Diffusion Modeling

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Modeling $N(x)$ → J → x

⇒ Dopants from points of high conc. move to points of low conc. w/ flux J

⇒ Question: What's $N(x,t)$? ← fcn of time

Fick's Law of Diffusion – (1st law)

$$J(x,t) = -D\frac{\partial N(x,t)}{\partial x} \quad (1)$$

J: flux [#/cm²·s]; D: Diffusion Coefficient

Continuity Equation for Particle Flux –

General Form: $\frac{\partial N(x,t)}{\partial t} = -\vec{\nabla}\cdot\vec{J}$

$\frac{\partial N}{\partial t}$: rate of increase of conc. w/ time; $-\vec{\nabla}\cdot\vec{J}$: negative of the divergence of particle flux

Diffusion Modeling (cont.)

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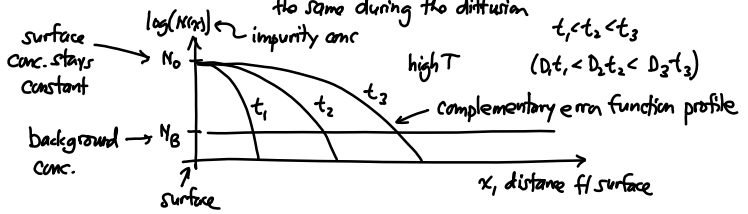
⇒ we're interested for now in the one-dimensional form:

$$\frac{\partial N(x,t)}{\partial t} = -\frac{\partial J}{\partial x} \quad (2)$$

[$\frac{\partial}{\partial x}$(1) and substitute (2) in (1)] ⇒ $\frac{\partial N(x,t)}{\partial t} = D\frac{\partial^2 N(x,t)}{\partial x^2}$ [Fick's 2nd Law of Diffusion in 1-D]

Solutions: → dependent upon boundary conditions
→ use variable separation or Laplace Xform techniques

Case 1: Predeposition → constant source diffusion · surface concentration stays the same during the diffusion



Diffusion Modeling (Predeposition)

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⇒ if plotted on a linear scale, would look like this:

⇒ Boundary Condition:

(i) $N(0,t) = N_0$
(ii) $N(\infty,t) = 0$

$$N(x,t) = N_0\left[1 - \frac{1}{\sqrt{\pi}}\int_0^{\frac{x}{2\sqrt{Dt}}} e^{-y^2}dy\right]$$

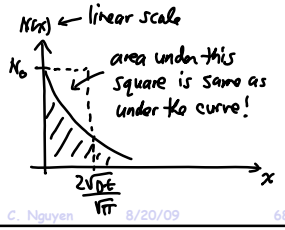
$$N(x,t) = N_0\,\mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

⇒ again, complementary error function (read tables or graph)

Dose, Q ≜ total # of impurity atoms per unit area in the Si
= area under the curve

$$Q = \int_0^\infty N(x,t)dx \Rightarrow \boxed{Q(t) = N_0\frac{2\sqrt{Dt}}{\sqrt{\pi}}\ \mathrm{cm}^{-2}}$$

$2\sqrt{Dt}$ ≜ characteristic diffusion length



Diffusion Modeling (Limited Source)

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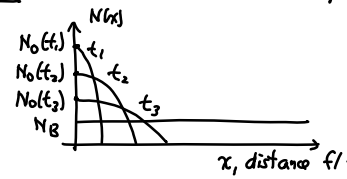
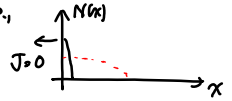
Case 2: Drive-in → limited source diffusion, i.e., constant dose Q



⇒ Boundary Condition:

(i) $N(\infty,t) = 0$ → Why? Constant Dose: $\int_0^\infty N(x,t)dx = Q$ ← const.

(ii) $\left.\frac{\partial N(x,t)}{\partial x}\right|_{x=0} = 0$ → This is equivalent to saying that there's no flux going out of the Si, i.e., and that's what this says!



Diffusion Modeling (Limited Source)

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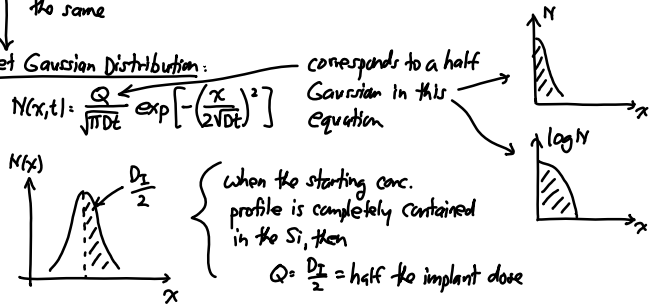
(iii) Usually make delta fcn. approx.: $N(x,0) = Q\,\delta(x)$

⇒ we can do this, because for sufficiently long diffusion times, no matter what the original shape of the dopant distribution, the diffused distribution will be the same

Get Gaussian Distribution:

$$N(x,t) = \frac{Q}{\sqrt{\pi Dt}} \exp\left[-\left(\frac{x}{2\sqrt{Dt}}\right)^2\right]$$

corresponds to a half Gaussian in this equation



When the starting conc. profile is completely contained in the Si, then

$Q = \frac{D_I}{2}$ = half the implant dose

Two-Step Diffusion

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- Two step diffusion procedure:
  - Step 1: predeposition (i.e., constant source diffusion)
  - Step 2: drive-in diffusion (i.e., limited source diffusion)
- For processes where there is both a predeposition and a drive-in diffusion, the final profile type (i.e., complementary error function or Gaussian) is determined by which has the much greater Dt product:

  $(Dt)_{predep} \gg (Dt)_{drive\text{-}in}$ ⇨ impurity profile is complementary error function

  $(Dt)_{drive\text{-}in} \gg (Dt)_{predep}$ ⇨ impurity profile is Gaussian (which is usually the case)

Successive Diffusions

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- For actual processes, the junction/diffusion formation is only one of many high temperature steps, each of which contributes to the final junction profile
- Typical overall process:
  1. Selective doping
     - Implant → effective $(Dt)_1 = (\Delta R_p)^2/2$ (Gaussian)
     - Drive-in/activation → D_2t_2
  2. Other high temperature steps
     - (eg., oxidation, reflow, deposition) → D_3t_3, D_4t_4, …
     - Each has their own Dt product
  3. Then, to find the final profile, use

$$(Dt)_{tot} = \sum_i D_i t_i$$

in the Gaussian distribution expression.

The Diffusion Coefficient

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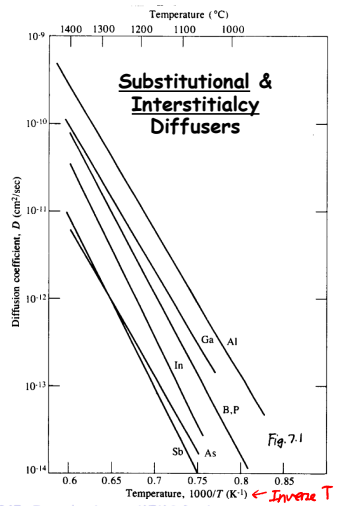
$$D = D_o \exp\left(-\frac{E_A}{kT}\right)$$ (as usual, an Arrhenius relationship)

Table 4.1 Typical Diffusion Coefficient Values for a Number of Impurities.

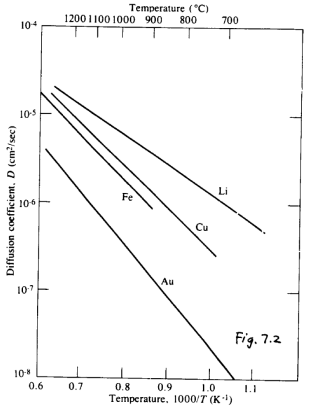
Element	$D_0(cm^2/sec)$	$E_A(eV)$
B	10.5	3.69
Al	8.00	3.47
Ga	3.60	3.51
In	16.5	3.90
P	10.5	3.69
As	0.32	3.56
Sb	5.60	3.95

Diffusion Coefficient Graphs



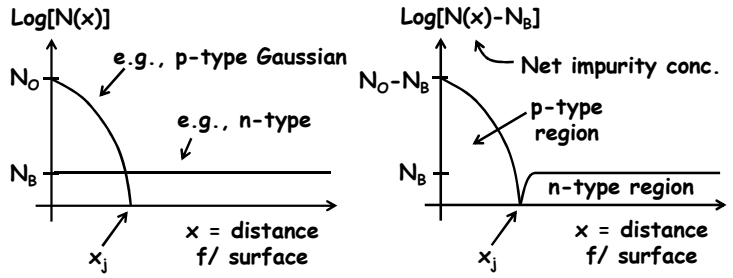
Interstitial Diffusers

↳ Note the much higher diffusion coeffs. than for substitutional



Metallurgical Junction Depth, x_j

x_j = point at which diffused impurity profile intersects the background concentration, N_B



Expressions for x_j

- Assuming a Gaussian dopant profile: (the most common case)

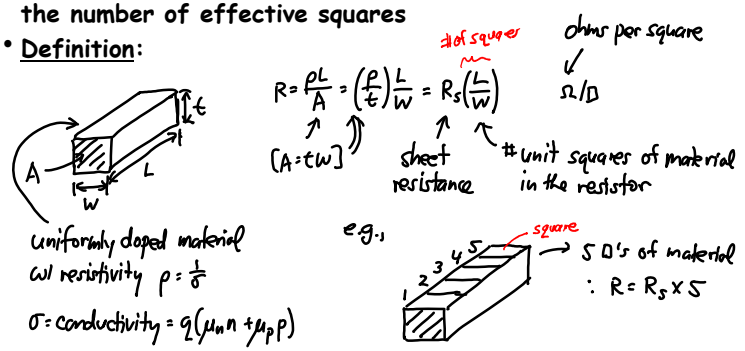
$$N(x_j,t) = N_o \exp\left[-\left(\frac{x_j}{2\sqrt{Dt}}\right)^2\right] = N_B \quad \rightarrow \quad x_j = 2\sqrt{Dt \ln\left(\frac{N_o}{N_B}\right)}$$

- For a complementary error function profile:

$$N(x_j,t) = N_o \operatorname{erfc}\left(\frac{x_j}{2\sqrt{Dt}}\right) = N_B \quad \rightarrow \quad x_j = 2\sqrt{Dt}\operatorname{erfc}^{-1}\left(\frac{N_B}{N_o}\right)$$

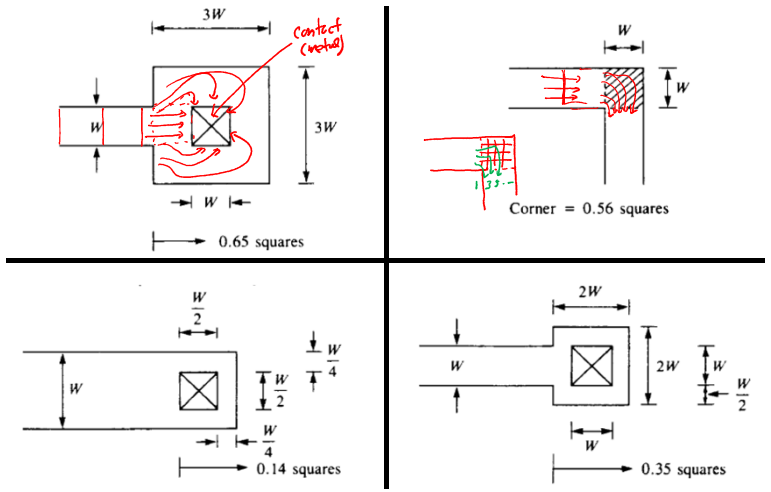
Sheet Resistance

- Sheet resistance provides a simple way to determine the resistance of a given conductive trace by merely counting the number of effective squares
- **Definition**:



- What if the trace is non-uniform? (e.g., a corner, contains a contact, etc.)

Squares From Non-Uniform Traces



Sheet Resistance of a Diffused Junction

- For diffused layers:

Majority carrier mobility

Sheet resistance

Effective resistivity

Net impurity concentration

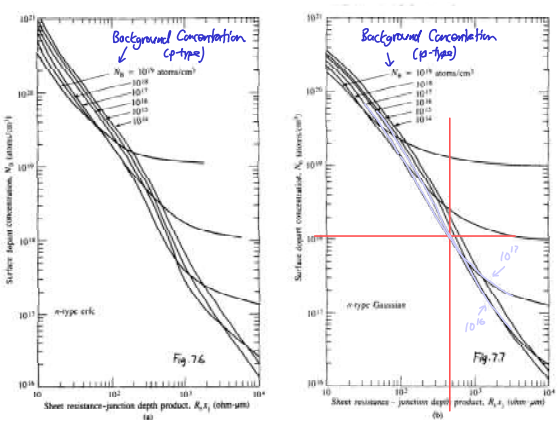
$$R_s = \frac{\bar{\rho}}{x_j} = \left[\int_o^{x_j} \sigma(x)dx\right]^{-1} = \left[\int_o^{x_j} q\mu N(x)dx\right]^{-1}$$

dopant decreases as we go deeper

[extrinsic material]

- This expression neglects depletion of carriers near the junction, x_j → thus, this gives a slightly lower value of resistance than actual
- Above expression was evaluated by Irvin and is plotted in "Irvin's curves" on next few slides
  - Illuminates the dependence of R_s on x_j, N_o (the surface concentration), and N_B (the substrate background conc.)

Irvin's Curves (for n-type diffusion)



Example.
Given: p-type
N_B = 3x10^{16} cm^{-3}
N_o = 1.1x10^{18} cm^{-3}
(n-type Gaussian)
x_j = 2.77 μm
Can determine these given known predep. and drive conditions

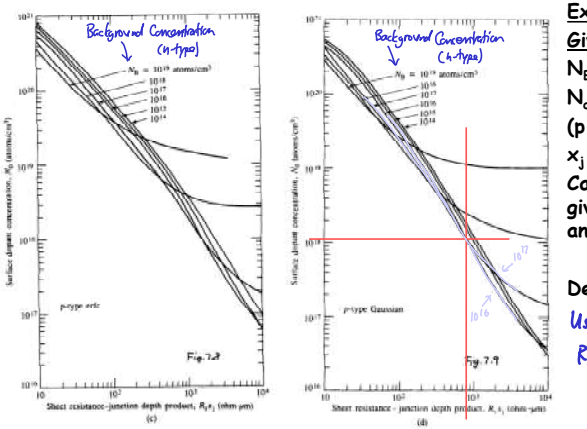
Determine the R_s.

Using Fig. 7.7:

$R_s x_j$ = 470 Ω·μm

$\therefore R_s = \frac{470}{2.77} = 170\ \Omega/\square$

Irvin's Curves (for p-type diffusion)



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x_j = 2.77 μm
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Determine the R_s.

Using Fig. 7.9:

$R_s x_j$ = 800 Ω·cm

$\therefore R_s = \frac{800}{2.77} = 289\ \Omega/\square$