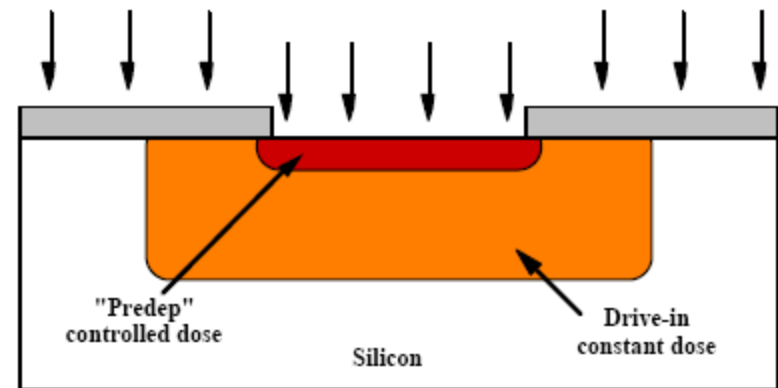


# Impurity diffusion

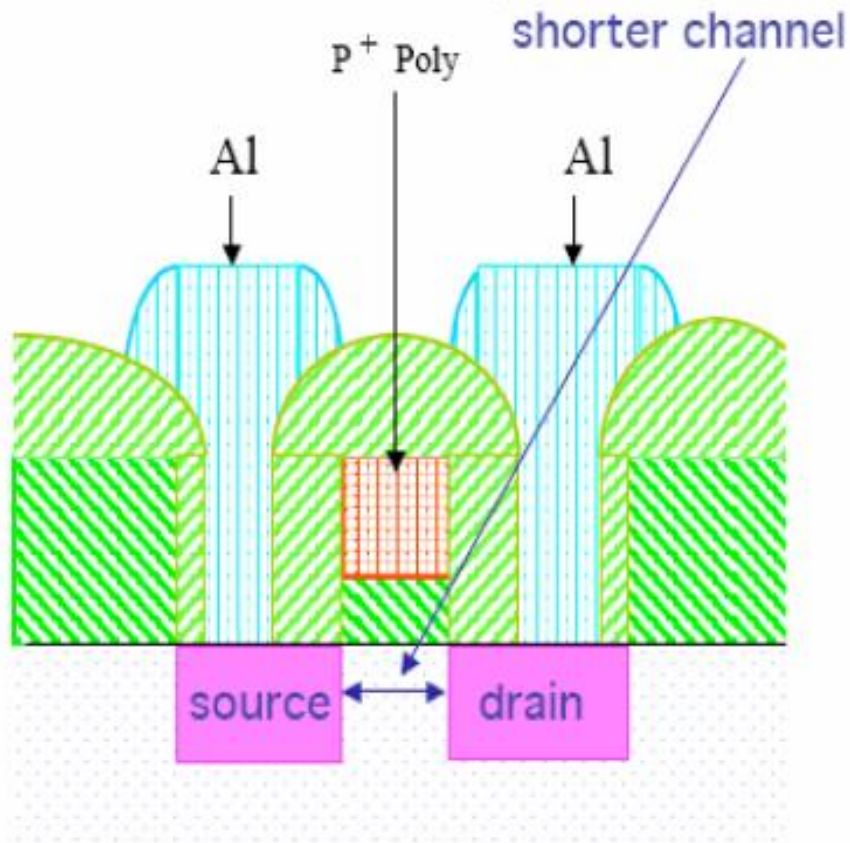
# Diffusion concepts

- ▶ Diffusion is the redistribution of atoms from regions of high concentration of mobile species to regions of low concentration. It occurs at all temperatures, but the diffusivity has an exponential dependence on  $T$ .
- ▶ Usually occurs in two steps:
  - **Predeposition:** doping often proceeds by an initial predep step to introduce the required dose of dopant into the substrate.
  - **Drive-In:** a subsequent drive-in anneal then redistributes the dopants giving the required surface concentration and diffusion depth

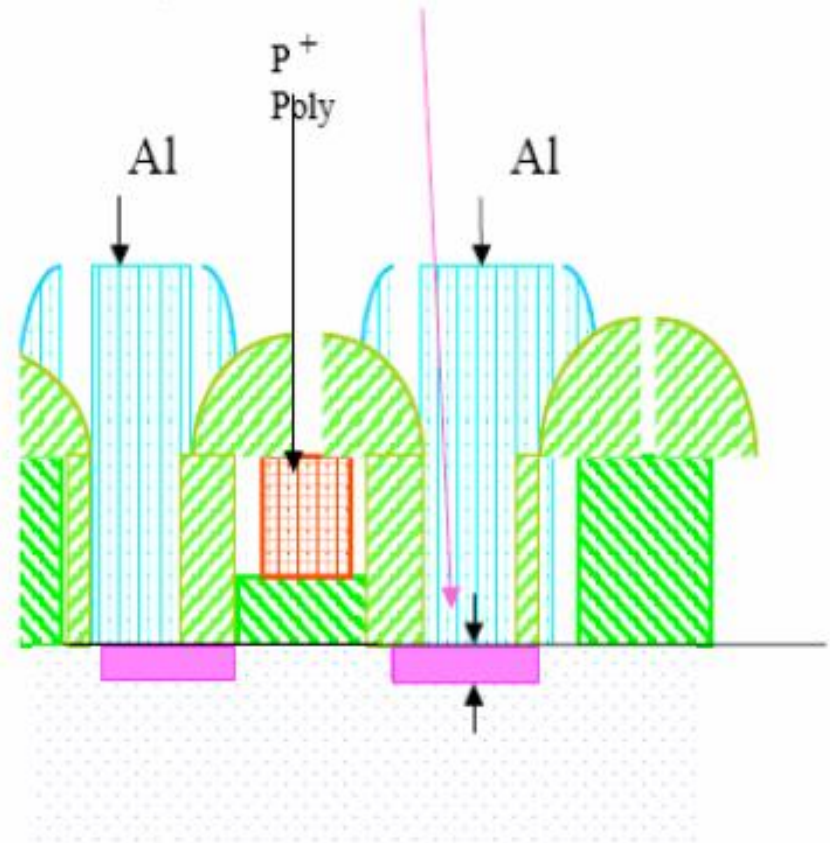


# Motivation

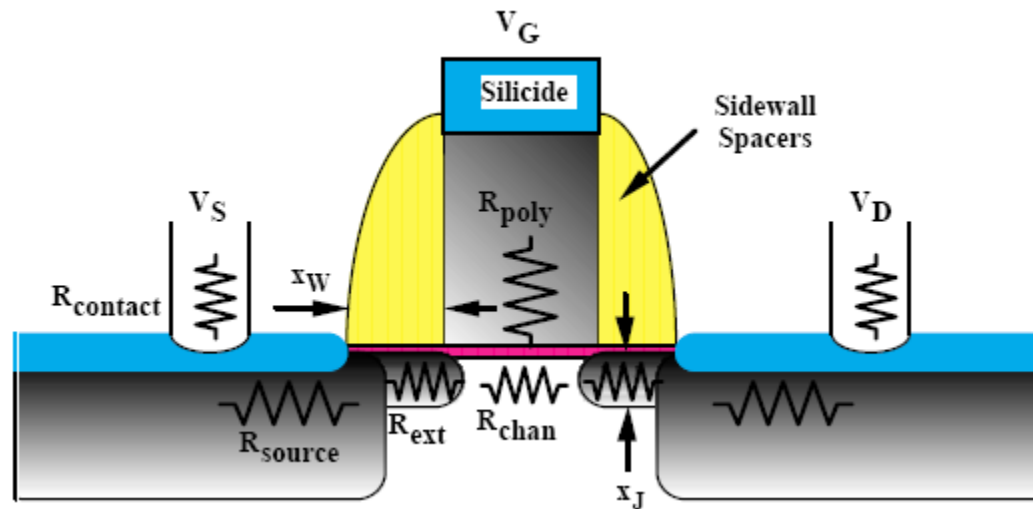
Faster MOSFET requires  
shorter channel



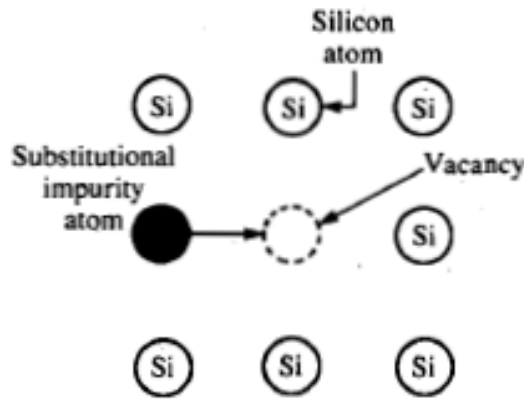
Requires shallower source, drain



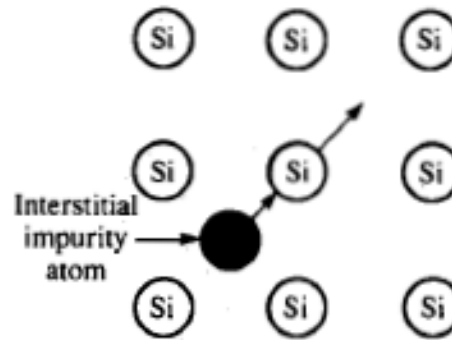
- ▶ Doping profiles determine many short-channel characteristics in MOS devices.
- ▶ Resistance impacts drive current.
- ▶ Scaling implies all lateral and vertical dimensions scale by the same factor.
- ▶ Generally doping levels need to increase and  $x_J$  values need to decrease.



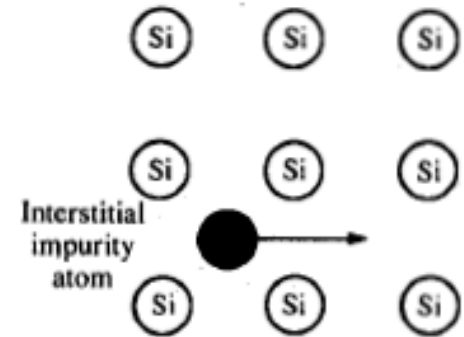
# Impurity diffusion in Si



Substitutional  
diffusion



Interstitial  
substitution



Interstitial  
diffusion

- ▶ In substitutional diffusion due to small no of vacancies, the process occurs at slow rate.
- ▶ Interstitial process has potentially high rate and rather uncontrollable due to large inter-atomic space in Si lattice

# Diffusion modelling

- ▶ Mathematically, one dimensional diffusion can be modelled by Fick's first law

$$J = -D \frac{\partial N}{\partial x}$$

- ▶ J is the diffusion flux, N is the impurity concentration and D is the diffusion factor
- ▶ On the other hand continuity equation implies that the divergence of flux (flux in-flux out=change in the concentration) is equal to the time variation of concentration. i.e.:

flux in-flux out=change in the concentration

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

## Diffusion modelling (Cont'd)

- ▶ Eliminating flux in the above two equations yields:

- ▶ Fick's Second law: 
$$\frac{\partial N}{\partial t} = D \frac{\partial^2 N}{\partial x^2}$$

- ▶ D is assumed to be position independent.
- ▶ In 3D diffusion, derivative operator is converted to the Laplacian operator ( $\nabla^2$ )
- ▶ The partial differential equation can be solved using standard methods (separation of variables), providing sufficient boundary conditions



# Boundary conditions

## ► Constant-source diffusion

- There is a constant-rate source of impurity at the surface of the wafer. This condition resembles the pre-deposition step.
- So for the solution in the form of  $N(x,t)$  the boundary condition would be:

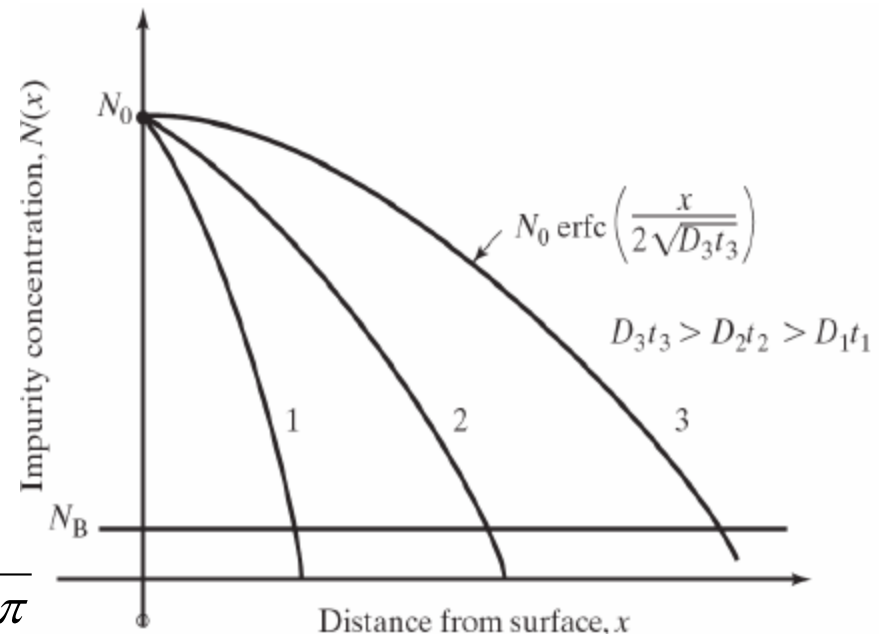
- $N(0,t)=N_0$   $N(\infty,t)=0$

- The associated solution is

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

- Dose: Total number of impurities per unit Si area:

$$Q = \int_0^{\infty} N(x, t) dx = 2N_0 \sqrt{Dt} / \pi$$





# Error function properties

$$\operatorname{erfc}(z) = 1 - \operatorname{erf}(z)$$

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp[-x^2] dx$$

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

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

$$\operatorname{erfc}(\infty) = 0$$

$$\operatorname{erfc}(0) = 1$$

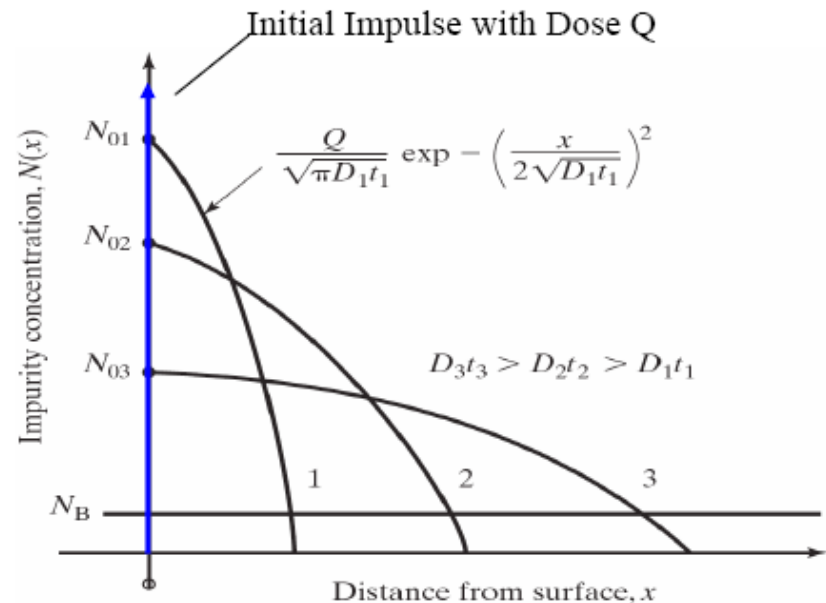
# Boundary condition (Cont'd)

## ► Limited-source diffusion

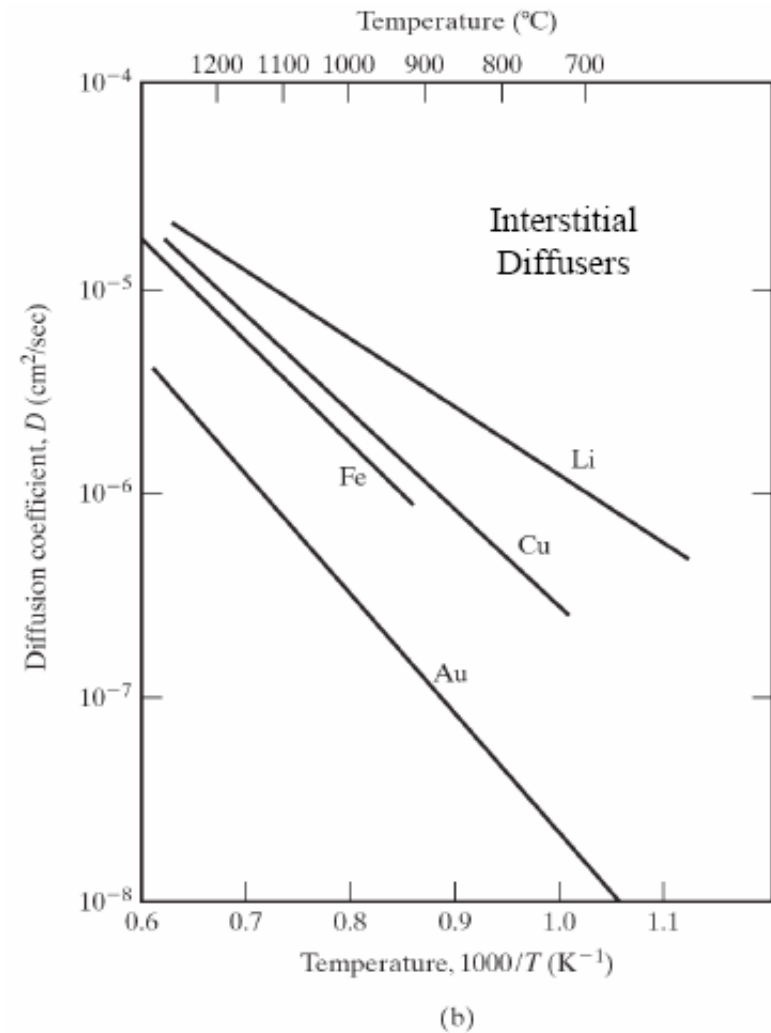
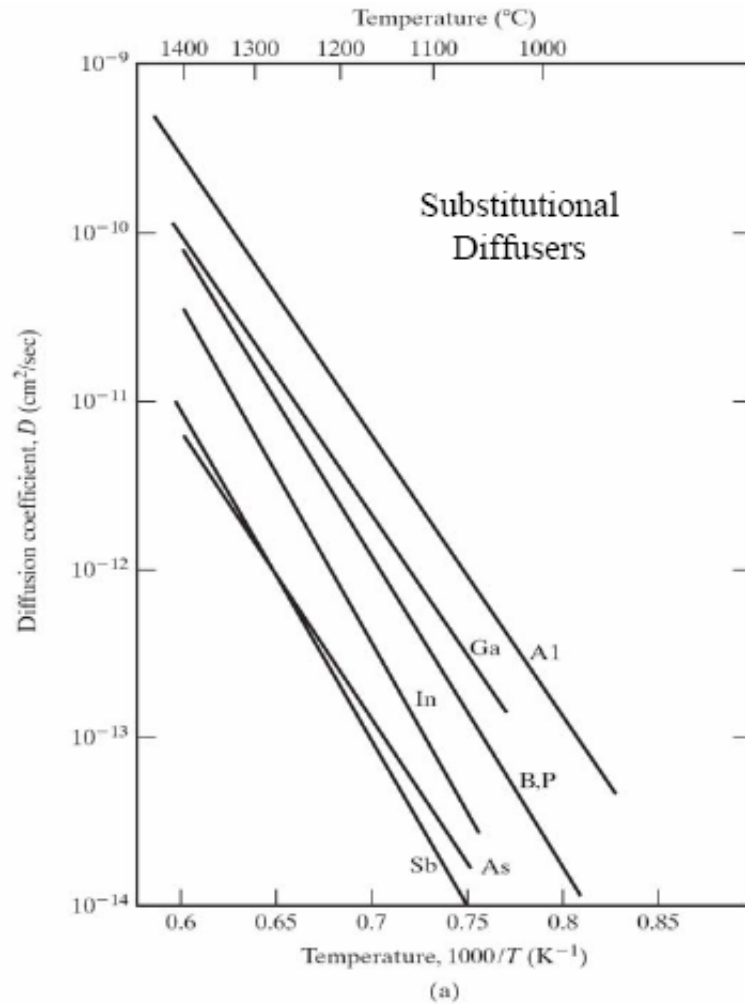
- The dose of impurities is constant along the diffusion
- Corresponds to Drive-In step of the diffusion
  - $Q(t)=\text{constant}$      $N(\infty,t)=0$
- The solution to the diffusion equation would be a Gaussian function as:

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

$$= N_0 \exp\left[-\left(\frac{x}{2\sqrt{Dt}}\right)^2\right]$$



# Diffusion coefficient



# Diffusion coefficient

$$D = D_0 \exp\left(-\frac{E_A}{kT}\right) \quad \text{Arrhenius Relationship}$$

$E_A$  = activation energy

$k$  = Boltzmann's constant =  $1.38 \times 10^{-23}$  J/K

$T$  = absolute temperature

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

Element	$D_0$ (cm <sup>2</sup> /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

## Example 4.1

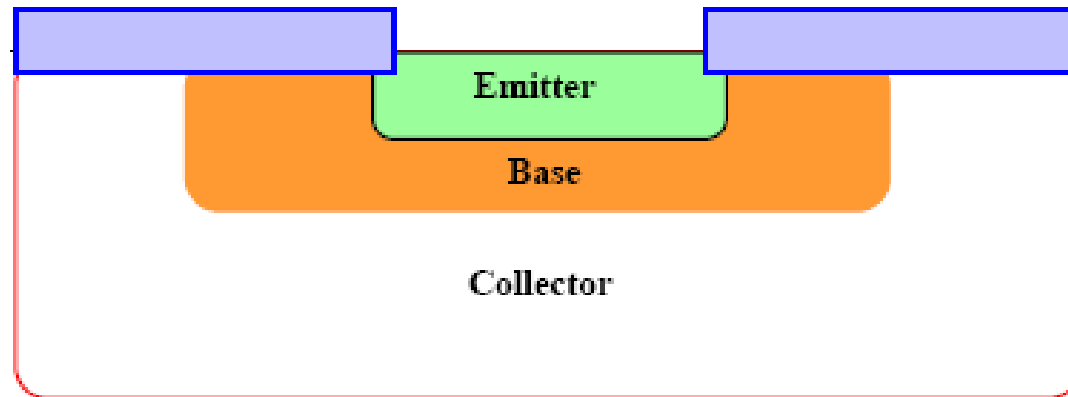
Calculate the diffusion coefficient for boron at 1100 °C.

**Solution:** From Table 4.1,  $D_0 = 10.5$  cm<sup>2</sup>/sec and  $E_A = 3.69$  eV.  $T = 1373$  K.

$$D = 10.5 \exp - \frac{3.69}{(8.614 \times 10^{-5})(1373)} = 2.96 \times 10^{-13} \text{ cm}^2/\text{sec}.$$

# Successive distribution

- ▶ Process steps may contain several steps of high temperature cycles. Diffusion could continue during all these steps
- ▶ Example: In a bipolar transistor, if the emitter profile is formed by a predep and the base profile by an implant + drive-in, then the junctions occur where net impurity concentration become zero



# Successive diffusion (Cont'd)

- ▶ Assume a dopant diffused at temperature  $T_1$  for time  $t_1$ , then followed by a later diffusion at  $T_2$  for  $t_2$  and so forth, the effective  $D.t$  product is the sum of all  $D_i t_i$ 's.  
i.e.:

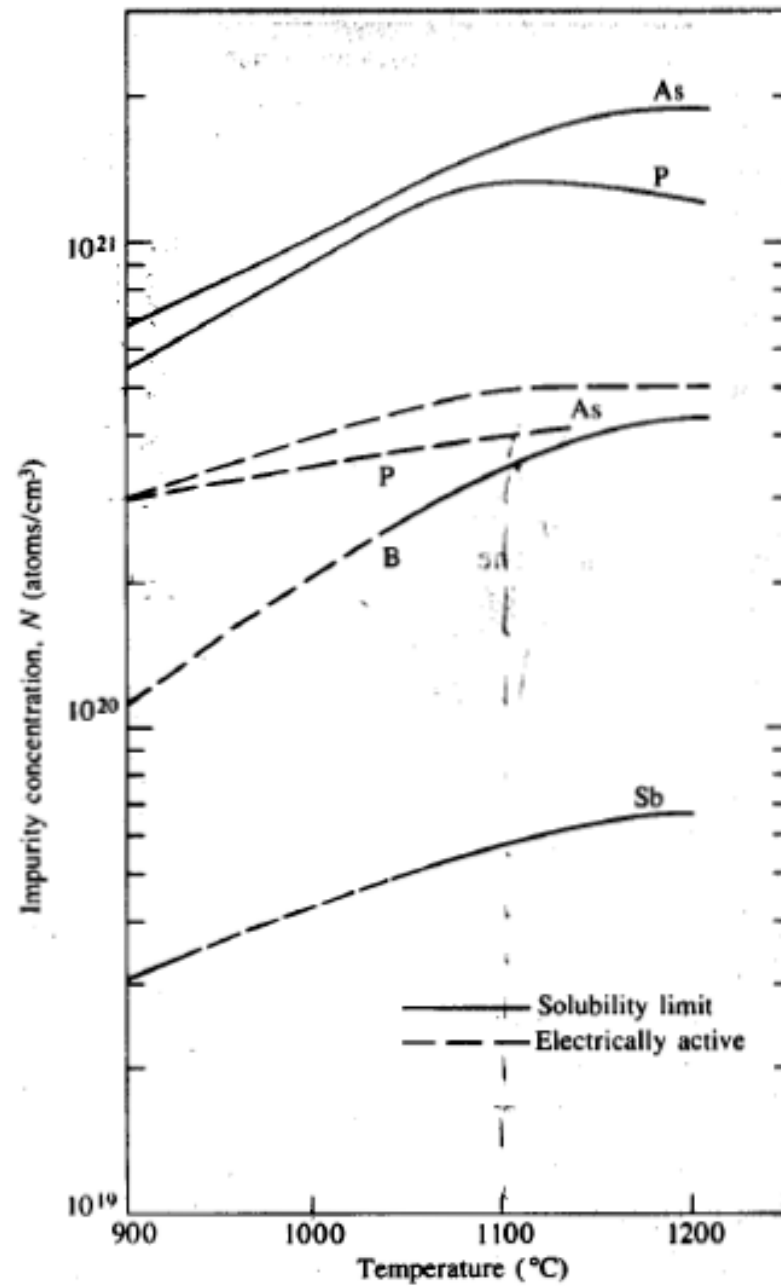
$$D.t_{\text{eff}} = \sum_{i=1}^n D_i t_i$$

- ▶ The Gaussian distribution is applicable if the predep period would be far less than further drive-in time.

# Solid solubility

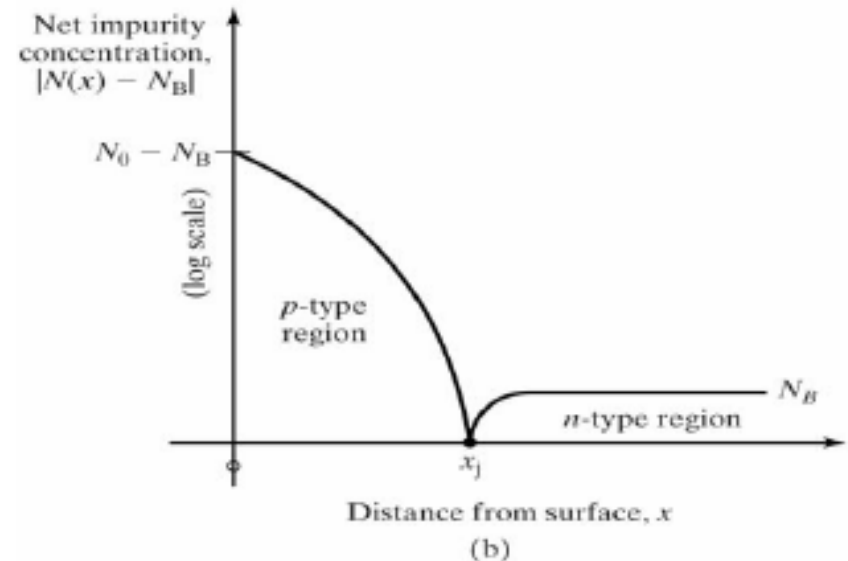
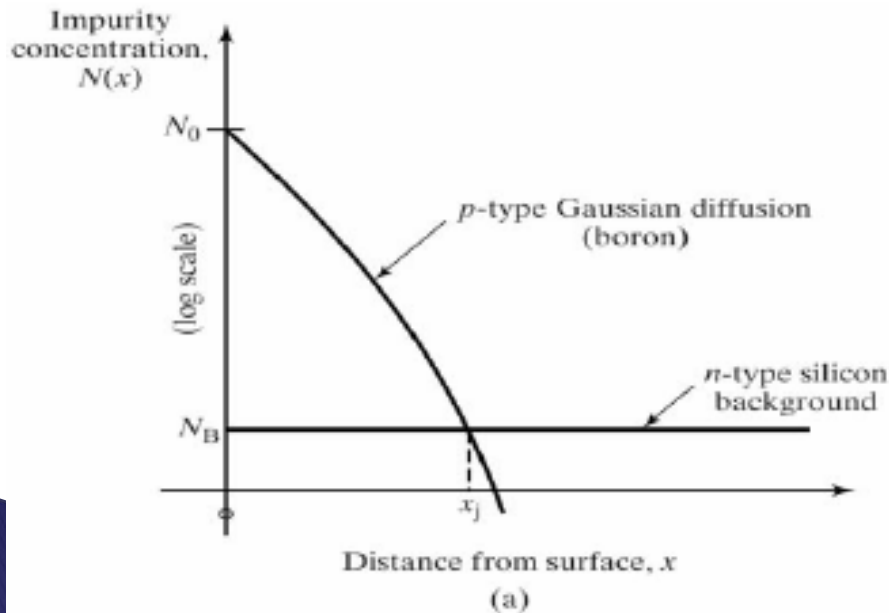
- ▶ When diffusing impurities, at any given temperature, there is a limit to the atoms successfully doped to the Si. In other words Si would have a certain acceptance limit for the impurity atoms.
- ▶ This limit on diffuser concentration is called Solid-solubility concentration and mostly depends on diffusers and temperature





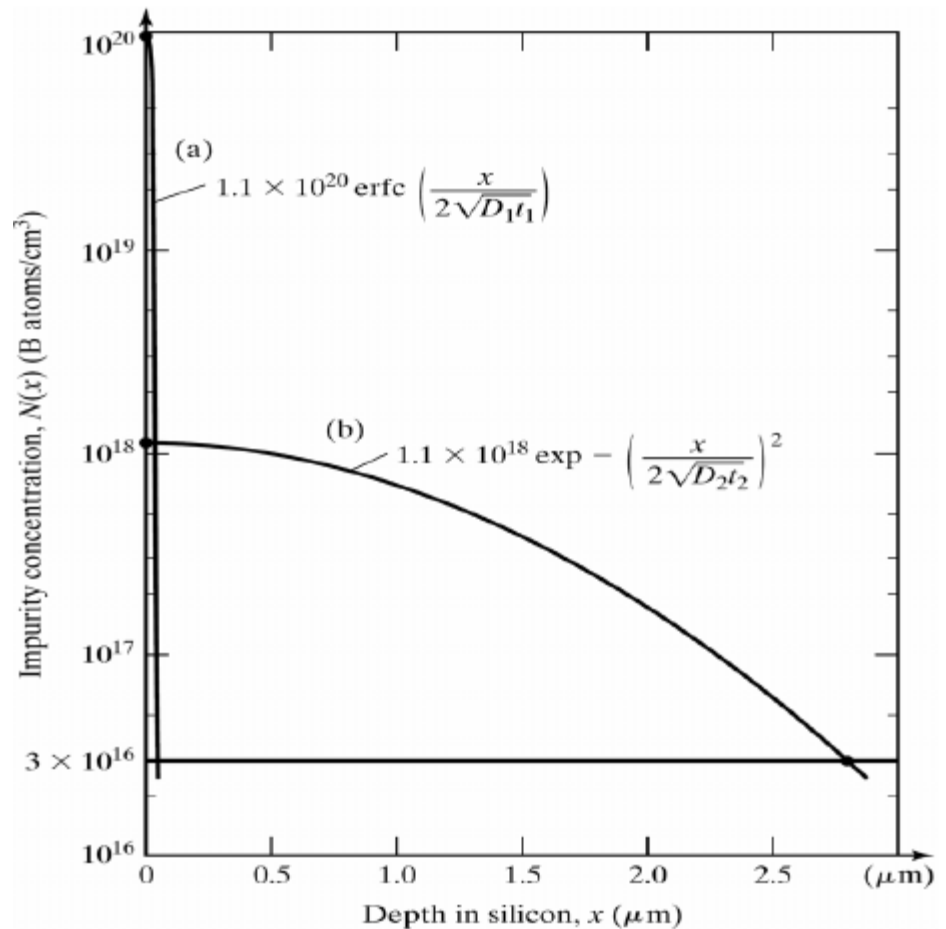
# Pn junction formation

- ▶ In most cases diffusion is used to form a pn junction by diffusing acceptor ions to a n-type material or vice versa.
- ▶ A so-called metallurgical junction is formed where the diffused layer reach to the background concentration.
- ▶ The net impurity concentration reached zero at that place



# Two step diffusion

- ▶ Short constant source diffusion used to establish dose  $Q$  (“Predep” step)
- ▶ Longer limited source diffusion drives profile in to desired depth (“drive in” step)
- ▶ Final profile is Gaussian



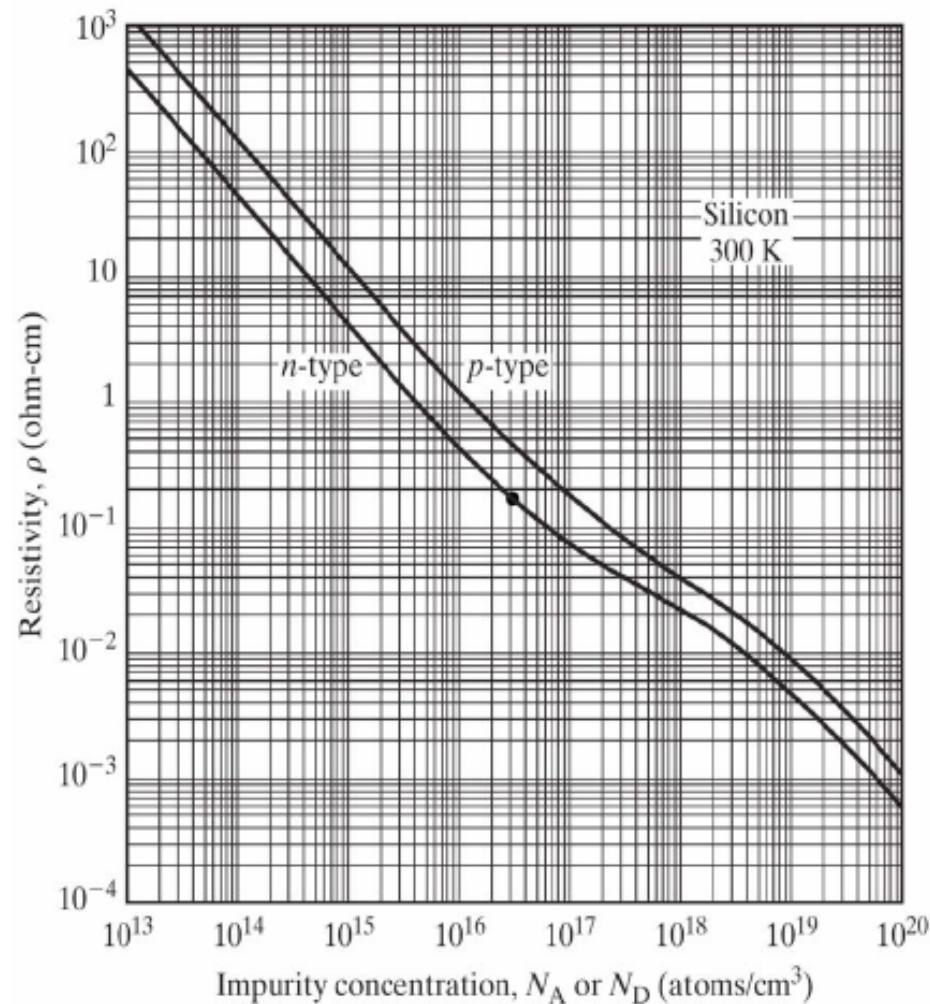
# Junction depth

- ▶  $x_j$ =Metallurgical Junction Depth

Gaussian Profile: 
$$x_j = 2\sqrt{Dt \ln\left(\frac{N_0}{N_B}\right)}$$

Error Function profile: 
$$x_j = 2\sqrt{Dt} \operatorname{erfc}^{-1}\left(\frac{N_0}{N_B}\right)$$

# Resistivity of doped si



$$\rho = \sigma^{-1} = [q(\mu_n n + \mu_p p)]^{-1}$$

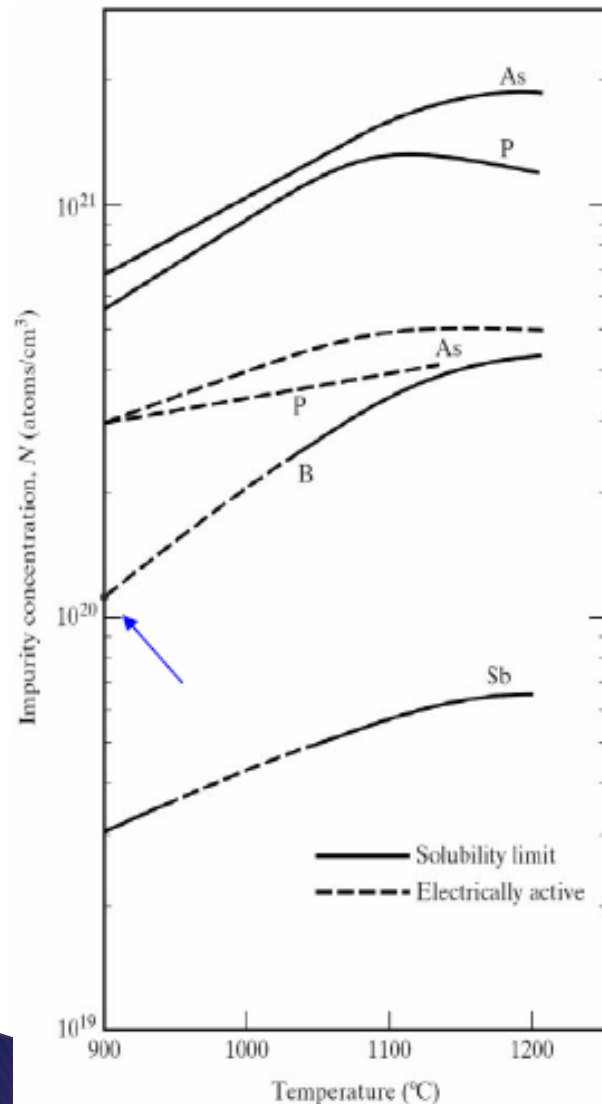
$$\text{n-type: } \rho \cong [q\mu_n(N_D - N_A)]^{-1}$$

$$\text{p-type: } \rho \cong [q\mu_p(N_A - N_D)]^{-1}$$

# Example: Boron diffusion

- ▶ A boron diffusion is used to form the base region of an npn transistor in a  $0.18\ \Omega\text{-cm}$  n-type silicon wafer. A solid-gas-phase boron predeposition in the solid-solubility-concentration is performed at  $900^\circ\text{C}$  for 15 min followed by a 5-hr drive-in at  $1100^\circ\text{C}$ . Find the surface concentration and junction depth (a) after the predep step and (b) after the drive-in step.

# Solution



Predeposition step is solid - solubility limited.

$$T_1 = 900^\circ\text{C} = 1173\text{ K} \rightarrow N_0 = 1.1 \times 10^{20} / \text{cm}^3$$

$$D_1 = 10.5 \exp\left[-\frac{3.69\text{ eV}}{(8.614 \times 10^{-5} \text{ eV/K}) 1173\text{ K}}\right] = 1.45 \times 10^{-15} \text{ cm}^2 / \text{sec}$$

$$t_1 = 15 \text{ min} = 900 \text{ sec} \quad D_1 t_1 = 1.31 \times 10^{-12} \text{ cm}^2$$

$$N(x) = 1.1 \times 10^{20} \operatorname{erfc}\left(\frac{x}{2.28 \times 10^{-6} \text{ cm}}\right) / \text{cm}^3$$

$$\text{Dose : } Q = 2N_0 \sqrt{\frac{D_1 t_1}{\pi}} = 1.42 \times 10^{14} / \text{cm}^2$$

$$T_2 = 1100^\circ\text{C} = 1373\text{ K}$$

$$D_2 = 10.5 \exp\left[-\frac{3.69\text{ eV}}{(8.614 \times 10^{-5} \text{ eV/K}) 1373\text{ K}}\right] = 2.96 \times 10^{-13} \text{ cm}^2 / \text{sec}$$

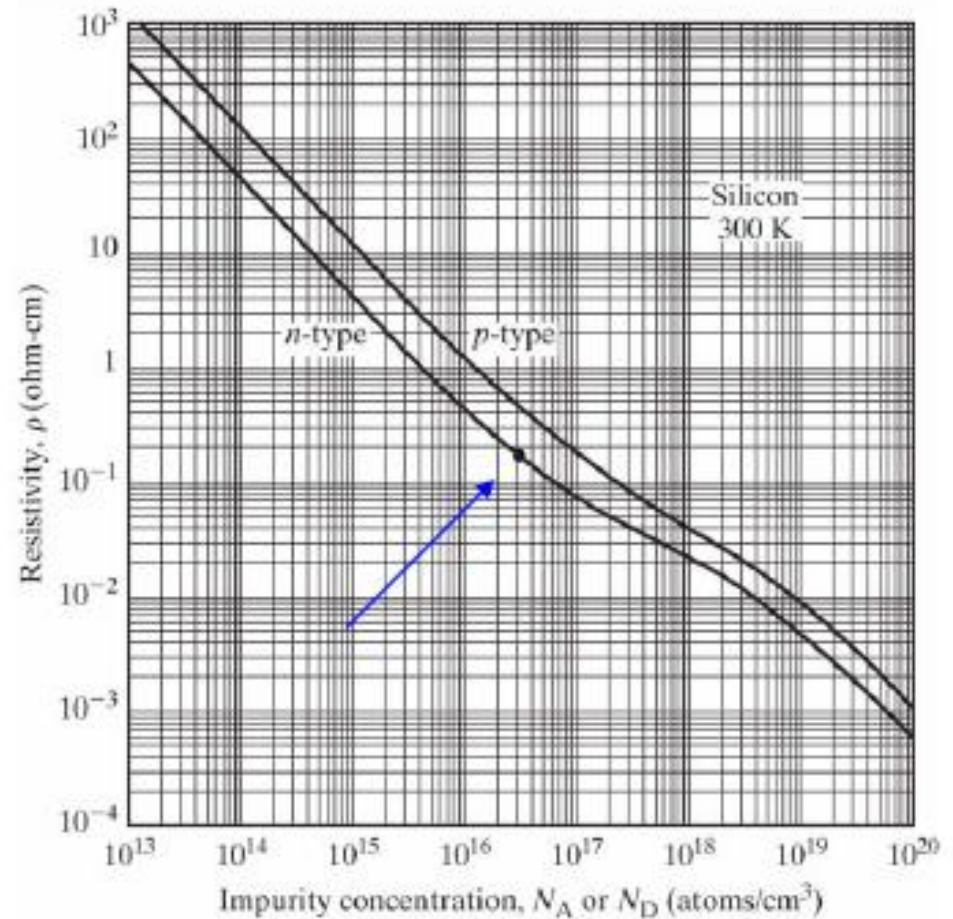
$$t_2 = 5 \text{ hr} = 18000 \text{ sec} \quad D_2 t_2 = 5.33 \times 10^{-9} \text{ cm}^2$$

$$N_2(x) = \frac{1.42 \times 10^{14} / \text{cm}^2}{\sqrt{\pi(5.33 \times 10^{-9} \text{ cm}^2)}} \exp\left(-\frac{x^2}{2\sqrt{D_2 t_2}}\right) = 1.1 \times 10^{18} \exp\left(-\frac{x}{1.46 \times 10^{-4}}\right)^2 / \text{cm}^3$$

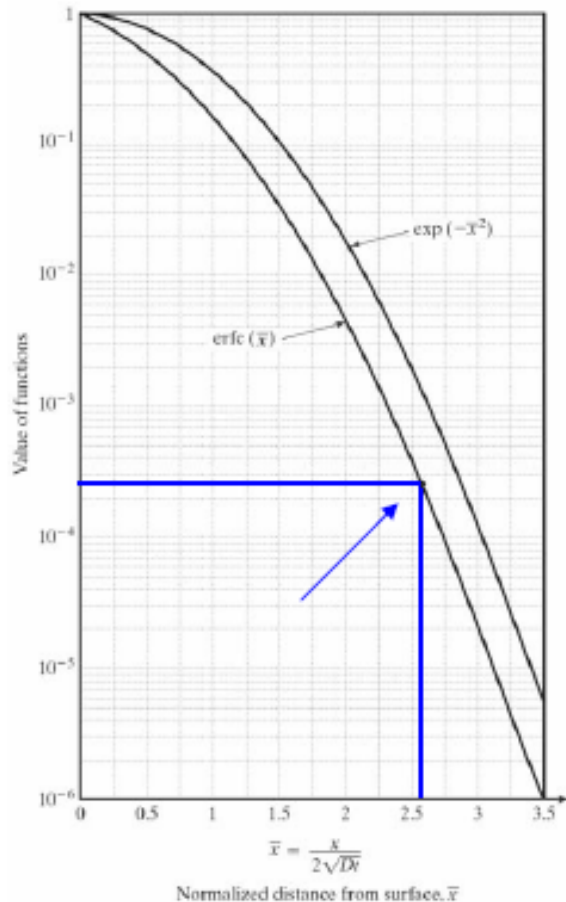


# Solution (cont'd)

- ▶ Starting wafer:
  - n-type  $0.18 \Omega\text{-cm}$
  - $N_D = 3 \times 10^{16}/\text{cm}^3$



# Solution ( Cont'd)



$$N_1(x) = 1.1 \times 10^{20} \text{erfc}\left(\frac{x}{2.28 \times 10^{-6} \text{cm}}\right) / \text{cm}^3$$

$$x_{j1} = 2\sqrt{D_1 t_1} \text{erfc}^{-1}\left(\frac{N_o}{N_B}\right) = (2.28 \times 10^{-6} \text{cm}) \text{erfc}^{-1}\left(\frac{3 \times 10^{16}}{1.1 \times 10^{20}}\right) = (2.28 \times 10^{-6} \text{cm}) \text{erfc}^{-1}(2.73 \times 10^{-4})$$

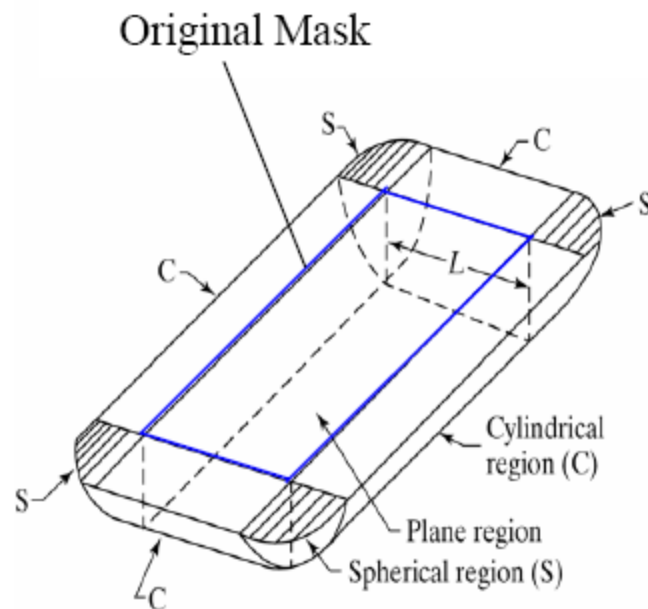
$$x_{j1} = (2.28 \times 10^{-6} \text{cm})(2.57) = 5.86 \times 10^{-6} \text{cm} = 0.058$$

$$N_2(x) = 1.1 \times 10^{18} \exp\left(-\frac{x}{1.46 \times 10^{-4}}\right)^2 / \text{cm}^3$$

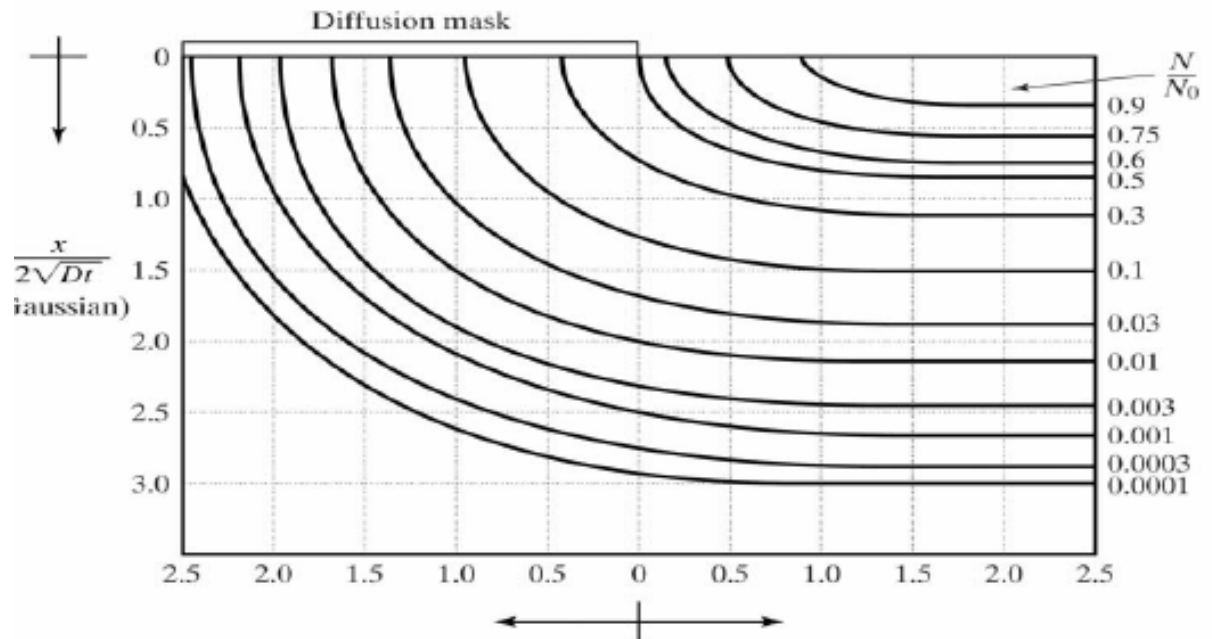
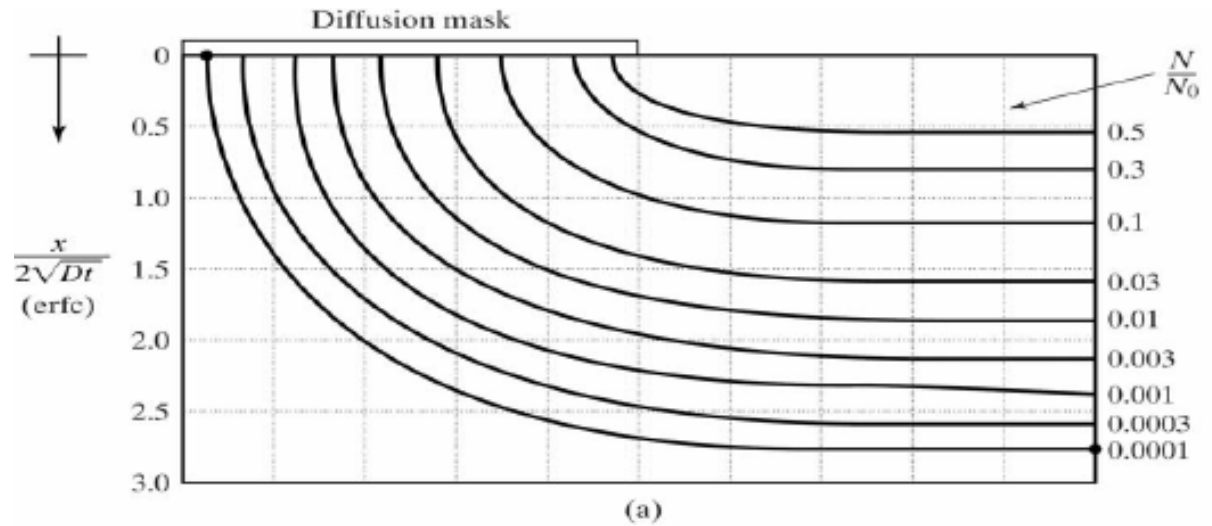
$$x_{j2} = 1.46 \times 10^{-4} \text{cm} \sqrt{\ln\left(\frac{1.1 \times 10^{18}}{3 \times 10^{16}}\right)} = 2.77 \times 10^{-4} \text{cm} = 2.77 \mu\text{m}$$

# Lateral diffusion

- ▶ Diffusion is really a 3-D process. As impurities diffuse vertically, they also diffuse horizontally in both directions.
- ▶ Diffusion proceeds laterally under the edge of the mask opening .



Lateral diffusion of dopants for two diffusion regimes:  
a) predep with erfc  
b) Drive-in with Gaussian



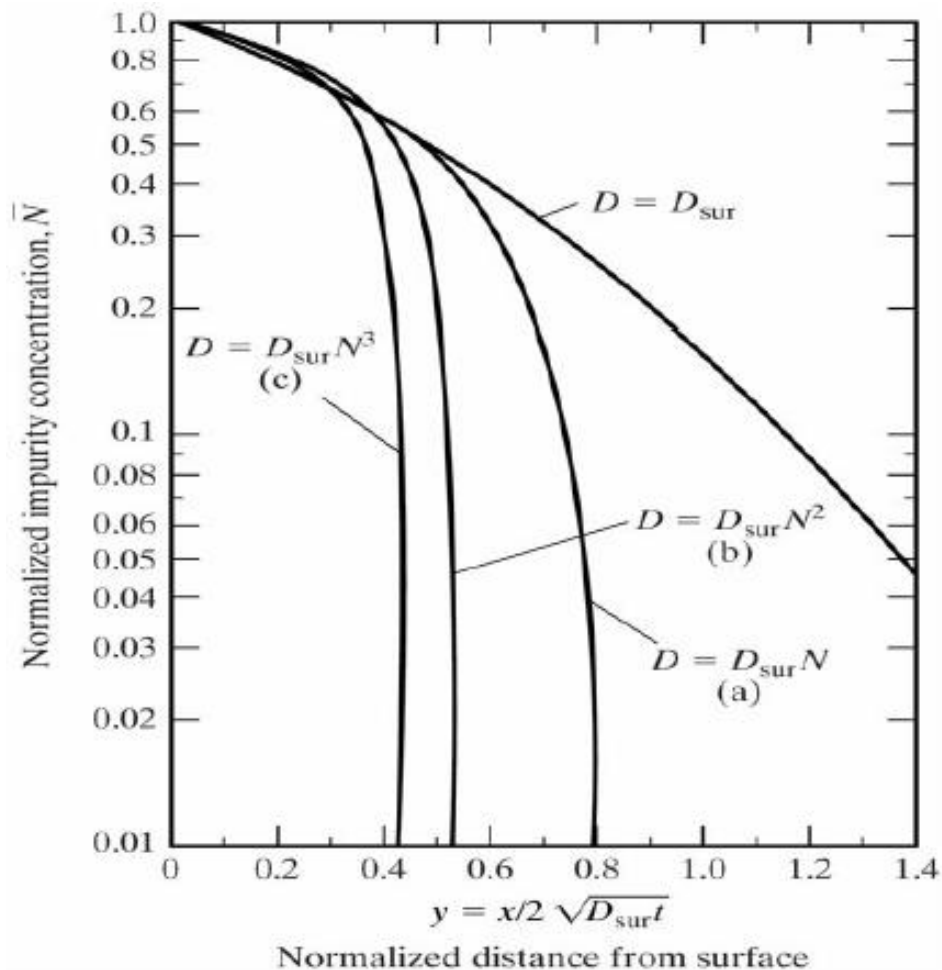
# Concentration dependent diffusion

- ▶ When considering diffusion model, it is assumed that diffusion occurs at concentration far less than intrinsic level ( $n_i$ )
- ▶ At higher concentration level, diffusion depends on layer concentration, results in variable  $D$ , the coefficient factor.
- ▶ Second law of diffusion has to be rewritten as:

$$\frac{\partial N}{\partial t} = \frac{\partial}{\partial x} D(x) \frac{\partial N}{\partial x}$$

- ▶ To be able to carry on equation solution, one may need some approximate model for  $D(x)$  See [...](#)
- ▶ So more defection would happen on the impurity distribution considering above correction.
- ▶ Some mathematical solutions are available for each shape of  $D(x)$

# Models for concentration dependent diffusion



- ▶ While B, As shows less dependency on concentration which is modelled by linear model in above diagram

TABLE 4.2 Properties of High-Concentration Arsenic and Boron Diffusions

Element	$x_j(\text{cm})$	$D(\text{cm}^2/\text{sec})$	$N_0(\text{cm}^{-3})$	$Q(\text{cm}^{-2})$
Arsenic	$2.29\sqrt{N_0Dt/n_i^*}$	$22.9 \exp(-4.1/kT)$	$1.56 \times 10^{17}(R_s x_j)^{-1}$	$0.55N_0 x_j$
Boron	$2.45\sqrt{N_0Dt/n_i^*}$	$3.17 \exp(-3.59/kT)$	$2.78 \times 10^{17}(R_s x_j)^{-1}$	$0.67N_0 x_j$

- ▶ But Phosphorous requires more complicated models



- Concentration dependent diffusion for phosphorous

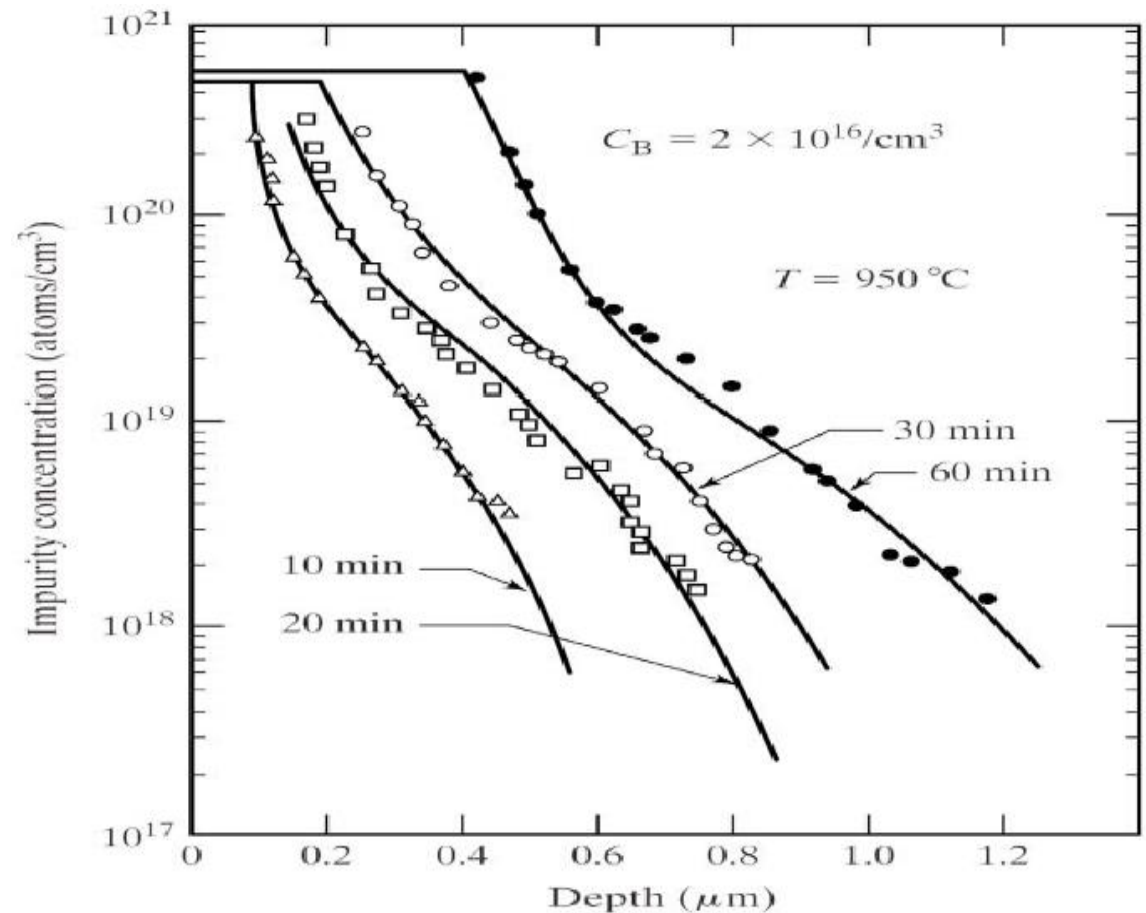
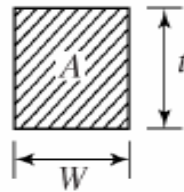
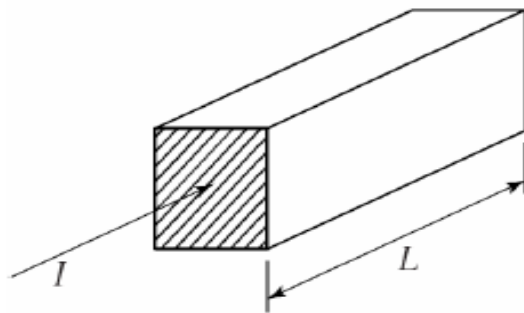


FIGURE 4.12

Shallow phosphorus diffusion profiles for constant-source diffusions at 950 °C. Copyright 1969 IEEE. Reprinted with permission from Ref. [10].

# Sheet resistance

- ▶ As already mentioned, sheet resistance is a conceptual term to specify resistance of a known depth resistor with given resistivity.
- ▶ Can be used to find resistance of any feature by knowing its  $L/W$  and counting squares of  $W \times W$  dimensions.



$$A = W \cdot t$$

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

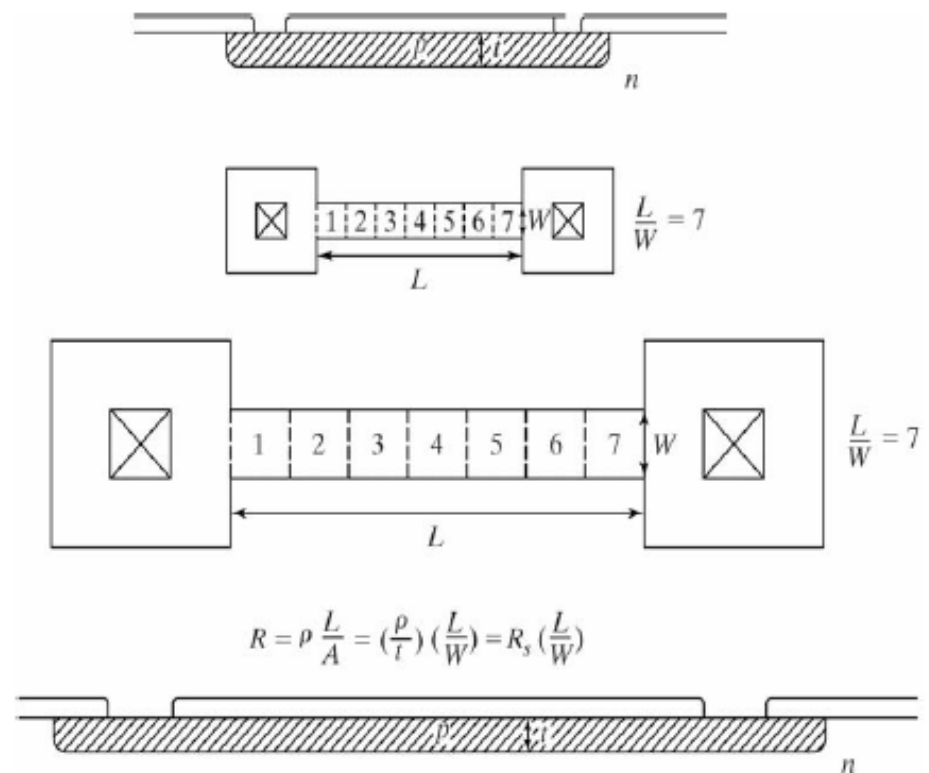
$$R_s = \frac{\rho}{t} = \text{Sheet Resistance [Ohms per Square]}$$

$$R = \rho \frac{L}{A} \quad \rho = \frac{1}{\sigma} \quad \sigma = q(\mu_n n + \mu_p p)$$

$$\left( \frac{L}{W} \right) = \text{Number of Squares of Material}$$

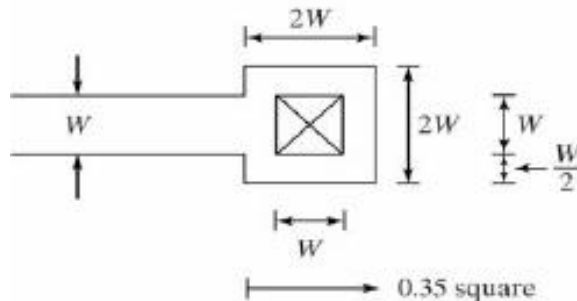
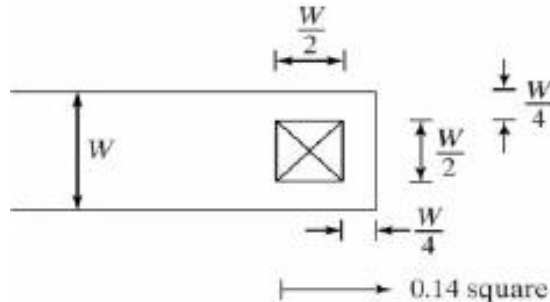
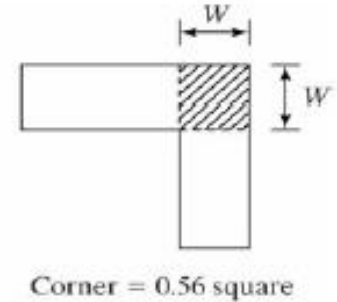
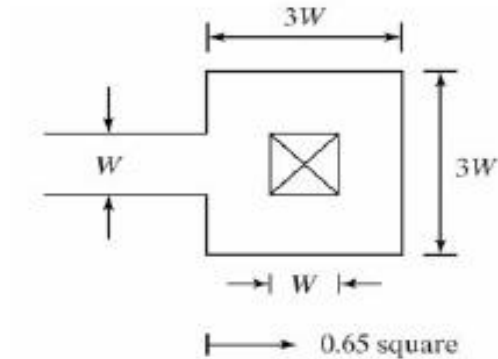
# Example of sheet resistance

- ▶ Top and side views of two resistors of different size
- ▶ Resistors have the same value of resistance
- ▶ Each resistor is  $7 \cdot \square$  in length
- ▶ Each end contributes approximately  $0.65 \square \bullet$
- ▶ Total for Each is  $8.3 \square \bullet$



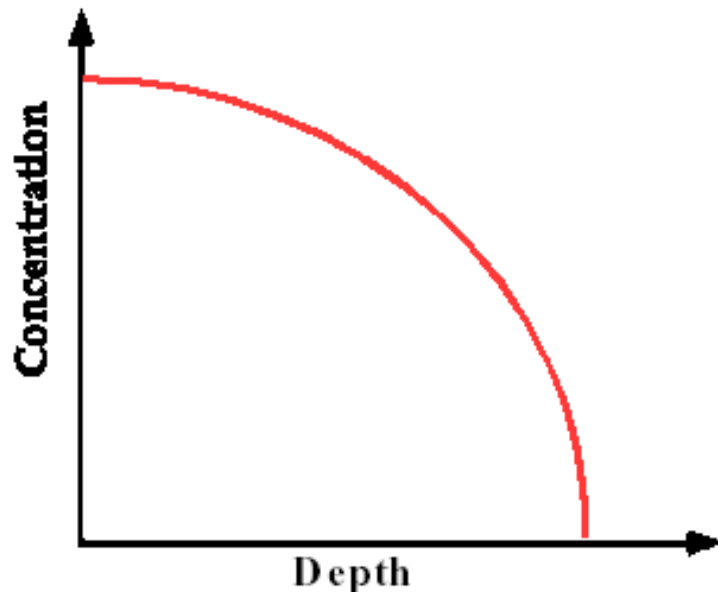
# Contact and corner contributions

- Effective contributions of various resistor end and corner configurations has been shown



# Sheet resistance of nonuniform resistive layers

- ▶ In diffused layers, resistivity is not uniform through any cross section (carrier distribution is not uniform) and depends on the depth of diffusion.
- ▶ Average resistivity(conductivity) is replaced.



$$R_s = \bar{\rho} / x_j = 1 / \bar{\sigma} . x_j$$

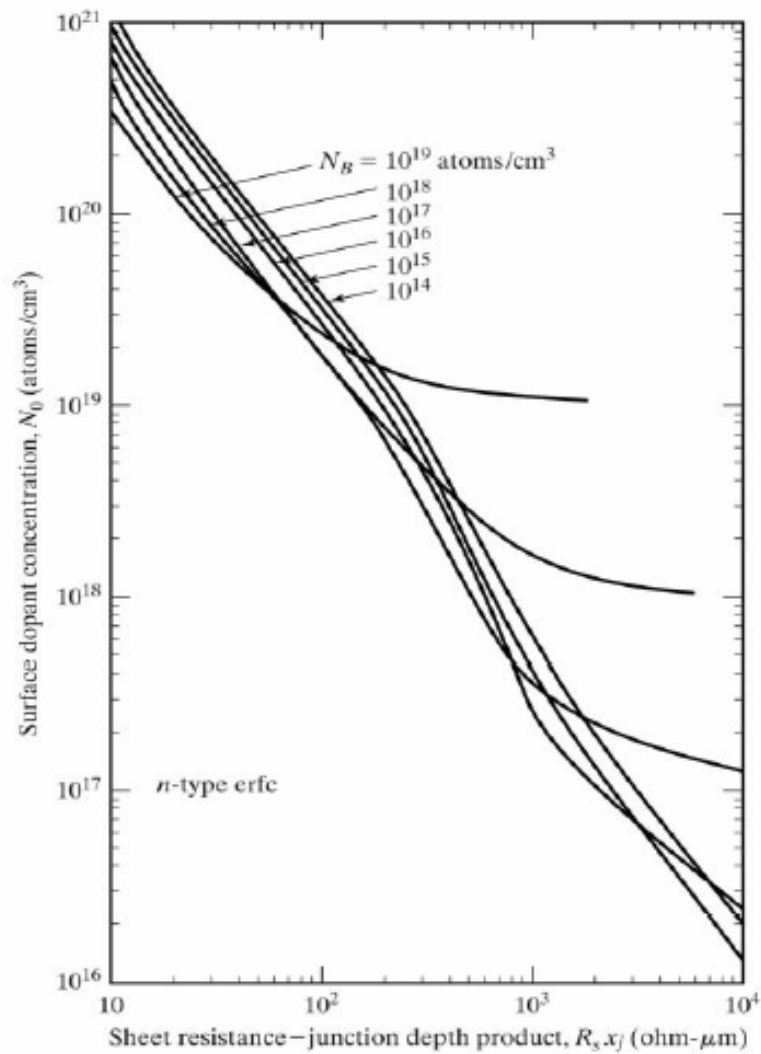
$$\bar{\sigma} = \frac{1}{x_j} \int_0^{x_j} \sigma . dx = \frac{q}{x_j} \int_0^{x_j} N(x) . \mu . dx$$

$$\Rightarrow \bar{\sigma} . x_j = q . \mu . \int_0^{x_j} N(x) . dx$$

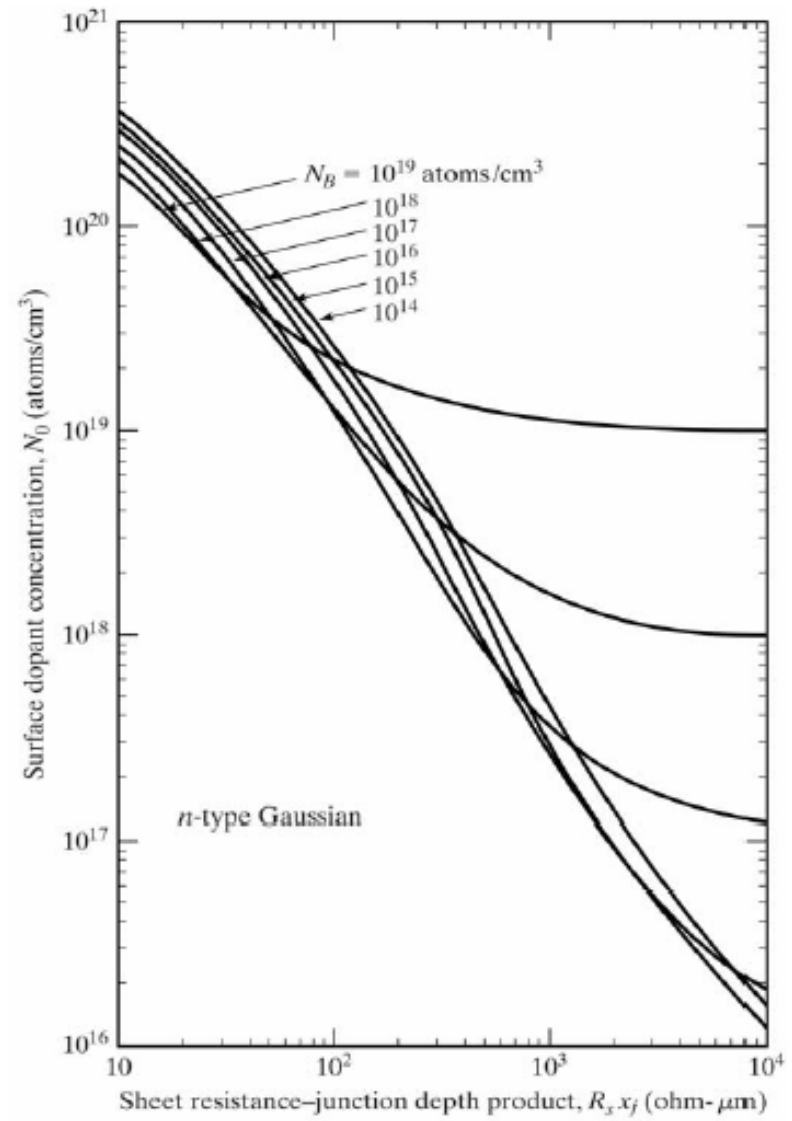
$$\Rightarrow R_s = \frac{1}{q . \mu . \int_0^{x_j} N(x) . \mu . dx}$$

# Irvin's curve

- ▶ In above expressions,  $N(x)$  is the net impurity concentration and can be written as  $N(x) = N_d(x) - N_B$
- ▶ Irvin has performed the integration above for given doping conditions and published in the form of four curve sets, surface concentration to sheet resistance-junction depth product ( $R_s \cdot \sigma$ ) to assist sheet resistance calculation.

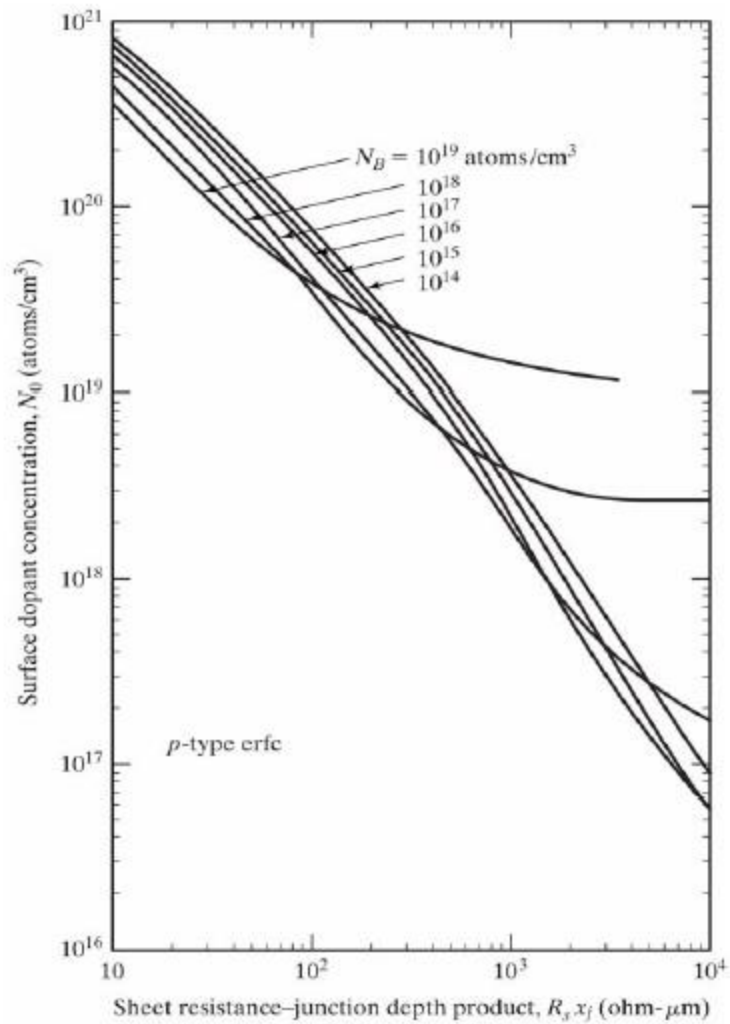


(a)

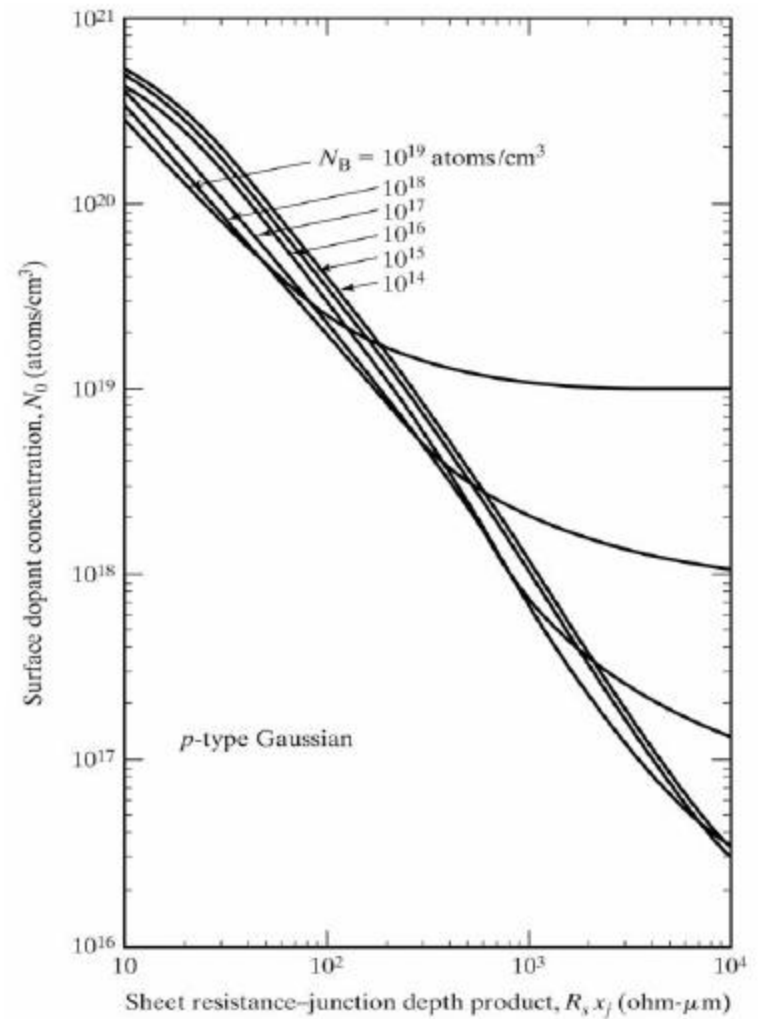


(b)



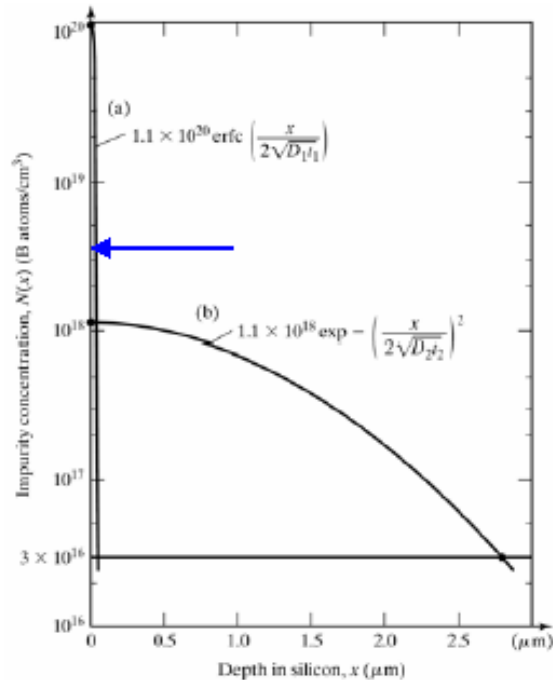


(c)



(d)

# Example of using Irvin's curve in a two step diffusion process: Predep step



Initial Profile

$$N_o = 1.1 \times 10^{20} / \text{cm}^3$$

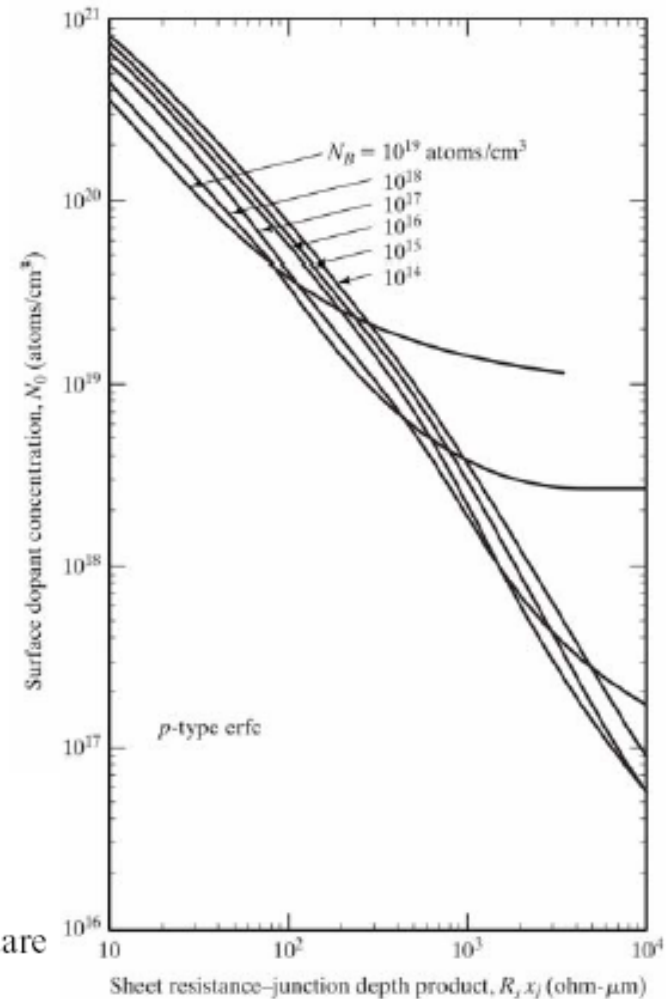
$$N_B = 3 \times 10^{16} / \text{cm}^3$$

$$x_j = 0.0587 \text{ } \mu\text{m}$$

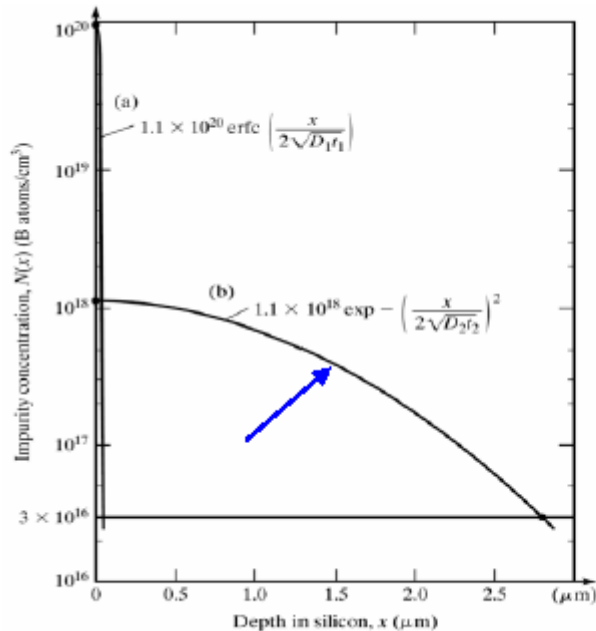
p-type erfc profile

$$R_S x_j = 50 \text{ } \Omega \cdot \mu\text{m}$$

$$R_S = \frac{32 \text{ } \Omega \cdot \mu\text{m}}{0.0587 \text{ } \mu\text{m}} = 850 \text{ } \Omega/\text{Square}$$



# Drive-in step:



Final Profile

$$N_o = 1.1 \times 10^{18} / \text{cm}^3$$

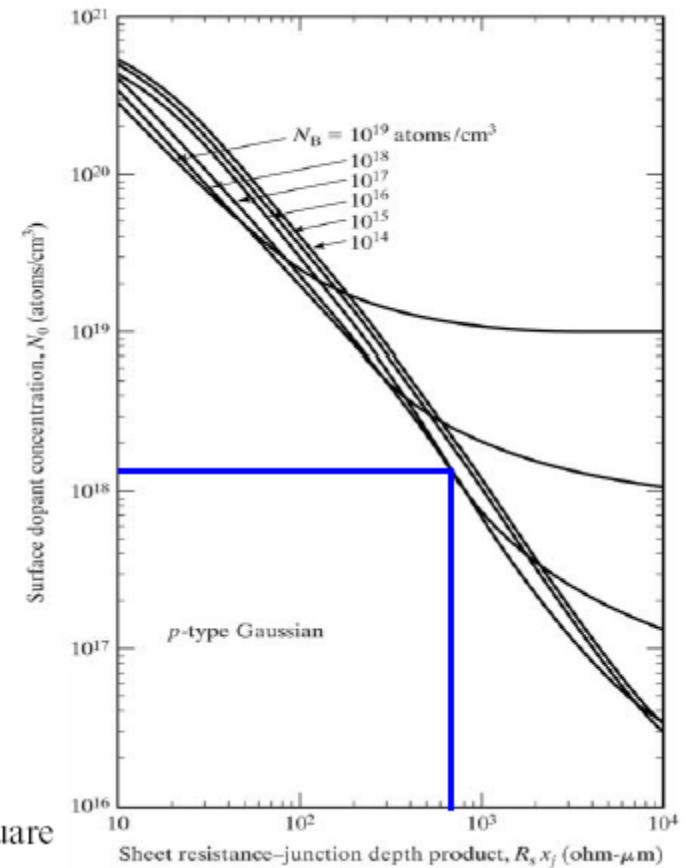
$$N_B = 3 \times 10^{16} / \text{cm}^3$$

$$x_j = 2.73 \text{ } \mu\text{m}$$

p-type Gaussian profile

$$R_S x_j = 700 \text{ } \Omega \cdot \mu\text{m}$$

$$R_S = \frac{700 \text{ } \Omega \cdot \mu\text{m}}{2.73 \text{ } \mu\text{m}} = 260 \text{ } \Omega/\text{Square}$$

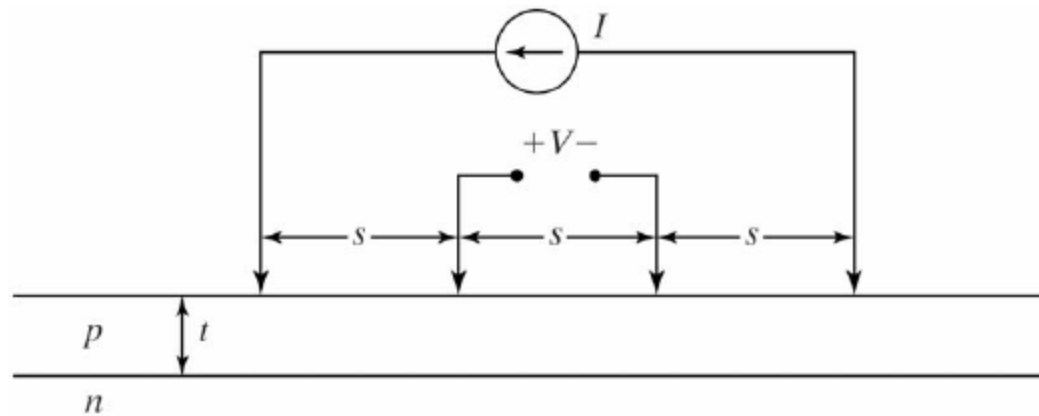


# Diffusion characterization

- ▶ In order to qualify diffusion process, various parameters such as junction depth and sheet resistance has to be measured experimentally.
- ▶ In practise, test wafers are used in parallel processes as the main wafer and can be used to evaluate the process.

# Resistivity measurement

## ► Four terminal probe:

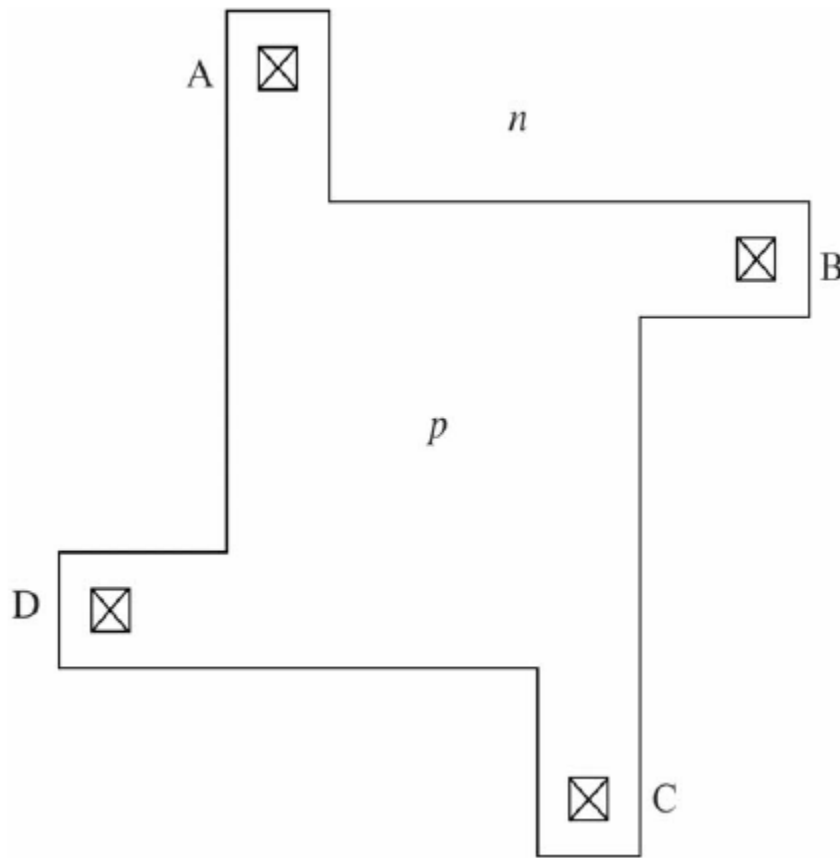


$$\rho = 2\pi s \frac{V}{I} \quad [\Omega \cdot \text{m}] \quad \text{for } t \gg s$$

$$\rho = \frac{\pi t}{\ln 2} \frac{V}{I} \quad [\Omega \cdot \text{m}] \quad \text{for } s \gg t$$

$$R_s = \frac{\rho}{t} = \frac{\pi}{\ln 2} \frac{V}{I} \cong 4.53 \frac{V}{I} \quad [\Omega/\text{square}]$$

# Resistivity measurement: Van der Pauw's method



Van der Pauw's Theory

Any Four - Terminal Region without Holes

$$\exp\left(-\pi t \frac{R_{AB,CD}}{\rho}\right) + \exp\left(-\pi t \frac{R_{BC,DA}}{\rho}\right) = 1$$

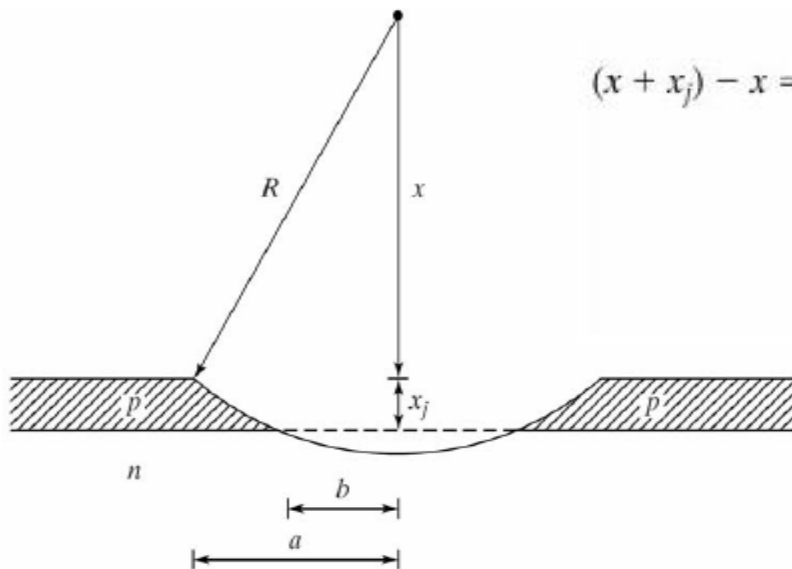
$$R_{AB,CD} = \frac{V_{CD}}{I_{AB}} \quad \text{and} \quad R_{BC,DA} = \frac{V_{DA}}{I_{BC}}$$

For symmetrical structure  $R_{AB,CD} = R_{AB,CD}$

$$R_s = \frac{\rho}{t} = \left(\frac{\pi}{\ln 2}\right) \frac{V_{CD}}{I_{AB}}$$

## Junction depth measurement

- ▶ Groove and stain method: A groove has been made on the wafer to a known depth using a grinding tool of radius  $R$
- ▶ The groove is then stained using concentrated HF with 0.1-0.5% Nitric acid to delineate the contact surface. The parameters  $a$  and  $b$  can then be measured by a microscope monitoring



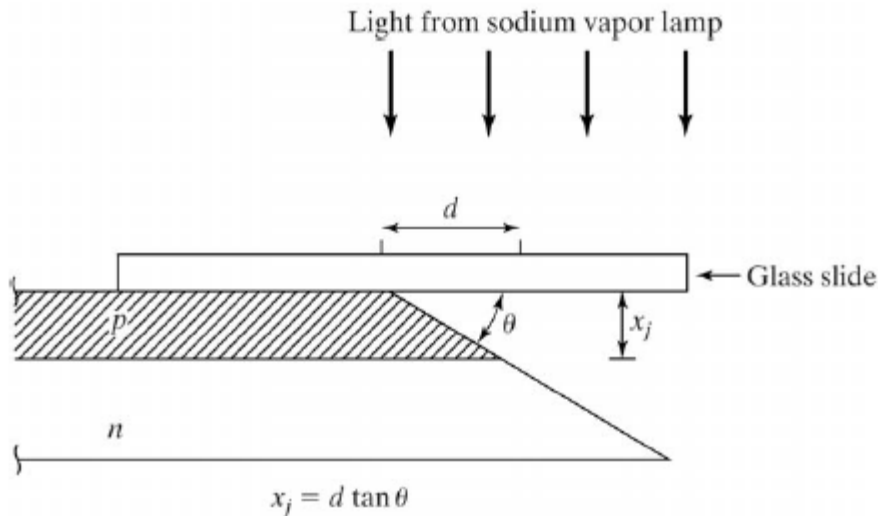
$$(x + x_j) - x = \sqrt{R^2 - b^2} - \sqrt{R^2 - a^2} = R \left( \sqrt{1 - \left(\frac{b}{R}\right)^2} - \sqrt{1 - \left(\frac{a}{R}\right)^2} \right)$$

$$\doteq R \left[ \left(1 - \frac{1}{2} \frac{b^2}{R^2}\right) - \left(1 - \frac{1}{2} \frac{a^2}{R^2}\right) \right] \quad \begin{matrix} R \gg a \\ R \gg b \end{matrix}$$

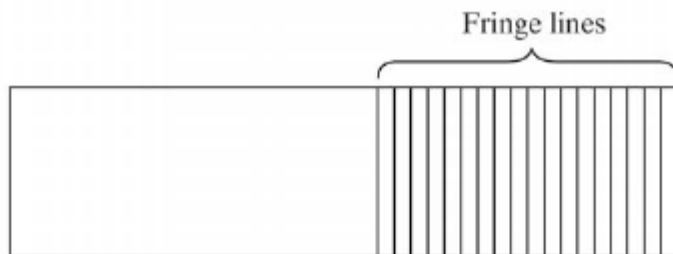
$$x_j \doteq \frac{a^2 - b^2}{2R} = \frac{(a+b)(a-b)}{2R}$$

# Junction depth measurement :Angle lap technique

- ▶ A piece of the wafer is fixed and lapped at an angle (1-5°). A glass slide is in contact with the wafer, and the setup is illuminated with monochrome light, results in interference fringes on the slide. Number of fringes depends on the junction depth ( $x_j$ )



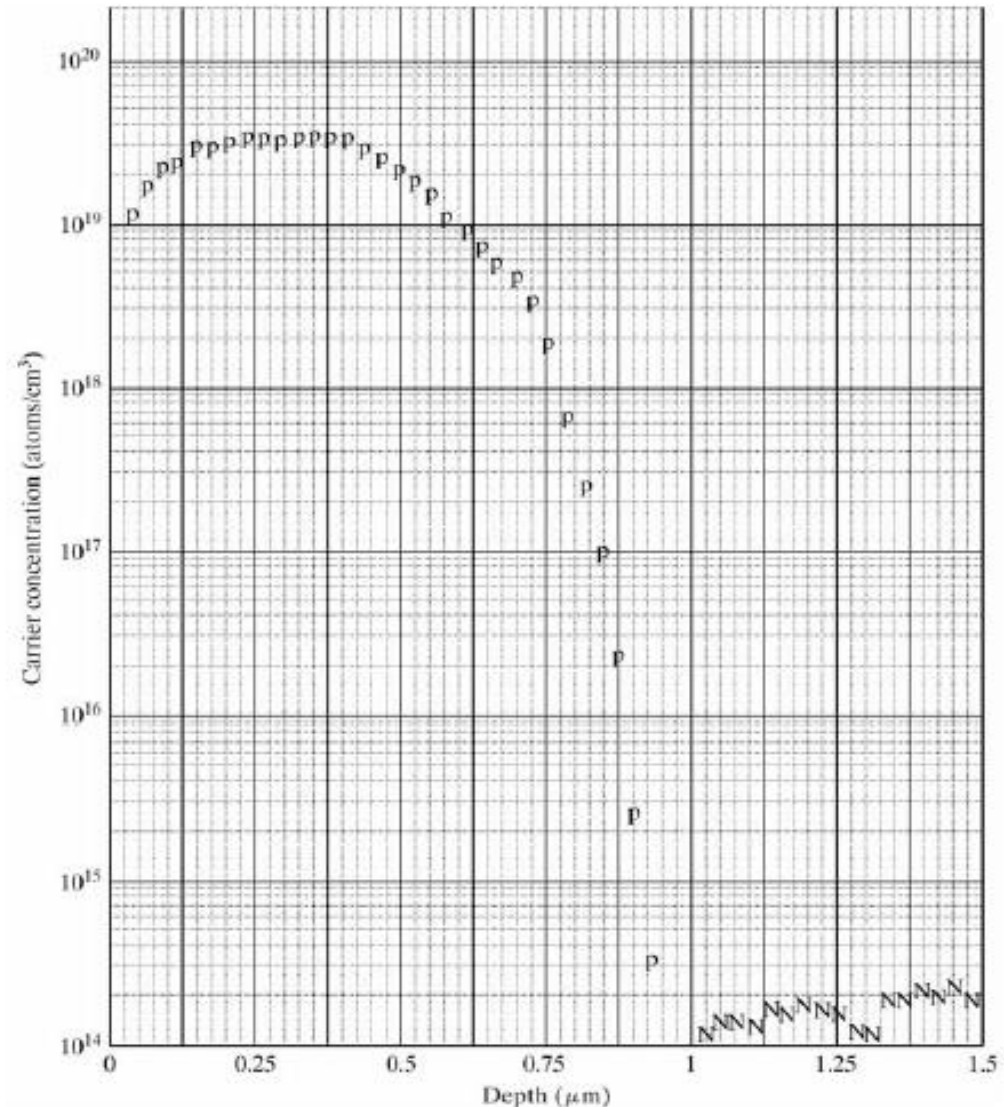
$$x_j = d \cdot \tan(\theta) = N \cdot \lambda / 2$$





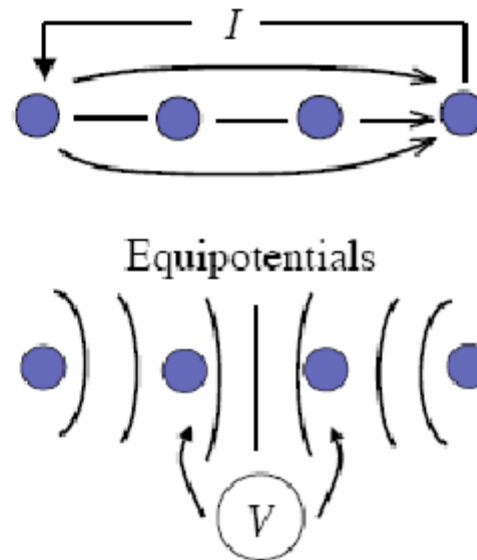
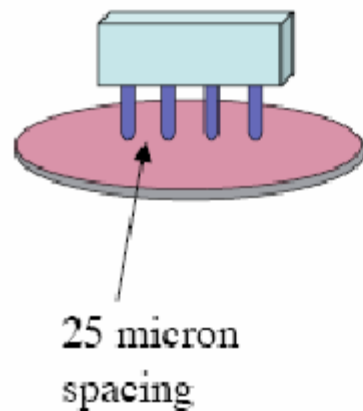
# Diffusion profile extraction

- ▶ Region angle-lapped
- ▶ Four-point probe resistance measurements vs. depth
- ▶ Profile Extracted

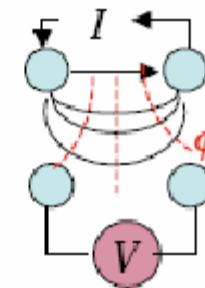


# Profile extraction process

## 4-point probe

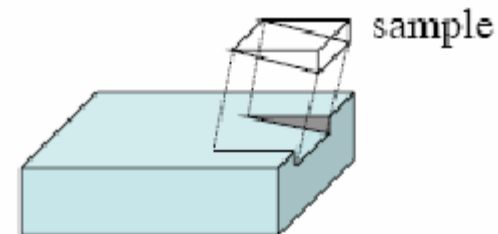
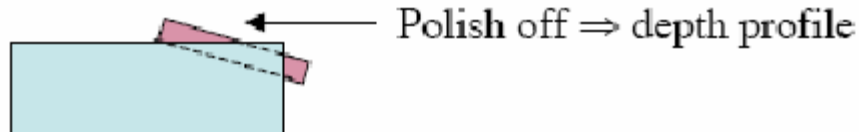


Also square array  
(Van der Pauw method)



These  $\Rightarrow$  average  $n$  if done from surface.

These are most useful if done on beveled wafer:



# Diffusion profile extraction : Secondary Ion Mass Spectroscopy (SIMS)

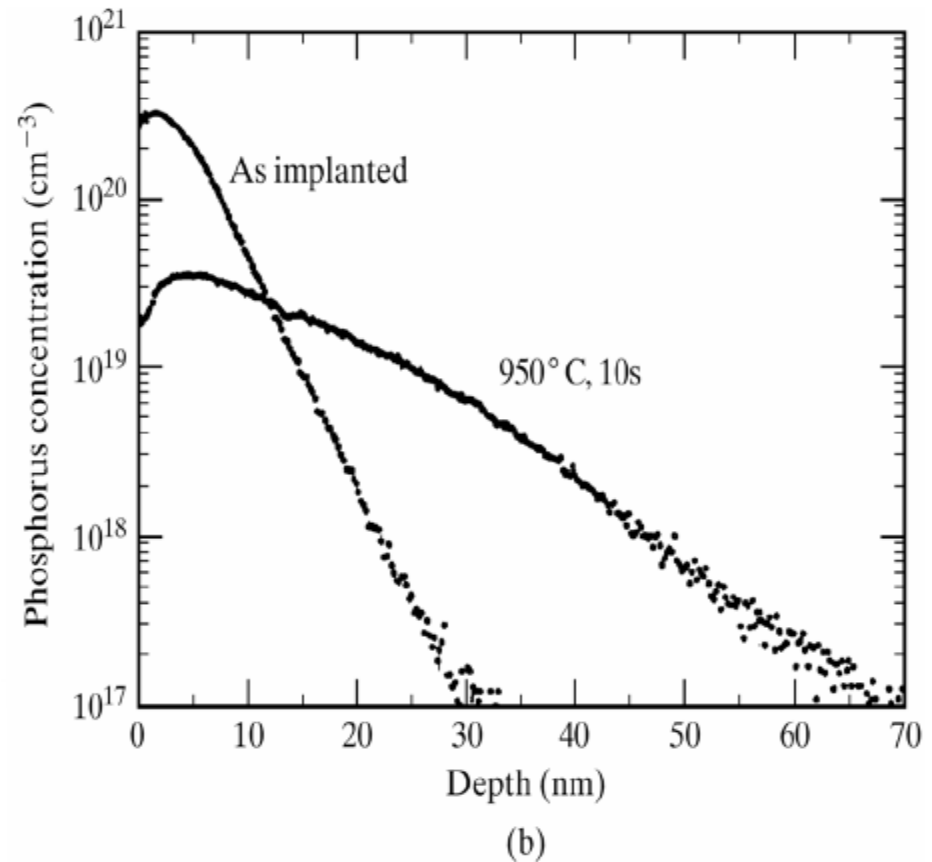
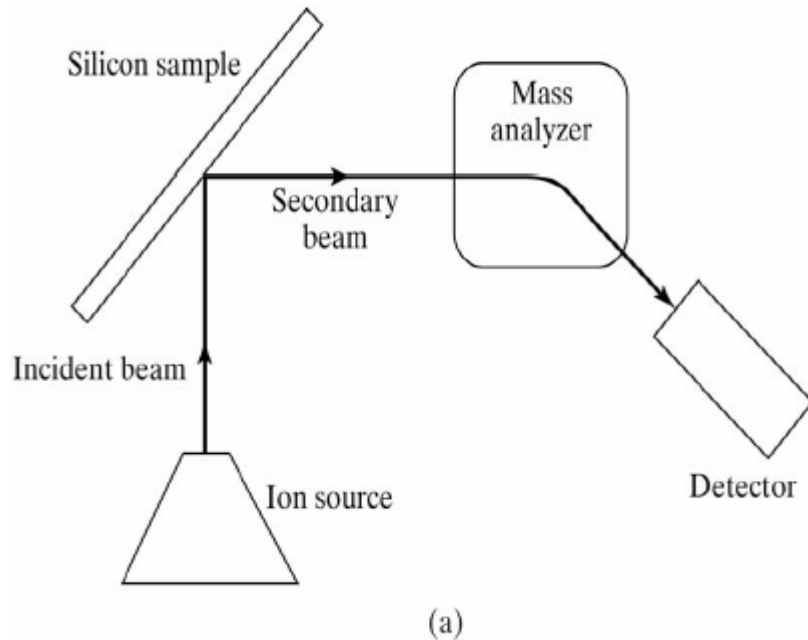
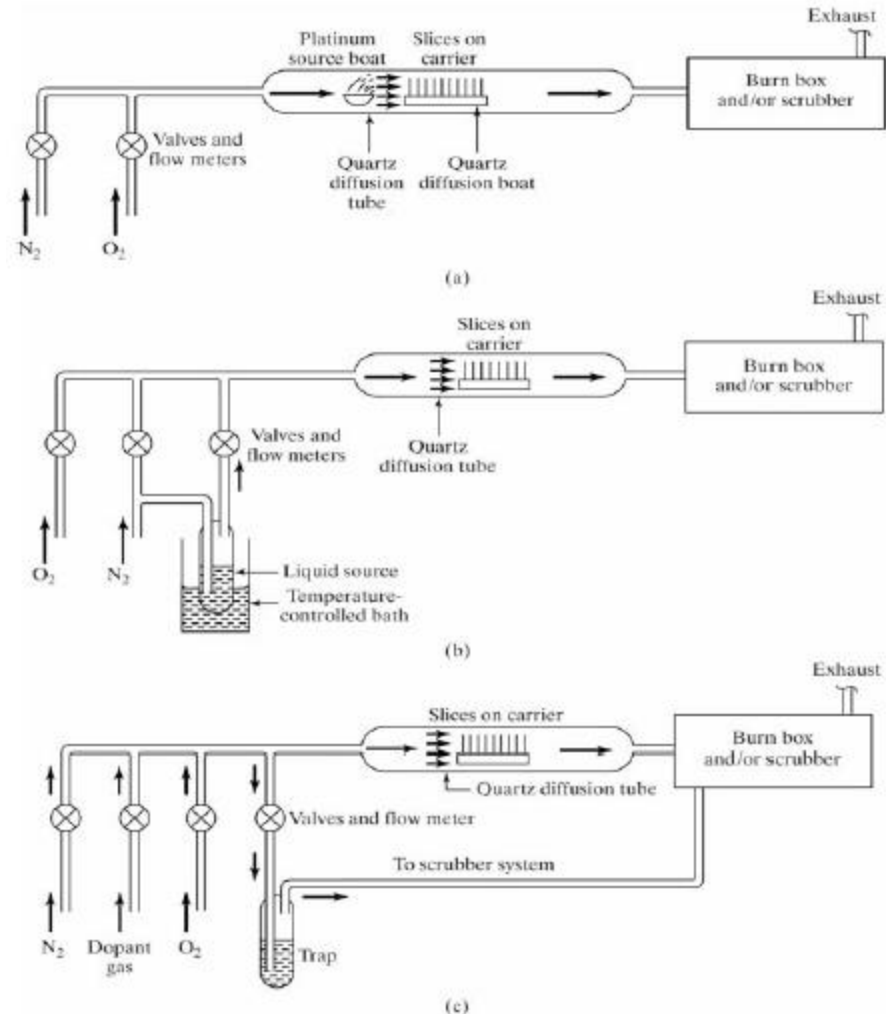


TABLE 4.3 SIMS Analysis in Silicon.

Element	Ion Beam	Sensitivity
Arsenic	Cesium	$5 \times 10^{14}/\text{cm}^3$
Boron	Oxygen	$1 \times 10^{13}/\text{cm}^3$
Phosphorus	Cesium	$5 \times 10^{15}/\text{cm}^3$
Oxygen	Cesium	$1 \times 10^{17}/\text{cm}^3$

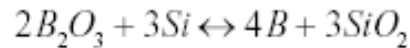
# Diffusion systems

- ▶ Open Furnace Tube systems
  - (a) Solid source in platinum source boat
  - (b) Liquid Source - carrier gas passing through bubbler
  - (c) Gaseous impurity source
- ▶ Wafers in Quartz Boat Scrubber at Output

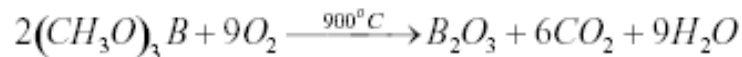


# Boron diffusion process

Surface Reaction :



Solid Sources : Boron Nitride & Trimethylborate (TMB)

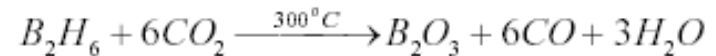
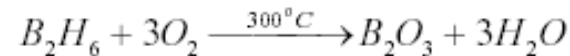


Class is using Boron Nitride Wafers

Liquid Sources : Boron Tribromide  $BBr_3$



Gaseous Source : Diborane  $B_2H_6$  (Extremely Toxic)

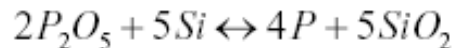


All systems need careful scrubbing!

$CO_2$     $BBr_3$     $CO$    TMB    $B_2H_6$

# Phosphorous diffusion

Surface Reaction :



Gaseous Source : Phosphine  $PH_3$  (Extremely Toxic)



Solid Sources :

Phosphorus Pentoxide

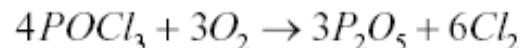
Ammonium monophosphate  $NH_4H_2PO_4$

Ammonium diphosphate  $(NH_4)_2H_2PO_4$

All systems need careful scrubbing!

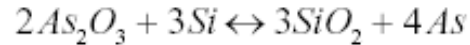


Liquid Source : Phosphorus Oxychloride  $POCl_3$



# Arsenic and Antimony diffusion

## Arsenic Surface Reaction

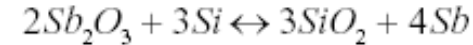


Solid Sources: Possible - Low Surface Concentrations

Gaseous Source: Arsine  $AsH_3$  (Extremely Toxic)

Ion – Implantation Is Normally Used for Deposition

## Antimony Surface Reaction



Liquid Source: Antimony Pentachloride  $Sb_3Cl_5$

Ion – Implantation Is Normally Used for Deposition