Ion Implantation and Diffusion
Overview

- Basic semiconductor physics: Most common application of ion implantation is doping silicon
- Ion implantation
- Dopant activation and Diffusion
Energy bands

Basic convention:

Kinetic energy:

\[ K.E. = E - E_C \]

Potential Energy:

\[ P.E. = -qV = E_C - E_{ref} \]

Electric field:

\[ e = -\nabla V, \text{ or in 1D } e = -\frac{dV}{dx} = \frac{1}{q} \frac{dE_C}{dx} \]
Basic semiconductor physics

- Semiconductor bands

Current density

\[ J_n = -q n v_e \]

\[ J = J_n + J_p = q \mu_n n \mathcal{E} + q \mu_p p \mathcal{E} \]

mobility 1400 cm²/V-s
Basic semiconductor physics

- Semiconductor bands

Current density

\[ J_n = -q n v_e \]

\[ J = J_n + J_p = q \mu_n n \mathcal{E} + q \mu_p p \mathcal{E} \]

mobility 1400 cm²/V-s

\[ \varepsilon = \frac{1}{q} \frac{dE_C}{dx} \]

**Figure 5:** Band diagram with an electric field.
Doping and resistivity

The graph shows the relationship between impurity concentration and resistivity. The x-axis represents the impurity concentration (in m/cm^3) on a log scale, ranging from $10^{-4}$ to $10^{21}$. The y-axis represents resistivity (in ohm-cm) on a log scale, ranging from $10^{-3}$ to $10^{0}$. The line demonstrates a decreasing trend in resistivity as the impurity concentration increases.
MOSFET is a four-terminal device. Basic device configuration is illustrated on the figures below.

**Side-view of the device**

- $V_{DS}$
- $V_{GS}$
- $V_{BE}$
- GATE
- n-SOURCE
- GATE OXIDE
- INVERSION LAYER
- DEPLETION LAYER
- p-SUBSTRATE
- BACK CONTACT

**Top-view of the device**

- $V_{DS}$
- $V_{GS}$
- $V_{BE}$
- GATE
- n-SOURCE
- n-DRAIN
- W
- L

**Basic device parameters:**

- Channel length $L$
- Channel width $W$
- Oxide thickness $d_{ox}$
- Junction depth $r_j$
- Substrate doping $N_A$
• The role of the Gate electrode for *n*-channel MOSFET:

\[ V_G = 0 \]

source \hspace{1cm} drain

\[ V_G > V_T \]

source \hspace{1cm} drain

Positive gate voltage does two things:

1. **Reduces the potential energy barrier** seen by the electrons from the source and the drain regions.
2. **Inverts the surface**, and increases the **conductivity** of the channel.
• The role of the **Drain** electrode for *n*-channel MOSFETs:

\[ V_G = 0, \ V_D > 0 \]

source \[\xrightarrow{\text{Large potential barrier allows only few electrons to go from the source to the drain}}\] drain

\[ E_C \]

Smaller potential barrier allows a large number of electrons to go from the source to the drain

\[ V_G > V_T, \ V_D > 0 \]

source \[\xrightarrow{\text{Smaller potential barrier allows a large number of electrons to go from the source to the drain}}\] drain

\[ E_C \]
There are basically four types of MOSFETs:

(a) *n*-channel, enhancement mode device

(b) *n*-channel, depletion mode device
(c) p-channel, enhancement mode device

(b) p-channel, depletion mode device
(A) Terminology and symbols

Bipolar Junction Transistor

PNP - transistor

NPN - transistor

- Both, \( pnp \) and \( npn \) transistors can be thought as two very closely spaced \( pn \)-junctions.
- The base must be small to allow interaction between the two \( pn \)-junctions.
(D) Types of transistors

- Discrete (double-diffused) $p^+np$ transistor

- Integrated-circuit $n^+pn$ transistor
Summary

- We need to control doping in XY and Z, and also in density
- Ion Implantation and diffusion give us the freedom to do this
Ion Implantation

Concentration Profile versus Depth is a single-peak function

Reminder: During implantation, temperature is ambient. However, post-implant annealing step (>900°C) is required to anneal out defects.
Advantages of Ion Implantation

- Precise control of dose and depth profile
- Low-temp. process (can use photoresist as mask)
- Wide selection of masking materials e.g. photoresist, oxide, poly-Si, metal
- Less sensitive to surface cleaning procedures
- Excellent lateral dose uniformity (< 1% variation across 12” wafer)

Application example: self-aligned MOSFET source/drain regions

\[ \text{As}^+ \quad \text{As}^+ \quad \text{As}^+ \]

\[ \text{Poly Si Gate} \]

\[ \text{n}^+ \quad \text{p-Si} \quad \text{n}^+ \]

\[ \text{SiO}_2 \]
Masking

Mask layer thickness can block ion penetration

- photoresist
- $\text{SiO}_2$,
- $\text{Si}_3\text{N}_4$,
- or others

Complete blocking

No blocking

Incomplete Blocking

SUBSTRATE
Ion Implanter

- e.g. AsH₃, As⁺, AsH⁺, H⁺, AsH₂⁺
- Magnetic Mass separation

Ion source → As⁺ → Accelerator Column → Ion beam (stationary)

- Accelerator Voltage: 1-200kV
- Dose: ~10¹¹-10¹⁶/cm²
- Accuracy of dose: <0.5%
- Uniformity <1% for 8” wafer

$3-4M/implanter

~60 wafers/hour

Translational wafer holder motion.

spinning wafer holder
Energetic ions penetrate the surface of the wafer and then undergo a series of collisions with the atoms and electrons in the target.
Monte Carlo Simulation of 50keV Boron implanted into Si

SRIM-2000 (v.09)

- Ion Type = B (11 amu)
- Ion Energy = 50 keV
- Ion Angle = 0 degrees

TARGET LAYERS

Layer 1
- Depth: 5000Å
- Density: 2.321

AtomColors=B/B

Ion Completed = 333 (99999)
Backscattered Ions =
Transmitted Ions =

Range Straggle

Longitudinal = 1775Å 511Å
Lateral Proj = 487Å 595Å
Radial = 753Å 365Å
Vac./Ion = 323.0

ENERGY LOSS (%) IONS RECOILS

Ionization → 68.00 7.08
Vacancies → 0.21 1.08
Phonons → 0.71 22.95
(1) Range and profile shape depends on the ion energy (for a particular ion/substrate combination)

(2) Height (i.e. Concentration) of profile depends on the implantation dose

\[ \text{[Conc]} = \frac{\text{# of atoms}}{\text{cm}^3} \]
\[ \text{[dose]} = \frac{\text{# of atoms}}{\text{cm}^2} \]

\[ \text{dose} \phi = \int_{0}^{\infty} C(x) \, dx \]

\[ C(x) \text{ in } \#/\text{cm}^3 \]

Depth x in cm
Simulation: SRIM

Monte Carlo Simulation of 50keV Boron implanted into Si

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TARGET LAYERS Depth Density
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ENERGY LOSS(%) IONS RECOILS
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X−Y Longitudinal Projection

http://www.srim.org/
Implantation Dose

For singly charged ions (e.g. As⁺)

\[
\Phi = \frac{\left( \text{Ion Beam Current in amps} \right)}{q \left[ \text{Implant area} \right]} \times \left( \text{Implant time} \right)
\]

\[
= \frac{\#}{cm^2}
\]

Over-scanning of beam across wafer is common. In general, Implant area > Wafer area
Practical Implantation Dosimetry

aperture for dose monitoring

Wafer holder wheel

ions\(^+\)

Faraday cup

Secondary electron effect eliminated

+V

+ bias applied to Faraday Cup to collect all secondary electrons. Cup current = Ion current

A

* (Charge collected by integrating cup current) / (cup area) = dose
Ion Implantation Energy Loss Mechanisms

Nuclear stopping

Crystalline Si substrate damaged by collision

Electronic stopping

Electronic excitation creates heat
Energy Loss and Ion Properties

Light ions/at higher energy → more electronic stopping

Heavier ions/at lower energy → more nuclear stopping

**EXAMPLES**

Implanting into Si:

- $\text{H}^+$ → Electronic stopping dominates
- $\text{B}^+$ → Electronic stopping dominates
- $\text{As}^+$ → Nuclear stopping dominates
\[ S_n \equiv \frac{dE}{dx}|_n \]
\[ S_e \equiv \frac{dE}{dx}|_e \]

More crystalline damage at end of range $S_n > S_e$

Less crystalline damage $S_e > S_n$

$E = E_o = \text{incident kinetic energy}$

$x \sim R_p$

Substrate

Surface
Figure 5.8  Nuclear and electronic components of $S(E)$ for several common silicon dopants as a function of energy (after Smith as redrawn by Seidel, “Ion Implantation,” reproduced by permission, McGraw-Hill, 1983).
Gaussian Approximation of One-Dimensional Implant Depth Profile

\[ C(x) = C_p \cdot e^{-\frac{(x-R_p)^2}{2(\Delta R_p)^2}} \]

\[ R_p = \text{projected range} \]

\[ \Delta R_p = \text{longitudinal straggle} \]

Note: For lateral positions far from masking boundaries, \( C(x) \) is independent of lateral position \( y \)
Projected Range and Straggle

$R_p$ and $\Delta R_p$ values are given in tables or charts
e.g. see pp. 113 of Jaeger

Note: this means 0.02 $\mu m$. 
Dose-Concentration Relationship

Using Gaussian Approximation:

\[ \text{Dose} = \phi = \int_{0}^{\infty} C(x) \, dx \]

\[ \approx \int_{-\infty}^{+\infty} C(x) \, dx \]

\[ = C_p \cdot \left[ \sqrt{2\pi \cdot \Delta R_p} \right] \]

\[ \therefore C_p = \frac{\phi}{\sqrt{2\pi \cdot \Delta R_p}} \approx \frac{0.4\phi}{\Delta R_p} \]
\[ C( x = x_j ) = N_B = \text{Bulk Conc.} \Rightarrow \text{Solution for } x_j \]

If Gaussian approx for \( C(x) \) is used, from

\[ C_p \exp \left[ - \left( x_j - R_p \right)^2 / 2(\Delta R_p)^2 \right] = C_B \]

we can solve for \( x_j \).
Sheet Resistance $R_s$ of Implanted Layers

Example:

n-type dopants implanted into p-type substrate

$$R_s = \frac{1}{\int_0^{x_j} q \cdot \mu(x) [C(x) - C_B] \, dx}$$

- Needs numerical integration to get $R_s$ value

$C(x)$ log scale

Total doping conc

$\mu_p$, $\mu_n$
Approximate Value for $R_s$

If $C(x) \gg C_B$ for most depth $x$ of interest and use approximation: $\mu(x) \sim \text{constant}$

$$R_s \approx \frac{1}{q \mu \phi}$$

This expression assumes ALL implanted dopants are 100% electrically activated

use the $\mu$ for the highest doping region which carries most of the current

$[R_s] = \text{ohm/square}$

or ohm/square
Example Calculations

200 keV Phosphorus is implanted into a p-Si ($C_B = 10^{16}/\text{cm}^3$) with a dose of $10^{13}/\text{cm}^2$.

From graphs or tables, $R_p = 0.254 \ \mu\text{m}$, $\Delta R_p = 0.0775 \mu\text{m}$

(a) Find peak concentration

$$C_p = \frac{(0.4 \times 10^{13})}{(0.0775 \times 10^{-4})} = 5.2 \times 10^{17}/\text{cm}^3$$

(b) Find junction depths

(b) $C_p \exp\left[-\frac{(x_j-0.254)^2}{2 \Delta R_p^2}\right] = C_B$ with $x_j$ in $\mu\text{m}$

$$\therefore \ (x_j - 0.254)^2 = 2 \times (0.0775)^2 \ln\left[5.2 \times 10^{17}/10^{16}\right]$$

or $x_j = 0.254 \pm 0.22 \ \mu\text{m}$; $x_{j1} = 0.032 \ \mu\text{m}$ and $x_{j2} = 0.474 \ \mu\text{m}$

(c) Find sheet resistance

From the mobility curve for electrons (using peak conc as impurity conc), $\mu_n = 350 \ \text{cm}^2/\text{V-sec}$

$$R_s = \frac{1}{q\mu_n \phi} = \frac{1}{1.6 \times 10^{-19} \times 350 \times 10^{13}} \approx 1780 \ \Omega/\text{square}.$$
After implantation, we need an annealing step. A typical \( \sim 900^\circ \text{C}, 30 \text{min} \) will:

1. Restore Si crystallinity.

2. Put dopants into Si substitutional sites for electrical activation.
Implantation Damage

Schematic of the disorder produced along the individual paths of light and heavy ions and the formation of an amorphous region.
Solid Epitaxial “Growth” through the Implant Damaged Region

Implanted amorphous silicon

$\dot{t}_r$ = regrown layer thickness

Anneal time
Solid Epitaxial "Growth" through the Implant Damaged Region – cont.

(1) Regrow the amorphous region at $T = 500-600^\circ C$ into single crystal. The substrate acts as a seed. If higher temperatures are used then nucleation within the amorphous layer takes place making it polycrystalline and crystal structure can never be regained. This temperature range also recovers most of the electrical activity.

(2) A further anneal at $T > 900^\circ C$ restores the crystal structure and electrical activity 100%.
Dopant Activation Versus Annealing Temp

$N_{Hall}/N_b$

Region I Region II Region III

$150 \text{ keV Boron}$
$T_s = 25^\circ C$
$t_a = 30 \text{ min}$

Interstitial-Vacancy recombination

Secondary defects Annealed out

Agglomeration of secondary defects

Figure 5.15 Fraction of implanted boron activated in silicon for several isochronal anneals (after Seidel and MacRae, reprinted by permission, Elsevier Science).
Transverse (or Lateral) Straggle ($\Delta R_t$ or $\Delta R_\perp$)

Lateral standard deviation of boron, phosphorus, arsenic and antimony in silicon
Lateral Scattering Causes Feature Enlargement

Lower concentration

Higher concentration

Implanted specie has lateral distribution, larger than mask opening

$C(y)$ at $x = R_p$
Transmission Factor of Implantation Mask

What fraction of dose gets into Si substrate?
Transmitted Fraction

\[ T = \int_{0}^{\infty} C(x) \, dx - \int_{0}^{d} C(x) \, dx \]

\[ = \frac{1}{2} \text{erfc} \left( \frac{d - R_p}{\sqrt{2} \Delta R_p} \right) \]

\[ \text{erfc}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-y^2} \, dy \]

Rule of thumb: Good masking thickness

\[ d = R_p + 4.3 \Delta R_p \]

\[ \frac{C(x = d)}{C(x = R_p)} \sim 10^{-4} \]

\( R_p, \Delta R_p \) are values of for ions into the masking material
Diffusion

- Motion of impurities inside the crystal
- Sometimes intentional
- Sometimes unintentional, as a byproduct of a thermal process
Dopant Diffusion

(1) Predeposition

- dopant gas
  - dose control
  - $\text{SiO}_2$
  - Doped Si region

(2) Drive-in

- profile control (junction depth; concentration)
  - Turn off dopant gas or seal surface with oxide

Note: Predeposition by diffusion can also be replaced by a shallow implantation step.
Dopant Diffusion Sources

(a) Gas Source: AsH$_3$, PH$_3$, B$_2$H$_6$

(b) Solid Source

(c) Spin-on-glass SiO$_2$+dopant oxide
Figure 3.20  A typical bubbler arrangement for doping a silicon wafer using a POCI source. The gas flow is set using mass flow controllers (MFC).
Si Native Point Defects

For reference only

1) Thermal-equilibrium values of Si neutral interstitials and vacancies at diffusion temperatures
<< doping concentration of interest
\((10^{15} - 10^{20}/\text{cm}^3)\)

\[ C_f^* \equiv 1 \times 10^{27} \exp\left(\frac{-3.8 \text{ eV}}{kT}\right) \]

\[ C_v^* \equiv 9 \times 10^{23} \exp\left(\frac{-2.6 \text{ eV}}{kT}\right) \]

At \(1000^\circ\text{C}\),
\( C_{f0}^* \sim 10^{12} \text{ /cm}^3 \)
\( C_{v0}^* \sim 10^{13} \text{ /cm}^3 \)

2) Diffusivity of Si interstitials and Si vacancies >> diffusivity of dopants

\[ d_f = 1.58 \times 10^{-1} \exp\left(\frac{-1.37}{kT}\right) \text{ cm}^2 \text{ sec}^{-1} \]

\[ d_v = 1.18 \times 10^{-4} \exp\left(\frac{-0.1}{kT}\right) \text{ cm}^2 \text{ sec}^{-1} \]
Diffusion Mechanisms in Si

(A) No Si Native Point Defect Required

Example: Cu, Fe, Li, H

(a) Interstitial Diffusion

![Diagram showing interstitial diffusion in silicon with an example involving Cu, Fe, Li, and H.](image)
Diffusion Mechanisms in Si

(B) Si Native Point Defects Required (Si vacancy and Si interstitials)

Example: Dopants in Si (e.g. B, P, As, Sb)

(a) Substitutional Diffusion

(b) Interstitialcy Diffusion

Figure 3.5 In interstitialcy diffusion an interstitial silicon atom displaces a substitutional impurity, driving it to an interstitial site where it diffuses some distance before it returns to a substitutional site.
(B) Si Native Point Defects Required (Si vacancy and Si interstitials) continued

(c) Kick-Out Diffusion
(d) Frank Turnbull Diffusion

Figure 3.6 The kick-out (left) and Frank–Turnbull mechanisms (right).
Diffusivity Comparison:
Dopants, Si interstitial, and interstitial diffusers

Figure 4-8  Diffusivities of various species in silicon. Au₆ refers to gold in substitutional form (on a lattice site); Au₇ to gold in an interstitial site. The silicon interstitial (I) diffusivity is also shown and will be discussed later. The gray area representing the I diffusivity indicates the uncertainty in this parameter. (After [4.10, 4.11].)
Mathematics of Diffusion

Fick’s First Law:

\[ J(x, t) = -D \cdot \frac{\partial C(x, t)}{\partial x} \]

\( D \): diffusion constant

\([ D ] = \text{cm}^2 \text{/sec}\)
Concentration independence of D

*If* D is independent of C (i.e., D is independent of x).

\[
\frac{\partial C(x, t)}{\partial t} = D \frac{\partial^2 C(x, t)}{\partial x^2}
\]

Concentration Independent Diffusion Equation

State of the art devices use fairly high concentrations, causing variable diffusivity and other significant side-effects (transient-enhanced diffusion, for example.)
Solid Solubility of Common Impurities in Si

$C_0 \text{ (cm}^{-3}\text{)}$

Figure 2.4  Solid solubility of common silicon impurities (all rights reserved, reprinted with permission, © 1960 AT & T).
A. Predeposition Diffusion Profile

• Boundary Conditions:
  
  \[ C(x = 0, t) = C_0 = \text{solid solubility of the dopant} \]
  
  \[ C(x = \infty, t) = 0 \]
  
  Justification:
  Si wafers are \(~500\text{um}\) thick, doping depths of interest are typically \(<\text{several um}\)

• Initial Condition:
  
  \[ C(x, t = 0) = 0 \]
  
  At time \(=0\), there is no diffused dopant in substrate
Diffusion under constant surface concentration

\[ C(x, t) = C_0 \cdot \left[ 1 - \frac{2}{\sqrt{\pi}} \int_0^{\frac{x}{2\sqrt{Dt}}} e^{-y^2} dy \right] \]

\[ = C_0 \cdot \text{erfc} \left( \frac{x}{2\sqrt{Dt}} \right) \]

\(2\sqrt{Dt} = \text{Characteristic distance for diffusion.}\)

\(C_0 = \text{Surface Concentration (solid solubility limit)}\)
**B. Drive-in Profile**

- **Boundary Conditions**: 
  \[ C(x = \infty, t) = 0 \]
  \[ \frac{\partial C}{\partial x} \bigg|_{x=0} = 0 \]
  Physical meaning of \( \frac{\partial C}{\partial t} = 0 \): No diffusion flux in/out of the Si surface. Therefore, dopant dose is conserved.

- **Initial Conditions**: 
  \[ C(x, t = 0) = Co \cdot \text{erfc} \left[ \frac{x}{2\sqrt{(Dt)}} \right] \]
  Predep’s (Dt)
Solution of Drive-in Profile with Shallow Predeposition Approximation:

\[ Q = \frac{C_0 \cdot 2\sqrt{(Dt)}_{\text{predep}}}{\sqrt{\pi}} \]

Approximate predep profile as a delta function at \( x=0 \)

\[ C(x,t=0) \]

\[ C(x,t) = \frac{Q}{\sqrt{\pi(Dt)}_{\text{drive-in}}} e^{-\frac{x^2}{4(Dt)_{\text{drive-in}}}} \]
Summary of Predeposition + Drive-in

\[ D_1 = \text{Diffusivity at Predeposition temperature} \]
\[ t_1 = \text{Predeposition time} \]
\[ D_2 = \text{Diffusivity at Drive-in temperature} \]
\[ t_2 = \text{Drive-in time} \]

\[ C(x) = \left( \frac{2C_0}{\pi} \right) \left( \frac{D_1 t_1}{D_2 t_2} \right)^{1/2} e^{-x^2/4D_2 t_2} \]

*This will be the overall diffusion profile after a “shallow” predeposition diffusion step, followed by a drive-in diffusion step.*
Diffusion of Gaussian Implantation Profile

\[ C(x, t) = \frac{\phi}{\sqrt{2\pi (\Delta R_p^2 + 2Dt)^{1/2}}} \cdot e^{-\frac{(x - R_p)^2}{2 (\Delta R_p^2 + 2Dt)}} \]

Note: \( \phi \) is the implantation dose
Diffusion of Gaussian Implantation Profile (arbitrary $R_p$)

The exact solutions with $\frac{\partial C}{\partial x} = 0$ at $x = 0$ (i.e. no dopant loss through surface) can be constructed by adding another full gaussian placed at $-R_p$ [Method of Images].

$$C(x, t) = \frac{\phi}{\sqrt{2\pi (\Delta R_p^2 + 2Dt)^{1/2}}} \cdot \left[ e^{-\frac{(x - R_p)^2}{2 (\Delta R_p^2 + 2Dt)}} + e^{-\frac{(x + R_p)^2}{2 (\Delta R_p^2 + 2Dt)}} \right]$$

We can see that in the limit $(Dt)^{1/2} \gg R_p$ and $\Delta R_p$.

$$C(x, t) \rightarrow \frac{\phi e^{-x^2/4Dt}}{(\pi Dt)^{1/2}} \quad \text{(the half-gaussian drive-in solution)}$$
Thermal Budget

$$(Dt)_{\text{effective}} = \sum_{\text{step } i} (Dt)_i$$

Example

$D_{t_{\text{total}}} \text{ of:}$

Well drive-in
and
S/D annealing

For a complete process flow, only those steps with high $Dt$ values are important