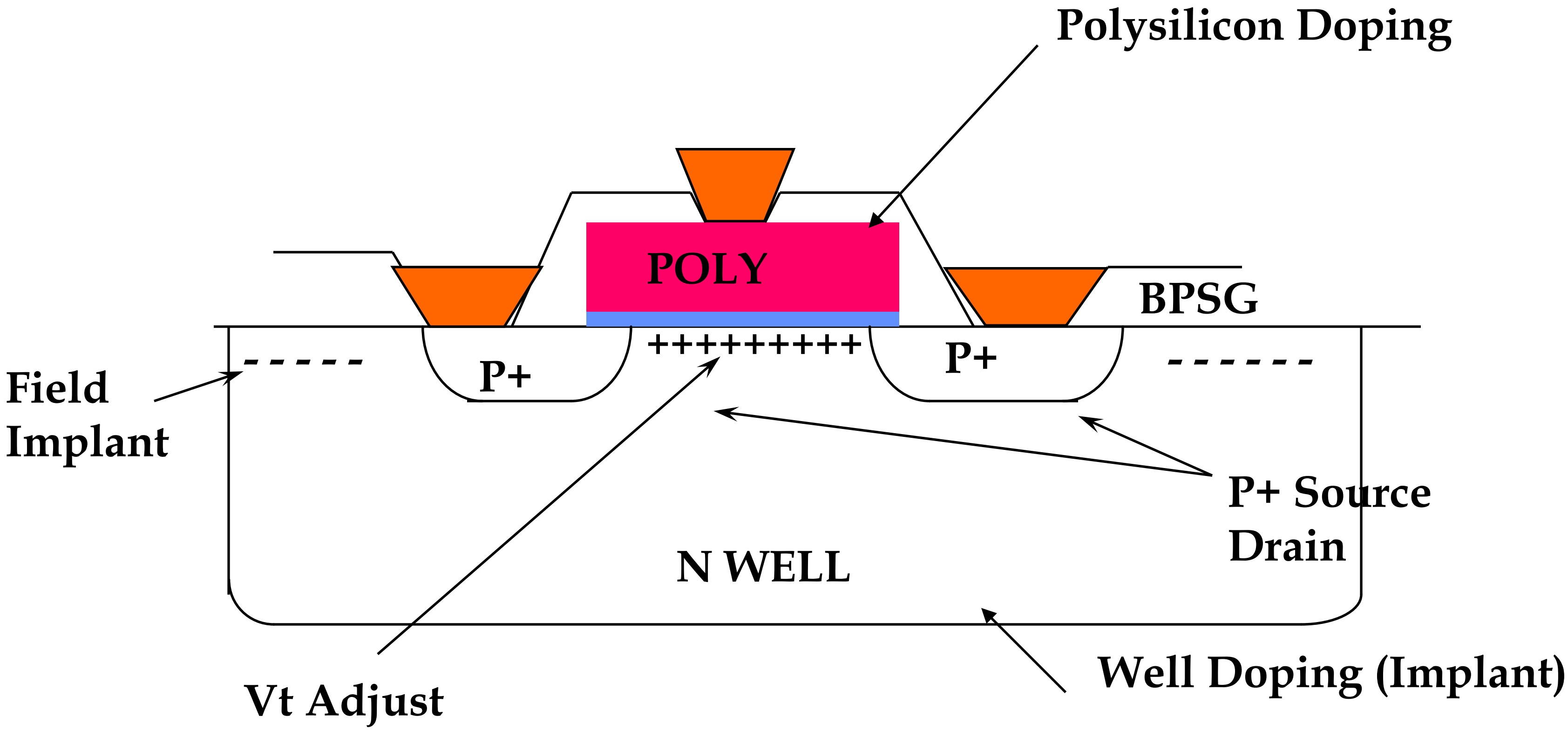
Diffusion

Contents

Introduction

- Introducing dopants into the silicon crystal can alter the “type” of the silicon
  - from n type to p type and vise versa
- Dopants are usually introduced in a two stage process
- Predeposition and Drive-in
- Implant and Drive-in (anneal)

Doping the Silicon



P- Substrate Doping (material as purchased)

Doping the Silicon 2

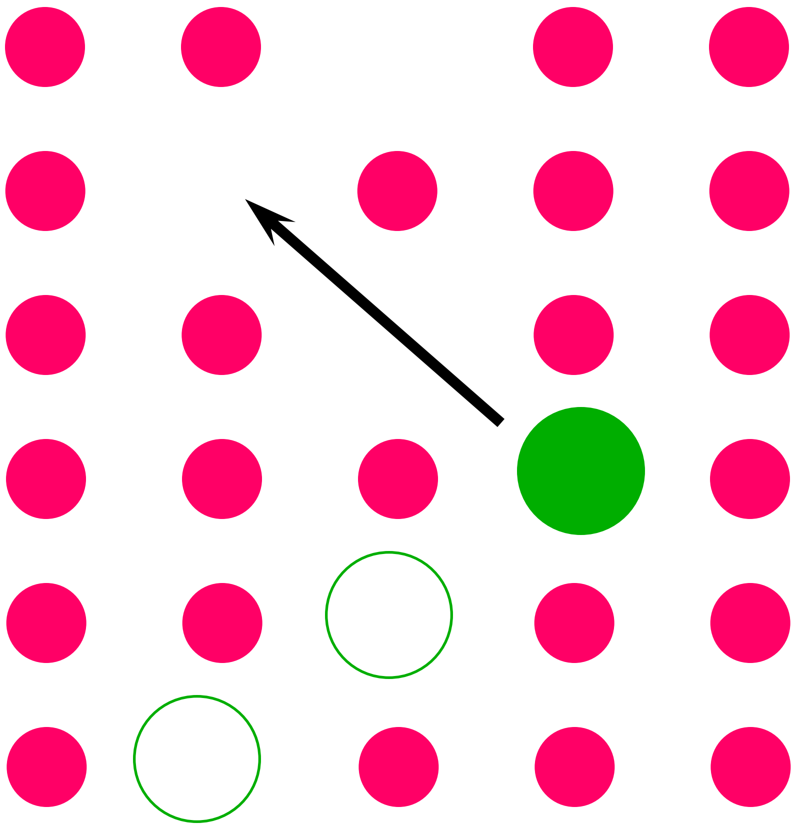
- In older processes the Source /Drain regions were doped using Thermal Diffusion
- With the maturing of implant technology CMOS processes became possible because of the greater control over the dopant quantities introduced to the silicon
- In modern CMOS processes all of the doping with the exception of the saturation doping of polysilicon is done by implantation
- In Sub-180nm processes even the polysilicon doping is done with implantation

Diffusion Mechanism

- Particles naturally diffuse (move) from areas of high concentration to areas of low concentration
- The mechanisms by which dopant atoms move in the silicon crystal are twofold
- Substitutional
  - movement of the atoms from vacancy to vacancy in the crystal
- Interstitial
  - Movement of small dopant atoms between the atoms of the silicon crystal

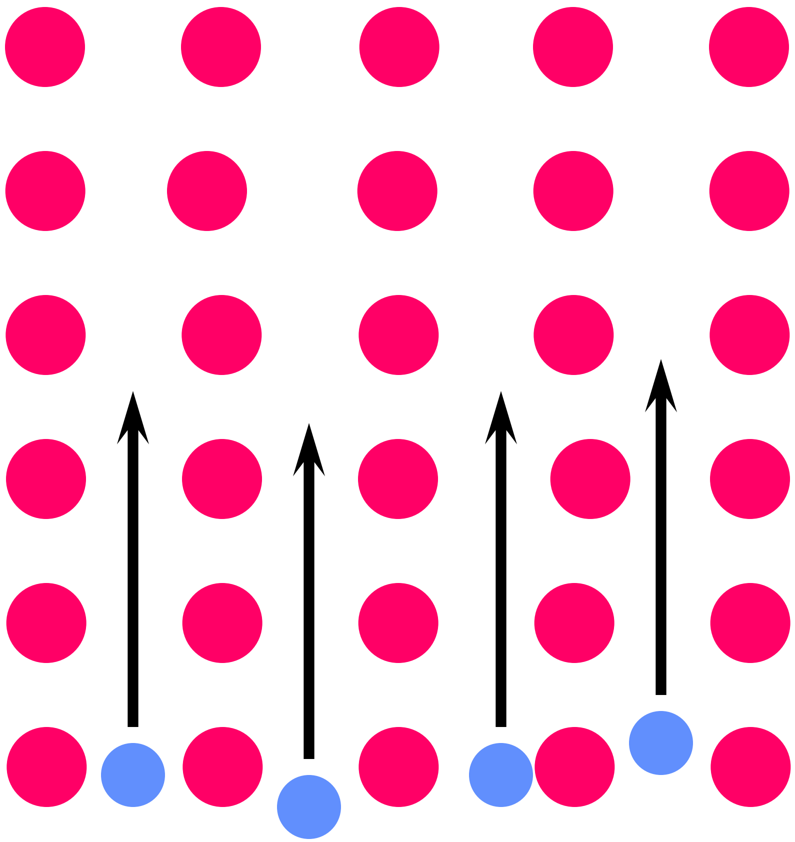
Substitutional Diffusion

- Dopant atoms move from vacancy to vacancy in the silicon crystal
- Thermal energy causes vibrations which dislocate silicon atoms from their position in the crystal
- At the elevated temperatures of diffusion furnaces there are sufficient vacancies to allow large dopant atoms to diffuse through the silicon



Interstitial Diffusion

- Some dopant atoms are small enough to move between the atoms of the silicon crystal
- They are not dependant on finding vacancies in the crystal for movement
- To become “electrically” active they must come to rest in a vacancy site
- Boron is one such dopant

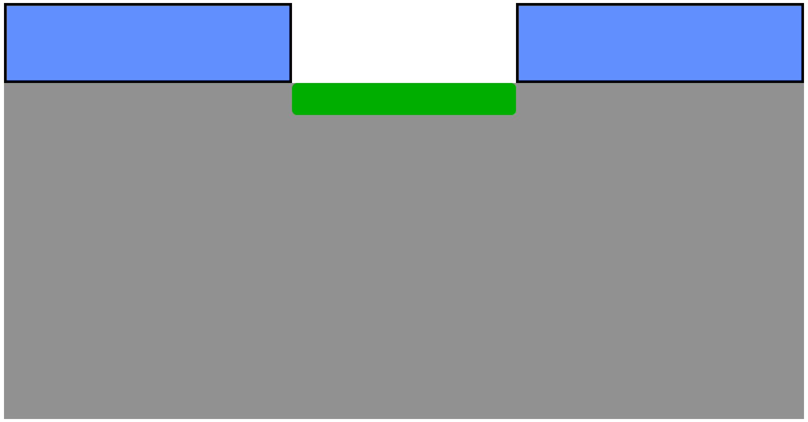


Two Stage Process

- Thermal introduction of dopant into the silicon is usually done as a two stage process
- The first of these steps is called predeposition
- Predeposition loads the surface of the silicon with a large quantity of dopant
- This dopant is then driven to the required depth during the drive in or diffusion stage
- The quantity of dopant introduced is somewhat uncontrolled as the surface of the silicon is saturation doped

Selective Doping

- P/N junctions are formed in selected areas through
  - oxidation
  - Photolithography
  - etching
- Holes are opened in the oxide the dopant can reach the silicon through these holes



- The oxide acts as a diffusion barrier to the dopant in the other areas

Equipment

Oxidation Furnace
(Silicon Valley Group - Thermco Systems)

- Same furnace arrangement as for oxidation
- Either vertical or horizontal furnace orientation can be used

Dopant Sources

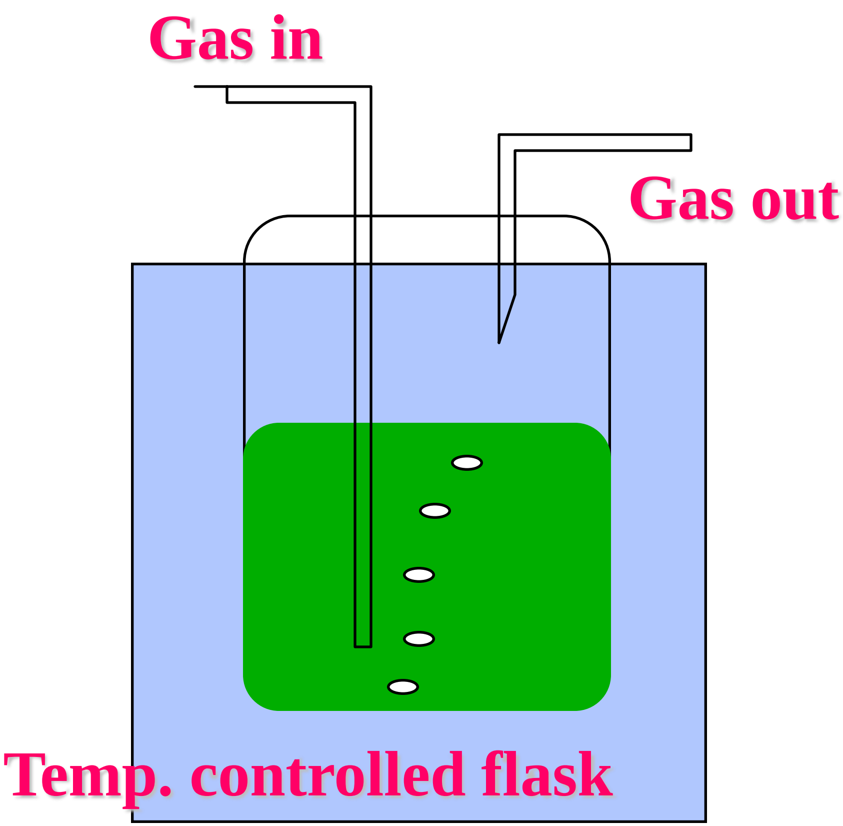
- During the predeposition stage the ambient in the furnace is rich in the dopant required
- This dopant can come from
  - solid sources
  - liquid sources
  - gas sources
- Most processes use either solid or liquid sources as gas sources for the type of materials in question are quite dangerous

Sources

- **Liquid sources**
  - Boron - BBr_3
  - Phosphorous - $POCl_3$
- **Solid sources**
  - Boron - Boron nitride or B_2O_3 disks
  - Phosphorous - P_2O_5 disks

Liquid Sources

- Liquid sources are usually delivered to the furnace from a bubbler system
- A carrier gas is passed through a temperature controlled flask of the liquid
- The gas (nitrogen) picks up some of the source chemical and delivers it down the furnace tube



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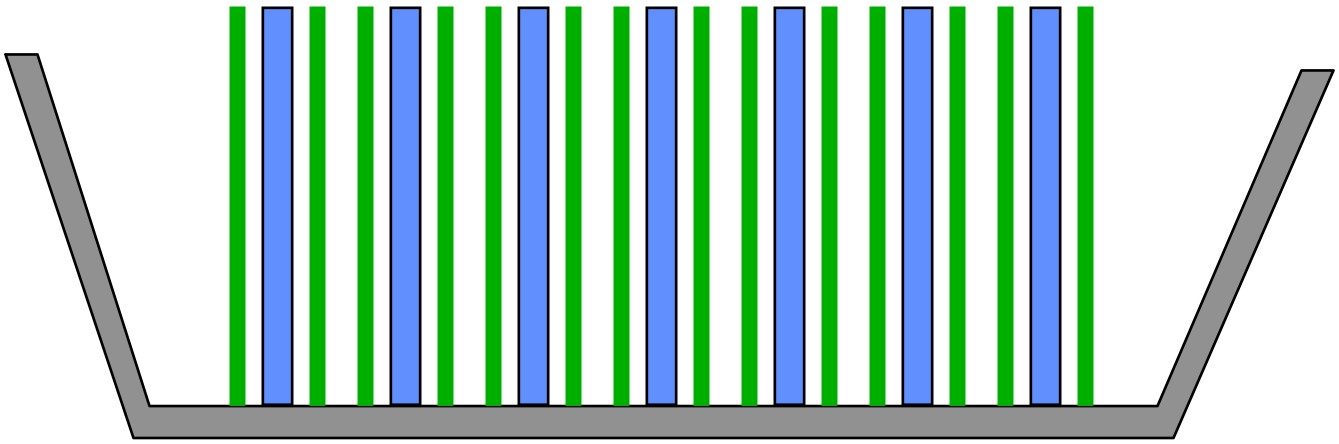
Solid Sources



Solid Source Disk

Silicon Wafer

Typical Reactions

- Boron
  - Liquid - 4 BBr_3 + $3O_2$ ---> $2B_2O_3$ + $6Br_3$
  - Solid - $2B_2O_3$ + 3Si ----> 4B + $3SiO_2$
- Phosphorous
  - Liquid - $4POCl_3$ + $3O_2$ ----> $2P_2O_5$ + 6HCl
- Most reactions involve the formation of an oxide of the dopant on the silicon surface this oxide then actually acts as the source of dopant into the silicon

Diffusion Model

- The model which describes the doping of silicon is based on Ficks Law

$$J = D\frac{\delta C_{(x,t)}}{\delta x} \qquad \textbf{1}$$

- From the law of the conservation of matter, the change in concentration over time must be the same as the decrease in the flux (local)

$$\frac{\delta C_{(x,t)}}{\delta t} = \frac{\delta J_{(x,t)}}{\delta x} \qquad \textbf{2}$$

- Substitute equation 1 into 2

$$\frac{\delta C_{(x,t)}}{\delta t} = D\frac{\delta^2 C_{(x,t)}}{\delta x^2} \qquad \textbf{3}$$

Model Assumptions

- We need to look at two sets of different initial conditions and Boundary condition assumptions for predeposition and drive-in
  - Predeposition - Constant Source Diffusion
  - Drive-in - Constant Total Dopant Diffusion

Predeposition Initial and Boundary Conditions

- **Initial Condition**
  - at $t=0$ $C_{(x,t)}=0$
- **Boundary Conditions**
  - $C_{(0,t)}=C_s$ -The surface concentration remains constant, at the solid solubility of the dopant in silicon at the process temperature
  - $C_{(\infty,t)}=0$ -At a point "very" deep into the silicon there is no dopant, the solution is for activity close to the surface

Predeposition Solution

- The solution to equation 3 which satisfies the initial and boundary conditions is:

$$C_{(x,t)} = C_s \, erfc\left[x \Big/ 2\sqrt{Dt} \right]$$

- As time progresses the dopant penetrates deeper into the silicon, the surface conc remains constant, so the total dopant quantity is increasing

$$Q_{(t)} = \int_0^{\infty} C_{(x,t)} dx \qquad Q_{(t)} = \frac{2}{\sqrt{\pi}} C_s \sqrt{Dt} \qquad Q_{(t)} = 1.13 C_s \sqrt{Dt}$$

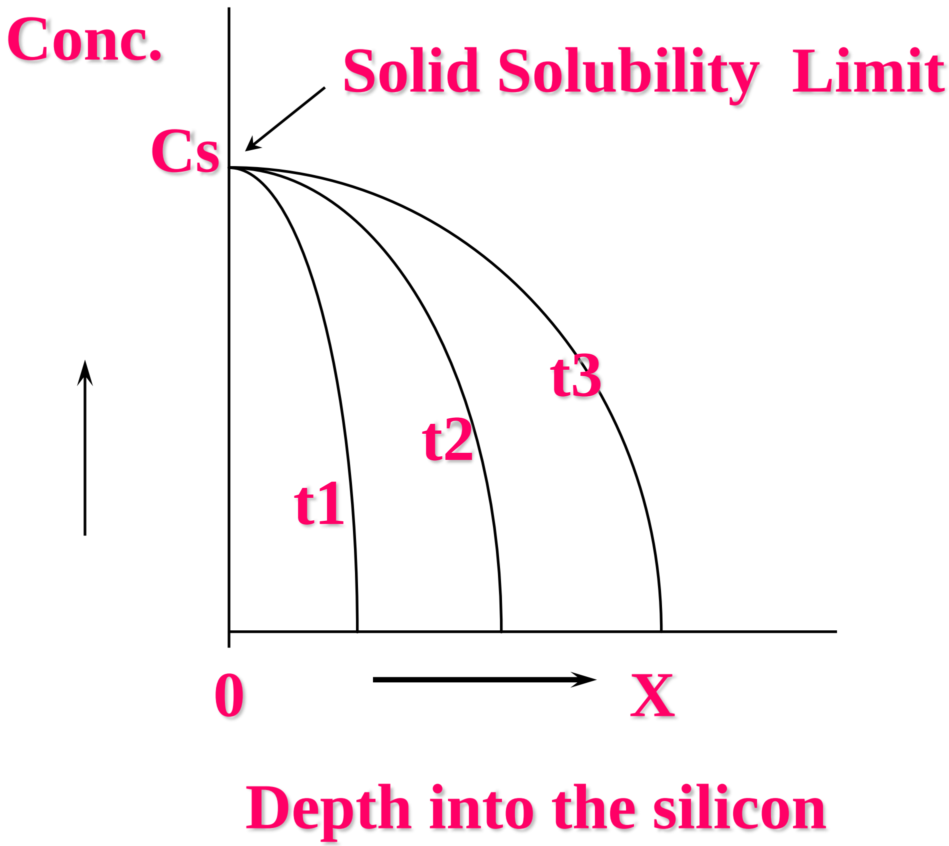
- The gradient is:

$$\left.\frac{dc}{dx}\right| x,t = -\frac{C_s}{\sqrt{\pi Dt}}$$

Predeposition

- The un limited supply of dopant means that the surface concentration goes to the solid solubility and remains at that for the duration of the furnacing

- The longer the wafers remain in the furnace the deeper into the silicon the dopant goes



Drive-In Initial and Boundary Conditions

- **Initial Condition**
  - at t=0 $C_{(x,0)}=0$
- **Boundary Conditions**
  - $\int_0^\infty C_{(x,t)}dx = S$ -No matter how long the process goes on there is only a constant amount of dopant available
  - $C_{(x,\infty)}=0$ -After a "very" long time the finite quantity of dopant would be so dispersed (diffused) as to be not there

Drive-In Solution

- The solution to equation 3 which satisfies the initial and boundary conditions is:

$$C_{(x,t)} = \frac{S}{\sqrt{\pi D t}} \exp\left[-x^2 / 4Dt\right]$$

- By setting x=0 we can get the surface concentration

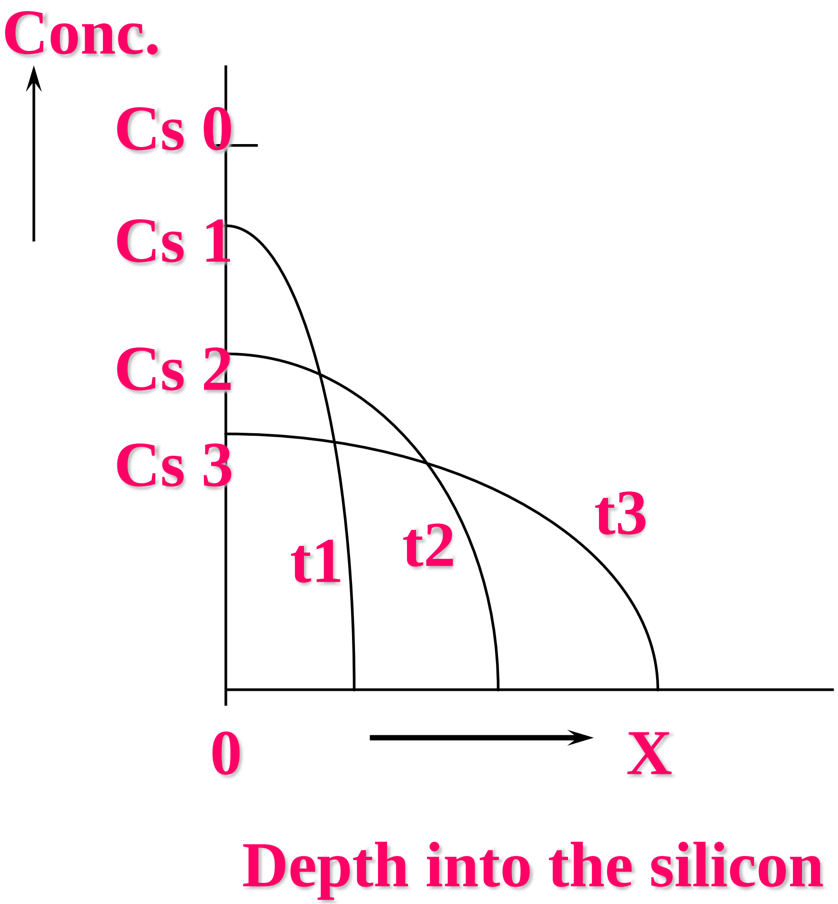
$$C_s = C_{(0,t)} = \frac{S}{\sqrt{\pi D t}}$$

- The gradient is

$$\left.\frac{dc}{dx}\right| x,t = -\frac{xS}{2\pi D t^{3/2}} \exp\left[\frac{-x^2}{4Dt}\right]$$

Drive-in

- A fixed amount of dopant remains in the silicon from the pre-deposition stage
- This is the only dopant available for diffusion
- As the dopant diffuses deeper into the silicon the surface concentration is reduced
- The total dopant quantity remains the same throughout the drive-in process
- The drive-in generally takes place in an oxygen environment which also re-oxidises the hole opened for the pre-deposition

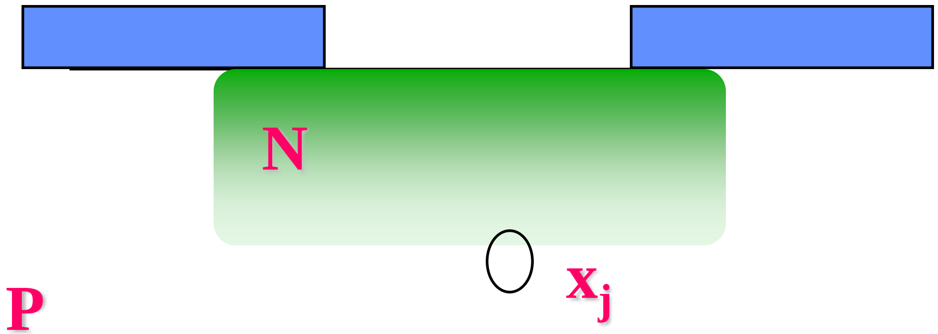


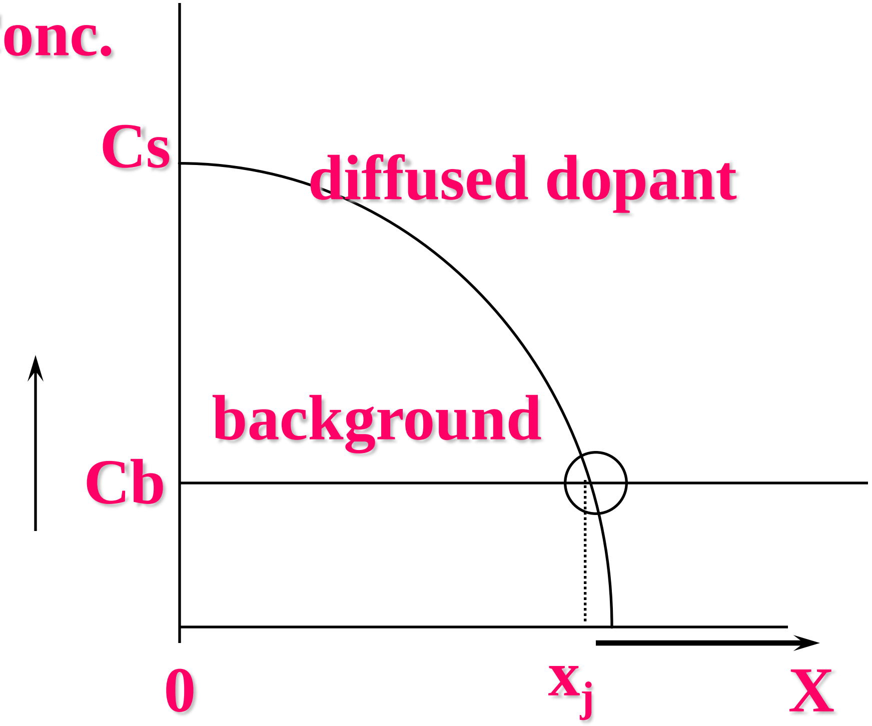
Full Process Flow

- Pre Furnace Clean
- Predeposition
- Deglaze
  - to remove the oxide/glass formed during predep
- Drive-in

Junction Formation

- The junction between the P/N region occurs where the concentration of the introduced dopant is equal to the background dopant concentration





Thermal Diffusion Summary

- In modern processes Predep/Diffusion is not used where control over the dopant quantity and surface concentration is important
- Is still used where saturation doping is needed (Polysilicon doping)
- Most processes would use an Implant/Thermal cycle