



공정 6. Diffusion

➤ 관련 과목	
➤ 관련 시험/과제	
➤ 강의 일자	
☰ 상태	정리중
📎 강의자료	Lecture6_Diffusion (Kwon).pdf

Purpose

Diffusion

- Diffusion has been **the primary method of introducing impurities** such as boron, phosphorus, and antimony into silicon. (doping해서 n-type, p-type 만들기)

Purpose

- Impurity control -> **resistivity** (MOSFET에서 drain, source 등)
- Majority carrier type
- Majority carrier concentration
- Diffusion depth

Process

high concentration으로 증착 후 높은 온도를 가해서 Si 안으로 확산되도록 함

- Deposition(증착) of a high concentration of the desired impurity
- At high temperature (900 to 1200 °C), the impurity atoms move from the surface into the silicon crystal

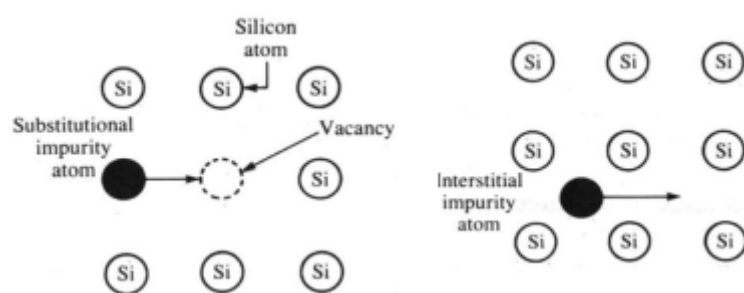
Mechanism

(1) Substitutional or vacancy diffusion

- vacancy : Si 간의 공유결합이 비어있는 공간, 그 자리로 impurity atom이 들어감
- Si lattice 안에는 vacancy가 존재할 수밖에 없으므로 가능
- 정해진 vacancy만큼 diffusion이 일어나므로 정확한 doping농도 계산하기 쉽다

(2) Interstitial diffusion

- Si 사이로 비집고 들어가는 것
- Interstitial diffusion은 substitutional diffusion보다 빠름
- impurity atom이 전류에 영향을 주려면 activation 공정 필요 (vacancy 안에 들어가도록)



Substitutional diffusion	Interstitial diffusion
Need vacancy supply	Diffusion without vacancy
Slow diffusion	Rapid diffusion
Good process control	Need activation*

* Impurity atoms needs to occupy substitutional site in the lattice in order to be act as donors or acceptors

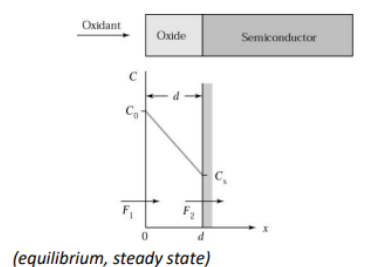
Modeling

유도 과정)

- oxidation은 시간에 따라 두께가 바뀌는 게 핵심이었는데
diffusion은 시간에 따라 concentration이 바뀜

Fick's law of diffusion

- the particle flow per unit area, F (particle flux), is directly proportional to the concentration gradient of the particle:



$$F = -D \frac{\partial C}{\partial x} \quad \text{Fick's 1st law}$$

where D is the diffusion coefficient and C is the particle concentration.

(one-dimensional continuity equation)

$$\begin{aligned} \text{Flux} &= \frac{\text{Num Change of atom}}{\text{Unit A} \times \text{Unit time}} \\ \frac{\partial F}{\partial x} &= \frac{\text{Unit L (x)}}{\text{Unit A} \times \text{Unit time} \times \text{Unit L(x)}} \\ &= \frac{\text{Num Change of atom}}{\text{Unit V} \times \text{Unit time}} \\ &= \frac{\partial C}{\partial t} \end{aligned}$$

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

Fick's diffusion equation (Fick's 2nd law)
: Fick's second law predicts how diffusion causes the concentration to change with time.

Diffusion Coefficient

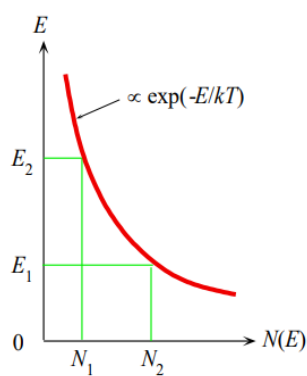
$$D = D_0 \exp\left(\frac{-E_a}{kT}\right)$$

E_a : activation energy

$k = (8.617) \times 10^{-5} \text{ eV/K}$ (볼츠만 상수)

T는 절대온도이므로 K 단위로 꼭 환산!!!

[Note] Boltzman Classical Statistics



Boltzman energy distribution : In statistical mechanics and mathematics, a Boltzmann distribution is a **probability distribution**, probability measure, or frequency distribution of particles in a system over various possible states.

Diffusion Profile: Constant Surface Concentration

erfc distribution



Boundary conditions:

i) $C(0,t) = C_s$, ii) $C(\infty, t) = 0$

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

Diffusion length

Total number of dopant atoms per unit area (dose):

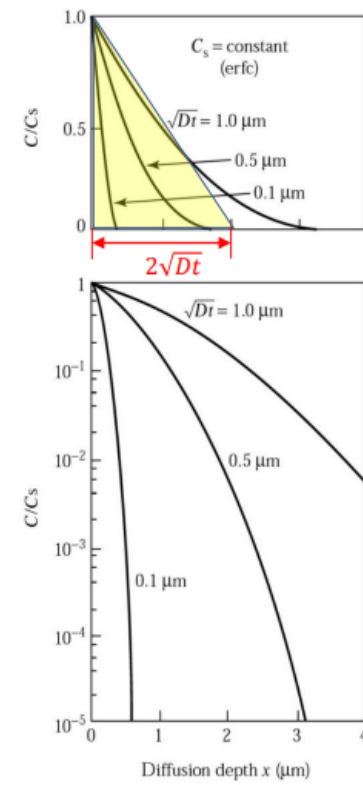
$$Q(t) = \int_0^\infty C(x,t) dx \rightarrow \text{Area under of the diffusion profile}$$

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

Correction constant

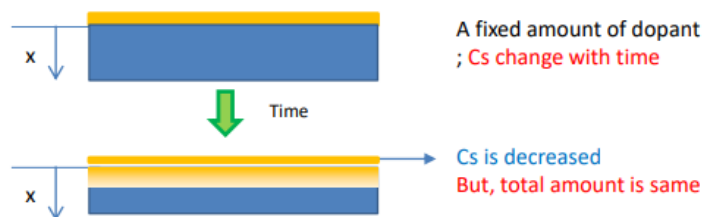
The gradient of diffusion profile (a related quantity):

$$\frac{\partial C}{\partial x} \Big|_{x,t} = \frac{C_s}{\sqrt{\pi Dt}} e^{-x^2/4Dt}$$



Diffusion Profile: Constant Total Dopant

Gaussian distribution



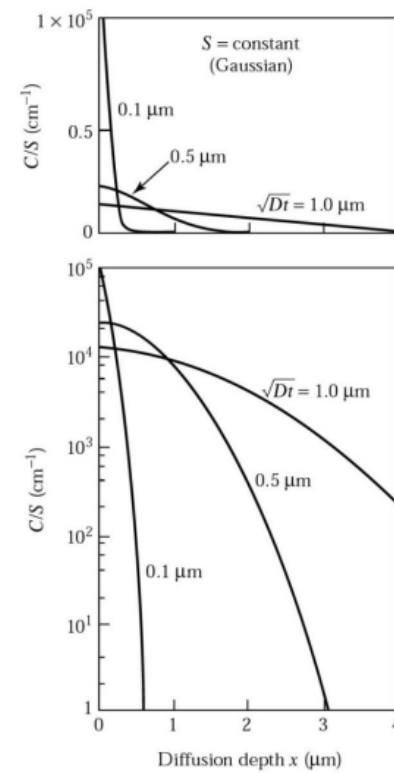
$$\int_0^\infty C(x,t) dx = Q \text{ (constant)}, \quad C(\infty, t) = 0$$

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

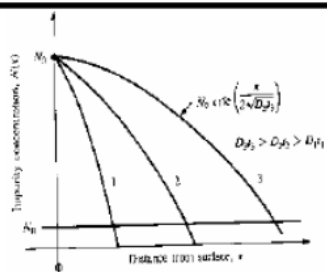
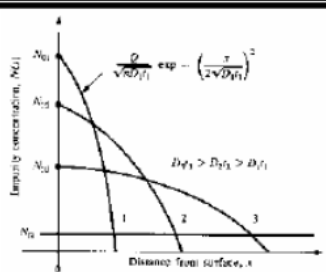
$$C(x,t) = \frac{Q}{\sqrt{\pi Dt}} \exp\left(\frac{-x^2}{4Dt}\right) \quad \text{C.F.) } C(x,t) = C_s \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$C(0,t) = \frac{Q}{\sqrt{\pi Dt}} \quad \text{Surface concentration decrease with time}$$

$$\frac{\partial C}{\partial x} \Big|_{x,t} = -\frac{xQ}{2\sqrt{\pi}(Dt)^{3/2}} = -\frac{x}{2Dt} C(0,t) \quad \text{The gradient of diffusion profile}$$



Summary: Diffusion Profile (중요!)

	Constant-source diffusion	Limited-source diffusion
Solution of equation (a)	$N(x,t) = N_0 \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$	$N(x,t) = \frac{Q_0}{\sqrt{\pi Dt}} \exp\left[-\left(\frac{x}{2\sqrt{Dt}}\right)^2\right]$
Impurity distribution	 <p>complementary error function</p>	 <p>Gaussian distribution</p>
Dose (Q) ≡ Total # of Impurity atoms per unit area [atom/cm ²]	$Q = \int_0^\infty N(x,t) dx = 2N_0 \sqrt{\frac{Dt}{\pi}}$	Q_0

3/29 → 3/31

Two-Step Diffusion

Two-step diffusion (general process)

1. Pre-deposition : Constant surface concentration (D_1t_1) ← short-time
2. Drive-in (Redistribution) : Constant total dopant (D_2t_2) ← long-time

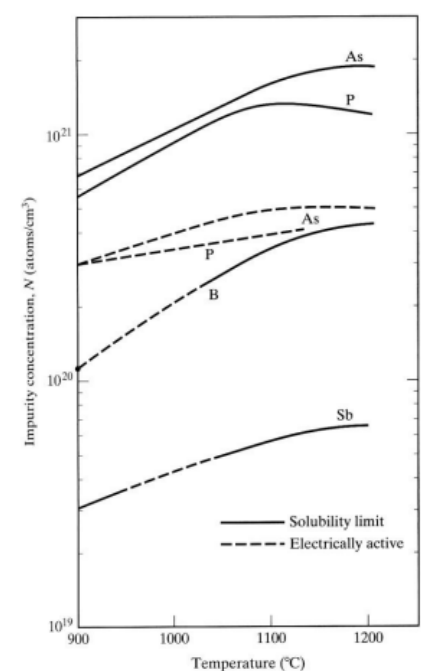
Successive diffusion

- We are interested in the **final impurity distribution** after all processing is complete.
- A wafer typically goes through many time-temperature cycles during predeposition, drive-in, oxide growth, CVD, etc.
- The effect of these steps is determined by calculating the total Dt for all ightemperature cycles affecting diffusion →

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

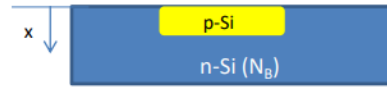
Solid Solubility Limits

- At a given temperature, there is an upper limit to the amount of an impurity which can be absorbed by silicon
- At high concentrations, only a fraction of the impurities actually contribute holes or electrons for conduction. The dotted line shows the “electrically active” portion of the impurity concentration.



Junction Formation

- Vertical diffusion and junction formation



i) Constant surface concentration (Erfc distribution)

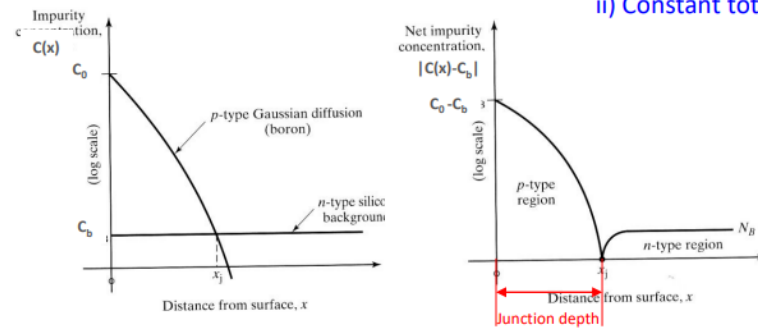
$$C(x, t) = C_s \operatorname{erfc} \left(\frac{x}{2\sqrt{Dt}} \right)$$

$$x_j = 2\sqrt{Dt} \operatorname{erfc}^{-1} \left(\frac{C_b}{C_s} \right)$$

ii) Constant total dopant (Gaussian distribution)

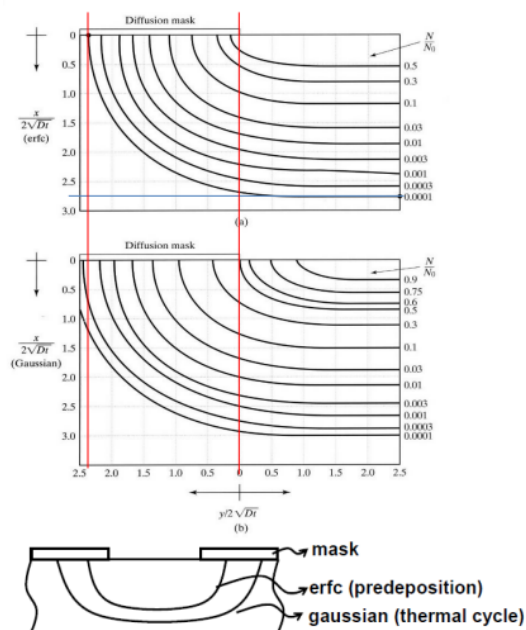
$$C(x, t) = \frac{Q}{\sqrt{\pi Dt}} \exp \left(\frac{-x^2}{4Dt} \right)$$

$$x_j = 2 \sqrt{Dt \cdot \ln \left(\frac{C_0}{C_b} \right)}$$

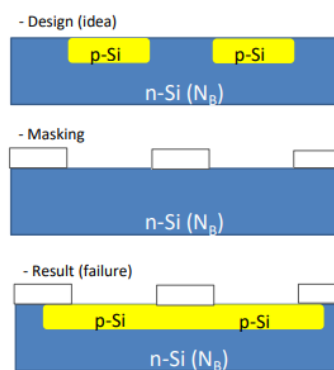


Direction: Lateral

Lateral diffusion



- During diffusion, impurities not only diffuse vertically but also move laterally under the edge of any diffusion layer: important factor for design



Q) Constant surface diffusion, Junction depth is 2um, $C_s=1 \times 10^{20}/\text{cm}^3$, $C_b=1 \times 10^{16}/\text{cm}^3$.
[the lateral diffusion underneath?](#)

$$2.75 : 2.4 = 2 : X$$

$$X = 1.74 \text{ um}$$

Mask for Diffusion : SiO₂

- Diffusion rate to SiO₂ \ll Diffusion rate to Si
 : Sb, As, B, P 에 좋은 diffusion mask
 : P보다 B에 더 효과적임
- SiO₂는 Ga, Al 에는 좋은 diffusion mask가 아님
 → Si₃N₄ 가 더 효과적

Evaluation of Diffusion Layers

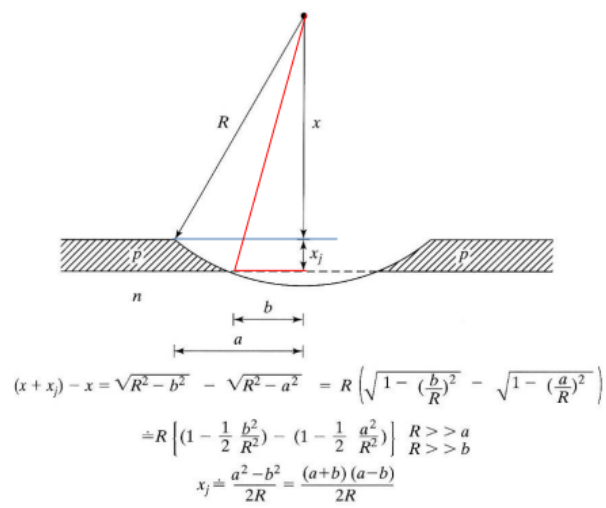
How to know the a, b value ?

- 0.1% HF + 0.5% HNO₃ with high intensity light : pn Junction color change
- Measure the a, b length using microscope

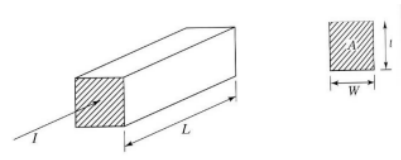
● Junction depth measurement

• Groove and stain method (Old method)

: Cylindrical groove is mechanically ground into the surface of the wafer



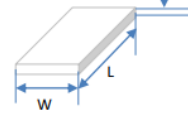
● Sheet resistance



Resistance

$$R = \rho L / A$$

Resistivity (material's own property)



$$R = \rho L / wt = (\rho / t) (L / w)$$

Sheet resistance : R_s

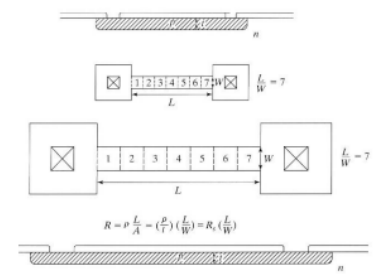
Unit - R: Ω R_s : Ω/\square

(\square , there is no meaning – to avoid confusion)

- Why we use sheet resistance for micro fabrication?

: Easy for design

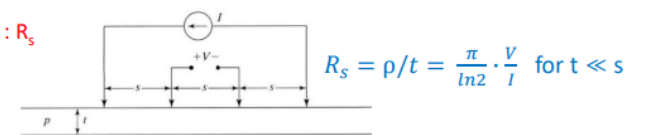
; a circuit designer need specify only the length and width of the resistance to define its value.



● Measuring sheet resistance

Measuring sheet resistance: four point probe

I : out side two probes, V; Inside two probes



Capacitance-voltage technique

Spreading-resistance profiling (SRP)

Secondary Ion Mass Spectroscopy (SIMS)