

### MATHEMATICS OF DOPING PROFILES

The diffusion equation with **constant D** :

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

has the general solution: 
$$C(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} F(x') e^{-\frac{(x-x')^2}{4Dt}} dx'$$

where  $F(x')$  is the  $C(x,t)$  profile at  $t=0$

#### A. Predeposition: (constant source diffusion)

(1)  $C(x,t) = C_0 \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$

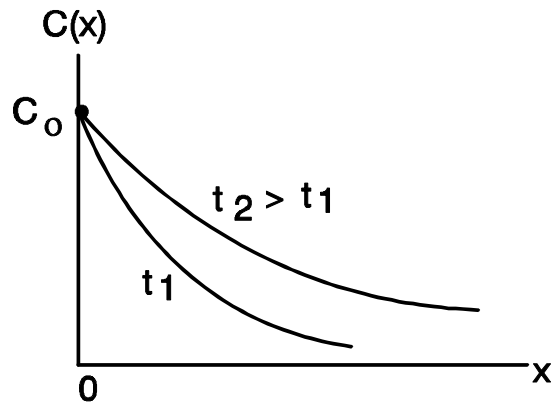
(2) Dopant dose incorporated  $Q = \int_0^{\infty} C(x,t) dx = \frac{2C_0\sqrt{Dt}}{\sqrt{\pi}}$

\* The dose incorporated depends on the square-root of predep time

(3) **Surface concentration**  $C_0 = C(0,t) = \text{solid solubility of dopant in Si for all times.}$

\* The surface concentration is independent of predeposition time. Use Fig. 4.6 of Jaeger for the  $C_0$  values.

(4) Concentration gradient  $\frac{\partial C(x,t)}{\partial x} = \frac{-C_0}{\sqrt{\pi Dt}} \exp[-x^2/4Dt]$



#### B. Drive-in (limited source diffusion)

Initial condition: At  $t=0$ , we approximate the initial distribution as a delta function of area  $Q$  located at  $x=0$ . This approximation applies to diffusion predeposition or ion implantation with small  $R_p$ .

(1)  $C(x,t) = \frac{Q}{\sqrt{\pi Dt}} \exp[-x^2/4Dt]$  for  $x>0$  "**half-gaussian**"

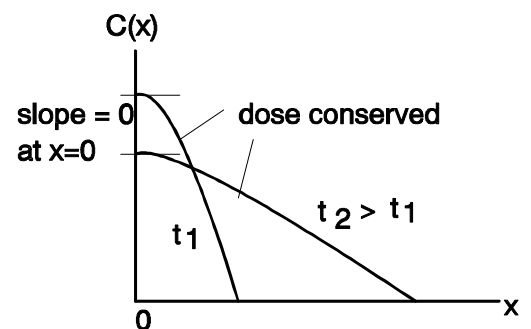
(2)  $Q(t) = \int_0^{\infty} C(x,t) dx = Q$  (at  $t=0$ ) for all times

\* **During drive-in, the dopant dose is conserved.**

(3) Surface concentration  $C(0,t) = \frac{Q}{\sqrt{\pi Dt}}$

\* During drive-in, the surface concentration decreases with time.

(4) Concentration gradient  $\frac{\partial C(x,t)}{\partial x} = \frac{-x}{2Dt} \times \frac{Q}{\sqrt{\pi Dt}} \exp[-x^2/4Dt]$



#### C. Ion Implantation

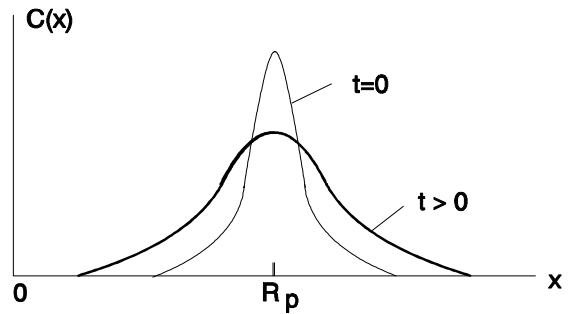
(1) Gaussian Approximation :  $C(x) = N_p \exp \left[ \frac{-(x-R_p)^2}{2(\Delta R_p)^2} \right]$  **"full gaussian"**

(2) Incorporated dose  $\phi = \int_{-\infty}^{\infty} C(x) dx \approx \int_0^{\infty} C(x) dx = N_p [\sqrt{2\pi}\delta R_p]$  if  $R_p$  is  $> 3\delta R_p$

(3) Peak concentration  $N_p = \frac{\phi}{\sqrt{2\pi}\Delta R_p} \approx \frac{0.4\phi}{\Delta R_p}$

(4) If  $R_p$  is sufficiently deep that the implant profile is close to a full gaussian, additional drive-in step for time  $t$  will just create a gaussian with larger straggle:

$$C(x,t) = \frac{N_p}{\left[1 + \frac{4Dt}{2(\Delta R_p)^2}\right]^{1/2}} \exp \left[ \frac{-(x - R_p)^2}{2(\Delta R_p)^2 + 4Dt} \right]$$



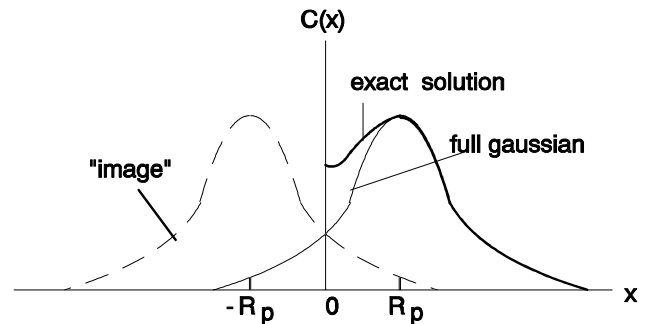
[Note: For long drive-in times, the left-side of the full gaussian piles up at the surface and the above equation is not valid. We can see in the limit that  $2\sqrt{Dt} \gg R_p$ ,  $C(x,t)$  develops into a half gaussian with:

$$C(x,t) = \frac{\phi}{\sqrt{\pi Dt}} \exp \left[ -x^2 / 4Dt \right] \text{ for } x > 0$$

(5)  $R_p$  close to surface

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 for  $(Dt)^{1/2} \gg R_p$  and  $\Delta R_p$ ,  $C(x,t) \rightarrow$

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

#### D. Common Dopant Diffusion Constants

Diffusion constants of dopants in Si reported in the literature are not consistent, probably due to variability of the processing conditions. High concentration diffusion effects (discussed later) also complicates the picture. Unless specified, we will use the following concentration independent diffusion constants for calculations:

$$D = D_0 \exp[-E_a/kT]$$

$D_0$  = Pre-exponent constant

$E_a$  = Activation Energy in eV

$k$  = Boltzmann Constant =  $8.62 \times 10^{-5}$  eV /K

Use Table 4.1 of Jaeger for the  $D_0$  and  $E_a$  values.

Dopant	$D_0$ (cm <sup>2</sup> /sec)	$E_a$ (eV)
<b>B</b>	<b>10.5</b>	<b>3.69</b>
<b>P</b>	<b>10.5</b>	<b>3.69</b>
<b>As</b>	<b>0.32</b>	<b>3.56</b>

### E. Multiple Drive-in steps

$(Dt)_{\text{effective}} = (Dt)_1 + (Dt)_2 + (Dt)_3, \dots$  will be used in the half-gaussian solution

**Proof:** The diffusion equation can be written as :  $\frac{\partial C}{\partial t} = D(t) \frac{\partial^2 C}{\partial x^2}$

$$\text{Let } \beta(t) \equiv \int_0^t D(t') dt' \quad \therefore D(t) = \frac{\partial \beta}{\partial t}$$

$$\text{Using } \frac{\partial C}{\partial t} = \frac{\partial C}{\partial \beta} \cdot \frac{\partial \beta}{\partial t}$$

$$\text{The diffusion equation becomes: } \frac{\partial C}{\partial \beta} \cdot \frac{\partial \beta}{\partial t} = \frac{\partial \beta}{\partial t} \cdot \frac{\partial^2 C}{\partial x^2} \quad \text{or} \quad \frac{\partial C}{\partial \beta} = \frac{\partial^2 C}{\partial x^2}$$

$$\text{The diffusion equation becomes: } \frac{\partial C}{\partial \beta} \cdot \frac{\partial \beta}{\partial t} = \frac{\partial \beta}{\partial t} \cdot \frac{\partial^2 C}{\partial x^2} \quad \text{or} \quad \frac{\partial C}{\partial \beta} = \frac{\partial^2 C}{\partial x^2}$$

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  $\beta$  will also satisfy the time-dependent D diffusion equation.

[Note} 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.

## F. Two-Dimensional Drive-in Diffusion Profile (Constant D)

### (a) Line Diffusion Source

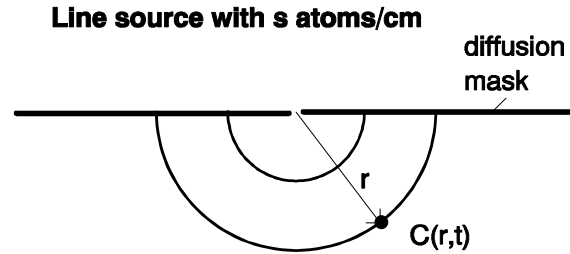
Consider a line diffusion source with  $s$  atoms/cm at  $r = 0$ , the diffusion equation in cylindrical coordinates is:

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

The 2-dimensional diffusion profile is equal to:

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

[Note:  $r^2 = x^2 + y^2$  in rectangular co-ordinates]



### (b) Semi-infinite plane Diffusion Source

For a half-plane of diffusion source at  $x=0$ ,  $0 \leq y < \infty$  (with surface concentration of  $Q$  atoms/cm<sup>2</sup>, the diffusion profile in  $x$ - $y$  coordinates is simply the **superposition** of all line sources located at  $(0, y')$  from  $0 \leq y' < \infty$  :

$$C(x, y, t) = K \cdot \int_0^{\infty} e^{-(x^2 + (y-y')^2)/4Dt} dy'$$

where  $K$  is a normalization factor.

$$\text{Let } z = \frac{y-y'}{2\sqrt{Dt}}, \therefore dz = \frac{-dy'}{2\sqrt{Dt}}$$

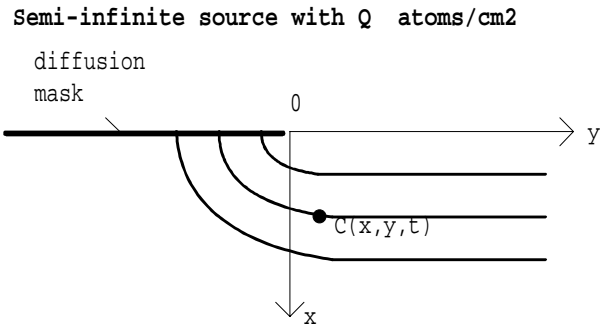
$$C(x, y, t) = K \cdot 2\sqrt{Dt} \cdot e^{-x^2/4Dt} \int_{-\infty}^{y/2\sqrt{Dt}} e^{-z^2} dz$$

$$= K \sqrt{\pi Dt} e^{-x^2/4Dt} \left[ 1 + \operatorname{erf}\left(\frac{y}{2\sqrt{Dt}}\right) \right]$$

To find  $K$ , we note that for  $y \rightarrow +\infty$  (far from the masking edge),  $C(x, y, t) \rightarrow \frac{Q}{\sqrt{\pi Dt}} e^{-x^2/4Dt}$  (i.e., the one-dimensional case). So  $K = Q / 2\pi Dt$

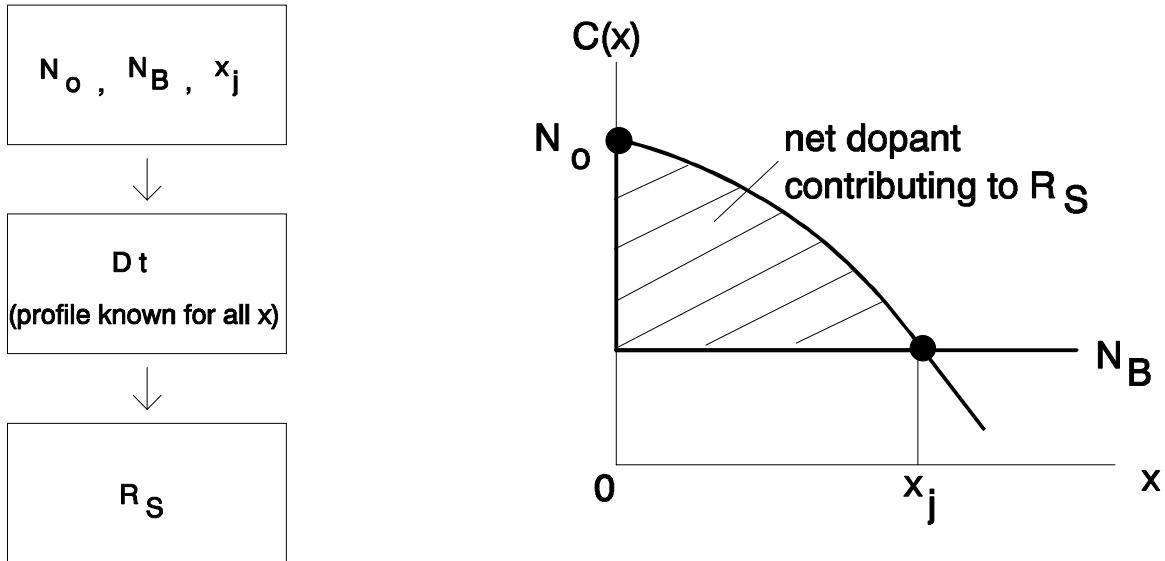
$$\text{Therefore } C(x, y, t) = \frac{Q}{2\sqrt{\pi Dt}} e^{-x^2/4Dt} \left[ 1 + \operatorname{erf}\left(\frac{y}{2\sqrt{Dt}}\right) \right]$$

- We will expect less dopants under the diffusion mask region since there is no supply of dopant from the surface.



### G. Interpretation of the Irvin's Curves

The purpose of generating the Irvin's curves is establish the *explicit* relationship between the four parameters :  $N_o$  (surface concentration) ,  $x_j$  (junction depth), background concentration ( $N_B$ ), and the  $R_S$  (sheet resistance), if the profile is known to be either an erfc function (predeposition) or a half-gaussian function (drive-in). **Once any three parameters are known, the fourth one can be determined.** The implicit relationship used to generate the curves is the dependence of the majority carrier mobility on the total dopant concentration (assumed to be universal for dopants in Si).



Keep in mind there are only two parameters which will *uniquely* determine the erfc or half-gaussian doping profiles :  $N_o$  and  $\sqrt{Dt}$ . Given  $N_o, N_B$ , and  $x_j$ ,  $\sqrt{Dt}$  can be solved for either of these two profiles. Since the depth dependence of the dopant concentration is known, the sheet resistance is simply an integral quantity of the (net concentration • mobility ) product :

$$R_S = \frac{\bar{\rho}}{x_j} = \frac{1}{\int_0^{x_j} q [N(x) - N_B] \mu(x) dx}$$

For IC process monitoring,  $x_j$  and  $R_S$  can easily be measured in the laboratory, not  $\sqrt{Dt}$ . The Irvin's curves are arranged in such a way ( i.e.,  $N_o$  versus  $R_S \cdot x_j$  ) such that  $N_o$  can be determined once  $R_S, x_j$  and  $N_B$  are known. Alternatively, if  $N_o$  can be measured ( with Hall Effect or Secondary Mass Ion Spectrometry),  $x_j$  can also be inferred.

### SOME PROPERTIES OF THE ERROR FUNCTION

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-y^2} dy$$

$$\text{erfc}(z) \equiv 1 - \text{erf}(z)$$

$$\text{erf}(0) = 0$$

$$\text{erf}(\infty) = 1$$

$$\text{erf}(-\infty) = -1$$

$$\text{erf}(z) \approx \frac{2}{\sqrt{\pi}} z \quad \text{for } z \ll 1$$

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

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

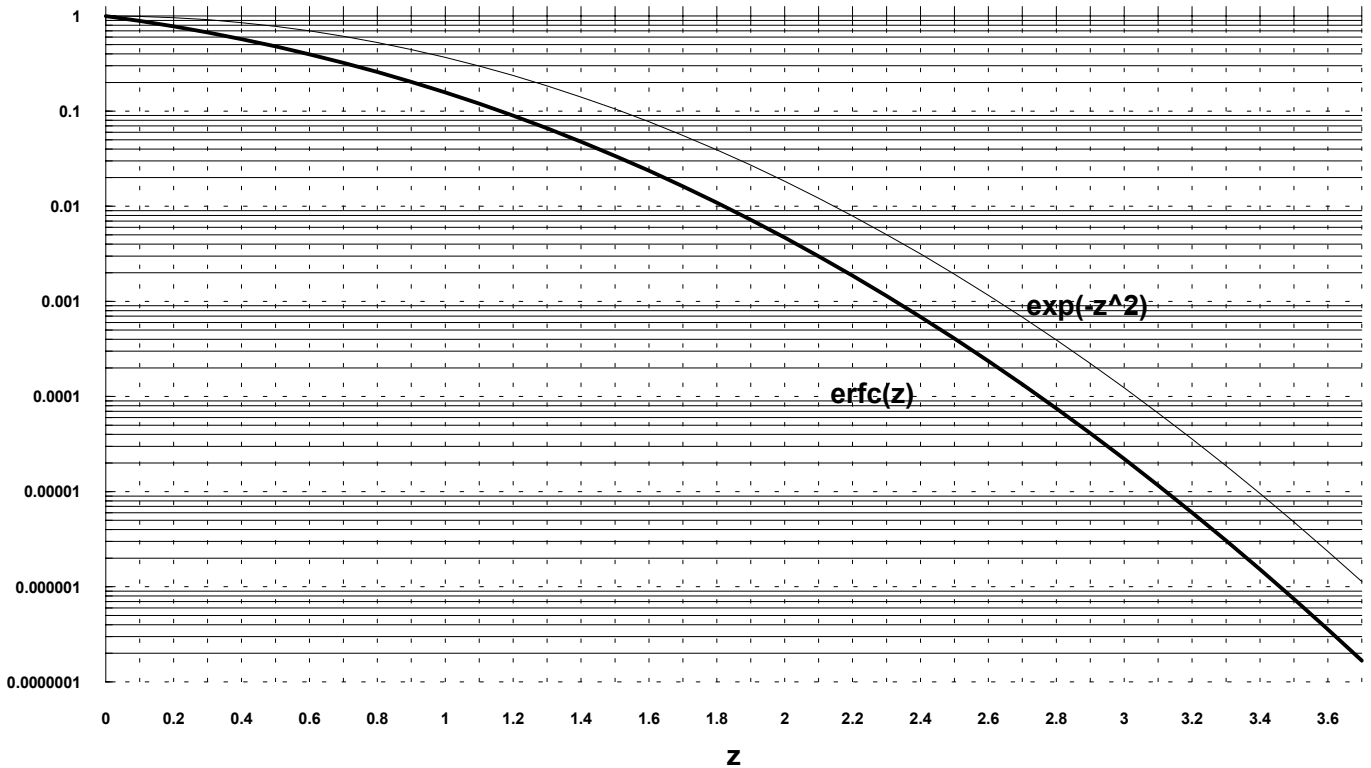
$$\int_0^z \text{erfc}(y) dy = z \text{erfc}(z) + \frac{1}{\sqrt{\pi}} (1 - e^{-z^2})$$

$$\int_0^{\infty} \text{erfc}(z) dz = \frac{1}{\sqrt{\pi}}$$

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<sup>7</sup>):  $\text{erf}(z) = 1 - (a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 + a_5 T^5) e^{-z^2}$

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

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



Another less-accurate but simpler approximation is  $\text{erf}(z) \approx [1 - e^{-\frac{4z^2}{\pi}}]^{1/2}$ . This approximation has error less than 1%. For calculations involving the difference of two erf functions, the 1% accuracy may not be adequate.