Semiconductor Fundamentals – (II)

2.3 Energy Bands

2.4 The doping of semiconductors

Material developed by Prof. C. Z. Zhao

HW-1: solution

- Si atomic density:

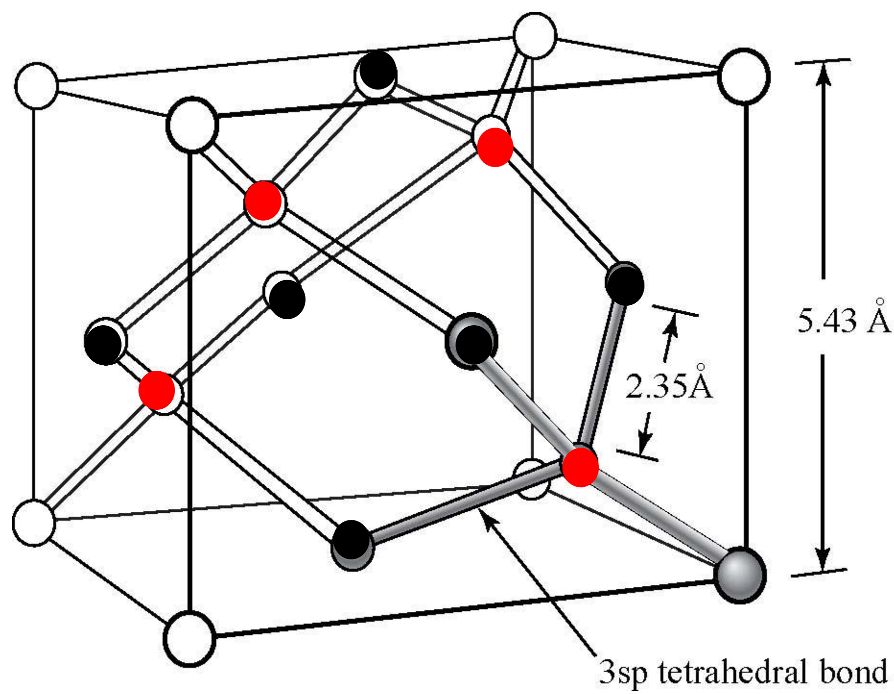
$$\frac{\#\,Atoms}{Volume} = \frac{8\times(1/8)+6\times(1/2)+4}{a_0^3} = \frac{8}{(5.43\times10^{-8}\,cm)^3} = 5\times10^{22}\,cm^{-3}$$

- **Number of atoms in a unit cell:**
  - **4 atoms completely inside cell**
  - **Each of the 8 atoms on corners are shared among cells → count as 1 atom inside cell**
  - **Each of the 6 atoms on the faces are shared among 2 cells → count as 3 atoms inside cell**

Total number inside the cell = 4 + 1 + 3 = 8

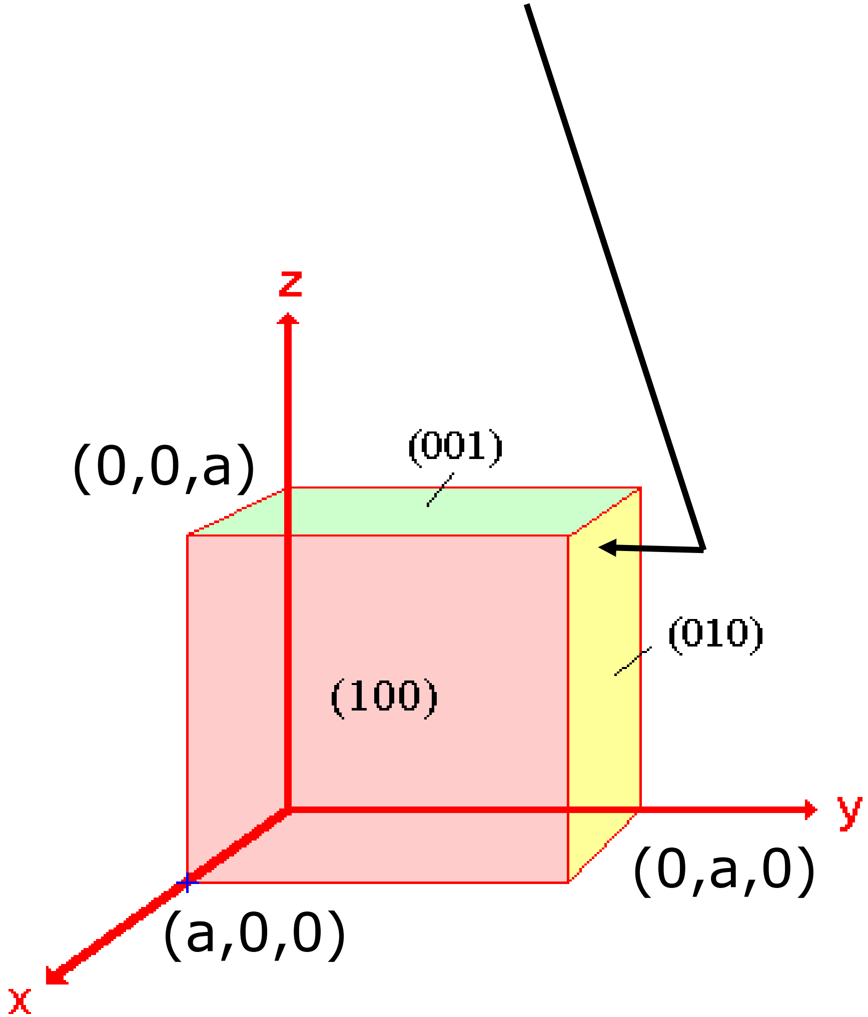
- **Cell volume:**

  $(.543\ \text{nm})^3 = 1.6 \times 10^{-22}\ \text{cm}^3$



HW-2: solution

Why the Miller indices of this plane is (010)?



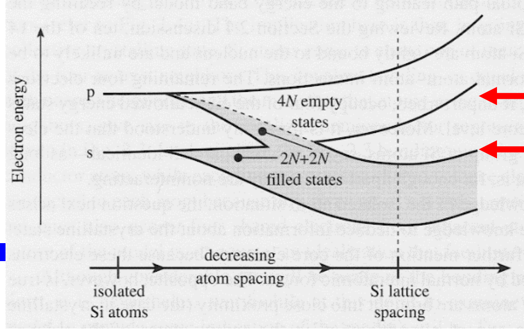
***x*-intercept of plane**
***y*-intercept of plane**
***z*-intercept of plane**

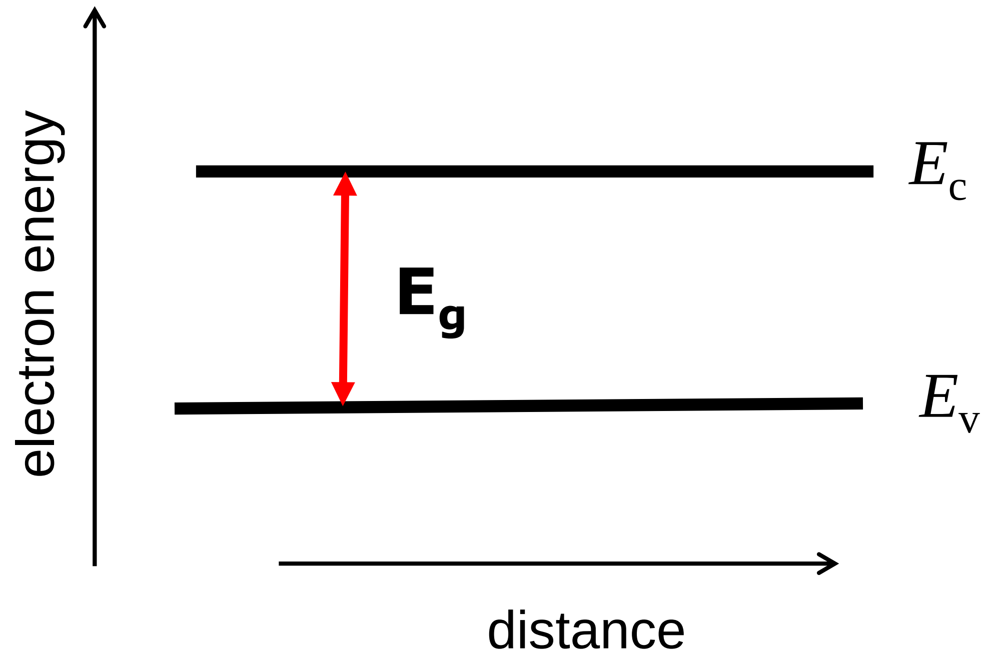
***h*: inverse *x*-intercept of plane**
***k*: inverse *y*-intercept of plane**
***l*: inverse *z*-intercept of plane**

***h*, *k* and *l* are reduced to 3 integers having the same ratio.**

(010)

Last lecture:





Simplified version of energy band model, indicating

- bottom edge of the conduction band (***E*$_c$**)
- top edge of the valence band (***E*$_v$**)

➢ E_c and E_v are separated by the **band gap energy *E*$_g$**

2.3 Energy Bands

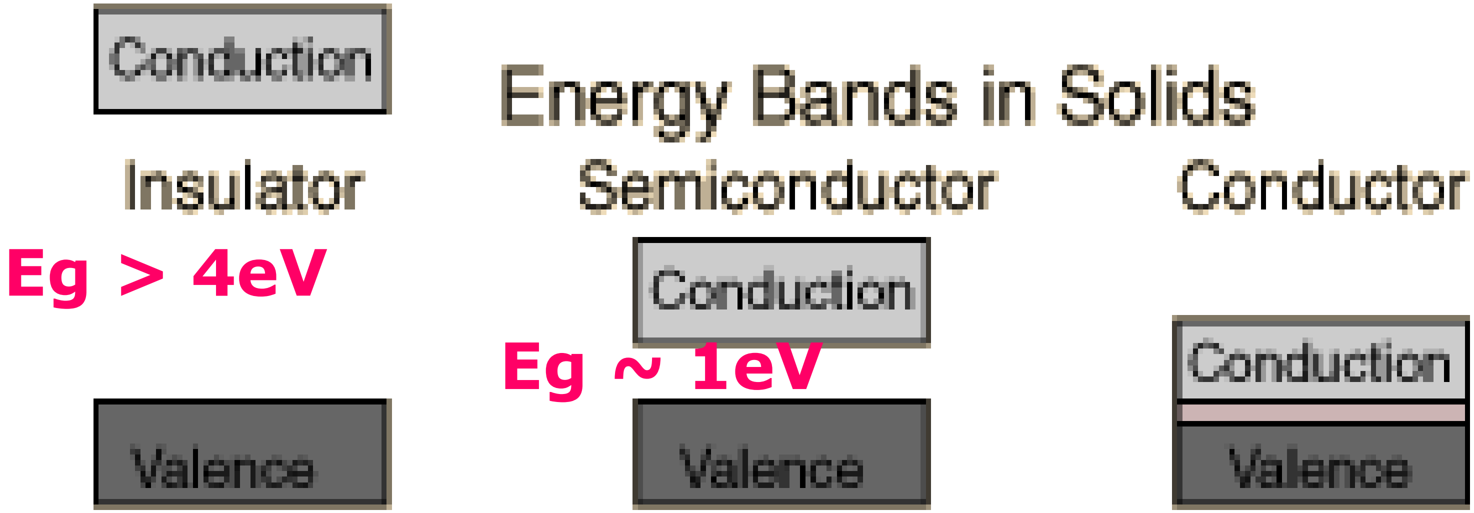
- Band theory
  - What's a Semiconductor
  - Fermi Level
  - Band model of *e* & *h*
  - Bond model of *e* & *h*
- Generation and recombination
- Intrinsic semiconductor

What is a Semiconductor?

- Low resistivity => "conductor" e.g. Al, Cu
- High resistivity => "insulator" e.g. SiO_2
- Intermediate resistivity => "semiconductor"
  - conductivity lies between that of conductors and insulators

Band Theory of Solids

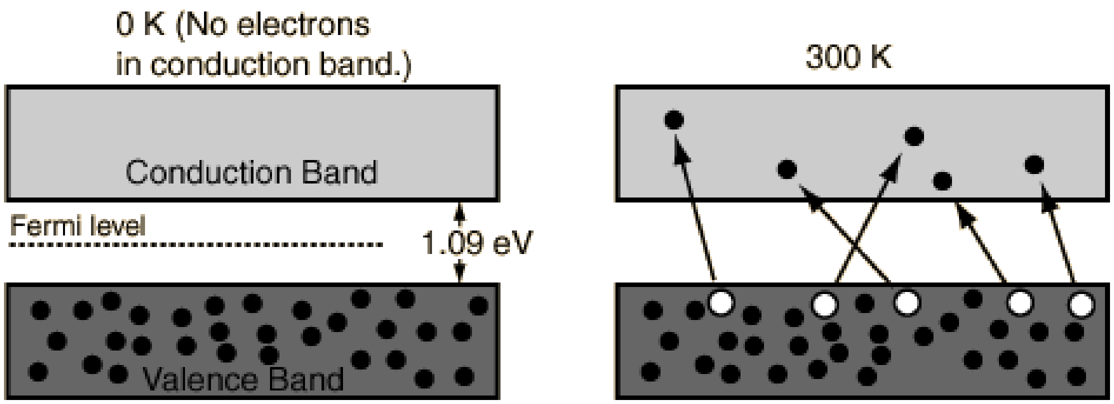
- A useful way to visualize the difference between conductors, insulators and semiconductors is to plot the available energies for electrons in the materials. In conductors the valence band overlaps the conduction band, and in semiconductors/insulator there is a small/big gap between the valence and conduction bands.
- An important parameter in the band theory is the Fermi level, the top of the available electron energy levels at low temperatures.



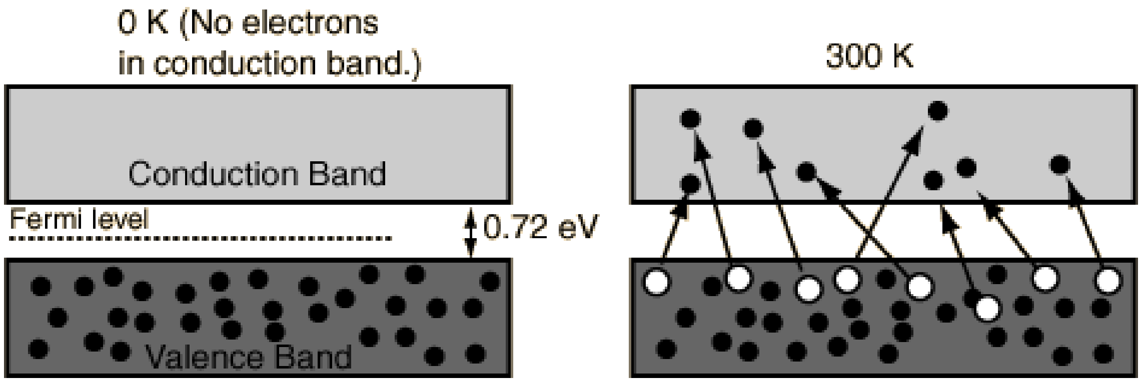
Energy Bands of Silicon & Germanium

- At finite temperatures, the number of electrons which reach the conduction band and contribute to current can be modeled by the Fermi function.

1) Fermi level?
2) "holes"?



Si



Ge

Fermi function and Fermi level

概率 Probability **that** a **state** at energy level, *E*, is occupied by one electron is,

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

Students → Electrons

Seat row → energy level, *E*.

Seat → state

Example: Students in a theatre class room.

Every row has different potential, *E*. For example, for row 7, its potential is *E7*.

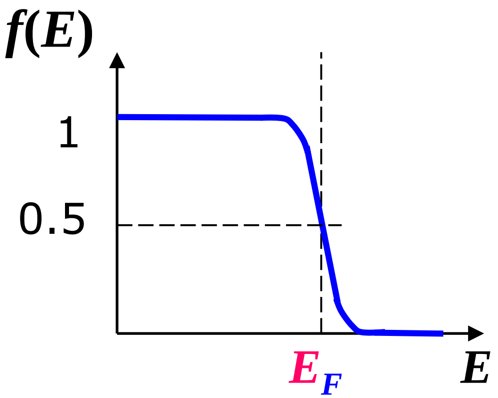
The probability for one **student** to occupy a **seat** on **row** 7 can be calculated by *f*(*E7*).

E_F is a energy level at which *f*(*E*) is 50%.

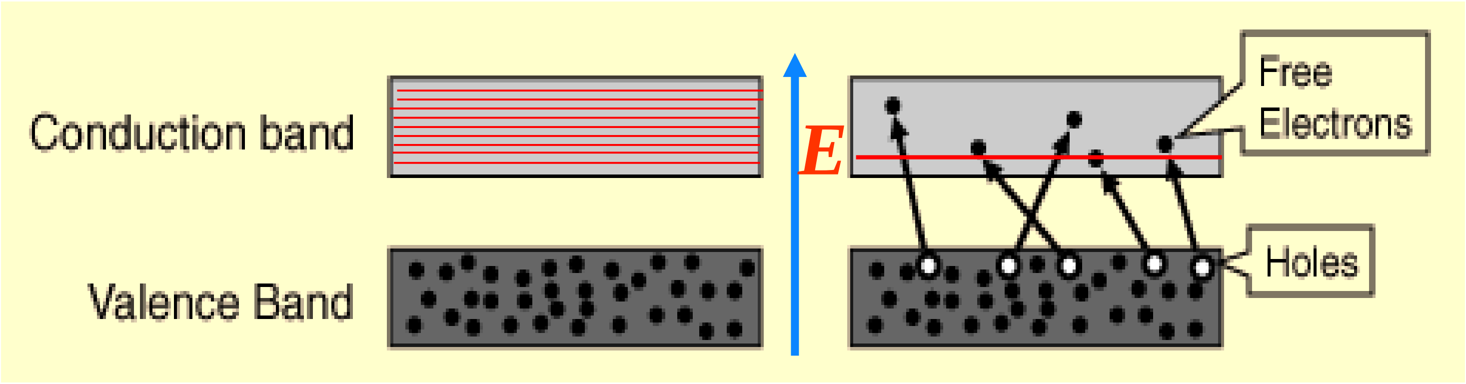
Fermi function and Fermi level

- Probability that a **state** at energy level, E, is occupied by one electron is,

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$



- $f(E)$: Fermi-Dirac function
- An increase in E will reduce $f(E)$
- **E_F --- Fermi-level**
  - **When $E = E_F$, $f(E=E_F) = 0.5$.**

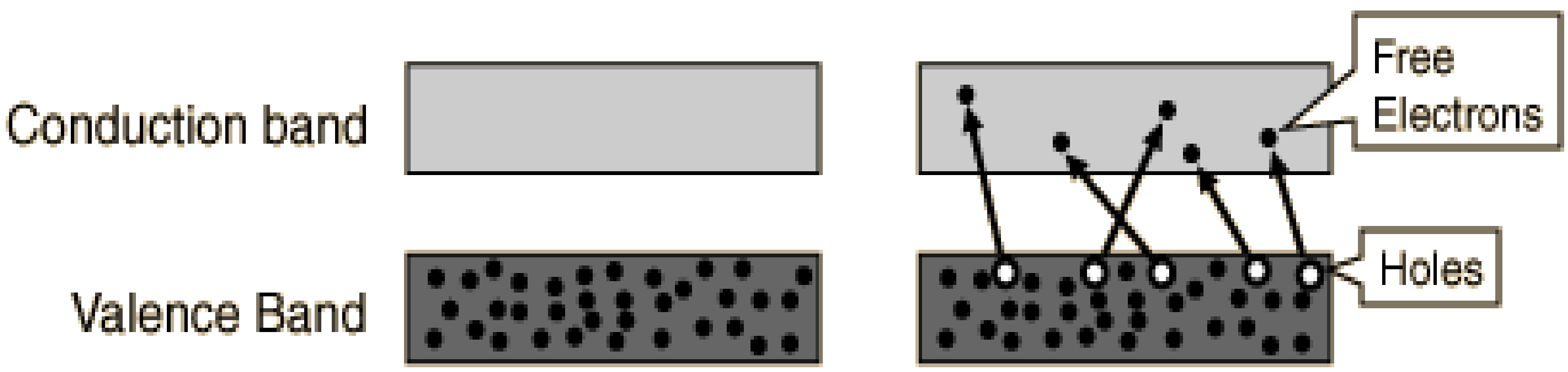


textbook

P.66

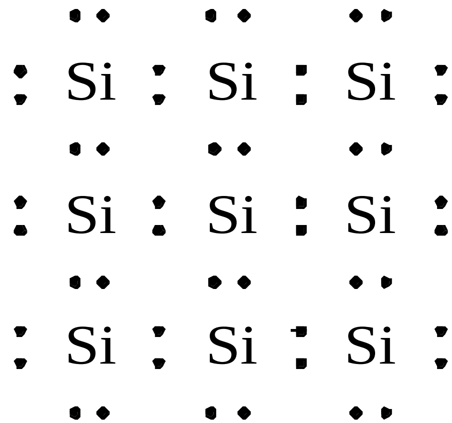
Band Model of Electrons and Holes

- In an pure semiconductor like silicon at temperatures above absolute zero, there will be some electrons which are excited across the band gap into the conduction band and which can produce current.
- When the electron in pure silicon crosses the gap, it leaves behind an **electron vacancy** or "**hole**" in the regular silicon lattice.
- Under the influence of an external voltage, both the electron and the hole can move across the material.

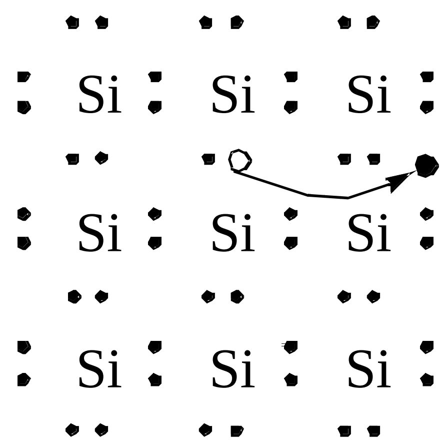


Bond Model of Electrons and Holes

2-D representation:
Covalent Bonds



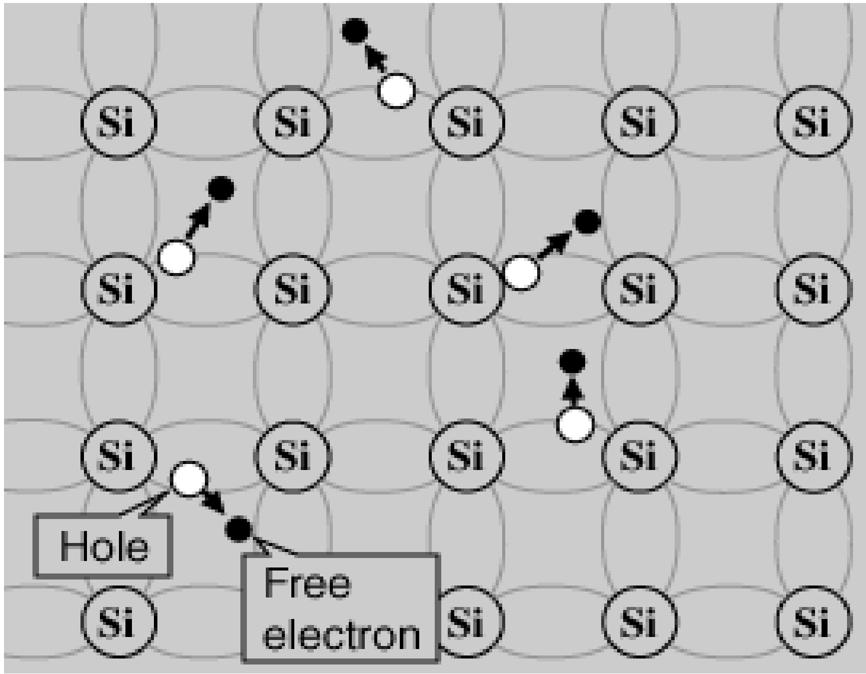
When an electron **breaks loose** and becomes a ***conduction electron***, a ***hole*** is also created.



Bond Model of Electrons and Holes

- When an electron **breaks loose** and becomes a ***conduction electron***, a ***hole*** is also created.
- A hole (along with its associated positive charge) is mobile!
- Hole density **=** electron density in a pure Si.

2-D representation:



Pure Si

2.3 Energy Bands

- Band theory
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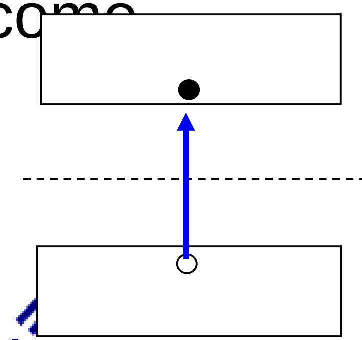
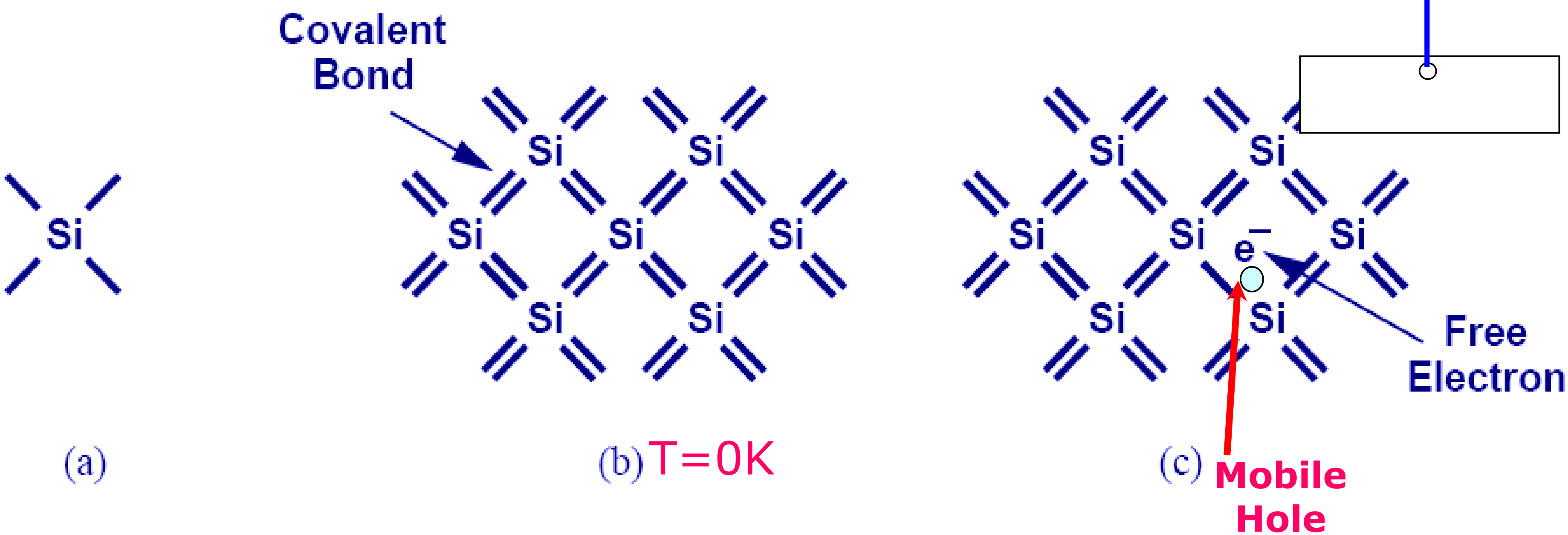
  - Bond model of *e* & *h*
- **Generation and recombination**
- Intrinsic semiconductor

Thermal Generation

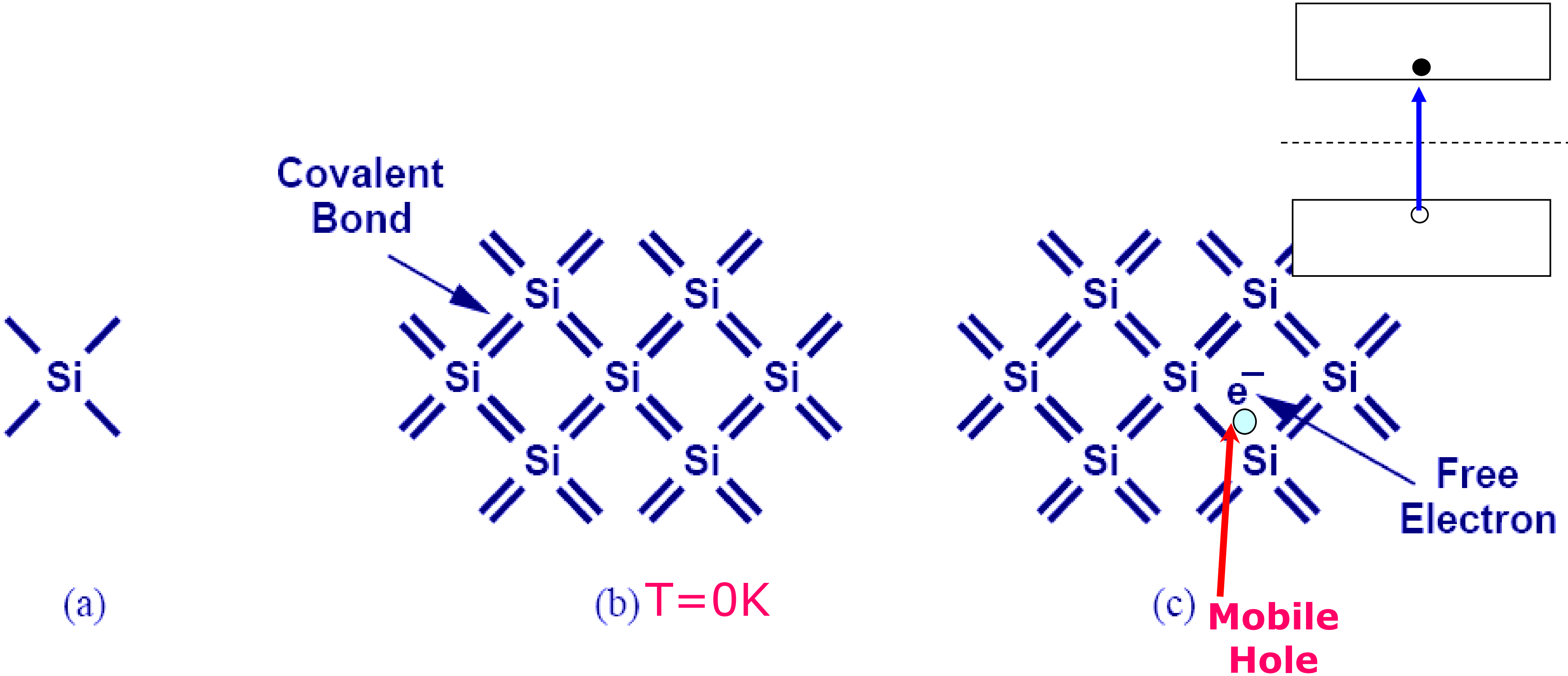
- Inverse process: recombination
- Si has four valence electrons. Therefore, it can form covalent bonds with four of its nearest neighbors.
- When temperature goes up, electrons can become free to move about the Si lattice.





Generation

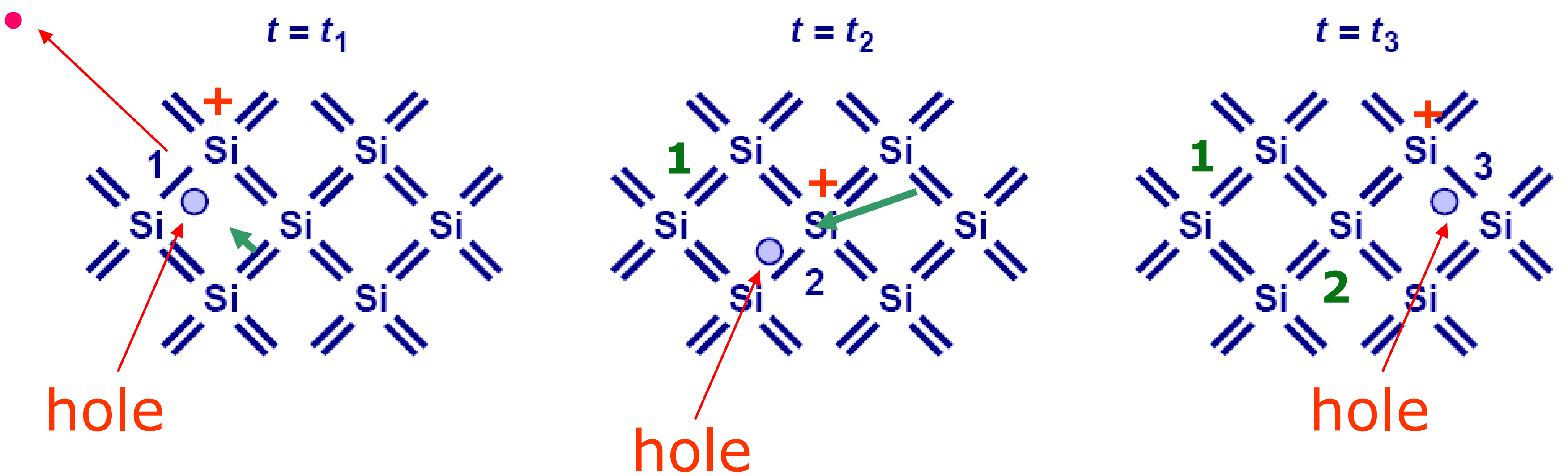
- **Generation: A process to create electron-hole pairs.**



Electron-Hole Pair Generation

- When a conduction electron is thermally generated, a “hole” is also generated.
- A hole is associated with a positive charge, and is free to move about the Si lattice as well.

A hole is **mobile!**



Generation

- We have seen that conduction (mobile) electrons and holes can be created in pure (intrinsic) silicon by ***thermal generation***.
  - Thermal generation rate increases exponentially with temperature ***T***
- Another type of generation process which can occur is ***optical generation***
  - The energy absorbed from a **photon** frees an electron from covalent bond
    - In Si, the minimum energy required is 1.1eV, which corresponds to ~1 μm wavelength (infrared region). 1 eV = energy gained by an electron falling through 1 V potential = $q_eV = 1.6 \times 10^{-19}$ C x 1 V = 1.6×10^{-19} J.
- Note that conduction electrons and holes are continuously generated, if $T > 0$

Light interactions with Semiconductors

Absorption of light in a semiconductor:

- For energies of light greater than the bandgap (***hv*** > E_g), light is absorbed
- For energies less than the bandgap ($hv<E_g$), light is out
- Silicon is transparent to IR (can see through it with an IR camera)
- Diamond is a wide bandgap semiconductor (transparent to visible light)

Solar cell

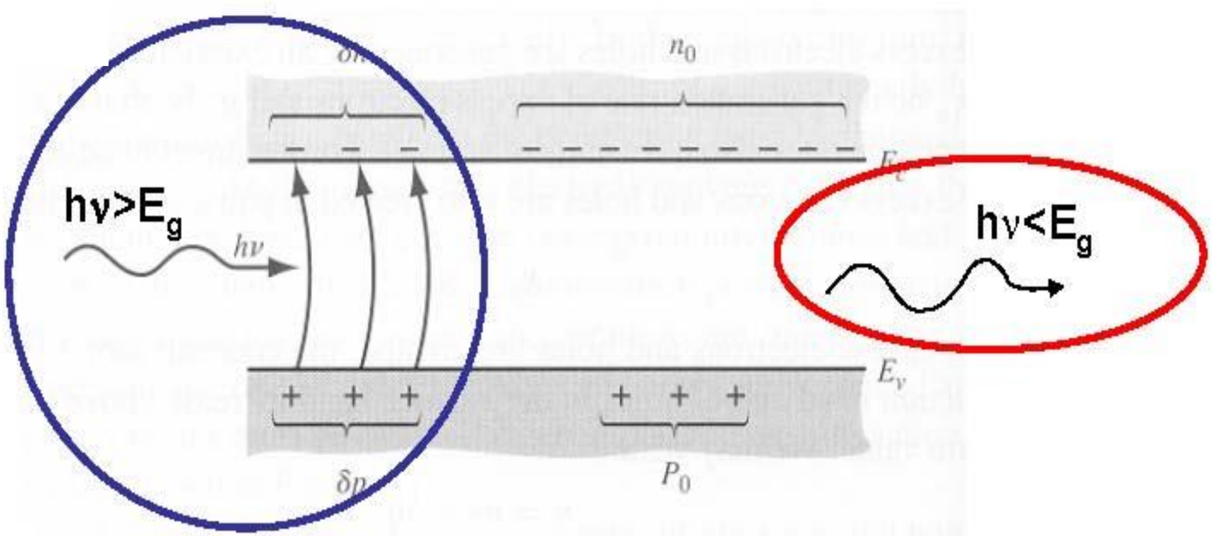


Figure 6.2 | Creation of excess electron and hole densities by photons.

Recombination

- When a conduction electron and hole meet, each one is eliminated, a process called “recombination”. The energy lost by the conduction electron (when it “falls” back into the covalent bond) can be released in two ways:

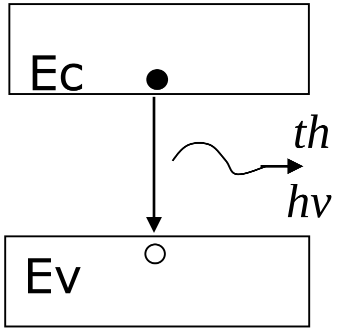
1. to the semiconductor lattice (vibrations)

   “thermal recombination” → semiconductor is heated

2. to photon emission

   “optical recombination” → light is emitted

   - It is the basis for light-emitting diodes and laser diodes.



LED

2.3 Energy Bands

- Band theory
  - What's a Semiconductor
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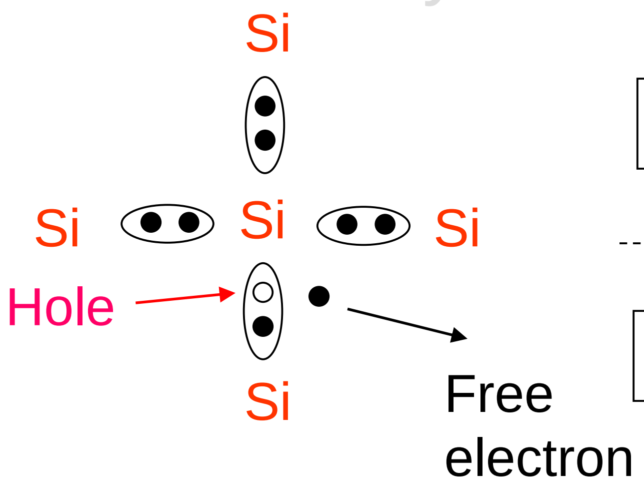
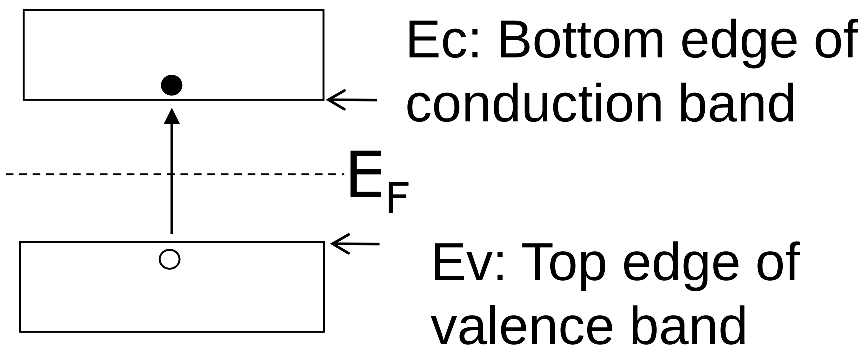
- **Intrinsic semiconductor**

Intrinsic semiconductors

- **Intrinsic**: **<u>pure semiconductor</u>**
- A hole is created simultaneously with a free electron
  - ***n***(free electron density) = ***p***(hole density)
- E_F is in the middle of the bandgap
- Its resistivity is too high for most of devices





Carrier Concentrations in Intrinsic Si

- The "band-gap energy" E_g is the amount of energy needed to remove an electron from a covalent bond.
- The concentration of conduction electrons in intrinsic silicon, n_i, depends exponentially on E_g and the absolute temperature (T):

E_g=1.12eV

$$n_i = 5.2\times10^{15} T^{3/2} \exp\frac{-E_g}{2kT} \quad \text{electrons/cm}^3$$

Boltzmann constant
8.62E-5 eV/K

$$n_i \cong 1\times10^{10} \text{ electrons/cm}^3 \text{ at 300K}$$

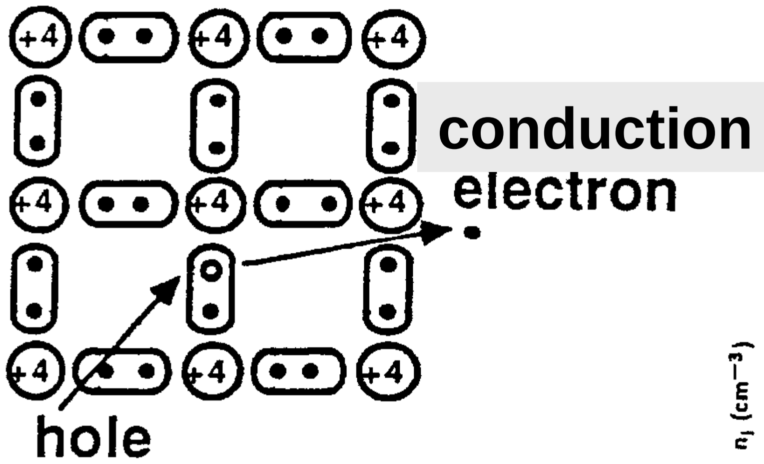
RT

$$n_i \cong 1\times10^{15} \text{ electrons/cm}^3 \text{ at 600K}$$

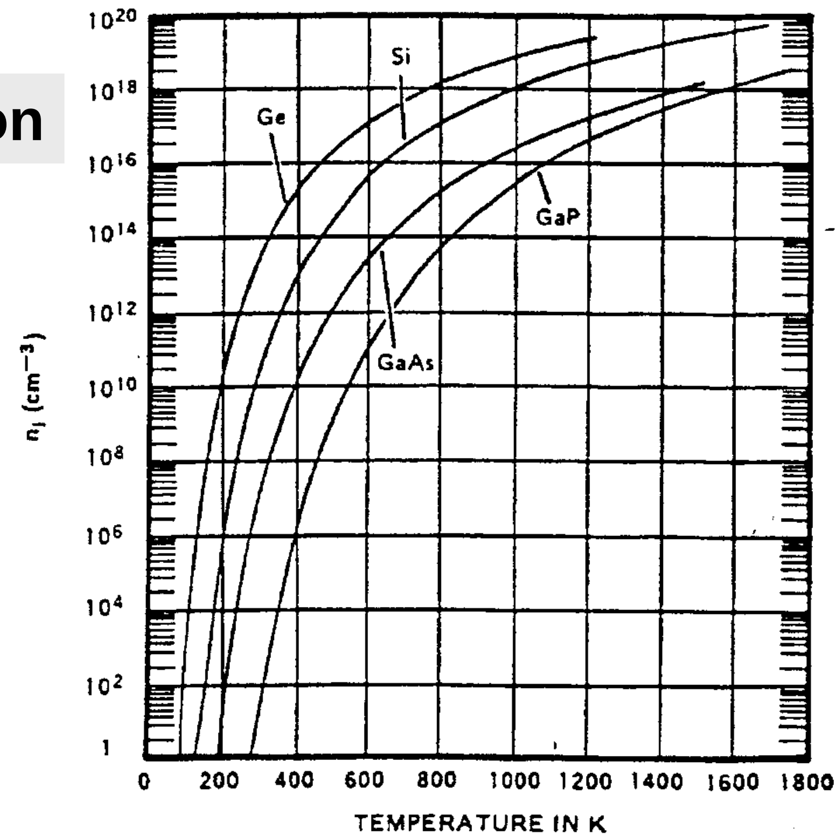
Pure Si

Thermal generation rate increases exponentially with temperature *T*

$$n_i = 5.2\times10^{15} T^{3/2} \exp\frac{-E_g}{2kT} \ \text{electrons/cm}^3$$



Covalent (shared e$^-$) bonds exists between Si atoms in a crystal. Since the e$^-$ are loosely bound, some will be free at any T, creating hole electron pairs.



Si:

$$n_i = 3.9\times10^{16} T^{3/2} e^{-\frac{0.605\text{eV}}{kT}} /\text{cm}^3$$

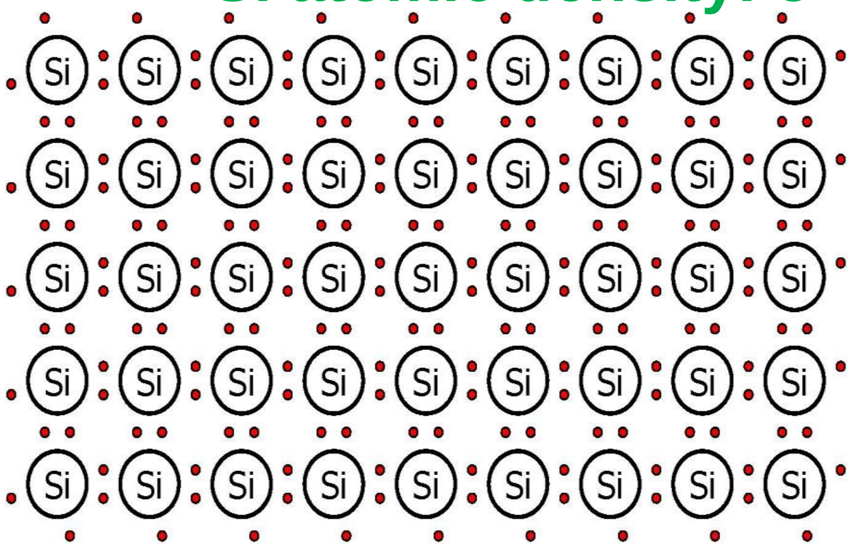
p.75

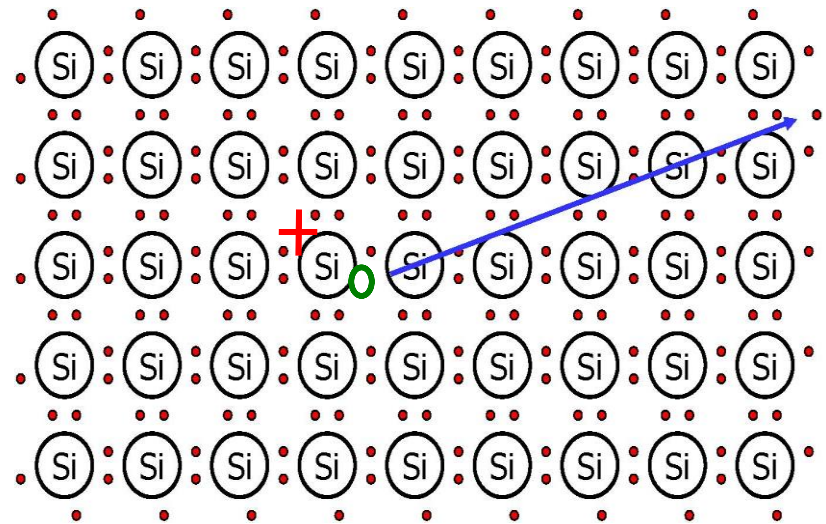
$n_i \cong$ 1.5$\times10^{10}$ cm^{-3} at room temperature

Intrinsic Semiconductor

Silicon has four valence electrons

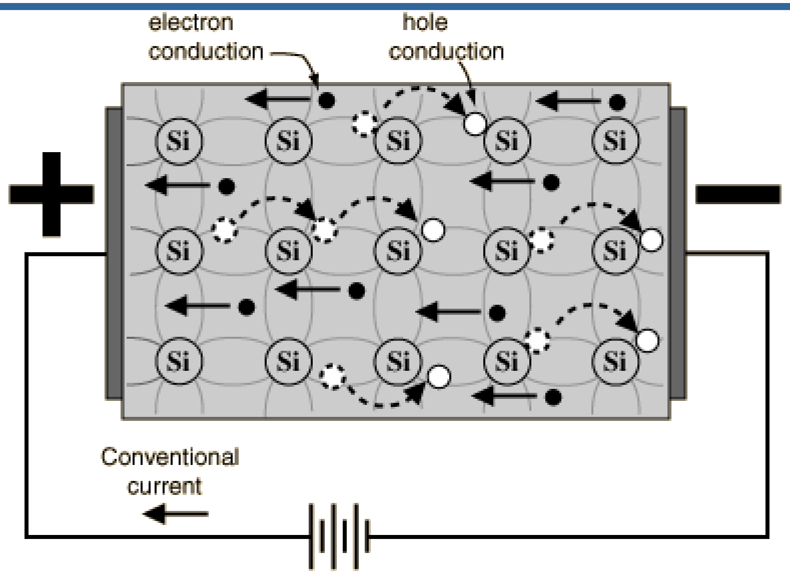
- It covalently bonds with 4 adjacent atoms in the crystal lattice
- Increasing Temperature Causes Creation of Free Carriers. 10^{10}cm^{-3} free carriers at 23^{o}C (out of 2x10^{23}cm^{-3}): Intrinsic Conductivity.
- **Si atomic density: 5 ×10^{22} cm^{-3}**





Semiconductor Current

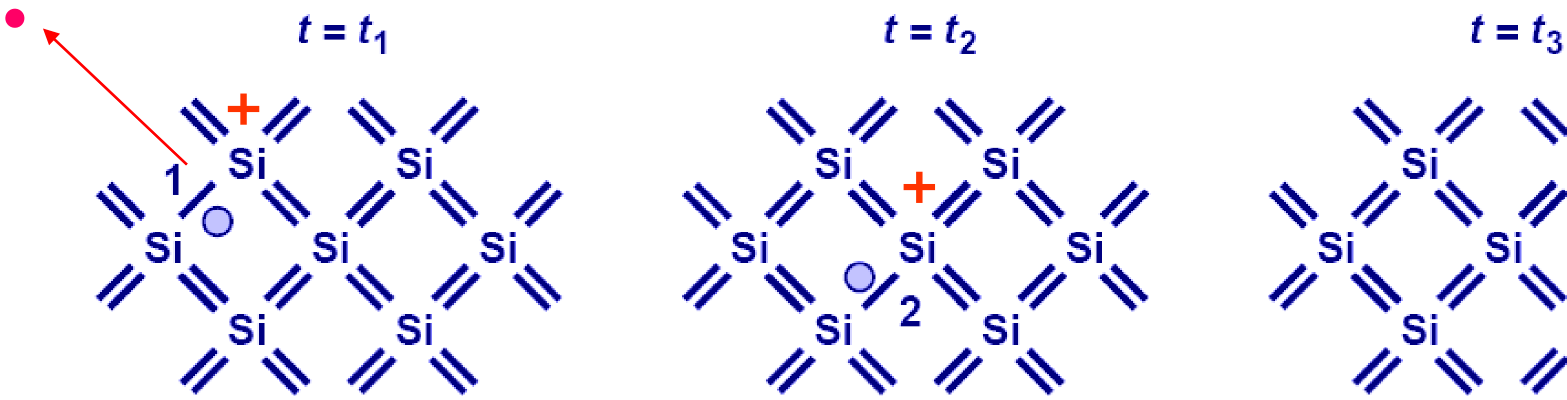
- Both electrons and holes contribute to current flow in an intrinsic semiconductor.



Electron-Hole Pair Generation

PL

- When a conduction electron is thermally generated, a “hole” is also generated.
- A hole is associated with a positive charge, and is free to move about the Si lattice as well.



Summary of Section 2.3

- In a pure Si crystal, conduction electrons and holes are formed in pairs.
  - Holes can be considered as positively charged mobile particles which exist inside a semiconductor.
  - Both holes and electrons can conduct current.
- Splitting of allowed atomic energy levels occurs in a crystal
  - Separation between energy levels is small, so we can consider them as bands of continuous energy levels
    - Highest nearly-filled band is the valence band
    - Lowest nearly-empty band is the conduction band
- The band gap energy is the energy required to free an electron from a covalent bond.
  - E_g for Si at 300K = 1.12eV

2.4 The doping of semiconductors

掺杂

- **Doping elements**
- Doping: N type
- Doping: P type
- Counter doping

补偿掺杂

The Doping

- The addition of a **small** percentage of foreign atoms in the regular crystal lattice of silicon or germanium produces dramatic changes in their electrical properties, producing **n-type** and **p-type** semiconductors.
- Definition of Terms:

n = number of electrons/cm^3

p = number of holes/cm^3

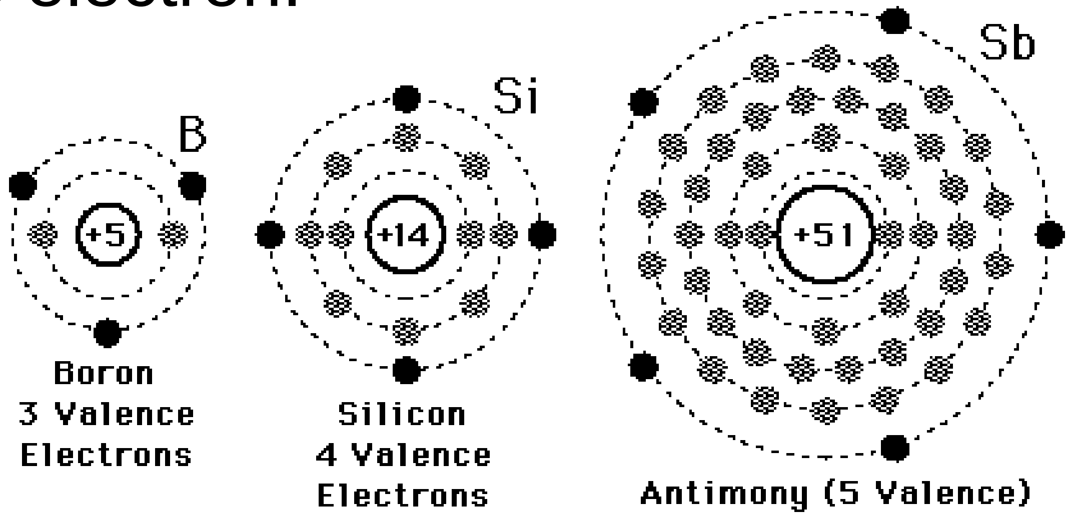
n_i = intrinsic carrier concentration

In a pure semiconductor,

$$n = p = n_i$$

Valence Electrons

- The electrons in the outermost shell of an atom are called valence electrons; they dictate the nature of the chemical reactions of the atom and largely determine the electrical nature of solid matter. The electrical properties of matter are pictured in the band theory of solids in terms of how much energy it takes to free a valence electron.

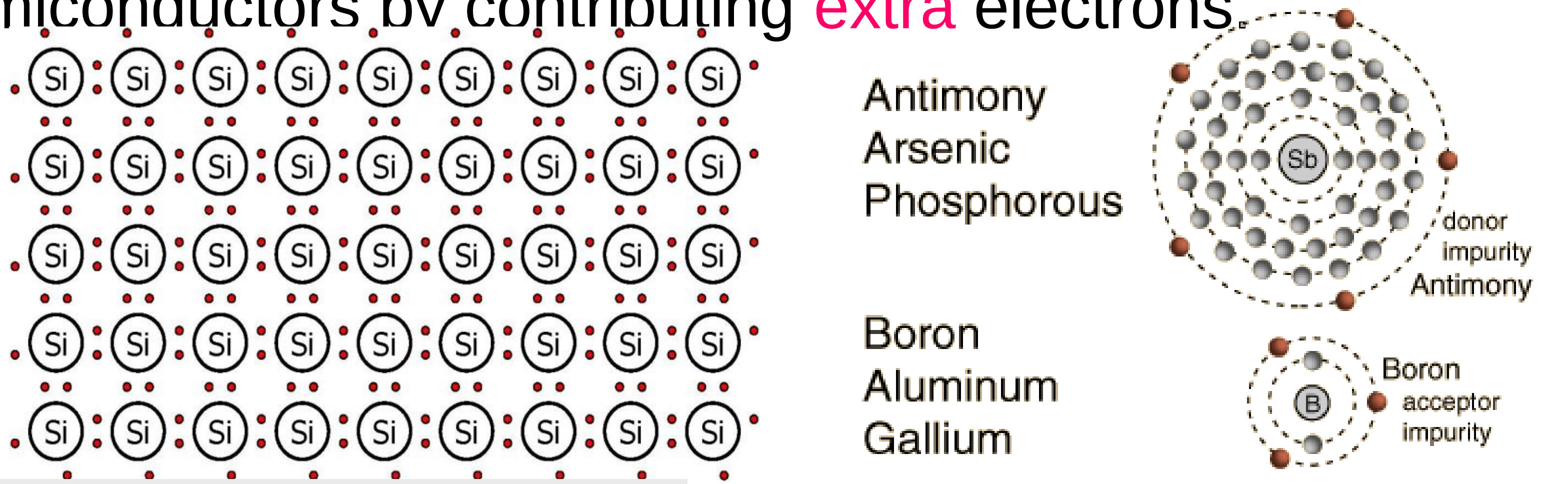


The Doping of Semiconductors

五价的杂质（施主杂质）

Pentavalent impurities (donor impurities = donors)

Impurity atom with 5 valence electrons produce **n-type** semiconductors by contributing extra electrons.



三价的杂质（受主杂质）

Trivalent impurities (acceptor impurities = acceptors)

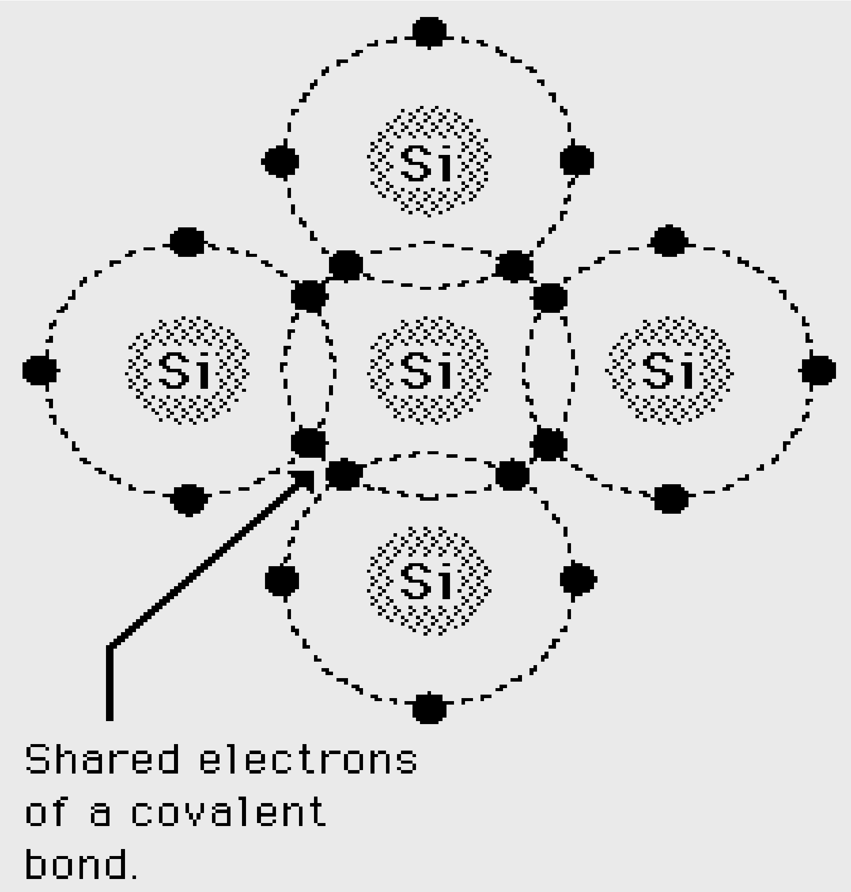
Impurity atoms with 3 valence electrons produce **p-type** semiconductors by producing a "hole" or electron deficiency.

2.4 The doping of semiconductors

- Doping elements
- **Doping: N type**
- **Doping: P type**
- Counter doping

Doping (N type)

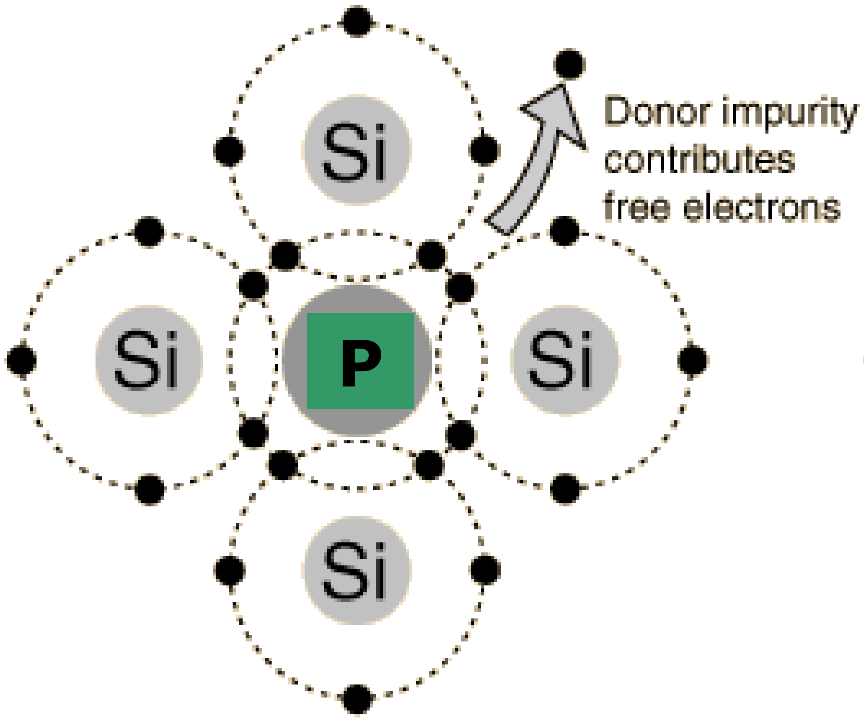
Column V elements are donors, e.g. P, As, Sb



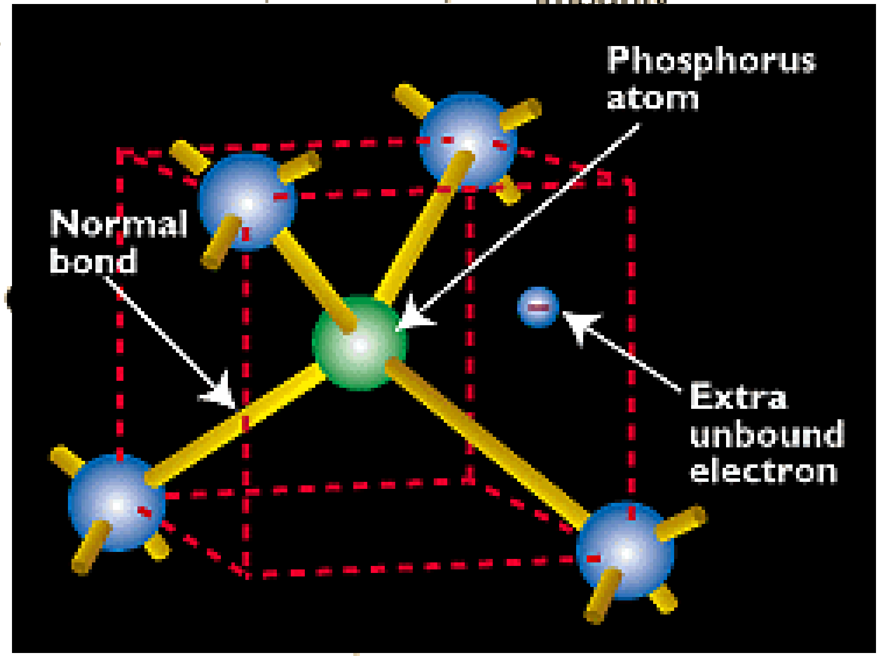
Doping (N type)

Column V elements are donors, e.g. P, As, Sb

By <u>substituting</u> a Si atom with a special impurity atom (Column V element), a conduction electron is created.

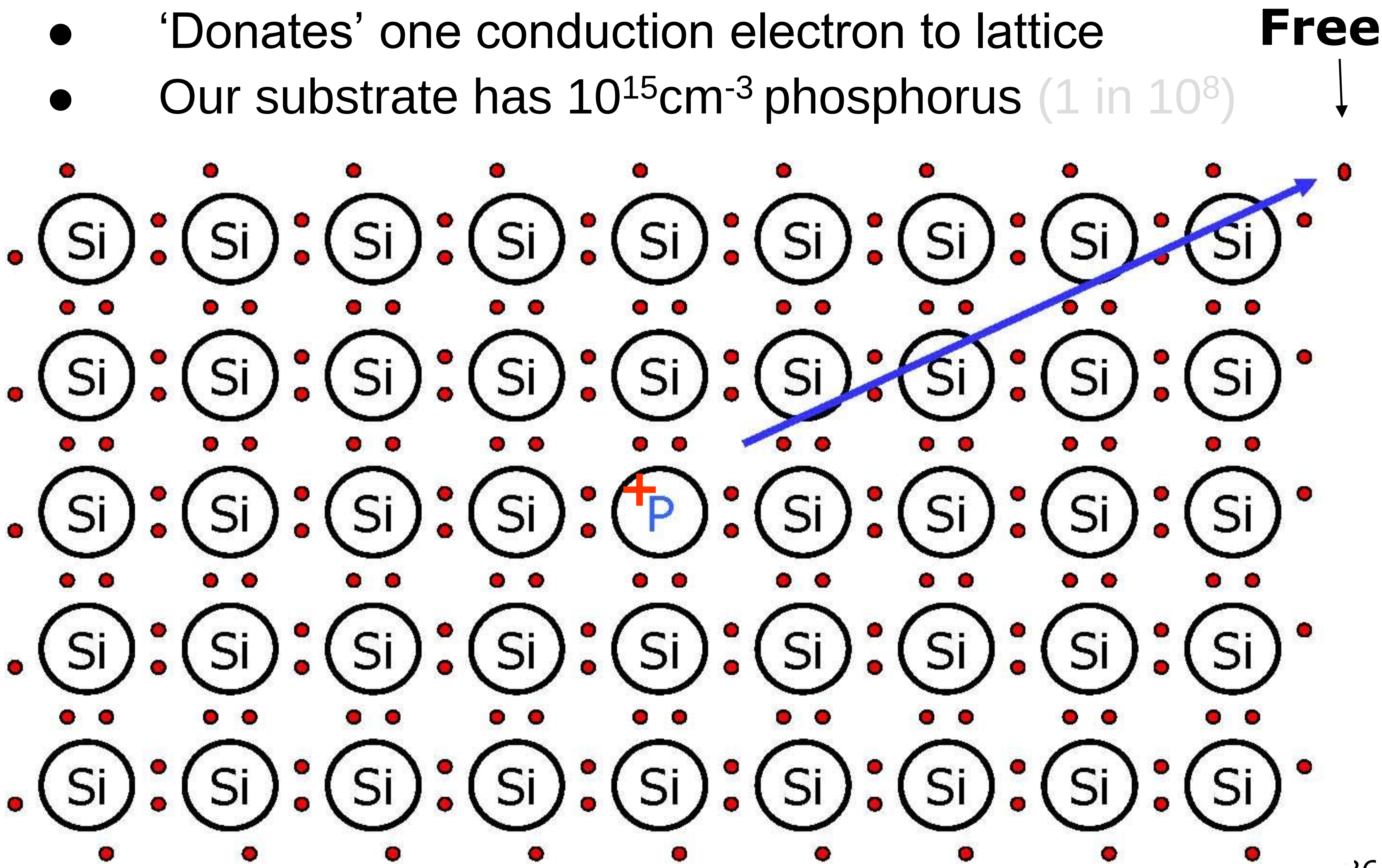


<u>Donors</u>: P, As, Sb



Phosphorus has 5 valence electrons

- ‘Donates’ one conduction electron to lattice
- Our substrate has $10^{15}cm^{-3}$ phosphorus (1 in 10^8)



Doping (N type)

- If Si is doped with phosphorus (P), each P atom can contribute a conduction electron, so that the Si lattice has more electrons than holes, *i.e.* it becomes "**N type**":

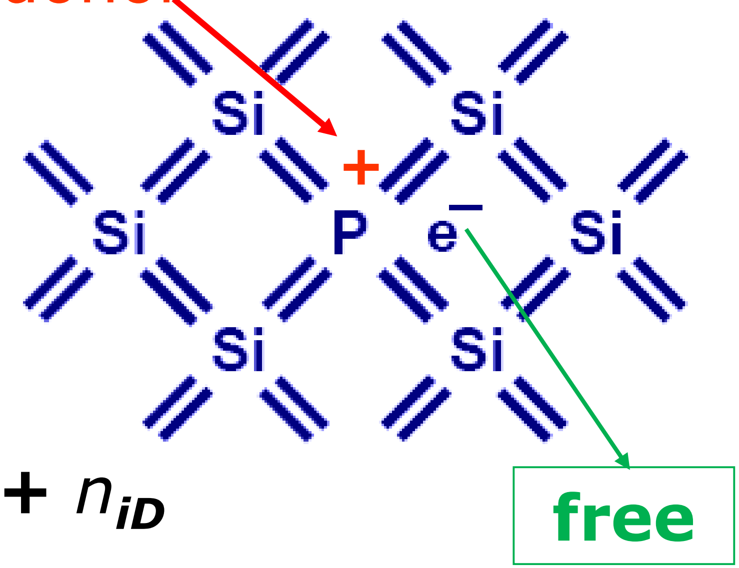
<u>Notation</u>:

N_D = Concentration of donors

n = electron concentration

N_D^+ = Concentration of ionized donors

Immobile ion: N_D^+
Ionized donor



n_{iD} **?**

$$n = N_D^+ + n_{iD}$$

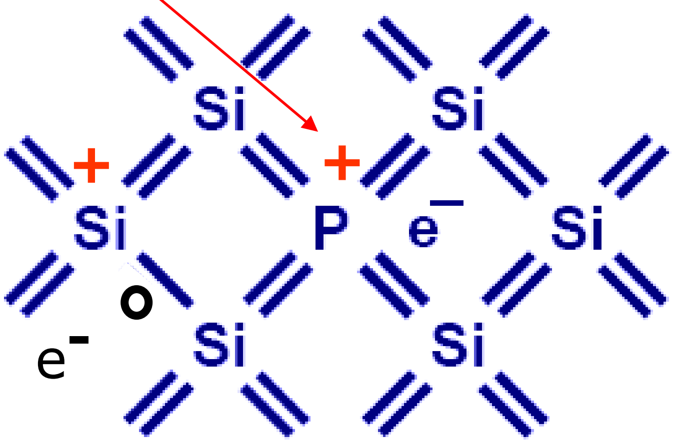
Ionization energy < 50meV:

At RT, $N_D \approx N_D^+ >> n_{iD}$

Doping (N type)

- If Si is doped with phosphorus (P), each P atom can contribute a conduction electron, so that the Si lattice has more electrons than holes, *i.e.* it becomes "**N type**":

Immobile ion: N_D^+
Ionized donor



n_{iD} ?

$$n = N_D^+ + n_{iD}$$

$$p = n_{iD} = ?$$

Notation:

N_D = Concentration of donors

n = electron concentration

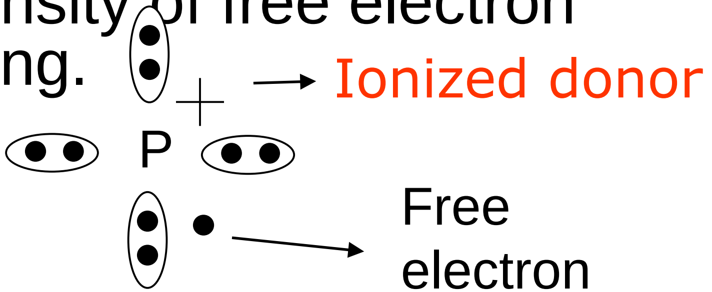
N_D^+ = Concentration of ionized donors

Ionization energy < 50meV:

At RT, $N_D \approx N_D^+ >> n_{iD}$

N-type

- Doped by impurities of 5 valence electrons (donors)
- At room temperature, one donor will create one free electron.
- Holes are not created
- $n = n_{iD} + N_D$
  - $n_{iD} << n_i$ = density of free electrons in the intrinsic semiconductor
  - N_D = density of donors
- Normally, $N_D > 10^{14}$ cm^{-3} and $n_i \approx 10^{10}$ cm^{-3}
- Since $N_D >> n_{iD}$, **$n \approx N_D$**. The density of free electron can be controlled through doping.



Electron and Hole Concentrations

No E field, no B field, no light

- Under thermal equilibrium conditions, the product of the conduction-electron density and the hole density is ALWAYS equal to the square of n_i:

$$np = n_i^2 = (10^{10})^2/cm^3 \text{ at RT}$$

N-type material at RT

$$n \approx N_D$$

$$p \approx \frac{n_i^2}{N_D}$$

Example: at RT

$N_D = 10^{15}/cm^3$

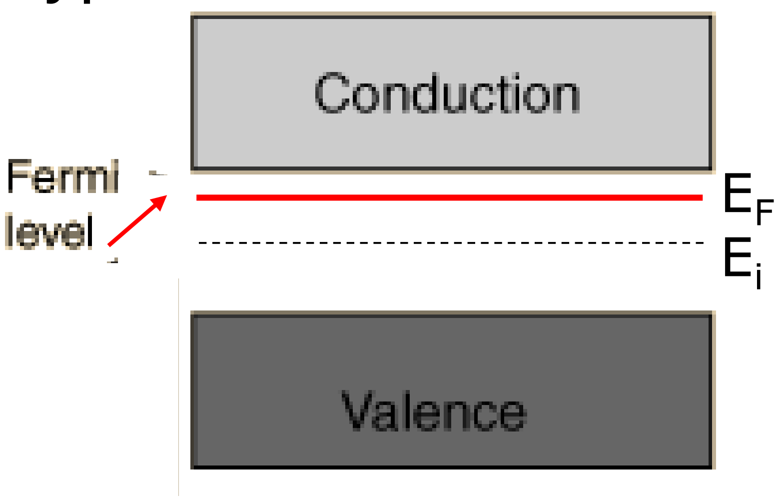
$n = 10^{15}/cm^3$

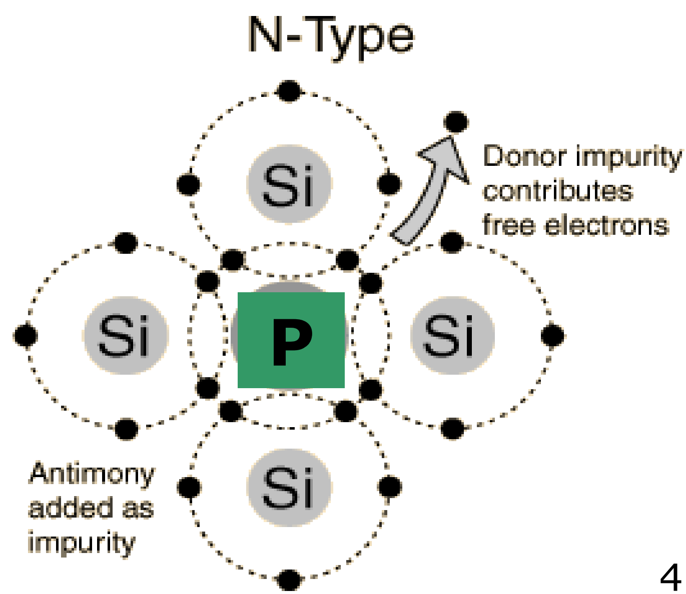
$N_D^+ = 10^{15}/cm^3$

$p = 10^5/cm^3$

N-Type Semiconductor

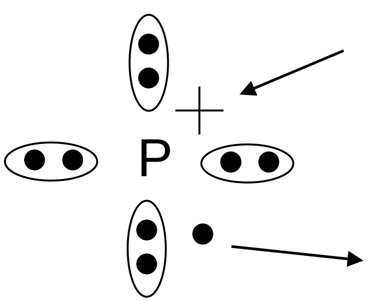
- The addition of pentavalent impurities such as Sb, As or P contributes free electrons, greatly increasing the conductivity of the intrinsic semiconductor.
- Phosphorus may be added by diffusion of phosphine gas (PH_3).
- E_F is shifted to the up-half of the bandgap for n-type.

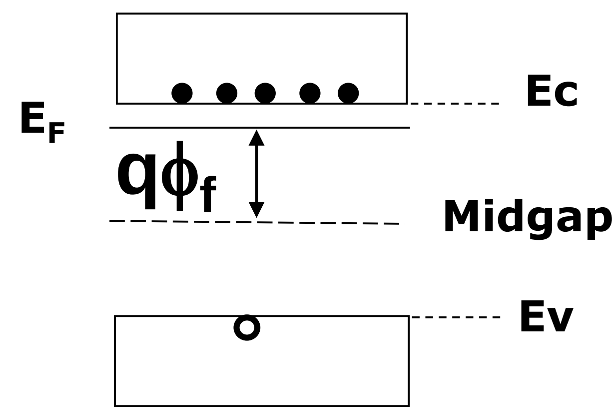




Properties of n-type

- n>>p, so "**n-type**".
- Electrons are '**majority**' charge carriers and holes are '**minority**' charge carriers.
- Space charge: when an electron is freed, it left a positively charged atom behind, which is fixed in space
- Fermi potential: ϕ_f
  - How 'strong' the n-type is



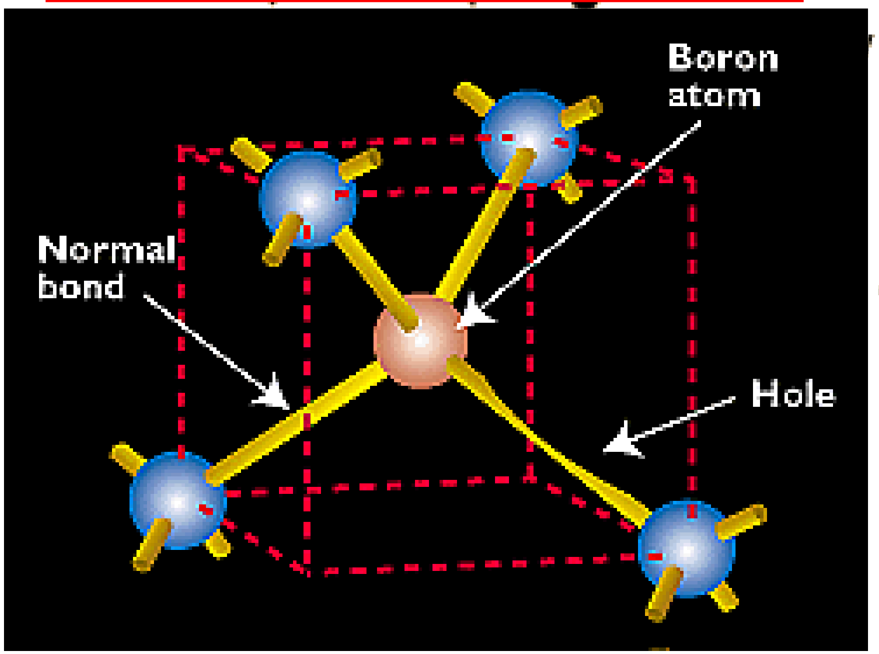


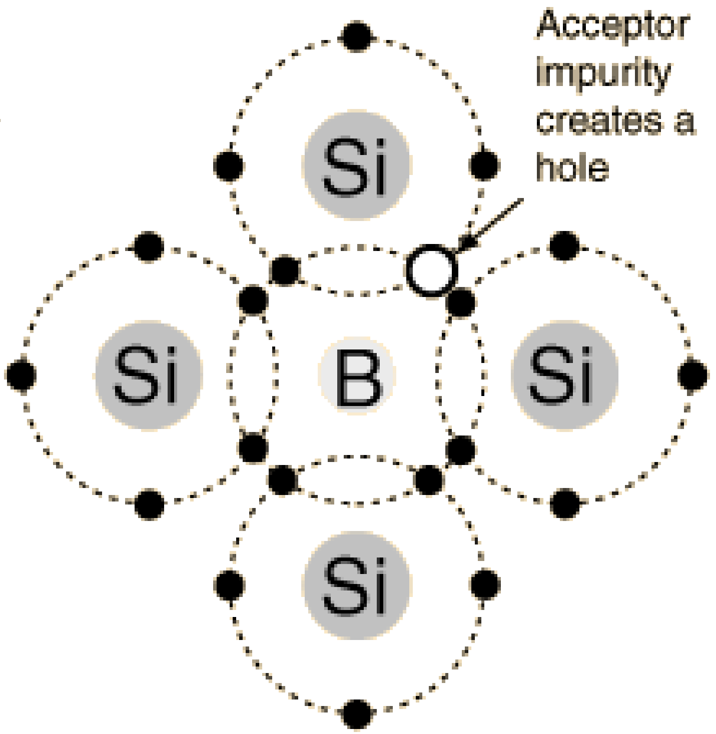
Doping (P type)

Column III elements are acceptors, e.g. B, Al, Ga

By <u>substituting</u> a Si atom with a special impurity atom (Column III element), a conduction hole is created.

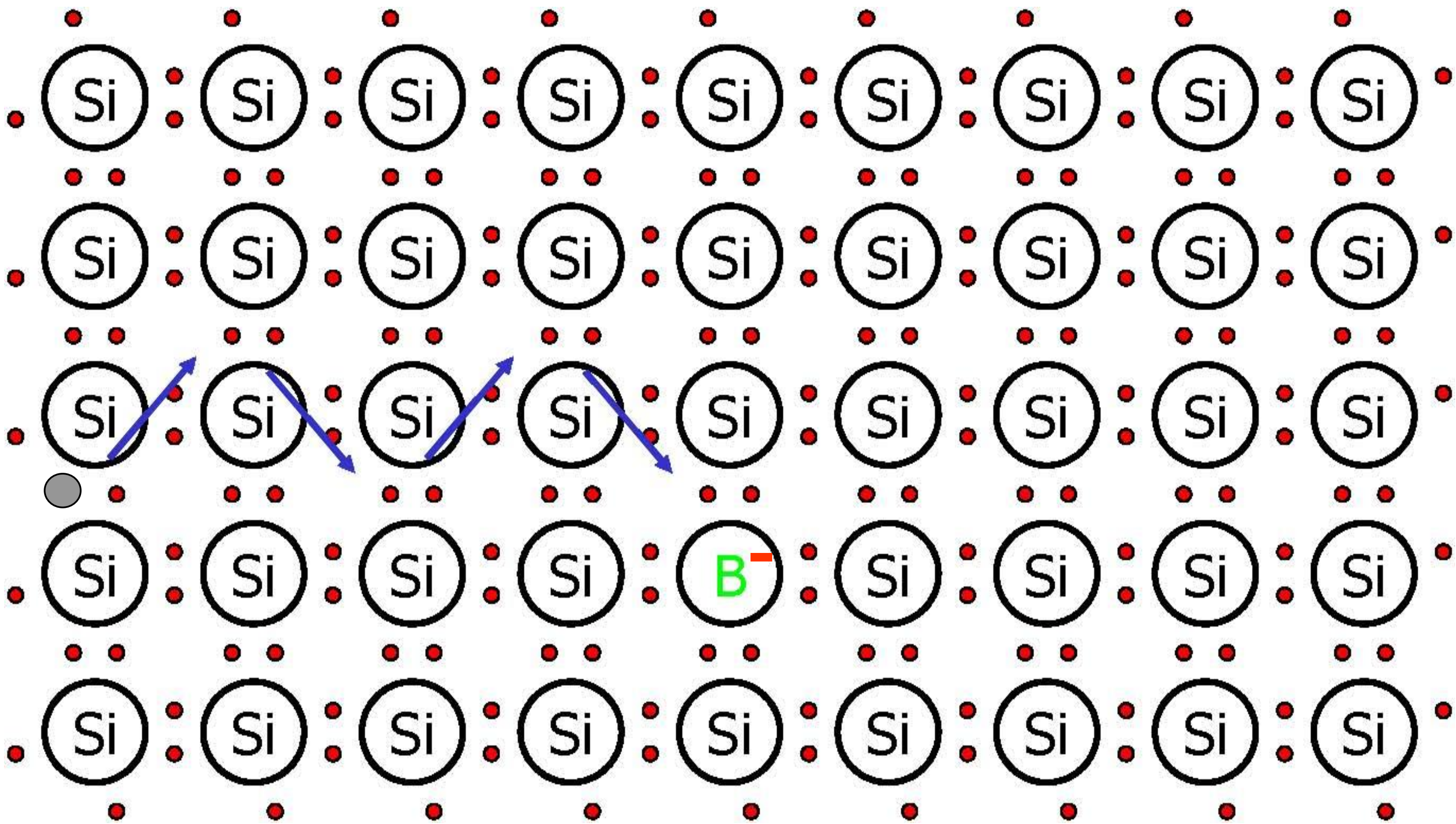
<u>Acceptors</u>: B, Al, Ga, **In**





Boron has 3 valence electrons

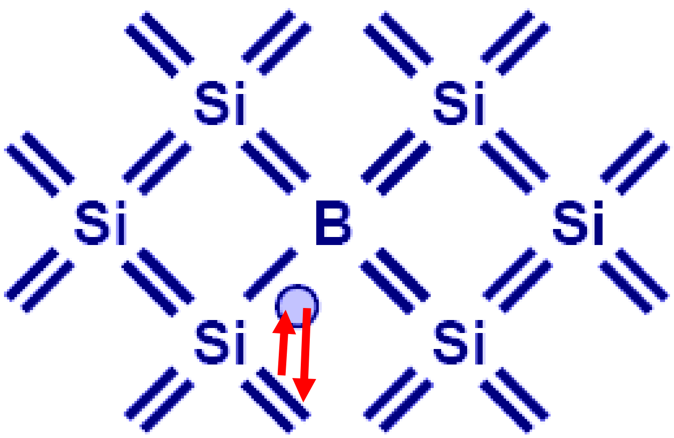
- ‘Accepts’ one electron from lattice
- Creates a ‘hole’



Doping (P type)

Column III elements are acceptors, e.g. B

- If Si is doped with Boron (B), each B atom can contribute a hole, so that the Si lattice has more holes than electrons, *i.e.* it becomes "P type":



Notation:

N_A = concentration of acceptors

p = hole concentration

N_A^- = concentration of ionized acceptors

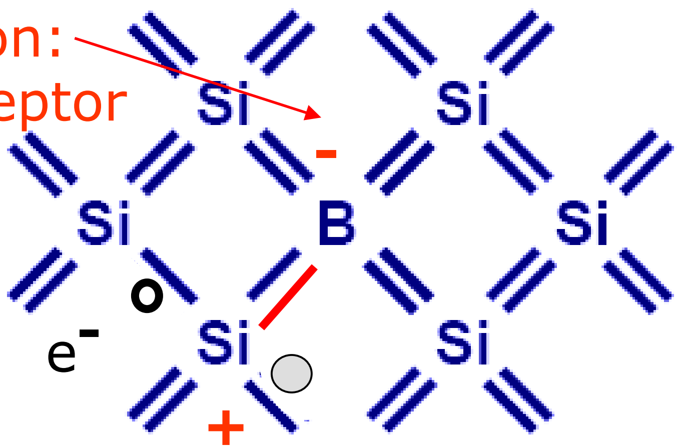
Hole is created when a neighboring valence electron moves to the B atom.

Doping (P type)

Column III elements are acceptors, e.g. B

- If Si is doped with Boron (B), each B atom can contribute a hole, so that the Si lattice has more holes than electrons, *i.e.* it becomes "P type":

Immobile ion: ionized acceptor



$n_{iA} = p_{iA}$

$$p = N_A^- + p_{iA}$$

Notation:

N_A = concentration of acceptors

p = hole concentration

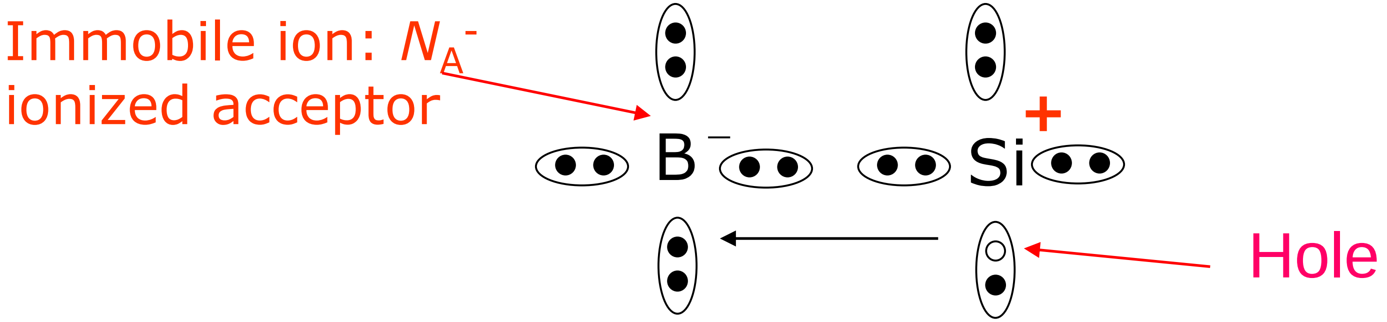
N_A^- = concentration of ionized acceptors

Ionization energy < 50meV:

At RT, $N_A \approx N_A^- >> p_{iA}$

P-type

- Doped by impurities of 3 valence electrons (acceptors)
- At room temperature, one acceptor will create one hole.
- Free electrons are not created
- $p = p_{iA} + N_A \approx N_A$.
  - $p_{iA} << p_i$ = density of holes in the intrinsic semiconductor
  - N_A = density of acceptors



Electron and Hole Concentrations

- Under thermal equilibrium conditions, the product of the conduction-electron density and the hole density is ALWAYS equal to the square of n_i:

$$np = n_i^2 = (10^{10})^2/\text{cm}^3 \textbf{ at RT}$$

<u>P-type material at RT</u>

$$p \approx N_A$$

$$n \approx \frac{n_i^2}{N_A}$$

Example: at RT

$N_A = 10^{15}/\text{cm}^3$

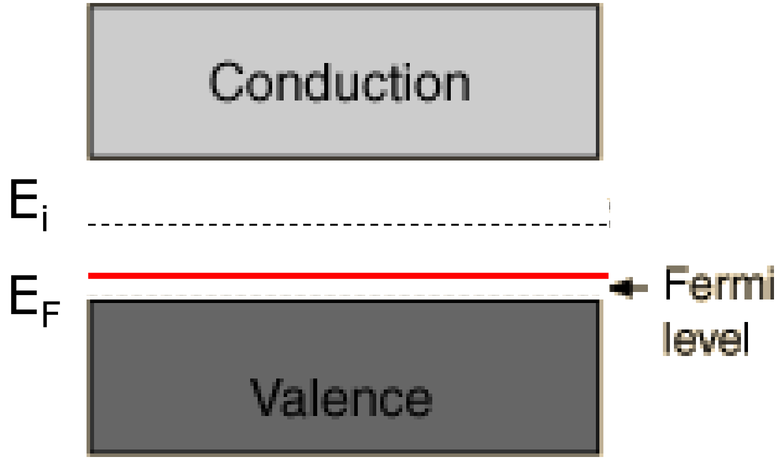
$\boldsymbol{p = 10^{15}/\text{cm}^3}$

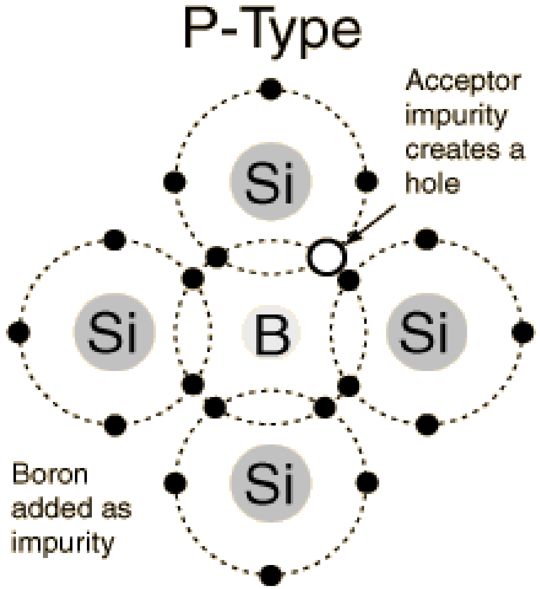
$N_A^- = 10^{15}/\text{cm}^3$

$\boldsymbol{n = 10^{5}/\text{cm}^3}$

P-Type Semiconductor

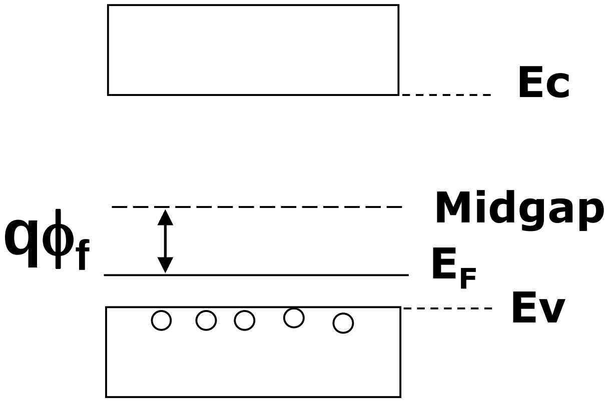
- The addition of trivalent impurities such as B, Al, or Ga to an intrinsic semiconductor creates deficiencies of valence electrons, called "holes".
- It is typical to use B_2H_6 diborane gas to diffuse boron into the silicon material.
- E_F is shifted to the down-half of the bandgap for p-type.





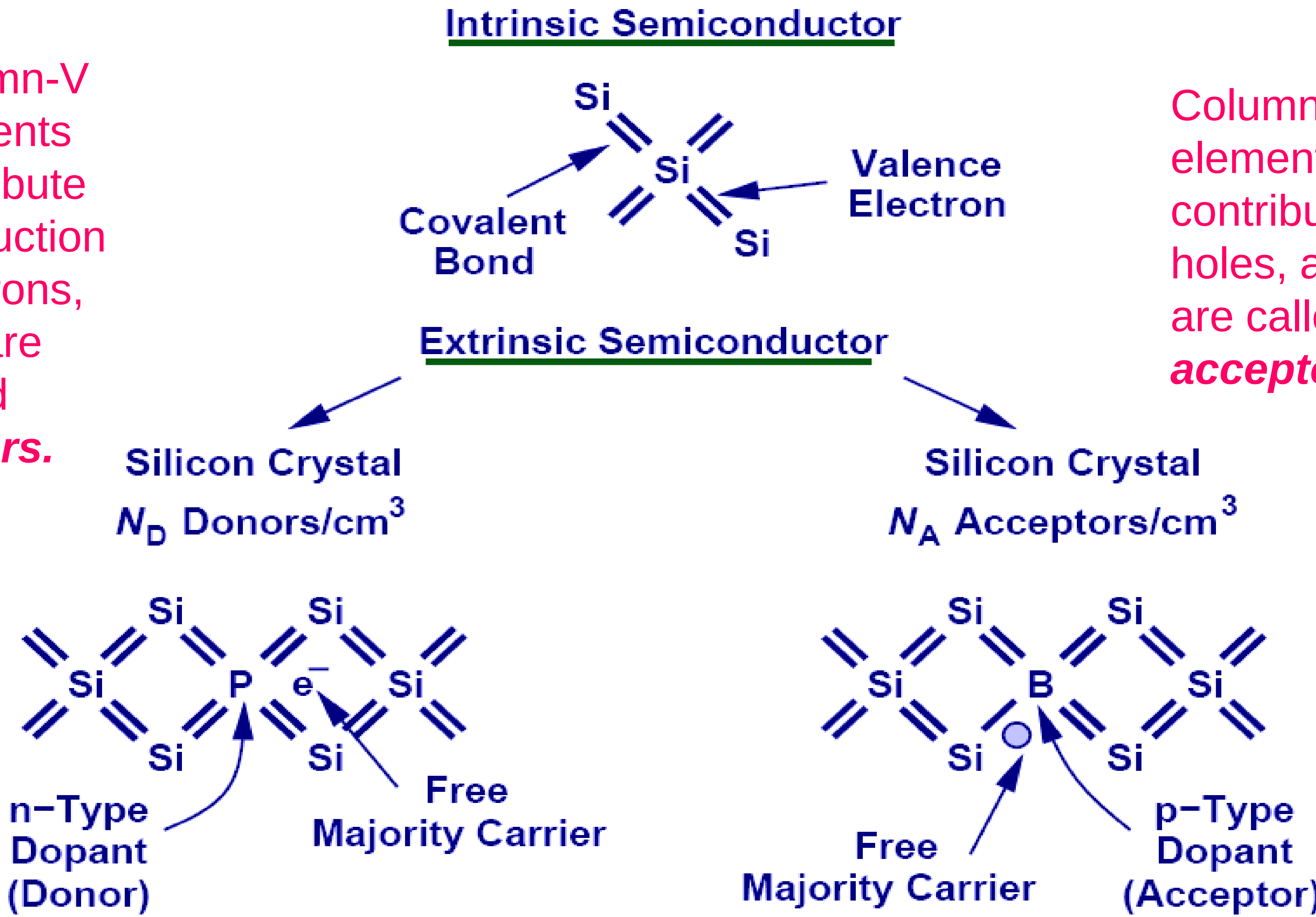
Properties of p-type

- p>>n, so “p-type”.
- **Holes are ‘majority’** charge carriers and **electrons are ‘minority’** charge carriers.
- Space charge: negative charges bonded to Boron atoms
- Fermi potential: ϕ_f
  - How ‘strong’ the p-type is



Summary of doping

Column-V elements contribute conduction electrons, and are called ***donors.***



Column-III elements contribute holes, and are called ***acceptors***

Types of charges in semiconductors

Hole	p	
Electron	n	

Mobile Charge Carriers

they contribute to current flow with electric field is applied.

Ionized Donor	N_D^+	
Ionized Acceptor	N_A^-	

Immobile Charges

they DO NOT contribute to current flow with electric field is applied. However, they affect the local electric field

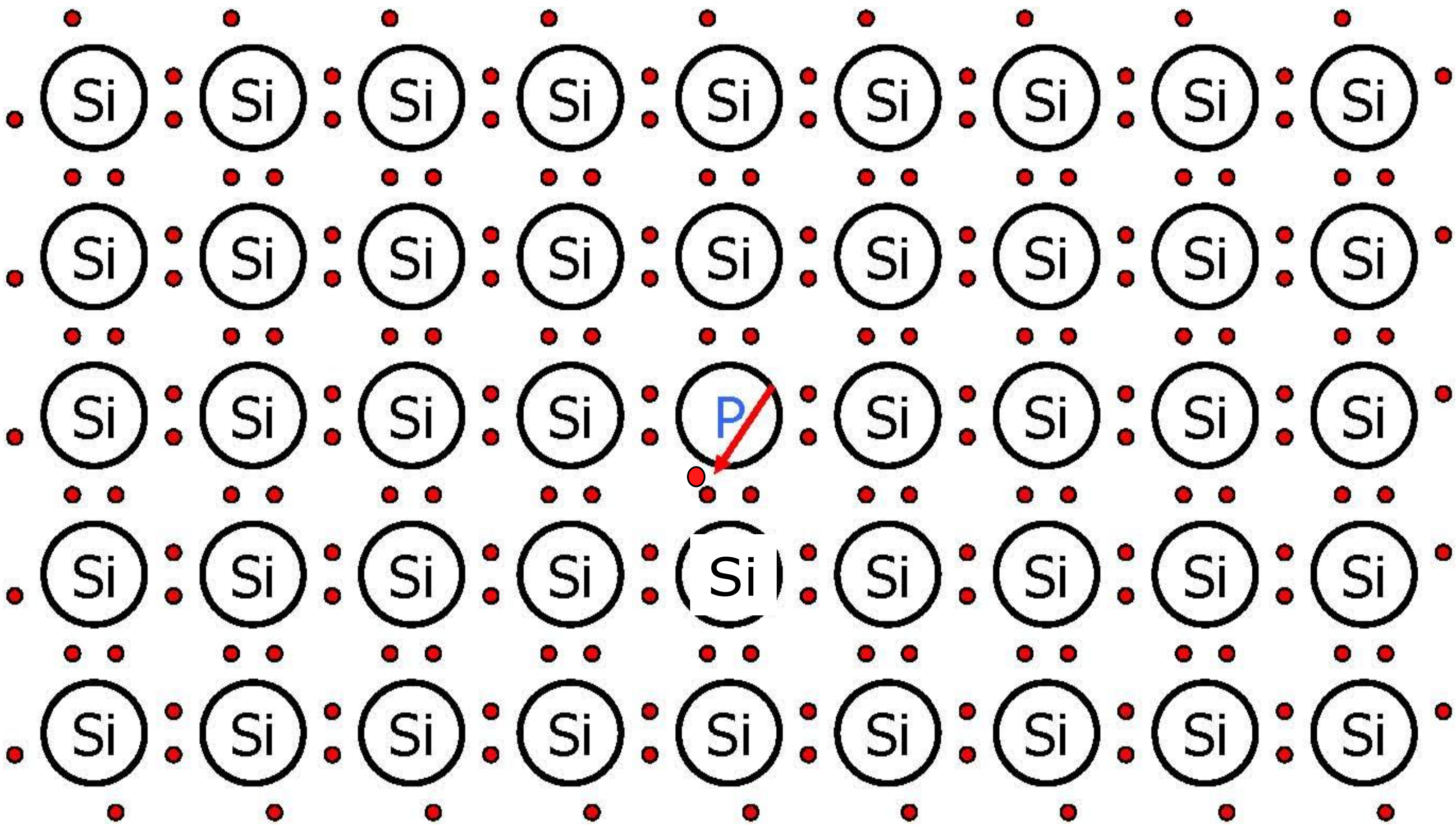
2.4 The doping of semiconductors

- Doping elements
- Doping: N type
- Doping: P type
- **Counter doping**

补偿掺杂

Counter Doping

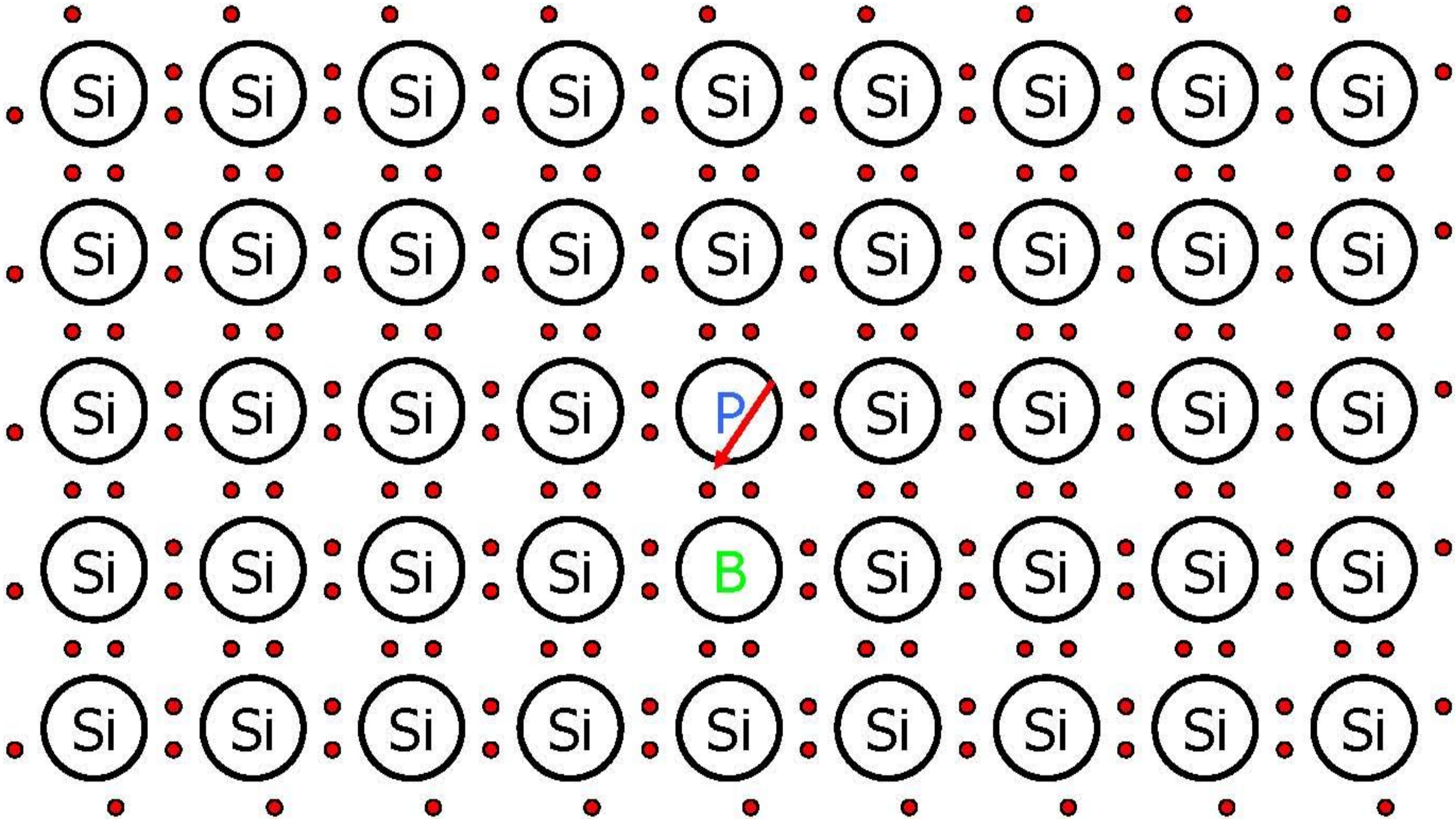
This is a n-type Si, $n = N_D + n_i$. Nomally $N_D >> n_i$, so $n = N_D$



Counter Doping

Adding the same **B** as **P** causes the doping type to change.

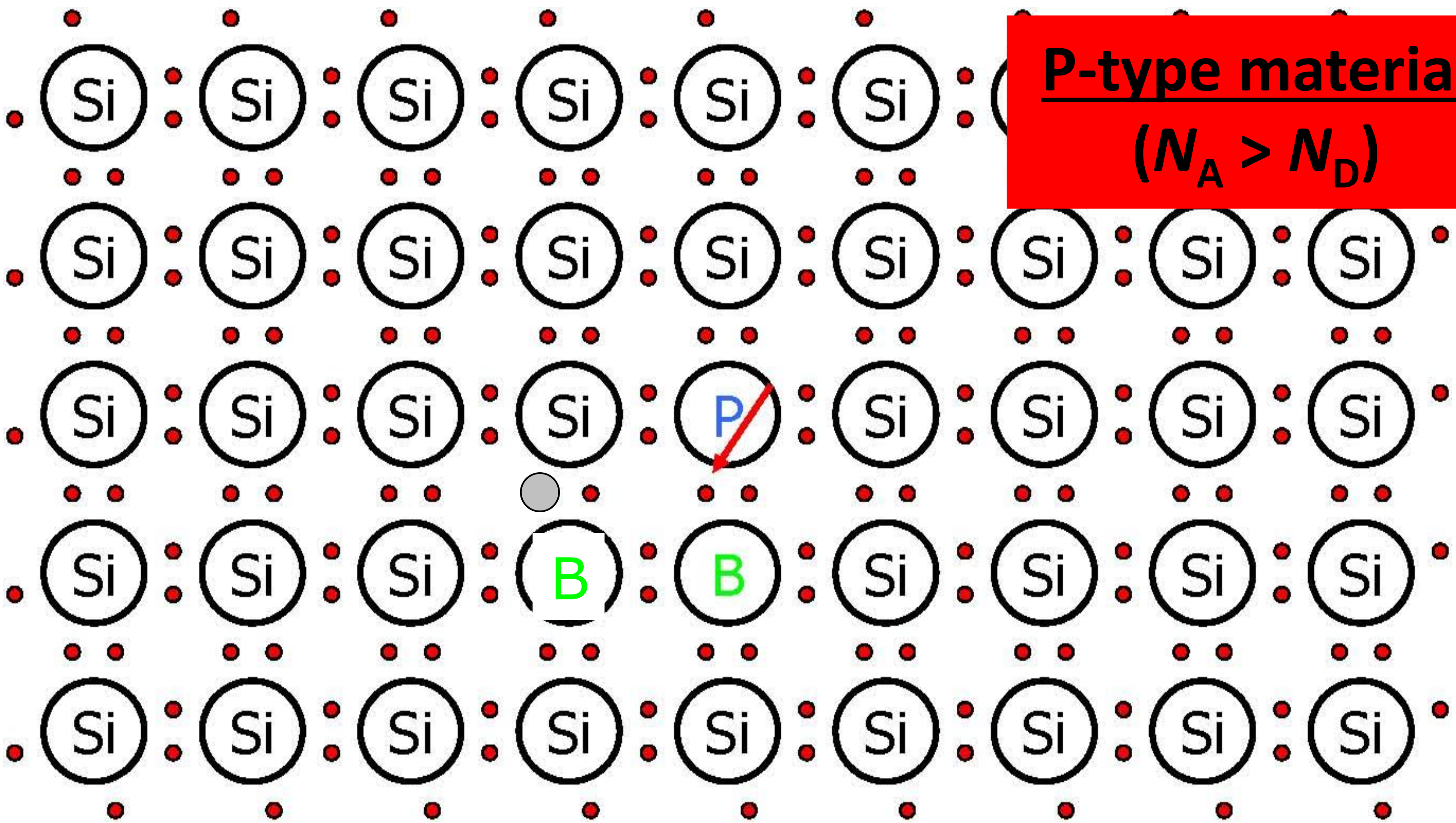
$n = p = N_D - N_A + n_i = n_i.$



Counter Doping

$$p \approx N_A - N_D, \quad n \approx \frac{n_i^2}{N_A - N_D}$$

The addition of one more B than P causes the doping type to change from n-type to p-type



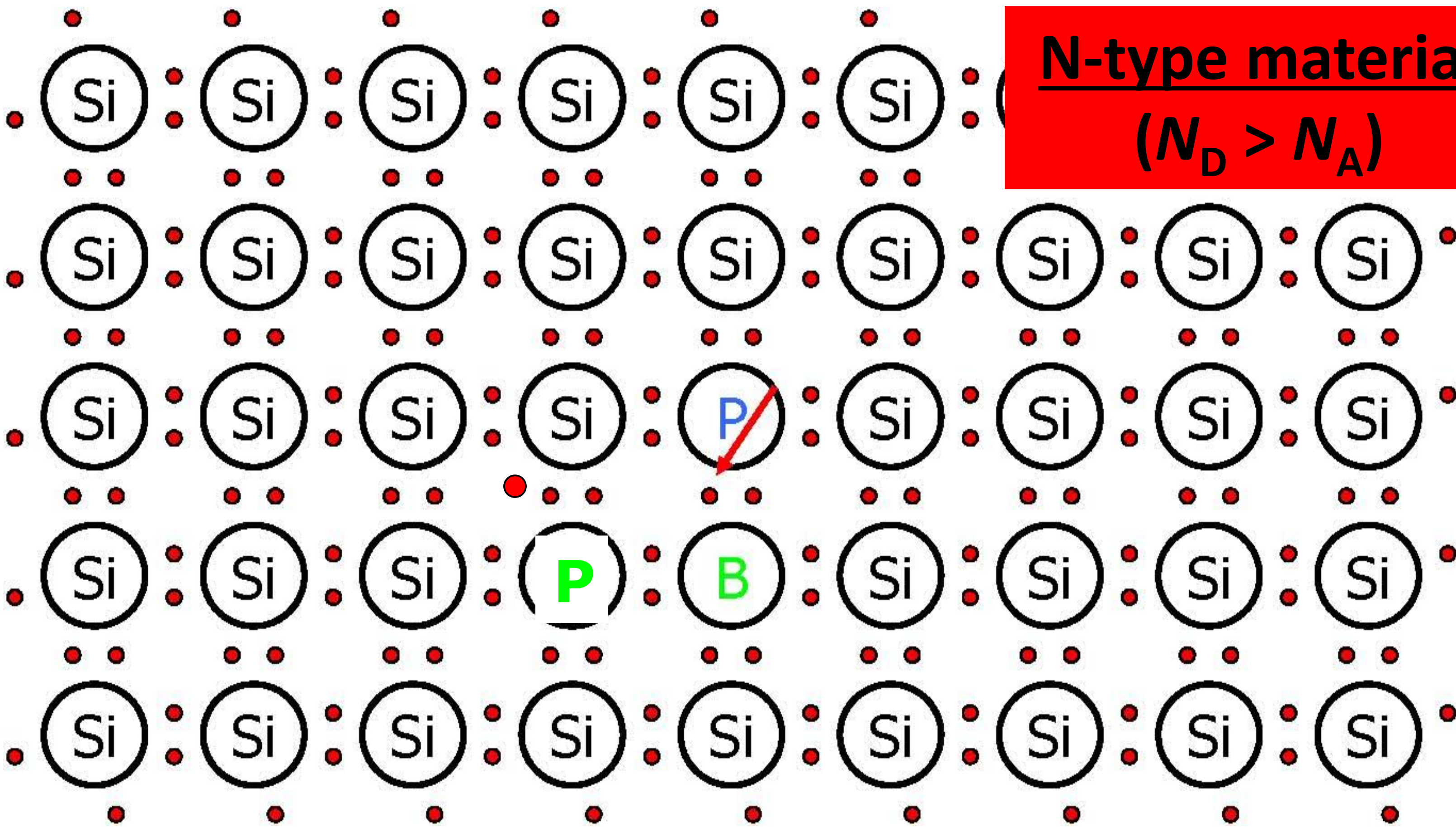
P-type material

($N_A > N_D$)

Counter Doping

$$n \approx N_D - N_A, \;\; p \approx \frac{n_i^2}{N_D - N_A}$$

The addition of one more P than B causes the doping type to change from p-type to n-type



N-type material
($N_D > N_A$)

Dopant Compensation

- An N-type semiconductor can be converted into P-type material by counter-doping it with acceptors such that $N_A > N_D$.
- A ***compensated semiconductor material*** has both acceptors and donors.

<u>N-type material</u>

$(N_D > N_A)$

$$n \approx N_D - N_A$$

$$p \approx \frac{n_i^2}{N_D - N_A}$$

"net doping"

<u>P-type material</u>

$(N_A > N_D)$

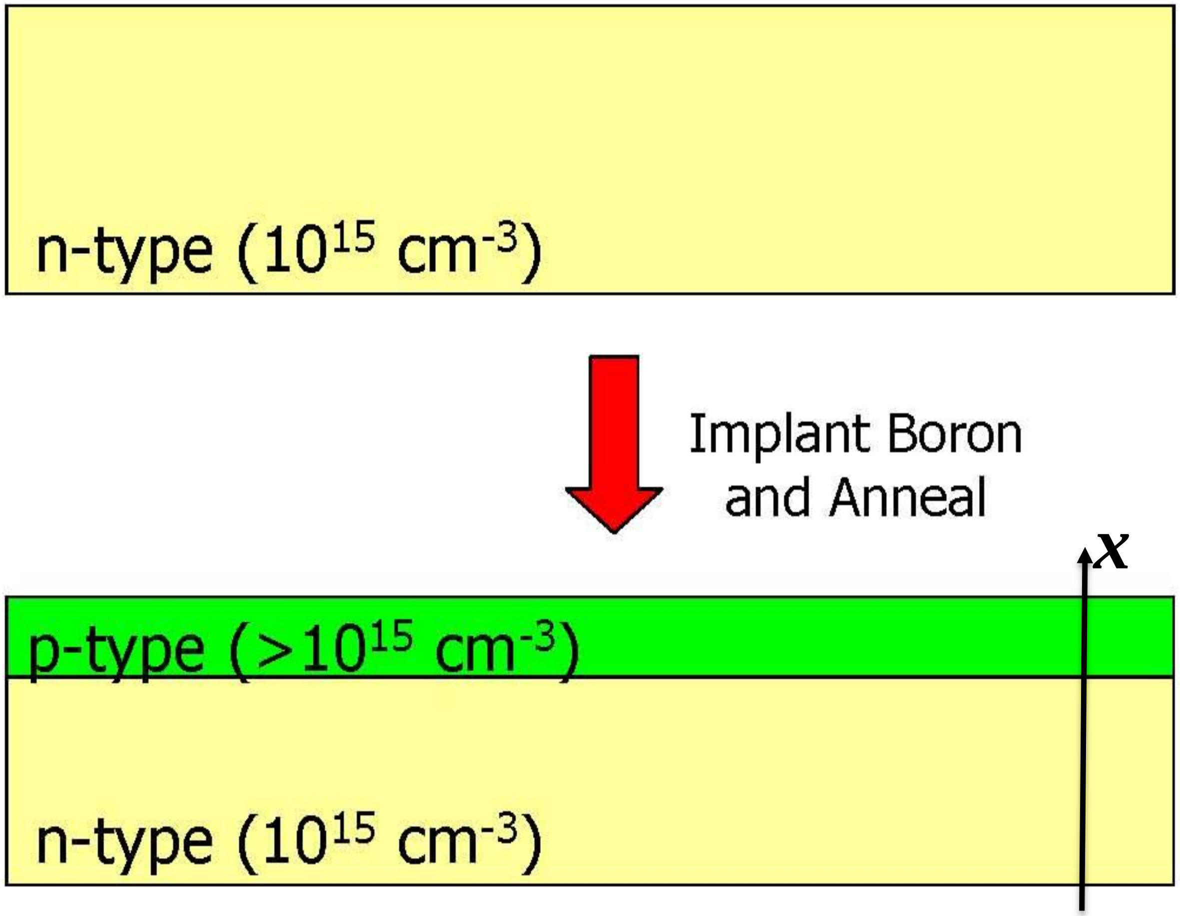
$$p \approx N_A - N_D$$

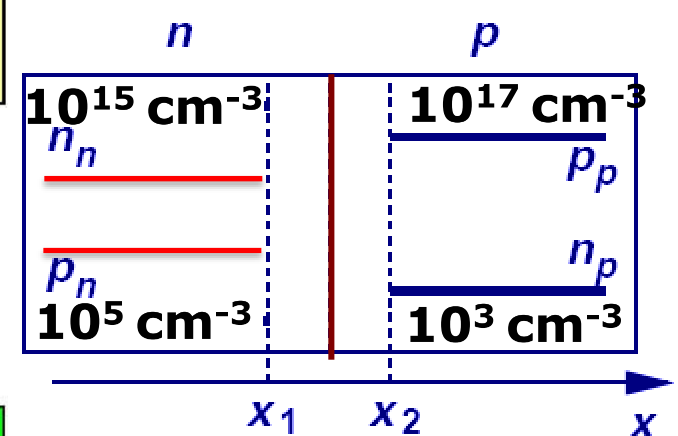
$$n \approx \frac{n_i^2}{N_A - N_D}$$

What is the relationship between E_F and n/p?

Counter Doping Process

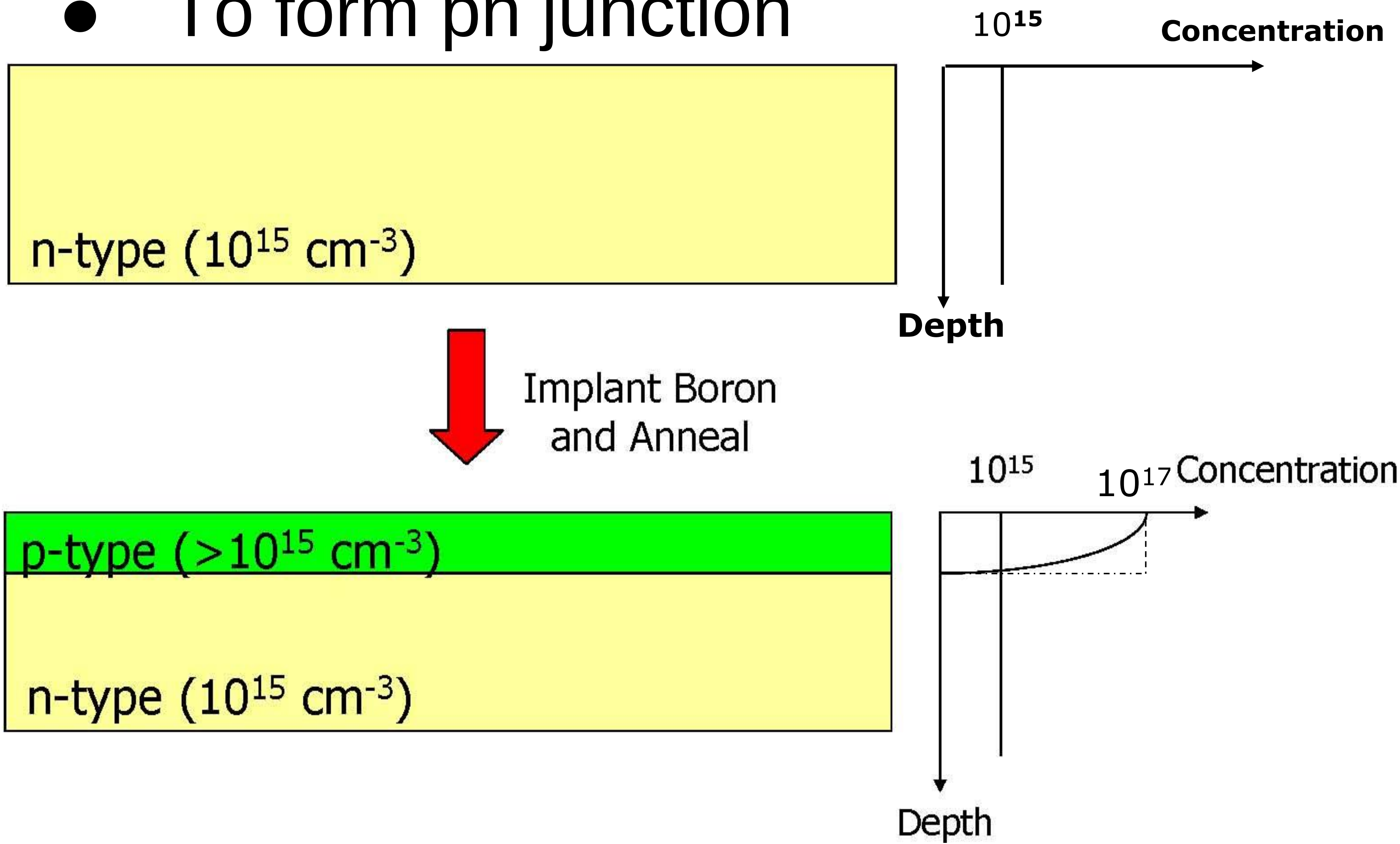
- To form pn junction





Counter Doping Process

- To form pn junction



Next week:

Semiconductor Fundamentals – (III)

2.5 Boltzmann approximation & E_F, n, p

2.6 Carrier drift and diffusion