

EE 143
Microfabrication Technology
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Lecture Module 6: Diffusion

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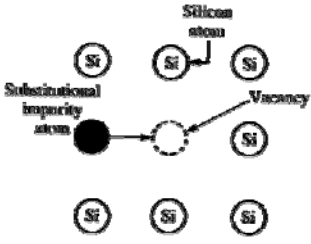
Diffusion

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Diffusion in Silicon

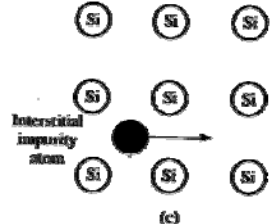
- Movement of dopants within the silicon at high temperatures
- Three mechanisms: (in Si)



(a)



(b)



(c)

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

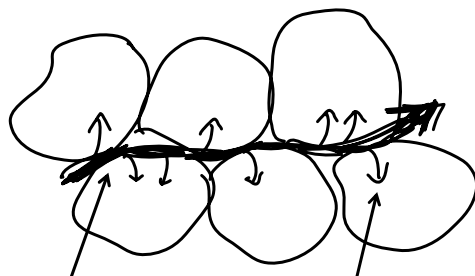
- Impurity atoms jump from one interstitial site to another
- Get rapid diffusion
 - ↳ Hard to control
 - ↳ Impurity not in lattice so not electrically active

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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



Fast diffusion through grain boundaries

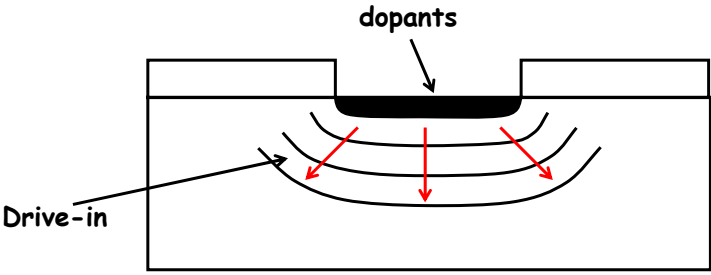
Regular diffusion into crystals

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

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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 $> 900^\circ\text{C}$ in N_2 or N_2/O_2
- Result:

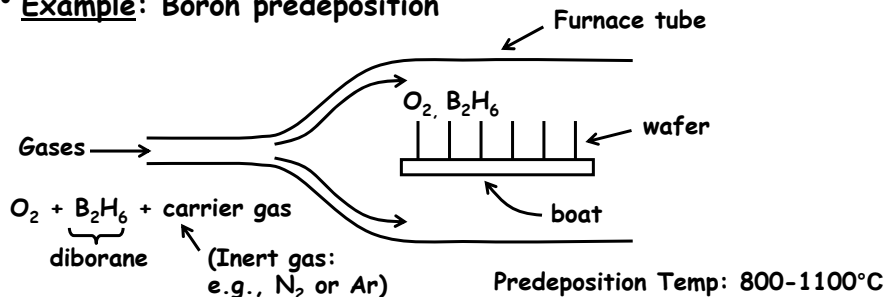


The diagram shows a cross-section of a semiconductor wafer with a central well. A black layer labeled 'dopants' is deposited in the well. Red arrows labeled 'Drive-in' point from the dopant layer into the substrate, indicating the diffusion process.

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Predeposition

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



The diagram illustrates a furnace tube system. Gases (O_2 , B_2H_6 , and carrier gas) enter from the left. The carrier gas is identified as diborane (B_2H_6) and an inert gas (e.g., N_2 or Ar). The gases flow through a furnace tube containing a boat with a wafer. The predeposition temperature is $800-1100^\circ\text{C}$.

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Ex: Boron Predeposition

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- Basic Procedure:
 1. Deposit B_2O_3 glass
 2. B diffuses from $B_2O_3 \rightarrow Si$

- 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

Furnace tube cross-section
Less B concentration

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Ex: Boron Predeposition (cont.)

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For better uniformity, use solid source:

Furnace tube
wafer
Boron/Nitride wafer
 \rightarrow 2% uniformity

Reactions:

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

$$Si + O_2 \rightarrow SiO_2$$

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General Comments on Predeposition

- Higher doses only: $Q = 10^{13} - 10^{16} \text{ cm}^{-2}$ (I/I is $10^{11} - 10^{16}$)
- Dose not well controlled: $\pm 20\%$ (I/I can get $\pm 1\%$)
- Uniformity is not good
 - ↪ $\pm 10\%$ w/ gas source
 - ↪ $\pm 2\%$ w/ solid source
- Max. conc. possible limited by solid solubility
 - ↪ Limited to $\sim 10^{20} \text{ cm}^{-3}$
 - ↪ No limit for I/I \rightarrow 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 \rightarrow introduces unbalanced stress \rightarrow warping of structures
 - ↪ I/I can do physical damage \rightarrow problem if annealing is not permitted
- Thus, predeposition is often preferred when doping MEMS

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Diffusion Modeling

Modeling $N(x)$

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

\Rightarrow Question: What's $N(x,t)$?
 τ fun of time

Fick's Law of Diffusion - (1st law)

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

↑ flux [$\#/\text{cm}^2 \cdot \text{s}$] ↑ Diffusion Coefficient

Continuity Equation for Particle Flux -

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

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

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Diffusion Modeling (cont.)

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

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

[$\frac{\partial}{\partial x}$ (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

surface conc. stays constant → N_0

background conc. → N_B

surface

x , distance from surface

$t_1 < t_2 < t_3$

high T ($D_1 t_1 < D_2 t_2 < D_3 t_3$)

complementary error function profile

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

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

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

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

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

$N(x)$ ← linear scale

area under this square is same as under the curve!

$2\sqrt{Dt}$

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Diffusion Modeling (Limited Source)

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

$N(x,t)$
 $N_0(t_1)$
 $N_0(t_2)$
 $N_0(t_3)$
 N_B
 x , distance x from the surface

\Rightarrow Boundary Condition:

(i) $N(\infty, t) = 0$
(ii) $\left. \frac{\partial N(x,t)}{\partial x} \right|_{x=0} = 0$

Why? Constant Dose: $\int_0^{\infty} N(x,t) dx = Q \leftarrow \text{const.}$

This is equivalent to saying that there's no flux going out of the Si, i.e., and that's what this says!

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Diffusion Modeling (Limited Source)

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

\Rightarrow 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:

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

corresponds to a half Gaussian in this equation

When the starting conc. profile is completely contained in the Si, then $Q = \frac{D_I}{2} = \text{half the implant dose}$


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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:
 - $(Dt)_{\text{predep}} \gg (Dt)_{\text{drive-in}} \Rightarrow$ impurity profile is complementary error function
 - $(Dt)_{\text{drive-in}} \gg (Dt)_{\text{predep}} \Rightarrow$ impurity profile is Gaussian (which is usually the case)

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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 \rightarrow effective $(Dt)_1 = (\Delta R_p)^2/2$ (Gaussian)
 - ↳ Drive-in/activation $\rightarrow D_2 t_2$
 2. Other high temperature steps
 - ↳ (eg., oxidation, reflow, deposition) $\rightarrow D_3 t_3, D_4 t_4, \dots$
 - ↳ Each has their own Dt product
 3. Then, to find the final profile, use

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

in the Gaussian distribution expression.

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The Diffusion Coefficient

$D = D_0 \exp\left(-\frac{E_A}{kT}\right)$ (as usual, an Arrhenius relationship)

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

Element	$D_0(\text{cm}^2/\text{sec})$	$E_A(\text{eV})$
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

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Diffusion Coefficient Graphs

Substitutional & Interstitial Diffusers

Fig. 7.1

Interstitial Diffusers

↳ Note the much higher diffusion coeffs. than for substitutional

Fig. 7.2

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Metallurgical Junction Depth, x_j

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

The left graph shows $\text{Log}[N(x)]$ on the y-axis and $x = \text{distance f/ surface}$ on the x-axis. A curve starts at N_o and decays towards a horizontal line at N_B . The intersection point is x_j . Labels include "e.g., p-type Gaussian" and "e.g., n-type".

The right graph shows $\text{Log}[N(x)-N_B]$ on the y-axis and $x = \text{distance f/ surface}$ on the x-axis. The curve starts at $N_o - N_B$ and decays towards zero. The intersection point is x_j . Labels include "Net impurity conc.", "p-type region", and "n-type region".

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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:

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

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Sheet Resistance

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

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

$\sigma = \text{conductivity} = q(\mu_n n + \mu_p p)$

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

$(A = tw)$

sheet resistance

ohms per square
 Ω/D

unit squares of material in the resistor

e.g.,

5 D's of material
 $\therefore R = R_s \times 5$
- What if the trace is non-uniform? (e.g., a corner, contains a contact, etc.)

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Squares From Non-Uniform Traces

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<p>0.65 squares</p>	<p>Corner = 0.56 squares</p>
<p>0.14 squares</p>	<p>0.35 squares</p>

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Sheet Resistance of a Diffused Junction

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- For diffused layers:

$$R_s = \frac{\rho}{x_j} = \left[\int_0^{x_j} \sigma(x) dx \right]^{-1} = \left[\int_0^{x_j} q\mu N(x) dx \right]^{-1}$$

[extrinsic material]

Majority carrier mobility

Net impurity concentration

Effective resistivity

Sheet resistance
- This expression neglects depletion of carriers near the junction, $x_j \rightarrow$ 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_0 (the surface concentration), and N_B (the substrate background conc.)

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Irvin's Curves (for n-type diffusion)

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(a)

(b)

Example. p-type

Given:

- $N_B = 3 \times 10^{16} \text{ cm}^{-3}$
- $N_0 = 1.1 \times 10^{18} \text{ cm}^{-3}$ (n-type Gaussian)
- $x_j = 2.77 \text{ } \mu\text{m}$

Can determine these given known predep. and drive conditions

Determine the R_s .

Using Fig. 7.7:

$R_s x_j = 470 \text{ } \Omega \cdot \mu\text{m}$

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

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