Diffusion

Topic covered:

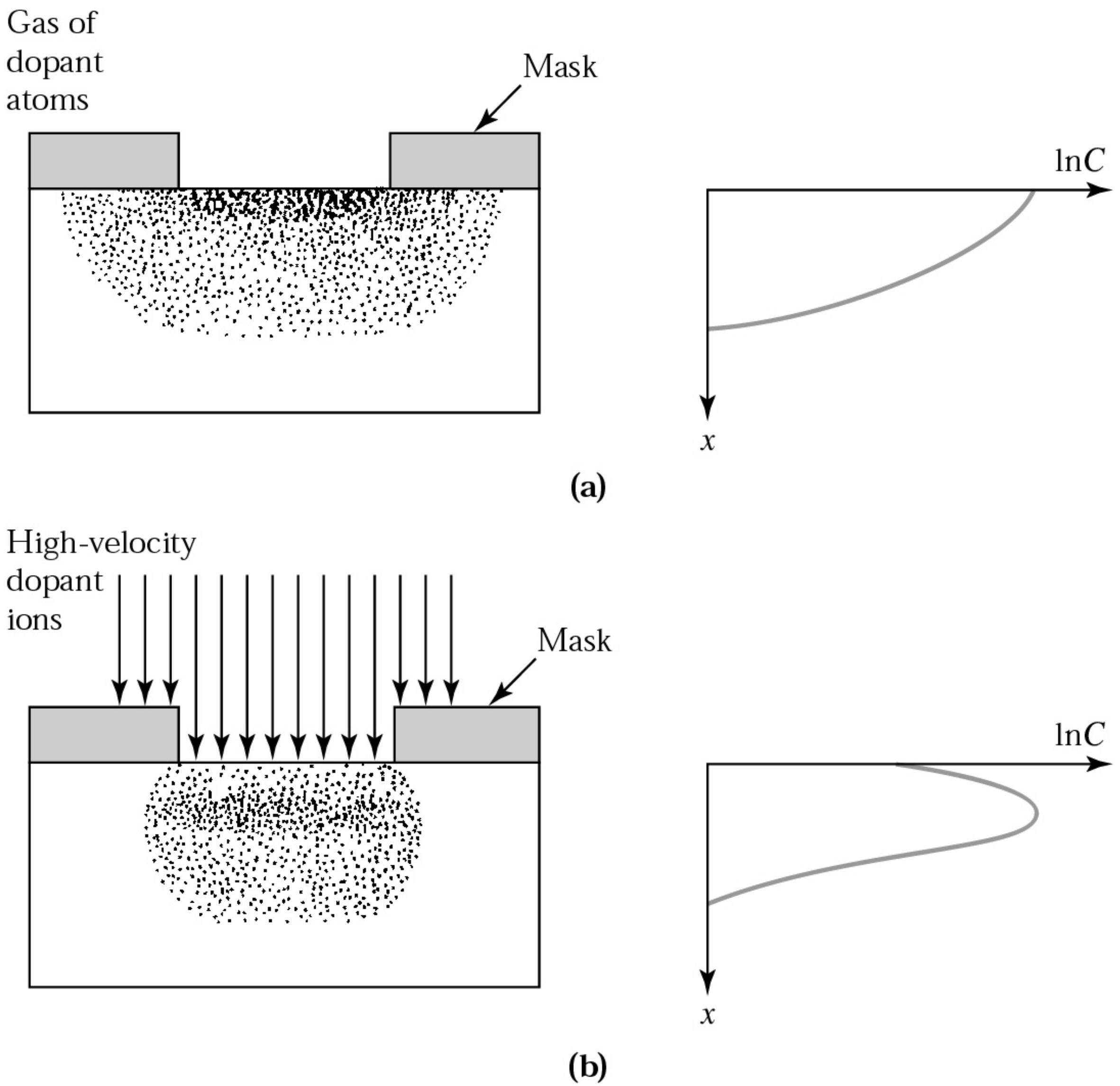
- Movement of Impurity Atoms in Crystal Lattice
- Impurity Profiles
- Impact of Lateral Diffusion and Impurity Redistribution
- Simulation of Diffusion

Impurity Doping

- An introduction of controlled amount of impurity dopants into semiconductors.
- Key methods of impurity doping are:
  - Diffusion
  - Ion implantation
- Both methods are used for fabricating discrete devices and integrated circuits because these processes complement each other.

Figure 1

Comparison of
(a) diffusion and (b) ion-implantation techniques for the selective introduction of dopants into the semiconductor substrate.



Basic Diffusion Process

- Semiconductor wafers are placed in a controlled, high-temperature quartz-tube furnace and passing a gas mixture that contains the desired dopant through it.
- Temperature ranges between 800ºC and 1200ºC for silicon and 600ºC and 1000ºC for gallium arsenide.
- For diffusion of silicon, boron is popular dopant for introducing a p-type impurity whereas arsenic and phosphorous are used as n-type dopants.
- For diffusion on gallium arsenide, the high vapor pressure of arsenic requires special methods to prevent the loss of arsenic by decomposition or evaporation.

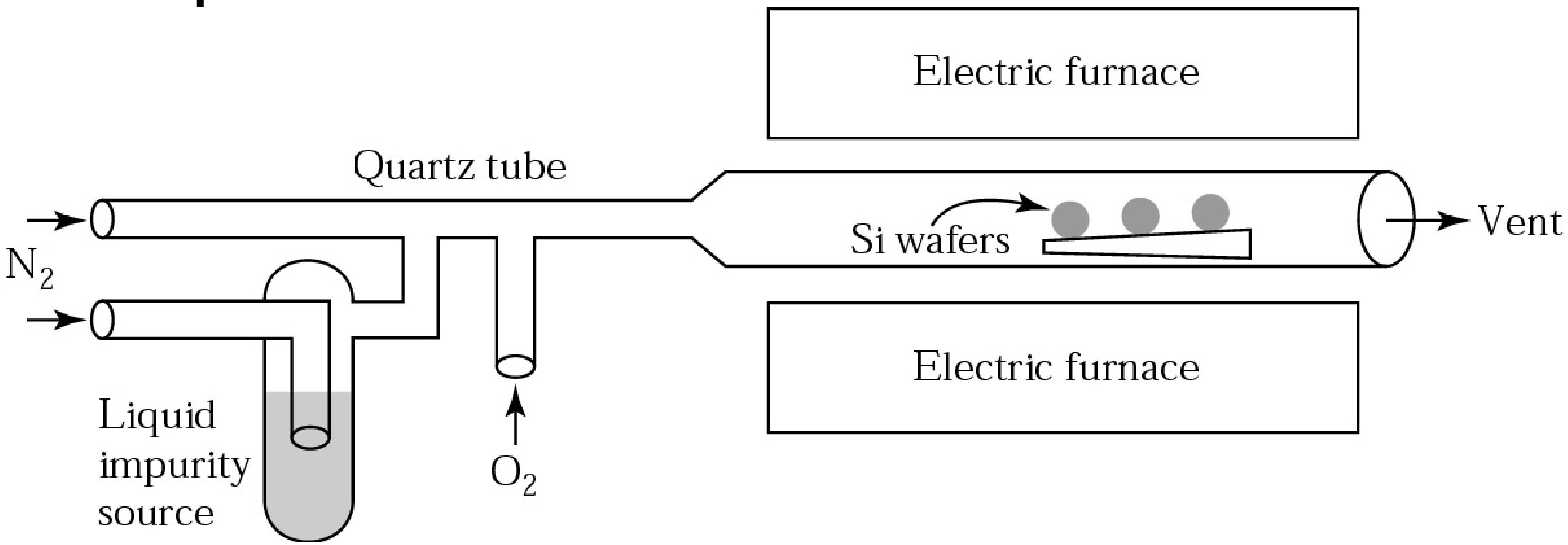


Figure 2

Schematic diagram of a typical open-tube diffusion system.

Diffusion Mechanism

- Diffusion can be visualized as the atomic movement of the diffusant in the crystal lattice by vacancy or interstitials.

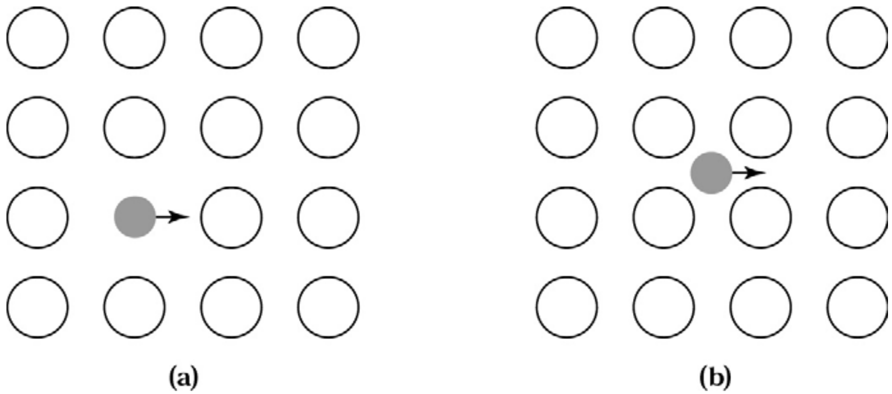


Figure 3

Atomic diffusion mechanisms for a two-dimensional lattice. (a) Vacancy mechanism. (b) Interstitial mechanism.

Diffusion Equation

- The basic diffusion process of impurity atoms is similar to that of charge carriers (electrons or holes).
- The flux, **F**, is define as the number of dopant atoms passing through a unit area, and **C** as the dopant concentration per unit volume.

$$F = -D \frac{\partial C}{\partial x} \qquad (1)$$

where **D** is the diffusion coefficient or diffusivity

- Note that the basic driving force of the diffusion process is the concentration gradient $\delta C / \delta x$.
- Substitute Eq.1 into the one-dimensional continuity equation under the condition that no materials are formed or consumed in the host semiconductor, we obtain:

$$\frac{\partial C}{\partial x} = -\frac{\partial F}{\partial x} = \frac{\partial}{\partial x}\left(D \frac{\partial C}{\partial x} \right) \qquad (2)$$

- When the concentration of dopant atoms is low, the diffusion coefficient can be considered independent of doping concentrations, and Eq.2 becomes

$$\frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} \qquad (3)$$

- Equation 3 is often referred to as Fick's diffusion equation or Fick's Law.

- The logarithm of the diffusion coefficient plotted against the reciprocal of the absolute temperature gives a straight line in most cases.
- The diffusion coefficients can be expressed as

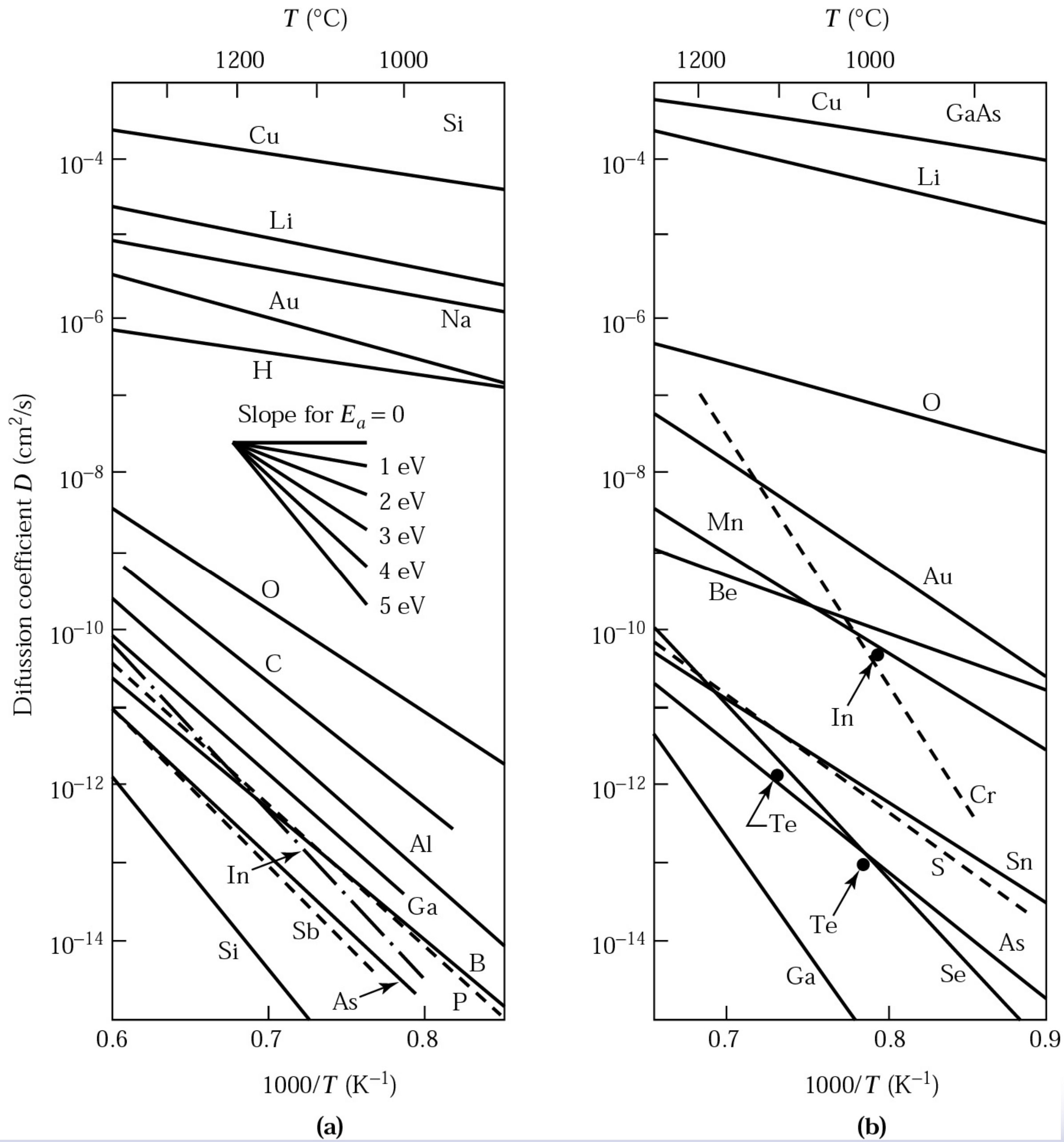
$$D = D_o \exp\left(\frac{-E_a}{kT}\right) \qquad (4)$$

where D_o is the diffusion coeffient in cm^2/s extrapolated to infinite temperature, and E_a is the activation energy.

Note: Values of E_a are found to be between 0.5 and 2eV in both silicon and gallium arsenide.

Figure 4

Diffusion coefficient (also called diffusivity) as a function of the reciprocal of temperature for (a) silicon and (b) gallium arsenide.



Diffusion Profiles

- Diffusion profile of the dopant atoms is dependent on the initial and boundary conditions.
- Two important cases:
  - Constant Surface Concentration Diffusion
  - Constant Total Dopant Diffusion

Constant Surface Diffusion

- Initial condition at t=0 is

$$C(x,0) \qquad (5)$$

- The boundary conditions are

and

$$C(0,t) = C_s \qquad (6a)$$

$$C(\infty,t) = 0 \qquad (6b)$$

where C_s is the surface concentration (at x=0), which is independent of time.

- The solution to Fick's diffusion equation that satisfies initial and boundary condition is given by

$$C(x,t) = C_s \, erfc\left(\frac{x}{2\sqrt{Dt}}\right) \qquad (7)$$

where erfc is the complementary error function and $\sqrt{Dt}$ is the diffusion length

- The total number of dopant atoms per unit area of the semiconductor is given by

$$Q(t) = \int_0^{\infty} C(x,t)\,dx \qquad (8)$$

Error Function Algebra

$$\mathrm{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2}\, dy$$

$$\mathrm{erfc}(x) \equiv 1 - \mathrm{erf}(x)$$

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

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

$$\mathrm{erf}(x) \cong \frac{2}{\sqrt{\pi}} x \quad \text{for } x << 1$$

$$\mathrm{erfc}(x) \cong \frac{1}{\sqrt{\pi}} \frac{e^{-x^2}}{x} \quad \text{for } x >> 1$$

$$\frac{d}{dx} \mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}$$

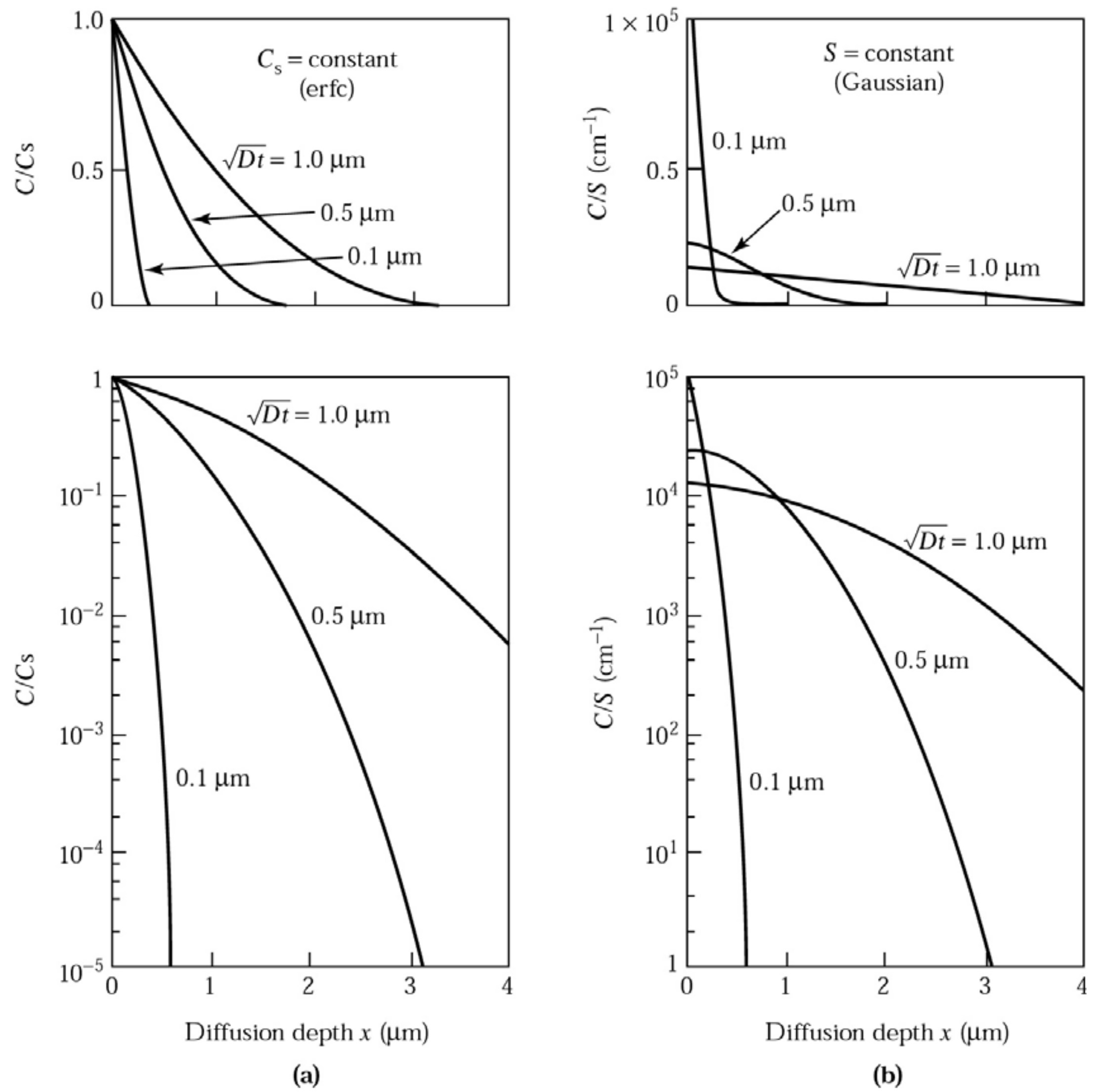
$$\frac{d^2}{dx^2} \mathrm{erf}(x) = -\frac{4}{\sqrt{\pi}} x e^{-x^2}$$

$$\int_0^x \mathrm{erfc}(y')\, dy' = x\, \mathrm{erfc}(x) + \frac{1}{\sqrt{\pi}} \left(1 - e^{-x^2}\right)$$

$$\int_0^\infty \mathrm{erfc}(x)\, dx = \frac{1}{\sqrt{\pi}}$$

Figure 5

Diffusion profiles. (a) Normalized complementary error function versus distance for successive diffusion times. (b) Normalized Gaussian function versus distance.



- Substitute Eq.7 to Eq.8, yields

$$Q(t) = \frac{2}{\pi} C_s \sqrt{Dt} \cong 1.13 C_s \sqrt{Dt} \qquad (9)$$

- A related quantity is the gradient of the diffusion profile $\delta C / \delta x$. The gradient can be obtained by differentiating Eq.7:

$$\left. \frac{\partial C}{\partial x} \right|_{x,t} = \frac{C_s}{\sqrt{\pi Dt}} e^{-x^2/4Dt} \qquad (10)$$

Constant Total Dopant

- A fixed (or constant) amount of dopant is deposited onto the semiconductor surface in a thin layer, and the dopant subsequently diffuses into the semiconductor.
- Initial condition is as Eq.5. The boundary conditions are

$$\int_0^\infty C(x,t) = S \qquad (11a)$$

and

$$C(\infty,t) = 0 \qquad (11b)$$

where **S** is the total amount of dopant per unit area.

- The solution to diffusion equation that satisfies the conditions is

$$C(x,t)=\frac{S}{\sqrt{\pi Dt}}e^{\left(-\frac{x^2}{4Dt}\right)} \qquad (12)$$

- This expression is the Gaussian distribution.
- The surface concentration at x=0 given by

$$C(x,t)=\frac{S}{\sqrt{\pi Dt}} \qquad (13)$$

- The gradient of diffusion profile is

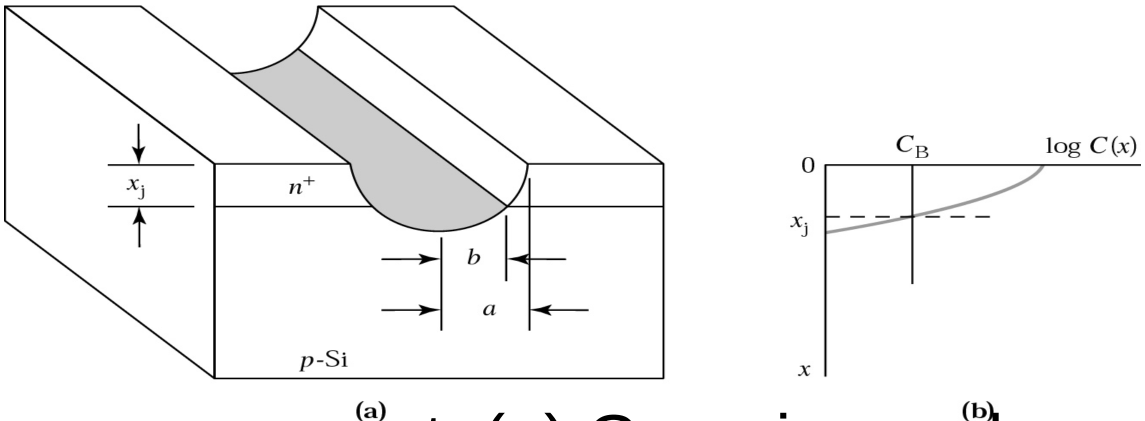
$$\left.\frac{\partial C}{\partial x}\right|_{x,t}=-\frac{xS}{2\sqrt{\pi}(Dt)^{3/2}}=-\frac{x}{2Dt}C(x,t) \qquad (14)$$

Evaluation of Diffused Layer

- The results of diffusion process can be evaluated by three measurements:
  - Junction Depth - delineated by cutting a groove into the semiconductor and etching the surface solution that stains the p-type darker than n-type region.
  - Sheet Resistance – layer are measured by four-point probe technique.
  - Dopant Profile – can be measured using capacitance-voltage technique.

Junction Depth

Figure 6



Junction-depth measurement. (a) Grooving and staining. (b) Position in which dopant and substrate concentrations are equal.

$$x_j = \sqrt{R_o^{\,2} - b^2} - \sqrt{R_o^{\,2} - a^2} \qquad (15)$$

If R_o is much larger than ***a*** and ***b***

$$x_j \cong \frac{b^2 - a^2}{2R_o} \qquad (16)$$

$$C(x_j) \cong C_B \qquad (17)$$

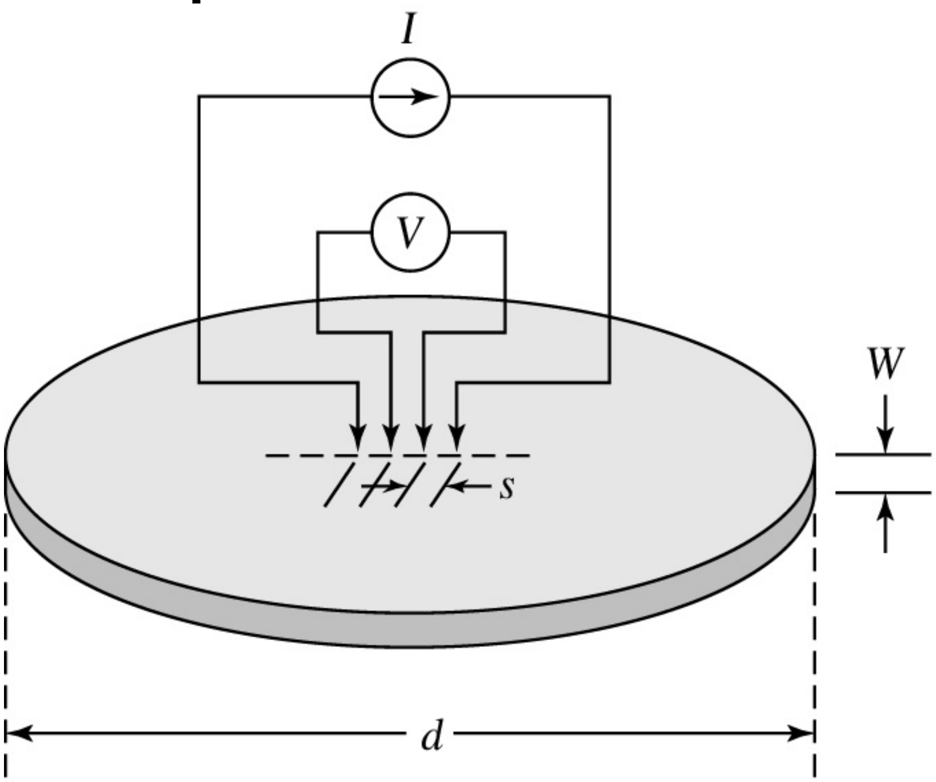


Figure 7

Measurement of resistivity using a four-point probe.

Sheet Resistance

- The probes are equally spaced. A small current ***I*** from a constant-current source is passed through the outer probes.

$$\rho = \frac{V}{I} * W * CF, \Omega - cm \qquad (18)$$

where CF is the correction factor, which is dependent of ratio of d/S. When d/S >20, CF approaches 4.54.

- The Sheet Resistance (R_s) is realted to junction depth (x_j), the carrier mobility (μ), and the impurity distribution C(x) is given by the following expression:

$$R_s = \frac{1}{q\int_0^j \mu C(x)dx} \qquad (19)$$

Doping Profile

- The majority carrier profile (n), which is equal to the impurity profile if impurities are fully ionized, can be determined by measuring reverse-bias capacitance of a p-n junction or a Schottky barrier diode as a function of applied voltage. This is due to the relationship

$$\boldsymbol{n} = \frac{2}{\boldsymbol{q}\varepsilon_s}\left[\frac{-1}{\boldsymbol{d}(1/\boldsymbol{C}'^2)/\boldsymbol{dV}}\right] \qquad (20)$$

Concentration-Dependent Diffusivity

$$C_v = C_i * e^{\left(\frac{E_F - E_i}{kT}\right)} \qquad (21)$$

where

C_V is the intrinsic vacancy density

E_F is the Fermi level

E_i is the intrinsic Fermi level

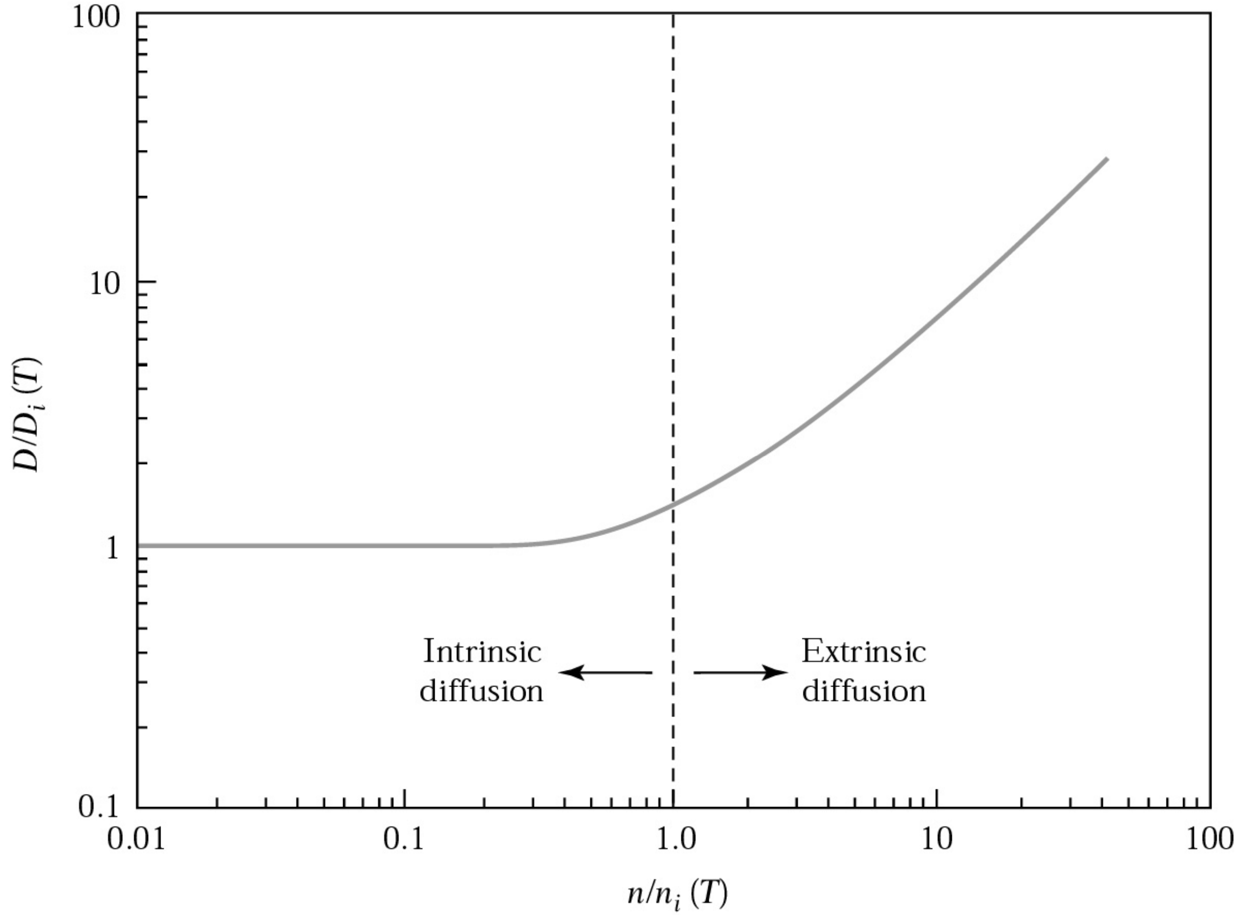
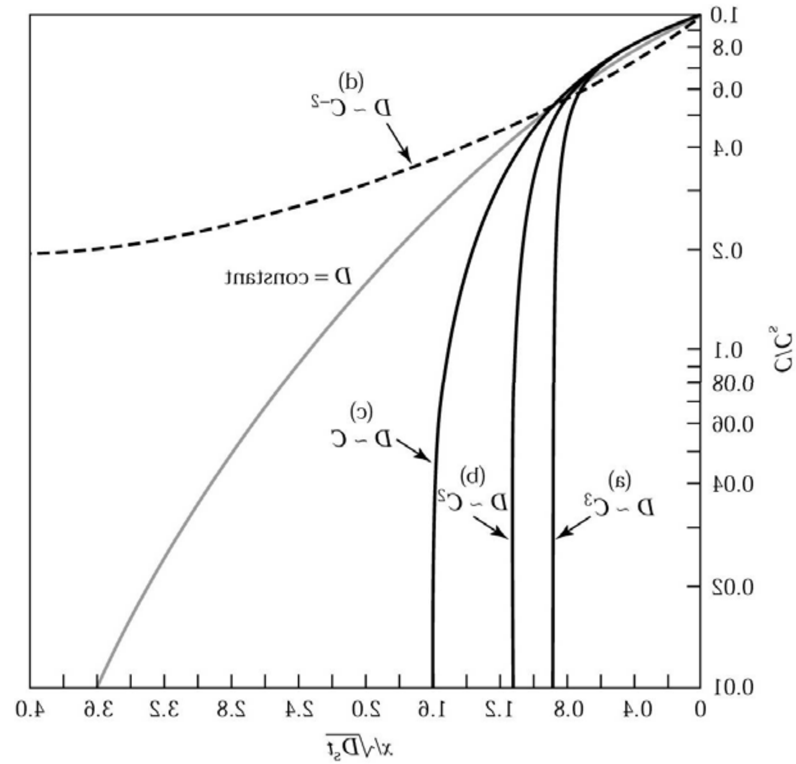


Figure 8

Donor impurity diffusivity versus electron concentration showing regions of intrinsic and extrinsic diffusion.

Figure9

Normalized diffusion profiles for extrinsic diffusion where the diffusion coefficient becomes concentration dependent.

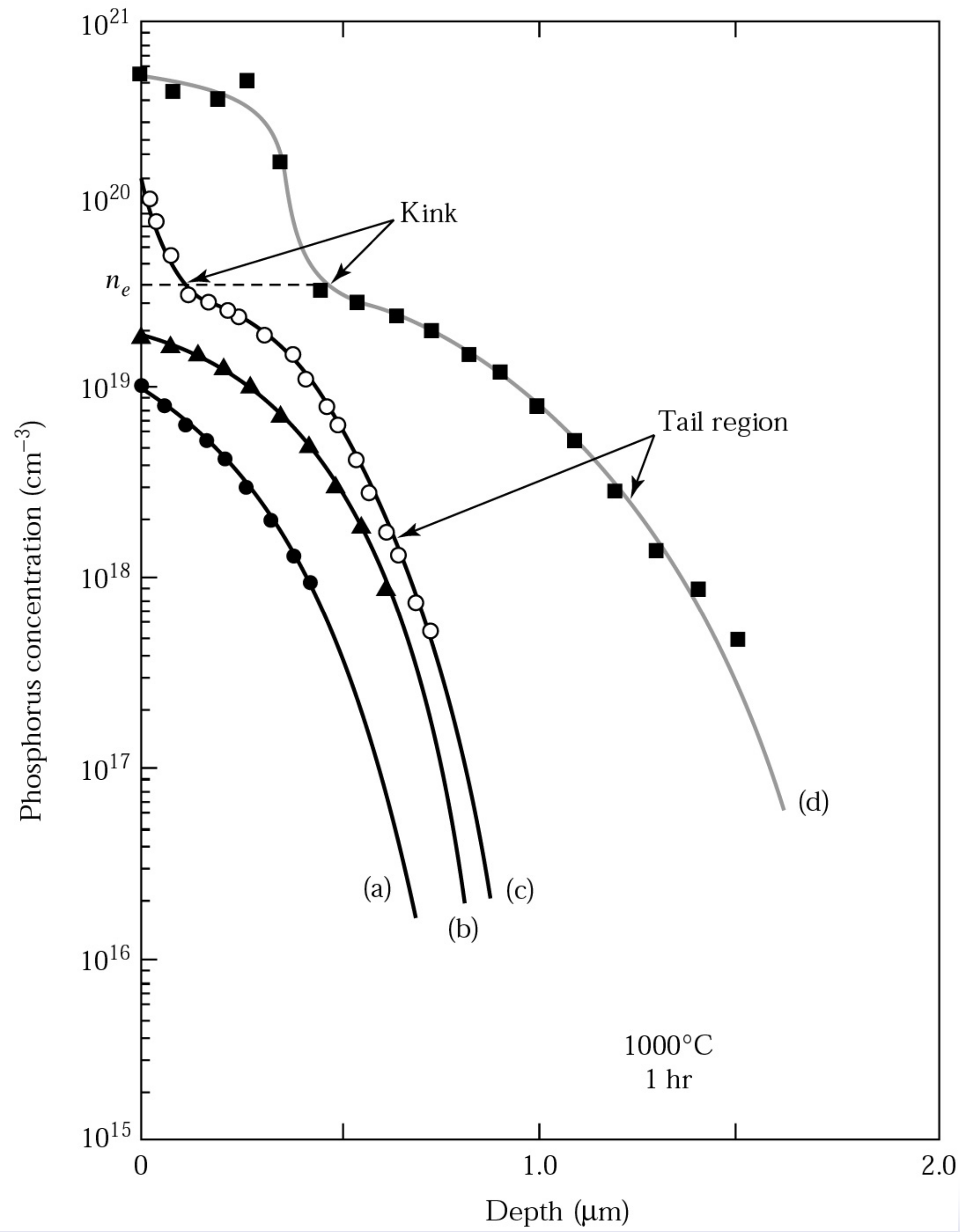


$$D = D_s \left(\frac{C}{C_s} \right)^{\gamma} \quad (22)$$

where C_s surface concentration, D_s diffusion coefficient at the surface, γ is the parameter of concentration-dependent

Figure 10

Phosphorus diffusion profiles for various surface concentrations after diffusion into silicon for 1 hour at 1000°C.



Lateral Diffusion

Figure 11

Diffusion profiles of zinc in GaAs after annealing at 1000°C for 2.7 hours. The different surface concentrations are obtained by maintaining the Zn source at temperatures in the range 600°C to 800°C.

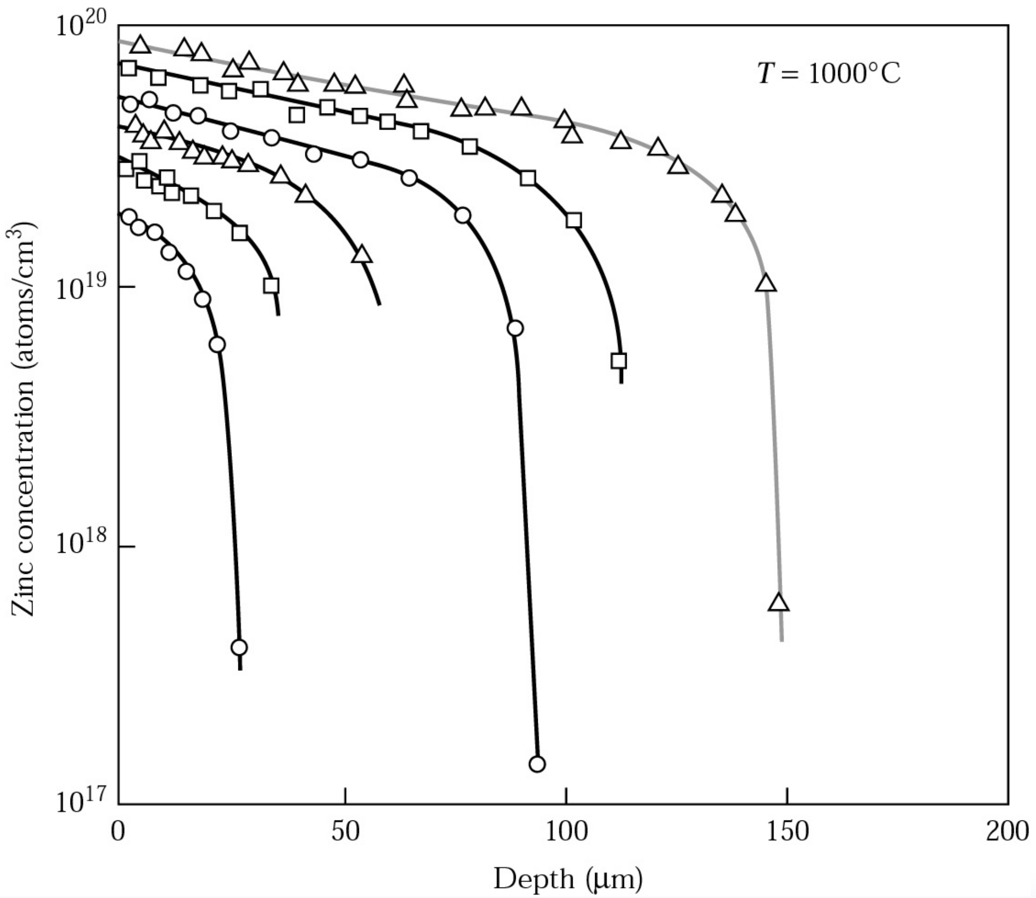
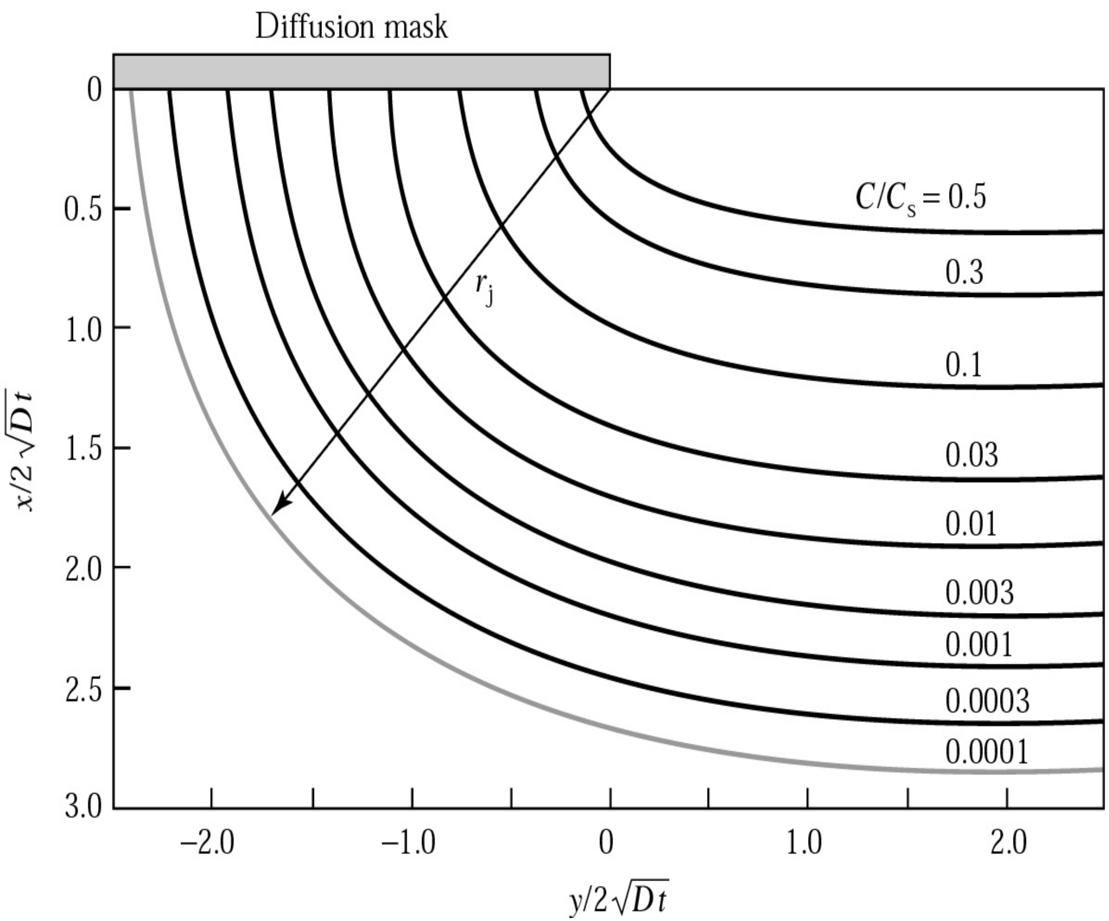


Figure 12

Diffusion contours at the edge of an oxide window; there r_j is the radius of curvature.



Example 1

For a boron diffusion in silicon at 1000^{o}C, the surface concentration is maintained at 10^{19} cm^{-3} and the diffusion time is hour. Find Q(t) and the gradient at x=0 and at a location where the dopant concentration reaches 10^{15} cm^{-3}.

Example 2

Arsenic was predeposited by arsine gas, and the resulting total amount of dopant per unit area was $1x10^{14}$ atoms/cm^2. How long would it take to drive the arsenic in to a junction depth of 1 um?

Assume a background doping C_B= $1x10^{15}$ atoms/cm^3 , and drive-in temperature of 1200^{o}C. As for diffusion, D_0=24cm^2/s and E_a=4.08eV.

Example 3: Simulation Problem

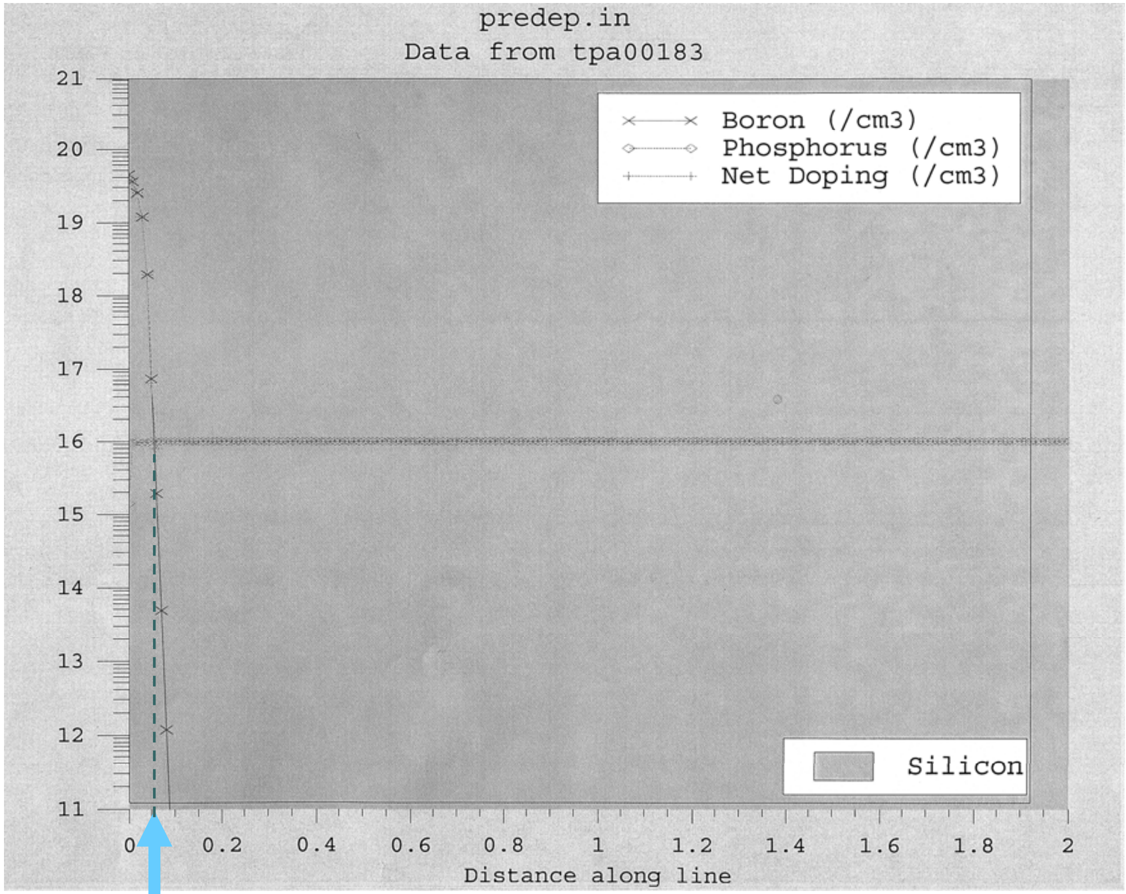
Suppose we want to simulate the predeposition of boron into an n-type <100> silicon wafer at 850^{o}C for 15 minutes. If the silicon substrate is doped with phosphorous at a level of 10^{16} cm^{-3}, use SUPREM to determine the boron doping profile and junction depth.

SUPREM Input Listing

TITLE	**Predeposition Example**
COMMENT	Initialize silicon substrate
INITIALIZE	**<100> Silicon Phosphor Concentration = 1e16**
COMMENT	Diffuse boron
DIFFUSION	**Time=15 Temperature=850 Boron Solidsol**
PRINT	**Layers Chemical Concentration Phospor-Boron Net**
PLOT	**Active Net Cmin=1e15**
STOP	**End Predeposition example**

Figure 13

Plot of boron concentration as a function of depth into the silicon substrate, using SUPREM.



Junction depth = 0.06um