EE 143
Microfabrication Technology
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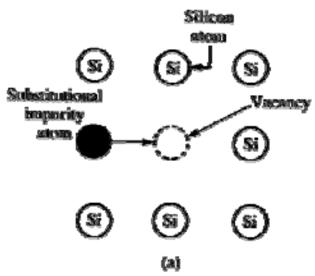
Lecture Module 6: Diffusion

Diffusion

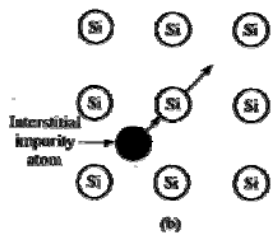
Diffusion in Silicon

- Movement of dopants within the silicon at high temperatures
- Three mechanisms: (in Si)



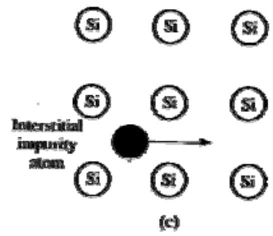
Substitutional Diffusion

- Impurity moves along vacancies in the lattice
- Substitutes for a Si-atom in the lattice



Interstitialcy Diffusion

- Impurity atom replaces a Si atom in the lattice
- Si atom displaced to an interstitial site

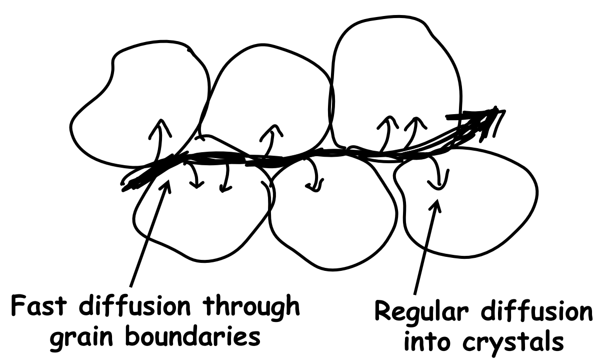


Interstitial Diffusion

- Impurity atoms jump from one interstitial site to another
- Get rapid diffusion
  - Hard to control
  - Impurity not in lattice so not electrically active

Diffusion in Polysilicon

- In polysilicon, still get diffusion into the crystals, but get more and faster diffusion through grain boundaries
- Result: overall faster diffusion than in silicon

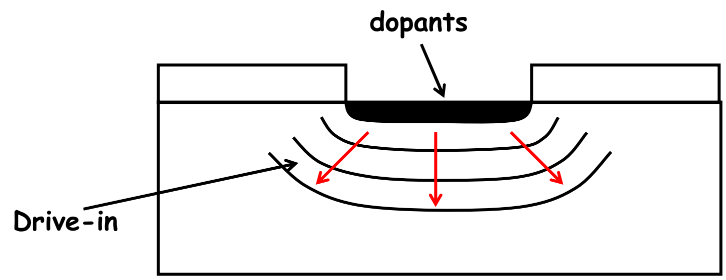


- In effect, larger surface area allows much faster volumetric diffusion

Basic Process for Selective Doping

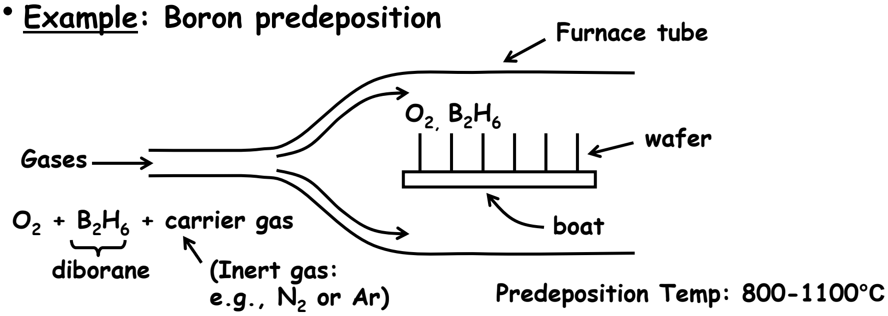
1. Introduce dopants (introduce a fixed dose Q of dopants)
   (i) Ion implantation
   (ii) Predeposition
2. Drive in dopants to the desired depth
   - High temperature > 900°C in N_2 or N_2/O_2

- Result:



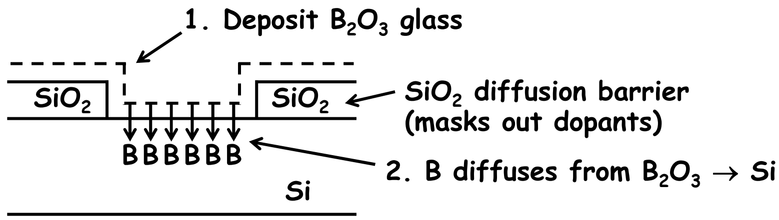
Predeposition

- Furnace-tube system using solid, liquid, or gaseous dopant sources
- Used to introduced a controlled amount of dopants
  - Unfortunately, not very well controlled
  - Dose (Q) range: 10^{13} – 10^{16} ± 20%
  - For ref: w/ ion implantation: 10^{11} – 10^{16} ± 1% (larger range & more accurate)
- Example: Boron predeposition

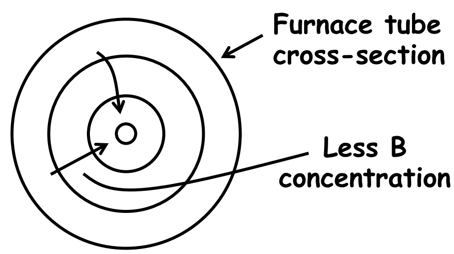


Ex: Boron Predeposition

- Basic Procedure:

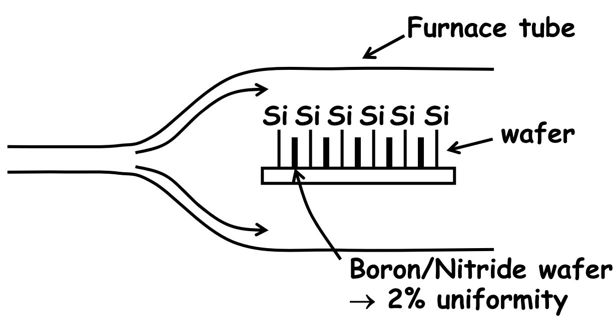


- Difficult to control dose Q, because it's heavily dependent on partial pressure of B_2H_6 gas flow
  - ↳ this is difficult to control itself
  - ↳ get only 10% uniformity



Ex: Boron Predeposition (cont.)

For better uniformity, use solid source:



Reactions:

$B_2H_6 + 3O_2 \rightarrow 3H_2O + B_2O_3$

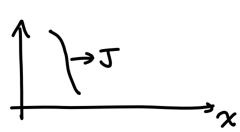
$Si + O_2 \rightarrow SiO_2$

General Comments on Predeposition

- Higher doses only: $Q = 10^{13} - 10^{16}$ cm^{-2} (I/I is $10^{11} - 10^{16}$)
- Dose not well controlled: ± 20% (I/I can get ± 1%)
- Uniformity is not good
  - ± 10% w/ gas source
  - ± 2% w/ solid source
- Max. conc. possible limited by solid solubility
  - Limited to ~10^{20} cm^{-3}
  - No limit for I/I → you force it in here!
- For these reasons, I/I is usually the preferred method for introduction of dopants in transistor devices
- But I/I is not necessarily the best choice for MEMS
  - I/I cannot dope the underside of a suspended beam
  - I/I yields one-sided doping → introduces unbalanced stress → warping of structures
  - I/I can do physical damage → problem if annealing is not permitted
- Thus, predeposition is often preferred when doping MEMS

Diffusion Modeling

Modeling



⇒ 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)

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

↑ flux [#/cm²·s] ↖ Diffusion Coefficient

Continuity Equation for Particle Flux –

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

↑ rate of increase of conc. w/ time ↖ negative of the divergence of particle flux

Diffusion Modeling (cont.)

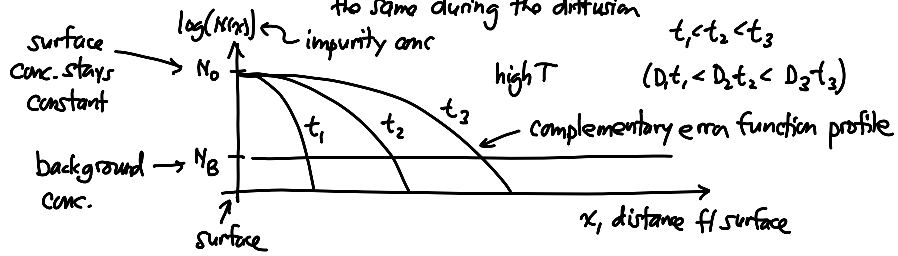
⇒ we're interested for now in the one-dimensional form:

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

$\left[\frac{\partial}{\partial x}(1) \text{ and substitute (2) in (1)}\right] \Rightarrow \frac{\partial N(x,t)}{\partial t} = D\frac{\partial^2 N(x,t)}{\partial x^2}$ [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)

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

⇒ Boundary Condition:
(i) $N(0,t) = N_0$
(ii) $N(\infty,t) = 0$

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

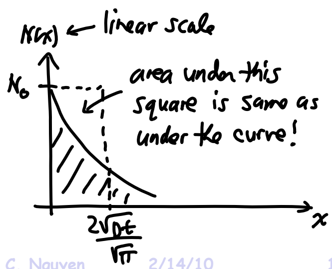
$$\boxed{N(x,t) = N_0 \, \mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)}$$

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

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

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

$\boxed{2\sqrt{Dt} \triangleq \text{characteristic diffusion length}}$



Diffusion Modeling (Limited Source)

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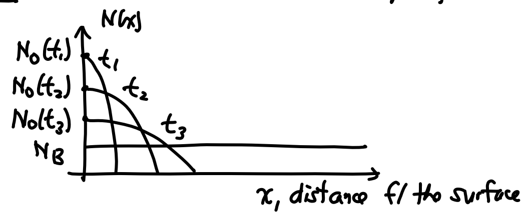
Case 2: Drive-in → limited source diffusion, i.e., constant dose Q

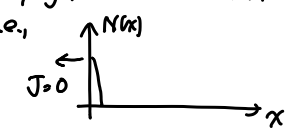


⇒ Boundary Condition:

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

(ii) $\left.\frac{\partial N(x,t)}{\partial x}\right|_{x=0} = 0$ → Why? Constant Dose: $\int_0^\infty N(x,t)\,dx = Q$ ← const.

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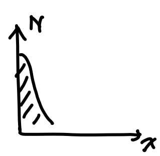
(iii) Usually make delta fcn. approx.: $N(x,0) = Q\,\delta(x)$

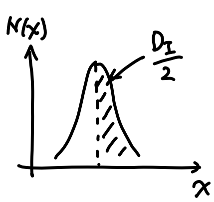
⇒ we can do this, because for sufficiently long diffusion times, no matter what the original shape of the dopant distribution, the diffused distribution will be the same

Get Gaussian Distribution:

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

← 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

- 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

- 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.

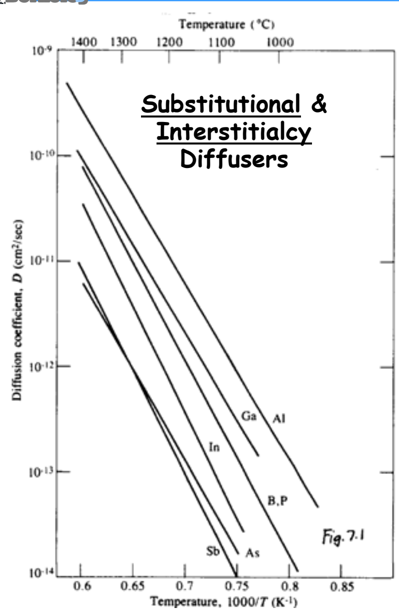
The Diffusion Coefficient

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

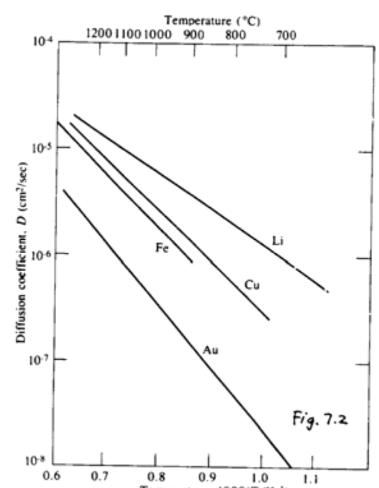
Table 4.1 Typical Diffusion Coefficient Values for a Number of Impurities.

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

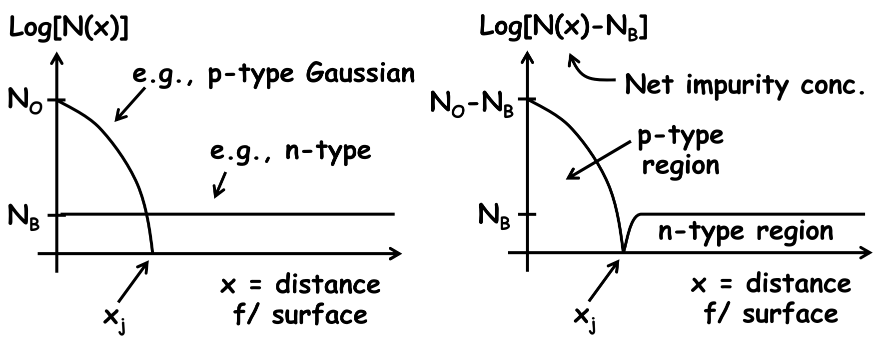


Interstitial Diffusers
- Note the much higher diffusion coeffs. than for substitutional



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)

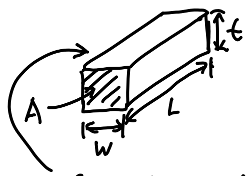
$$N(x_j,t) = N_o \exp\left[-\left(\frac{x_j}{2\sqrt{Dt}}\right)^2\right] = N_B \rightarrow x_j = 2\sqrt{Dt \ln\left(\frac{N_o}{N_B}\right)}$$

- For a complementary error function profile:

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

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**:



$$R = \frac{\rho L}{A} = \left(\frac{\rho}{t}\right)\frac{L}{W} = R_s\left(\frac{L}{W}\right)$$

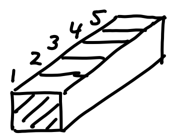
[$A = tW$] — sheet resistance — # unit squares of material in the resistor

ohms per square: $\Omega/\square$

uniformly doped material w/ resistivity $\rho = \frac{1}{\sigma}$

σ = conductivity = $q(\mu_n n + \mu_p p)$

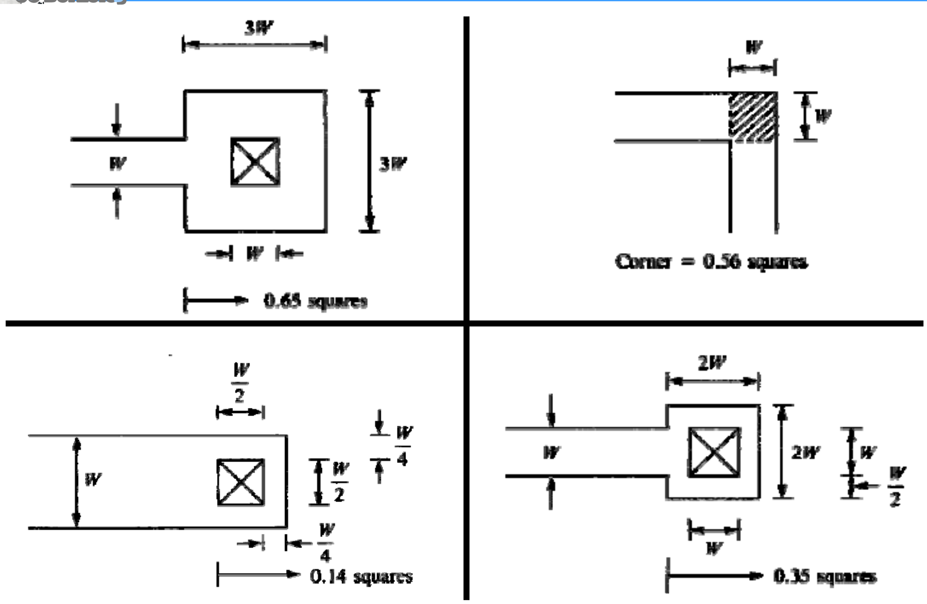
e.g.,



→ 5 $\square$'s of material $\therefore R = R_s \times 5$

- 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:

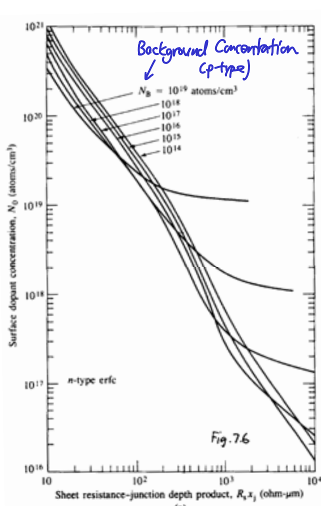
Sheet resistance — Effective resistivity — Majority carrier mobility — Net impurity concentration

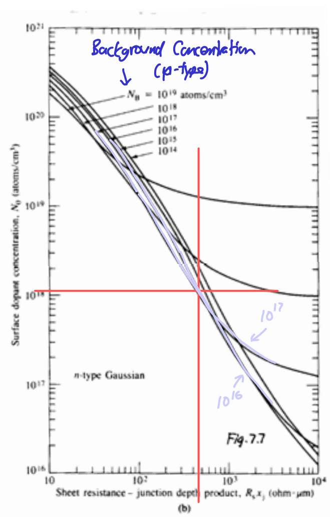
$$R_s = \frac{\bar{\rho}}{x_j} = \left[\int_o^{x_j} \sigma(x)dx\right]^{-1} = \left[\int_o^{x_j} q\mu N(x)dx\right]^{-1}$$

[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)



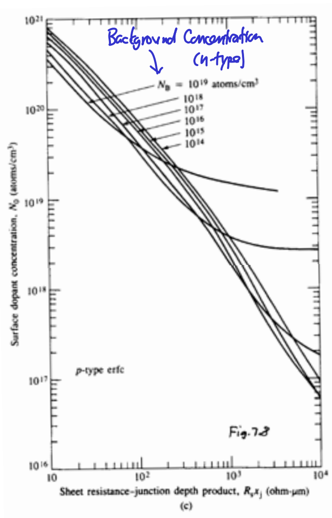


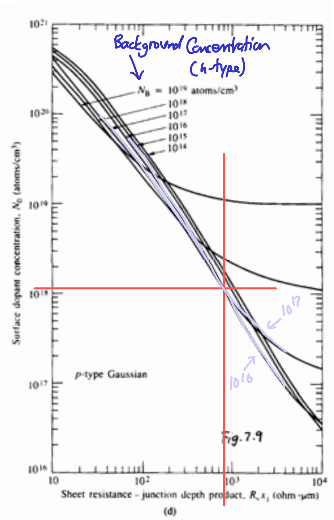
Example.
Given: (p-type)
N_B = 3x10^{16} cm^{-3}
N_o = 1.1x10^{18} cm^{-3} (n-type Gaussian)
x_j = 2.77 μm
Can determine these given known predep. and drive conditions

Determine the R_s.

Using Fig. 7.7:
$R_s x_j = 470\ \Omega/\square \cdot \mu m$
$\therefore R_s = \frac{470}{2.77} = 170\ \Omega/\square$

Irvin's Curves (for p-type diffusion)





Example.

Given: (n-type)

N_B = 3x10^{16} cm^{-3}

N_o = 1.1x10^{18} cm^{-3}

(p-type Gaussian)

x_j = 2.77 μm

Can determine these given known predep. and drive conditions

Determine the R_s.

Using Fig. 7.9:

$R_s x_j = 800\ \Omega/\square \cdot \mu m$

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