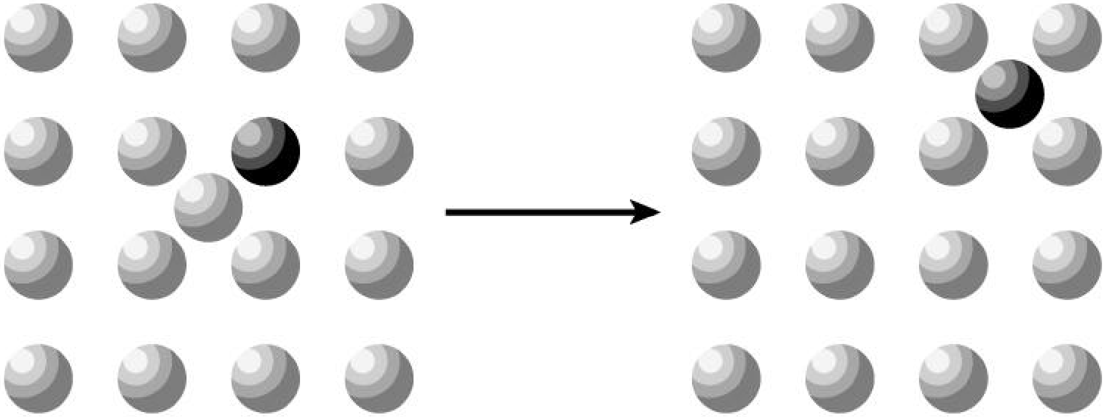


Figure 3.5 In interstitialcy diffusion an interstitial silicon atom displaces a substitutional impurity, driving it to an interstitial site where it diffuses some distance before it returns to a substitutional site.

Diffusion Mechanisms : (d) Kick-Out, (e) Frank Turnbull

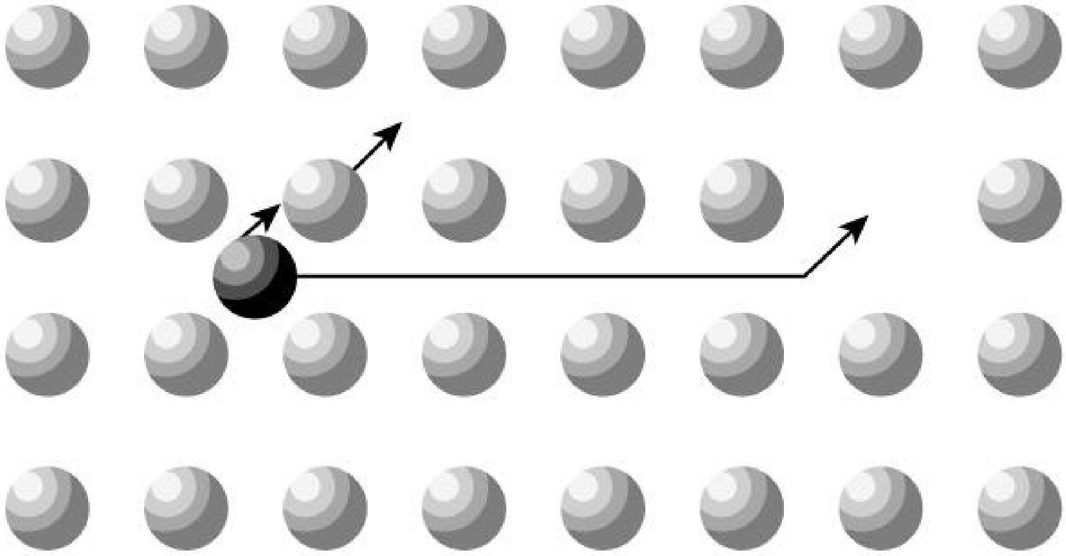
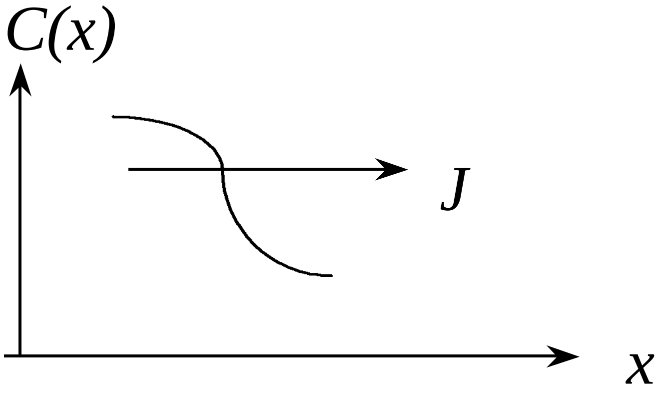


Figure 3.6 The kick-out (left) and Frank–Turnbull mechanisms (right).

Mathematics of Diffusion



Fick's First Law:

$$J(x,t) = -D \cdot \frac{\partial C(x,t)}{\partial x}$$

$$D : diffusion \quad constant$$

$$[D] = cm^2 / \sec$$

Using the Continuity Equation

$$\frac{\partial C(x,t)}{\partial t} + \nabla \cdot J(x,t) = 0$$

$$\Rightarrow \frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x} = \frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x} \right)$$

Diffusion Equation

If D is independent of C
(i.e., C is independent of x).

$$\frac{\partial\, C(x,t)}{\partial\, t} = D\,\frac{\partial^{2} C(x,t)}{\partial\, x^{2}}$$

Concentration Independent Diffusion Equation

Temperature Dependence of D

$$D = D_0 e^{-E_A/kT}$$

$$E_A = \text{activation energy in eV}$$

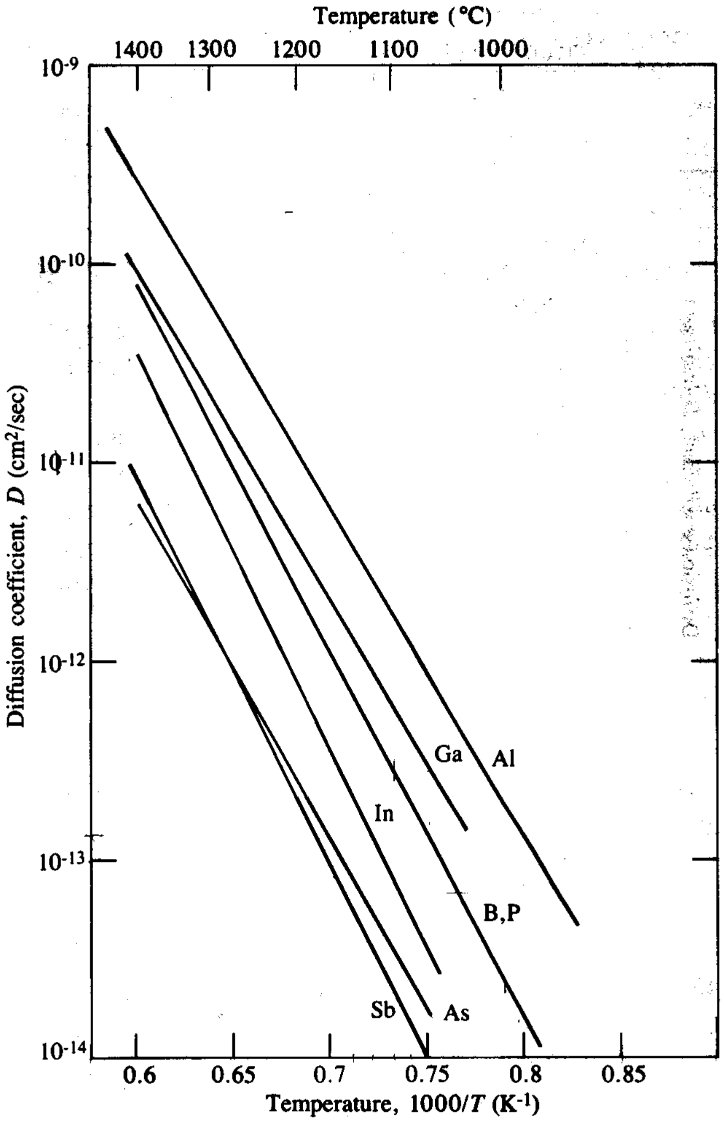
$$k = \text{Boltzman constant}$$

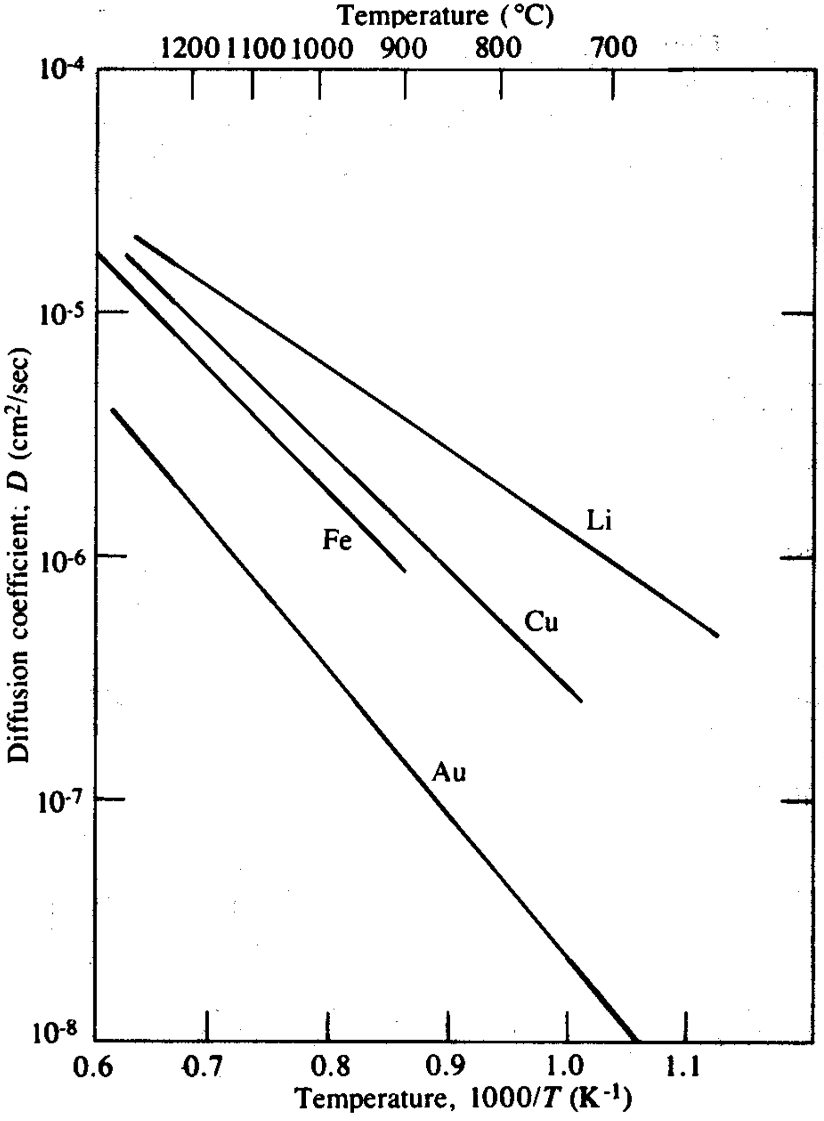
$$= 8.6 \times 10^{-5}\ eV / kelvin$$

$$D_0, E_A \text{ are tabulated.}$$

Diffusion Coefficients of Impurities in Si

$$D = D_O e^{-E_A/kT}$$





A. Predeposition Diffusion Profile

- *Boundary Conditions*:

$$C(x = 0, t) = C_0 = solid\ solubility\ of\ the\ dopant$$

$$C(x = \infty, t) = 0$$

- *Initial Condition*:

$$C(x, t = 0) = 0$$

Solid Solubility of Common Impurities in Si

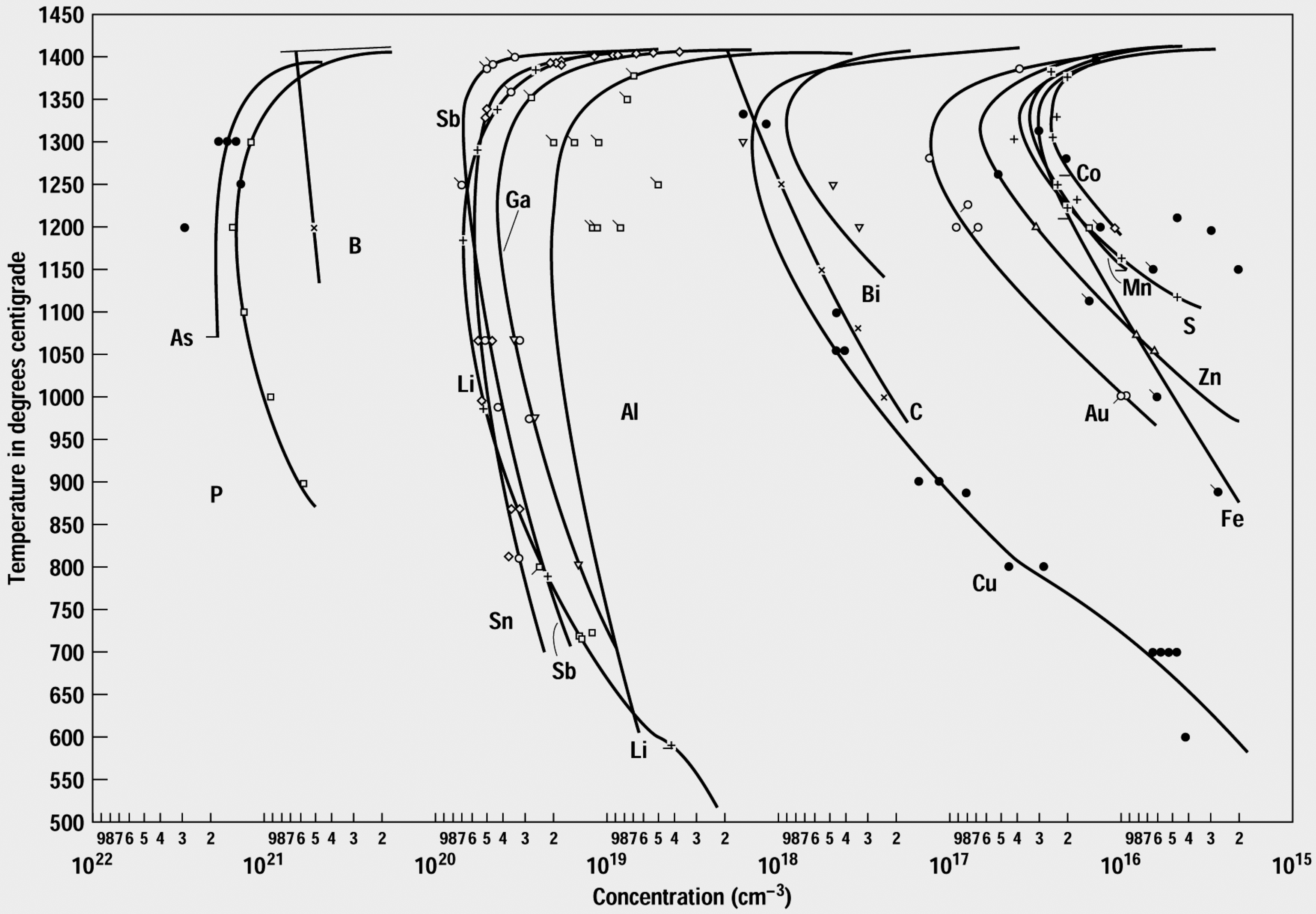


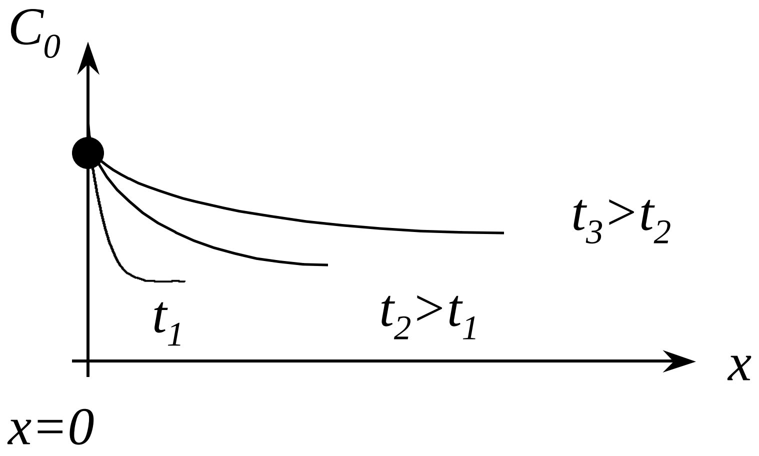
Figure 2.4 Solid solubility of common silicon impurities *(all rights reserved, reprinted with permission, © 1960 AT & T).*

$$C\left(x,t\right)=C_0\cdot\left[1-\frac{2}{\sqrt{p}}\int_0^{\frac{x}{2\sqrt{Dt}}}e^{-y^2}dy\right]$$

$$=C_0\cdot erfc\left(\frac{x}{2\sqrt{Dt}}\right)$$

$2\sqrt{Dt}$ = *Characteristic distance for diffusion.*

$C_0 \equiv$ *Surface Concentration (solid solubility limit)*



[1] Predeposition dose

$$Q(t) = \int_0^\infty C(x,t)\,dx$$

$$= \frac{C_0 \cdot 2\sqrt{Dt}}{\sqrt{p}} \quad \propto \quad \sqrt{t}$$

[2] Conc. gradient

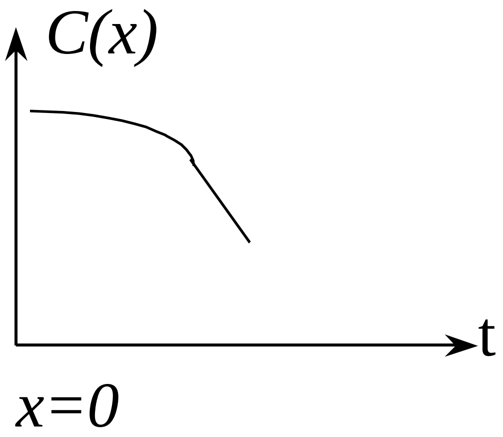
$$\frac{\P C}{\P x} = -\frac{Co}{\sqrt{p}\sqrt{Dt}}\, e^{-x^2/4Dt}$$

B. Drive-in Profile

- ***Boundary Conditions*** :

$$C\left(x=\infty, t\right)=0$$

$$\left.\frac{\partial C}{\partial X}\right|_{x=0}=0$$

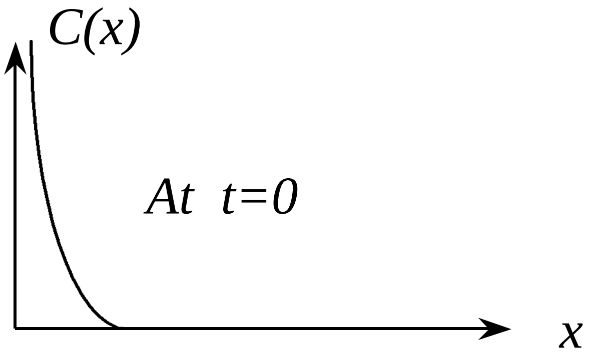


- ***Initial Conditions*** :

$$C\left(x, t=0\right)=Co\cdot erfc\left[\frac{x}{2\sqrt{\left(Dt\right)}}\right]$$

Predep's (Dt)

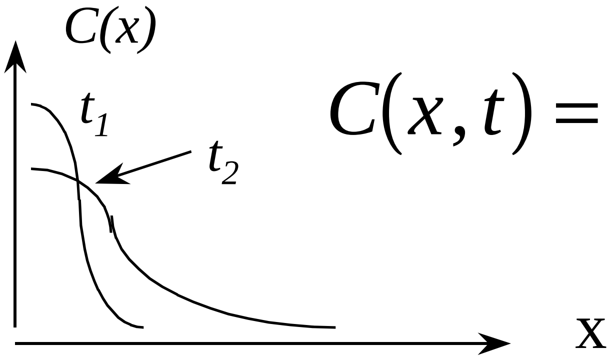
Shallow Predep Approximation:



$$C(x, t=0) \approx Q \cdot \delta(x)$$

$$Q = \frac{C_0 \cdot 2\sqrt{(Dt)}_{predep}}{\sqrt{\pi}}$$

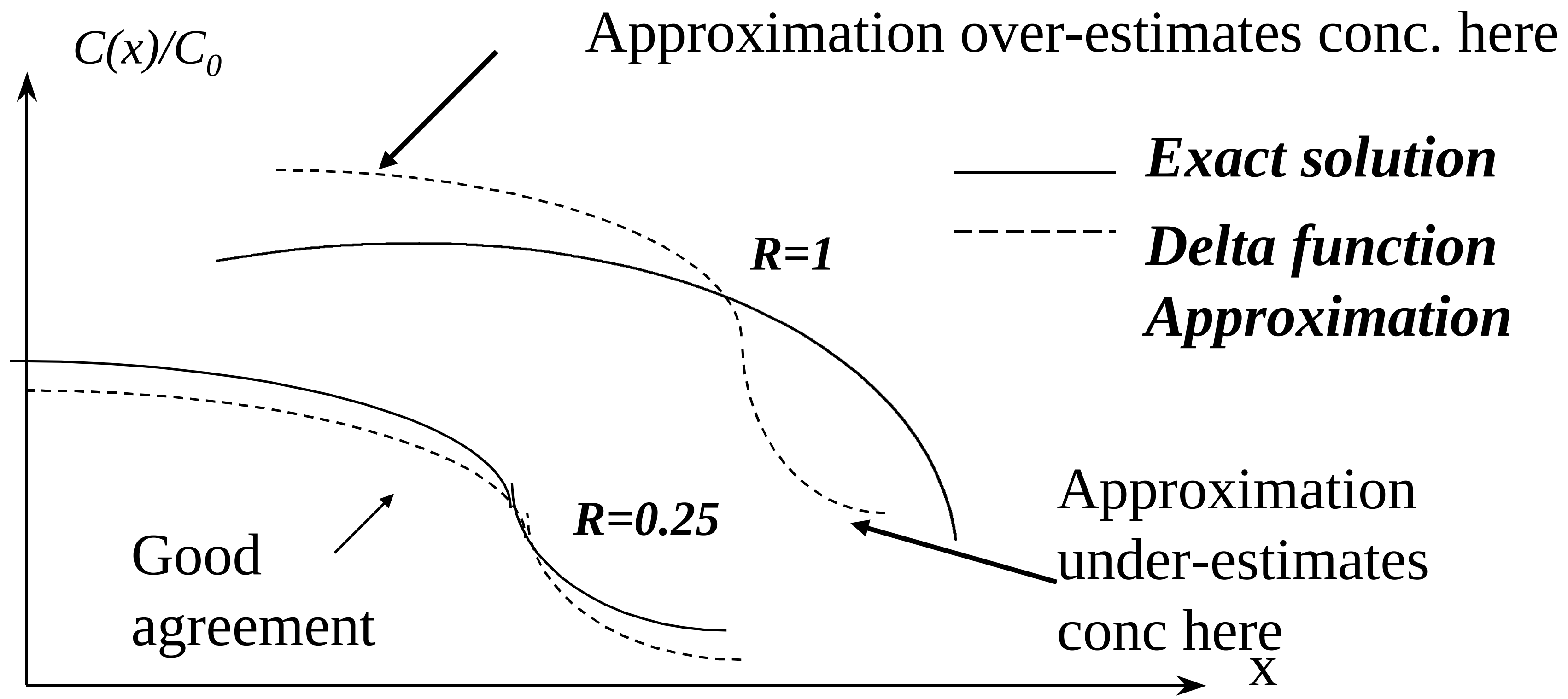
Solution of Drive-in Profile :



$$C(x,t) = \frac{Q}{\sqrt{\pi (Dt)_{drive-in}}} e^{-x^2 / 4(Dt)_{drive-in}}$$

How good is the δ(x) approximation ?

$$R = \frac{\sqrt{Dt}_{\,predep}}{\sqrt{Dt}_{\,drive-in}}$$



Summary of Predep + Drive-in

$D_1 = \text{Diffusivity at Predep temperature}$

$t_1 = \text{Predep time}$

$D_2 = \text{Diffusivity at Drive-in temperature}$

$t_2 = \text{Drive-in time}$

$$C(x) = \left(\frac{2C_0}{p}\right)\left(\frac{D_1 t_1}{D_2 t_2}\right)^{1/2} e^{-x^2 / 4D_2 t_2}$$

Semilog Plots of normalized Concentration versus depth

Predep

Drive-in

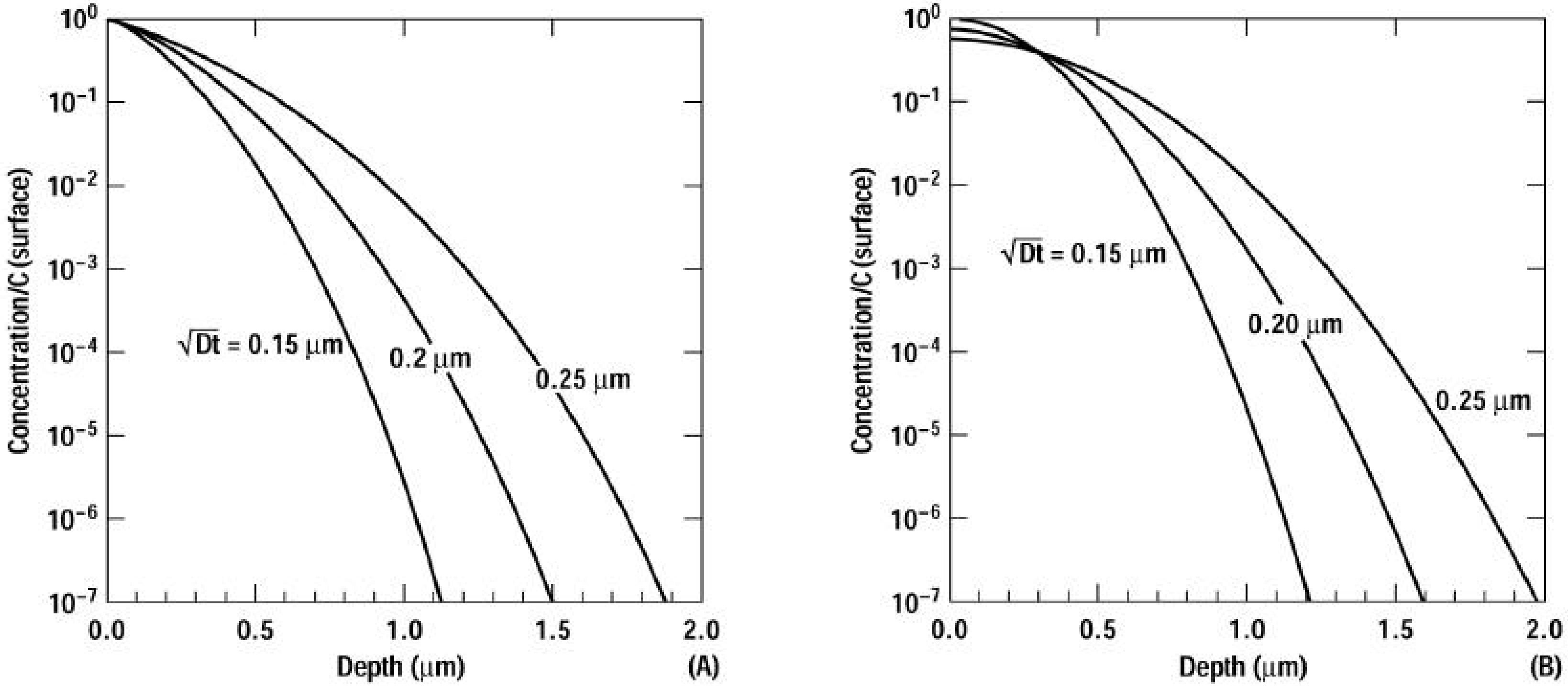
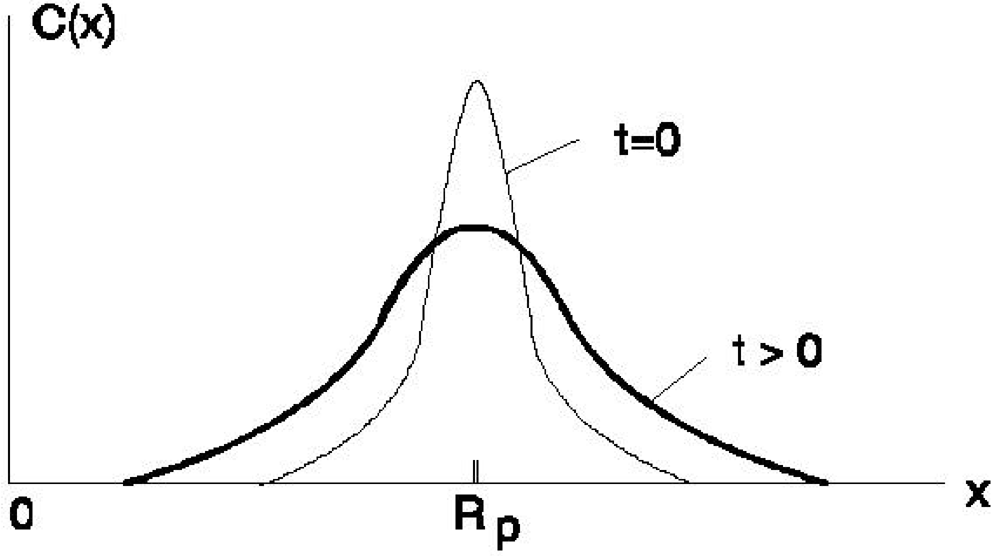


Figure 3.7 Concentration as a function of depth for (A) predeposition and (B) drive in diffusions for several values of the characteristic diffusion length.

Diffusion of Gaussian Implantation Profile



$$C(x,t) = \frac{\phi}{\sqrt{2\pi}\,(\Delta R_p^2 + 2Dt)^{1/2}} \cdot e^{-\frac{(x - R_p)^2}{2\,(\Delta R_p^2 + 2Dt)}}$$

Note: ϕ is the implantation dose

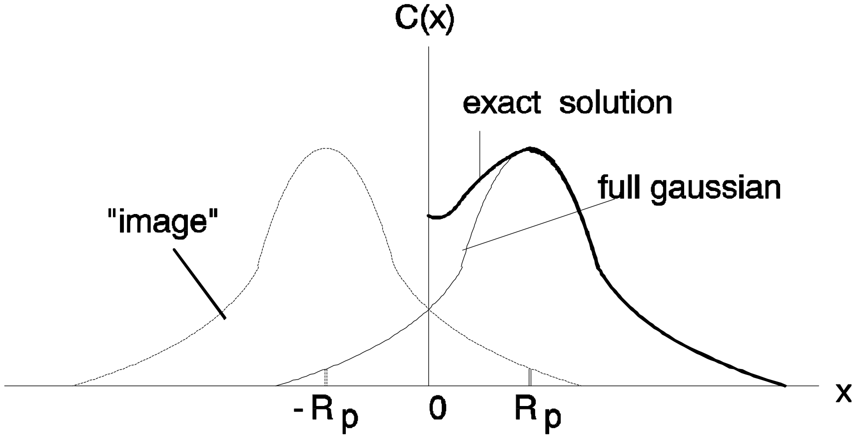
Diffusion of Gaussian Implantation Profile (arbitrary R_p)

The exact solutions with $\frac{\partial C}{\partial x} = 0$ at x = 0 (.i.e. no dopant loss through surface) can be constructed by adding another full gaussian placed at $-R_p$ [Method of Images].

$$C(x, t) = \frac{\phi}{\sqrt{2\pi}\,(\Delta R_p^2 + 2Dt)^{1/2}} \cdot \left[e^{-\frac{(x - R_p)^2}{2\,(\Delta R_p^2 + 2Dt)}} + e^{-\frac{(x + R_p)^2}{2\,(\Delta R_p^2 + 2Dt)}} \right]$$

We can see that in the limit $(Dt)^{1/2} >> R_p$ and ΔR_p ,

$$C(x,t) \rightarrow \frac{\phi e^{-x^2/4Dt}}{(\pi Dt)^{1/2}} \qquad \text{(the half-gaussian drive-in solution)}$$



The Thermal Budget

Dopants will redistribute when subjected to various thermal cycles of IC processing steps. If the diffusion constants at each step are independent of dopant concentration, the diffusion equation can be written as :

$$\frac{\partial C}{\partial t} = D(t)\,\frac{\partial^2 C}{\partial x^2}$$

Let $\beta(t) \equiv \int_0^t D(t')dt'$

$$\therefore\ D(t) = \frac{\partial \beta}{\partial t}$$

Using $\dfrac{\partial C}{\partial t} = \dfrac{\partial C}{\partial \beta} \bullet \dfrac{\partial \beta}{\partial t}$

The diffusion equation becomes: $\dfrac{\partial C}{\partial \beta} \bullet \dfrac{\partial \beta}{\partial t} = \dfrac{\partial \beta}{\partial t} \bullet \dfrac{\partial^2 C}{\partial x^2}$ or $\dfrac{\partial C}{\partial \beta} = \dfrac{\partial^2 C}{\partial x^2}$

When we compare that to a standard diffusion equation with D being time-independent: $\frac{\partial C}{\partial (Dt)} = \frac{\partial^2 C}{\partial x^2}$, we can see that replacing the (Dt) product in the standard solution by β will also satisfy the time-dependent D diffusion equation.

Example

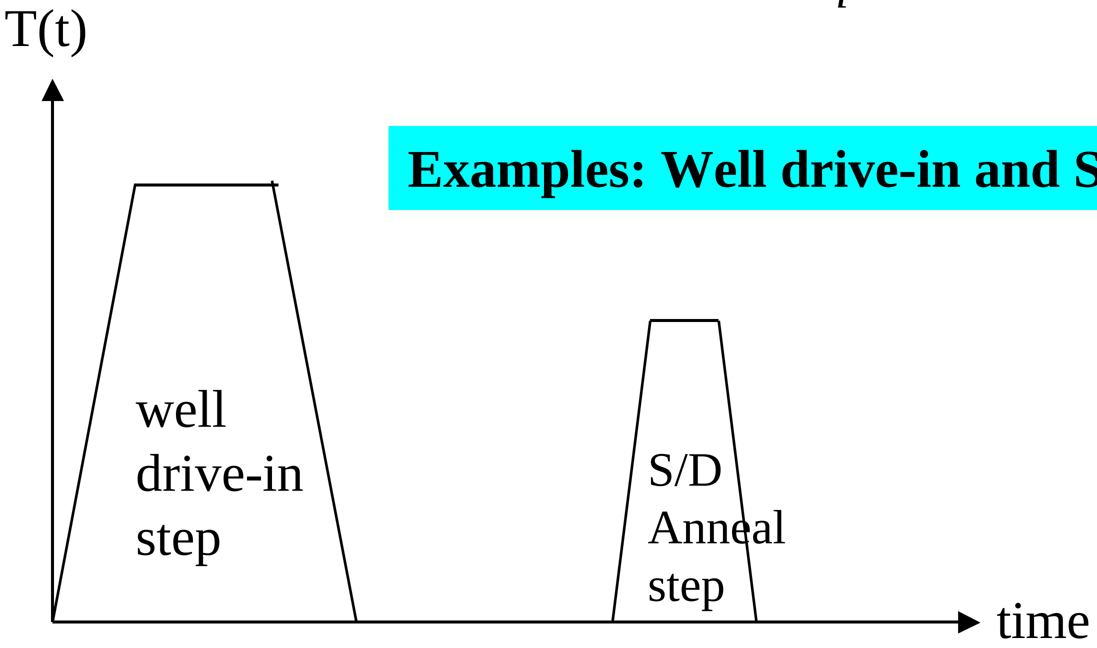
Consider a series of high-temperature processing cycles at { temperature T_1, time duration t_1} ,{ temperature T_2, time duration t_2}, etc. The corresponding diffusion constants will be D_1, D_2,... . Then, $\beta = D_1t_1+D_2t_2 +\ldots.. = (Dt)_{\text{effective}}$

** The sum of Dt products is sometimes referred to as the “thermal budget” of the process. For small dimension IC devices, dopant redistribution has to be minimized and we need low thermal budget processes.

Thermal Budget

$$(Dt)_{effective} = \sum_i (Dt)_i$$

Examples: Well drive-in and S/D annealing steps

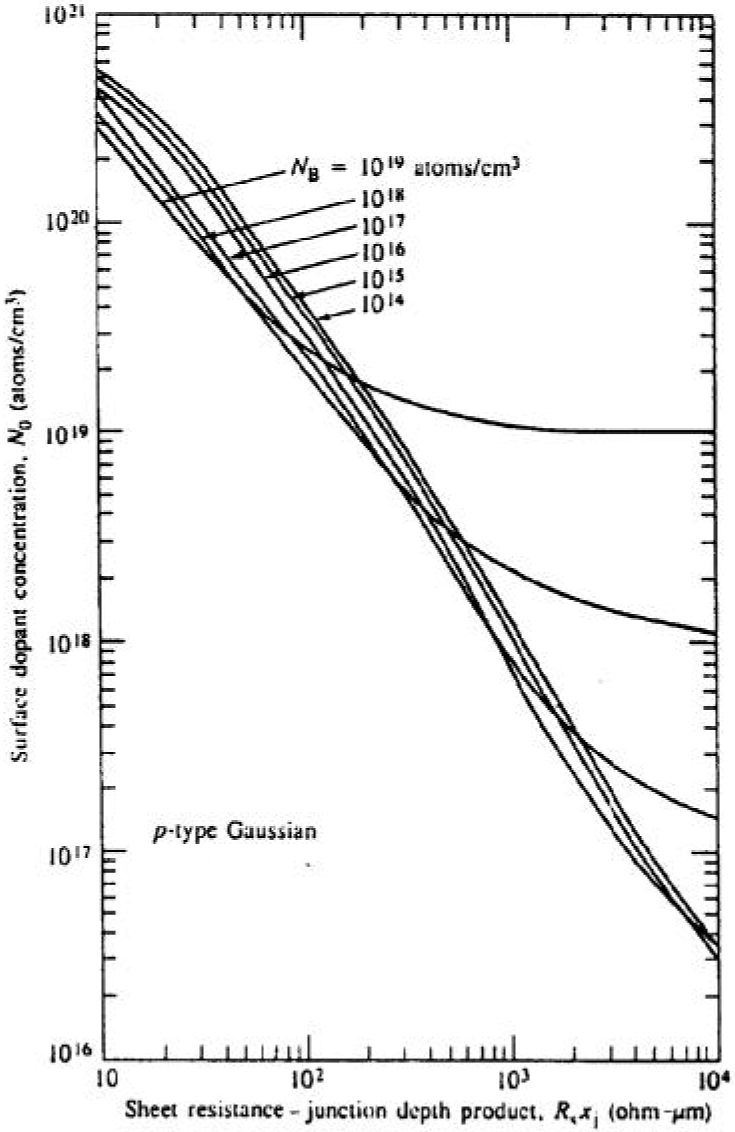


*** For a complete process flow, only those steps with high Dt values are important**

Irvin’s Curves

* 4 sets of curves
See Jaeger text

- p-type Erfc
- n-type Erfc
- p-type half-gaussian
- n-type half-gaussian



Establish the ***explicit*** relationship between:

N_o (surface concentration) ,

x_j (junction depth),

N_B (background concentration),

R_S (sheet resistance),

Once any three parameters are known, the fourth one can be determined.

Motivation to generate the Irvin's Curves

Both N_B(4-point-probe), R_S (4-point probe) and x_j (junction staining) can be conveniently measured experimentally but not N_o (requires secondary ion mass spectrometry). However, these four parameters are related.

Approach

1) The dopant profile (erfc or half-gaussian)can be uniquely determined if one knows the concentration values at ***two*** depth positions.

2) We will use the concentration values N_o at x=0 and N_B at $x=x_j$ to determine the profile C(x). (i.e., we can determine the Dt value)

3) Once the profile C(x) is known, the sheet resistance R_S can be integrated numerically from:

$$Rs = \frac{1}{\int_0^{x_j} q \cdot m(x)\left[C(x) - N_B\right] dx}$$

4) The Irvin's Curves are plots of N_o versus ($R_s \bullet x_j$) for various N_B.

Figure illustrating the relationship of N_o,N_B,x_j, and R_S

N_o , N_B , x_j

↓

Dt

(profile known for all x)

↓

R_S