

# **Lecture 2**

# 1 INTRODUCTION TO SEMICONDUCTOR

## 1.1 Electronic configuration of atoms

- Table 1.1 is the periodic table of the elements.
- The construction of electronic configuration in atoms is discussed in Appendix A (*advanced topic, not required in exam*).
- The electronic configurations of some common elements in semiconductors are given.

# Table 1.1 Periodic table of elements

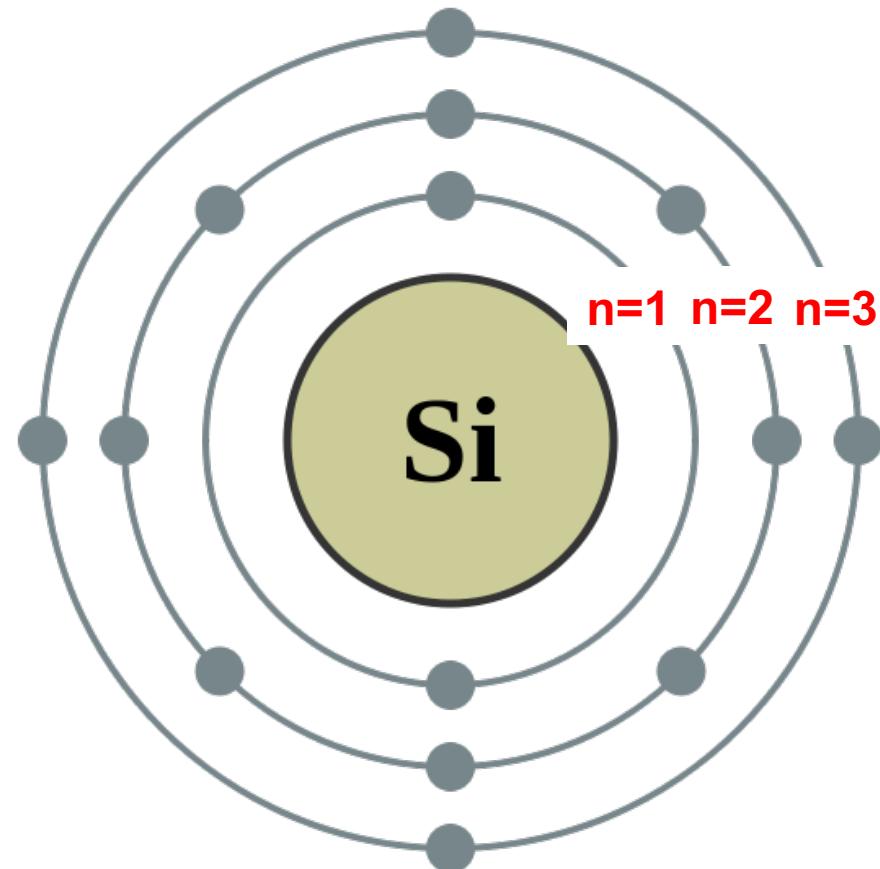
**Periodic Table of the Elements**

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H																									He
Li	Be																								Ne
Na	Mg																								Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn		Ga	Ge	As	Se	Br							Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd		In	Sn	Sb	Te	I							Xe	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg		Tl	Pb	Bi	Po	At							Rn	
Fr	Ra	Ac	Unq	Unp	Unh	Uns	Uno	Une	Unn																
		58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu										
		90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr										

- The understanding and knowledge of electronic configurations of atoms are required to understand, for example:
  - the atomic bonding in semiconductors (discussed in section 1.2);
  - the construction of energy band diagram (discussed in Chapter 3);
  - the behavior of impurity/dopant atoms in semiconductors (discussed in Chapter 4);
  - and many other things...

# Electronic configuration of silicon



[https://commons.wikimedia.org/wiki/File:Electron\\_shell\\_014\\_Silicon\\_no\\_label.svg](https://commons.wikimedia.org/wiki/File:Electron_shell_014_Silicon_no_label.svg)

## Available quantum states in atoms

<b><i>n</i></b>	<b>Subshell</b>	<b>No. of states</b>	<b>Max. No. of electrons</b>
1	<b>s</b>	2 (2x1)	2
2	<b>s</b>	2 (2x1)	2
	<b>p</b>	6 (2x3)	6
3	<b>s</b>	2 (2x1)	2
	<b>p</b>	6 (2x3)	6
	<b>d</b>	10 (2x5)	10

## How about $n = 4$ ?

$n$	Subshell	No. of states	Max. No. of electrons
4	<b>s</b>		
	<b>p</b>		
	<b>d</b>		

Atom	1s	2s	2p			Electron Configuration
Li						$1s^2 2s^1$
Be						$1s^2 2s^2$
B						$1s^2 2s^2 2p^1$
C						$1s^2 2s^2 2p^2$
N						$1s^2 2s^2 2p^3$
O						$1s^2 2s^2 2p^4$
F						$1s^2 2s^2 2p^5$
Ne						$1s^2 2s^2 2p^6$

**Table 1.2** Electronic configuration of some common elements in semiconductors

<b>Element</b>	<b>Symbol</b>	<b>Atomic number</b>	<b>Electronic configuration</b>
Boron	B	5	$1s^2 2s^2 2p^1$
Silicon	Si	14	$1s^2 2s^2 2p^6 \underline{3s^2 3p^2}$
Phosphorus	P	15	-
Gallium	Ga	31	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$
Germanium	Ge	32	-
Arsenic	As	33	-

**Table 1.2** Electronic configuration of some common elements in semiconductors

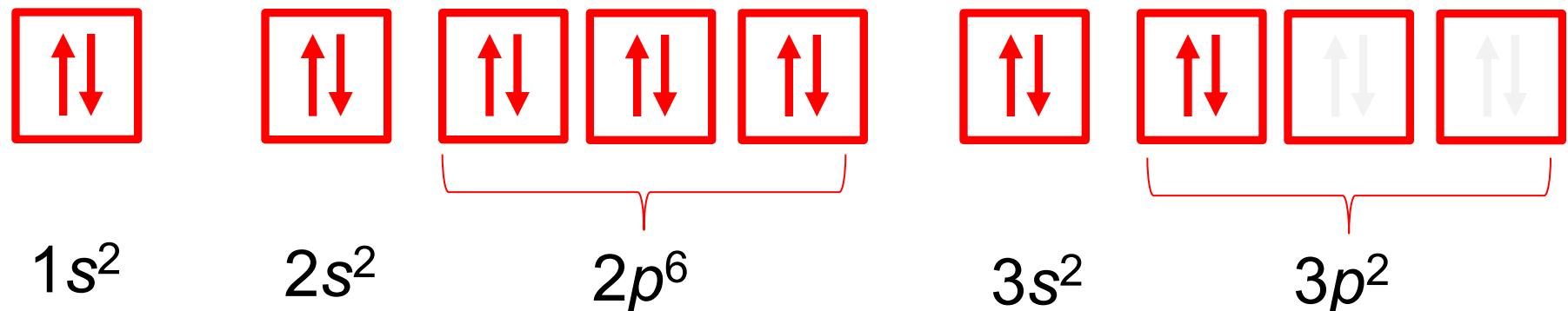
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Gallium	Ga	31	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$
Germanium	Ge	32	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$
Arsenic	As	33	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$

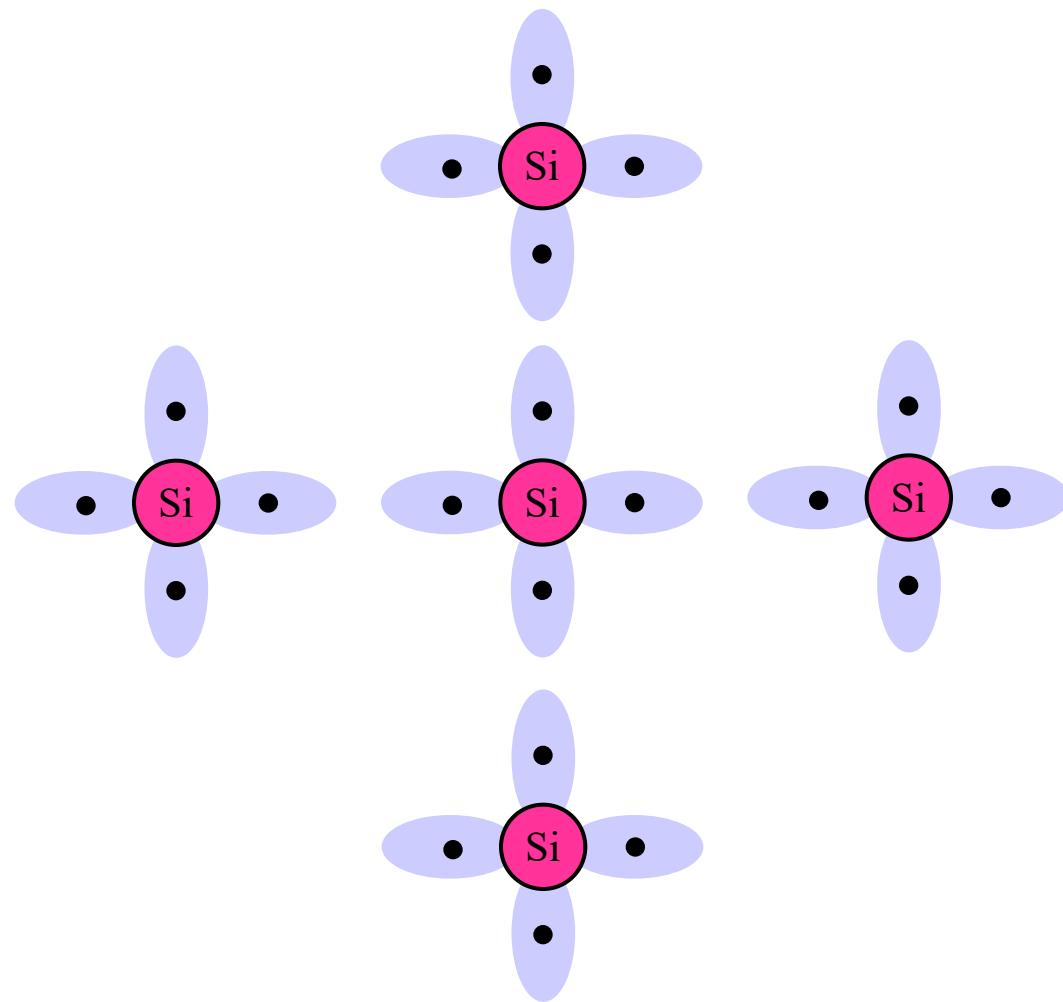
## 1.2 Atomic bonding in semiconductor

- A solid can be conductor or dielectric depends on the types of bonds, or interaction, between its atoms.
- Solids are mostly formed by ionic, covalent and metallic bonds.
- Semiconductor materials (e.g. Si, Ge, GaAs....etc.) have covalent bonds.
- Covalent bond:
  - formed by sharing the electrons between atoms so that the atoms achieve a stable electron configuration (i.e. complete subshells)

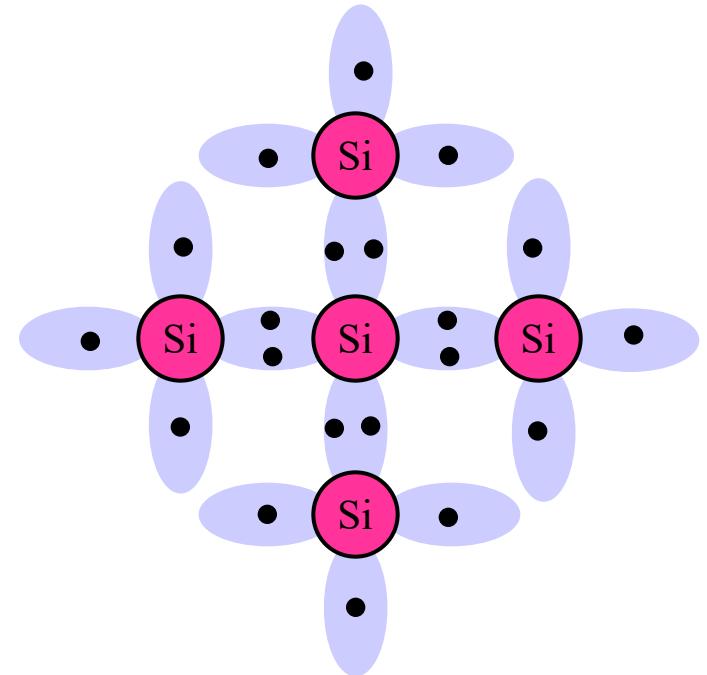
- Consider Si:  $1s^2 2s^2 2p^6 \underline{3s^2 3p^2}$

- To have complete subshells each Si atom needs four more electrons.
- This is achieved by making bonds with four nearest neighbors of Si atoms, with each Si atom contribute one electron.
- This is conveniently illustrated in 2-dimensional representation in Fig.1.1.





(a)

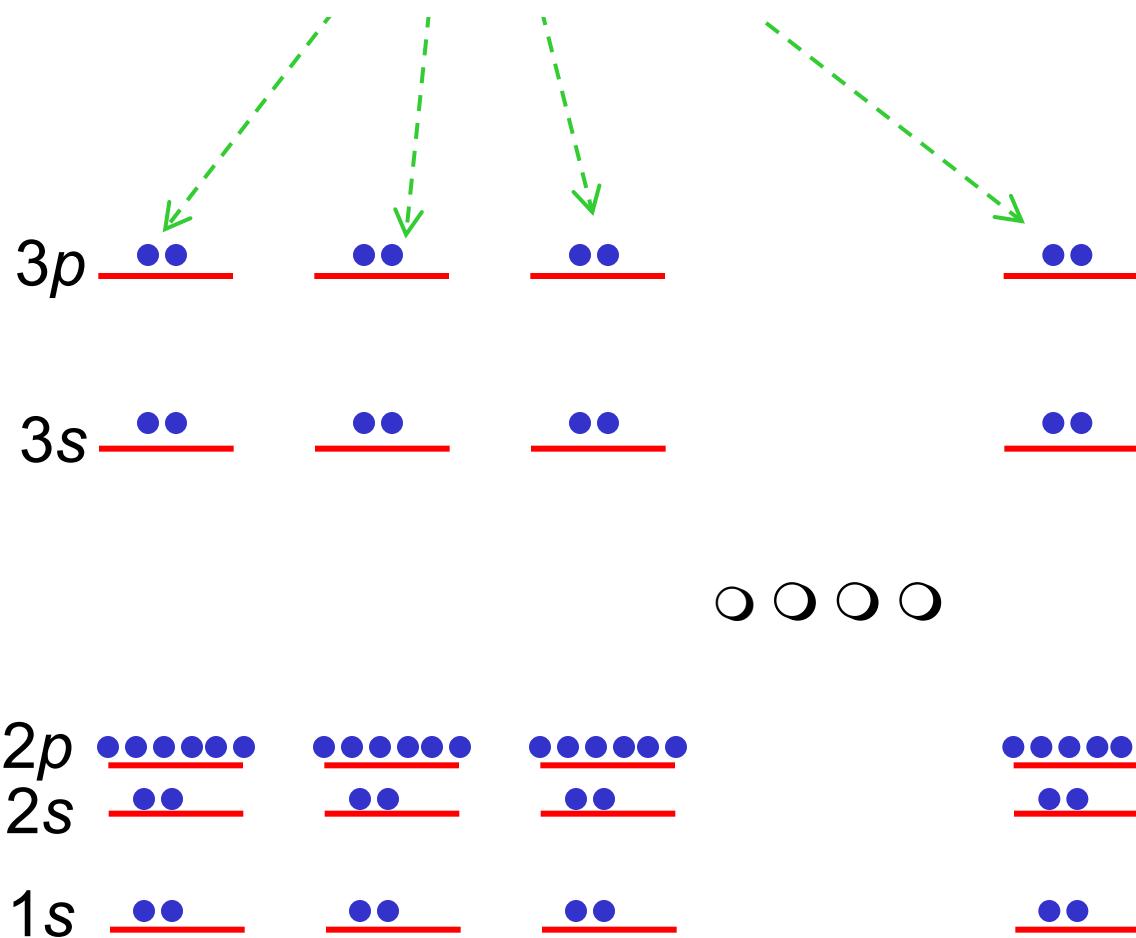


(b)

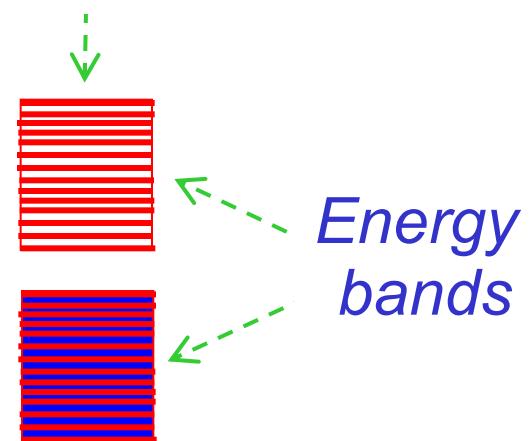
**Fig. 1.1** Illustration of (a) silicon valence electrons (b) covalent bonding in the silicon crystal

$\text{Si} - 1s^2 2s^2 2p^6 3s^2 3p^2$

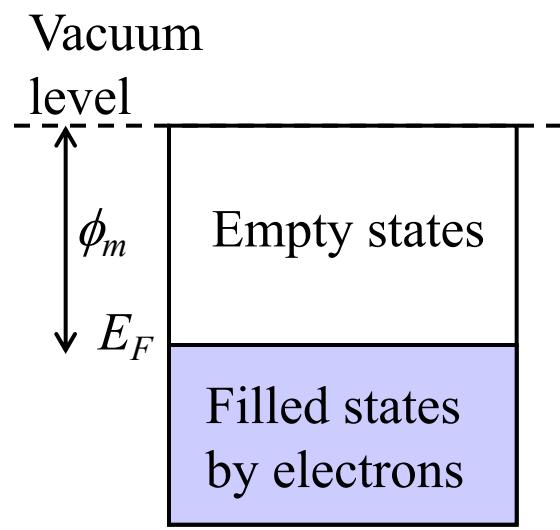
*Individual Si atoms*



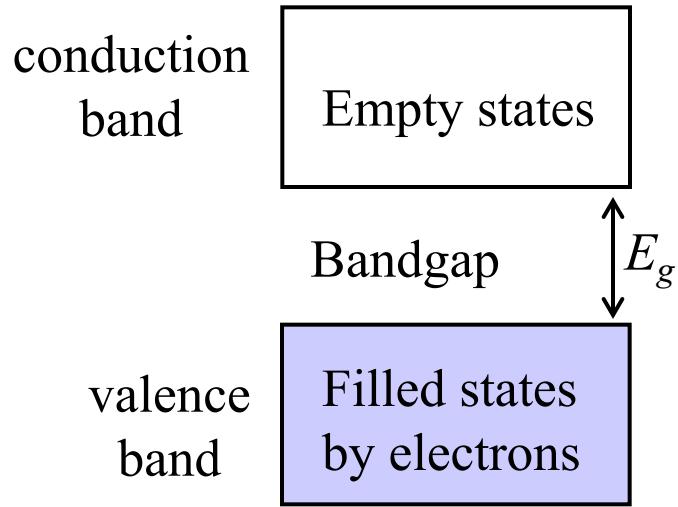
*Atoms making bonds  
Valence electrons  
interact forming energy  
bands*



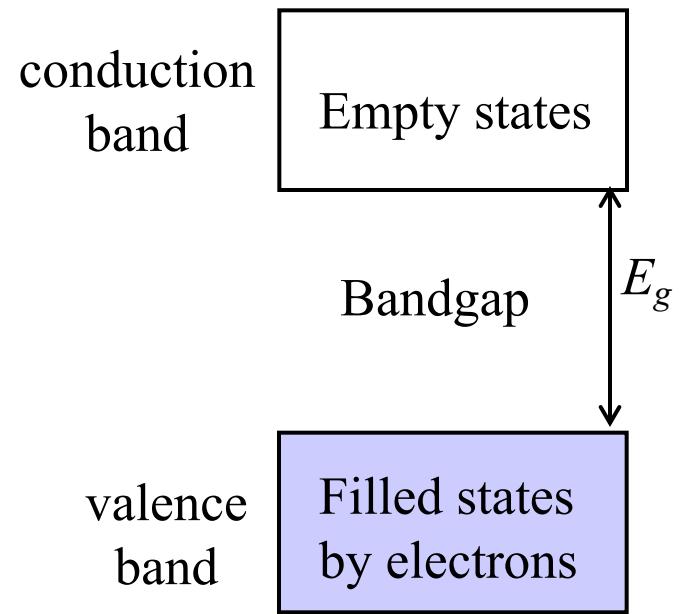
- When atoms are brought together, the interaction of valence electrons lead to the formation of an electron energy band (discussed in Chapter 3).
- The electrical properties of a solid are the consequence of the energy band structure:
  - The electrical conduction can only take place when there is empty states in the energy band.
  - Typical energy band diagrams of metals, semiconductors and insulators are shown in Fig. 1.2



(a)



(b)



(c)

**Fig. 1.2** Energy band structure of (a) metal, (b) semiconductor and (c) insulator

- In **metals**, the energy band is partially filled with electrons:
  - The energy of the highest occupied state at 0 K is referred to as the Fermi energy  $E_F$  .
  - Very little energy is required to promote electrons to the adjacent empty states.
  - Therefore metals are very good electrical conductors.
  - The minimum energy required for an electron to escape from a metal is called work function  $\phi_m$  (energy from the Fermi level  $E_F$  to the vacuum level)

- For **semiconductors & insulators**, there are two bands separated by an energy gap or a bandgap  $E_g$ .
  - No *quantum states* in the energy gap  $\Rightarrow$  no electron is allowed there!
- For **insulators**,  $E_g$  is typically  $> 3\text{eV}$ .

$$1 \text{ eV} = 1.60 \times 10^{-19} \text{ J} = 3.83 \times 10^{-20} \text{ calories}$$

100 g of French fries  $\rightarrow$  300 Calories

- For **semiconductors**,  $E_g$  is typically tenths of fractions to  $2 \sim 3\text{eV}$ .
  - At 0 K, all states in the lower band (*valence band*) are fully occupied by electrons & the upper band (*conduction band*) is empty. Hence, no electrical conduction.
  - For electrical conduction, electrons from the valence band have to be promoted to the empty conduction band.
  - Owing to their relatively small  $E_g$ , thermal energy at room temperature may excite some electrons from the valence band to the conduction band.

## 1.3 Main characteristics of a semiconductor

- Conductivity is neither very large nor very small
  - smaller than conductivity of good metals such as copper,
  - but much greater than insulators like glass.
- The conductivity can be varied over orders of magnitude by changes in temperature, optical excitation, electric field, and impurity content.

“Actors” in the conductivity process are:

- Electrons
  - An electron is a particle carrying an elementary charge of negative  $1.6 \times 10^{-19}$  Coulomb
- Holes
  - A hole is a “particle” in semiconductors that are able to produce current. A hole carries an elementary charge of positive  $1.6 \times 10^{-19}$  Coulomb
  - A hole is merely absence of an electron where it should be

# Two general classifications of semiconductors

- Elemental semiconductors
  - Found in group IV of periodic table (see Table 1.1)
  - For examples, Silicon (most commonly used for ICs) and Germanium (used to make the first transistors and semiconductor diodes)
- Compound semiconductors
  - Special combinations of group III and group V elements
  - Two element, or binary, compounds. For example, gallium arsenide (GaAs) and indium phosphide (InP)
  - Three element, or ternary, compounds. For example aluminium gallium arsenide (AlGaAs)

## **Some questions to think about...**

- (1) Would it be possible to mix Si and Ge to form another type of semiconductor?
- (2) Name one application for Si, Ge and GaAs.

# Key takeaways (Lecture #2)

- Electronics configuration:

- Each quantum state is unique, the higher the quantum state, the higher the energy of the electron
- Incomplete subshell makes an atom chemically unstable

- Silicon:

- Incomplete  $3p$  subshell, need 4 more valence electrons
- Form covalent bond (i.e. sharing of electron pairs) with 4 other Si atoms
- Discrete quantum state → energy band

- Conduction in Silicon:

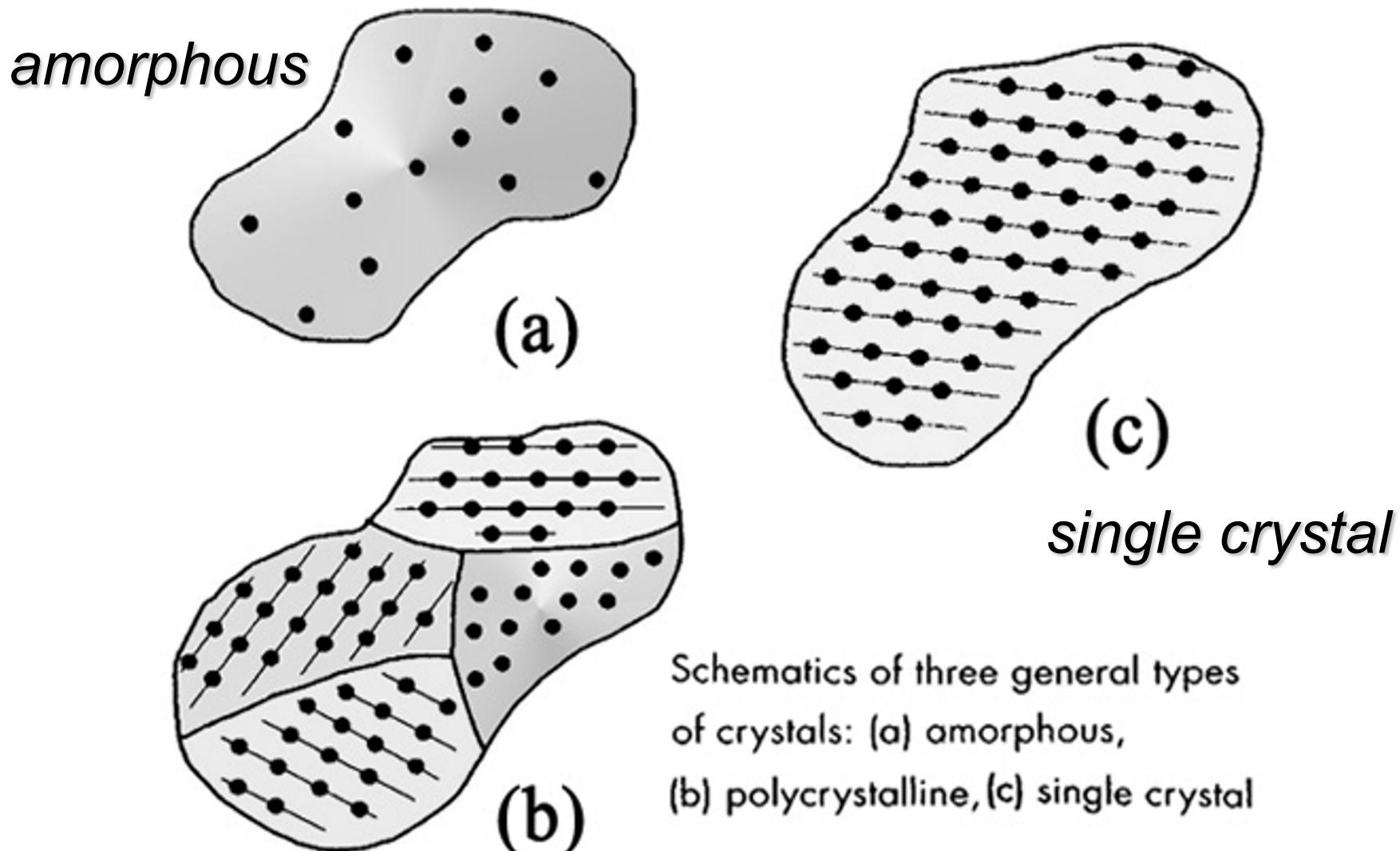
- Valence band and conduction band are separated by a bandgap
- Need empty state and electron/hole in these bands for conduction

# **Lecture 3**

# 2 SEMICONDUCTOR CRYSTAL STRUCTURE

## 2.1 Types of Solids

- Solids are characterized by the size of an ordered region within the material.
- The ordered region is a spatial volume in which atoms or molecules have a regular geometric arrangement, or periodicity.
- Three general types of solids (see Fig. 2.1)



Schematics of three general types  
of crystals: (a) amorphous,  
(b) polycrystalline, (c) single crystal

*polycrystalline*

**Fig.2.1**

- Amorphous materials

- Ordered region is only within a few atomic or molecular dimensions (a few to tens of angstrom;  $1\text{\AA} = 10^{-10} \text{ m}$ )

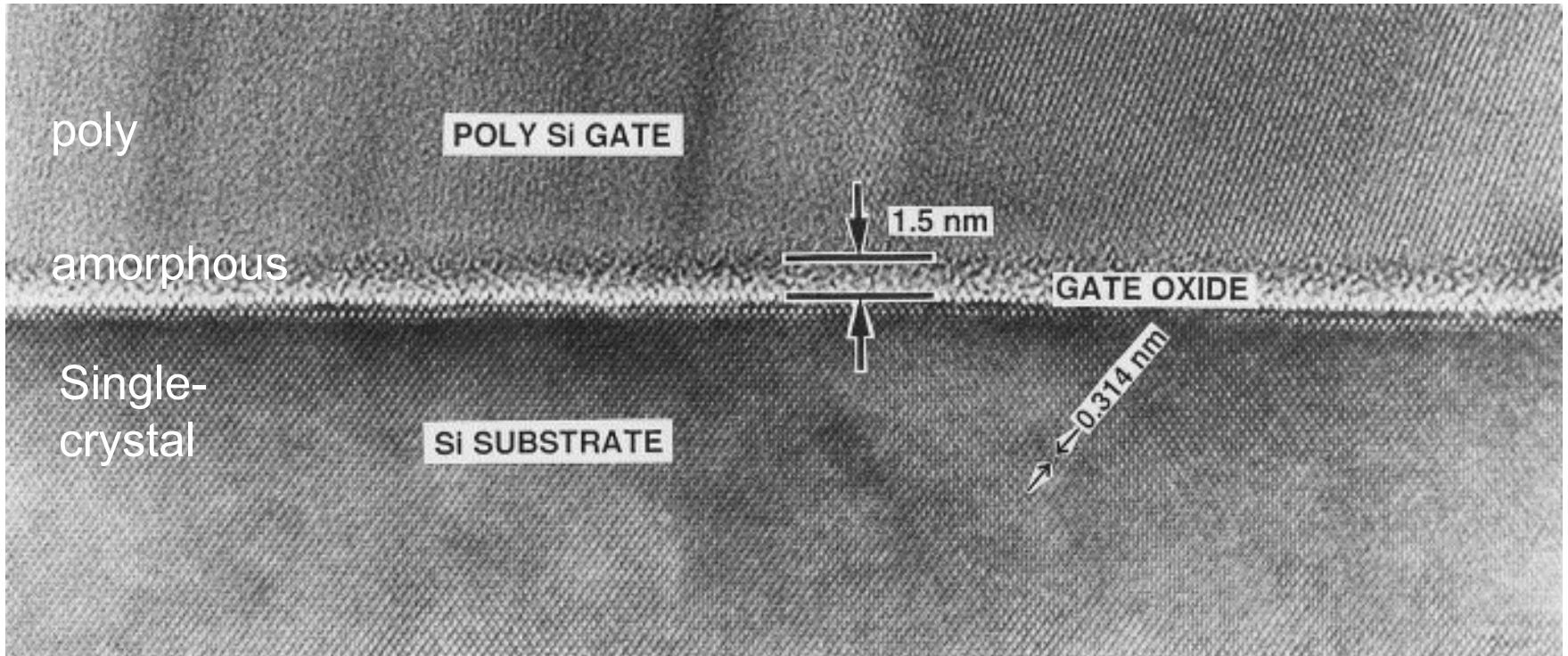
- Polycrystalline materials

- High degree of order over many atomic or molecular dimensions
- Ordered regions (or single crystal regions) vary in size & orientation with respect to one another.
- These single crystal regions are called *grains* & are separated from one another by grain boundaries.

- Single crystal

- High degree of order, or regular geometric periodicity, throughout entire volume of material
- Electrical properties are superior to those of non-single crystal materials (because grain boundaries degrade electrical characteristics)

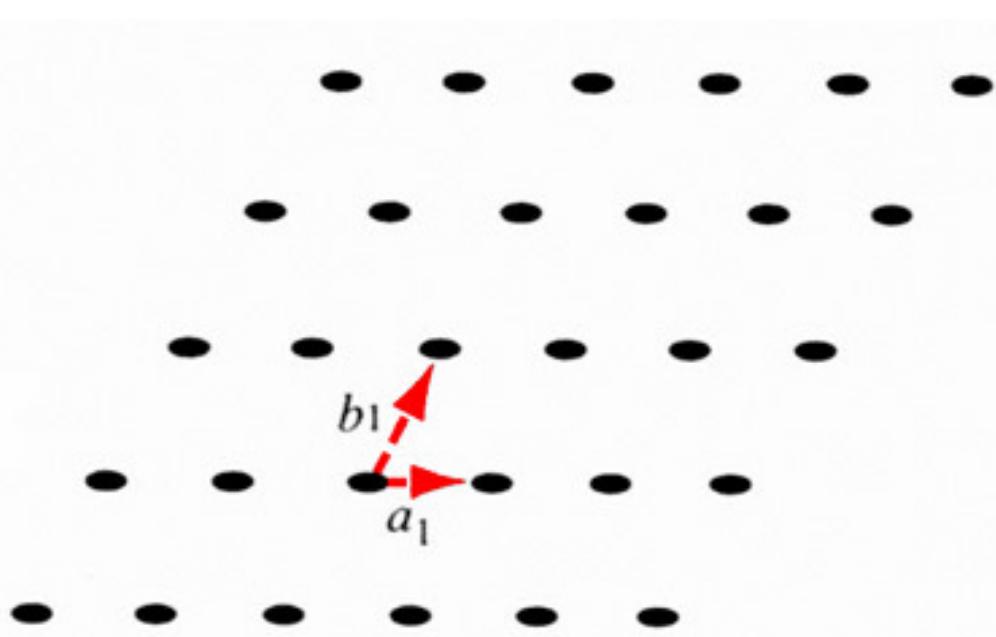
# Image of an MOS capacitor



Momose et al, Microelectronics Reliability, Volume 38, Issue 9,  
September 1998, Pages 1413–1423

## 2.2 Space Lattice, Primitive and Unit Cell

- Consider a single crystal
- Periodic arrangement of points in a space is called a lattice. The point is called a lattice point.



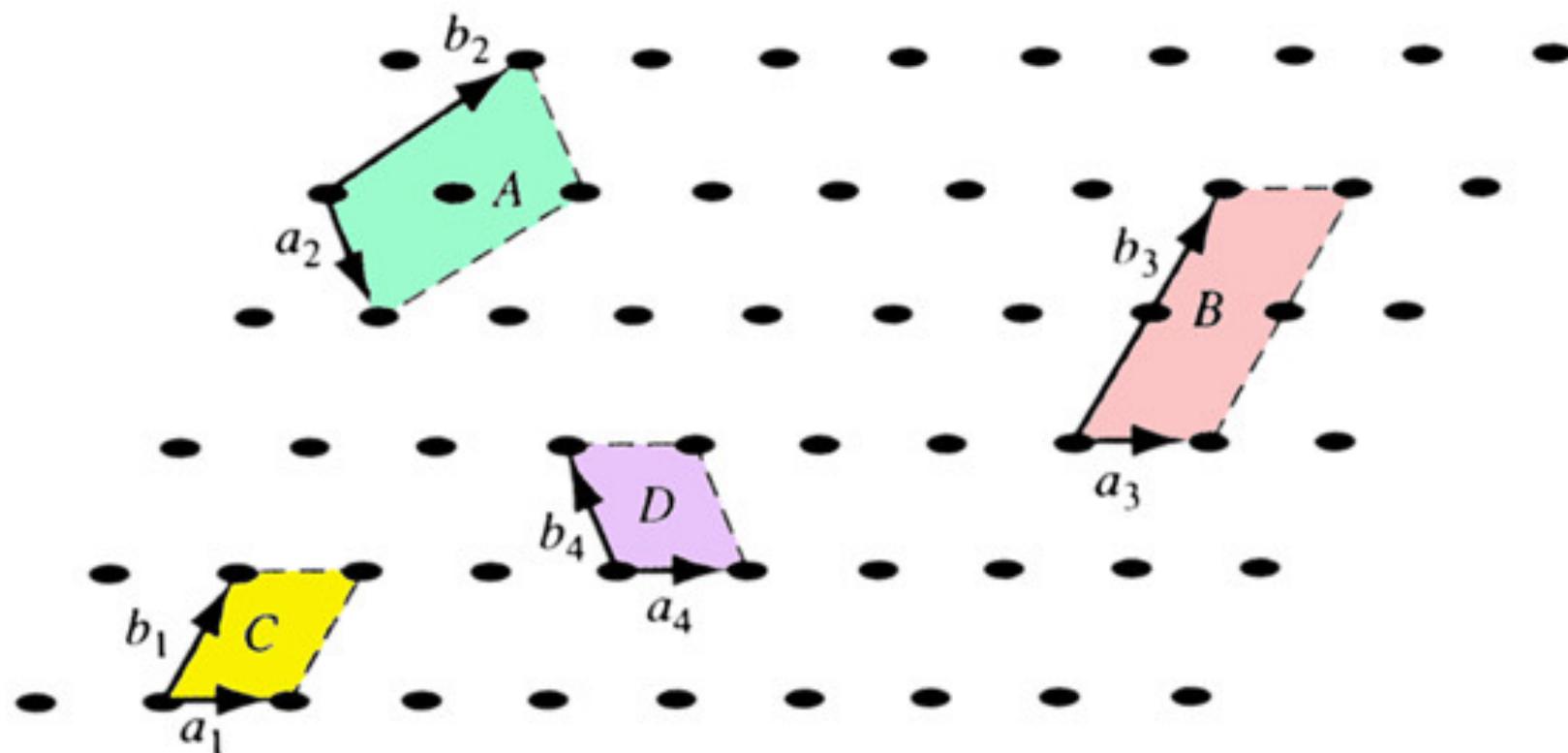
Two-dimensional representation  
of a single-crystal lattice

**Fig. 2.2** shows an infinite 2-D array of lattice points.

- Each lattice point can be translated a distance  $a_1$  and a distance  $b_1$  in a second non-colinear direction to generate the 2-D lattice.
- A third non-colinear translation will produce the three dimensional (3-D) lattice. The lattice directions need not be perpendicular
- A crystal structure is formed when an atom, group of atoms/molecules is attached identically to each lattice point

When considering a lattice,

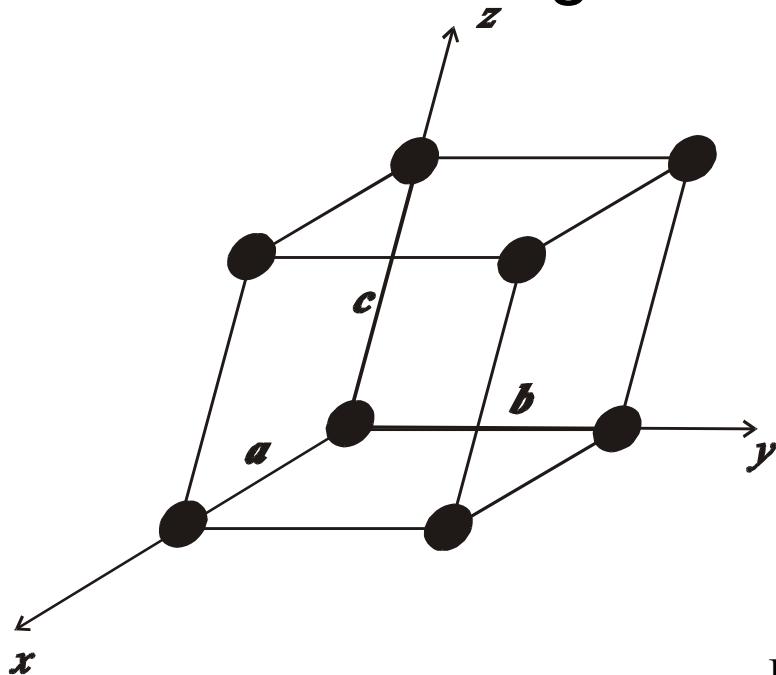
- Do not need to consider the entire lattice. Need to look only at a fundamental unit that is being repeated
- A unit cell is a small volume of crystal that can be used to reproduce the entire crystal. It is a representative of the entire lattice. We can generate the entire lattice by repeating the unit cell throughout the crystal
  - A unit cell is not unique entity
  - Several possible unit cell in 2-D lattice is shown in Fig. 2.3



**Fig. 2.3**

Two-dimensional representation of a single-crystal lattice showing various possible unit cells

- A primitive cell is the smallest unit cell that can be repeated to form lattice
- In many cases, more convenient to use a unit cell
  - They can be chosen to have orthogonal sides, whereas sides of primitive cell may not be orthogonal as shown in Fig. 2.4.

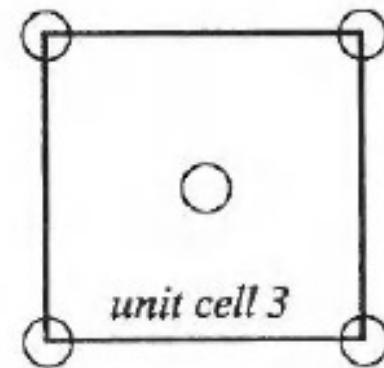
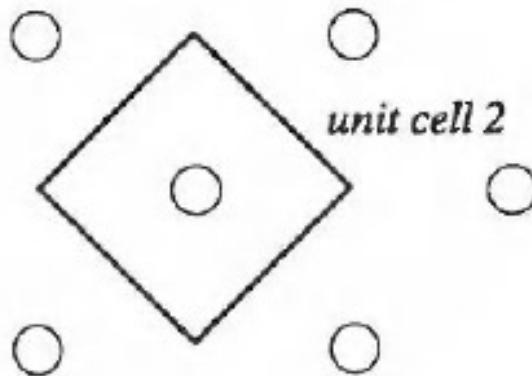
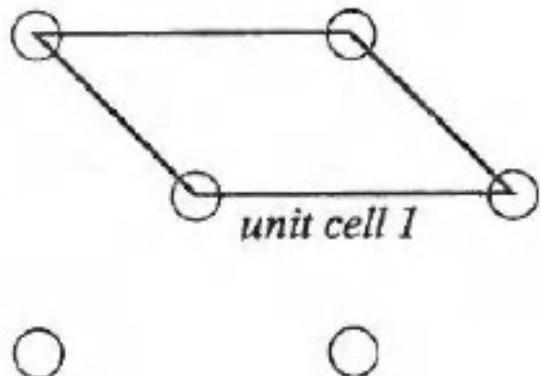


**Fig. 2.4** A generalized primitive unit cell

# Question (BG Streetman)

Which of the following three unit cells are *primitive cells* for the two-dimensional lattice? Circle the correct combination **in bold** below.

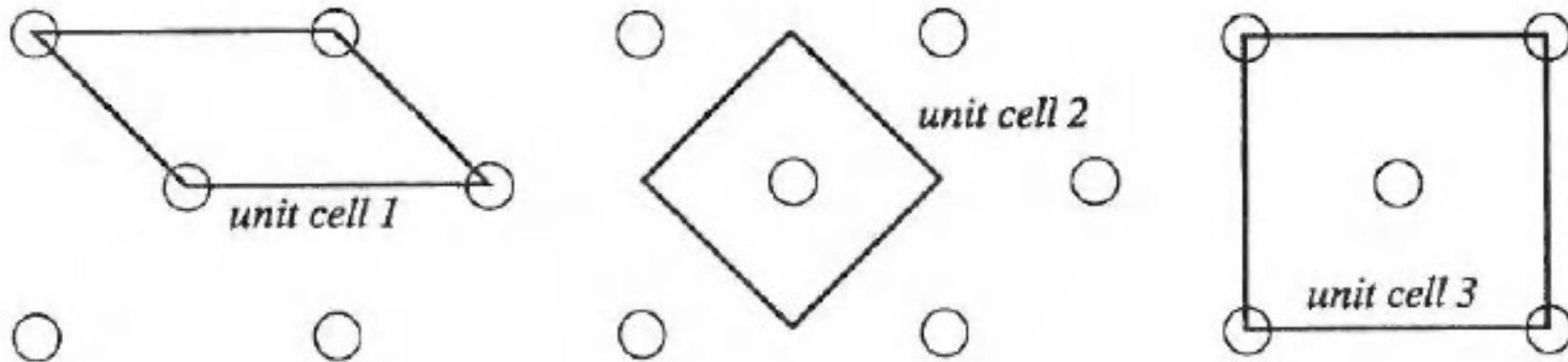
*1 / 2 / 3 / 1 and 2 / 1 and 3 / 2 and 3 / 1, 2, and 3*



# Question (BG Streetman)

Which of the following three unit cells are *primitive cells* for the two-dimensional lattice? Circle the correct combination **in bold** below.

*1 / 2 / 3 / 1 and 2 / 1 and 3 / 2 and 3 / 1, 2, and 3*



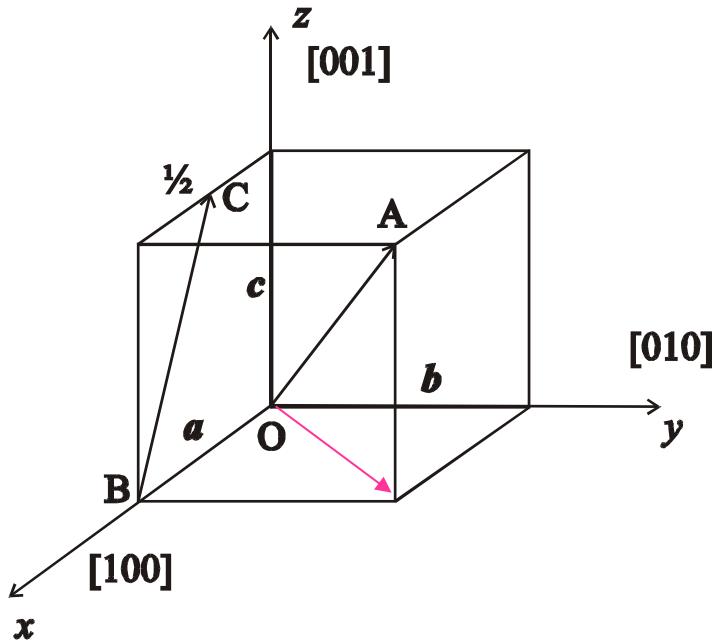
**1 and 2:** 1 and 2 each contain a single atom and may be repeated to form the lattice. 3 may be repeated to form the lattice, but it contains 2 atoms.

## 2.3 Crystallographic directions and planes

- Consider a unit cell defined by 3 vectors  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{c}$ . The dimensions  $a$ ,  $b$  and  $c$  are unit cell dimensions or lattice constant. For cubic unit cell the dimensions  $a = b = c$ .
- A crystallographic direction is defined as a line between two points, a vector. To determine the crystallographic directions:
  - determine the origin
  - determine the initial and the final positions of the vector in terms of the lattice constant  $a$ ,  $b$  and  $c$

- determine the vector: (final position) – (initial position)
- write down the vector in terms of the numbers of the lattice constant
- multiply or divide these numbers by a common factor to reduce them to the smallest integer values
- the three indices are enclosed in square brackets  $[uvw]$ . The  $u$ ,  $v$  and  $w$  integers correspond to the reduced projections along  $x$ ,  $y$  and  $z$
- negative indices are represented by a bar over the appropriate index

# Examples 2.1



In most Si transistor, current flows in the [110] direction

## Vector OA

	$x$	$y$	$z$
Final position	$1a$	$1b$	$1c$
Initial position	$0a$	$0b$	$0c$
Vector OA	$1a$	$1b$	$1c$
Vector OA (numbers only)	1	1	1
Reduction	1	1	1
Enclosure	[111]		

## Vector BC

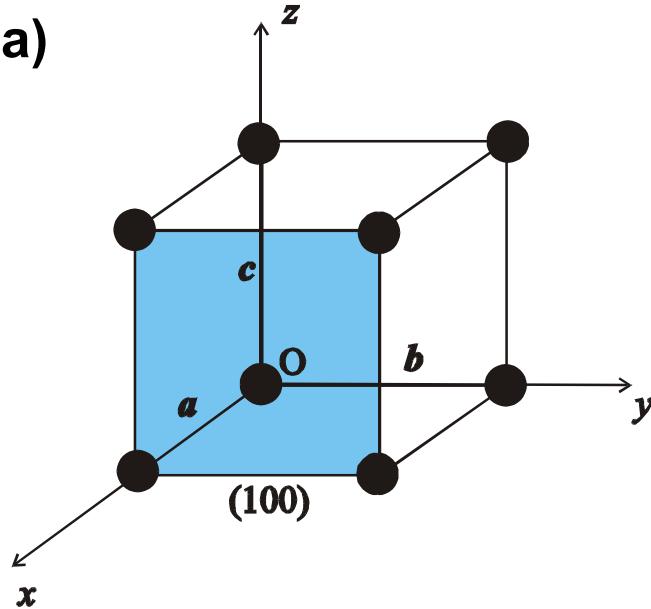
	$x$	$y$	$z$
Final position	$1/2a$	$0b$	$1c$
Initial position	$1a$	$0b$	$0c$
Vector BC	$-1/2a$	$0b$	$1c$
Vector BC (numbers only)	$-1/2$	0	1
Reduction	-1	0	2
Enclosure	[ $\bar{1}02$ ]		

- Planes in a crystal are specified by Miller indices ( $hkl$ ).
- To determine the Miller indices of the planes:
  - determine the origin, make sure that the planes do not pass through the origin
  - determine the intercepts on the axes in terms of the lattice constant  $a$ ,  $b$  and  $c$
  - write down the intercepts in terms of the numbers of the lattice constant

- take the reciprocal of these numbers
- multiply or divide the reciprocal to reduce them to usually smallest three integers
- the integers are enclosed in parentheses ( $hkl$ )
- again, negative indices are represented by a bar over the appropriate index

## Example 2.2

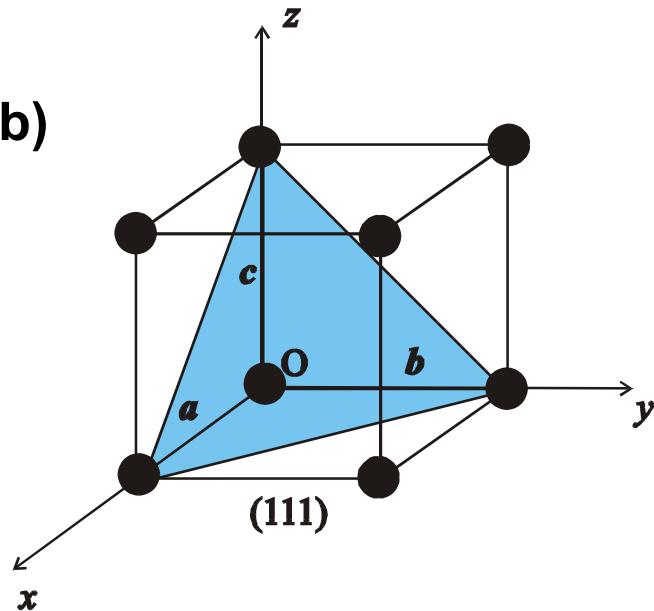
(a)



(100) plane (origin at O)

	$x$	$y$	$z$
Intercepts	$1a$	$\infty b$	$\infty c$
Intercepts (numbers only)	1	$\infty$	$\infty$
Reciprocal	1	0	0
Reduction	1	0	0
Enclosure	(100)		

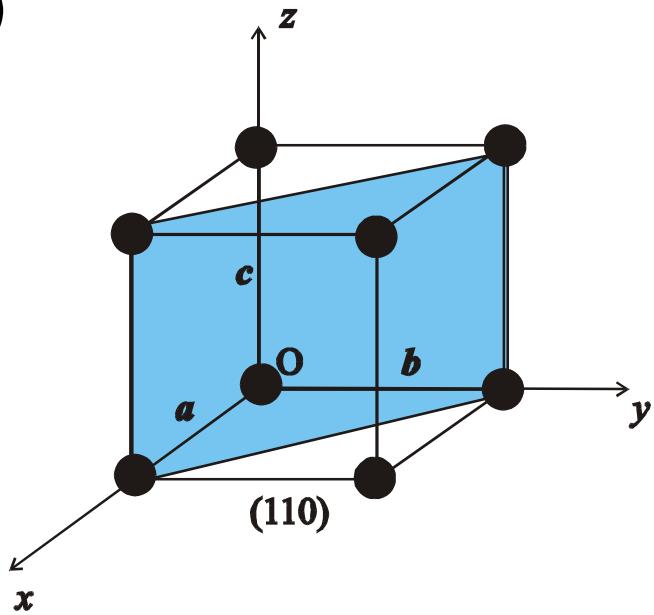
(b)



(111) plane (origin at O)

	$x$	$y$	$z$
Intercepts	$1a$	$1b$	$1c$
Intercepts (numbers only)	1	1	1
Reciprocal	1	1	1
Reduction	1	1	1
Enclosure	(111)		

(c)



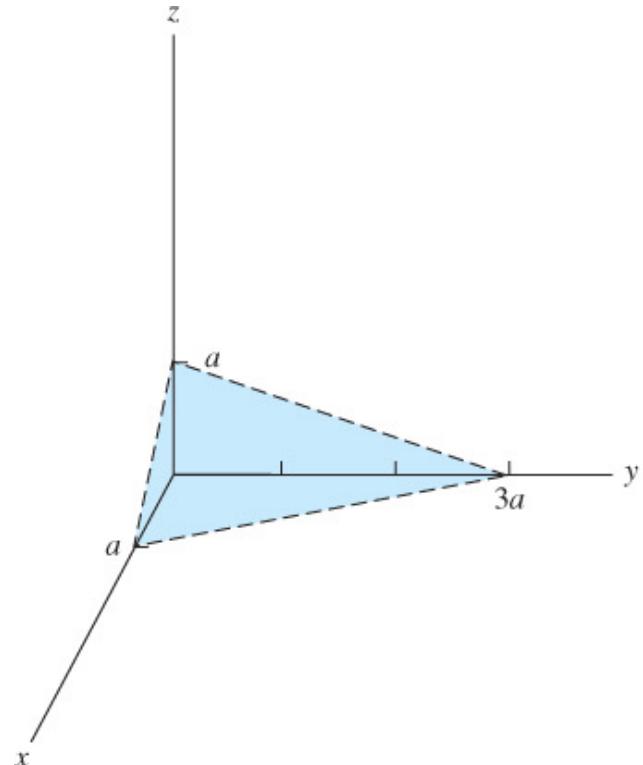
### (110) plane (origin at O)

	$x$	$y$	$z$
Intercepts	$1a$	$1b$	$\infty c$
Intercepts (numbers only)	1	1	$\infty$
Reciprocal	1	1	0
Reduction	1	1	0
Enclosure	(110)		

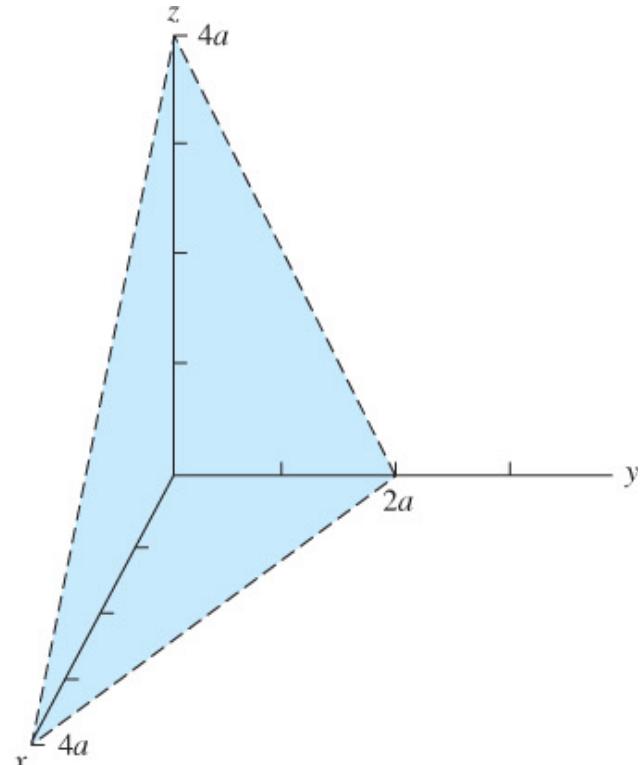
Silicon wafer surface is classified as (100) or (111)

# Problem 1

Determine the Miller indices for the planes shown below. [1.16]



(a)



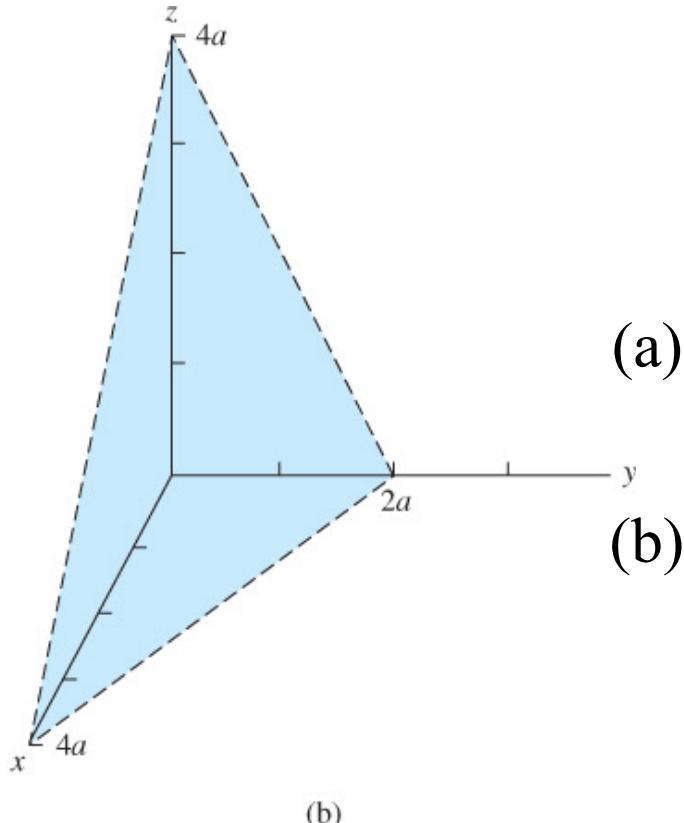
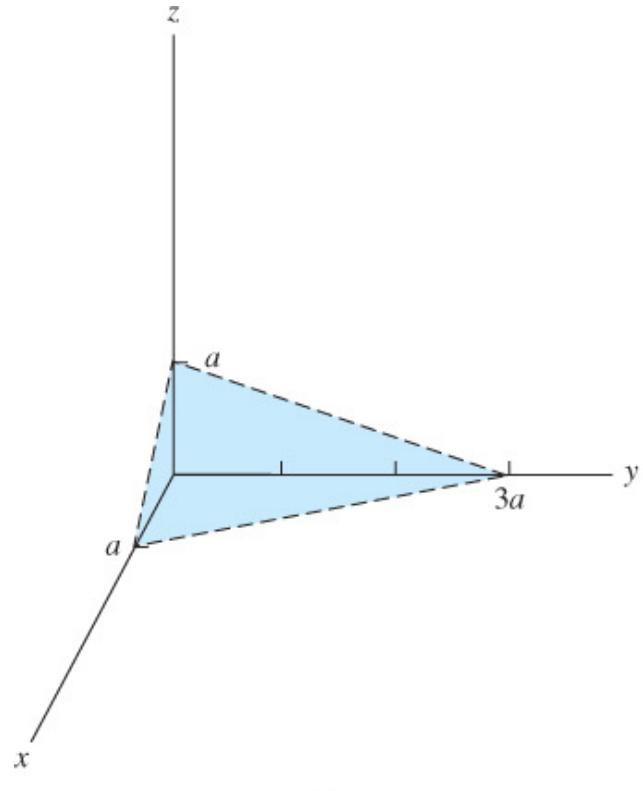
(b)

**Figure P1.16** | Figure for Problem 1.16.



# Problem 1

Determine the Miller indices for the planes shown below. [1.16]

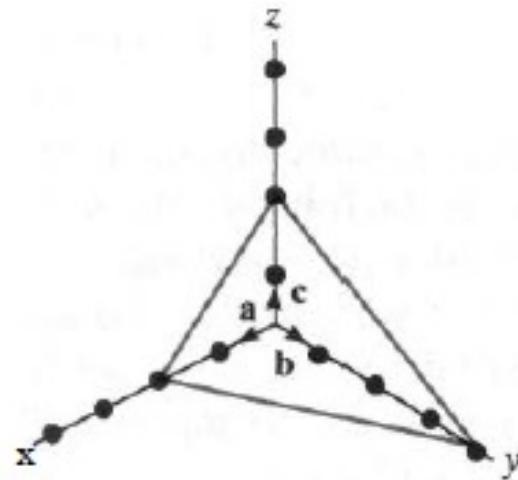
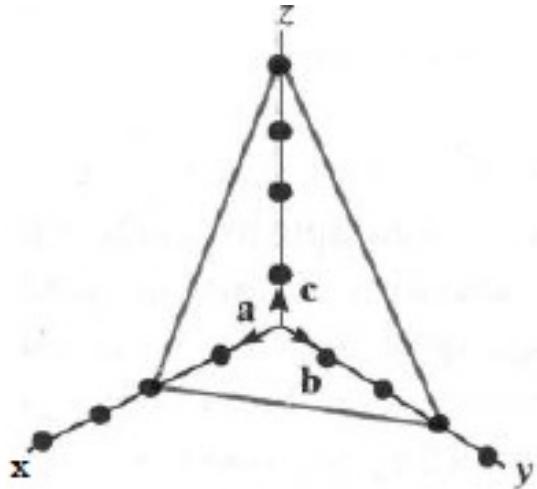


$$(a) \left( \frac{1}{1}, \frac{1}{3}, \frac{1}{1} \right) \Rightarrow (313)$$
$$(b) \left( \frac{1}{4}, \frac{1}{2}, \frac{1}{4} \right) \Rightarrow (121)$$

Figure P1.16 | Figure for Problem 1.16.

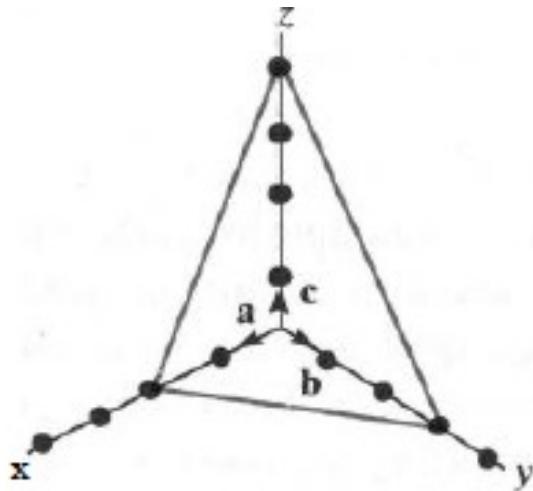
## Problem 2

Determine the Miller indices for the planes shown below.

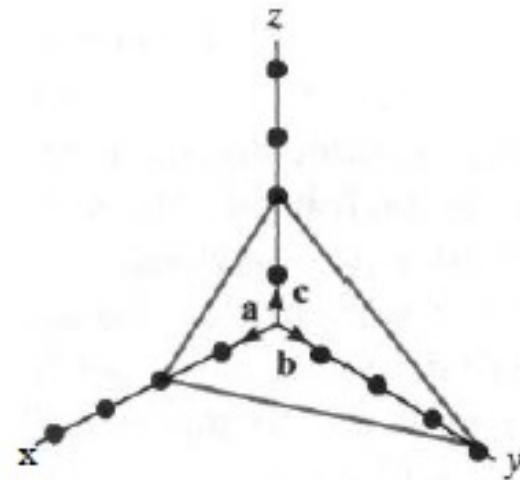


## Problem 2

Determine the Miller indices for the planes shown below.



x	y	z
2	3	4
1/2	1/3	1/4
6	4	3



x	y	z
2	4	2
1/2	1/4	1/2
2	1	2

How do you determine the Miller indices for a plane that intercepts the origin?

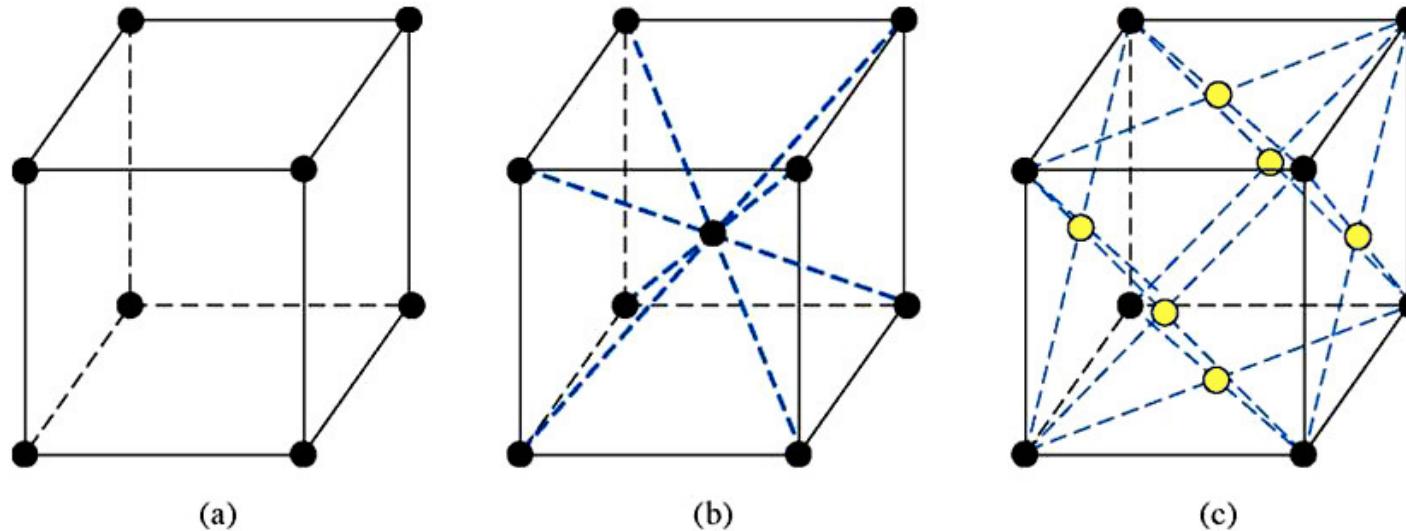
## Key takeaways (Lecture #3)

- Types of solid:
  - Amorphous, poly-crystalline, crystalline
- A unit cell is a small volume of crystal that can be used to reproduce the entire crystal.
- A crystallographic direction is defined as a line between two points, a vector.
- Planes in a crystal are specified by Miller indices.

# **Lecture 4**

## 2.4 Basic Crystal Structures

Three simple structures are shown in Fig. 2.6:



Three lattice types: (a) simple cubic, (b) body-centered cubic, (c) face-centered cubic

<http://www.dawgsdk.org/crystal/en/library/>

Fig. 2.6

The vectors  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{c}$  of the unit cells are perpendicular to each other and have equal lengths.

- for simple cubic crystal structure
  - *one lattice point located at each corner of the cube*
- for body-centered cubic crystal structure
  - *one lattice point located at each corner of the cube & an additional lattice point at the center of the cube*
- for face-centered cubic crystal structure
  - *one lattice point located at each corner of the cube & additional lattice points on each face plane*

- To have a crystal, one or more atoms/molecules can be placed identically at each lattice point
- Length of the cube side is termed as the **lattice constant**
- By knowing the crystal structure & the lattice dimensions, we are able to determine the *surface density* (# atoms/cm<sup>2</sup>) & *volume density* of atoms (# atoms/cm<sup>3</sup>)

## Problems

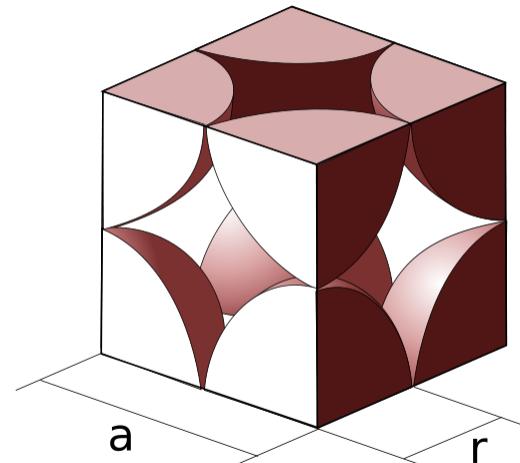
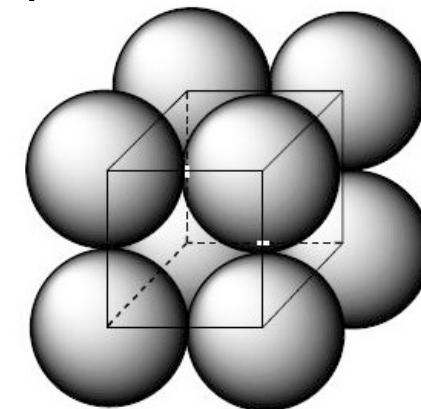
Q1: The volume density of atoms for a simple cubic lattice is  $4 \times 10^{22} \text{ cm}^{-3}$ . Assume that the atoms are hard spheres with each atom touching its nearest neighbor. Determine the lattice constant and the radius of the atom. (TYU 1.1)

$$\text{Number of atoms per unit cell} = 8 \times \frac{1}{8} = 1$$

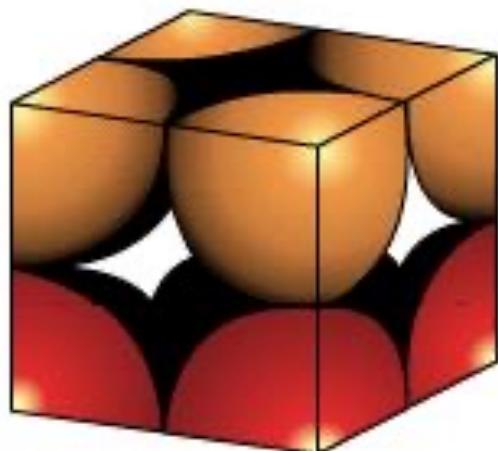
$$\text{Volume Density} = 4 \times 10^{22} = \frac{1}{a^3}$$

$$\Rightarrow a = 2.92 \times 10^{-8} \text{ cm} = 2.92 \text{ } \overset{\circ}{\text{\AA}}$$

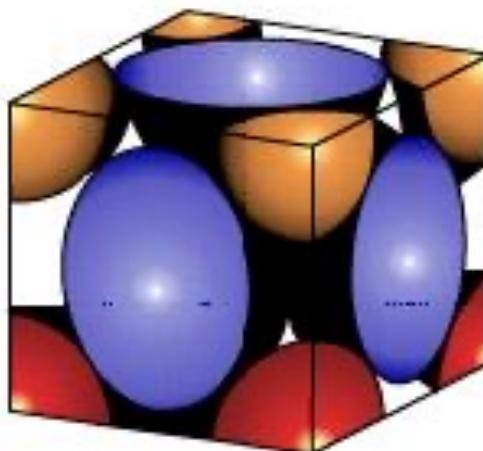
$$\text{Radius} = r = a/2 = 1.46 \text{ } \overset{\circ}{\text{\AA}}$$



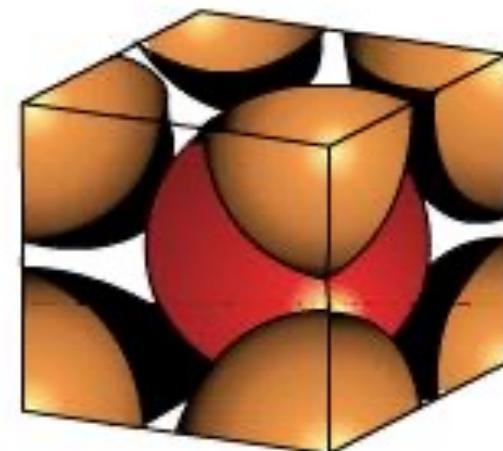
# Effective number of atom



(a) Simple cubic



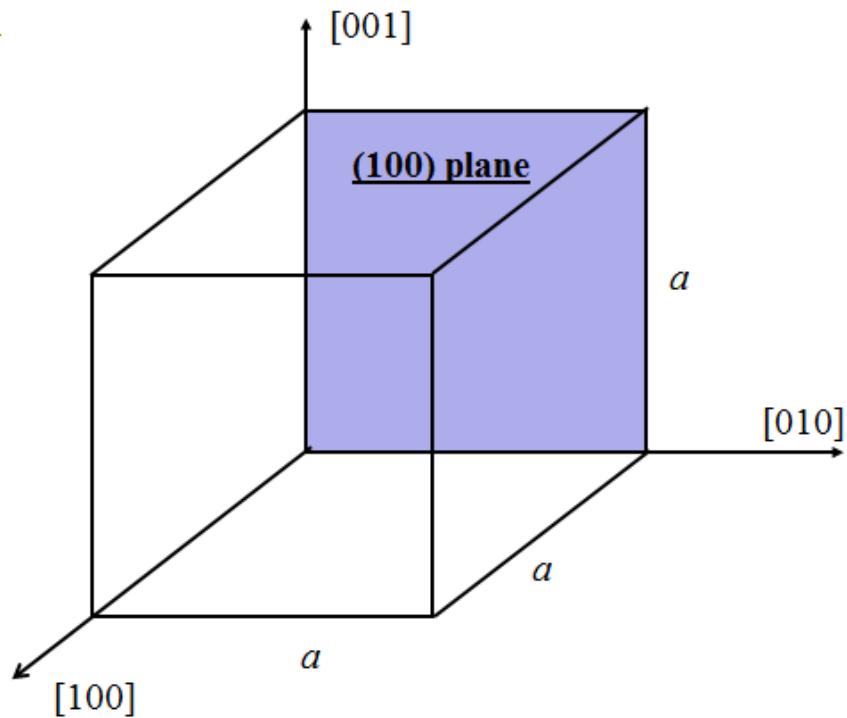
(b) Face centred cubic



(c) Body centred cubic

Three dimensional view showing the number of atoms per unit cell

Q2: Consider a simple cubic structure with a lattice constant of  $a = 4.56\text{\AA}$ . Determine the surface density of atoms in the (a) (100) plane, (b) (110), plane and (c) (111) plane. (TYU 1.2)



Number of atoms per (100) lattice plane

$$= 4 \times \frac{1}{4} = 1$$

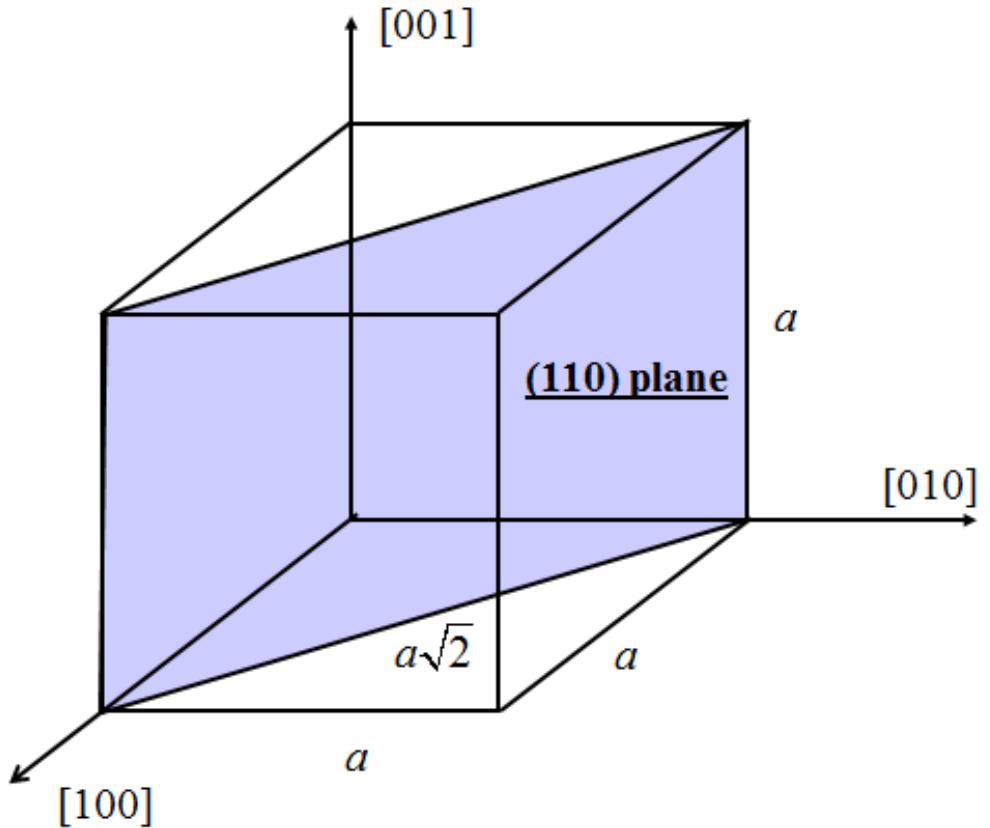
$$\begin{aligned}\text{Surface Density} &= \frac{1}{a^2} = \frac{1}{(4.65 \times 10^{-8})^2} \\ &= 4.62 \times 10^{14} \text{ cm}^{-2}\end{aligned}$$

(b) Number of atoms per (110) lattice plane

$$= 4 \times \frac{1}{4} = 1$$

Surface Density

$$\begin{aligned} &= \frac{1}{(a)(a\sqrt{2})} = \frac{1}{(4.65 \times 10^{-8})^2 \sqrt{2}} \\ &= 3.27 \times 10^{14} \text{ cm}^{-2} \end{aligned}$$



(c) Number of atoms per (111) lattice plane

$$= 3 \times \frac{1}{6} = \frac{1}{2}$$

$$\text{Lattice plane area} = \frac{1}{2} b h$$

$$\text{where } b = a\sqrt{2}$$

$$h = \left[ (a\sqrt{2})^2 - \left( \frac{1}{2} a\sqrt{2} \right)^2 \right]^{1/2}$$

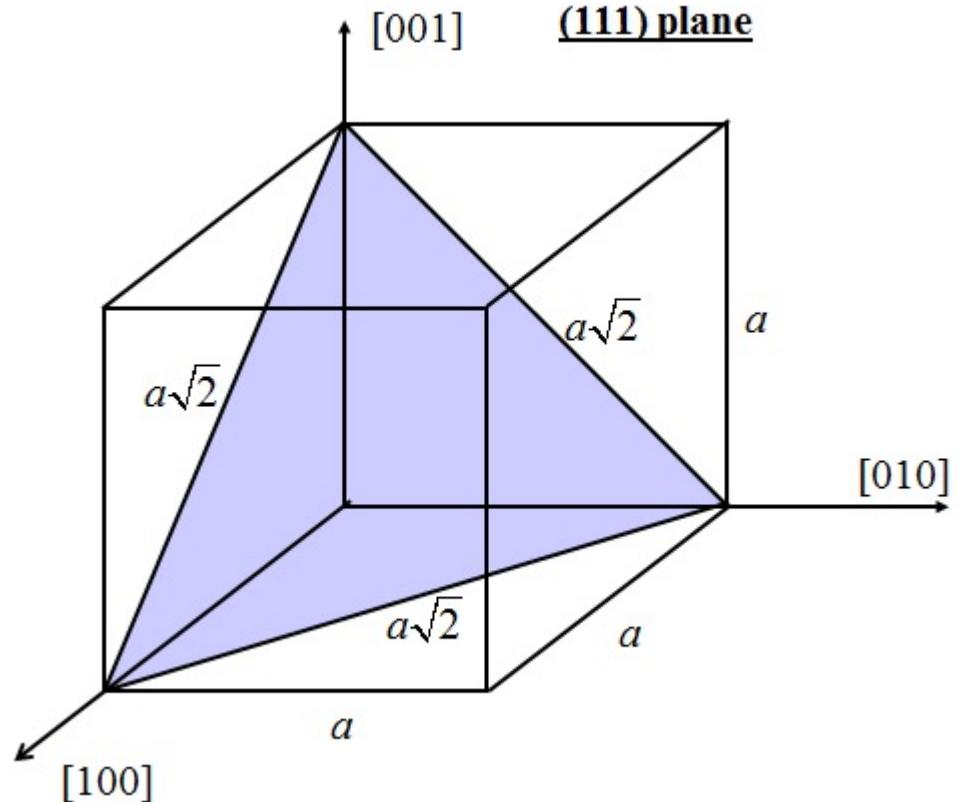
$$= \left[ 2a^2 - \frac{1}{2}a^2 \right]^{1/2} = a\sqrt{\frac{3}{2}}$$

Then lattice plane area

$$= \frac{1}{2} \left( a\sqrt{2} \right) \left( a\sqrt{\frac{3}{2}} \right) = \frac{\sqrt{3}}{2} a^2$$

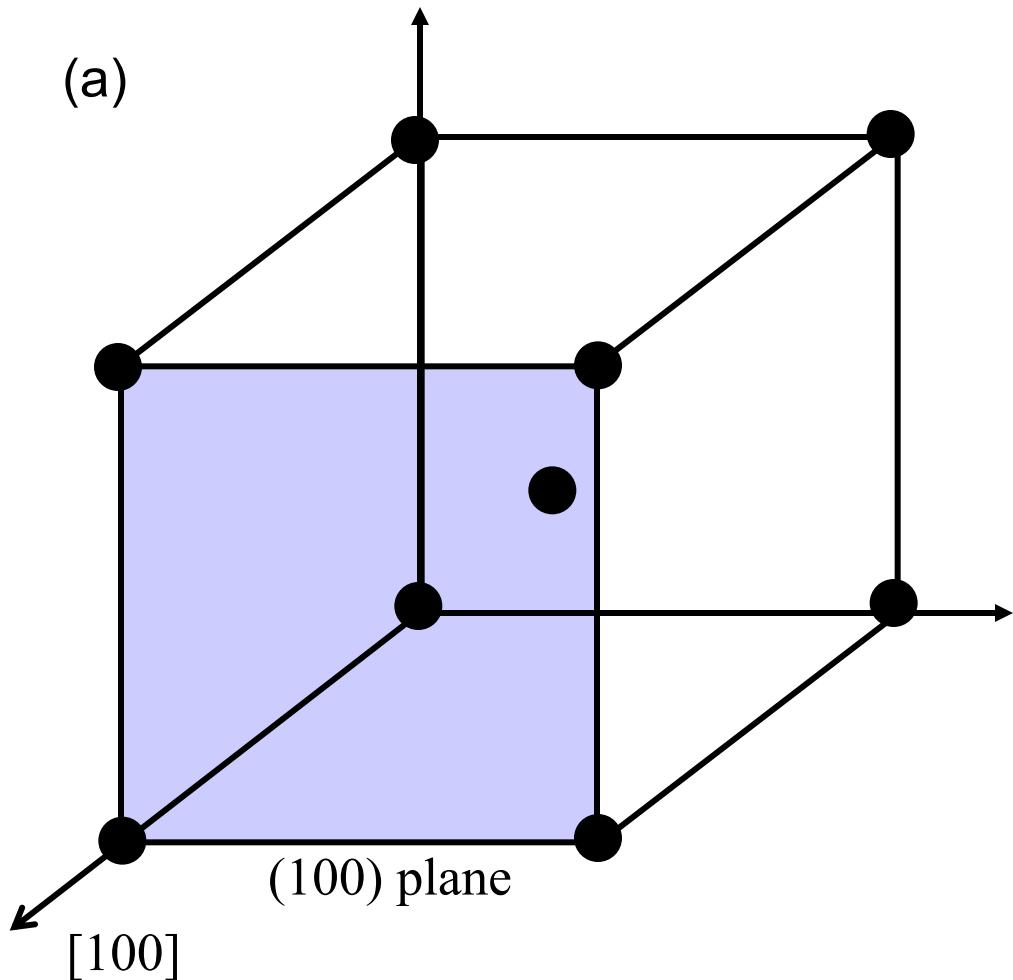
Surface Density

$$= \frac{\frac{1}{2}}{\frac{\sqrt{3}}{2} \left( 4.65 \times 10^{-8} \right)^2} = 2.67 \times 10^{14} \text{ cm}^{-2}$$

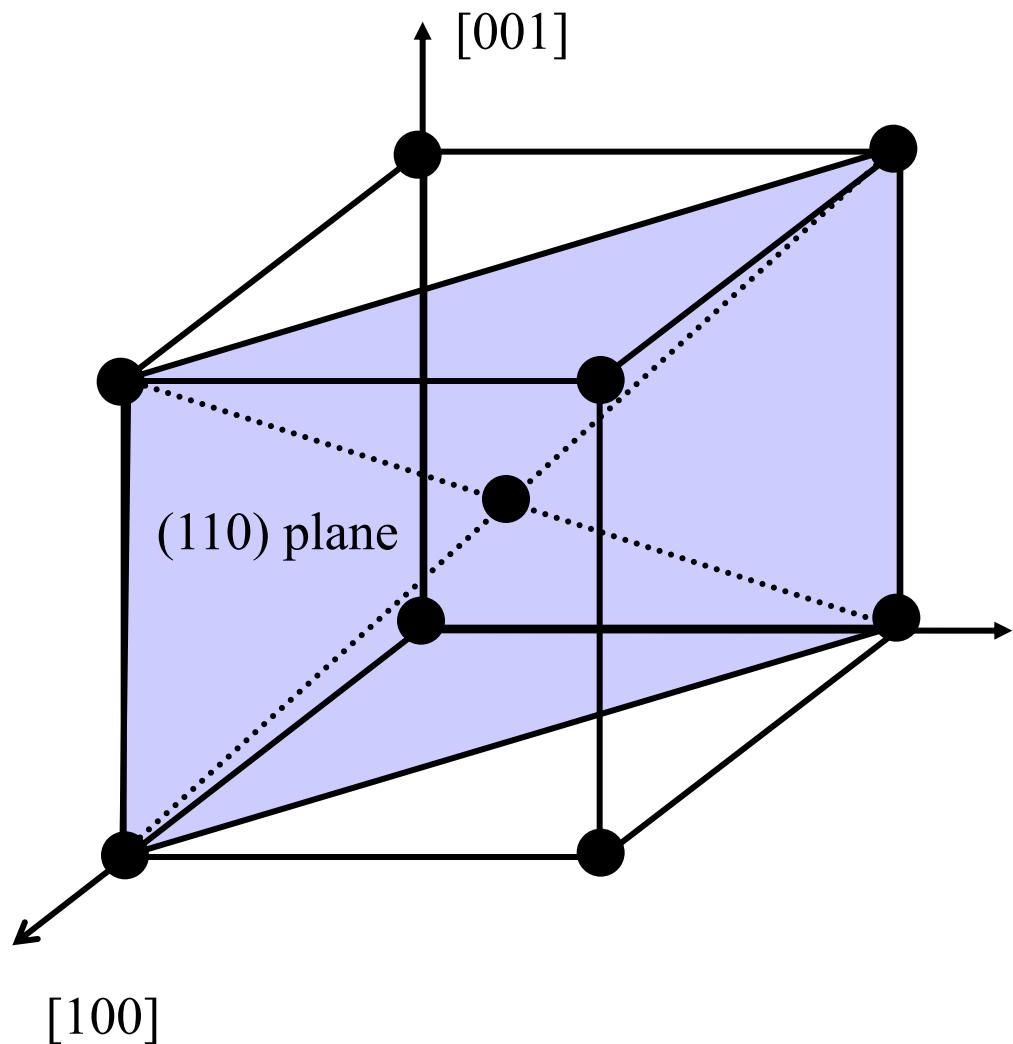


*For SC, (100) has the highest surface density of atoms. How about BCC and FCC? (See Tutorial 1)*

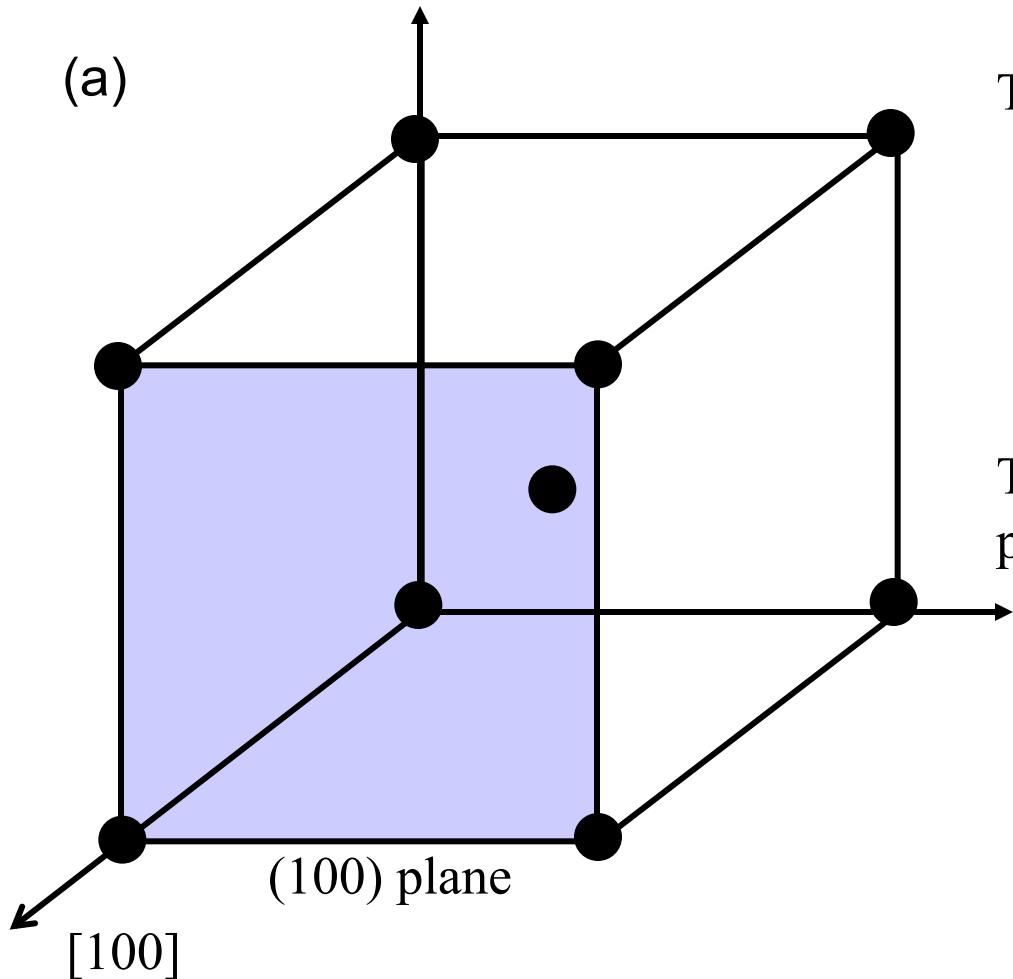
Q3. The lattice constant of a body-centered cubic structure is 4 Å. Calculate the surface density of atoms for (a) a (100) plane and (b) a (110) plane.



(b)



Q3. The lattice constant of a body-centered cubic structure is 4 Å. Calculate the surface density of atoms for (a) a (100) plane and (b) a (110) plane.



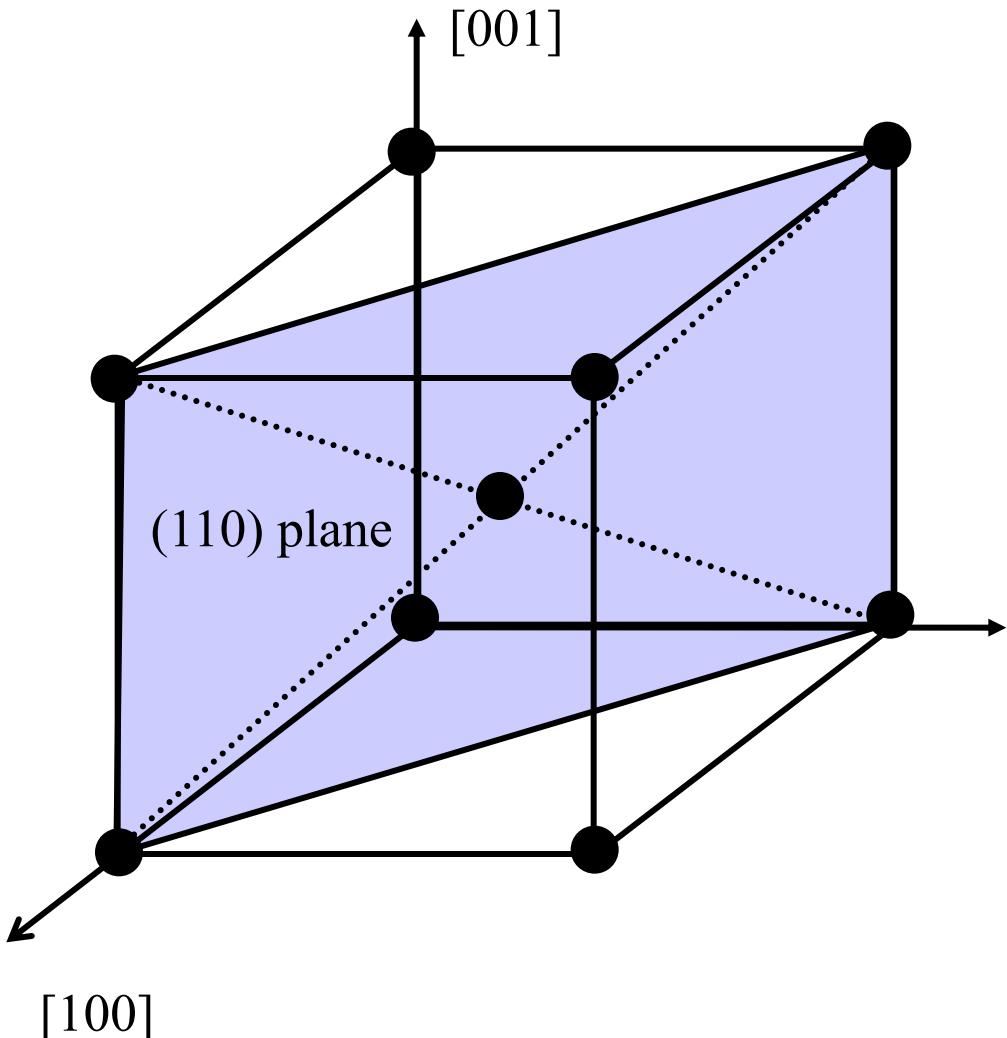
The surface area of (100) plane =

$$(4 \times 10^{-8})^2 = 1.6 \times 10^{-15} \text{ cm}^2$$

The surface density of atoms on (100) plane =

$$\frac{4 \times 1/4}{1.6 \times 10^{-15}} = 6.25 \times 10^{14} / \text{cm}^2$$

(b)



The surface area of (110) plane =

$$(4 \times 10^{-8}) (4\sqrt{2} \times 10^{-8}) = 2.26 \times 10^{-15} \text{ cm}^2$$

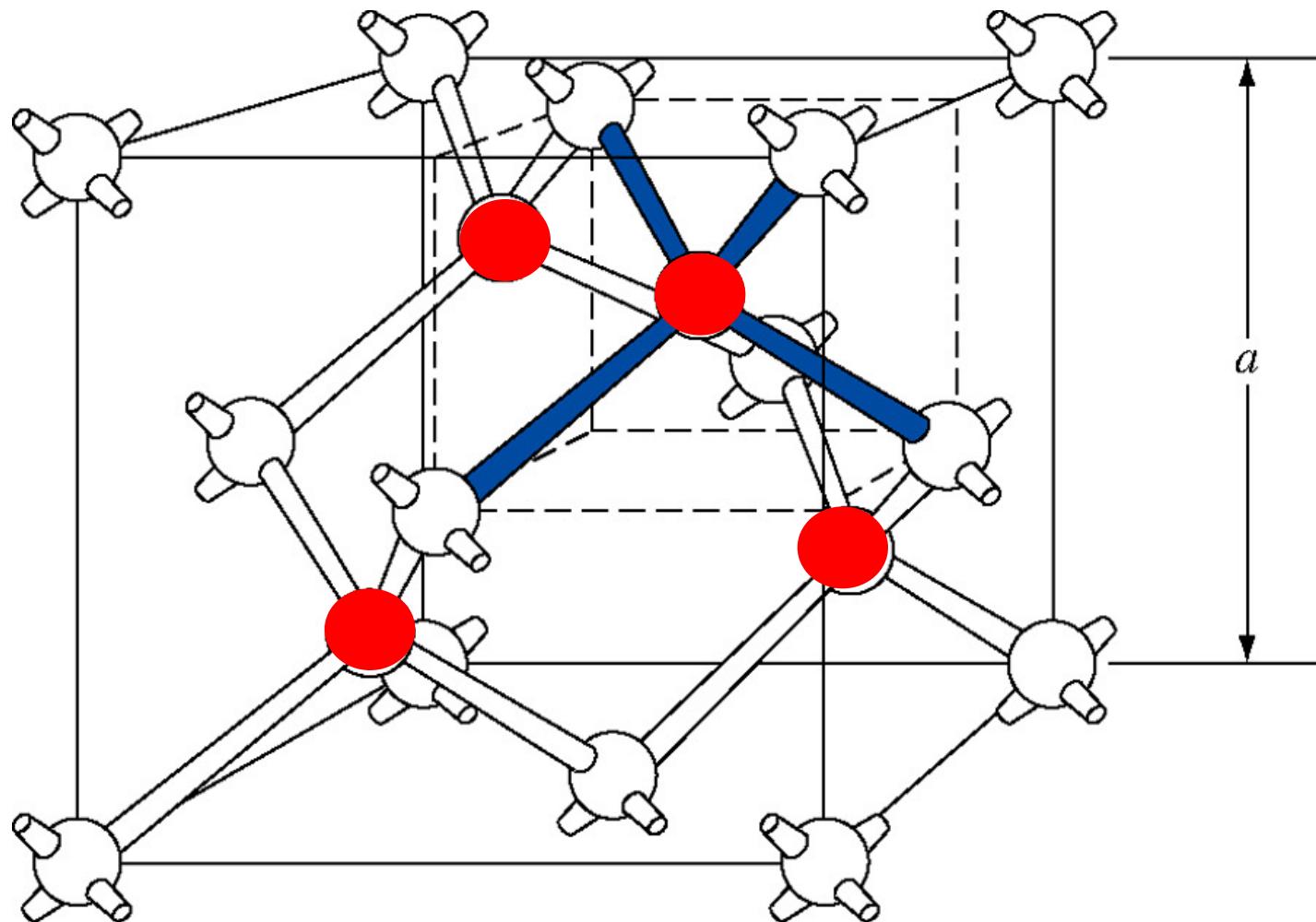
The surface density of atoms on (110) plane =

$$\frac{4 \times 1/4 + 1}{2.26 \times 10^{-15}} = 8.85 \times 10^{14} / \text{cm}^2$$

## 2.5 Semiconductor Crystals

Fig. 2.7 shows diamond crystal structure

- Silicon and Germanium have this structure
- All atoms are of the same species
- Any atom within the diamond structure will have four nearest neighboring atoms
  - they are bonded by covalent bonding



**Fig. 2.7** The diamond structure

<http://www.dawgsdk.org/crystal/en/library/>

- Silicon crystal can be regarded as a face-centered cubic structure with 2 silicon (Si) atoms at each lattice point
  - the relative position of the Si atoms at each lattice point are  $(0,0,0)$  and  $(a/4,a/4,a/4)$

Fig. 2.8

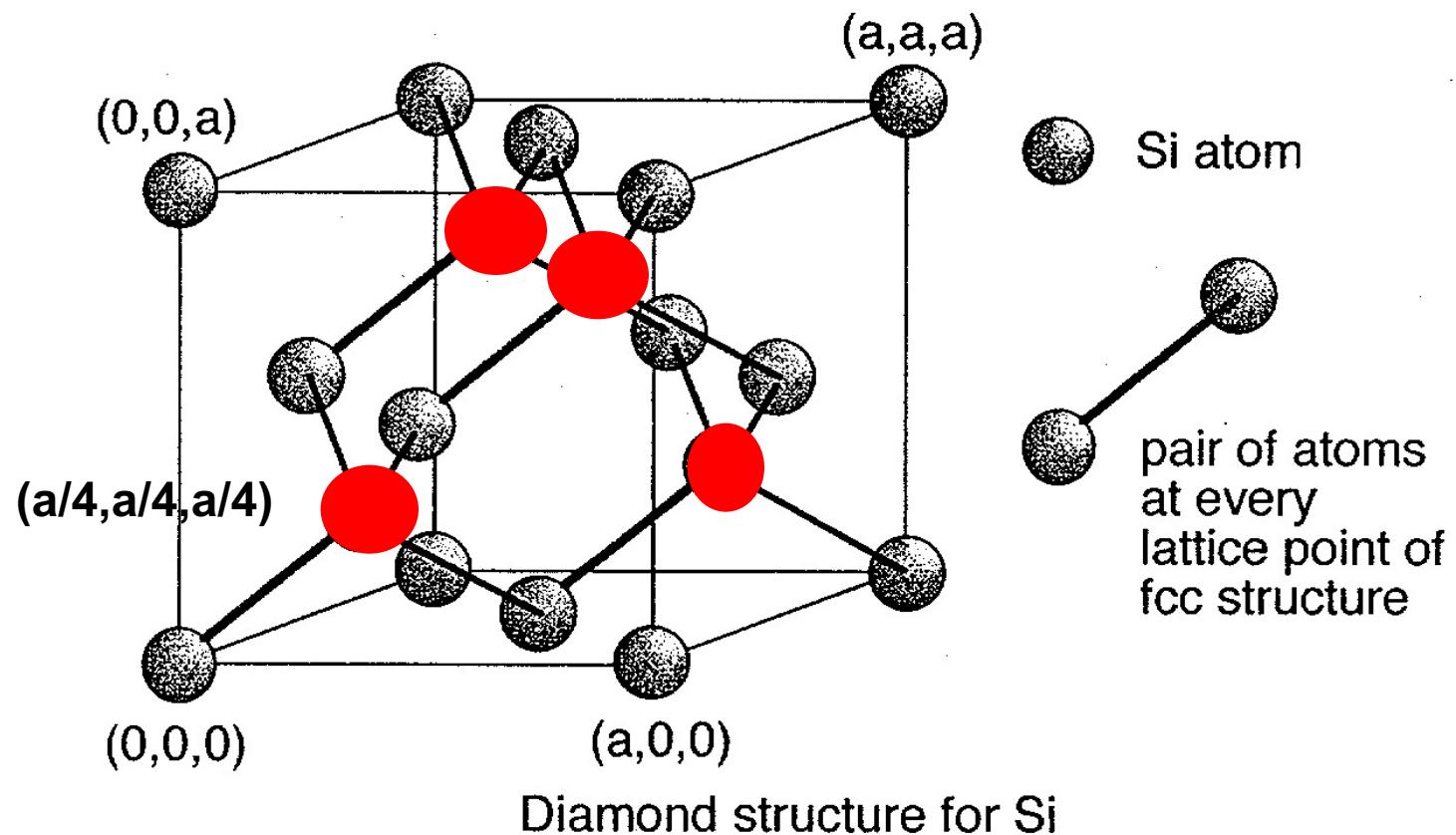
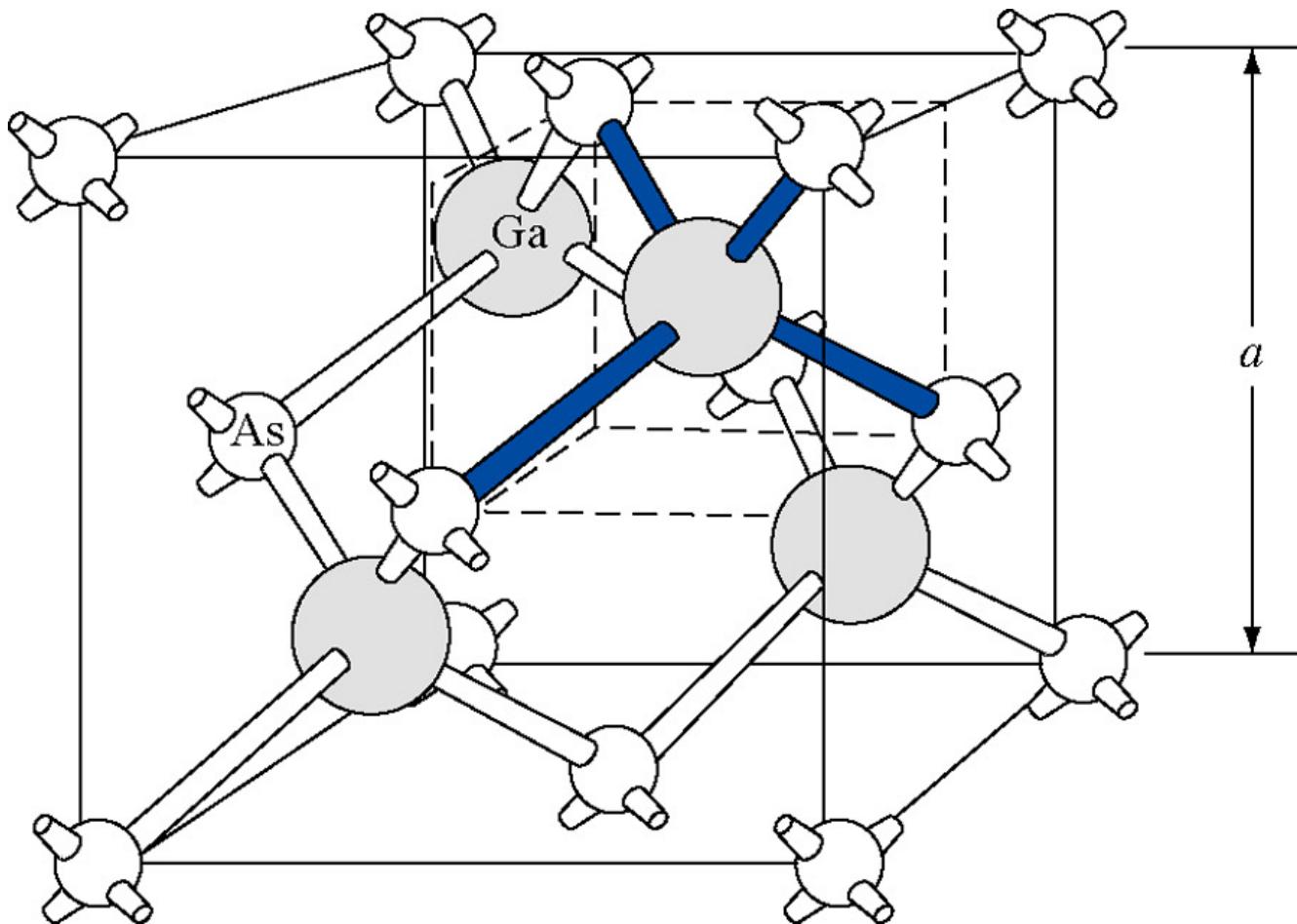


Fig. 2.9 shows a zincblende (sphalerite) crystal structure:

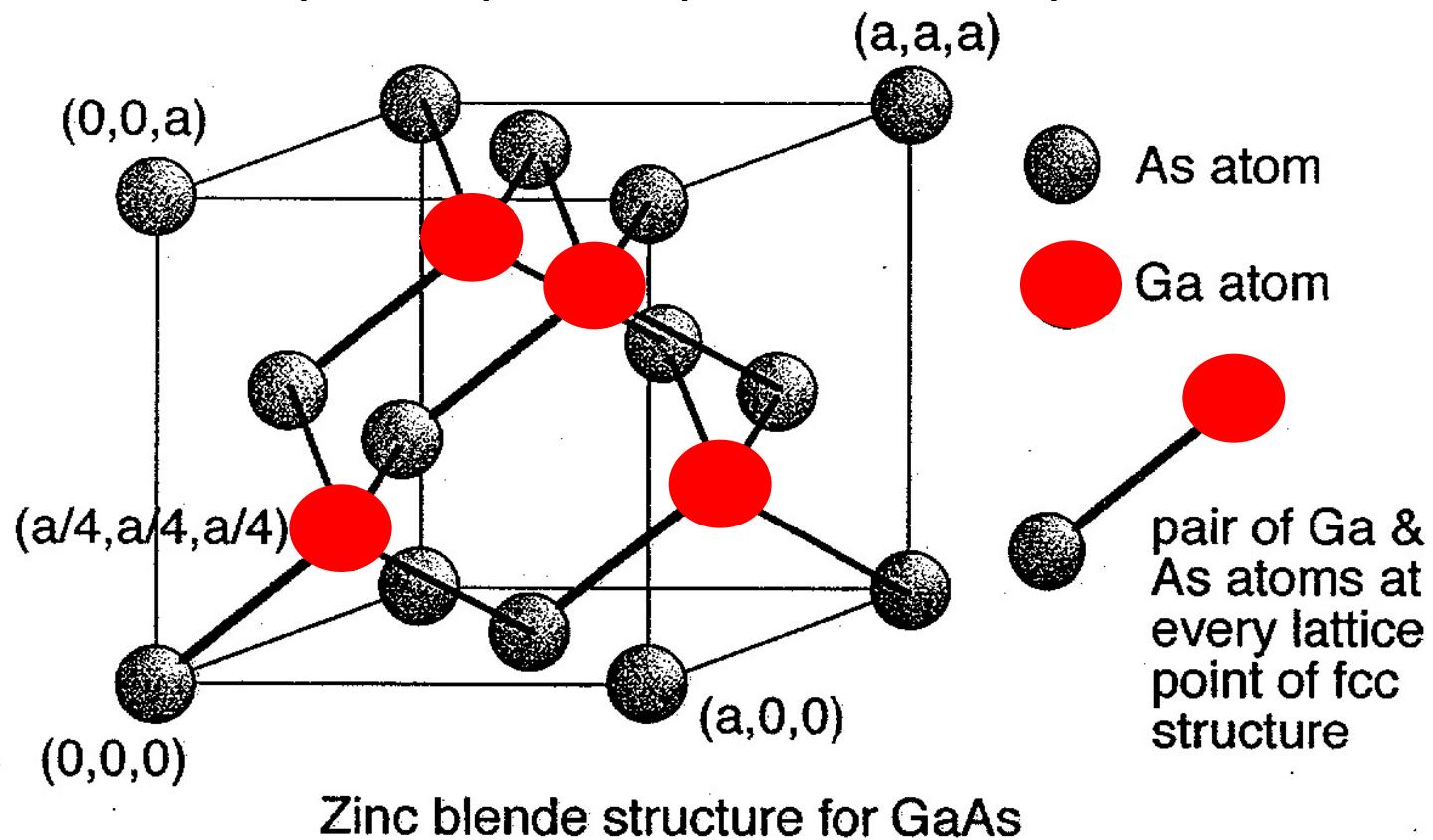
- This structure differs from the diamond structure only in that there are two different types of atoms in the lattice
- Most compound semiconductors, e.g. GaAs (gallium arsenide) and InP (indium phosphide) have this structure
- For a GaAs crystal, each Ga atom has 4 nearest As neighbors and each As atom has 4 nearest Ga neighbors
  - they are bonded by covalent bonding



**Fig. 2.9** The zincblende (sphalerite) lattice of GaAs

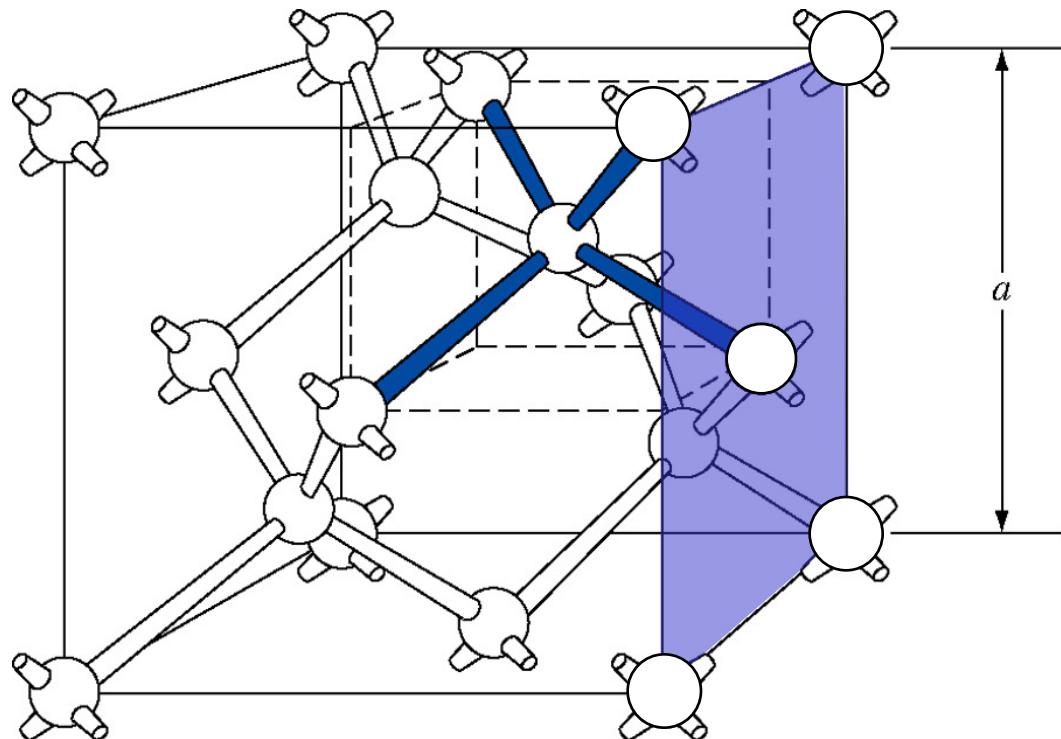
<http://www.dawgsdk.org/crystal/en/library/>

- GaAs crystals can also be considered as face-centered cubic with one Ga atom and one As atom at each lattice point
  - the relative position of the Ga and As atoms at each lattice point are  $(0,0,0)$  and  $(a/4,a/4,a/4)$

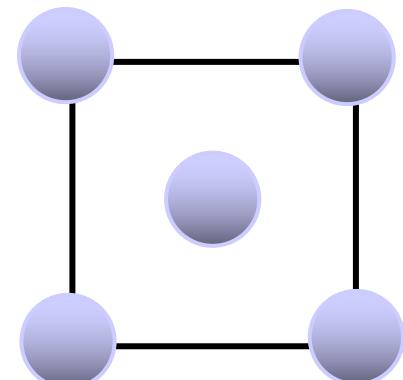


## Example 2.3

Calculate the surface density of atoms (# atoms/cm<sup>2</sup>) on the shaded plane [(010) plane] of a silicon crystal shown. The lattice constant for silicon is 5.43Å (1Å = 10<sup>-10</sup> m).



The silicon crystal has the face-centered cubic structure. The indicated plane can be redrawn as :



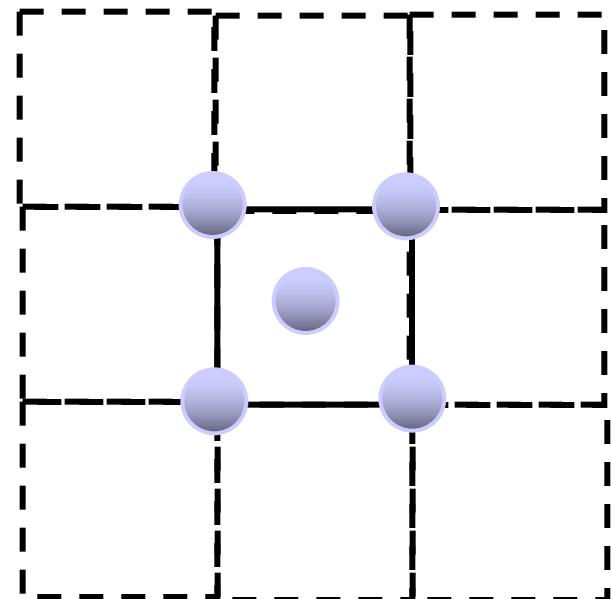
Notice that the atom at each corner is shared by 4 similar equivalent lattice planes, so each corner atom effectively contributes  $1/4$  atom to the indicated lattice plane.

The atom in the middle of the plane is not shared by any other plane.

Hence, no. of atoms on the plane is  
 $4(1/4) + 1 = 2$  atoms

Therefore,

$$\text{Surface density} = \frac{\text{No. of atoms}}{a^2} = \frac{2}{(5.43 \times 10^{-8} \text{ cm})^2}$$
$$= 6.78 \times 10^{14} \text{ atoms/cm}^2$$



# Problems

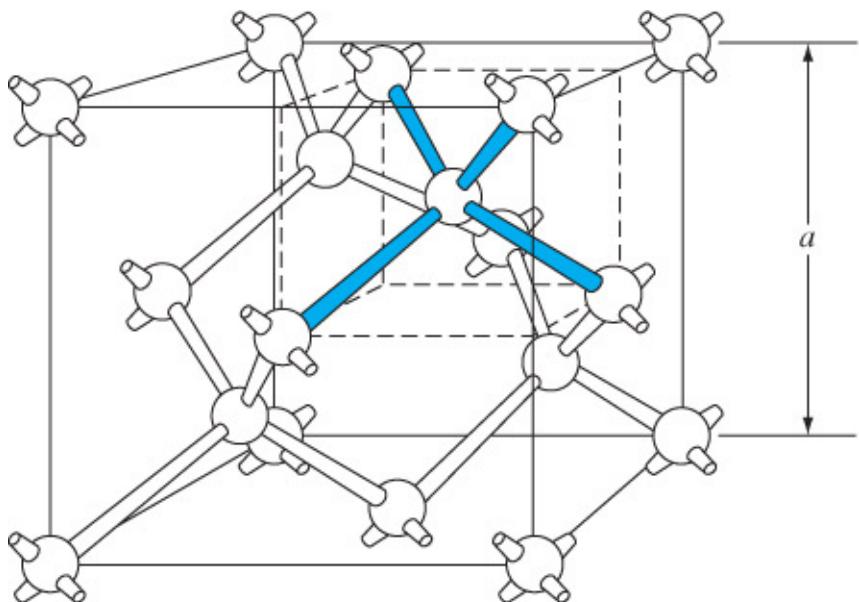


Figure 1.11 | The diamond structure.

Q1: Consider the diamond unit cell shown in Fig. 1.11. Determine the (a) number of corner atoms, (b) number of face-centered atoms, and (c) number of atoms totally enclosed in the unit cell. (TYU 1.4)

- (a) 8 corner atoms
- (b) 6 face-centered atoms
- (c) 4 atoms totally enclosed

Q2: The lattice constant of silicon is 5.43Å. Calculate the volume density of silicon atoms.

Number of atoms in the unit cell

$$= 8 \times \frac{1}{8} + 6 \times \frac{1}{2} + 4 = 8$$

$$\begin{aligned}\text{Volume Density} &= \frac{8}{a^3} = \frac{8}{(5.43 \times 10^{-8})^3} \\ &= 5 \times 10^{22} \text{ cm}^{-3}\end{aligned}$$

Q3: Calculate the density of valence electrons in silicon. (1.22)

Density of silicon atoms =  $5 \times 10^{22} \text{ cm}^{-3}$  and  
4 valence electrons per atom, so

Density of valence electrons =  $2 \times 10^{23} \text{ cm}^{-3}$

Q4: The structure of GaAs is the zincblende lattice. The lattice constant is  $5.65\text{\AA}$ . Calculate the valence electrons in GaAs. (1.23)

Density of GaAs atoms

$$= \frac{8}{(5.65 \times 10^{-8})^3} = 4.44 \times 10^{22} \text{ cm}^{-3}$$

An average of 4 valence electrons per atom,

So

Density of valence electrons

$$= 1.77 \times 10^{23} \text{ cm}^{-3}$$

Q5: Calculate the mass density of GaAs. The lattice constant is 5.65Å.

GaAs:  $a = 5.65 \cdot 10^{-8}$  cm, 4 each Ga, As atoms/cell

$$\frac{4}{a^3} = \frac{4}{(5.65 \cdot 10^{-8} \text{ cm})^3} = 2.22 \cdot 10^{22} \frac{1}{\text{cm}^3}$$

$$\text{density} = \frac{2.22 \cdot 10^{22} \frac{1}{\text{cm}^3} \cdot (69.7 + 74.9) \frac{\text{g}}{\text{mol}}}{6.02 \cdot 10^{23} \frac{1}{\text{mol}}} = 5.33 \frac{\text{g}}{\text{cm}^3}$$

## Key takeaways (Lecture #4)

- Three basic types of crystal structure:
  - SC, BCC, FCC
- It is essential to determine the effective number of atoms on a surface and within the unit cell
- Silicon and Germanium both have the diamond structure, while GaAs has the zinc blonde structure

# Lecture 5

# 3 ENERGY BAND OF SEMICONDUCTOR

## 3.1 Molecular orbitals and energies (*for illustration, not required for exam*)

- First, consider the formation of energy levels when two hydrogen atoms are brought together to form a hydrogen molecule ( $H_2$ ). The  $H_2$  molecule are bonded by the covalent bonding.
- The electronic configuration of H atoms is



- The wave function of the 1s state:  $\Psi_{1s}$
- The energy of the 1s state:  $E_{1s}$

- When two hydrogen atoms, A and B, approach each other, the 1s wave function  $\Psi_{1s}$  of each individual H atom interact producing two new wave functions,  $\Psi_a$  and  $\Psi_b$ , with energies  $E_a$  and  $E_b$  respectively.

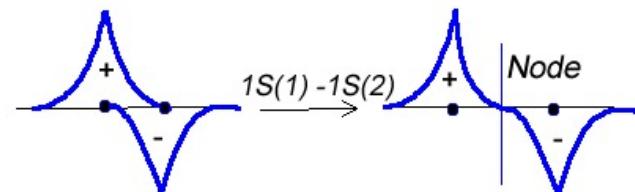
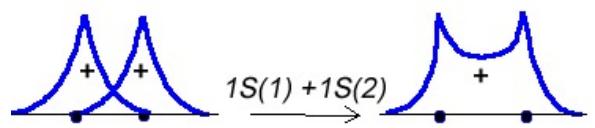
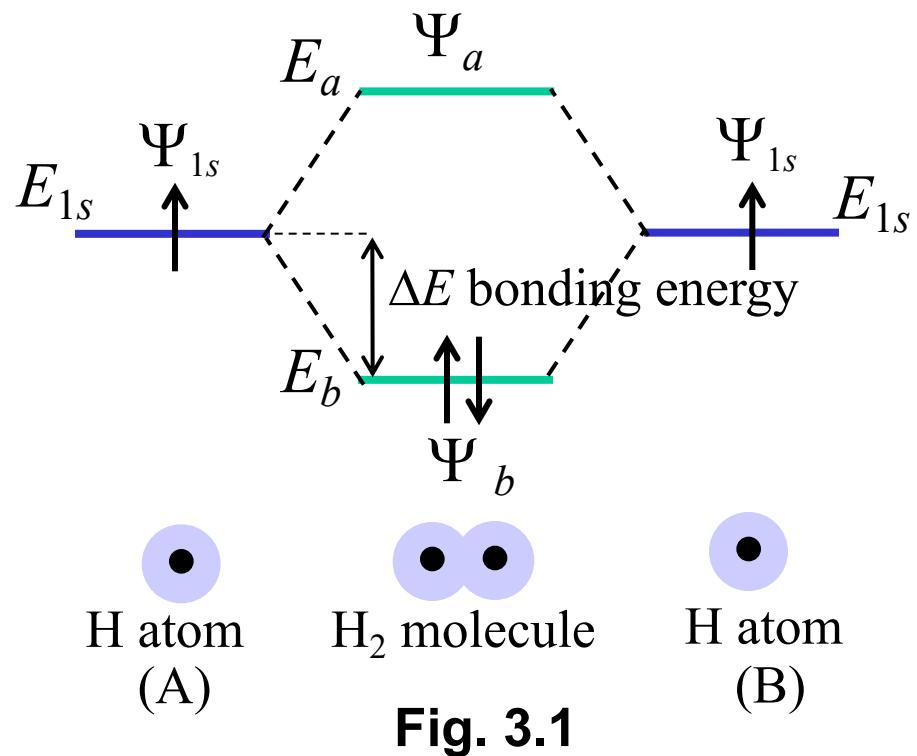
$\Psi\Psi$  Psi

- The wave functions  $\Psi_a$  and  $\Psi_b$  are obtained by linear combination of the individual atomic orbitals/wave functions (LCAO)

$$\Psi_a = \Psi_{1s}(A) + \Psi_{1s}(B) \quad (3.1)$$

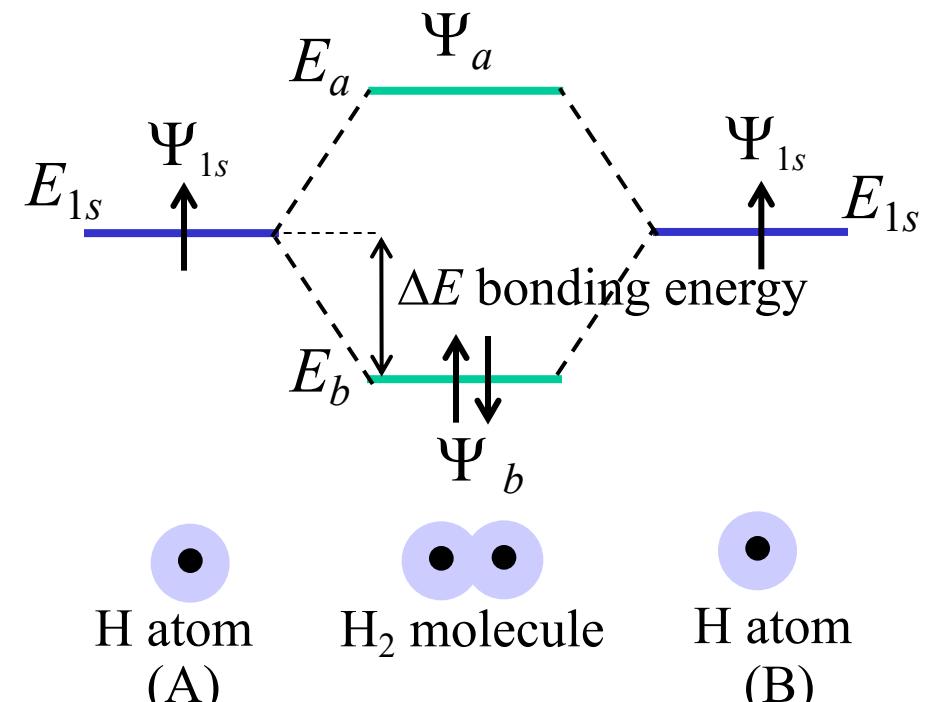
$$\Psi_b = \Psi_{1s}(A) - \Psi_{1s}(B)$$

$\Psi_{1s}(A)$  and  $\Psi_{1s}(B)$  are the 1s wave function of H atoms A and B respectively.



- The formation of the two new wave functions  $\Psi_a$  and  $\Psi_b$  is consistent with the Pauli exclusion principle, that is: this means we cannot have two identical  $\Psi_{1s}$  wave functions in the  $H_2$  molecule.
- The wave functions  $\Psi_a$  and  $\Psi_b$  are called the molecular orbital.
- Each wave function will have two distinct states: one spin up and one spin down. In other words, each wave function can accommodate two electrons.

- Before the interaction, each individual H atom has one electron in the 1s state/wave function.
- After the interaction, in the ground state, the two electrons will occupy the lowest energy wave function  $\Psi_b$ , one electron with spin up and the other electron with spin down.



- The lowering of the original energy before the interaction ( $E_{1s}$ ) and the ground state energy after the interaction ( $E_b$ ) is the bonding energy of the  $H_2$  molecule ( $\Delta E$ ).
- The formation of  $E_b$  and  $E_a$ , from the original energy  $E_{1s}$  is referred to as energy splitting

- The energy splitting, in other words is the separation of  $E_a$  and  $E_b$ , varies with the interatomic distance  $r$  between the two H atoms as shown in Fig. 3.2

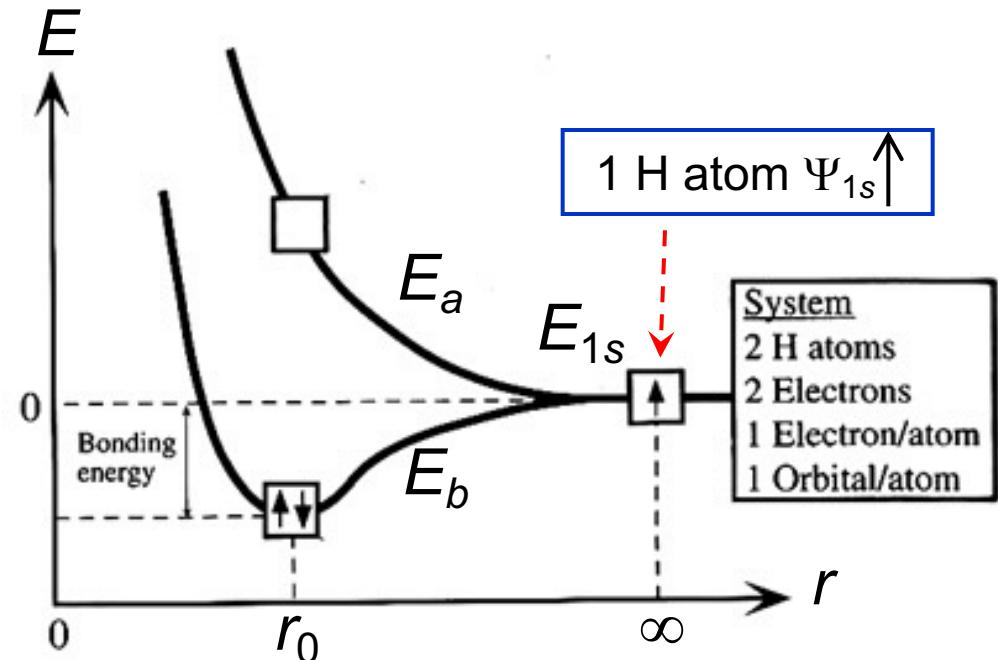
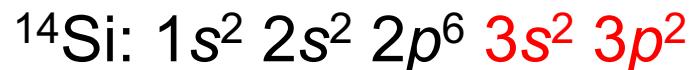


Fig. 3.2

- It is important to note here that:
  - the number of quantum states before interaction = the number of quantum states after interaction
  - the number of electrons before interaction = the number of electrons after interaction

## 3.2 Energy band: conduction and valence bands

- We can now look into the energy band formation in semiconductor crystals.
- Consider a silicon crystal consisting of  $N$  silicon atoms. The electronic configuration of an isolated silicon atom is

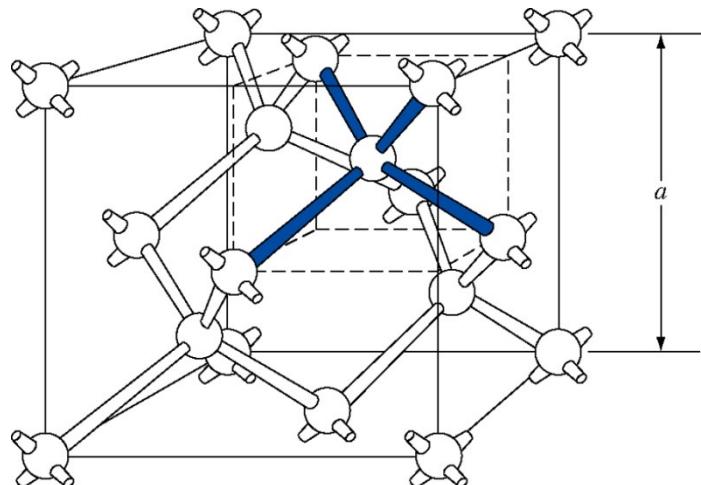


**Table 3.1**

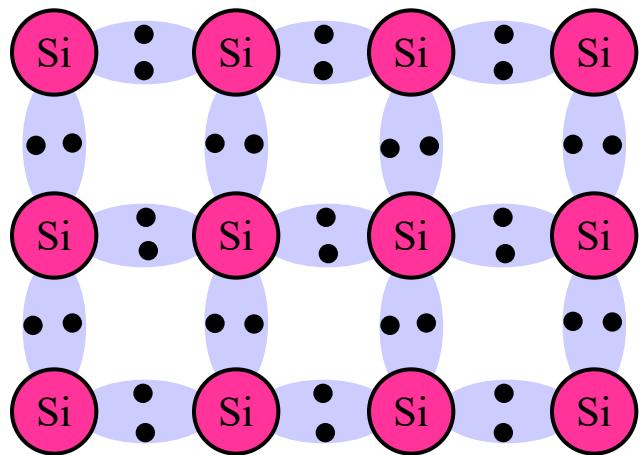
States	No. of states	No. of electrons
$1s$	$2N$	$2N$
$2s$	$2N$	$2N$
$2p$	$6N$	$6N$
$\textcolor{red}{3s}$	$\textcolor{red}{2N}$	$\textcolor{red}{2N}$
$\textcolor{red}{3p}$	$\textcolor{red}{6N}$	$\textcolor{red}{2N}$

- The number of states and electrons of  $N$  isolated Si atoms is given in Table 3.1

- The  $N$  silicon atoms are now brought together to form silicon crystal.
- Each Si atom shares its four valence electrons (2 electrons from each 3s and 3p states) with the four nearest neighbors to form stable configuration or to complete their subshells. As a result each Si atom is surrounded by 8 electrons.

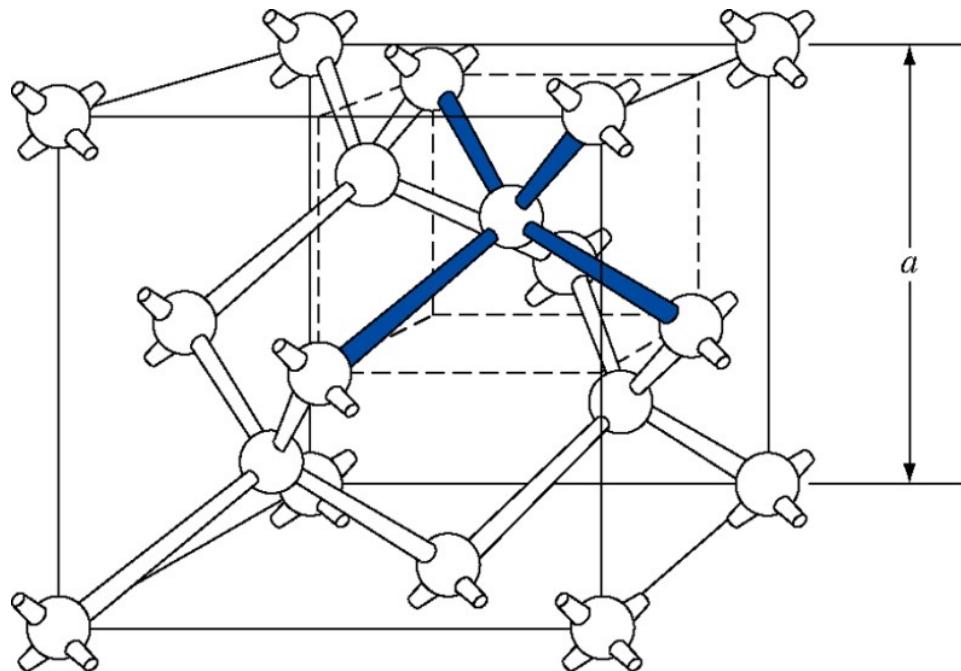


(a) 3-dimensional representation of the covalent bonding in Si crystal at 0 K



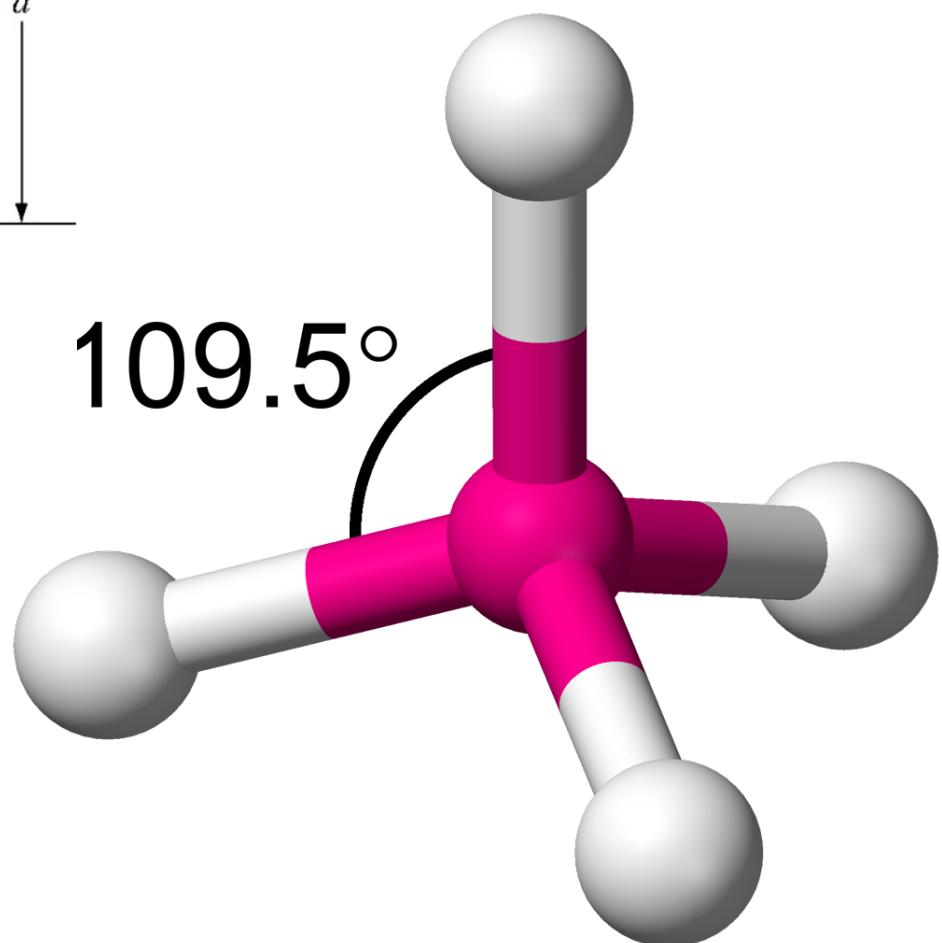
(b) 2-dimensional representation of the covalent bonding in Si crystal at 0 K

**Fig. 3.3 Covalent bonding of silicon crystal**



Tetrahedral

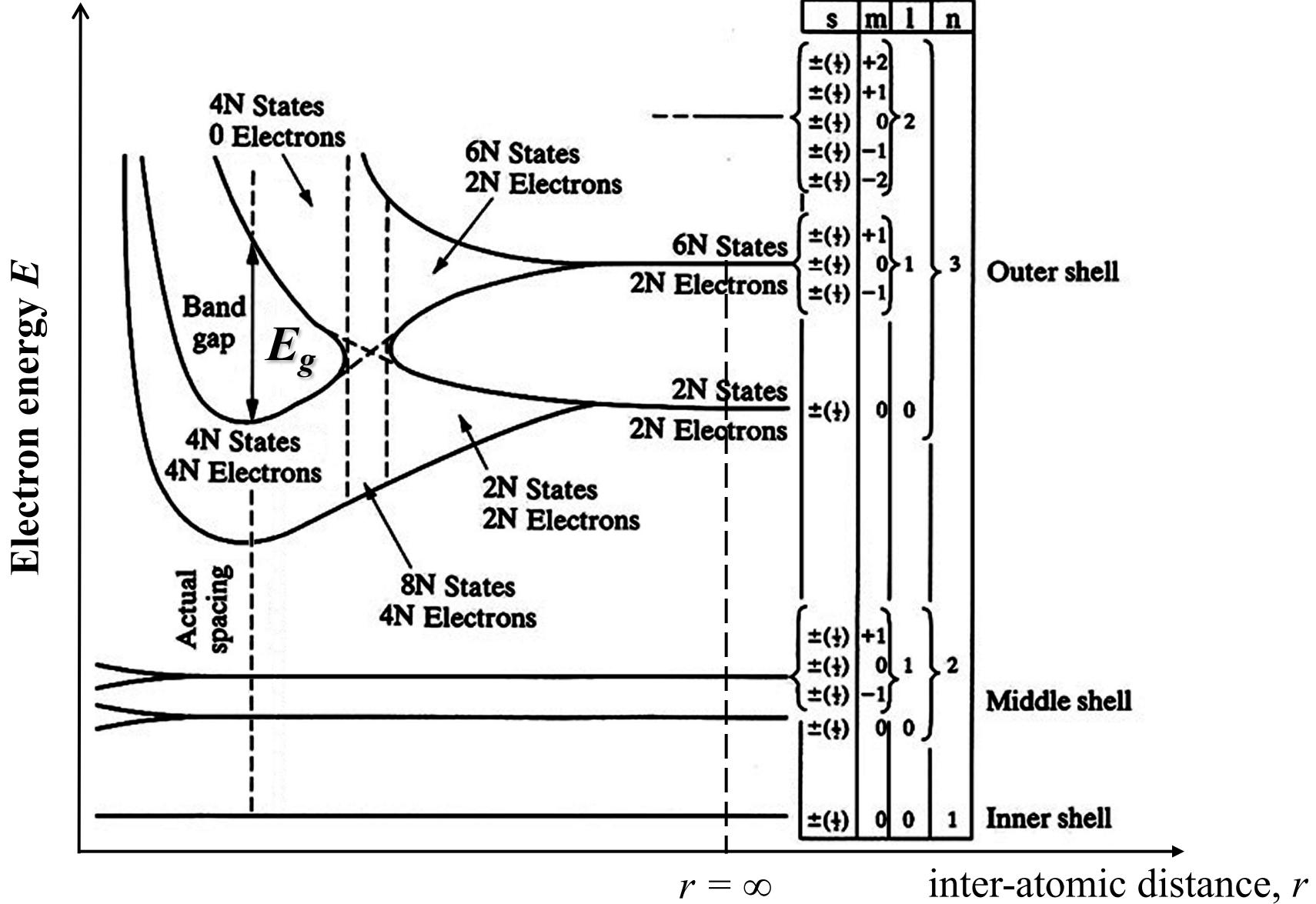
109.5°



- The formation of the energy band in Si crystal can be described as follow based on Fig. 3.4.
- As the inter-atomic distance decreases the outer shells  $3s$  and  $3p$  states interact:
  - The  $2N$  states of  $3s$  interact. The energy levels split forming  $3s$  band. There are  $2N$  states and  $2N$  electrons in the  $3s$  band.
  - The  $6N$  states of  $3p$  interact. The energy levels split forming  $3p$  band. There are  $6N$  states and  $2N$  electrons in this band.
  - The degree of the energy splitting increases with decreasing inter-atomic spacing.
  - Pauli exclusion principle: no two electrons in a given system may have the same quantum states.

- As the inter-atomic spacing decreases further, the  $3s$  and  $3p$  bands grow and merge into a single band composed of mixture of energy levels. This  $3s$ - $3p$  band contains  $8N$  states and  $4N$  electrons.
- Further decreasing the inter-atomic distance, approaching the equilibrium inter-atomic spacing, the  $3s$ - $3p$  band splits into two bands separated by an energy gap or a bandgap  $E_g$ .
  - The upper band, called the conduction band, contains  $4N$  states
  - and the lower band, called the valence band, also contains  $4N$  states.
- In a perfect crystal, there are no allowed energy levels (quantum states) in the bandgap for electrons to occupy. The bandgap is also called a “forbidden band”.

- At 0 K, the electrons will occupy the lowest energy states and therefore all  $4N$  available electrons occupy all  $4N$  states in the valence band.
- In other words, at 0 K the valence band is fully occupied and the conduction band is empty. In this state, the semiconductor is an insulator, no electrical conduction can take place.
  - for the electrical conduction to take place, electrons must be able to move into empty states. It follows that for the electrical conduction, the electrons must be excited to the conduction band.



**Fig. 3.4** Variation of electron energy with inter-atomic spacing

- The energy of the conduction and valence bands versus the physical distance  $x$  of the semiconductor sample can be represented by an energy band diagram as shown in Fig. 3.5
  - the energy refers to the electron energy
  - the physical distance  $x$  is normally not indicated
  - $E_c$  is the energy of the bottom of the conduction band, very often called the conduction band edge
  - $E_v$  is the energy of the top of the valence band, very often called the valence band edge

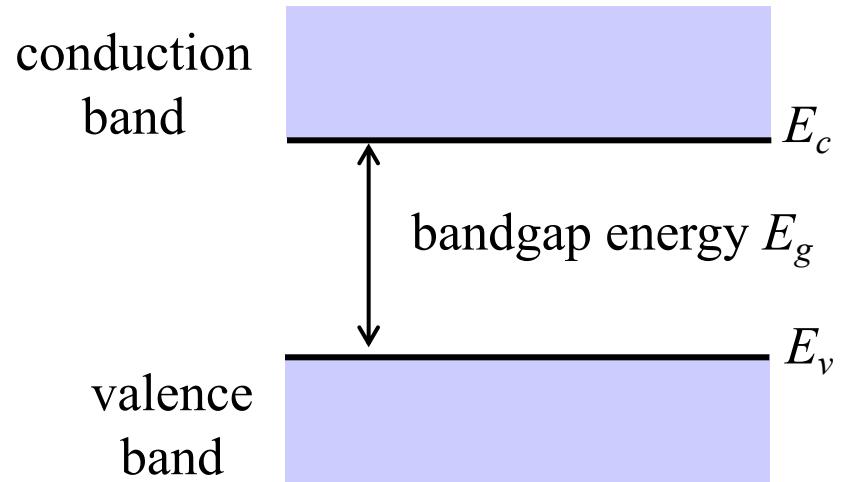
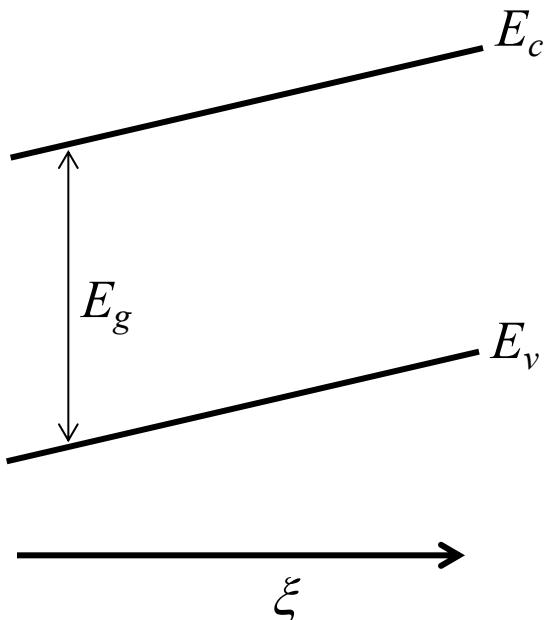


Fig. 3.5

- If an electric field  $\xi$  is applied to the semiconductor sample
  - the energy band is not flat anymore
  - the energy bands will be inclined at a gradient proportional to the electric field according to equation (3.2). The energy band diagram is shown in Fig. 3.6

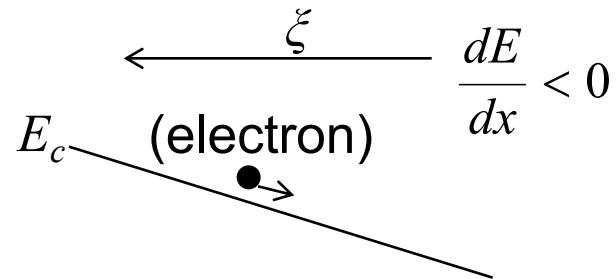


$$\xi = \frac{1}{q} \frac{dE}{dx} \quad (3.2)$$

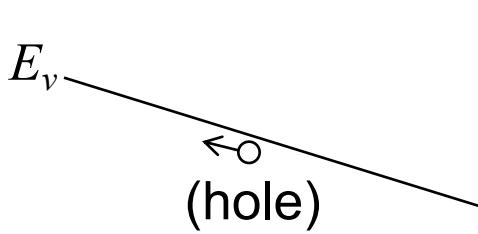
Fig. 3.6



$E_c$  —————



$E_v$  —————



Without electric field

With electric field  $\xi$

$$\xi = -\frac{dV}{dx}$$

$$E = -qV$$

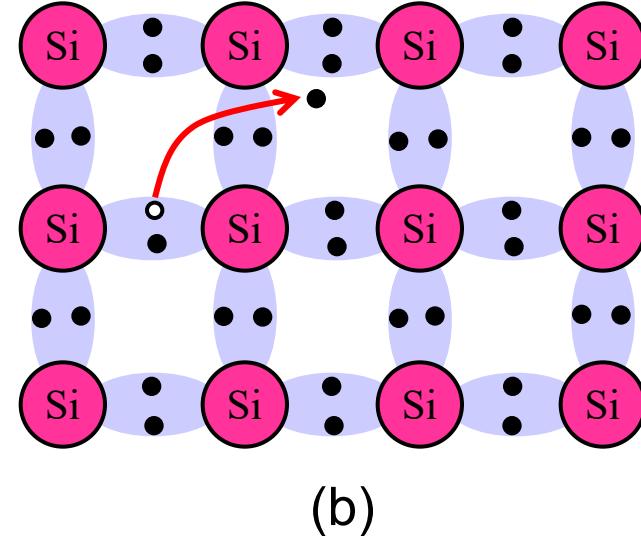
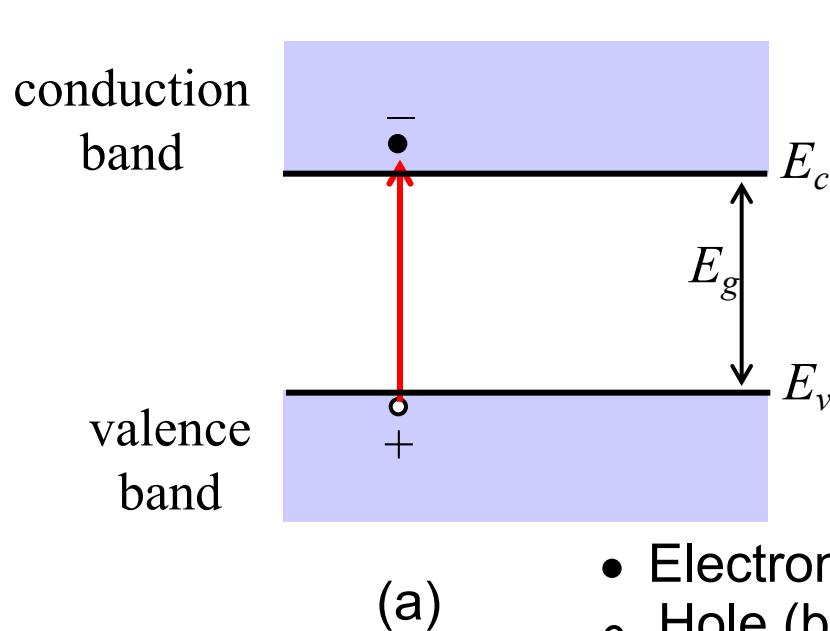
$$\xi = \frac{1}{q} \frac{dE}{dx}$$

We will learn more about this  
in Tutorial 4

### 3.3 Electrons and holes

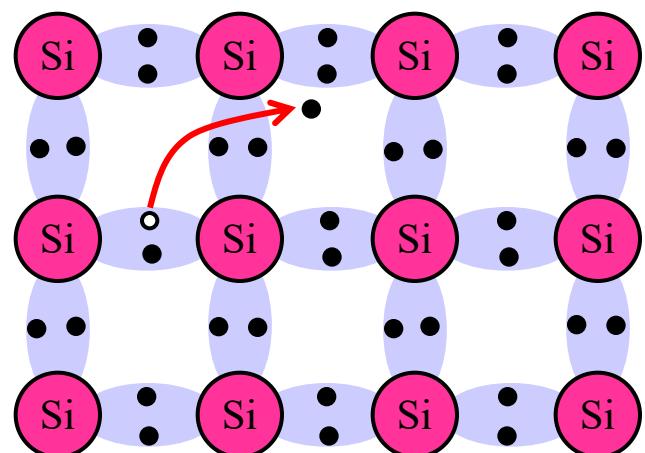
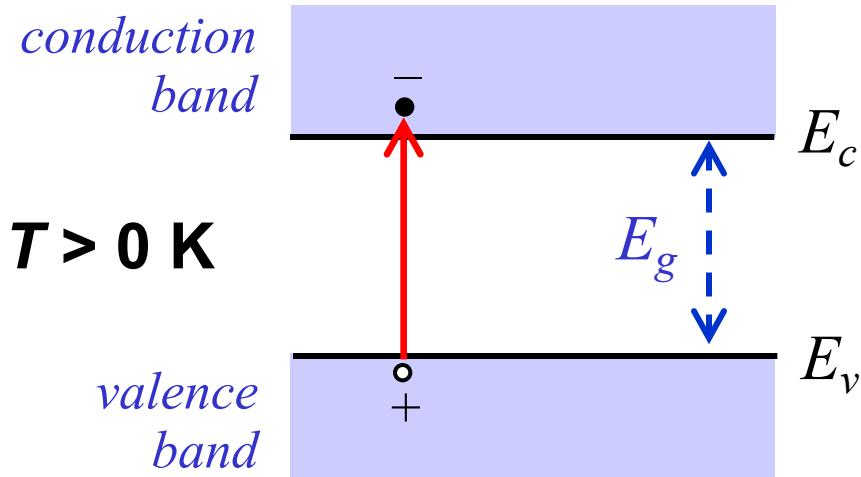
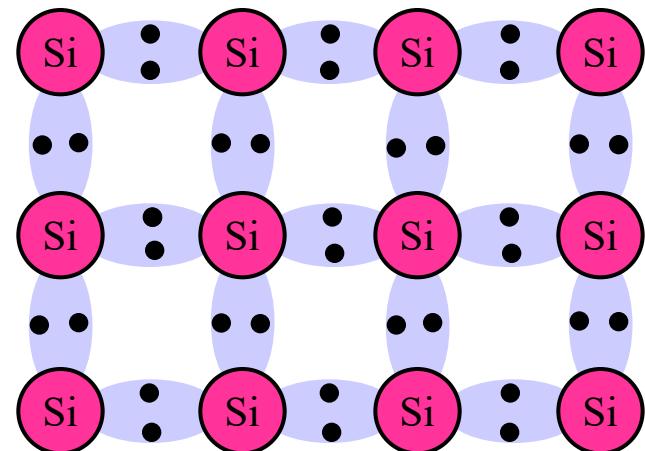
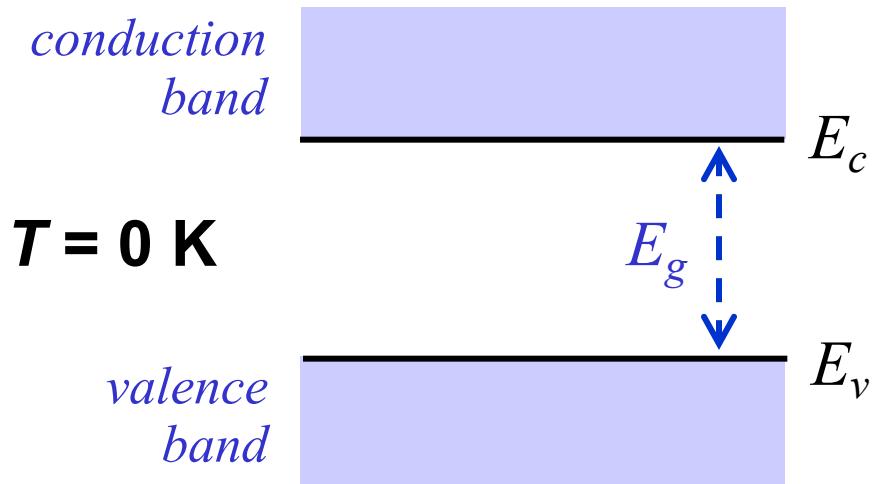
- At  $T = 0 \text{ K}$ , the valence band is fully occupied by electrons and the conduction band is empty. The semiconductor behaves like an insulator.
- The electrons in the valence band can be excited to the conduction by
  - increasing the temperature
  - illuminating crystal with light of a suitable wavelength

- As the temperature of the semiconductor is raised above 0 K, i.e.  $T > 0 \text{ K}$ 
  - some electrons in the valence band gain enough thermal energy to be excited across the bandgap to the conduction band.
  - This process corresponds to the electrons breaking the Si-Si covalent bonds leaving behind broken bonds. (Fig. 3.7)



- Electron, negatively charged ( $-1.6 \times 10^{-19} \text{ C}$ )
- Hole (broken bond), positively charged ( $+1.6 \times 10^{-19} \text{ C}$ )

Fig. 3.7



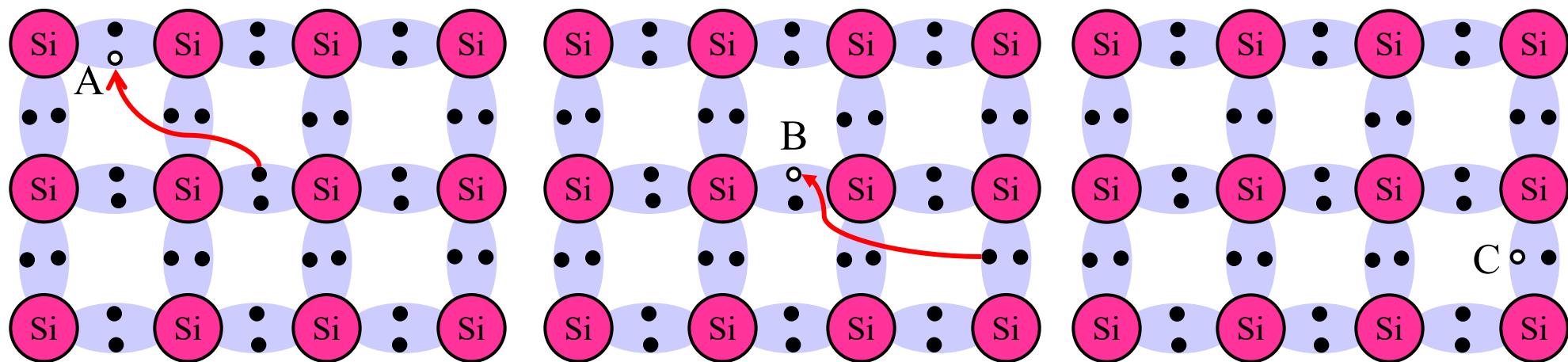
(a)

Fig. 3.7a

- Electron, negatively charged ( $-1.6 \times 10^{-19} \text{ C}$ )
- Hole (broken bond), positively charged ( $+1.6 \times 10^{-19} \text{ C}$ )

- Some of the states in the conduction band is now occupied by electrons and some of the states in the valence band is now empty.
- An empty state in the valences band is referred to as a **hole**, it corresponds to the broken bond in the Si-Si bonding. The hole is positively charged with a value of  $1.6 \times 10^{-19}$  C.
- The electrons and holes can “freely” move throughout the crystal, under the influence of periodic potential formed by the atoms/ions in the crystal (compare to the real free electron in vacuum).
- The electrons and holes can only move freely for a short period of time, after which they will collide with vibrating atoms, impurity atoms and defects.

- The movement of the hole is actually the movement of the electron from the Si-Si bond to the broken bond. This is illustrated in Fig. 3.8.
- It is easier and convenient to think in terms of the displacement of holes rather than the actual displacement of electrons from Si-Si bonds to the broken bonds.



**Fig. 3.8** The hole has moved from A to B to C

- The electrons and holes are created by the excitation of electrons from the valence band to the conduction band. This direct excitation of electrons from the valence band to the conduction band is referred to as direct band-to-band generation.
- Obviously, the number of hole in the valence band = the number of electrons in the conduction band. Since the electrons and holes are created in pair, they are also called electron-hole pairs (EHP).
- There are empty states in the conduction and valence bands, therefore the electrons and holes are able to perform a directed motion under the action of an external electric field, conducting an electric current.

- The electrons in the valence band can also be excited to the conduction band, creating electron-hole pairs, by illuminating the semiconductor with light having a photon energy  $E_{ph}$  equal or greater than the bandgap energy  $E_g$ . This is illustrated in Fig. 3.9.

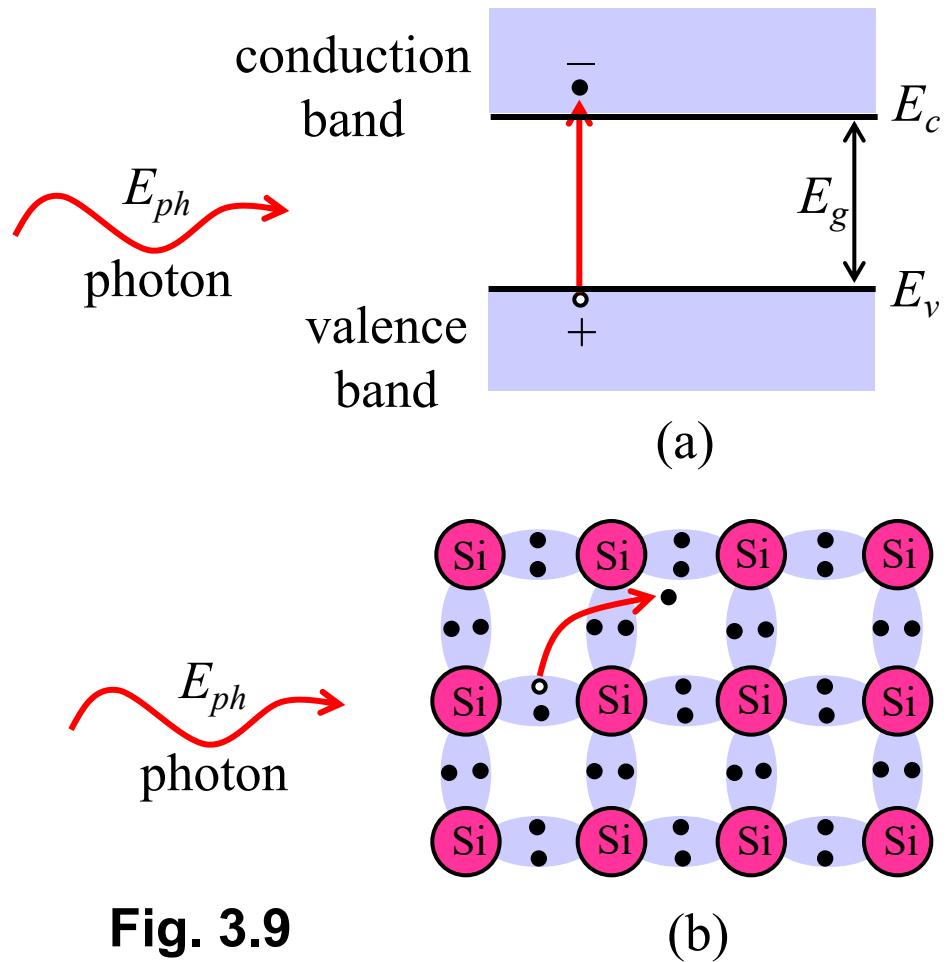
$$E_{ph} \geq E_g \quad (3.3)$$

$$E_{ph} = h\nu = \frac{hc}{\lambda} \quad (3.4)$$

$$\frac{hc}{\lambda} \geq E_g$$

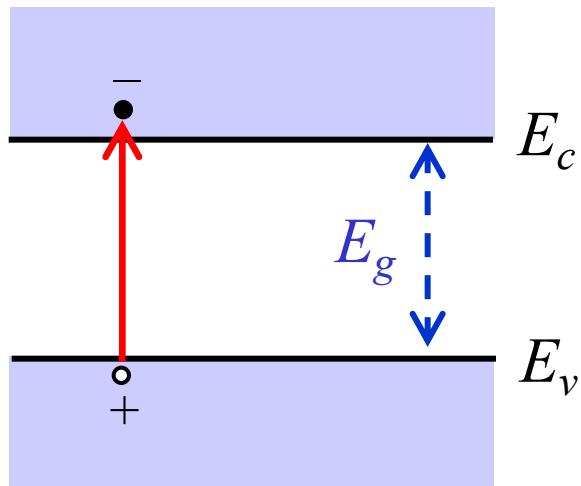
$$\frac{1240}{\lambda} \geq E_g \quad (3.5)$$

where  $\lambda$  in nm and  $E_g$  in eV

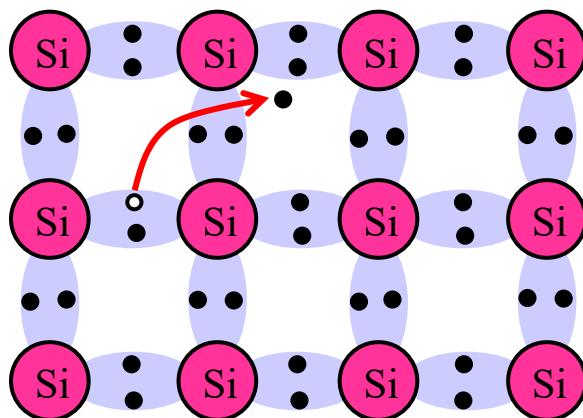


## Sample at temperature $T$

conduction  
band

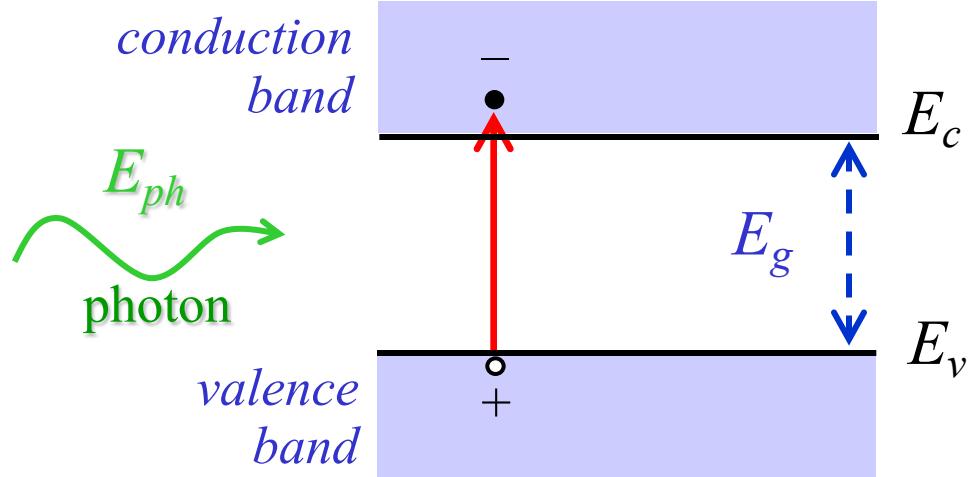


valence  
band

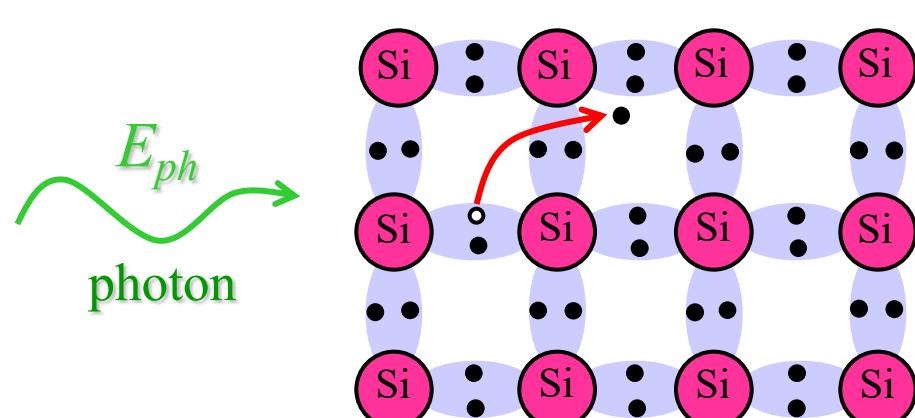


## Sample subjected to light

conduction  
band



valence  
band



# Problems

Q1: Determine the energy (in eV) of a photon having a wavelength of (a) 10 nm, and (b) 450 nm. (Ex 2.1)

$$(a) \quad E = h\nu = \frac{hc}{\lambda} = \frac{(6.625 \times 10^{-34})(3 \times 10^{10})}{100 \times 10^{-8}}$$
$$= 1.9875 \times 10^{-17} \text{ J}$$

$$\text{or} \quad E = \frac{1.9875 \times 10^{-17}}{1.6 \times 10^{-19}} = 124 \text{ eV}$$

$$(b) \quad E = \frac{hc}{\lambda} = \frac{(6.625 \times 10^{-34})(3 \times 10^{10})}{4500 \times 10^{-8}}$$
$$= 4.417 \times 10^{-19} \text{ J}$$

$$\text{or} \quad E = \frac{4.417 \times 10^{-19}}{1.6 \times 10^{-19}} = 2.76 \text{ eV}$$

Q2: The work function of a material refers to the minimum energy required to remove an electron from the material. Assume that the work function of gold is 4.90 eV and that of cesium is 1.90 eV. Calculate the maximum wavelength of light for the photoelectric emission of electrons for gold and cesium. (2.5)

Q2: The work function of a material refers to the minimum energy required to remove an electron from the material. Assume that the work function of gold is 4.90 eV and that of cesium is 1.90 eV. Calculate the maximum wavelength of light for the photoelectric emission of electrons for gold and cesium. (2.5)

$$E = h\nu = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{E}$$

$$\text{Gold: } E = 4.90 \text{ eV} = (4.90)(1.6 \times 10^{-19}) \text{ J}$$

So,

$$\lambda = \frac{(6.625 \times 10^{-34})(3 \times 10^{10})}{(4.90)(1.6 \times 10^{-19})} = 2.54 \times 10^{-5}$$

cm

or

$$\lambda = 0.254 \mu \text{m}$$

$$\text{Cesium: } E = 1.90 \text{ eV} = (1.90)(1.6 \times 10^{-19}) \text{ J}$$

So,

$$\lambda = \frac{(6.625 \times 10^{-34})(3 \times 10^{10})}{(1.90)(1.6 \times 10^{-19})} = 6.54 \times 10^{-5}$$

cm

or

$$\lambda = 0.654 \mu \text{m}$$

## Key takeaways (Lecture #5)

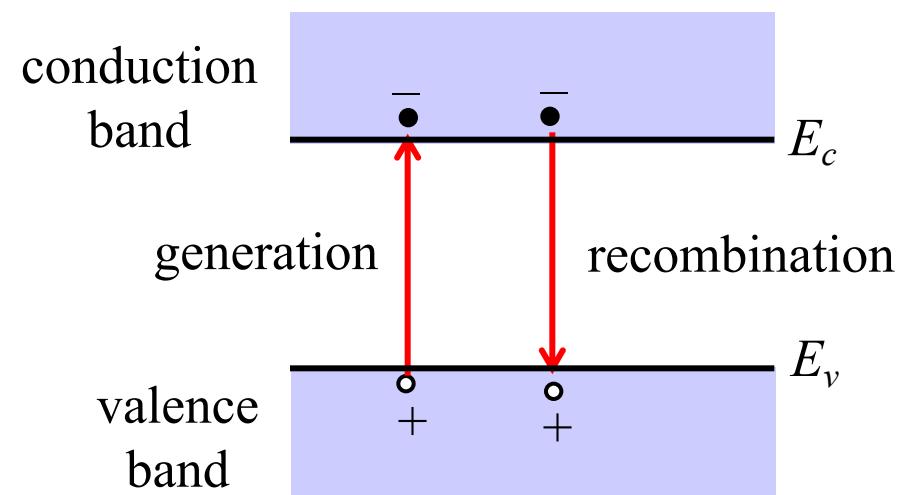
- When Silicon atoms form covalent bonds with four nearest atoms, discrete 3s and 3p energy states form continuous conduction band and valence band, separated by a bandgap;
- At 0K, the valence bond is fully occupied by electrons, the conduction band is empty → no current conduction;
- To achieve conduction, electrons in the valence band can be excited to the conduction band (direct band to band generation):
  - increasing the temperature
  - illuminating crystal with light of a suitable wavelength
  - The number of hole in the valence band = the number of electrons in the conduction band. Since the electrons and holes are created in pair, they are also called electron-hole pairs (EHP).

# Lecture 6

### 3.3.1 Direct band-to-band generation and recombination

- If a semiconductor is subjected to a certain temperature  $T$ , or illuminated with light ( $E_{ph} \geq E_g$ ) or both,
  - Do these generated electron-hole pairs keep increasing continuously?
  - The answer is certainly “NO”, otherwise we will observe that all the covalent bonds of the semiconductor will be broken simply by putting a sample at room temperature.

- The reason is that as electron-hole pairs are generated, they also can recombine. In this process the electrons and holes are annihilated (i.e. disappear). The process is called recombination. (Fig. 3.10)
- The direct generation and recombination processes from band-to-band shown in Fig. 3.10 is called direct band-to-band generation and recombination.



**Fig. 3.10**

- A steady state will be established when

$$\text{generation rate } G = \text{recombination rate } R \quad (3.6)$$

- The generation rate  $G$  is the number of electron-hole pairs created per unit volume per second (units: #/cm<sup>3</sup>-s).
  - *The generation is the sum of the thermal generation rate and the generation rate by the external excitation (if any)*
- The recombination rate  $R$  is the number of electron-hole pairs recombining per unit volume per second (units: #/cm<sup>3</sup>-s).
  - *It is expected that the recombination rate is proportional to the electron concentration in the conduction band and the hole concentration in the valence band.*
- Obviously, in the steady state, the electron and hole concentrations are constant with time.

- When a semiconductor is at temperature  $T$  and there is no external disturbance/excitation (e.g. external electric field, magnetic field or light illumination), the electrons and holes are solely created by thermal energy.
- An equilibrium will be established, and this equilibrium state is called thermal equilibrium since there is only thermal energy involved.
- In thermal equilibrium:
  - thermal generation rate  $G_{th}$  = recombination rate  $R$
  - there exist thermal equilibrium electron and hole concentrations,  $n_0$  and  $p_0$  respectively.

## 3.4 Direct and Indirect Bandgap Semiconductors

The electron energy  $E$  can also be related to its momentum  $p$  (or, in crystal, more precisely, it is called crystal momentum). This relation will lead to direct and indirect bandgap semiconductors.

### 3.4.1 $E$ versus $k$ ( $E - k$ ) for free electrons and electrons in crystals

- From appendix D [eqn (D.8)], the relation of  $E$  with  $p$  for a free electron in an one dimensional (1-D) system is parabolic and given by

$$E = \frac{\hbar^2 k_x^2}{2m} \quad (3.7)$$

where  $k_x$  is the wave vector

and the momentum  $p$  is given by

$$p_x = \hbar k_x \quad (3.8), \text{ here } \hbar = \frac{h}{2\pi} \quad (3.9)$$

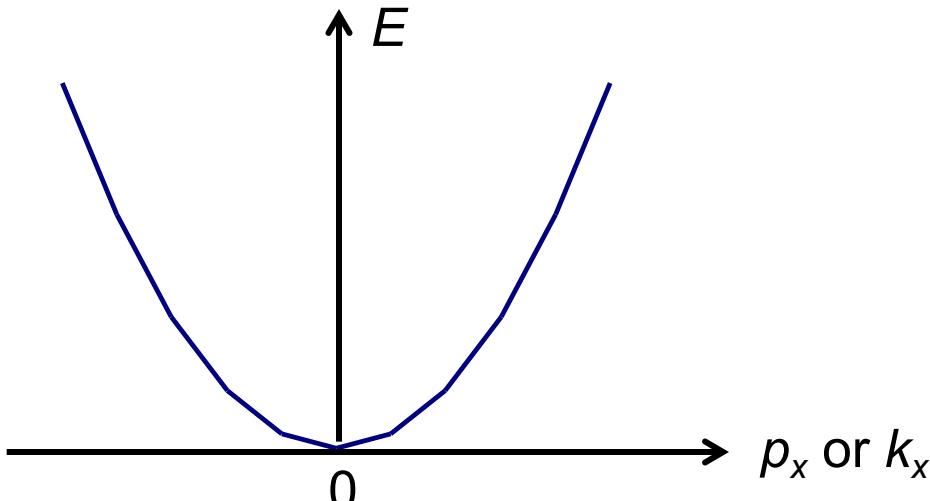


Fig. 3.11  $E$  vs  $p_x$  or  $k_x$  is parabolic

- In crystals, there is interaction between the electrons and the periodic potential in the lattice (see Appendix D section D.2).
- Taking this interaction into account, the Schrödinger equation, as shown in eqn. (D.1), becomes

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{dx^2} + U(x)\Psi = E\Psi \quad (3.10)$$


periodic potential energy

where  $U(x)$  is periodic potential energy and given by

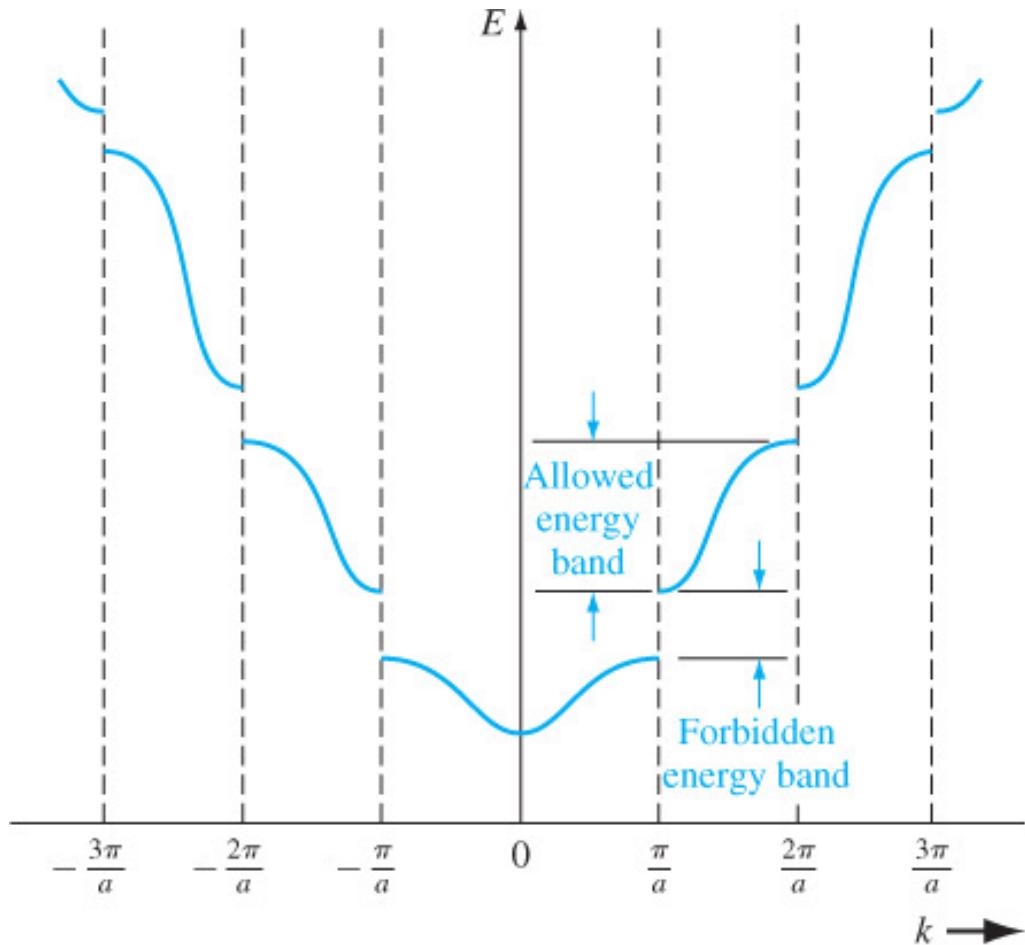
$$U(x) = U(x + n_x a) \quad (3.11 \text{ or see D.9})$$

$n_x$  is integer

- Due the interaction of the electrons with the periodic potential, the solution of the Schrödinger equation in eqn. (3.10) will lead to the forbidden energy band (energy bandgap) and allowed energy band.
- The electron energy  $E$  versus  $k$  ( $E - k$ ) relation is shown in Fig. 3.12.a. The parameter  $a$  is the period of the lattice or the lattice constant. The  $E - k$  relation is called the energy band structure.
  - Here the quantity  $p = \hbar k$  **(3.12)**

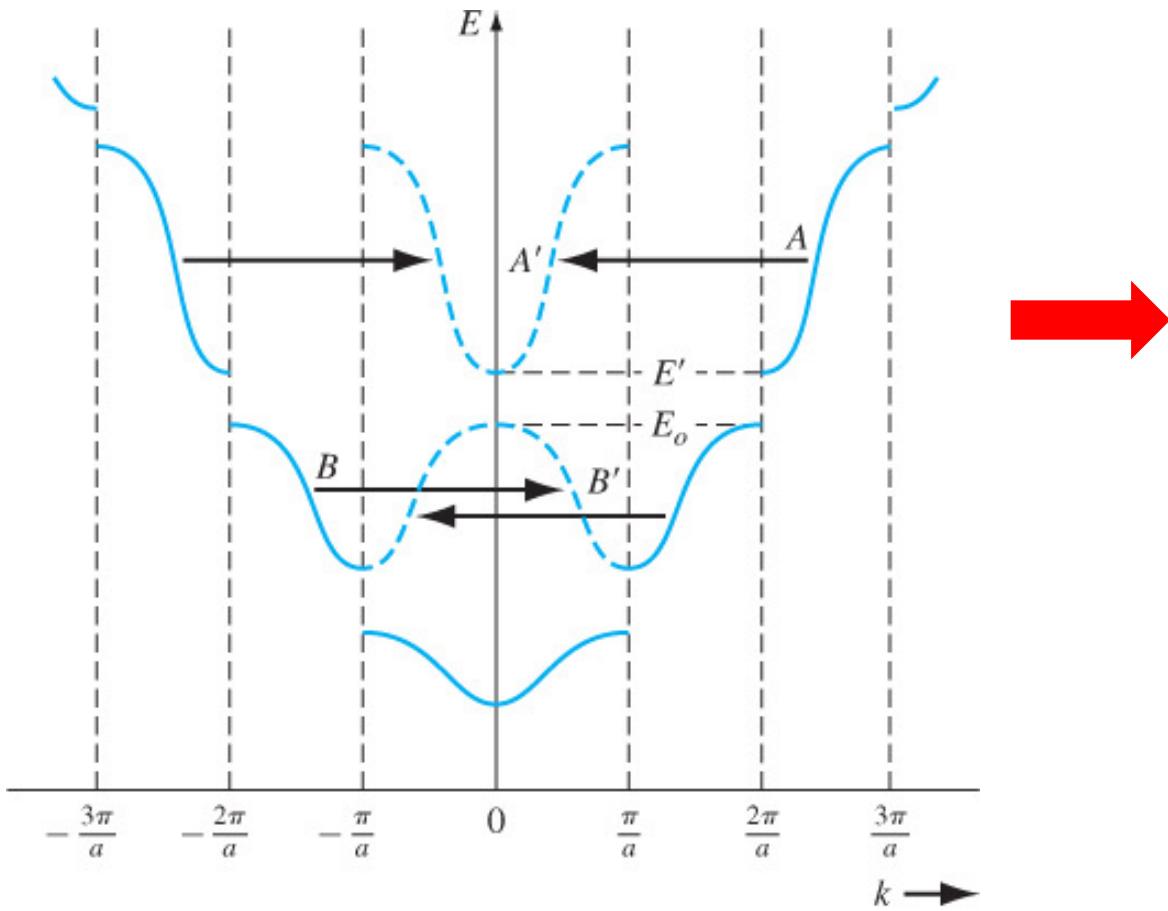
is called crystal momentum. This is not the actual momentum of the electron in the crystal, but it describes the motion of the electron that includes the interaction between the electron and the crystal (see Appendix D, section D.2).

- Note that the  $E$ - $k$  relation is no longer parabolic as that of a free particle shown in Fig. 3.11.

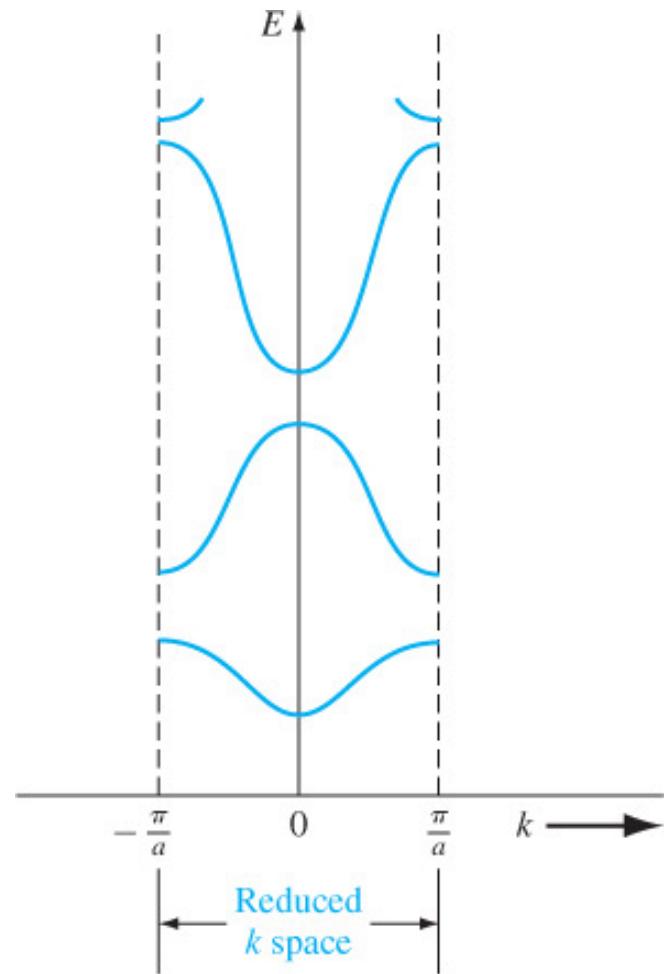


**Fig.3.12.a**  $E - k$  relation with the forbidden and allowed energy bands

- It is customary to plot the  $E$ - $k$  relation within  $-\pi/a < k < \pi/a$  by displacing the curve by multiple of  $2\pi/a$ . This is shown in Fig. 3.12.b & referred to as a reduced  $k$ -space diagram.

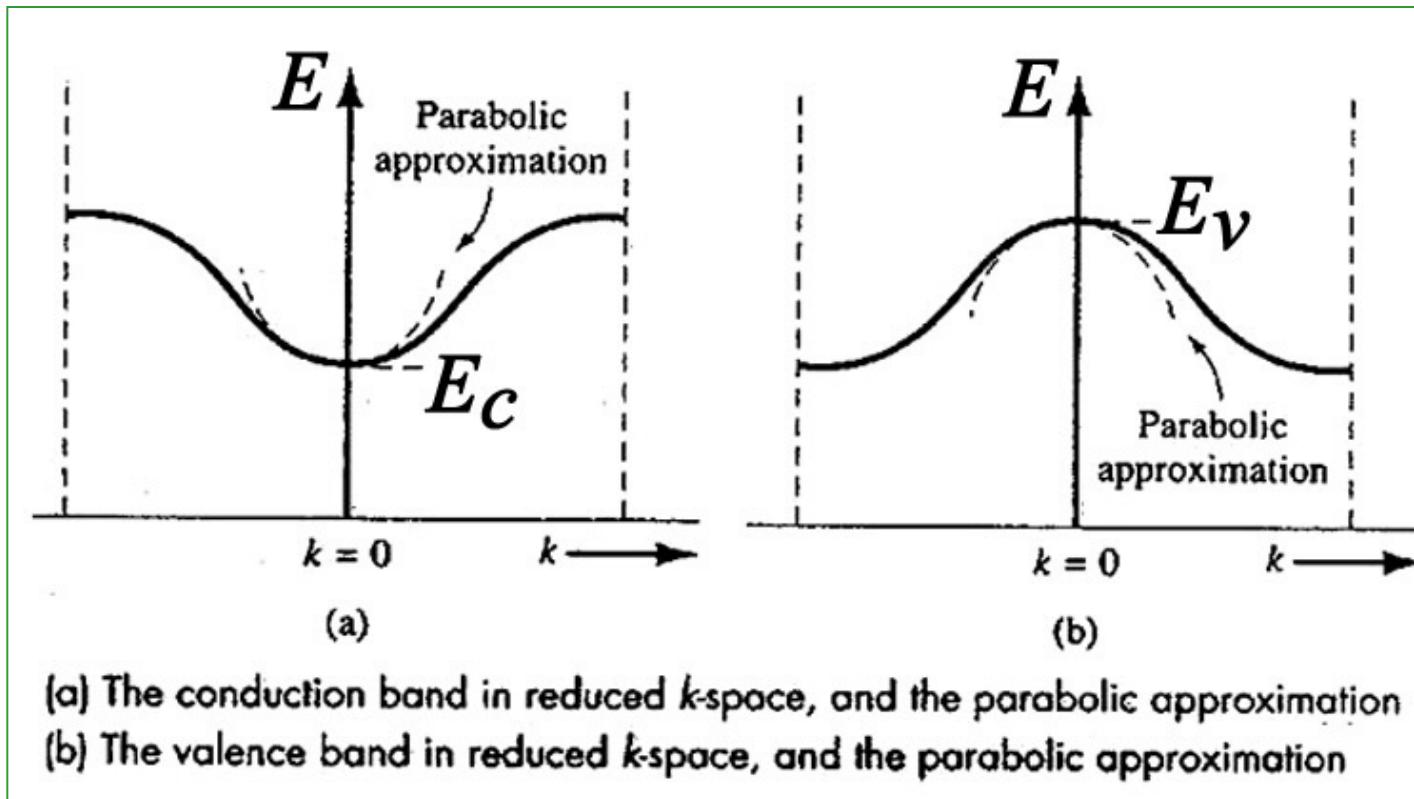


**Figure 3.10** | The  $E$  versus  $k$  diagram showing  $2\pi$  displacements of several sections of allowed energy bands



**Fig.3.12.b**  $E$ - $k$  relation in the reduced  $k$ -space diagram

- We have seen that because of the interaction of the electrons with the periodic potential in the lattice, the  $E$ - $k$  relation is **no longer parabolic** (see Fig.3.12) as in the free electron case.
- However, near the conduction band minima & the valence band maxima, it can be approximated by a *parabolic relation*. This is shown in Fig. 3.13.



## The concept of Effective Mass

- From equation (3.7),

$$E = \frac{\hbar^2 k_x^2}{2m}$$

- If we take the first and second derivative:

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m}$$

$$\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{1}{m}$$

Whereby  $m$  is the mass of a free particle.

- In a crystal, there are internal forces that act on the particle (such as electron) besides the external force due to positively charged ions or protons and negatively charged electrons.

- Hence, we modify the mass of the particle to an effective mass  $m^*$ , to take into account the particle mass as well as the effect of internal force. (*Analogy: marbles in water and oil*)

$$\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{1}{m^*}$$

- Since the energy near the minimum (or maximum) of the  $E$ - $k$  diagram can be approximated by a parabola, we may write the following for electron:

$$E - E_c = C_1(k^2)$$

- Whereby  $C_1$  is a coefficient. Hence:

$$\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} = \frac{1}{m^*} = \frac{2C_1}{\hbar^2}$$

## Problems

Q1: A simplified parabolic  $E$  vs.  $k$  curve for an electron in the conduction band is given. The value of  $a$  is 1 nm. Determine the relative effective mass. (TYU 3.3)

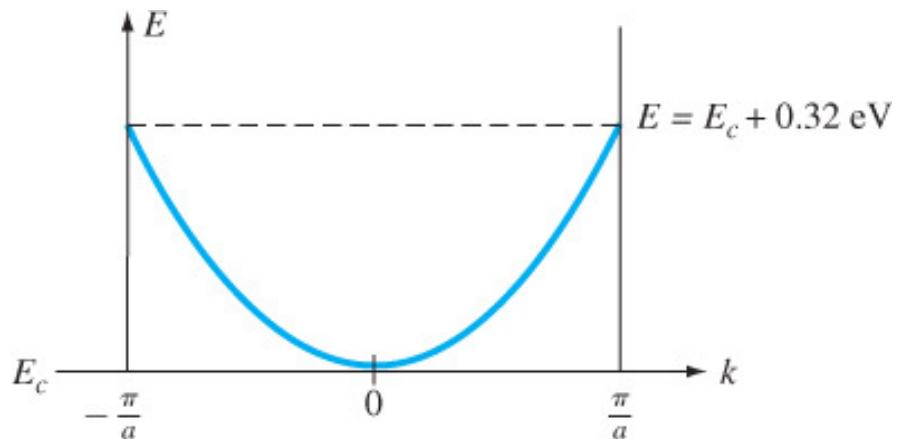


Figure 3.22 | Figure for Exercise TYU 3.3.

$$\begin{aligned} \text{We have } E - E_c &= C_1 k^2 \\ (E_c + 0.32 - E_c) (1.6 \times 10^{-19}) &= C_1 \left( \frac{\pi}{10 \times 10^{-10}} \right)^2 \end{aligned}$$

$$\text{so that } C_1 = 5.1876 \times 10^{-39}$$

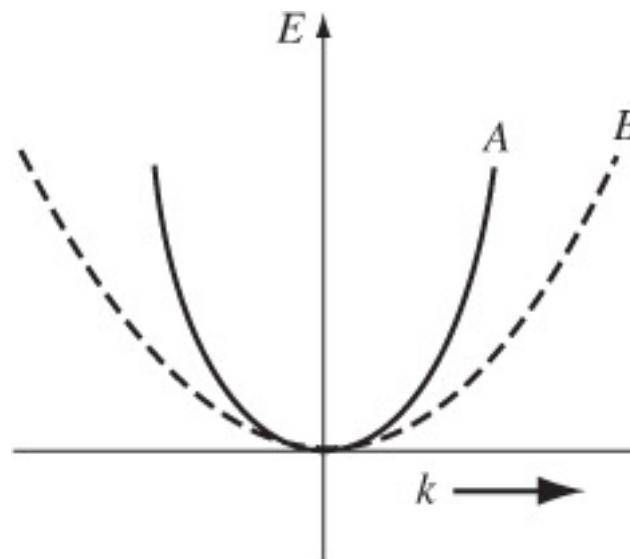
We have

$$\begin{aligned} m^* &= \frac{\hbar^2}{2C_1} \Rightarrow \frac{m^*}{m_o} = \frac{\hbar^2}{2m_o C_1} \\ &= \frac{(1.054 \times 10^{-34})^2}{2(9.11 \times 10^{-31})(5.1876 \times 10^{-39})} \end{aligned}$$

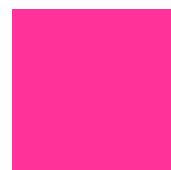
or

$$\frac{m^*}{m_o} = 1.175$$

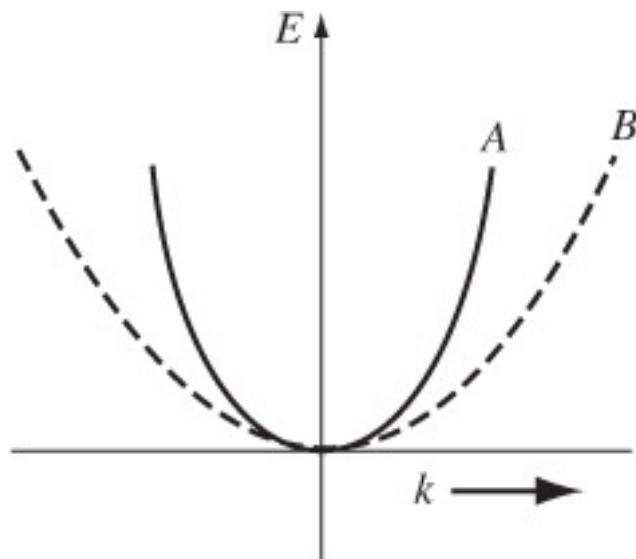
Q2: Two possible conduction bands are shown in figure. State which band will result in the heavier electron effective mass and why? (3.13)



**Figure P3.13** | Conduction bands for Problem 3.13.



Q2: Two possible conduction bands are shown in figure. State which band will result in the heavier electron effective mass and why? (3.13)



**Figure P3.13** | Conduction bands for Problem 3.13.

The effective mass is given by

$$m^* = \left( \frac{1}{\hbar^2} \cdot \frac{d^2 E}{dk^2} \right)^{-1}$$

We have

$$\frac{d^2 E}{dk^2} (\text{curve } A) > \frac{d^2 E}{dk^2} (\text{curve } B)$$

$$\text{so that } m^*(\text{curve } A) < m^*(\text{curve } B)$$

### 3.4.2 $E$ versus $k$ ( $E$ - $k$ ) for Si and GaAs

Consider the energy  $E$  versus  $k$  ( $E$  -  $k$ ) for silicon and gallium arsenide (GaAs).

- $E$  -  $k$  is symmetric in  $k$  and that no new information is obtained by displaying the negative axis.
- It is a normal practice to plot  $E$  -  $k$  along positive [100] direction to the right and along positive [111] direction to the left.

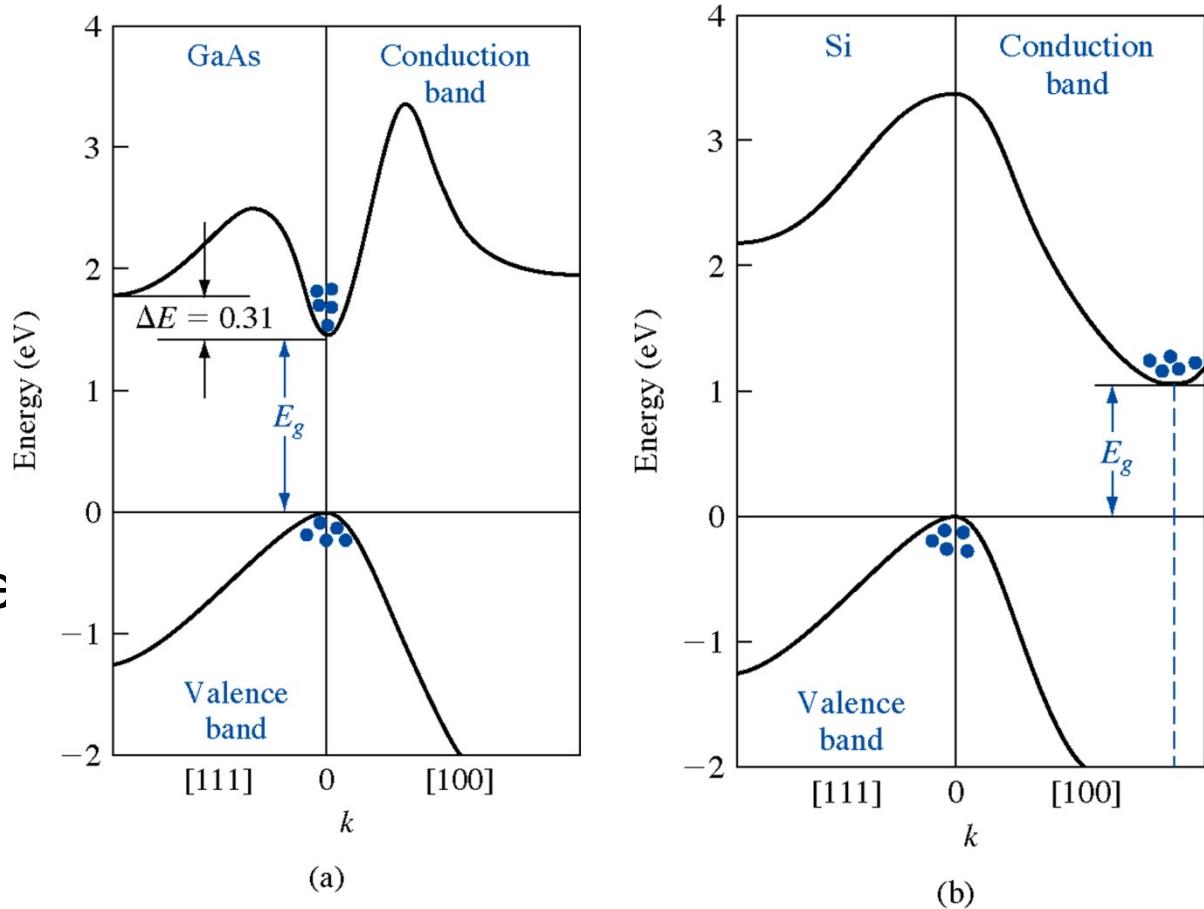
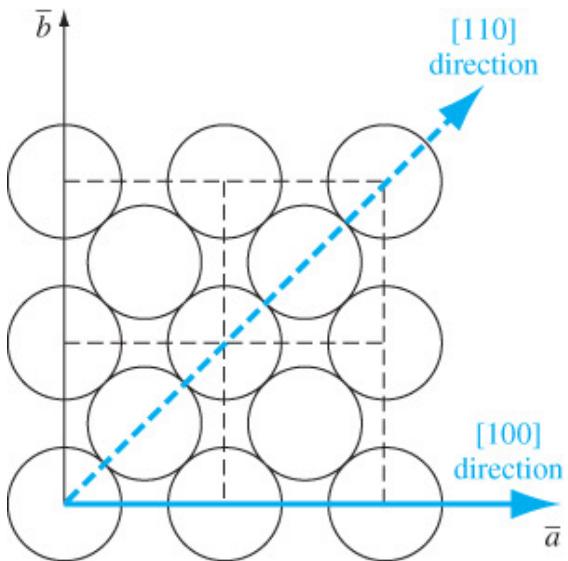


Fig.3.14 Energy band structure of (a) GaAs and (b) Si



**Figure 3.24** | The (100) plane of a face-centered cubic crystal showing the [100] and [110] directions.

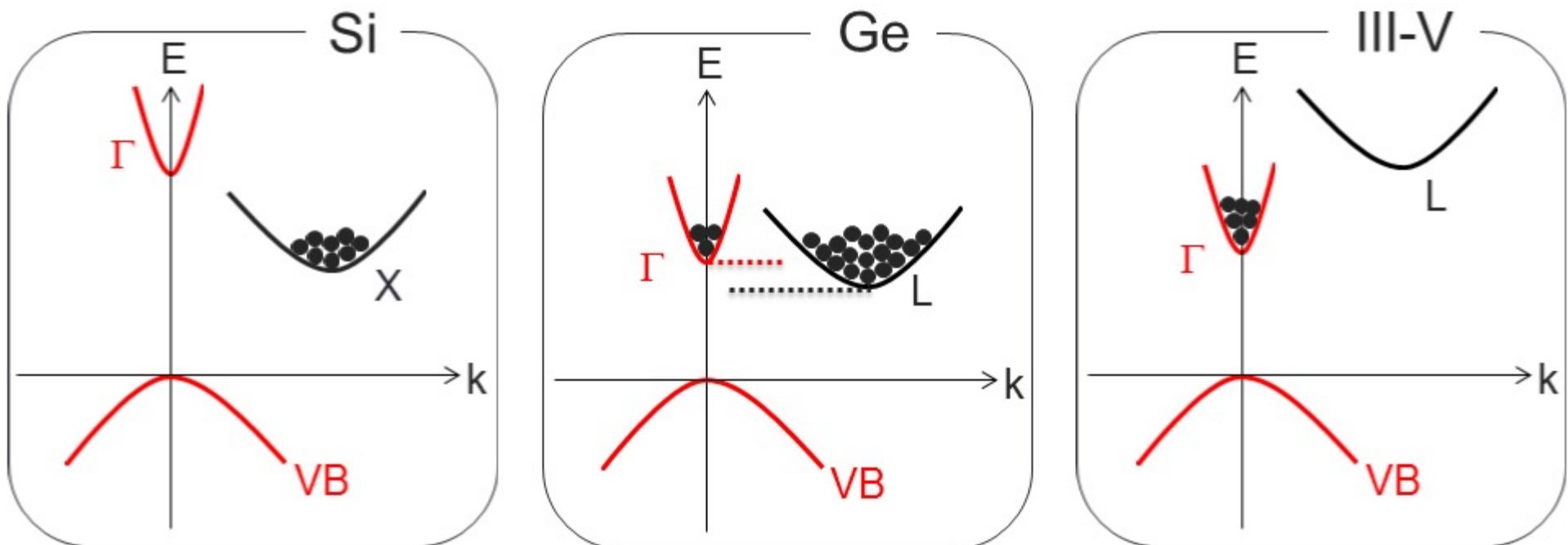
- In the  $E - k$  diagrams we see that
  - the majority of electrons occupy the bottom of the conduction band
  - and the majority of holes occupy the top of the valence band
  - the bandgap energy  $E_g$  is the energy difference between the conduction band minimum and the valence band maximum

- The  $E$  -  $k$  diagram for GaAs
  - Conduction band minimum and valence band maximum both occur at same  $k$ -value (in this case at  $k = 0$ ). A semiconductor with this property is called a direct bandgap semiconductor.
  - The electron transitions from conduction band to valence band or vice versa require the conservation of energy and momentum.
  - In the direct bandgap semiconductor, the transitions do not require changes in the crystal momentum. Therefore, the transitions are very efficient. For the transitions from the conduction band to the valence band, the energy is given off as photon (light).
  - Consequently, the direct band gap semiconductors are suitable for light producing optical devices (e.g. semiconductor laser)

- The  $E$  -  $k$  diagram for Si

- Conduction band minimum and valence band maximum do not occur at same  $k$ -value. A semiconductor with this property is called an indirect bandgap semiconductor.
- The electron transitions from the conduction band to the valence band require changes in the crystal momentum.
- The crystal momentum change can be satisfied, in principle, through the involvement of **phonons (lattice vibration)** in the transition process. Because of the need of the phonons involvement, this type of transitions are not efficient.
- In the presence of the **defect states**, the transitions of electrons from the conduction to the valence band are more likely through defect states and the energy is given out as heat.
- This is why the indirect semiconductor materials are not suitable for light producing devices.

## Is Ge a direct or indirect band-gap semiconductor?



## Key takeaways (Lecture #6)

- At thermal equilibrium (un-doped semiconductor):
  - thermal generation rate  $G_{th}$  = recombination rate  $R$
  - thermal equilibrium electron and hole concentrations,  $n_0 = p_0$
- $E$ - $k$  diagram for electrons in a crystal can be approximated as parabola curves around the conduction band min and valence band max;
- The effective mass of electron is inversely proportional to the curvature:
$$m^* = \left( \frac{1}{\hbar^2} \cdot \frac{d^2 E}{dk^2} \right)^{-1}$$
- Si = indirect band-gap, GaAs = direct bandgap

# Lecture 7

# 4 DOPING OF SEMICONDUCTORS

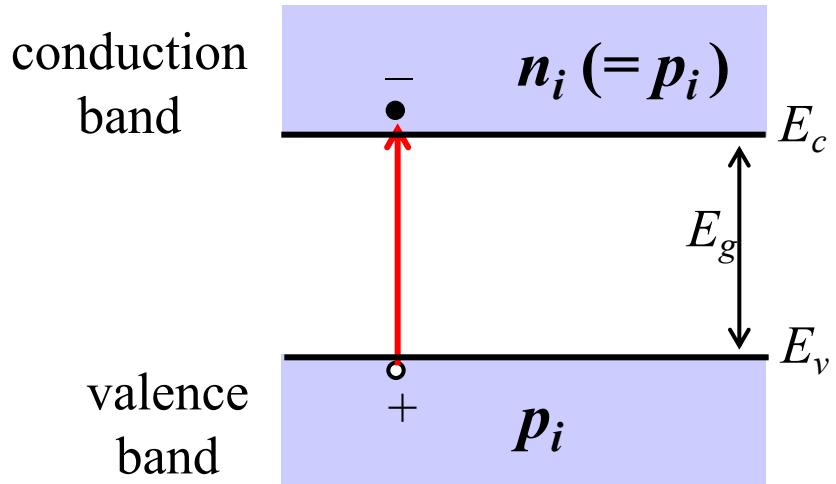
## 4.1 Intrinsic Material

- Essentially, it is a pure crystal with no impurity atoms or defects.
- As the temperature is raised above 0 K:
  - Valence electrons in the bonds gain thermal energy
  - Some electrons in valence band gain sufficient energy to jump to conduction band become conduction of “free” electrons.
  - This process corresponds to the electrons breaking the covalent bonds leaving behind broken bonds
  - As a result, broken bonds, empty states, or holes are created.
  - The electrons and holes are created in pairs by thermal energy

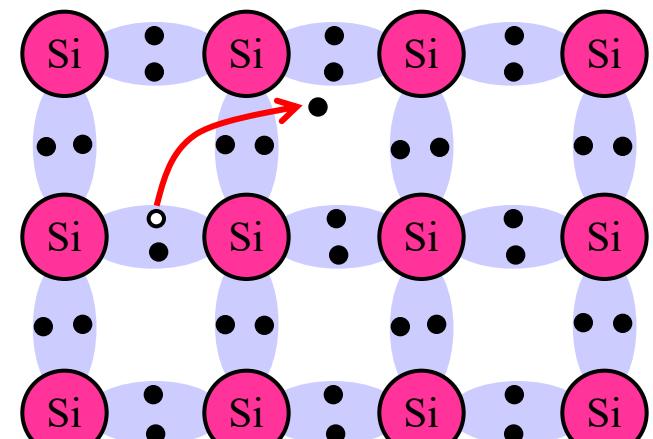
- Obviously, the number of electrons in the conduction band is equal to the number of holes in the valence band.

- The concentration of these electrons and holes is called intrinsic concentration  $n_i$ .
- It is expected that  $n_i$  increases with increasing temperature  $T$ .

The above processes are illustrated in Fig.4.1 for silicon semiconductor.



(a)



(b)

Fig.4.1

- In Silicon:

Density of silicon atoms =  $5 \times 10^{22} \text{ cm}^{-3}$  and

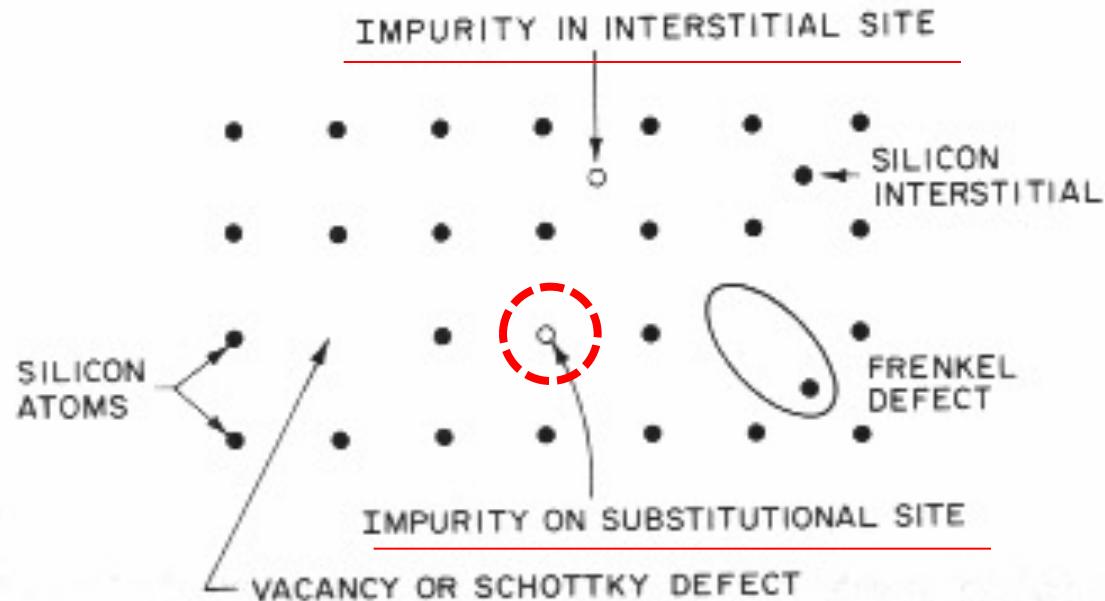
4 valence electrons per atom, so

Density of valence electrons =  $2 \times 10^{23} \text{ cm}^{-3}$  (Slides 2-45, 2-46)

- The value of  $n_i$  for silicon at 300 K is  $1.5 \times 10^{10} / \text{cm}^3$
- The properties (e.g. conductivity) of the semiconductor can be changed by adding controlled amounts of specific impurity atoms, called dopant atoms, to the semiconductor crystal
- Such doped material is then called an extrinsic material.

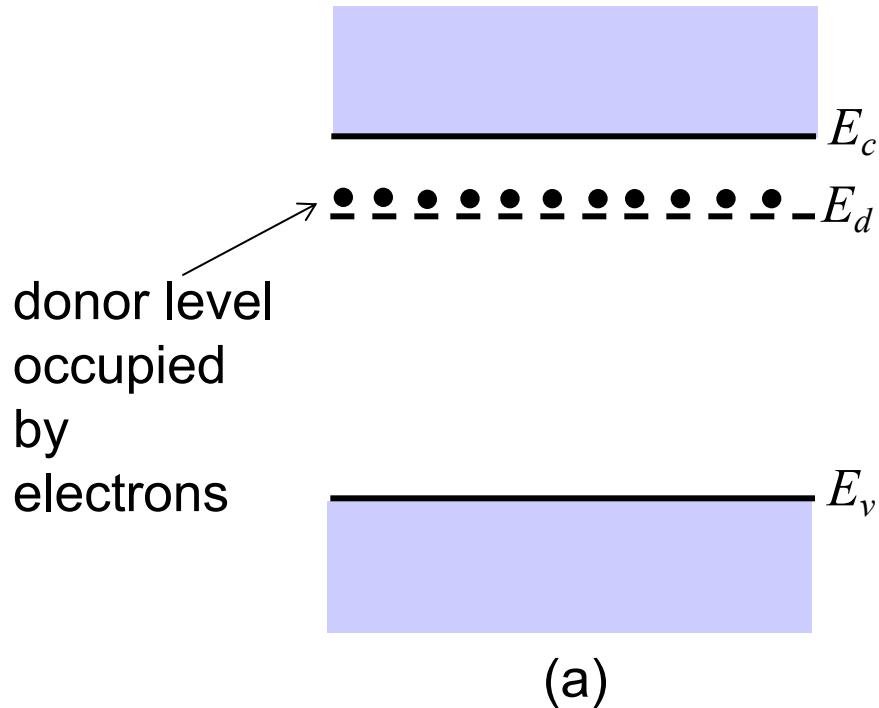
## 4.2 Donor Impurity

- Supposing a silicon crystal is doped with impurity atoms from group V in the periodic table (e.g. P, As, Sb).
- In the crystal, the group V atoms occupy the Si atom sites, or in other words substituting or replacing the host Si atoms.

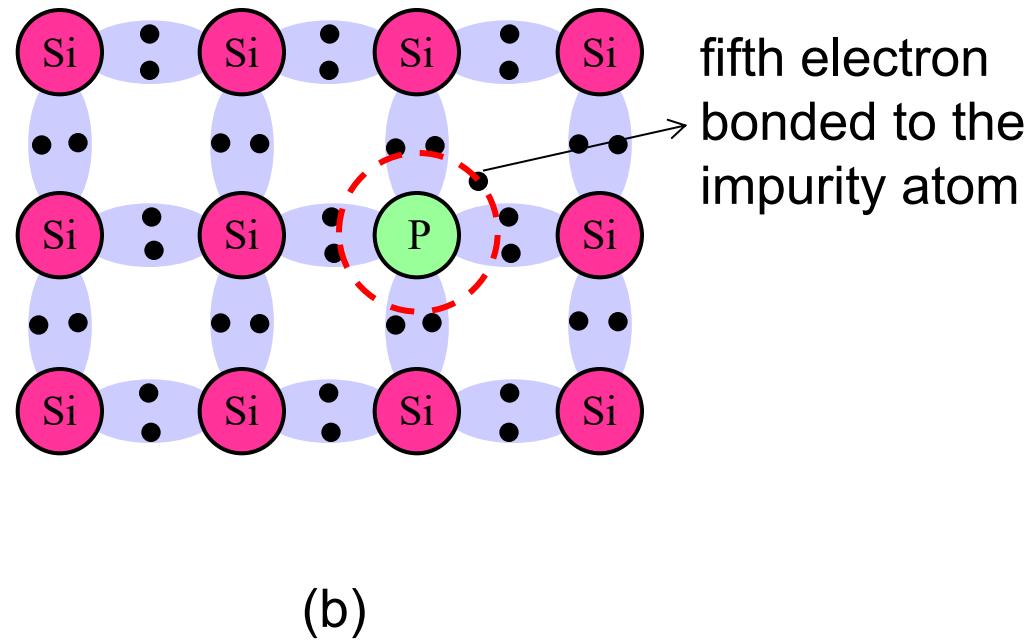


- The group V atoms in silicon crystals are called donor impurities/atoms for the reason which will be clear later.
- Consider now a group V atom, say a P atom, inside a silicon crystal (see Fig. 4.2)
  - Silicon atom has 4 valence electrons, but the phosphorus atom, P, has 5 valence electrons
  - Four valence electrons of P atom make covalent bonds with the neighboring Si atoms

- The fifth electron is held by the P atom, but much more weakly than the other 4 electrons forming the covalent bonds with the neighboring atoms
- The binding energy of the fifth electron to the P atom can be estimated using the hydrogen atom model. It is much smaller than bandgap energy  $E_g$  (the energy necessary to break Si-Si bond to create an electron-hole pair)
- The impurity P atoms introduce an energy level  $E_d$  in the bandgap below the conduction band edge  $E_c$ . The energy level  $E_d$  is called a donor level.
- The energy difference  $E_c - E_d$  corresponds to the binding energy of the fifth electron to the P atom. It is the energy required to excite an electron from the donor level to the conduction band.
- Typically, the donor levels  $E_d$  lie about 0.01 eV below  $E_c$  in Ge and about 0.03 – 0.06 eV below  $E_c$  in Si.



(a)



(b)

**Fig.4.2**

- At 0 K, the donor level is occupied by the electrons, which corresponds to the fifth electrons being bonded to the impurity atoms.

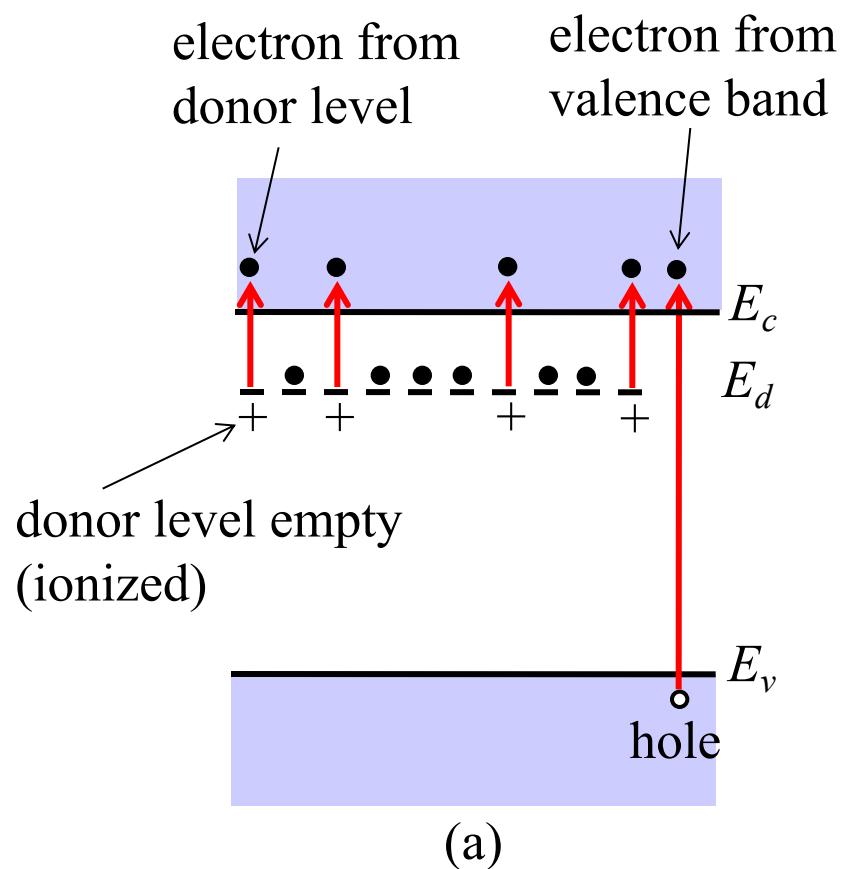
- Above 0 K, the electrons in the donor level and the valence band gain thermal energy. The following processes occur (see Fig. 4.3):
  - Electrons from donor level are excited to the conduction band. This corresponds to the fifth electrons breaking the bonds with the impurity atoms becoming conduction electrons.
  - The impurity atoms then become positively charged or ionized. Each ionized impurity carries a charge of  $+1.6 \times 10^{-19}$  C, because the initially neutral impurity atom donates one electron, the fifth electron, to the conduction band.
  - Since the impurity atoms donate the electrons to the conduction, they are called donor impurities/atoms.
  - Note that in this case electrons are donated to the conduction band without creation of holes in the valence band.

**Table 4.1** The bandgap and ionization energies at 300 K

	Ionization energy (eV)				$E_g$ (eV)	
	Donors		Acceptors			
	P	As	B	Al		
Si	0.045	0.05	0.045	0.06	1.11	
Ge	0.012	0.0127	0.0104	0.0102	0.67	

- The number of electrons excited to the conduction band from the valence band (creating electron-hole pairs) is much smaller than those excited from the donor level, this is because the energy gap  $E_g$  is much larger than the energy required to excite the electrons from the donor level to the conduction band  $E_c - E_d$  (see Table 4.1).
- Since the excitation of the electrons from the donor level to the conduction band ionizes the donor atoms, the energy difference  $E_c - E_d$  is also called the ionization energy of the donor atoms.

As  $T$  increases slightly above 0 K,



fifth electron detached from the donor atom becoming conduction electron

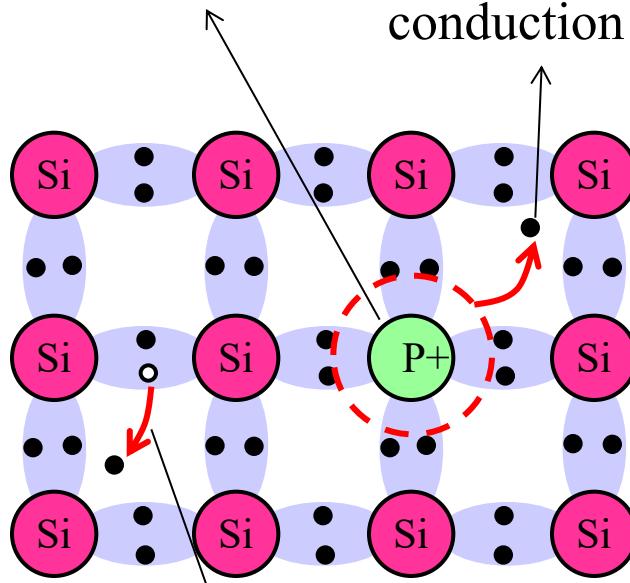
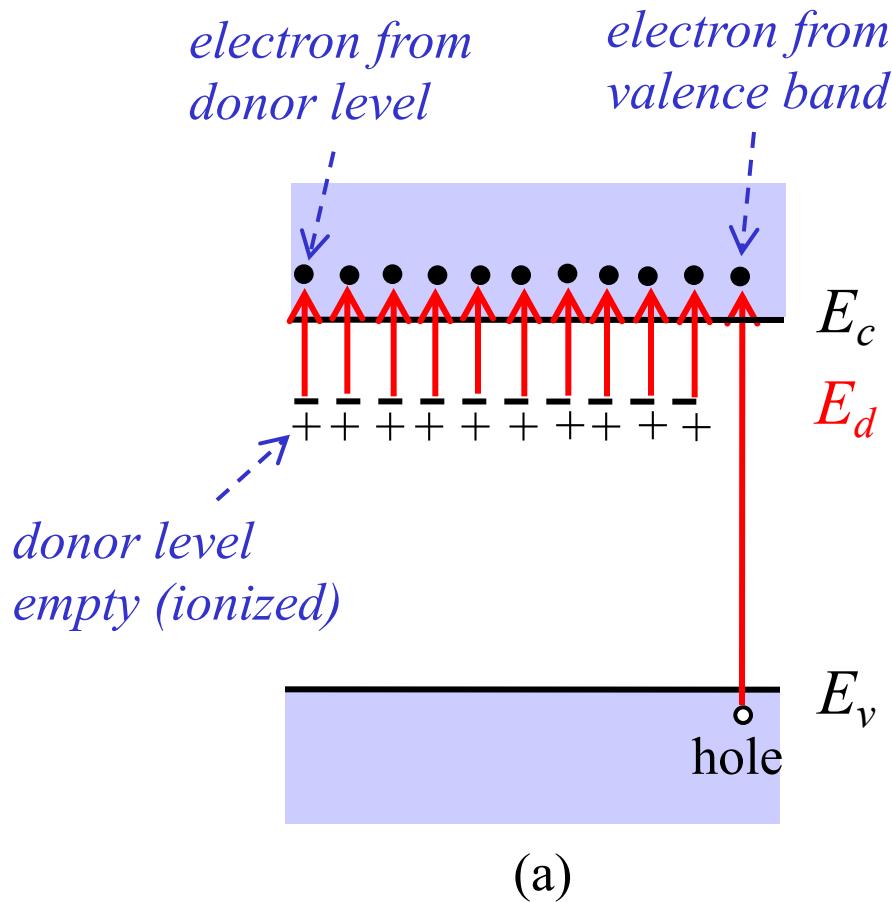


Fig.4.3

$$N_d = 5 \times 10^{16} \text{ cm}^{-3}$$
$$\text{Si: } 5 \times 10^{22} \text{ cm}^{-3}$$



At sufficiently high  $T$  whereby  
all donor impurities are  
ionized:

$$n_0 = N_d + p_0$$

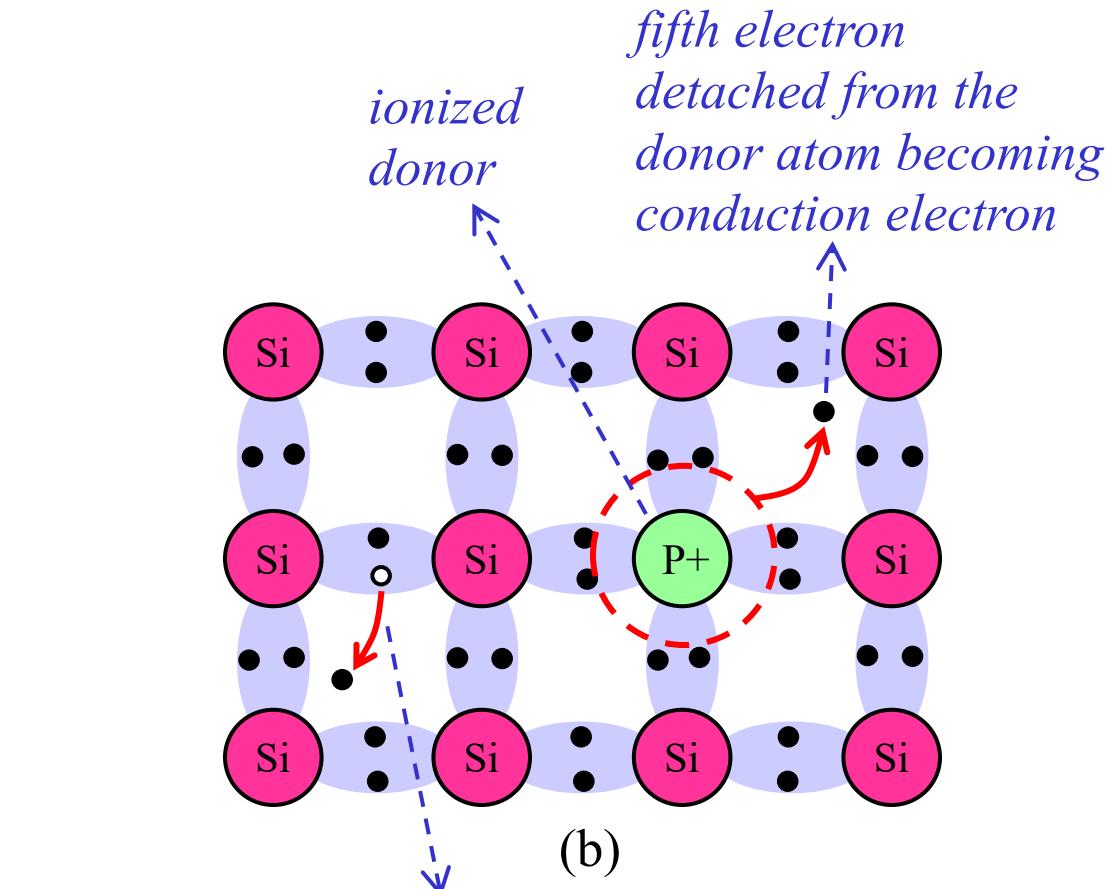


Fig.4.3a

$$N_d = 5 \times 10^{16} \text{ cm}^{-3}$$

$$\text{Si: } 5 \times 10^{22} \text{ cm}^{-3}$$

- At temperatures  $T$  whereby all the donor impurity atoms are ionized,
  - this phenomenon is called “impurity saturation (exhaustion)”

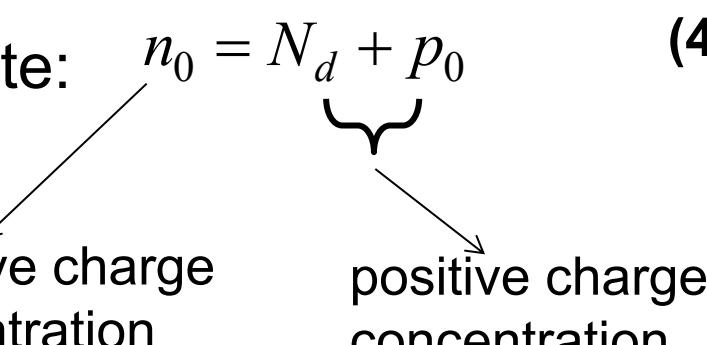
$T = 300 \text{ K}$  (room temperature) corresponds to impurity saturation region (see Chapter 4.4)

- We can now ask a question:

If a semiconductor is doped with donor atoms to a concentration  $N_d$ , what is the thermal equilibrium electron concentration in the conduction band  $n_0$  at temperature  $T$  whereby all the donor impurity atoms are ionized?

- The thermal equilibrium electron concentration in the conduction band  $n_0$  is the sum of
  - Electron concentration excited from the donor level to the conduction band. This electron concentration is equal to the donor concentration  $N_d$  since all donor impurity atoms are ionized. And consequently, all the donor impurities become positive ions.
  - Electron concentration excited from the valence band to the conduction band. This electron concentration is equal to the hole concentration in the valence band  $p_0$  since they are created in pairs.

Mathematically, we write:  $n_0 = N_d + p_0$  (4.1)

negative charge concentration

positive charge concentration

- The total charge concentration at thermal equilibrium is zero.
- We have established here the charge neutrality condition at thermal equilibrium.
- The positively charged ionized donor atoms are fixed in the crystal (covalently bonded with the neighboring atoms).
- They play important roles in the operation of devices, but do not participate in the electrical conduction.
- The electrical conduction in semiconductors is carried out by electrons and holes only.

- In the presence of donor atoms, the electrons from the donor atoms are donated to the conduction band without the creation of holes. It follows that

$$n_0 > p_0$$

This type of semiconductor, where  $n_0 > p_0$ , is called n-type semiconductor,

- the electrons are referred to as majority carriers and
- the holes are referred to as minority carriers

## Example 4.1

Estimate the donor binding energy for GaAs, given that the effective mass of electron  $m_n^* = 0.067 m_0$  and the relative permittivity  $\varepsilon_r$  of GaAs is 13.2

For hydrogen atom, the electron energy is [see Appendix A, eqn. (A.3.b)]

$$E_n = -\frac{q^4}{2(4\pi \hbar)^2} \left( \frac{m_0}{\varepsilon_0^2} \right) \frac{1}{n^2} = -\frac{13.6}{n^2} \text{ eV} \quad (4.2)$$

$$n = 1, 2, \dots, \infty$$

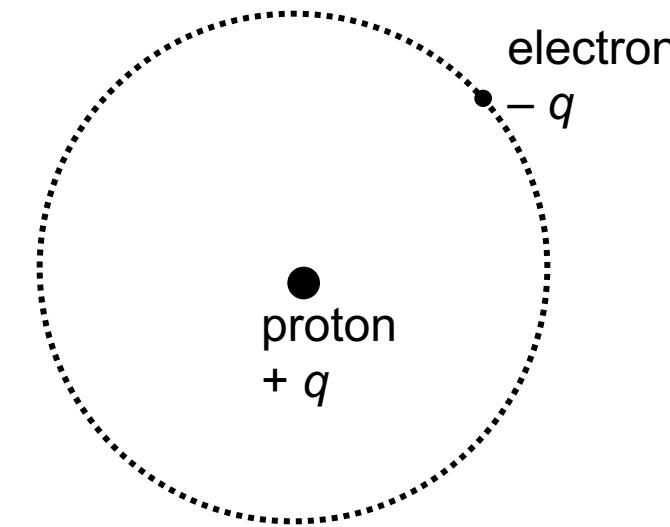


Fig.4.4

here,  $m_0$  is the electron rest mass  
and  $\varepsilon_0$  is the permitivity of free space or vacuum

The donor atom with its donor electron in GaAs resembles the hydrogen atom. Therefore, we can estimate the donor electron energy using eqn. (4.2), but with the following modification:

- use the electron effective mass  $m_n^* = 0.067 m_0$  instead of electron rest mass  $m_0$
- use and permitivity of GaAs  $\varepsilon = \varepsilon_r \varepsilon_0 = 13.2 \varepsilon_0$  instead of permitivity of free space  $\varepsilon_0$

Eqn. (4.2) becomes

$$E_n = -\frac{q^4}{2(4\pi \hbar)^2} \left( \frac{m_n^*}{\varepsilon_r^2 \varepsilon_0^2} \right) \frac{1}{n^2} \quad (4.3)$$

$$E_n = -\left( \frac{0.067}{13.2^2} \right) \frac{13.6}{n^2} = -\frac{0.0052}{n^2} \text{ eV} \quad (4.4)$$

for  $n = 1$ ,  $E_1 = -0.0052 \text{ eV}$

for  $n = \infty$ ,  $E_\infty = 0$

The energy required to excite the electron from the ground state ( $n = 1$ ) to the free state ( $n = \infty$ ) is

$$E_{\infty} - E_1 = 0.0052 \text{ eV} \quad (4.5)$$

which corresponds to the energy difference  $E_c - E_d$ , the ionization energy or the binding energy.

# Key takeaways (Lecture #7)

- Intrinsic semiconductor:
  - number of electrons in the conduction band = number of holes in the valence band
  - $n_i$  increases with increasing temperature  $T$
- Extrinsic semiconductor:
  - The properties (e.g. conductivity) of the semiconductor can be changed by adding controlled amounts of specific impurity atoms, called dopant atoms
  - Group V (such as Phosphorous, P) atoms in silicon crystals are called donor impurities/atoms
  - Electrons are donated to the conduction band without creation of holes in the valence band
  - Since  $n_0 > p_0$ , this semiconductor is called n-type semiconductor

$$n_0 = N_d + p_0$$

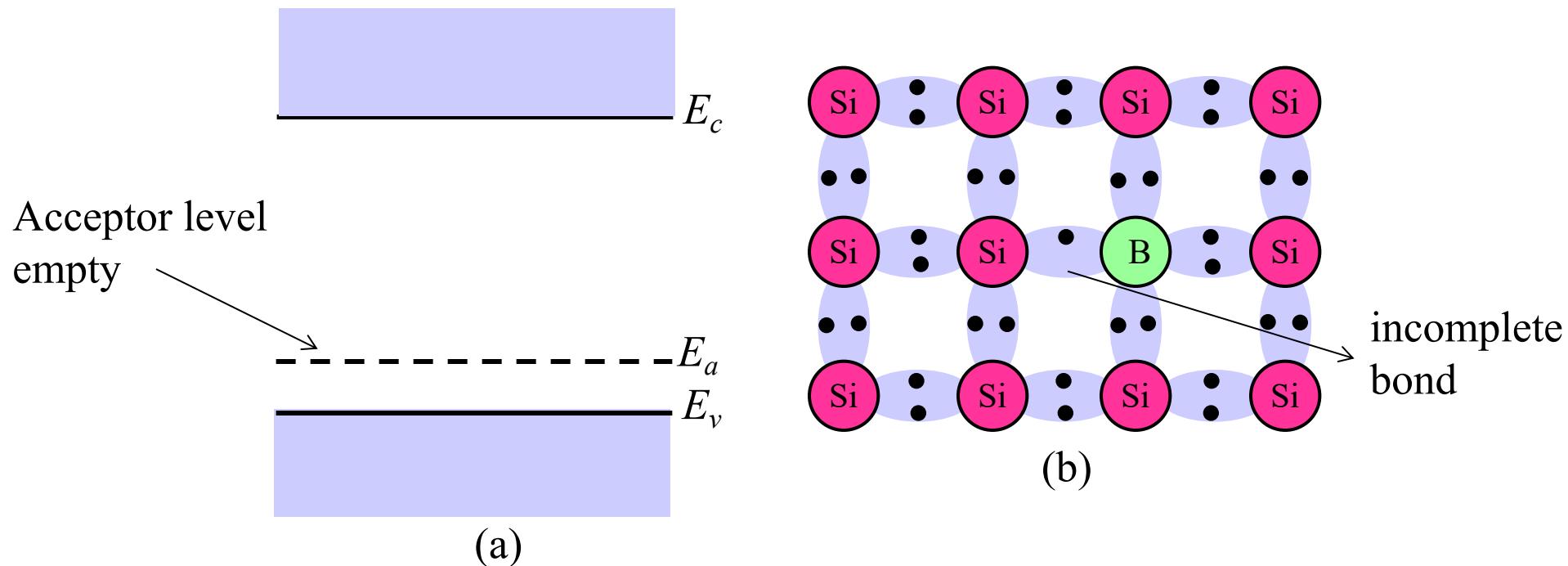
# Lecture 8

## 4.3 Acceptor Impurity

- We will now consider a situation where a silicon crystal is doped with impurity atoms from group III in the periodic table (e.g. B, Al, Ga).
- The group III atoms substitute the host Si atoms. The group III atoms in silicon crystals are called acceptor impurities/atoms, the reason will be clear later

- Consider now a group III atom, say a B atom, inside a silicon crystal (see Fig. 4.5)
  - Silicon atom has 4 valence electrons, but the boron atom, B, has only 3 valence electrons
  - In making covalent bonding with the neighboring Si atoms, the B atom only contributes 3 electrons thereby leaving one incomplete bond.
  - The impurity B atom introduces an energy level  $E_a$  in the energy gap above the valence band edge  $E_v$ . This energy level is called an acceptor level.
  - The energy difference  $E_a - E_v$  is the energy required to excite an electron from the valence band to the acceptor level.
  - This corresponds to the electron from the Si-Si covalent bond to move to the incomplete Si-B bond. The energy difference  $E_a - E_v$  is much smaller than the bandgap energy  $E_g$ .

- In Si, the acceptor levels  $E_a$  generally lie about 0.03-0.06 eV above  $E_v$ , whereas in Ge, the the acceptor levels lie about 0.01 eV above  $E_v$
- At 0 K, the acceptor level is empty. This corresponds to the incomplete Si-B covalent bond.



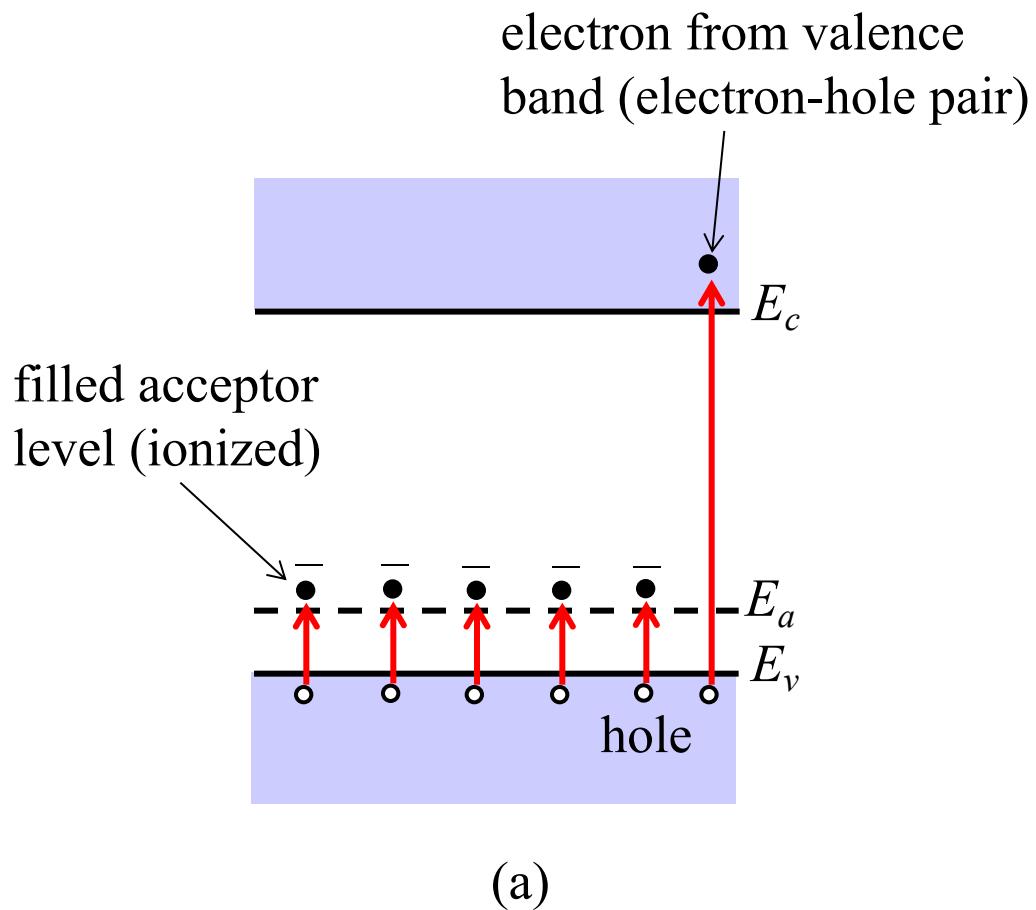
**Fig.4.5**

- Above 0 K, the electrons in the valence band gain thermal energy. The following processes occur (see Fig. 4.6):
  - Some electrons from the valence band are excited to the acceptor level creating holes in the valence band.
  - This corresponds to the electrons from the Si-Si bonds move occupying the incomplete Si-B bonds.
  - The impurity B atoms then become negatively charged or ionized. Each ionized impurity carries a charge of  $-1.6 \times 10^{-19}$  C, because the initially neutral impurity atom accepts one electron from the valence band.
  - Since the impurity atoms accept electrons, they are called acceptor impurities.
  - Note that in this case holes are created in the valence band without creation of electrons in the conduction band.

**Table 4.1** The bandgap and ionization energies at 300 K

	Ionization energy (eV)				$E_g$ (eV)	
	Donors		Acceptors			
	P	As	B	Al		
Si	0.045	0.05	0.045	0.06	1.11	
Ge	0.012	0.0127	0.0104	0.0102	0.67	

- Relatively much smaller number of electrons from the valence band are excited to the conduction band creating electron-hole pairs, simply because the energy gap  $E_g$  is much larger than the energy required to excite the electrons from the valence band to the acceptor level  $E_a - E_v$  (see Table 4.1)
- Here, the ionization energy of the acceptor atoms is the energy difference  $E_a - E_v$



At  $T > 0 \text{ K}$  whereby all acceptor impurities are ionized:

$$p_0 = N_a + n_0$$

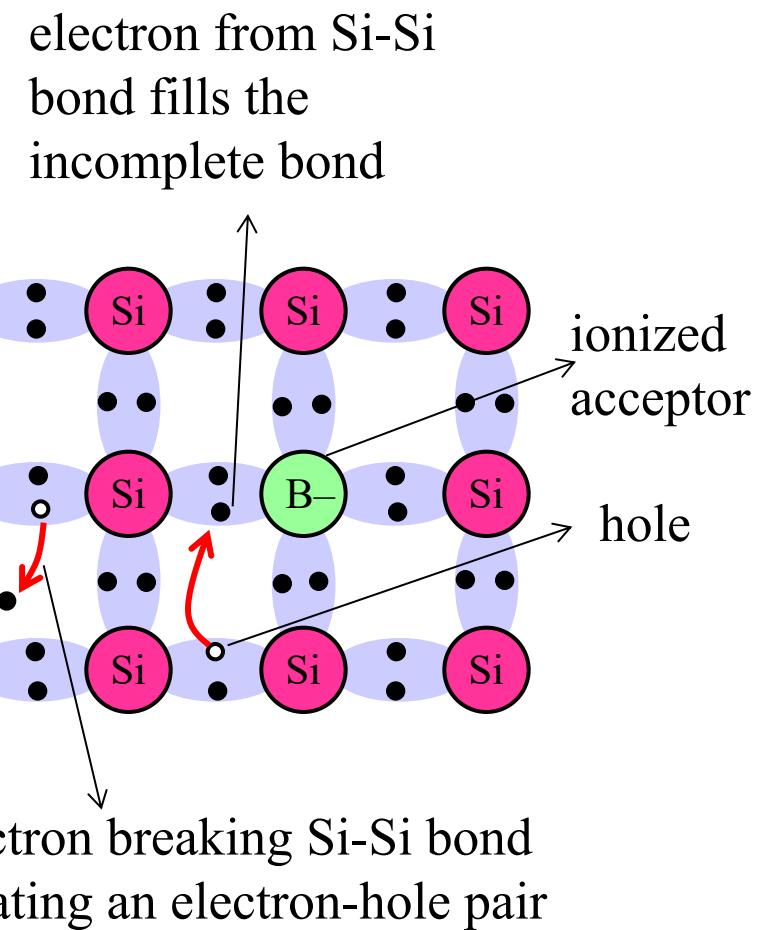


Fig.4.6

- Consider the situation at temperatures  $T$  whereby all the acceptor impurity atoms are ionized.
  - The semiconductor enters the impurity saturation (exhaustion) region (see section 4.4).
  - If the acceptor atom concentration is  $N_a$ , the thermal equilibrium hole concentration in the valence band  $p_0$  at  $T$  is the sum of
    - hole concentration due to the excitation of electron from the valence band to the acceptor level. This hole concentration is equal to the acceptor atom concentration  $N_a$  since all acceptor impurities are ionized. And consequently, all acceptor impurities become negative ions.
    - hole concentration due to the excitation of electrons from the valence band to the conduction band. This hole concentration is equal to the electron concentration in the conduction band  $n_0$  since they are created in pairs.

- Mathematically, we write:

$$p_0 = N_a + n_0 \quad (4.6)$$

The equation  $p_0 = N_a + n_0$  is shown. A curly brace underlines the sum  $N_a + n_0$ . Two arrows point from this brace to the labels "positive charge concentration" and "negative charge concentration".

- Again, eqn. (4.6) satisfies the charge neutrality condition.
- In Chapter 5 we will use the charge neutrality condition to calculate the thermal equilibrium electron and hole concentrations when donor, acceptor or both impurities are present.

- In the presence of acceptor concentration, holes in the valence band are created without the creation of electrons in the conduction band, and therefore

$$p_0 > n_0$$

This type of semiconductor, where  $p_0 > n_0$ , is called p-type semiconductor,

- the holes are referred to as majority carriers and
- the electrons are referred to as minority carriers

## 4.4 Temperature dependence of carrier concentration

Fig. 4.7 shows the thermal majority carrier concentration of an n-type semiconductor as a function of temperature  $T$ .

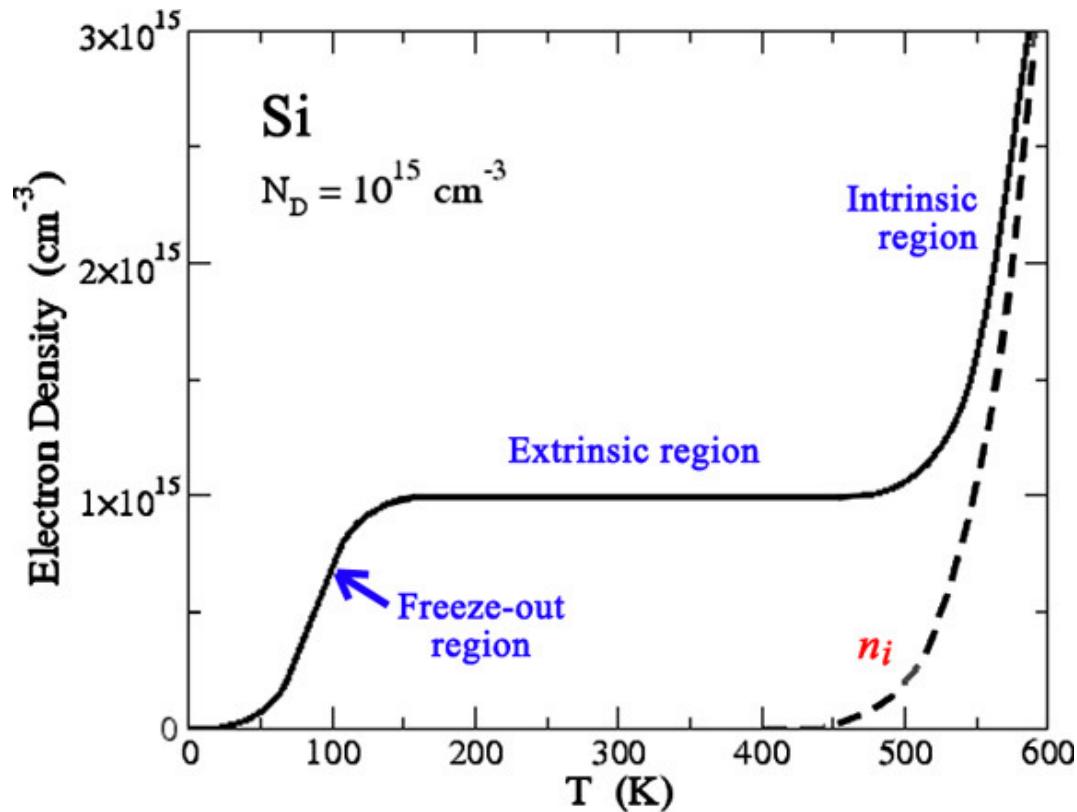


Fig. 4.7

- At 0 K, there is no excitation of electrons from the donor level and the valence band to the conduction band (see Fig. 4.2). Hence, the electron and hole concentrations are both zero.

- From 0 K to  $\sim$  150 K, the electron concentration in the conduction band increases. Above 0 K, the electrons gain thermal energy and the following processes occur (see also Fig. 4.3).
  - Electrons at the donor level are excited to the conduction band
  - There are some electrons excited from the valence band to the conduction band creating the electron-hole pairs. The number of these electrons are much smaller than those from the donor level because the energy gap  $E_g$  is much larger than  $(E_c - E_d)$ .
- From about 150 K to 450 K, the electron concentration is nearly constant. The reason is that the donor atoms are fully ionized and, yet, at this temperature range the electrons excited from the valence band to the conduction band, creating electron-hole pairs, are still much smaller than those excited from the donor level.

- Above 450 K, the electron concentration increases sharply. This corresponds to the increasing number of electrons being excited from the valence band to the conduction band creating electron-hole pairs. Here, the number of electrons from the donor level remain constant since the donor atoms have been fully ionized.
- As the electron-hole pair concentration increases and becomes much larger than the donor concentration, the semiconductor reverts to an intrinsic semiconductor.
- For fully ionized donor impurities, we can also see the variation of the electron concentration with temperature from eqn. (4.1)

$$n_0 = N_d + p_0 \quad (4.1)$$

negative charge concentration      positive charge concentration

- At about 150 K to 450 K, where the electron concentration is approximately constant

$$p_0 \ll N_d$$

$$\therefore n_0 \approx N_d$$

- Above 450 K, where the electron concentration increases sharply

$$p_0 \gg N_d$$

$\therefore n_0 \approx p_0 \longrightarrow$  intrinsic semiconductor

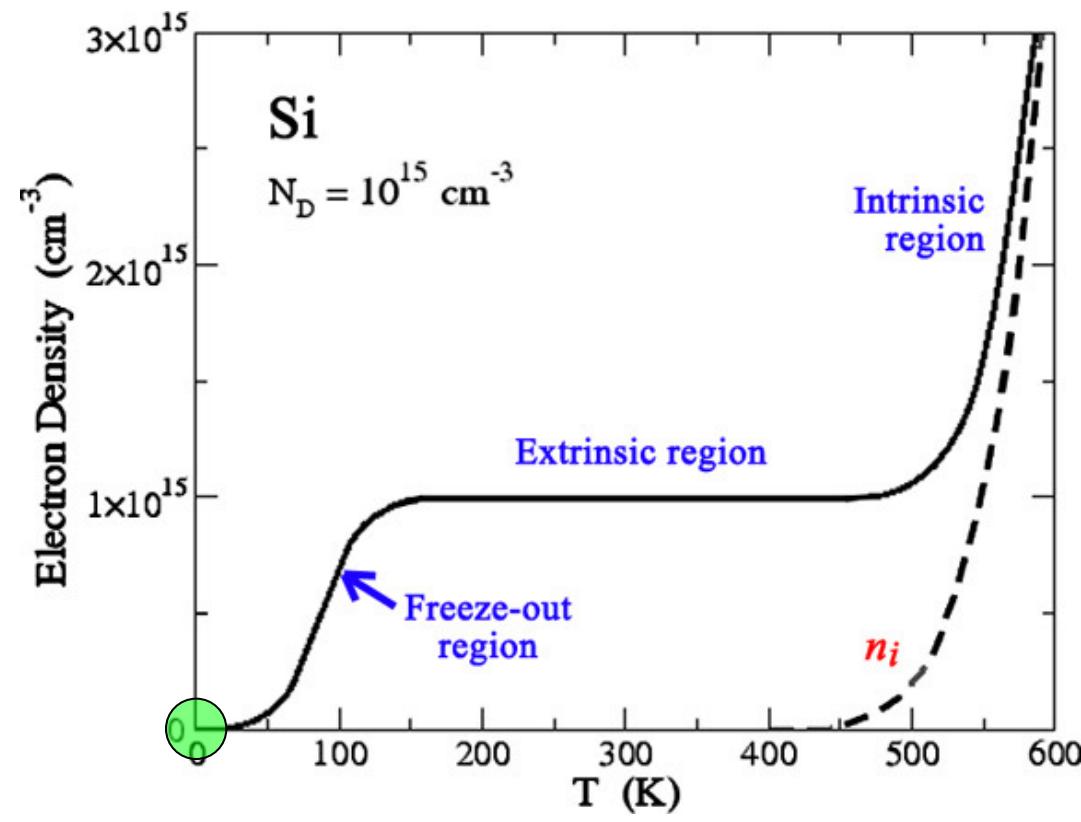
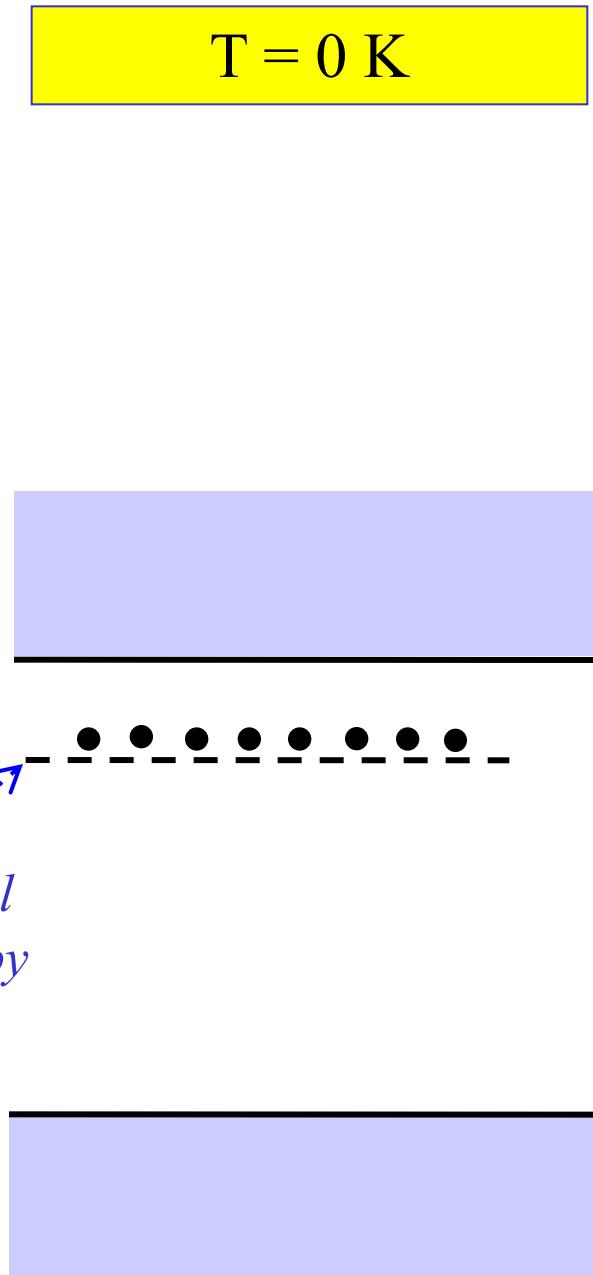


Fig. 4.7

*donor level  
occupied by  
electrons*



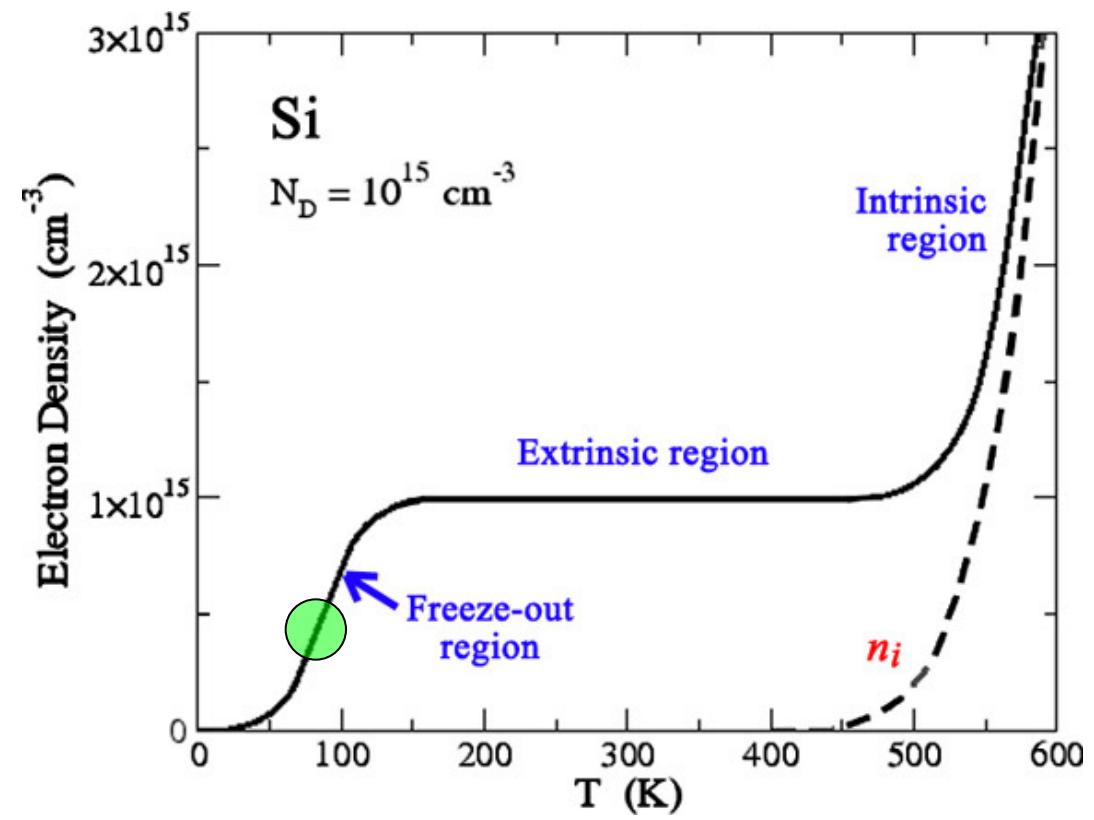
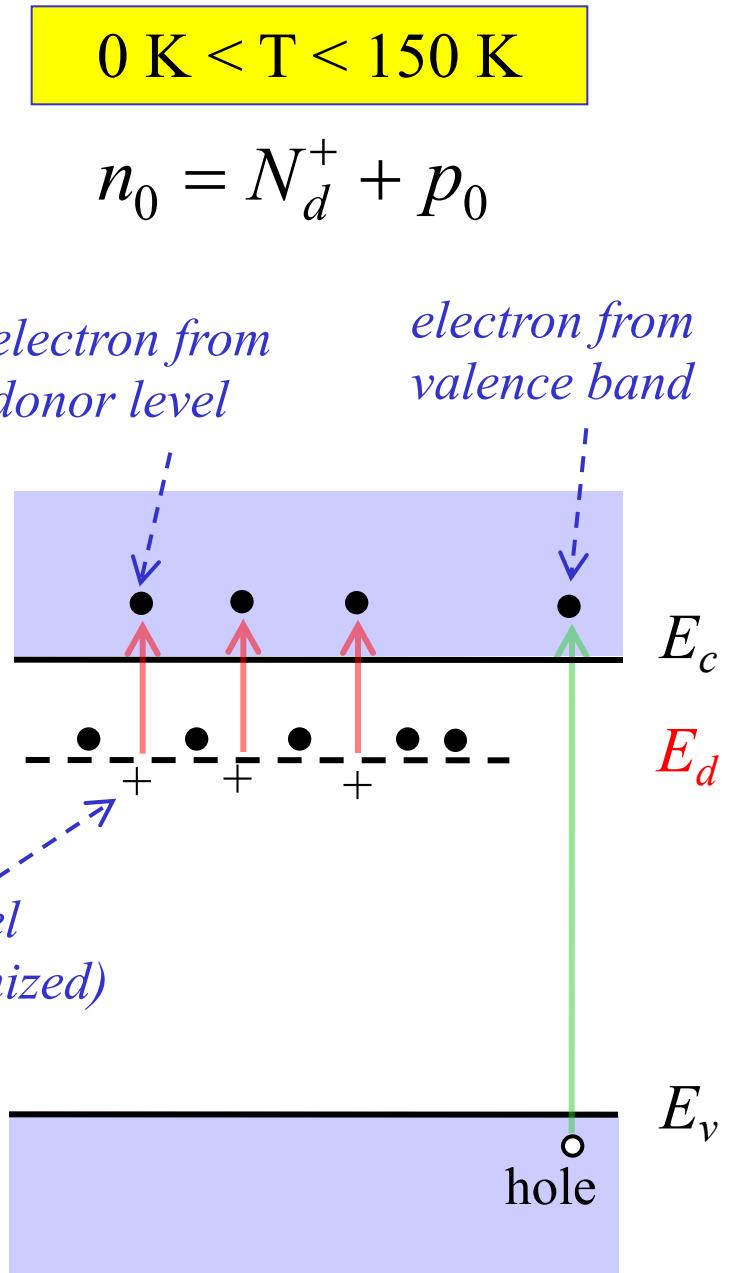


Fig. 4.7



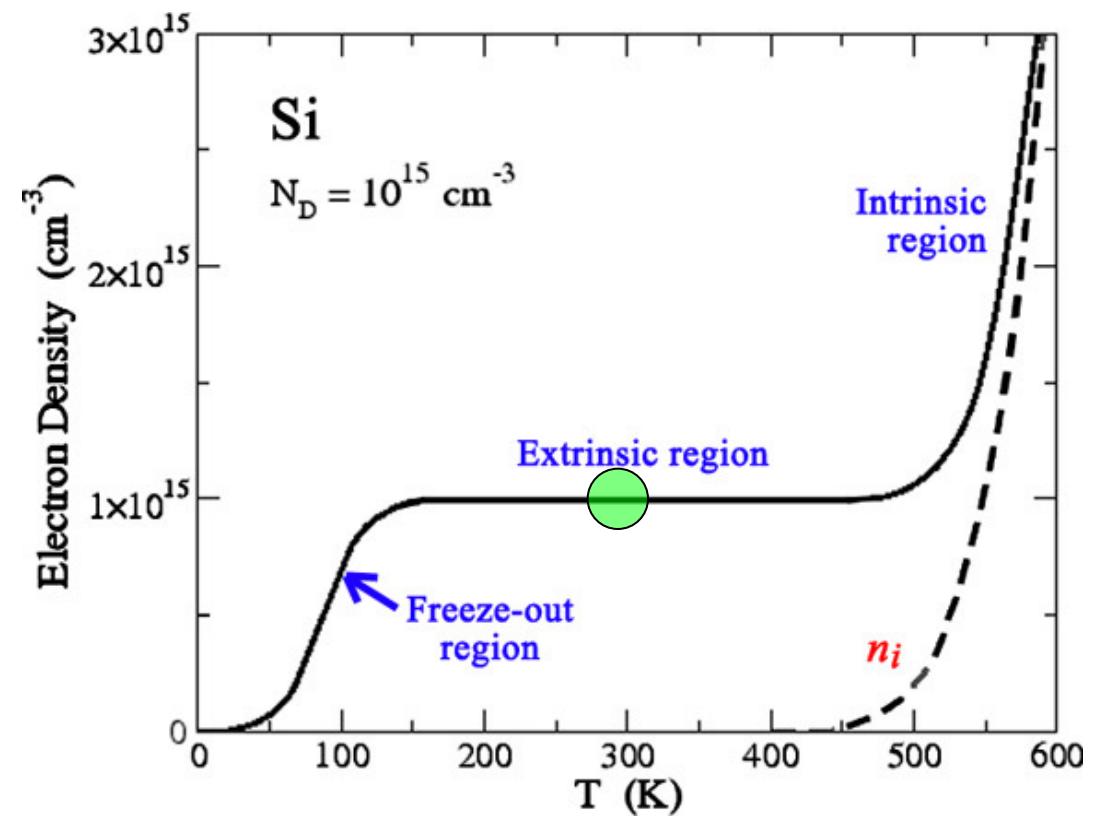


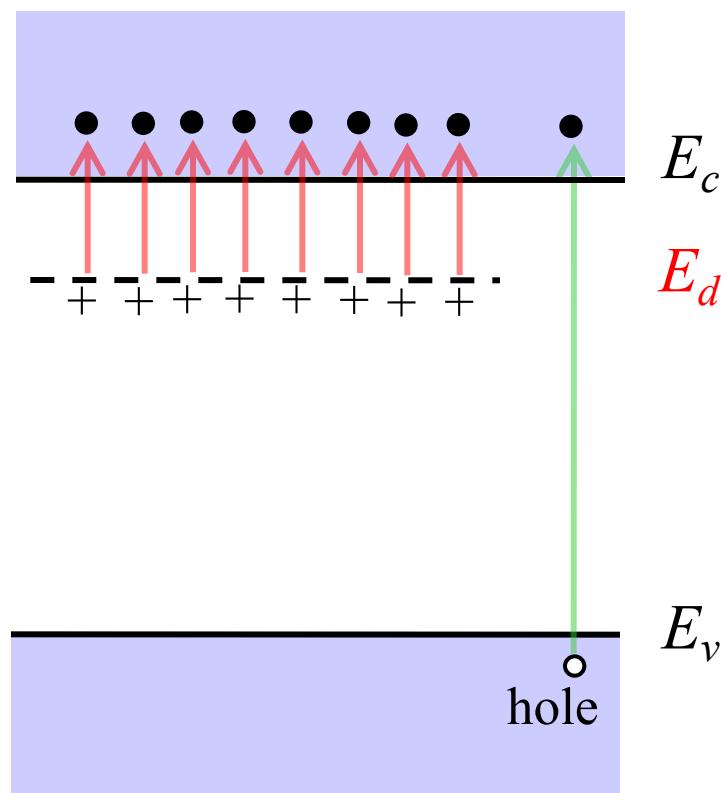
Fig. 4.7

150 K < T < 450 K

$$n_0 = N_d + p_0$$

$$N_d \gg p_0$$

$$n_0 \approx N_d$$



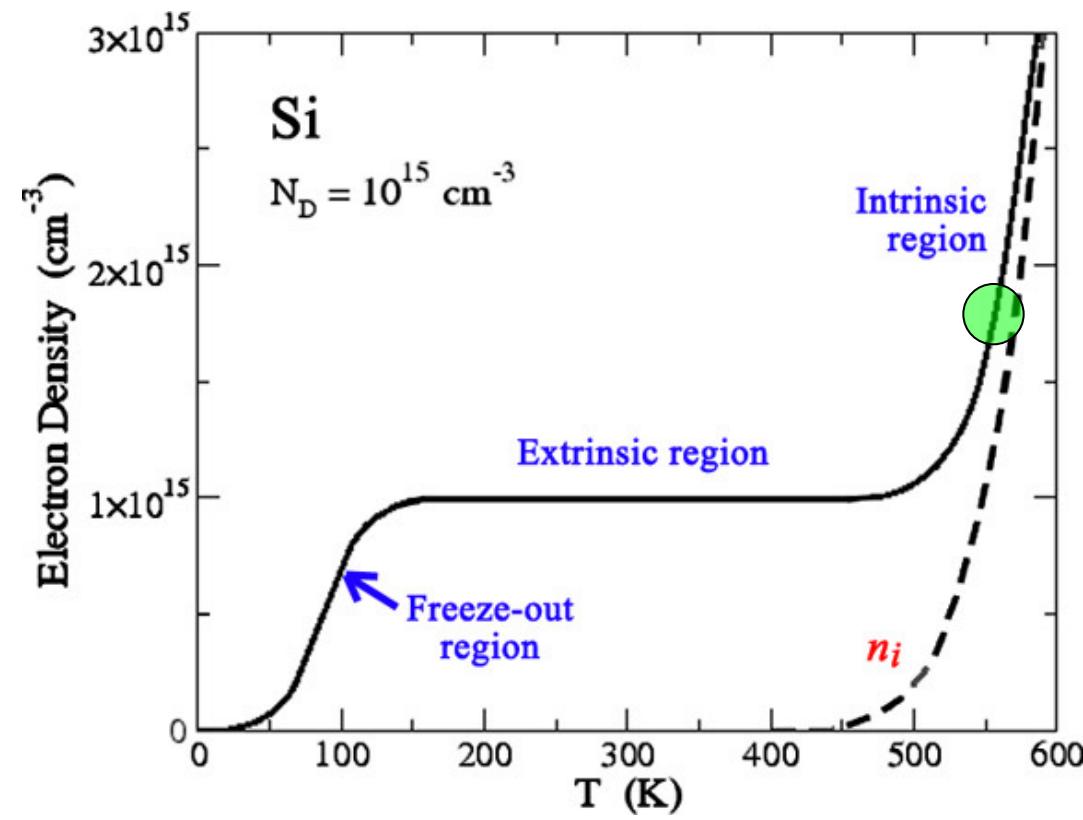
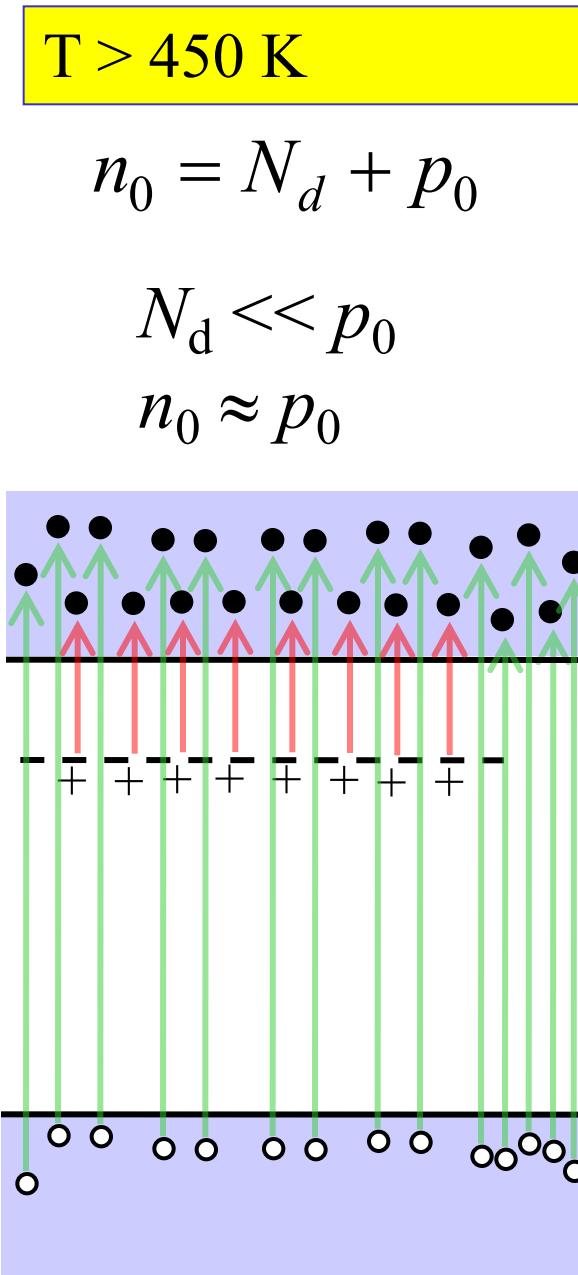


Fig. 4.7



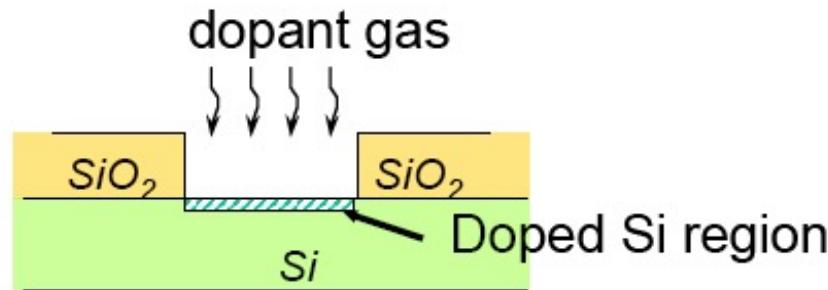
# Doping Technology

(not required for exam)

## (1) Diffusion

### (1) Predeposition

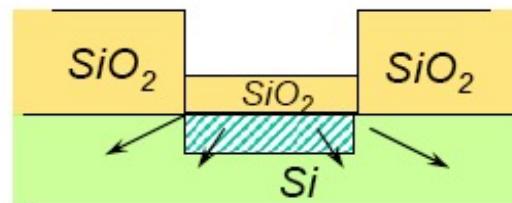
dose control



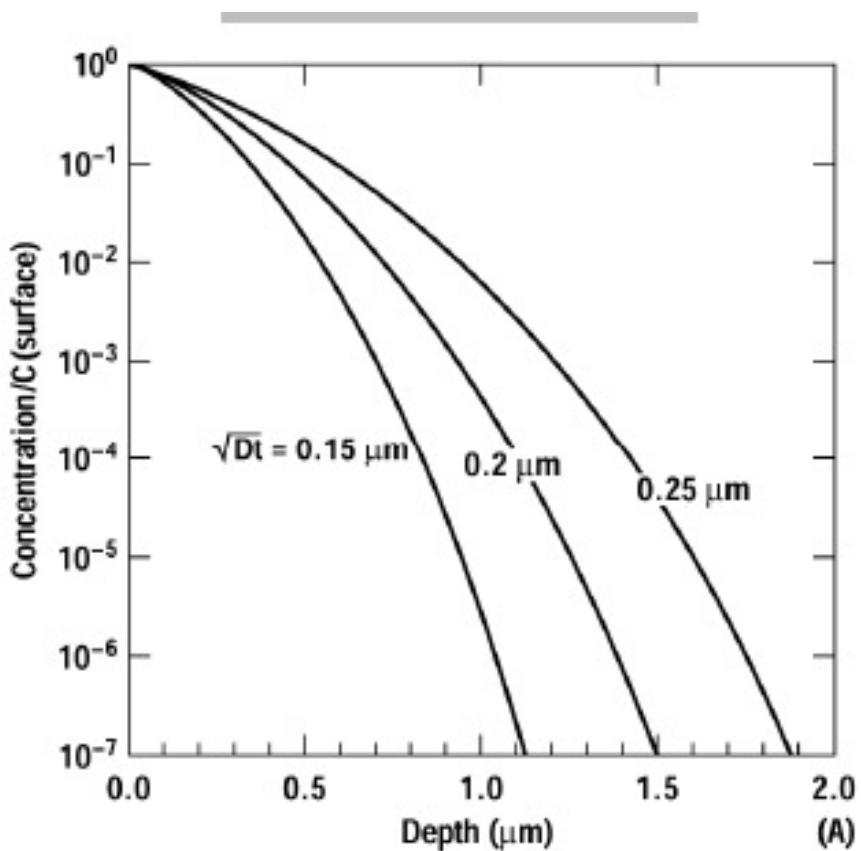
### (2) Drive-in

profile control  
(junction depth;  
concentration)

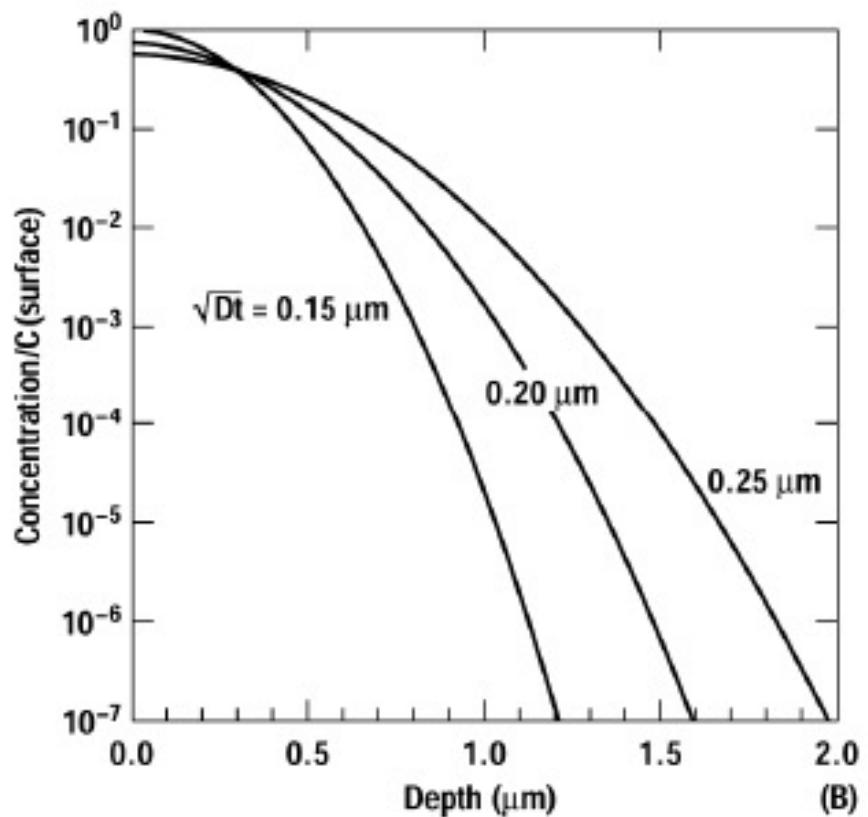
Turn off dopant gas  
or seal surface with oxide



# Doping profiles

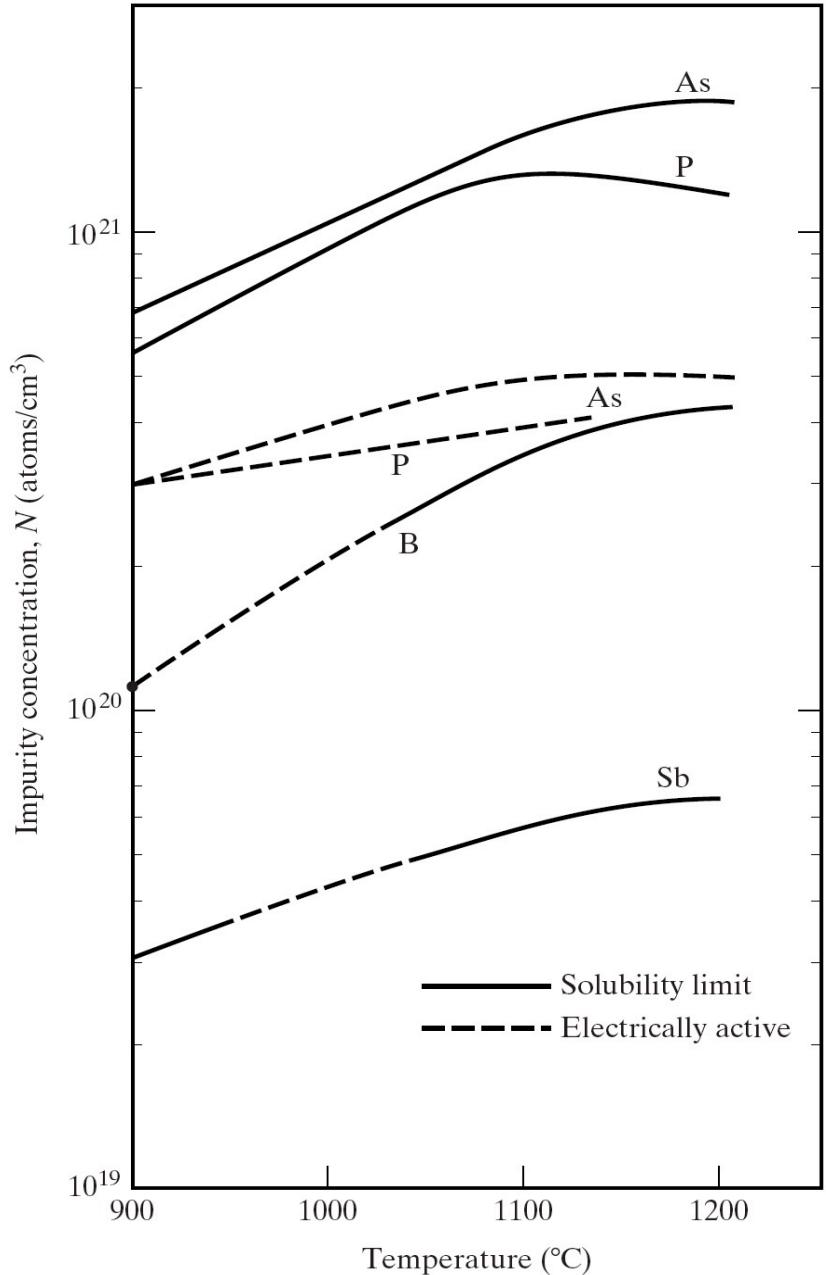


Pre-deposition



Drive-in

# Diffusion - Solid Solubility Limits

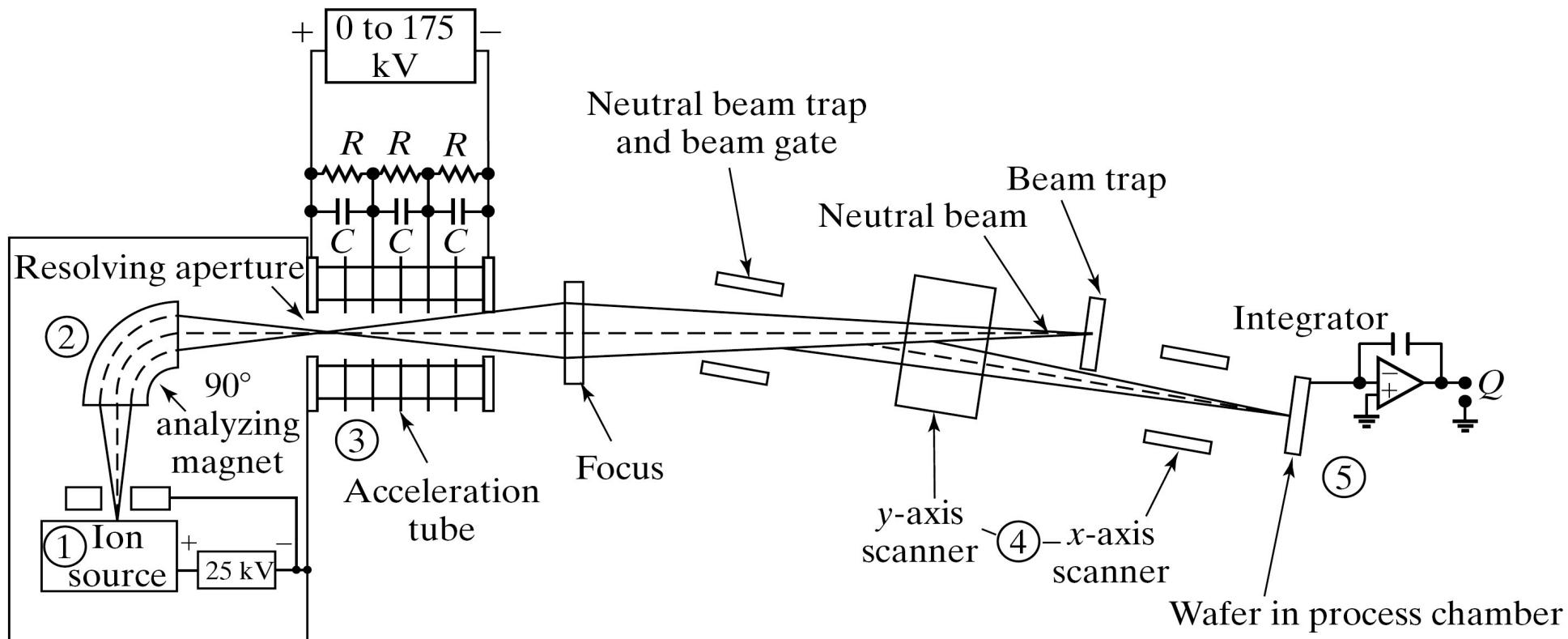


- There is a limit to the amount of a given impurity that can be “dissolved” in silicon (the Solid Solubility Limit)
- At high concentrations, all of the impurities introduced into silicon will not be electrically active

**FIGURE 4.6**

The solid-solubility and electrically active impurity-concentration limits in silicon for antimony, arsenic, boron, and phosphorus. Reprinted with permission from Ref. [29]. This paper was originally presented at the 1977 Spring Meeting of The Electrochemical Society, Inc., held in Philadelphia, Pennsylvania.

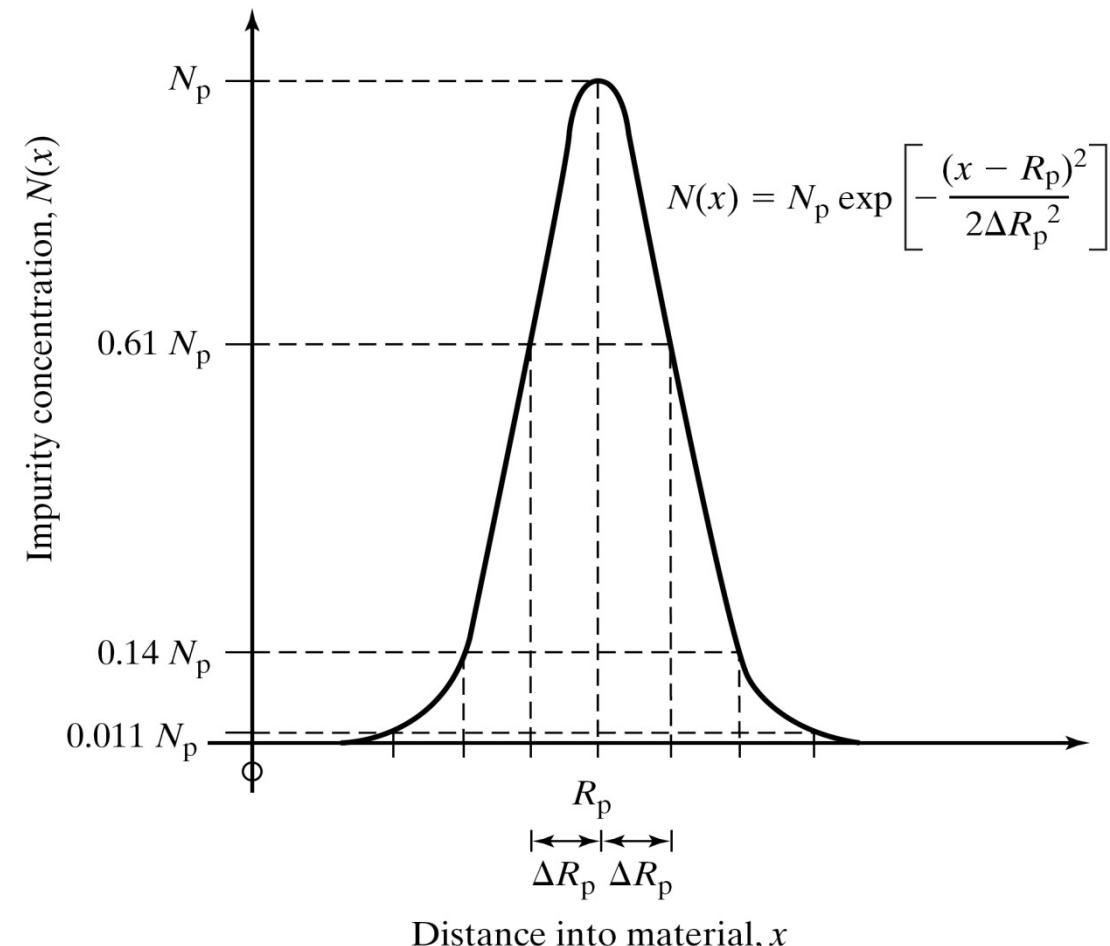
## (2) Ion implantation



- Ion implantation
- Rapid annealing

# Ion Implantation Mathematical Model

## Gaussian Profile



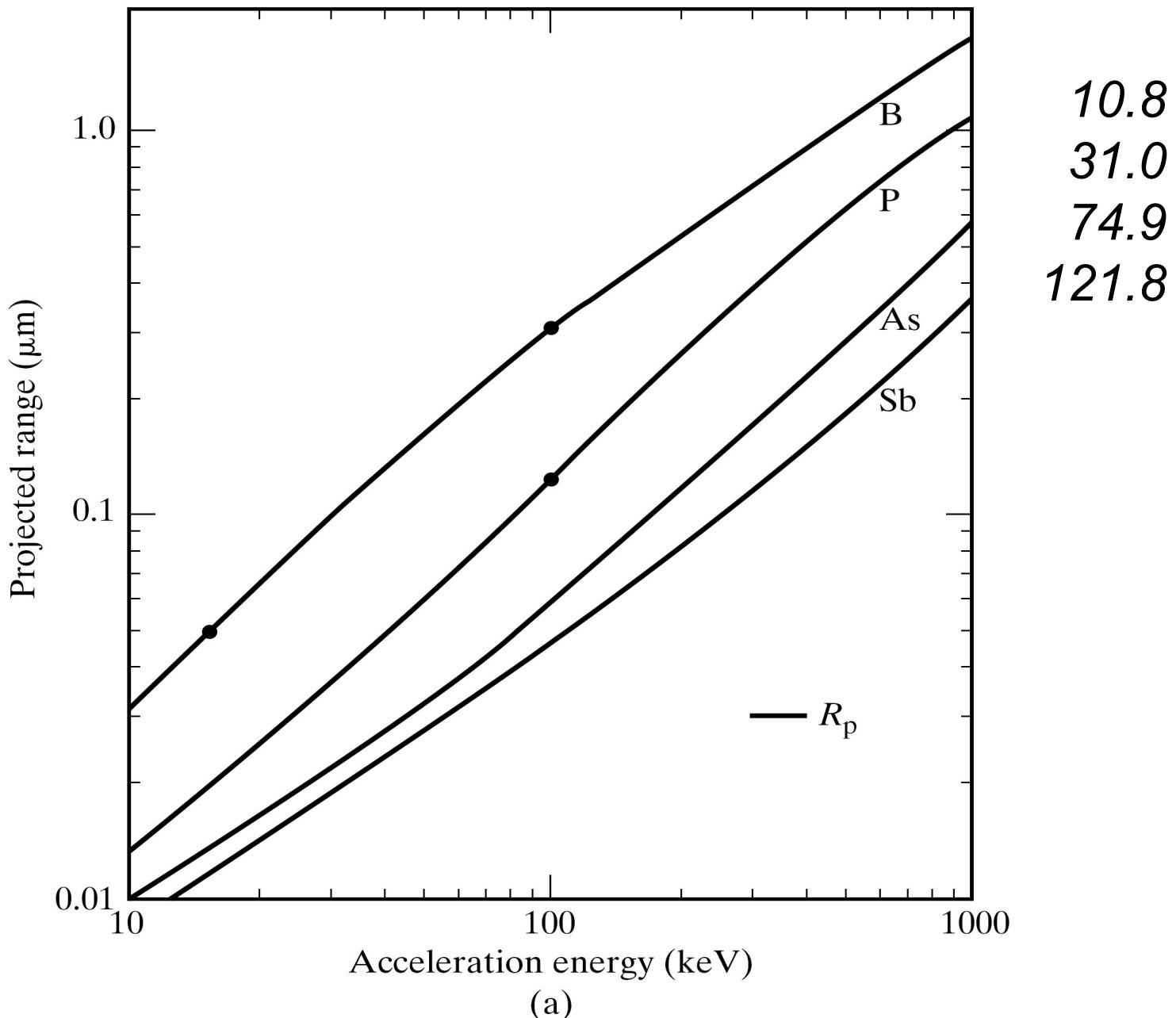
$$N(x) = N_p \exp\left[-\frac{(x - R_p)^2}{2\Delta R_p^2}\right]$$

$R_p$  = Projected Range

$\Delta R_p$  = Straggle

Dose  $Q = \int_0^\infty N(x)dx = \sqrt{2\pi}N_p\Delta R_p$

# Projected Range



# Resistivity vs. Doping

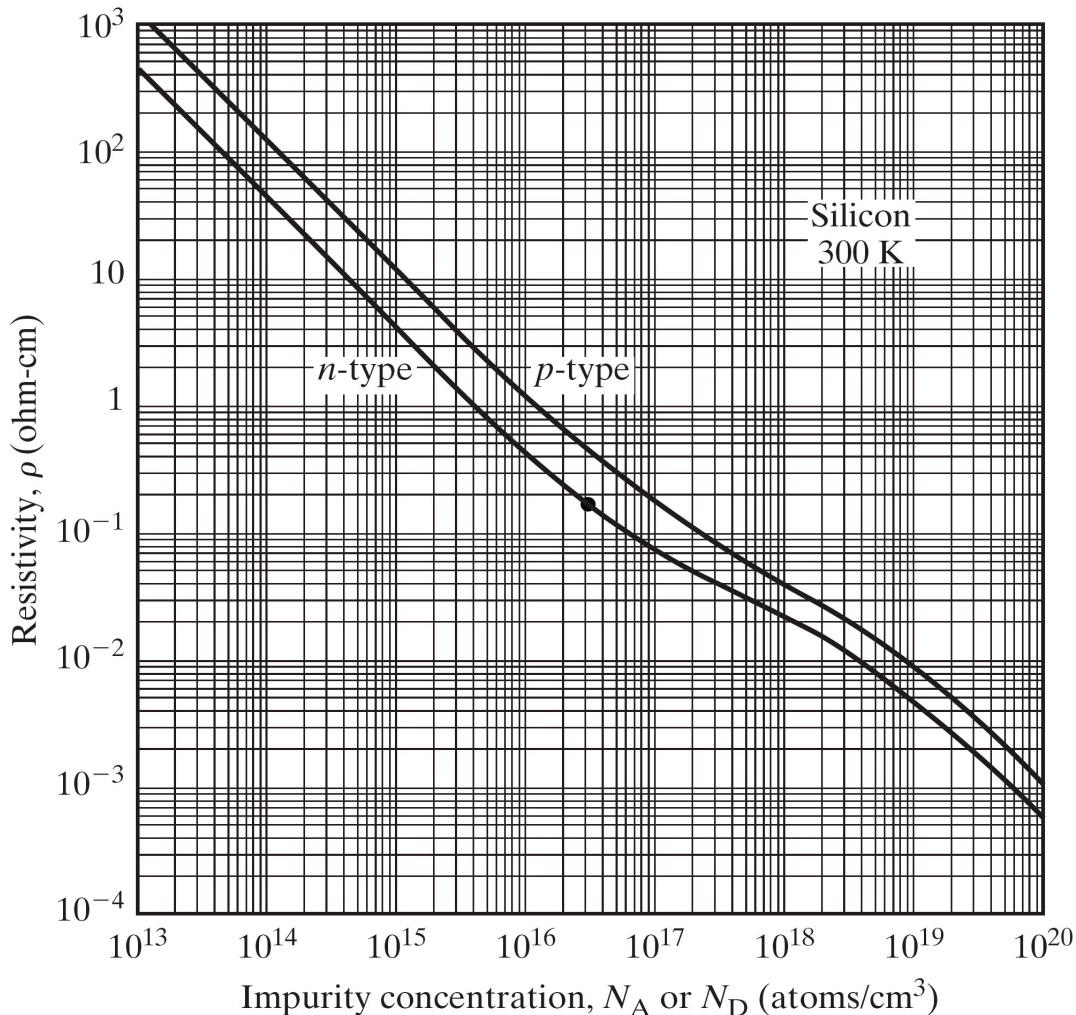


FIGURE 4.8

Room-temperature resistivity in *n*- and *p*-type silicon as a function of impurity concentration. (Note that these curves are valid for either donor or acceptor impurities but not for compensated material containing both types of impurities.)

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## Key takeaways (Lecture #8)

- Extrinsic semiconductor (p-type):
  - Group III (such as Boron, B) atoms in silicon crystals are called acceptor impurities/atoms
  - Electrons from the valence band are excited to the acceptor level creating holes in the valence band
  - Note that in this case holes are created in the valence band without creation of electrons in the conduction band

$$p_0 = N_a + n_0$$

- Since  $p_0 > n_0$  , this semiconductor is called p-type semiconductor

# Lecture 9

# 5 SEMICONDUCTOR IN EQUILIBRIUM

- Interested in determining the current-voltage characteristics of semiconductor devices.
- Current is due to net flow of charges, there is a need to determine the number of charge carriers available for generating the currents, i.e. the electron concentration in the conduction band and hole concentration in the valence band.
- Therefore, first of all, we will look at the electrons and hole concentrations in thermal equilibrium at temperature  $T$ 
  - Thermal equilibrium implies that no external forces, such as voltages, electric fields, magnetic fields or **temperature gradients** are acting on the semiconductor.

- However, if the presence of external forces do not create excess electrons in the conduction band and holes in the valence band, i.e. the electrons and holes are solely created by the thermal energy, then we can use the thermal equilibrium electron and hole concentrations to analyze the behavior of the semiconductor in the presence of the external forces.
- In thermal equilibrium, all properties of semiconductor will be independent of time

To determine the thermal equilibrium electron and hole concentrations at temperature  $T$ , essentially we need to know the following:

- The density of quantum states, that is the number of quantum states per unit volume of the crystal per unit energy, in the conduction and valence bands
- The probability of a quantum states at energy  $E$  is occupied by an electron at temperature  $T$

## 5.1 Fermi-Dirac Distribution Function

The probability that a quantum state is occupied by an electron at temperature  $T$  is given by the Fermi-Dirac distribution function.

The Fermi-Dirac probability function describes the distribution of electrons over a range of allowed energy levels at thermal equilibrium.

To develop this probability function, we must consider the following:

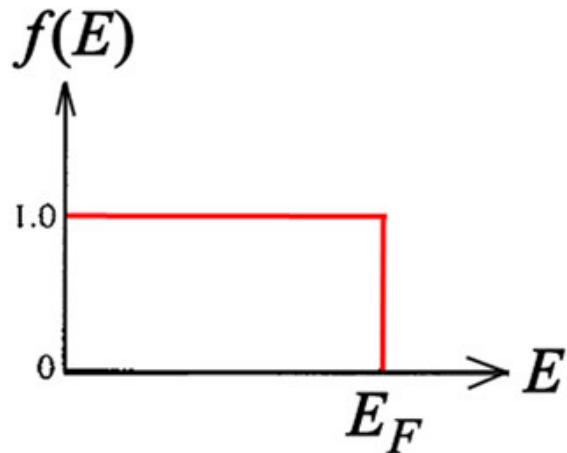
- The quantum nature of electrons
- Electrons are indistinguishable
- Only one particle is permitted in each quantum state (Pauli's exclusion principle)

- The Fermi-Dirac probability function is given by

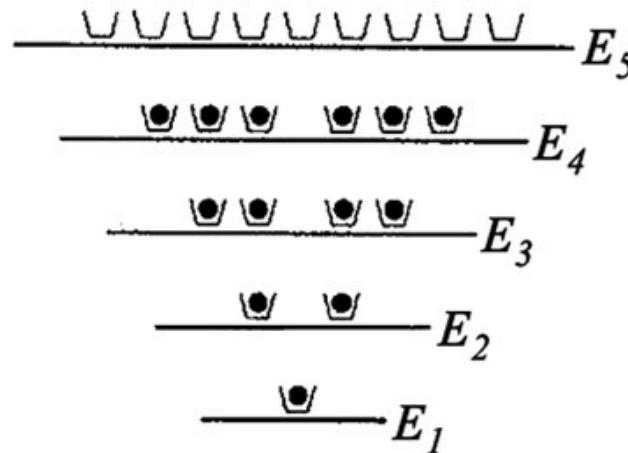
$$f(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]} \quad (5.1)$$

- it gives the probability that a quantum state at energy  $E$  will be occupied by an electron at temperature  $T$
- it is also the ratio of the filled states to the total quantum states at energy  $E$

$E_F$  is called the Fermi energy level. It determines the statistical distribution of electrons and does not have to correspond to an allowed energy state. The Fermi level is an important reference level.



**Fig. 5.1** The Fermi probability function versus energy for  $T = 0^\circ\text{K}$



Discrete energy states and quantum states for a particular system at  $T=0^\circ\text{K}$

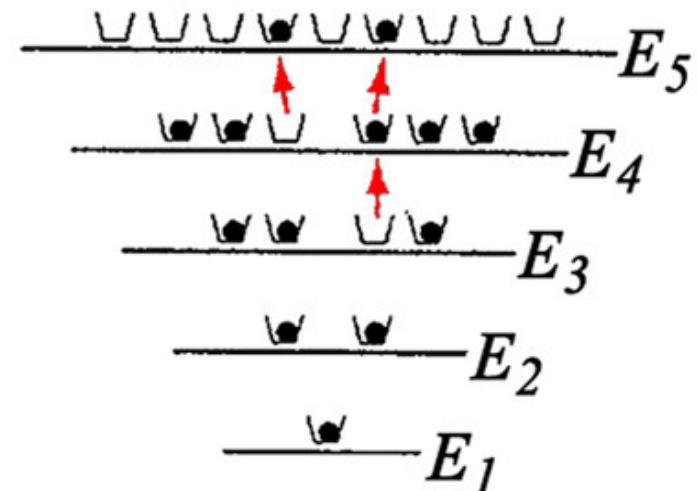
**At  $T = 0 \text{ K}$ ,**

$$f(E) = \begin{cases} 1 & \text{for } E < E_F \\ 0 & \text{for } E > E_F \end{cases} \quad (5.2)$$

- all electrons are in their lowest possible energy levels, up to the Fermi level
- probability of quantum states being occupied is unity for  $E < E_F$

At  $T > 0$  K,

- electrons gain a thermal energy so that some of them can jump to higher energy levels
  - change in distribution of electrons among available energy states
- At  $E > E_F$ , the Fermi-Dirac distribution in eqn. (5.1) is no longer zero. This means that some probabilities exists for a state above  $E_F$  is occupied by an electron.
- At  $E < E_F$ , the Fermi-Dirac distribution in eqn. (5.1) is no longer unity. This means that some probabilities exists for a state below  $E_F$  is empty.



**Fig. 5.2** Discrete energy states and quantum states for the same system at  $T > 0^\circ\text{K}$

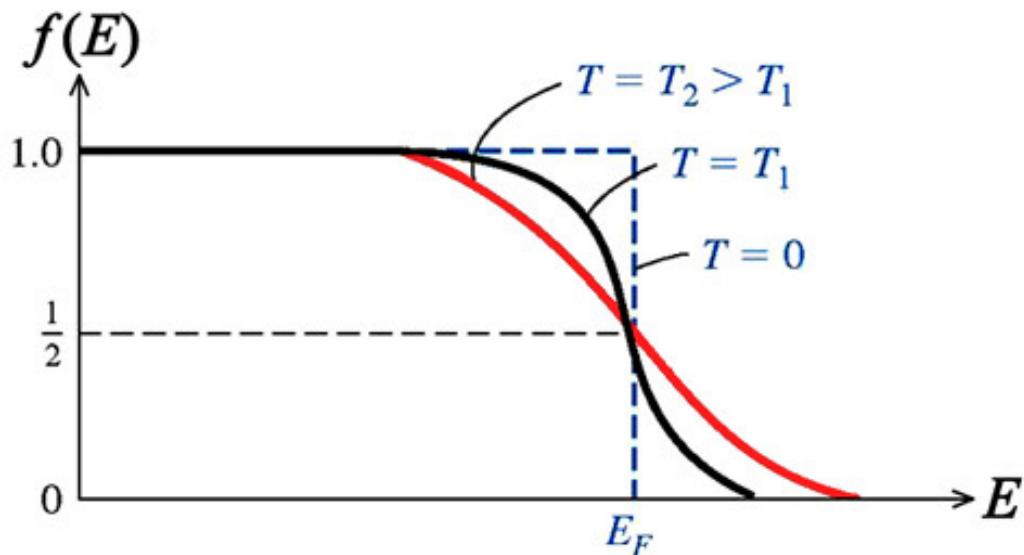
- At  $E = E_F$ , the Fermi-Dirac distribution is

$$f(E = E_F) = \frac{1}{1 + \exp(0)} = \frac{1}{2} \quad (5.3)$$

i.e. the probability of a state having energy  $E = E_F$  being occupied by an electron is  $\frac{1}{2}$

**Fig. 5.3**

The Fermi probability function vs energy for different temperatures



- Fig. 5.3 shows the Fermi-Dirac distribution function at various temperature  $T$ 
  - **symmetrical** about the Fermi energy  $E_F$  at all temperature.

- Consider the Fermi-Dirac function at temperature  $T_2$  in Fig. 5.3
  - The probability of a state having energy  $\Delta E$  above  $E_F$ , ( $E_F + \Delta E$ ), to be occupied by an electron is  $f(E_F + \Delta E)$
  - The probability of a state having energy  $\Delta E$  below  $E_F$ , ( $E_F - \Delta E$ ), to be empty is  $[1 - f(E_F - \Delta E)]$
  - Since the Fermi-Dirac function is symmetrical about the Fermi energy  $E_F$ , it follows that the probability of a state having energy  $\Delta E$  above  $E_F$  is occupied is the same as the probability of a state having energy  $\Delta E$  below  $E_F$  is empty.
  - mathematically, this means (and can be easily proved)

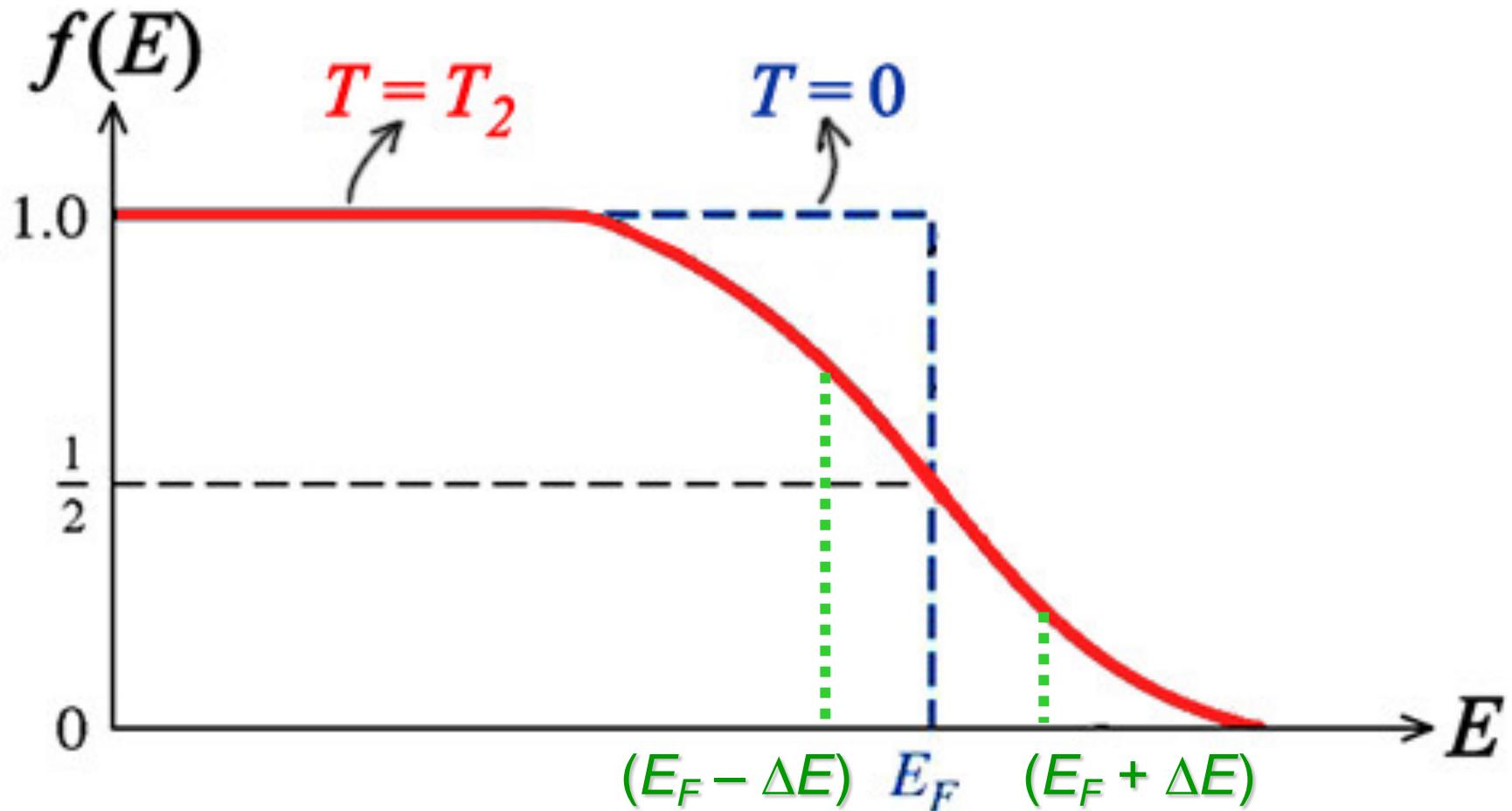
$$f(E_F + \Delta E) = 1 - f(E_F - \Delta E) \quad (5.4)$$


  
 probability of a state  
 having energy  $\Delta E$  above  
 $E_F$  is occupied


  
 probability of a state  
 having energy  $\Delta E$  below  
 $E_F$  is empty

**Tutorial #3**

- In terms of electrons and holes, we can say that probability of not finding an electron at energy  $E$ ,  $[1 - f(E)]$ , is the probability of finding a hole at energy  $E$ .



## Example 5.1

Calculate the probability that an energy state 0.56 eV above the Fermi energy is occupied by an electron for temperatures of 0 °C and 100 °C.

The probability of an energy state  $E = E_F + 0.56$  eV to be occupied by an electron is

$$f(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]} = \frac{1}{1 + \exp\left[\frac{0.56 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23} T}\right]}$$

Hence, for  $T = 0$  °C = 273 K,  $f(E) = 4.69 \times 10^{-11}$ ,

and for  $T = 100$  °C = 373 K,  $f(E) = 2.76 \times 10^{-8}$

Note that as temperature increases by 100 °C, the probability increases by  $\sim 600$  times. This shows the great sensitivity of this probability on temperature

## 5.2 Density of States

In addition to the Fermi-Dirac distribution function, we also need to consider the density of quantum states available for electrons to occupy.

### 5.2.1 Free electrons

To discuss the density of states of electrons in a crystal, let us start with the density of states of free electrons in 3-dimensions (3-D).

- Density of states is the number of quantum states per unit volume of the crystal per unit energy.
- The density of states  $g(E)$  for free electrons in 3-D is derived in Appendix B. It is given by

$$g(E) = \frac{4\pi(2m)^{3/2}}{h^3} \sqrt{E} \quad (5.5)$$

where the energy  $E$  is the free electron energy in 3-D [see Appendix B, eqn. (B.3)], that is

$$E = \frac{\hbar^2 k^2}{2m}$$

so, alternatively we can write eqn. 5.5 as

$$g(E) = \frac{4\pi(2m)^{3/2}}{h^3} \sqrt{\frac{\hbar^2 k^2}{2m}} \quad (5.6)$$

## 5.2.2 Electrons in crystals

The electrons in a crystal are not completely free , they interact with the periodic potential formed by the ions and electrons.

In section 3.4.4, we have seen that the effective mass takes into account the interaction of charge carriers with the lattice, which then allow us to regard the charge carriers as free carriers.

Consider now electrons in the conduction band

- Near the conduction band minima the  $E - k$  relation is approximately parabolic (see Fig. 5.4). The electrons behave like free electrons with effective mass  $m_n^*$ . Therefore we can express the energy  $E$  as

$$E - E_c = \frac{\hbar^2 k^2}{2m_n^*} \quad (5.7)$$

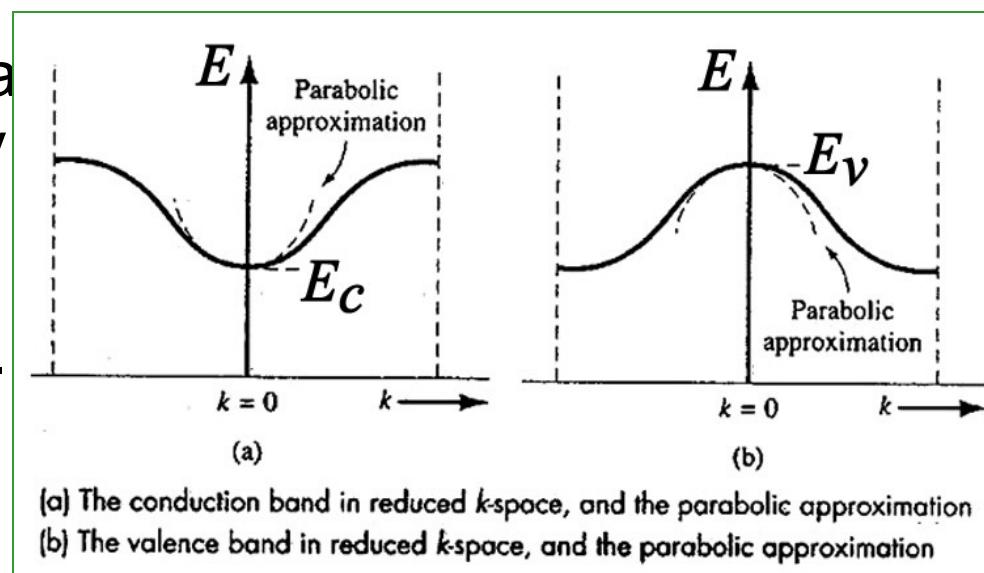


Fig.5.4

- Using eqn. (5.7) and the effective mass  $m_n^*$  in eqn. (5.6), we obtain the density of states in the conduction band  $g_c(E)$

$$g_c(E) = \frac{4\pi}{h^3} \left(2m_n^*\right)^{3/2} \sqrt{E - E_c} \quad (5.8)$$

We can obtain the density of states in the valence band  $g_v(E)$  in the same way as we obtain the density of states in the conduction band

- Near the top of the valence band, the  $E - k$  relation is also approximately parabolic (see Fig. 5.4) with the effective mass  $m_p^*$ . The energy  $E$  is then

$$E_v - E = \frac{\hbar^2 k^2}{2m_p^*} \quad (5.9)$$

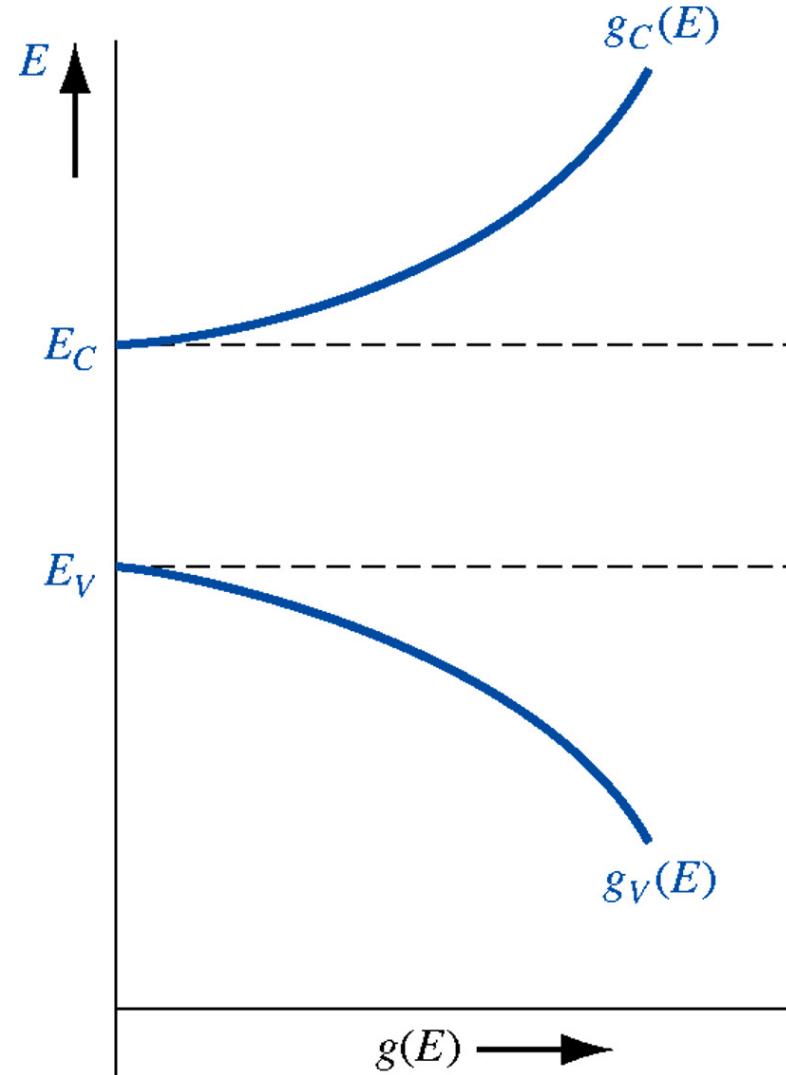
- Therefore, the density of states in the valence band is

$$g_v(E) = \frac{4\pi}{h^3} \left(2m_p^*\right)^{3/2} \sqrt{E_v - E} \quad (5.10)$$

Fig. 5.5 shows the density of states in the conduction and valence bands as function of energy  $E$

If quantum states do not exist within forbidden energy band, the density of states

$$g(E) = 0 \text{ for } E_v < E < E_c$$

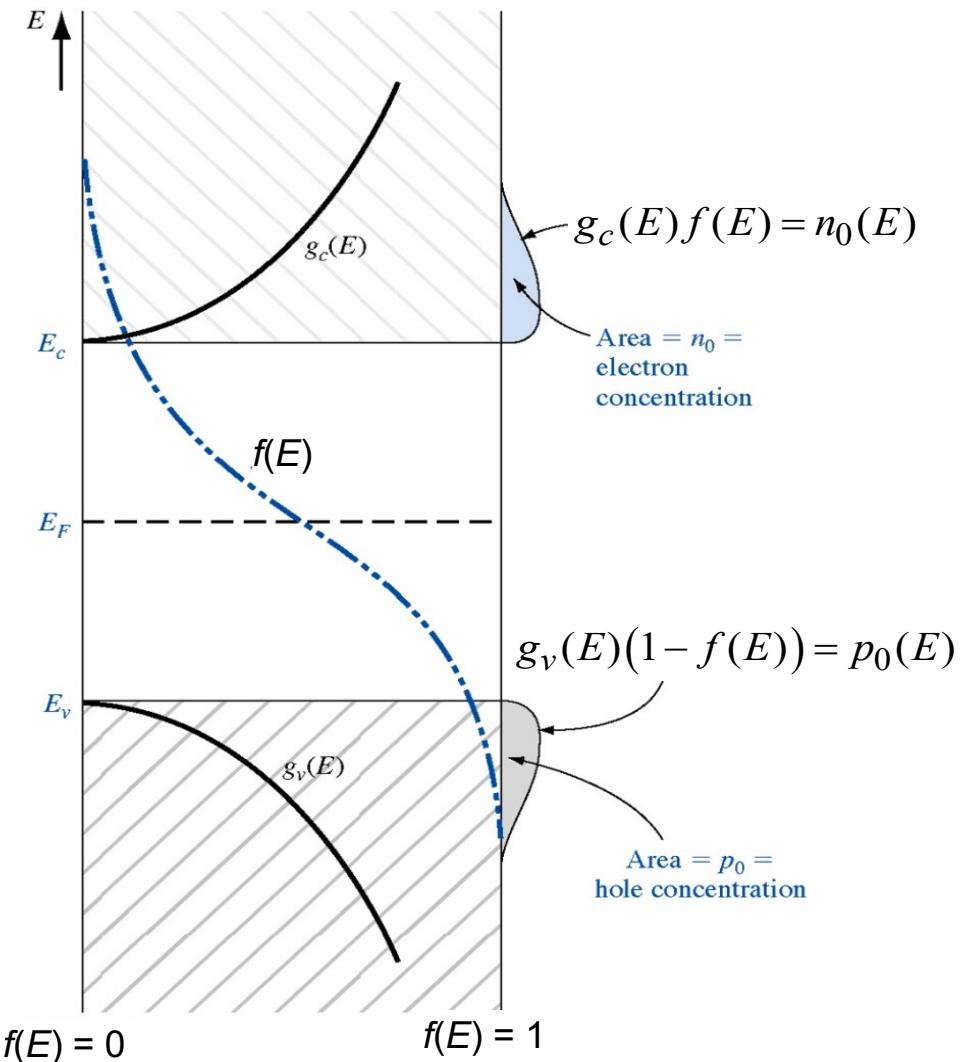


**Fig. 5.5**

## 5.3 Thermal equilibrium carrier concentrations

- At thermal equilibrium, the electron concentration at energy  $E$  in the conduction band, denoted by  $n_0(E)$ , is :

$$n_0(E) = g_c(E)f(E) \quad (5.11)$$



**Fig. 5.6**

Density of states function, Fermi-Dirac probability function, and areas representing electron and hole concentration for the case  $E_F$  is near the midgap

- The thermal equilibrium electron concentration in the conduction band  $n_0$  is then given by the integration over all the energies  $E$  in the entire conduction band, i.e. from the bottom of the conduction band  $E_c$  to  $\infty$

$$n_0 = \int_{E_c}^{\infty} n(E) dE = \int_{E_c}^{\infty} g_c(E) f(E) dE \quad (5.12)$$

- We will calculate the thermal equilibrium electron concentration  $n_0$  for the Fermi energy  $E_F$  within the bandgap below the conduction band edge  $E_c$ , such that

$$E_c - E_F \gg k_B T \quad (5.13)$$

To satisfy eqn. (5.13), it is sufficient to take  $E_c - E_F > 3k_B T$

- The energy of electrons in the conduction band  $E$  is above  $E_c$ , it follows

$$E - E_F \gg k_B T \quad (5.14)$$

The Fermi-Dirac distribution can then be reduced as follow

$$f(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]} \approx \exp\left[-\frac{E - E_F}{k_B T}\right] \quad (5.15)$$

- Now, we evaluate the thermal equilibrium electron concentration  $n_0$  in eqn. (5.12) using the density of states  $g_c(E)$  in eqn. (5.8) and the reduced  $f(E)$  in eqn. (5.15). We obtain

$$n_0 = N_c \exp\left[-\frac{E_c - E_F}{k_B T}\right] \quad (5.16)$$

where  $N_c$  is the effective density of states in the conduction band, given by

$$N_c = 2 \left( \frac{2\pi m_n^* k_B T}{h^2} \right)^{3/2} \quad (5.17)$$

# Problem

Q1: Determine the probability that a quantum state energy  $E = E_c + kT$  is occupied by an electron, and calculate the electron concentration in GaAs at  $T= 300\text{K}$  if the Fermi level is 0.25 eV below  $E_c$ . (Ex 4.1)



# Problem

Q1: Determine the probability that a quantum state energy  $E = E_c + kT$  is occupied by an electron, and calculate the electron concentration in GaAs at  $T= 300\text{K}$  if the Fermi level is 0.25 eV below  $E_c$ . (Ex 4.1)

$$\begin{aligned}f_F &\equiv \exp\left[\frac{-(E - E_F)}{kT}\right] \\&= \exp\left[\frac{-(E_c + kT - E_F)}{kT}\right] \\&= \exp\left[\frac{-(0.25 + 0.0259)}{0.0259}\right]\end{aligned}$$

$$f_F = 2.36 \times 10^{-5}$$

$$\begin{aligned}n_o &= N_c \exp\left[\frac{-(E_c - E_F)}{kT}\right] \\&= (4.7 \times 10^{17}) \exp\left[\frac{-0.25}{0.0259}\right]\end{aligned}$$

$$n_o = 3.02 \times 10^{13} \text{ cm}^{-3}$$



## Key takeaways (Lecture #9)

- To determine the thermal equilibrium electron and hole concentrations at temperature  $T$ , we need:
  - The density of quantum states in the conduction and valence bands
  - The probability of a quantum states at energy  $E$  is occupied by an electron at temperature  $T$
- Fermi-Dirac Distribution Function: 
$$f(E) = \frac{1}{1 + \exp\left[\frac{E - E_F}{k_B T}\right]}$$
- Equilibrium electron concentration  $n_0$  in CB:

$$n_0 = N_c \exp\left[-\frac{E_c - E_F}{k_B T}\right] \quad N_c = 2 \left( \frac{2\pi m_n^* k_B T}{h^2} \right)^{3/2}$$

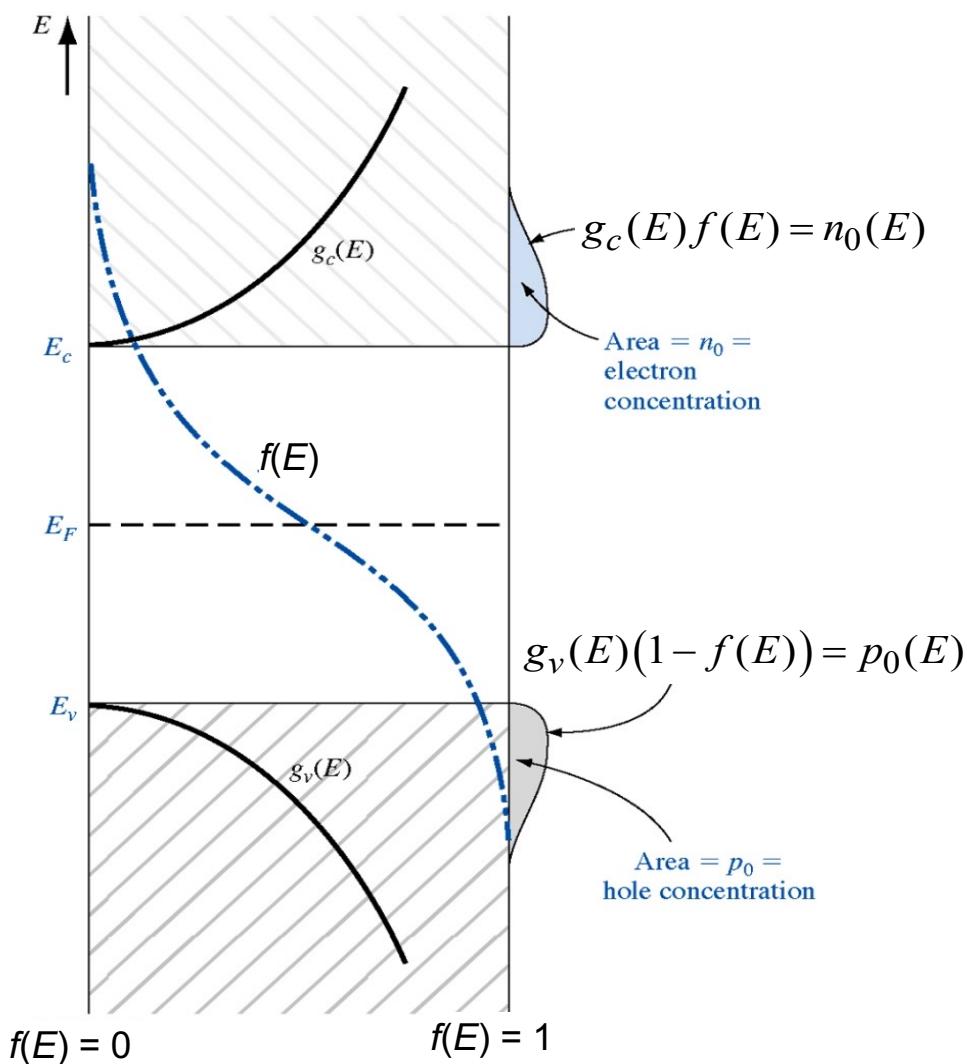
# Lecture 10

In a similar way, we can obtain the thermal equilibrium hole concentration in the valence band, denoted by  $p_0$ .

- The thermal equilibrium hole concentration at energy  $E$  in the valence band,  $p_0(E)$ , is

$$p_0(E) = g_v(E) \{1 - f(E)\} \quad (5.18)$$

the probability of a state at energy  $E$  is not occupied by an electron



Density of states function, Fermi-Dirac probability function, and areas representing electron and hole concentration for the case  $E_F$  is near the midgap

- The thermal equilibrium holes concentration in the valence band is then given by

$$p_0 = \int_{-\infty}^{E_v} g_v(E) \{1 - f(E)\} dE \quad (5.19)$$

the integration is over all the energy  $E$  in the valence band, i.e. from  $-\infty$  to the top of valence band  $E_v$ .

- Now, we evaluate  $p_0$  for the Fermi energy  $E_F$  above the valence band edge  $E_v$ , such that

$$E_F - E_v \gg k_B T \quad (5.20)$$

Again,  $E_F - E_v > 3k_B T$  is sufficient to satisfy eqn. (5.20)

- Since the energy  $E$  in the valence band is below  $E_v$ , it follows

$$E_F - E \gg k_B T \quad (5.21)$$

Using eqn. (5.21), the term  $\{1 - f(E)\}$  in eqn. (5.19) can then be approximated as follow

$$1 - f(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \approx \exp\left(-\frac{E_F - E}{k_B T}\right) \quad (5.22)$$

- We can now evaluate the thermal equilibrium hole concentration  $p_0$  in eqn. (5.19) using the density of states  $g_v(E)$  in eqn. (5.10) and the reduced  $\{1 - f(E)\}$  in eqn. (5.22). We obtain

$$p_0 = N_v \exp\left[-\frac{E_F - E_v}{k_B T}\right] \quad (5.23)$$

where  $N_v$  is the effective density of states in valence band and given by

$$N_v = 2 \left( \frac{2\pi m_p^* k_B T}{h^2} \right)^{3/2} \quad (5.24)$$

Semiconductors with electron and hole concentrations described by eqn. (5.16) and (5.23) respectively are called nondegenerate semiconductors. It is obvious, for nondegenerate semiconductors the position of the Fermi level  $E_F$  in the bandgap follows eqns. (5.13) and (5.20).

It is important to note the following

- The assumption used in deriving the thermal equilibrium electron and hole concentrations is that the Fermi energy  $E_F$  is not too close to the conduction and valence band edges,  $E_c$  and  $E_v$ , respectively.
- So long as this assumption is valid, the expressions for the thermal equilibrium electron and hole concentrations,  $n_0$  and  $p_0$ , are valid for intrinsic and extrinsic semiconductors.
- $n_0$  and  $p_0$  are directly related to the effective density of states and to the Fermi energy level
  - temperature factor present in the effective density of states and the exponential term (representative of probability)
  - hence, thermal equilibrium concentrations will be very sensitive to the temperature

## 5.4 Intrinsic Material

For an intrinsic semiconductor,

- concentration of electrons in conduction band is equal to concentration of holes in valence band
- if we denote the electron and hole concentrations in an intrinsic semiconductor as  $n_i$  and  $p_i$  (subscript  $i$  refers to intrinsic), then

$$n_i = p_i \quad (5.25)$$

- the Fermi energy level of an intrinsic semiconductor is called the intrinsic Fermi energy,  $E_i$ . We understand that the expression of the thermal equilibrium electron and hole concentrations, eqns. (5.16) and (5.23) respectively, valid for both intrinsic and extrinsic semiconductors. If we apply eqns. (5.16) and (5.23) to an intrinsic semiconductor we obtain

$$n_i = N_c \exp\left[-\frac{E_c - E_i}{k_B T}\right] \quad (5.26)$$

and

$$p_i = N_v \exp\left[-\frac{E_i - E_v}{k_B T}\right] \quad (5.27)$$

- Now, multiply eqn. (5.26) with eqn. (5.27) and use the condition in eqn. (5.25) we obtain

$$n_i^2 = N_c N_v \exp\left[-\frac{E_c - E_v}{k_B T}\right] = N_c N_v \exp\left[-\frac{E_g}{k_B T}\right] \quad (5.28)$$

$$n_i = \sqrt{N_c N_v} \exp\left[-\frac{E_g}{2k_B T}\right] \quad (5.29)$$

It is very important to note here, that for a given semiconductor material at a constant temperature, the value of the intrinsic carrier concentration,  $n_i$ , is a constant and is independent of the Fermi energy.

This is true regardless whether the semiconductor is intrinsic (undoped) or extrinsic (doped).

- Recall eqns. (5.16) and (5.23), the thermal equilibrium electron and hole concentrations,  $n_0$  and  $p_0$ . The product of  $n_0$  and  $p_0$  is

$$n_0 p_0 = N_c N_v \exp\left[-\frac{E_c - E_v}{k_B T}\right] = N_c N_v \exp\left[-\frac{E_g}{k_B T}\right] \quad (5.30)$$

We see that the product of  $n_0$  and  $p_0$  is a constant for a particular material and temperature  $T$ . This is exactly the same as the expression for  $n_i^2$  in equation (5.28). We, therefore, obtain

$$n_0 p_0 = n_i^2 \quad (5.31)$$

This equation valid for intrinsic and extrinsic semiconductors.

- At a particular temperature  $T$ , the value of  $n_i$  is dependent on material parameters, like electron and hole effective masses,  $m_n^*$  and  $m_p^*$  respectively, and the bandgap energy  $E_g$ .

- For example, silicon at 300 K

$m_n^* = 1.08 m_0$  and  $m_p^* = 0.56 m_0$ , where  $m_0$  is the free electron rest mass.  $E_g = 1.12$  eV.

Using equations (5.17) and (5.24),

$$N_c = 2.8 \times 10^{19} / \text{cm}^3 \text{ and } N_v = 1.05 \times 10^{19} / \text{cm}^3$$

and then using equation (5.29)

$$n_i = 6.84 \times 10^9 / \text{cm}^3$$

- experimentally, the accepted value of  $n_i$  for silicon at 300 K is  $1.5 \times 10^{10} / \text{cm}^3$ . The discrepancy is due to the simple theoretical model adopted.

- Table 5.1 lists the value of  $n_i$  for some semiconductors at 300 K. We see that  $n_i$  increases with decreasing energy gap  $E_g$ . This is expected since  $n_i$  is exponentially dependent on  $E_g$  (see eqn. 5.29)

**Table 5.1**

Materials	$n_i$ (/cm <sup>3</sup> )	$E_g$ (eV)
GaAs	$1.8 \times 10^6$	1.43
Si	$1.5 \times 10^{10}$	1.11
Ge	$2.4 \times 10^{13}$	0.67

- If we substitute the effective density of states  $N_c$  in eqn. (5.17) and  $N_v$  in eqn. (5.24) into the intrinsic carrier concentration  $n_i$  in eqn. (5.29), we obtain

$$n_i = 2 \left( \frac{2\pi k_B T}{h^2} \right)^{3/2} \left( m_n^* m_p^* \right)^{3/4} \exp \left[ -\frac{E_g}{2k_B T} \right] \quad (5.32)$$

relatively constant over temperature range dominant term

- In eqn. (5.32), we note that, for a given material, all the parameters, except  $T$ , are constant
  - temperature  $T$  appears twice in eqn. (5.32):  $T^{3/2}$  and  $\exp(-1/T)$ .
  - the dominant term is the exponential term, the  $T^{3/2}$  term is relatively constant over a temperature range.

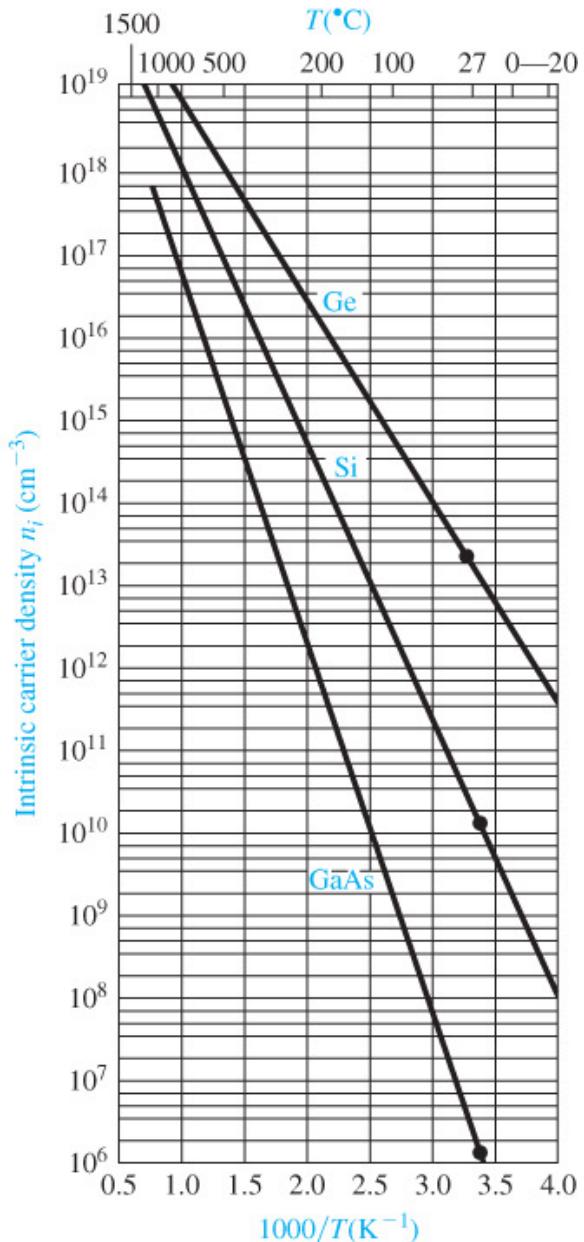
Hence, we could write

$$n_i \approx \text{constant} \times \exp\left[-\frac{E_g}{2k_B T}\right]$$

$$\ln n_i = \ln(\text{constant}) - \frac{E_g}{2k_B T} \quad (5.33)$$

this is a straight line equation, so if we plot  $\ln n_i$  versus  $1/T$ , we will get a straight line with the slope of  $-E_g / 2k_B$

- The plot of eqn. (5.33) for some semiconductors is shown in Fig. 5.7.



**Figure 4.2** | The intrinsic carrier concentration of Ge, Si, and GaAs as a function of temperature.  
(From Sze [14].)

- To calculate the exact position of the intrinsic Fermi level  $E_i$ , we equate  $n_i$  in eqn. (5.26) and  $p_i$  in eqn. (5.27). We obtain

$$n_i = N_c \exp\left[-\frac{E_c - E_i}{k_B T}\right] \quad (5.26)$$

$$E_i = \frac{1}{2}(E_c + E_v) + \frac{1}{2}k_B T \ln\left(\frac{N_v}{N_c}\right) \quad (5.34)$$

Using the expressions of  $N_c$  and  $N_v$  in eqns. (5.17) and (5.24) respectively, we change the ratio of the effective density of states into the ratio of the effective masses

$$E_i = E_{mid} + \frac{3}{4}k_B T \ln\left(\frac{m_p^*}{m_n^*}\right) \quad (5.35)$$

where  $E_{mid} = \frac{1}{2}(E_c + E_v)$  (5.36)

**Example:** Calculate the displacement of  $E_i$  from  $E_{mid}$  at 300 K, assuming the electron and hole effective masses are  $1.1 m_0$  and  $0.56 m_0$  respectively.

The displacement of the intrinsic Fermi energy from the center of the bandgap at 300 K is

$$E_i - E_{mid} = \frac{3k_B T}{4} \ln \left( \frac{\frac{m_p^*}{m_n^*}}{} \right)$$

$$E_i - E_{mid} = \frac{3 \times 1.38 \times 10^{-23} \times 300}{4 \times 1.6 \times 10^{-19}} \ln \left( \frac{0.56}{1.1} \right)$$

$$E_i - E_{mid} = -0.013 \text{ eV}$$

At room temperature the displacement of the intrinsic Fermi level from the centre of the bandgap is very small.  $E_i$  is very close to the center of the bandgap.

- From eqn. (5.36), we see that the intrinsic Fermi level is exactly in the middle of the bandgap, i.e.  $E_i = E_{mid}$ , if
  - the temperature  $T = 0$  K or
  - $m_n^* = m_p^*$
- The deviation of  $E_i$  from  $E_{mid}$  is very small and in many cases the position  $E_i$  can be considered to be at the center of the bandgap.

- To express  $n_0$  and  $p_0$ , in terms of the intrinsic carrier concentration  $n_i$  and the intrinsic Fermi level  $E_i$ , we can easily do that by dividing eqn. (5.16) with eqn. (5.26) and eqn. (5.23) with eqn. (5.27). We obtain

$$n_0 = n_i \exp\left[\frac{E_F - E_i}{k_B T}\right] \quad (5.37)$$

$$p_0 = n_i \exp\left[\frac{E_i - E_F}{k_B T}\right] \quad (5.38)$$

Multiplying eqn. (5.37) with eqn. (5.38) will give us

$$n_0 p_0 = n_i^2$$

which is exactly the same result as we obtained in eqn. (5.31).

## Interpreting the relative position of Fermi level

$$n_0 = N_c \exp\left[-\frac{E_c - E_F}{k_B T}\right]$$

$$n_0 = n_i \exp\left[\frac{E_F - E_i}{k_B T}\right]$$

$$p_0 = N_v \exp\left[-\frac{E_F - E_v}{k_B T}\right]$$

$$p_0 = n_i \exp\left[\frac{E_i - E_F}{k_B T}\right]$$

<http://www.acsu.buffalo.edu/~wie/applet/applet.old>

Three applets for the concept of Fermi Level:

## Key takeaways (Lecture #10)

- Equilibrium hole concentration  $p_0$  in VB :

$$p_0 = N_v \exp\left[-\frac{E_F - E_v}{k_B T}\right] \quad N_v = 2 \left(\frac{2\pi m_p^* k_B T}{h^2}\right)^{3/2}$$

- $n_i$  increases with decreasing energy gap  $E_g$  :

$$n_i = \sqrt{N_c N_v} \exp\left[-\frac{E_g}{2k_B T}\right]$$

- The product of  $n_0$  and  $p_0$  is a constant for a particular material and temperature  $T$ :

$$n_0 p_0 = n_i^2$$

# Lecture 11

## 5.5 Extrinsic materials

In this section we will calculate the thermal equilibrium electron and hole concentrations,  $n_0$  and  $p_0$ , as a function of the impurity concentration.

### 5.5.1 Donor impurity

Let us start with an n-type semiconductor where donor concentration is  $N_d$ . The majority carrier is electrons.

From section 4.2.:

- The thermal equilibrium majority electron concentration  $n_0$  is the sum of the electron concentration from the donor impurity and the electron concentration due to the excitation from the valence band to the conduction band creating the electron-hole pairs.

- At temperature  $T$  where all donor atoms are all ionized we have (recall eqn. 4.1)

$$n_0 = N_d + p_0 \quad (4.1)$$

negative charge concentration      positive charge concentration

- How can we now calculate  $n_0$  and  $p_0$  ?

We first calculate the majority carrier concentration  $n_0$  by simply using eqn. (5.31)

$$n_0 p_0 = n_i^2$$

to substitute  $p_0$  in eqn. (4.1) in terms of  $n_0$  and  $n_i$ .

We obtain

$$n_0 = N_d + \frac{n_i^2}{n_0} \quad (5.39)$$

Multiplying eqn. (5.39) throughout by  $n_0$  and rearranging the equation, we get

$$n_0^2 - N_d n_0 - n_i^2 = 0 \quad (5.40)$$

this is a quadratic equation in  $n_0$ . The solution of this equation is

$$n_0 = \frac{N_d \pm \sqrt{N_d^2 + 4n_i^2}}{2} \quad (5.41)$$

- We only take the positive solution in eqn. (5.41). The negative solution is omitted since it has no physical meaning.

- So, the thermal equilibrium majority electron concentration is

$$n_0 = \frac{N_d + \sqrt{N_d^2 + 4n_i^2}}{2} \quad (5.42)$$

- It is important to note the following in eqn. (5.42):
  - If the doping concentration is much larger than the intrinsic carrier concentration, that is

$$N_d \gg n_i \quad (5.43)$$

then the  $4n_i^2$  term in eqn. (5.42) can be ignored and  $n_0$  is approximately equal to  $N_d$ ,

$$n_0 \approx N_d \quad (5.44)$$

- If the doping concentration is not much larger than the intrinsic carrier concentration, then  $n_0$  cannot be approximated to  $N_d$ , and eqn. (5.42) needs to be used to calculate  $n_0$ .
- Once we obtain  $n_0$ , the thermal equilibrium minority hole concentration can be calculated using eqn. (5.31)

$$p_0 n_0 = n_i^2$$

- Using the value of  $n_0$ , the position of the Fermi level  $E_F$  in the bandgap can be determined using either eqn. (5.16) or eqn. (5.37), depending on the question, of course

$$n_0 = N_c \exp\left[-\frac{E_c - E_F}{k_B T}\right] \quad (5.16)$$

$$n_0 = n_i \exp\left[\frac{E_F - E_i}{k_B T}\right] \quad (5.37)$$

- At thermal equilibrium, the position of the Fermi level in the bandgap can also be determined using the value of  $p_0$ . In this case, we use either eqn. (5.23) or eqn. (5.38).

$$p_0 = N_v \exp \left[ -\frac{E_F - E_v}{k_B T} \right] \quad (5.23)$$

$$p_0 = n_i \exp \left[ \frac{E_i - E_F}{k_B T} \right] \quad (5.38)$$

At thermal equilibrium, the position of the Fermi level  $E_F$  is the same regardless we use  $n_0$  or  $p_0$  (see example 5.2)

- For n-type semiconductor ( $n_0 > p_0$ ),  $E_F$  is above the intrinsic Fermi level  $E_i$ . The Fermi level  $E_F$  moves up as  $n_0$  increases. This is clear from eqns. (5.16) and (5.37) and illustrated in Fig. 5.8.

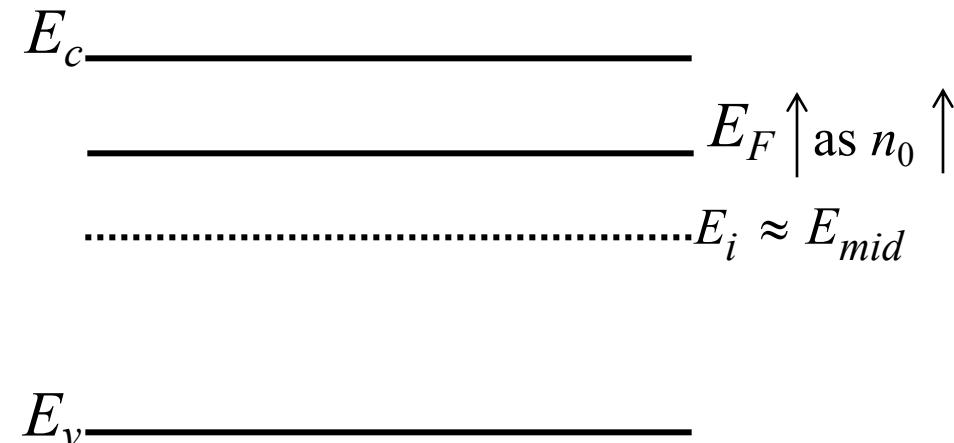


Fig. 5.8

## Example 5.2

Consider a Si sample doped with  $10^{16}$  P atoms/cm<sup>3</sup> at 300 K. The intrinsic carrier concentration is  $1.5 \times 10^{10}$ /cm<sup>3</sup>. Calculate

- i) the thermal equilibrium minority concentration
- ii) and the position of the Fermi level relative to the intrinsic Fermi level

The impurity P atom is from Group V in the periodic table. So, in the Si sample, the P atom acts as donor and hence the majority carrier is electrons.

Using eqn. (5.42) we obtain the majority carrier concentration

$$n_0 = \frac{10^{16} + \sqrt{(10^{16})^2 + 4(1.5 \times 10^{10})^2}}{2} = 10^{16} / \text{cm}^3$$

From the above calculation we show that for  $N_d \gg n_i$ ,  $n_0 = N_d$

From eqn. (5.31), the thermal equilibrium minority hole concentration is

$$n_0 p_0 = n_i^2$$

$$p_0 = \frac{(1.5 \times 10)^2}{10^{16}} = 2.25 \times 10^4 \text{ /cm}^3$$

The position the Fermi level can be obtained using either the value of  $n_0$  (eqn. 5.37) or  $p_0$  eqn. (eqn. 5.38)

Using the value of  $n_0$

$$n_0 = n_i \exp\left[\frac{E_F - E_i}{k_B T}\right] \quad (5.37)$$

$$E_F - E_i = k_B T \ln\left(\frac{n_0}{n_i}\right) = 1.38 \times 10^{-23} \times 300 \times \ln\left(\frac{10^{16}}{1.5 \times 10^{10}}\right) = 5.55 \times 10^{-20} \text{ J}$$

$$1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}, \quad \therefore E_F - E_i = 0.347 \text{ eV}$$

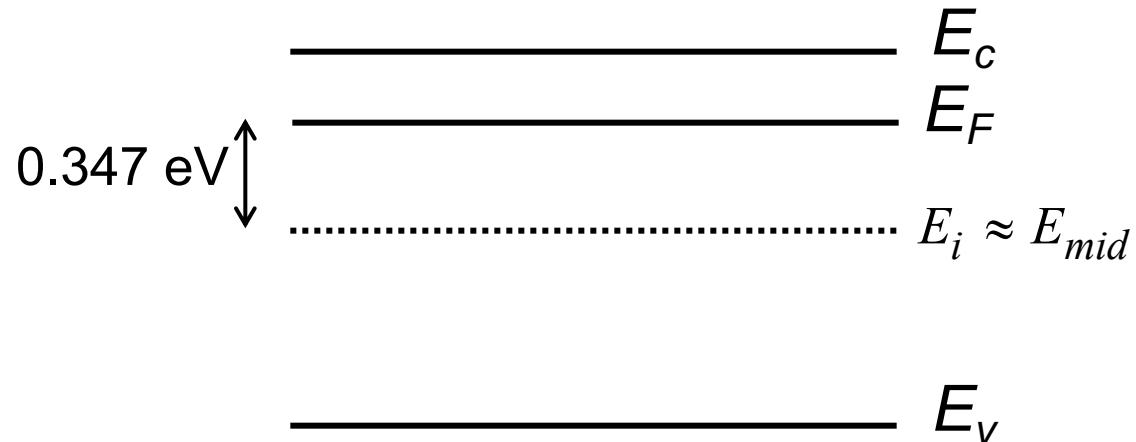
Using the value of  $p_0$

$$p_0 = n_i \exp\left[\frac{E_i - E_F}{k_B T}\right] \quad (5.38)$$

$$E_i - E_F = k_B T \ln\left(\frac{p_0}{n_i}\right) = 1.38 \times 10^{-23} \times 300 \times \ln\left(\frac{2.25 \times 10^4}{1.5 \times 10^{10}}\right) = -5.55 \times 10^{-20} \text{ J}$$

$$E_i - E_F = -0.347 \text{ eV} \text{ or } E_F - E_i = 0.347 \text{ eV}$$

This is exactly the same result as obtained previously using eqn.  
(5.37)



## Example 5.3

Consider a germanium sample at 330 K in which  $N_d = 5 \times 10^{13} / \text{cm}^3$ . Assume  $n_i = 2.4 \times 10^{13} / \text{cm}^3$ , calculate the thermal equilibrium majority and minority concentration.



### Example 5.3

Consider a germanium sample at 330 K in which  $N_d = 5 \times 10^{13} / \text{cm}^3$ . Assume  $n_i = 2.4 \times 10^{13} / \text{cm}^3$ , calculate the thermal equilibrium majority and minority concentration.

At 330 K, the donor impurity is fully ionized. From eqn. (5.42), the majority carrier concentration is

$$n_0 = \frac{5 \times 10^{13} + \sqrt{(5 \times 10^{13})^2 + 4(2.4 \times 10^{13})^2}}{2} = 5.97 \times 10^{13} / \text{cm}^3$$

Notice that, since  $N_d$  is not much larger than  $n_i$ ,  $n_0 \neq N_d$

From eqn. (5.31), the minority carrier concentration is

$$p_0 = \frac{n_i^2}{n_0} = \frac{(2.4 \times 10^{13})^2}{5.97 \times 10^{13}} = 9.65 \times 10^{12} / \text{cm}^3$$

## 5.5.2 Acceptor impurity

Let us now consider a p-type semiconductor with acceptor concentration  $N_a$ . Here, the majority carrier is holes.

From section 4.3:

- The thermal equilibrium majority hole concentration  $p_0$  is the sum of the holes created due to the excitation of electrons from the valence band to the acceptor level and the excitation of electron from the valence band to the conduction band.
- At  $T$  where all acceptor atoms are fully ionized we have (see eqn. 4.6)

$$p_0 = N_a + n_0 \quad (4.6)$$

The equation  $p_0 = N_a + n_0$  is shown. A curly brace under the terms  $N_a$  and  $n_0$  is connected by two arrows pointing downwards to the labels "positive charge concentration" and "negative charge concentration" respectively.

- We can obtain the majority carrier concentration  $p_0$  and the minority carrier concentration  $n_0$  by using the same procedure as we did in section 5.5.1.
- Firstly, we calculate the majority carrier concentration  $p_0$  by substituting the minority carrier concentration  $n_0$  in eqn. (4.6) in terms of  $p_0$  and  $n_i$ . Of course, we use eqn. (5.31). We obtain

$$p_0 = N_a + \frac{n_i^2}{p_0} \quad (5.45)$$

from eqn. (5.45), the majority carrier concentration is

$$p_0 = \frac{N_a + \sqrt{N_a^2 + 4n_i^2}}{2} \quad (5.46)$$

- Again, using eqn. (5.31), the minority carrier concentration is

$$n_0 = \frac{n_i^2}{p_0}$$

- For  $N_a \gg n_i$ ,  $p_0 \approx N_a$  (5.47)
- Having obtained  $p_0$  and  $n_0$ , the position of the Fermi level can be easily determined as discussed in section 5.5.1.
  - Using the value of  $p_0$  we use

either  $p_0 = N_v \exp\left[-\frac{E_F - E_v}{k_B T}\right]$  (5.23)

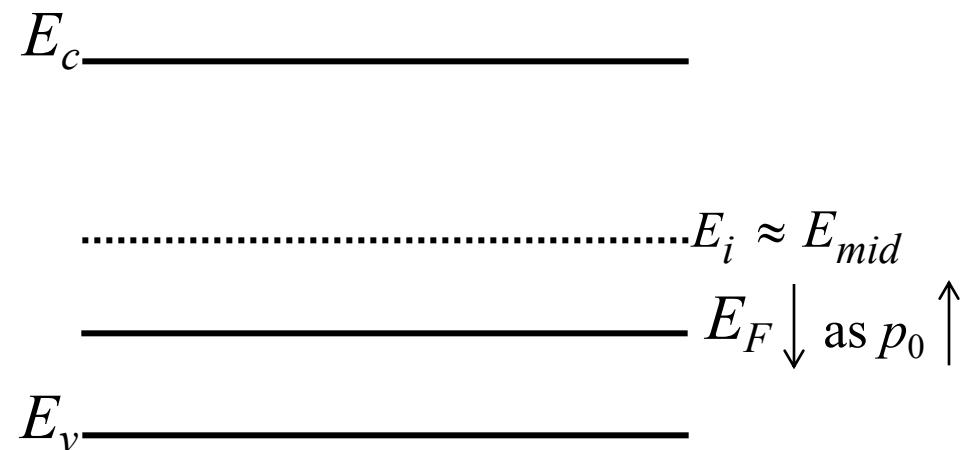
or  $p_0 = n_i \exp\left[\frac{E_i - E_F}{k_B T}\right]$  (5.38)

- Using the value of  $n_0$  we use

either  $n_0 = N_c \exp\left[-\frac{E_c - E_F}{k_B T}\right]$  (5.16)

or  $n_0 = n_i \exp\left[\frac{E_F - E_i}{k_B T}\right]$  (5.37)

- For p-type semiconductor ( $p_0 > n_0$ ),  $E_F$  is below  $E_i$ . The Fermi level  $E_F$  moves down with increasing  $p_0$ . This is clear from eqns. (5.23) and (5.38) and illustrated in Fig. 5.9.



**Fig. 5.9**

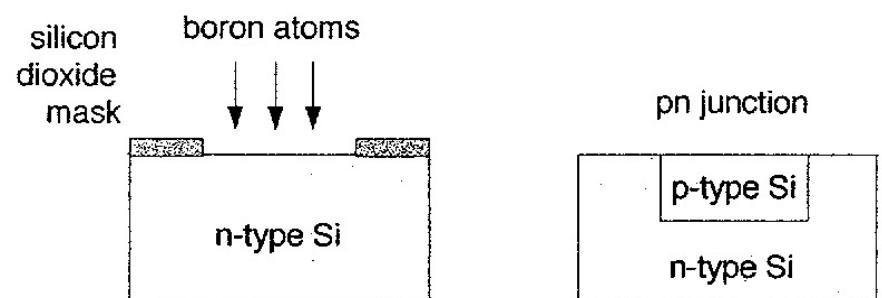
### 5.5.3 Compensated semiconductor

A compensated semiconductor is a semiconductor that contains both donor and acceptor impurity atoms in the same region.

- It can be formed by diffusing acceptor impurities into n-type material or donor impurities into a p-type material
- Considering all impurities are fully ionized
  - n-type is created when  $N_d > N_a$
  - p-type is created when  $N_a > N_d$
  - Intrinsic is created when  $N_d = N_a$

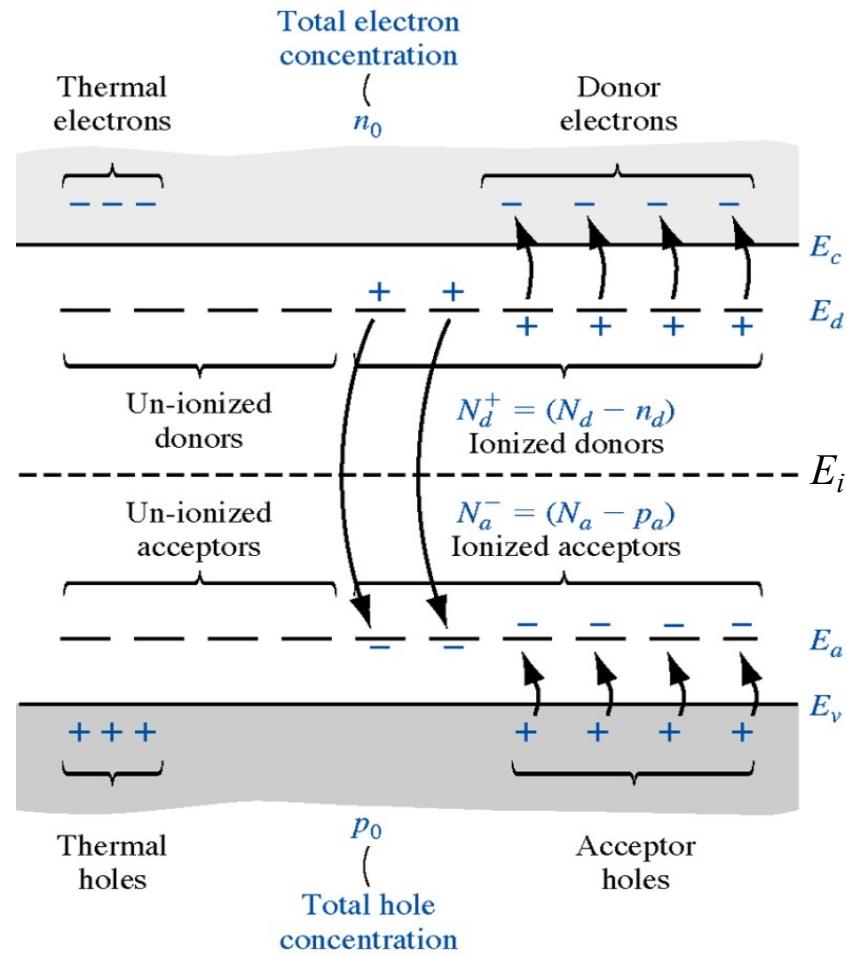
- Compensated semiconductors are created naturally during device fabrication.

Fig. 5.10 shows the formation a p-type semiconductor by diffusing acceptor boron impurities into an n-type Si sample thereby forming a p-n junction.



**Fig. 5.10**

- We will now calculate the thermal equilibrium carrier concentration,  $n_0$  and  $p_0$ , where both donor and acceptor impurities are present.
- At thermal equilibrium the semiconductor is electrically neutral. As we did in previous sections (sections 5.5.1 and 5.5.2) we will use the charge neutrality condition to obtain the thermal equilibrium carrier concentrations.



Energy-band diagram of a compensated semiconductor showing ionized and un-ionized donors and acceptors

Fig. 5.11

- The charge neutrality (often referred to as the space charge neutrality):

The sum of positive charges = the sum of negative charges

- The general form of the charge neutrality condition is

$$p_0 + N_d^+ = n_0 + N_a^- \quad (5.48)$$

**sum of  
positive  
charges**

**sum of  
negative  
charges**

Here, for generality, we have considered a relatively low temperature where the impurities are not fully ionized. So, we have in eqn. (5.48)

- $N_d^+$  : ionized donor concentration
- $N_a^-$  : ionized acceptor concentration

- At temperature  $T$  where all impurities are ionized eqn. (5.48) becomes

$$p_0 + N_d = n_0 + N_a \quad (5.49)$$

Note that, when only donor impurity is present, i.e.  $N_a = 0$ , eqn. (5.49) reduces to eqn. (4.1)

$$p_0 + N_d = n_0$$

and when only acceptor impurity is present, i.e  $N_d = 0$ , eqn. (5.49) reduces to eqn. (4.6)

$$p_0 = n_0 + N_a$$

- Let us calculate the thermal equilibrium carrier concentration where both donor and acceptor impurities are present and consider only the case where the temperature is high enough so that all impurities are ionized.

We start with eqn. (5.49):  $p_0 + N_d = n_0 + N_a$

- Consider first a case where  $N_d > N_a$ , i.e. n-type semiconductor. As before, we express  $p_0$  in eqn. (5.49) in terms of  $n_0$  and  $n_i$  using eqn. (5.31), we obtain

$$n_0^2 - (N_d - N_a)n_0 - n_i^2 = 0 \quad (5.50)$$

The solution this quadratic equation is

$$n_0 = \frac{(N_d - N_a) + \sqrt{(N_d - N_a)^2 + 4n_i^2}}{2} \quad (5.51)$$

as usual we obtain the minority carrier concentration  $p_0$  from eqn. (5.31)

- For  $N_a > N_d$ , i.e. p-type semiconductor, we express  $n_0$  in terms of  $p_0$  and  $n_i$ . We can then write eqn. (5.49) as follow

$$p_0^2 - (N_a - N_d)p_0 - n_i^2 = 0 \quad (5.51)$$

The solution is

$$p_0 = \frac{(N_a - N_d) + \sqrt{(N_a - N_d)^2 + 4n_i^2}}{2} \quad (5.52)$$

the minority carrier concentration  $n_0$  is then obtained from eqn. (5.31)

- It is important to note here that the charge neutrality equation is always true and can be used to determine the carrier concentrations in a semiconductor sample regardless
  - whether there is only one type of impurity or two types of impurities present
  - and whether the concentrations of the impurities are much larger or in the order of  $n_i$
- From eqns. (5.42), (5.46), (5.51) or (5.52), we see that the majority carrier concentration is not a simple sum of dopant concentration and intrinsic carrier concentration.

## Example 5.4

A piece of germanium crystal is doped with donor impurities to a concentration of  $5.8 \times 10^{14} /cm^3$ , as well as acceptor impurities to a concentration of  $5.4 \times 10^{14} /cm^3$ . Taking the intrinsic concentration at 300 K to be  $2.4 \times 10^{13} /cm^3$ , calculate the thermal equilibrium electron and hole concentrations.

Material has 2 types of impurities  $N_d = 5.8 \times 10^{14} /cm^3$

$$N_a = 5.4 \times 10^{14} /cm^3$$

Since  $N_d > N_a$ , the material is an n-type compensated material.

From eqn. (5.51), the majority carrier concentration is

$$n_0 = \frac{(N_d - N_a) + \sqrt{(N_d - N_a)^2 + 4n_i^2}}{2}$$

$$n_0 = \frac{(5.8 \times 10^{14} - 5.4 \times 10^{14}) + \sqrt{(5.8 \times 10^{14} - 5.4 \times 10^{14})^2 + 4(2.4 \times 10^{13})^2}}{2}$$

$$n_0 = 5.12 \times 10^{13} \text{ /cm}^3$$

From eqn. (5.31), the minority carrier concentration is

$$p_0 = \frac{(2.4 \times 10^{13})^2}{5.12 \times 10^{13}} = 1.125 \times 10^{13} \text{ /cm}^3$$

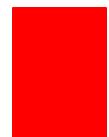
# Problem

**Q1:** Consider a compensated GaAs semiconductor at  $T = 300\text{K}$  doped at  $N_d = 5 \times 10^{15} \text{ cm}^{-3}$  and  $N_a = 2 \times 10^{16} \text{ cm}^{-3}$ . Calculate the thermal equilibrium electron and hole concentration. (TYU 4.11)

$$\begin{aligned} p_o &= N_a - N_d = 2 \times 10^{16} - 5 \times 10^{15} \\ &= 1.5 \times 10^{16} \text{ cm}^{-3} \end{aligned}$$

Then

$$\begin{aligned} n_o &= \frac{n_i^2}{p_o} = \frac{(1.8 \times 10^6)^2}{1.5 \times 10^{16}} \\ &= 2.16 \times 10^{-4} \text{ cm}^{-3} \end{aligned}$$



**Q2:** For a particular semiconductor,  $E_g = 1.50$  eV,  $m_p^* = 10m_n^*$ ,  $T=300K$ , and  $n_i = 1 \times 10^5$  cm $^{-3}$ . (a) Determine the position of the intrinsic Fermi energy level with respect to the center of the bandgap. (b) Impurity atoms are added so that the Fermi energy level is 0.45 eV below the center of the bandgap: (i) Are acceptor or donor atoms added? (ii) What is the concentration of impurity atoms added? (4.53)

$$(a) E_{Fi} - E_{midgap} = \frac{3}{4} kT \ln\left(\frac{m_p^*}{m_n^*}\right)$$

$$= \frac{3}{4} (0.0259) \ln(10)$$

or

$$E_{Fi} - E_{midgap} = +0.0447 \text{ eV}$$

(b) Impurity atoms to be added so

$$E_{midgap} - E_F = 0.45 \text{ eV}$$

(i) p-type, so add acceptor atoms

$$(ii) E_{Fi} - E_F = 0.0447 + 0.45 = 0.4947 \text{ eV}$$

Then

$$p_o = n_i \exp\left(\frac{E_{Fi} - E_F}{kT}\right)$$

$$= (10^5) \exp\left(\frac{0.4947}{0.0259}\right)$$

or

$$p_o = N_a = 1.97 \times 10^{13} \text{ cm}^{-3}$$

## Key takeaways (Lecture #11)

- The general form of the charge neutrality condition in compensated (counter-doped) semiconductor (assuming full ionization):

$$p_0 + N_d = n_0 + N_a$$

- when only donor impurity is present, i.e.  $N_a = 0$  (*n*-type)

$$p_0 + N_d = n_0$$

- when only acceptor impurity is present, i.e.  $N_d = 0$  (*p*-type)

$$p_0 = n_0 + N_a$$

# **Lecture 12**

# 6 CARRIER TRANSPORT

Net flow of electrons and holes in a semiconductor generate currents, and the process by which these charged particles move is called transport.

The carrier transport phenomena is the foundation for determining the current-voltage characteristic of semiconductor devices.

- There are two basic transport mechanisms in a semiconductor crystal depending on the driving force:
  - Drift : movement of charge due to electric fields
  - Diffusion : flow of charge due to concentration gradients
- In addition, the electrons and holes are in constant motion due to thermal energy. However, the motion due to the thermal energy is random and does not lead to current flow.

- Strictly speaking, when there is a net current flow due to drift and/or diffusion phenomena, the semiconductor is no longer in equilibrium.

In this chapter, however, we will assume that the thermal equilibrium condition is not substantially disturbed. The presence of an electric field does not generate extra or excess carriers (electrons and/or holes).

## 6.1 Thermal motion

Above 0 K, there is always random motion of particles due to thermal energy.

- The higher the temperature, the greater the thermal energy causing the thermal motion
- At temperature  $T$ , the average thermal energy of particles in 3 dimensions (3-D) is

$$E_{thermal\,(3-D)} = \frac{3}{2} k_B T \quad (6.1)$$

( $1/2 k_B T$  per degree of freedom)

- The average thermal velocity  $v_{th}$  of the particle can be obtain by equating eqn. (6.1) to the kinetic energy of the motion

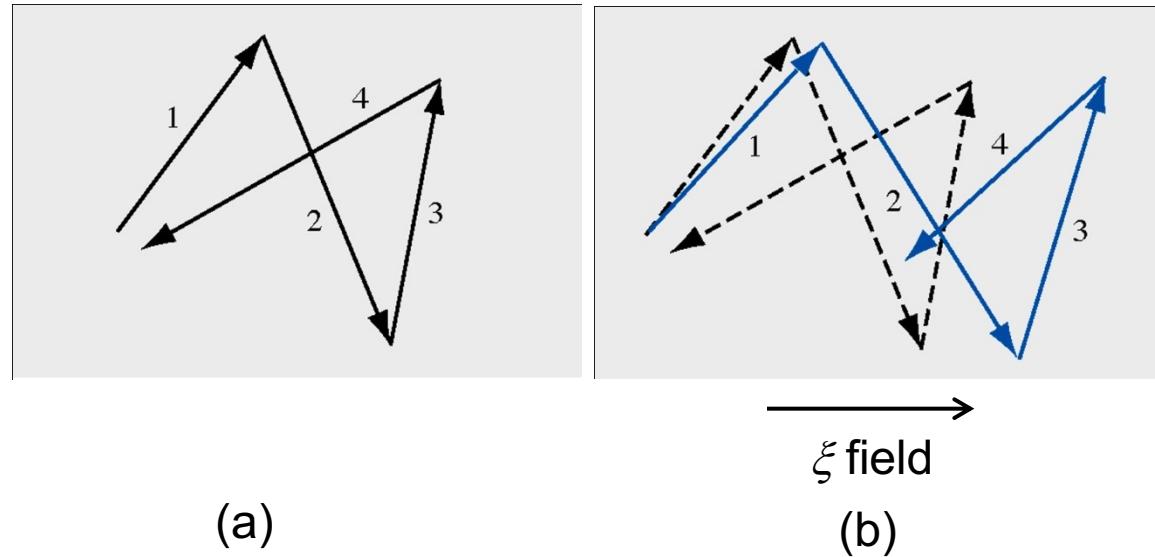
$$\frac{3}{2}k_B T = \frac{1}{2}mv_{th}^2 \quad \therefore v_{th} = \sqrt{\frac{3k_B T}{m}} \quad (6.2)$$

- From eqn. (6.2), the average thermal velocity of electrons at room temperature ( $T = 300$  K) is about  $10^5$  m/s (360,000 km/h). Here, we have used the electron rest mass.
  - this electron kinetic energy corresponds only to several hundredths of an electron volt, and it is not sufficient for electron even to leave semiconductor crystal
- In the absence of any external forces/influences, the electron (or hole) takes part only in the random thermal motion
- there is no directed motion whatsoever, there being no fixed direction which the electron (or hole) would prefer.

- although electrons (or holes) move randomly with a very great velocity, the velocity of the directed motion equals zero.

Fig. 6.1 illustrates the motion of a hole in a semiconductor with and without an electric field  $\xi$ .

- without the electric field, there is not net movement of the hole
- with the electric field, there is net movement of the hole



**Fig. 6.1** Typical motion behavior of a hole in a semiconductor a) without an electric field and b) with an electric field

<http://pveducation.org/pvcdrrom/pn-junction/movement-of-carriers-in-semiconductors>

## 6.2 Drift current

An electric field applied to a semiconductor produces a force on electrons and holes so that they will experience net acceleration and net movement.

- Directed motion is added on top of the thermal random motion of the carriers. This is illustrated in Fig. 6.1.b.
- Net movement of charge due to an electric field is called drift
- Net drift of charges give rise to a drift current

## 6.2.1 Mobility

Consider the motion of a hole in the presence of an electric field  $\xi$ . The equation of motion is

$$F = q\xi = m_p^* a \quad (6.3)$$

Here,  $F$  is the force experienced by the hole,  $q$  is the magnitude of the electric charge,  $a$  is the acceleration,  $\xi$  is the electric field and  $m_p^*$  is the effective mass of the hole

- If the electric field  $\xi$  is constant with time (i.e. does not change with time), velocity will increase linearly with time. Remember, the velocity at time  $t$  is

$$v(t) = v_0 + at \quad (6.4)$$

where  $v_0$  is the initial velocity (velocity at  $t = 0$ )

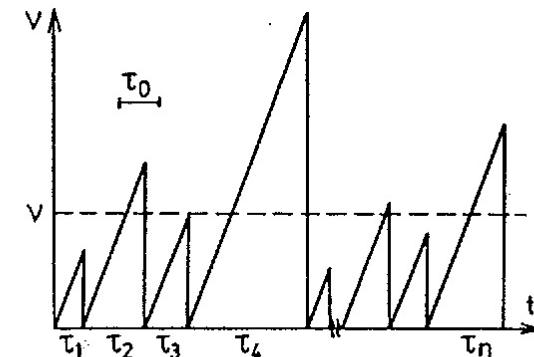
- however, charged carriers in a semiconductor will experience collisions with
  - thermally vibrating lattice atoms
  - ionized impurity atoms and
  - defects
- after a collision the carrier can move in any direction, and this means that the velocity of directed motion after the collision is equal to zero.
- It follows, from eqn. (6.4), the velocity in the directed motion at time  $t$  is

$$v(t) = at \quad (6.5)$$

- Let us denote the time between collisions be  $\tau$ . Since the collisions are quite accidental, the times between collisions  $\tau$  can also be quite different.

The velocity of the directed motion of a charge carrier  $v(t)$  in the presence of an electric field  $\xi$  versus time  $\tau$  is shown in Fig. 6.2.

- Although the times between collisions are not the same (as shown in Fig. 6.2), there is an average time between collisions which may be denoted by  $\tau_c$ . Consequently, there is corresponding average velocity in the directed motion, called drift velocity,  $v_d$ . From eqn. (6.5), we then have



The velocity of the directed motion of the electron (or the hole) in the electric field versus time at random scatterings.

**Fig. 6.2**

$$v_d = a \tau_c \quad (6.6)$$

- For a hole, we may then use the expression in eqn. (6.3) to substitute the acceleration  $a$  in eqn. (6.6). We obtain the drift velocity for hole

$$v_{dp} = \frac{q \tau_{cp}}{m_p^*} \xi \quad (6.7)$$

where  $\tau_{cp}$  is the mean time between collisions for holes

- Note that in deriving eqn. (6.7) we have assumed low electric fields where  $\tau_{cp}$  does not depend on  $\xi$ .

In eqn. (6.7), the hole drift velocity  $v_{dp}$  is directly proportional to the electric field  $\xi$ . We can define the hole mobility  $\mu_p$  by writing

$$v_{dp} = \mu_p \xi \quad (6.8)$$

where 
$$\mu_p = \frac{q \tau_{cp}}{m_p^*} \quad (6.9)$$

- mobility describes how well a particle will move due to an electric field
- unit of mobility is usually expressed in  $\text{cm}^2/\text{V}\cdot\text{s}$

We can apply the same analysis for electrons. Since electrons are negatively charged, the equation of motion of an electrons in the presence of an electric field  $\xi$  is

$$F = -q\xi = m_n^* a \quad (6.10)$$

- The electron drift velocity is

$$v_{dn} = a \tau_{cn} \quad (6.11)$$

where  $\tau_{cn}$  is the mean time between collisions for electrons.

From eqn. (6.10), we obtain

$$v_{dn} = -\frac{q \tau_{cn}}{m_n^*} \xi \quad (6.12)$$

- We then write

$$v_{dn} = -\mu_n \xi \quad (6.13)$$

where  $\mu_n = \frac{q \tau_{cn}}{m_n^*} \quad (6.14)$

- From eqn. (6.13), the electron drift velocity is in opposite direction to the applied electric field.
- From eqn. (6.14), the electron mobility  $\mu_n$  is a positive quantity

Table 6.1 lists typical mobility values at  $T = 300$  K of some semiconductors with low doping concentration

We see that  $\mu_p < \mu_n$ , this means for the same electric field, electrons move faster than holes.

**Table 6.1**

	$\mu_n$ (cm <sup>2</sup> /V-s)	$\mu_p$ (cm <sup>2</sup> /V-s)
Si	1350	480
GaAs	8500	400
Ge	3900	1900

Let us now look at the behavior of the mobility.

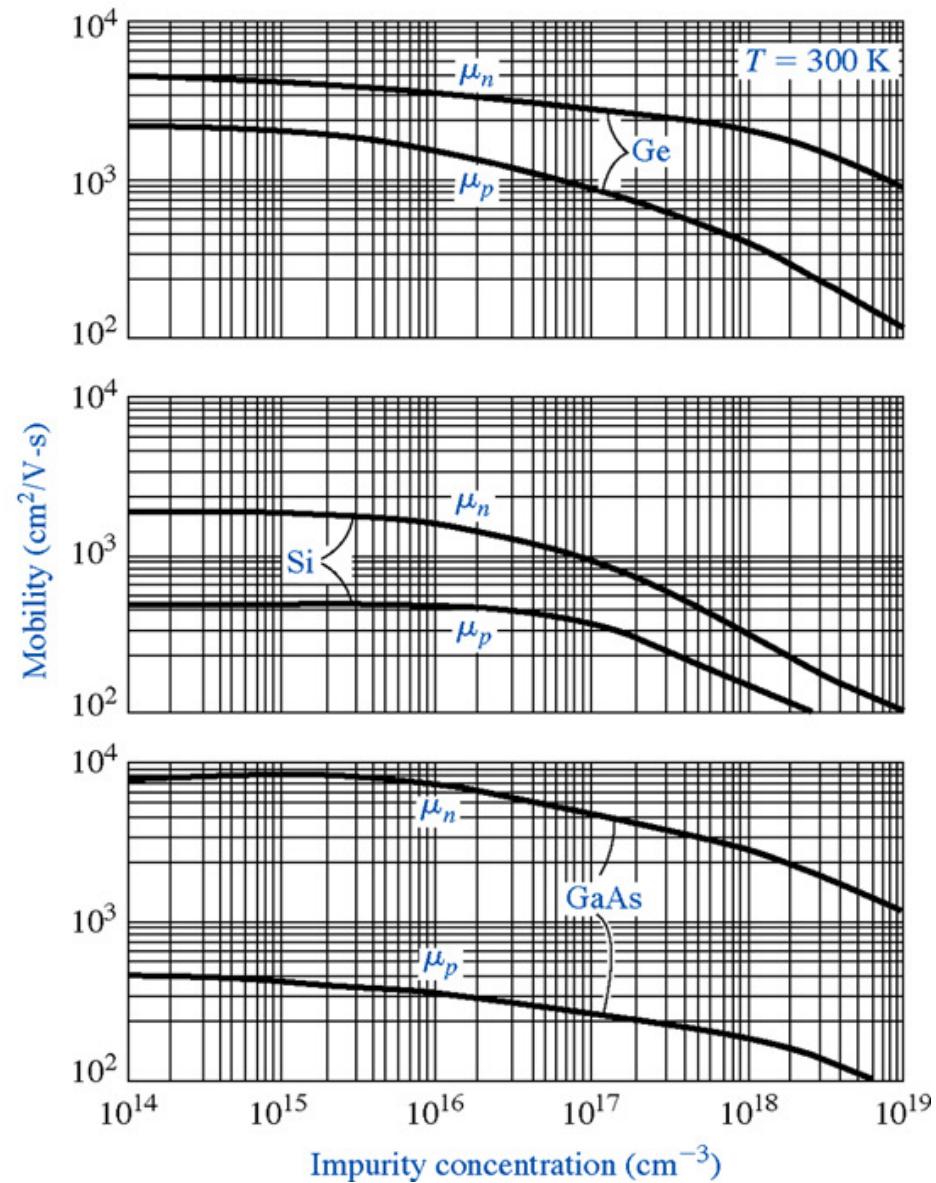
- We have earlier seen that charged particles in a semiconductor will be involved in collisions or scatterings with
  - thermally vibrating lattice atoms
  - ionized impurity atoms, and
  - defects

- It is interesting and important to note here, that the thermal vibration of lattice atoms, impurity atoms and defects disrupt the perfect periodic potential in the crystal.
  - The scattering is caused by the imperfection of the periodic potential.
  - A perfect periodic potential will allow the charge carriers (electrons and holes) to move unimpeded, or with no scattering, in the crystal. This can be understood from the wavefunctions discussed in Appendix D section D.2..
- Let us now discuss the scattering due to lattice vibrations in more detail.
  - Above 0 K, the atoms in a semiconductor vibrate about their lattice position in the crystal.
  - The thermal vibrations cause disruption of the periodic potential, resulting in an interaction between electrons or holes and the vibrating atoms and hence scattering.

- This type of scattering is referred to **lattice scattering** or phonon scattering.
  - The lattice vibrations are expected to increase with increasing temperature, which implies that the number of scatterings per unit time increases. Consequently, the average time between collision decreases and hence, from eqns. (6.9) or (6.14), the mobility decreases.
- 
- Next, let us discuss the scattering due to impurity atoms.
  - As we have seen earlier, the impurity atoms are all ionized at room temperature
  - Again, the ionized impurities disrupt the periodic potential causing the scattering. Here, the interaction between the carriers and the ionized impurities is the coulomb interaction.
  - This scattering is referred to **ionized impurity scattering**.

- We will expect that the number of scatterings per unit time to increase with increasing impurity concentration, which implies that the average time between scattering decreases. Again, from eqns. (6.9) or (6.14), the mobility will decrease.

Fig. 6.3 shows the electron and hole mobilities versus impurity concentrations of some semiconductor materials at 300 K.

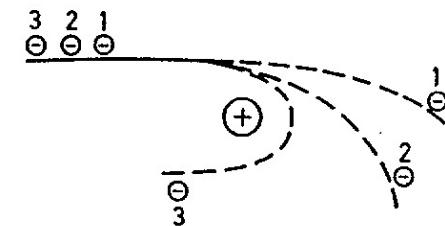


Electron and hole mobilities versus impurity concentration for Ge, Si and GaAs at 300 K

**Fig. 6.3**

- We now ask a question, what is the effect of temperature on the impurity scattering.

- As the temperature increases, the random thermal velocity of carriers increases.
- This would reduce the time the carriers spend in the vicinity of the ionized impurity center.
- The less time spent in the vicinity of a coulomb force, the smaller the scattering effect and thus increasing the mobility due to the impurity scattering. Fig. 6.4 shows the schematic of the scattering effect with the carrier velocity.
- So, in contrast to the lattice scattering, the mobility due to the impurity scattering increases with increasing temperature.



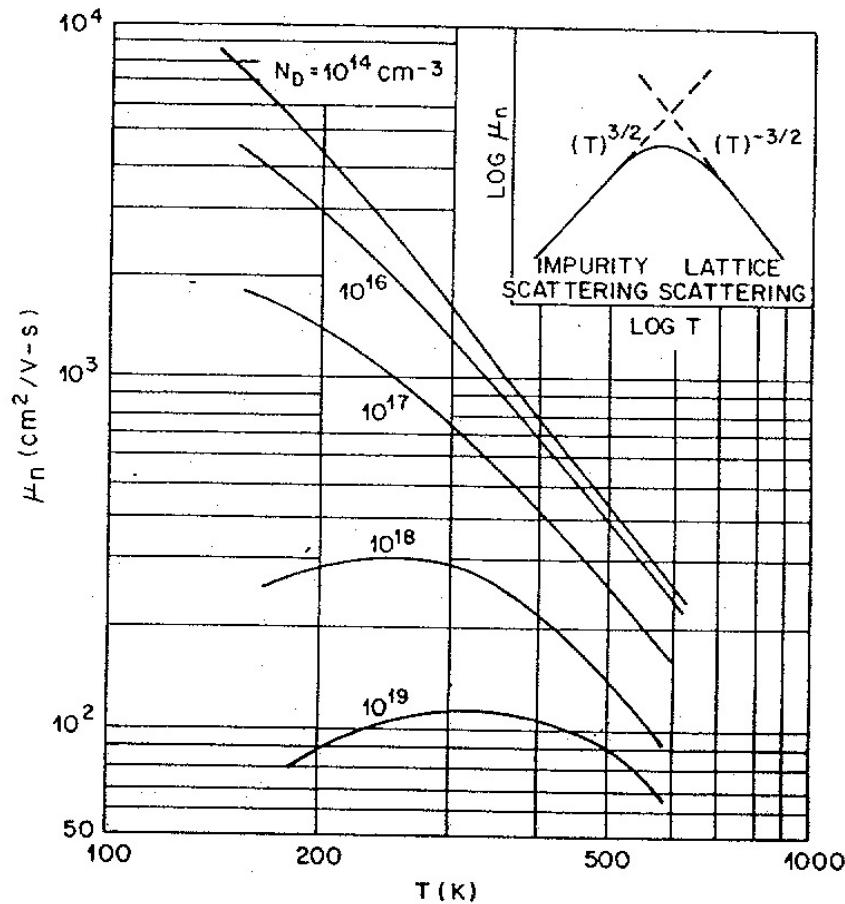
The carrier scattering by a charged impurity center. Electrons (1, 2 and 3) fly up to the impurity center along the same trajectory but with different velocities. Electron 1 has the greatest velocity; the attraction of the impurity atom in practice does not affect its initial trajectory. Electron 3 has the lowest velocity; the attraction of the charged impurity makes it change its route backwards.

**Fig. 6.4**

- We have discussed the effect of temperature on the mobility due to the lattice and ionized impurity scatterings.

Fig. 6.5 shows the electron mobility versus temperature of an n-type semiconductor.

- We firstly see that the mobility increases as the donor concentration decreases. This behavior has been discussed earlier (see Fig. 6.3).



Electron mobility in silicon versus temperature for various donor concentrations.  
Insert shows the theoretical temperature dependence of electron mobility.

**Fig. 6.5**

- For each mobility curve, we see that the mobility first increases and then on reaching a maximum begins to fall. So, we can divide into two regions, low and high temperature regions
- At high temperature region, the mobility decreases with increasing temperature. This indicates that at this region, the lattice scattering dominates.
- At low temperature region, the mobility increases with increasing temperature, this shows that at this region the impurity scattering dominates.

## Key takeaways (Lecture #12)

- There are two basic transport mechanisms in a semiconductor crystal depending on the driving force:
  - Drift : movement of charge due to electric fields
  - Diffusion : flow of charge due to concentration gradients

- Drift velocity:

$$v_{dp} = \frac{q \tau_{cp}}{m_p^*} \xi \quad v_{dp} = \mu_p \xi$$

$$v_{dn} = -\frac{q \tau_{cn}}{m_n^*} \xi \quad v_{dn} = -\mu_n \xi$$

- At high temperature region, the mobility decreases with increasing temperature → lattice scattering dominates
- At low temperature region, the mobility increases with increasing temperature → impurity scattering dominates

# Lecture 13

## 6.2.2 Drift current density

Consider a semiconductor sample with hole density  $p$  moving with drift velocity  $v_{dp}$  in the presence of an electric field  $\xi$

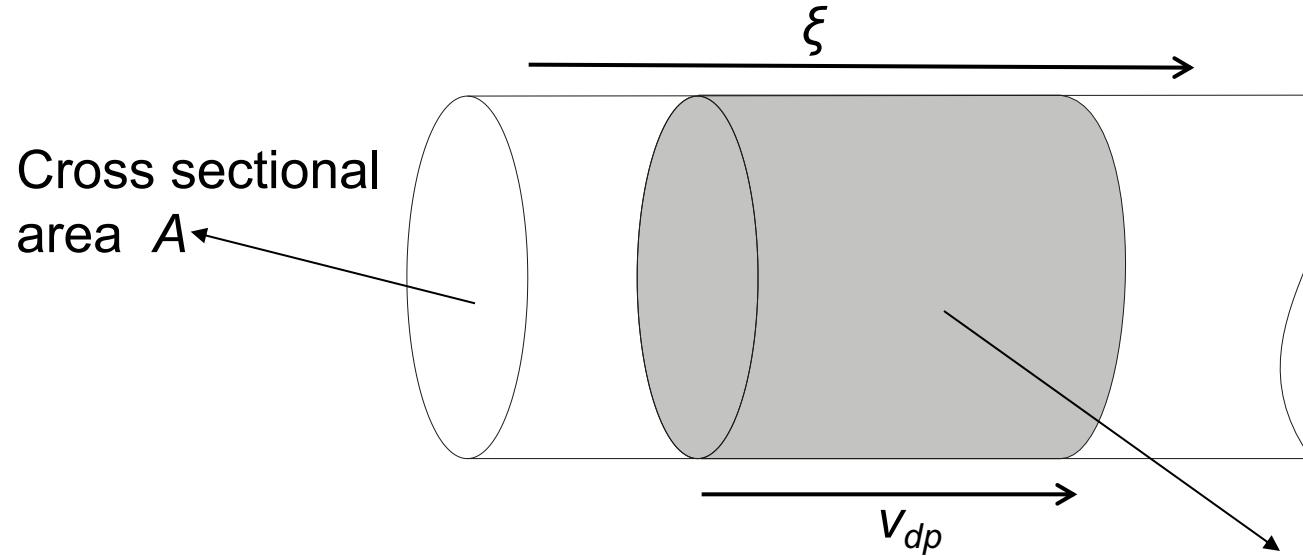


Fig. 6.6

$$\text{Volume} = A \times v_{dp}$$

$$\text{Charges } Q = q p A v_{dp}$$

- From Fig. 6.6, the number of charges in the volume  $A \times v_{dp}$  is

$$Q = q p A v_{dp} \quad (6.15)$$

- Since the drift velocity is  $v_{dp}$ , in one second, the charges Q in the volume will cross the cross sectional A.
  - By the definition of a current = the number of charge crossing an area per second
  - It follows that the hole drift current

$$I_{p\,drift} = q \ p \ A \ v_{dp} \quad (6.16)$$

- Hence, the hole drift current density is

$$J_{p\,drift} = q \ p \ v_{dp} \quad (6.17)$$

Remember, the current density is the number of charge crossing a unit area per second.

- Using eqn. (6.8), we can substitute  $v_{dp}$  in eqn. (6.17). We then obtain

$$J_{p\,drift} = q \ p \ \mu_p \ \xi \quad (6.18)$$

We can apply the same analysis for electrons.

- If we do that we obtain the electron drift current density

$$J_{n\,drift} = - q \ n \ v_{dn} \quad (6.19.a)$$

Here, the negative (- ve) sign is because the electron is negatively charged. The electron drift current density  $J_{n\,drift}$  is in the opposite direction to the electron drift velocity  $v_{dn}$ .

- From the expression for  $v_{dn}$  in eqn. (6.13), we get

$$J_{n\,drift} = -q n (-\mu_n \xi) = q n \mu_n \xi \quad (6.19.b)$$

- In semiconductors the electrical conduction is due to both electron and hole currents.
  - Therefore, the total drift current density  $J_{drift}$  is the sum of the individual electron and hole drift current densities

$$\begin{aligned} J_{drift} &= J_{n\,drift} + J_{p\,drift} \\ J_{drift} &= q \mu_n n \xi + q \mu_p p \xi = (q \mu_n n + q \mu_p p) \xi \end{aligned} \quad (6.20)$$

- We may write the total drift current density  $J_{drift}$  in eqn. (6.20) as

$$J_{drift} = \sigma \xi \quad (6.21)$$

where  $\sigma = q\mu_n n + q\mu_p p$  (6.22)

- $\sigma$  is the electrical conductivity of the semiconductor material.
- the unit is  $(\text{ohm}\cdot\text{cm})^{-1}$  or  $(\Omega\cdot\text{cm})^{-1}$
- Resistivity  $\rho$  is the reciprocal of conductivity

$$\rho = \frac{1}{\sigma} = \frac{1}{q\mu_n n + q\mu_p p} \quad (6.23)$$

- the unit is  $(\text{ohm}\cdot\text{cm})$  or  $(\Omega\cdot\text{cm})$

- For the case of an extrinsic semiconductor, where the majority carrier concentration greatly exceeds the minority carrier concentration, we can write as follow

- For p-type where  $p \gg n$ ,  $\rho = \frac{1}{\sigma} = \frac{1}{q\mu_p p}$  (6.24.a)

- For n-type where  $n \gg p$ ,  $\rho = \frac{1}{\sigma} = \frac{1}{q\mu_n n}$  (6.24.b)

## Example 6.1

Consider a bar of semiconductor as shown in Fig. 6.7 with an applied voltage  $V$  that produces a current  $I$ . Using eqn. (6.21) derive the expression  $V = IR_R$  where  $R_R$  is the resistance of the semiconductor.

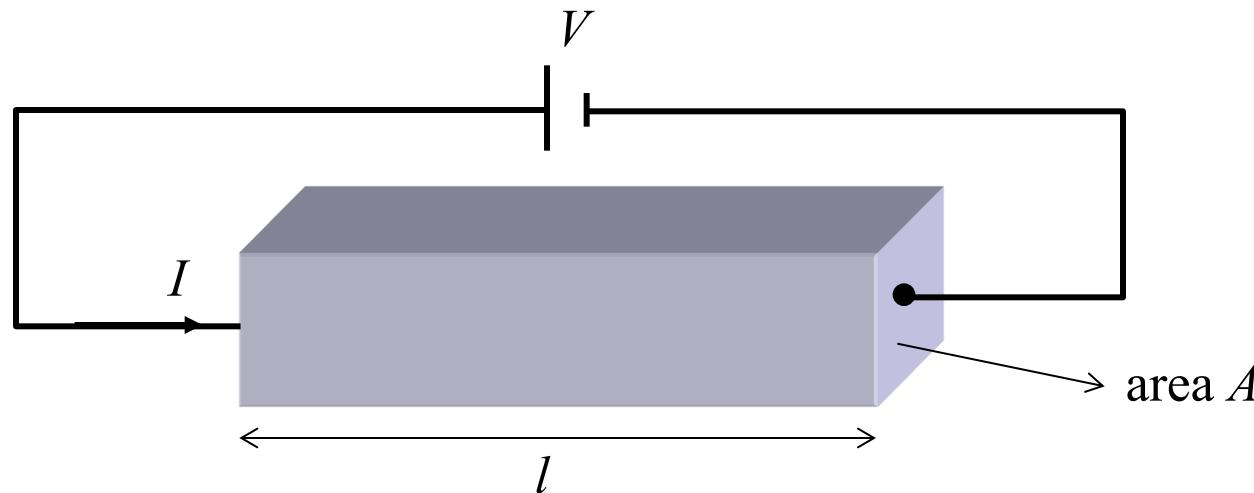


Fig. 6.7

The current density is  $J = \frac{I}{A}$  and the electric field is  $\xi = \frac{V}{l}$

From eqn. (6.21)       $J = \sigma \xi$

$$\frac{I}{A} = \sigma \frac{V}{l}$$

$$V = \left( \frac{1}{\sigma} \frac{l}{A} \right) I$$

$$V = \left( \rho \frac{l}{A} \right) I = IR_R \quad \text{which is Ohm's law}$$

where       $R_R = \rho \frac{l}{A}$

<http://pveducation.org/pvcdrrom/pn-junction/drift>

## 6.3 Diffusion current

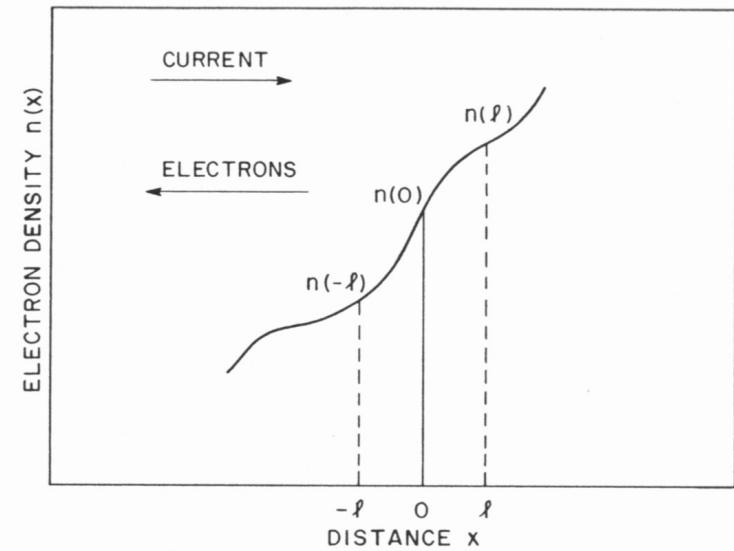
The word *diffusion* comes from Latin word “*diffusio*” (overflow, penetration). This notion can be applied to gases, liquids and solids.

- Diffusion is a flow of particles (e.g. electrons and holes) from a high concentrations region towards a low concentration region. This process is a consequence of random thermal motions of particles (atoms, molecules, electrons, holes etc.)
- To analyse the diffusion process, consider one-dimensional case where an electron density of a semiconductor varies in the  $x$ -direction as shown in Fig. 6.8.
- Here, the semiconductor temperature is assumed to be uniform, so that the average thermal energy, and hence the average thermal velocity  $v_{th}$ , of electrons is independent of  $x$ .

- Having a thermal velocity  $v_{th}$  and a mean time between collisions  $t_{cn}$ , the electron will consequently have a mean free path  $l$ , that is the average distance an electron travels between collisions. This is given by

$$l = v_{th} \tau_{cn} \quad (6.25)$$

- We can express the electron concentration at  $x = l$  and  $x = -l$  about the electron concentration at  $x = 0$  (linear approximate and consider the slope in Fig. 6.8)



Electron concentration versus distance;  $l$  is the mean free path. The directions of electron and current flows are indicated by arrows.

**Fig. 6.8**

$$n(+l) = n(0) + l \frac{dn}{dx} \quad (6.26.a)$$

$$n(-l) = n(0) - l \frac{dn}{dx} \quad (6.26.b)$$

- On the average, at any instant of time, half of the electron concentration at  $x = l$  will be traveling to the left and half of the electron concentration at  $x = -l$  will be traveling to the right crossing the  $x = 0$  plane.

Therefore, the average number of electrons crossing the plane at  $x = 0$  per unit area per unit time in the  $+x$  direction (or the electron flux) is

$$\varphi_n = \frac{1}{2} n(-l) v_{th} - \frac{1}{2} n(l) v_{th} \quad (6.27)$$

Using eqn. (6.26)  $\varphi_n = \frac{1}{2} v_{th} \left\{ \left[ n(0) - l \frac{dn}{dx} \right] - \left[ n(0) + l \frac{dn}{dx} \right] \right\}$

$$\varphi_n = -v_{th} l \frac{dn}{dx} = -D_n \frac{dn}{dx} \quad (6.28)$$

where  $v_{th} l = D_n \quad (6.29)$

is the electron diffusivity or the electron diffusion coefficient. The unit is  $\text{cm}^2/\text{s}$ .

- Since each electron has a charge of  $-q$ , the electron diffusion current density is

$$J_{n \text{ diff}} = -q\varphi_n = q D_n \frac{dn}{dx} \quad (6.30)$$

- We can apply the same analysis to holes. We obtain the average number of holes crossing the plane at  $x = 0$  per unit area per unit time in the  $+x$  direction (or the hole flux) is

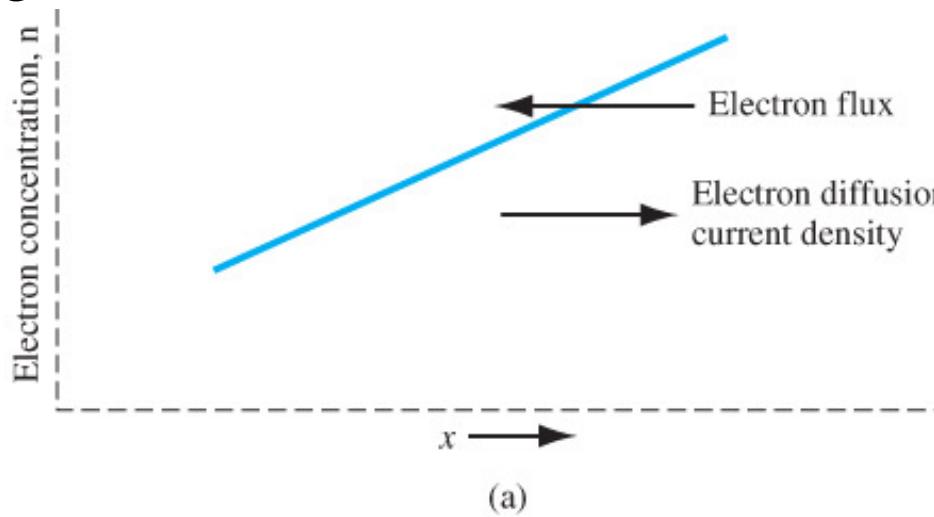
$$\varphi_p = -D_p \frac{dp}{dx} \quad (6.31)$$

Since each hole has a charge of  $+q$ , the hole diffusion current density is

$$J_{p \text{ diff}} = q\varphi_p = -q D_p \frac{dp}{dx} \quad (6.32)$$

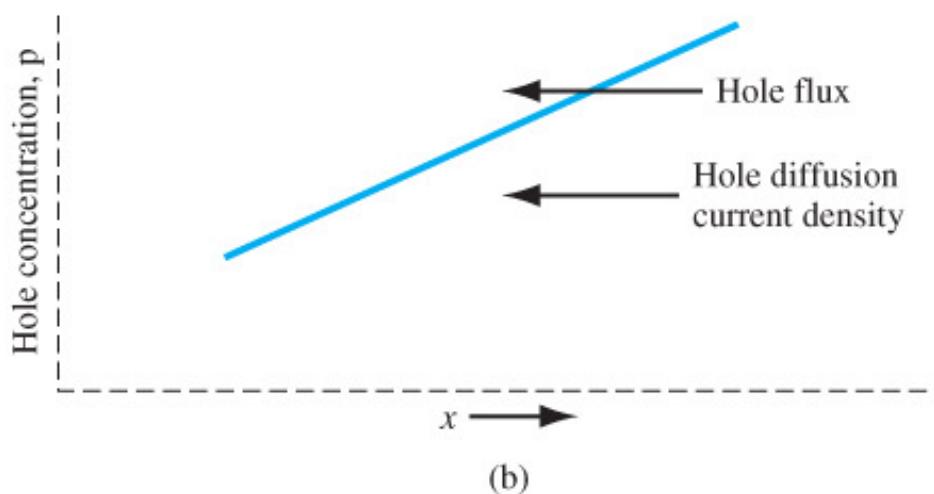
here  $D_p$  is the hole diffusivity or the hole diffusion coefficient and has units of  $\text{cm}^2/\text{s}$ .

- Fig. 6.9 shows the diffusion current density and the concentration of charge carriers.



(a)

**Fig. 6.9**



(b)

**Figure 5.11** | (a) Diffusion of electrons due to a density gradient. (b) Diffusion of holes due to a density gradient.

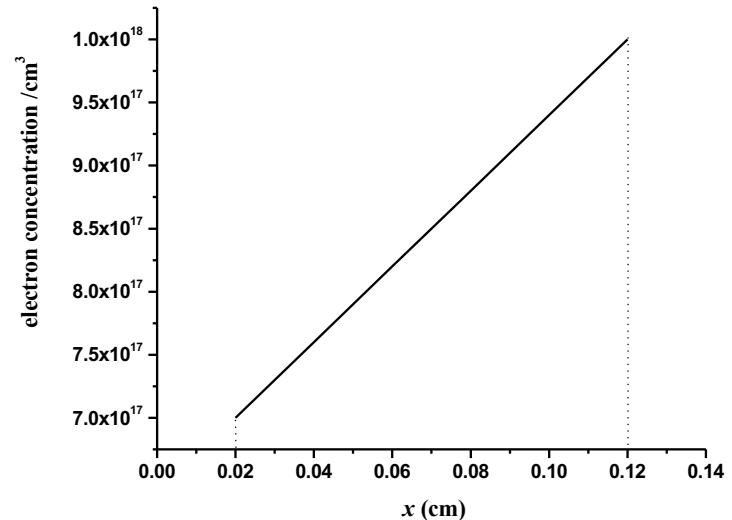
- For electrons (see Fig. 6.9.a) the concentration gradient ( $dn/dx$ ) is positive. The electrons diffuse from high to low concentration, i.e. in the negative  $x$  direction. Since electrons are negatively charged, the current is in the positive  $x$  direction.
- In Fig. 6.9.b, the hole concentration gradient ( $dp/dx$ ) is again positive. The holes diffuse from high to low concentration, i.e. in the negative  $x$  direction. Since holes are positively charged, the current is in the negative  $x$  direction.

<http://pveducation.org/pvcdrom/pn-junction/diffusion>

## Example 6.2

In an n-type GaAs semiconductor at  $T = 300$  K, the electron concentration varies linearly from  $7 \times 10^{17} /cm^3$  to  $1 \times 10^{18} /cm^3$  over a distance of 0.10 cm. Calculate the electron diffusion current density given that the electron diffusion coefficient  $D_n$  is  $225\text{ cm}^2/\text{s}$ .

From eqn. (6.30)



## Example 6.2

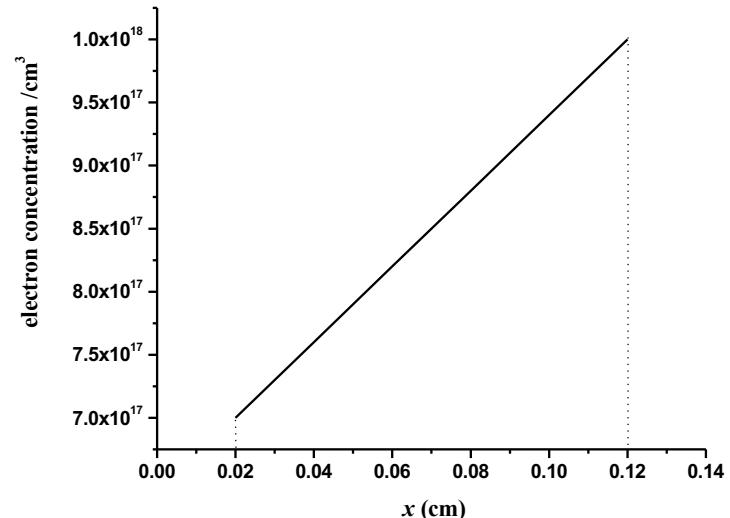
In an n-type GaAs semiconductor at  $T = 300$  K, the electron concentration varies linearly from  $7 \times 10^{17} /cm^3$  to  $1 \times 10^{18} /cm^3$  over a distance of 0.10 cm. Calculate the electron diffusion current density given that the electron diffusion coefficient  $D_n$  is  $225\text{ cm}^2/\text{s}$ .

From eqn. (6.30)

$$J_{n\ diff} = q D_n \frac{dn}{dx}$$

$$J_{n\ diff} = (1.6 \times 10^{-19}) (225) \frac{(1 \times 10^{18} - 7 \times 10^{17})}{0.10}$$

$$J_{n\ diff} = 108\text{ A/cm}^2$$



Having obtained the drift and diffusion current density for electrons and holes, we can have the total current density

- The total electron current density is

$$J_n = J_{n \text{ drift}} + J_{n \text{ diff}} = q \mu_n n \xi + q D_n \frac{dn}{dx} \quad (6.33)$$

- The total hole current density is

$$J_p = J_{p \text{ drift}} + J_{p \text{ diff}} = q \mu_p p \xi - q D_p \frac{dp}{dx} \quad (6.34)$$

In semiconductors the charge carriers are electrons and holes, therefore the total current density is

$$J_{total} = J_n + J_p \quad (6.35)$$

## 6.4 The Einstein Relation

There is a simple relation between diffusion coefficient of any particle and its mobility.

- We recall the electron diffusion coefficient in eqn. (6.29)

$$v_{th} / = D_n$$

- Using eqn. (6.25) we can write the electron diffusion coefficient as

$$D_n = v_{th}^2 \tau_{cn} \quad (6.36)$$

- For one dimensional case, the average thermal energy at temperature  $T$  is

$$E_{thermal(1-D)} = \frac{1}{2} k_B T \quad (6.37)$$

- Hence, the electron kinetic energy is

$$\frac{1}{2} m_n^* v_{th}^2 = \frac{1}{2} k_B T \quad (6.38)$$

and  $\therefore v_{th}^2 = \frac{k_B T}{m_n^*}$  (6.39)

- Substituting  $v_{th}$  in eqn. (6.39) into eqn. (6.36), we obtain

$$D_n = \frac{k_B T}{m_n^*} \tau_{cn} \quad (6.40)$$

- Recall eqn. (6.14), the electron mobility is  $\mu_n = \frac{q \tau_{cn}}{m_n^*}$

combining eqns. (6.14) and (6.40) we obtain  $D_n = \frac{k_B T}{q} \mu_n$

(6.41.a)

- Similarly, the hole diffusion coefficient and mobility is related by

$$D_p = \frac{k_B T}{q} \mu_p \quad (6.41.b)$$

- The relation between the diffusion coefficient and mobility in eqn. (6.41) is known as the Einstein relation. The diffusion coefficient and mobility are not independent parameters.
  - The motion of charge carriers under an electric field and the diffusion process are based on the same mechanism: by the collisions of the charge carriers which occur within the average time intervals  $\tau_{cn}$  (or  $\tau_{cp}$ ) with the average thermal velocity  $v_{th}$

Table 6.2 lists typical mobility and diffusion coefficient values of electrons and holes at  $T = 300$  K (mobility in  $\text{cm}^2/\text{V}\cdot\text{sec}$  and diffusion coefficient in  $\text{cm}^2/\text{sec}$ )

**Table 6.2**

	$\mu_n$	$D_n$	$\mu_p$	$D_p$
Silicon	1350	35	480	12.4
Gallium Arsenide	8500	220	400	10.4
Germanium	3900	101	1900	49.2

## Problems

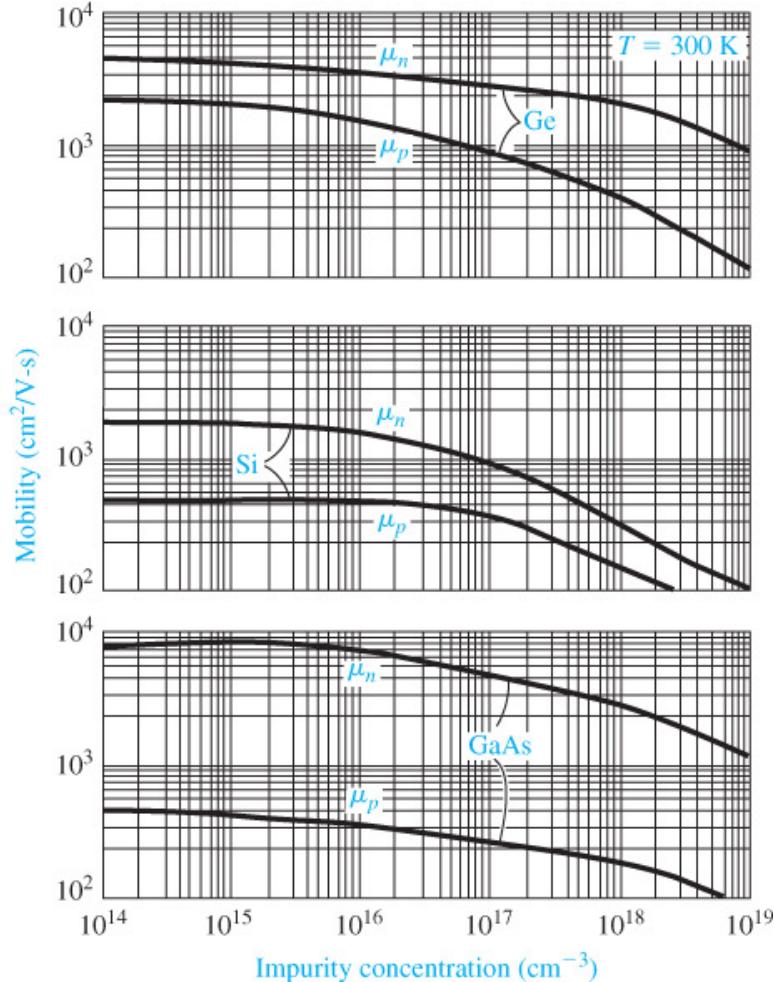
Q1: A drift current density of 75 A/cm<sup>2</sup> is required in a device using p-type silicon when an electric field of 120 V/cm is applied at 300K. Determine the required impurity doping concentration to achieve this specification. (Ex 5.1)

$$J_{drf} \cong e\mu_p p_o E = e\mu_p N_a E$$

$$75 = (1.6 \times 10^{-19}) (480) N_a (120)$$

$$\text{which yields } N_a = 8.14 \times 10^{15} \text{ cm}^{-3}$$

Q2: A compensated p-type silicon material at  $T = 300\text{K}$  has impurity doping concentration of  $N_a = 2.8 \times 10^{17} \text{ cm}^{-3}$  and  $N_d = 8 \times 10^{16} \text{ cm}^{-3}$ . Determine the (a) hole mobility, (b) conductivity, and (c) resistivity. (Ex 5.3)



**Figure 5.3** | Electron and hole mobilities versus impurity concentrations for germanium, silicon, and gallium arsenide at  $T = 300\text{ K}$ .  
(From Sze [14].)

(a) For

$$\begin{aligned} N_I &= N_a + N_d = 2.8 \times 10^{17} + 8 \times 10^{16} \\ &= 3.6 \times 10^{17} \text{ cm}^{-3}, \\ \Rightarrow \mu_p &= 200 \text{ cm}^2/\text{V-s} \end{aligned}$$

$$\begin{aligned} (\text{b}) \sigma &= e\mu_p(N_a - N_d) \\ &= (1.6 \times 10^{-19})(200)(2 \times 10^{17}) \\ \sigma &= 6.4(\Omega\text{-cm})^{-1} \end{aligned}$$

$$(\text{a}) \rho = \frac{1}{\sigma} = \frac{1}{6.4} = 0.156 \Omega\text{-cm}$$

Q3: The hole density in silicon is given by  $p(x) = 10^{16} \exp(-x/L_p)$  for  $x \geq 0$  where  $L_p = 2 \times 10^{-4}$  cm. Assume that the hole diffusion coefficient is  $D_p = 8$  cm<sup>2</sup>/s. Determine the hole diffusion current density at (a)  $x=0$ , (b)  $x=2 \times 10^{-4}$  cm, and (c)  $x=10^{-3}$  cm. (Ex 5.5)

$$\begin{aligned}
 J_p &= -eD_p \frac{dp}{dx} \\
 &= -eD_p \frac{d}{dx} \left[ 10^{16} e^{-x/L_p} \right] \\
 &= -eD_p \left( 10^{16} \left( \frac{-1}{L_p} \right) e^{-x/L_p} \right. \\
 &\quad \left. + \frac{eD_p (10^{16})}{L_p} e^{-x/L_p} \right) \\
 &= \frac{(1.6 \times 10^{-19})(8)(10^{16})}{2 \times 10^{-4}} e^{-x/L_p} \\
 J_p &= 64 \exp\left(\frac{-x}{L_p}\right)
 \end{aligned}$$

(a) For  $x = 0$ ,

$$J_p = 64 \text{ A/cm}^2$$

(b) For  $x = 2 \times 10^{-4}$  cm,

$$J_p = 64 \exp\left(\frac{-2 \times 10^{-4}}{2 \times 10^{-4}}\right) = 23.54$$

$$\text{A/cm}^2$$

(c) For  $x = 10^{-3}$  cm,

$$J_p = 64 \exp\left(\frac{-10^{-3}}{2 \times 10^{-4}}\right) = 0.431 \text{ A/cm}$$

Q4: In GaAs, the donor impurity concentration varies as  $N_{do} \exp(-x/L)$  for  $0 \leq x \leq L$ , where  $L = 0.1 \mu\text{m}$  and  $N_{do} = 5 \times 10^{16} \text{ cm}^{-3}$ . Assume  $\mu_n = 6000 \text{ cm}^2/\text{Vs}$  and  $T = 300\text{K}$ . (a) Derive the expression for the electron diffusion current density vs. distance over the given range of  $x$ . (b) Determine the induced electric field that generates a drift current density that compensates the diffusion current density.

(5.43)

(a) We have

$$J_{diff} = eD_n \frac{dn}{dx} = eD_n \frac{dN_d(x)}{dx}$$

$$= \frac{eD_n}{(-L)} \cdot N_{do} \exp\left(\frac{-x}{L}\right)$$

We have

$$D_n = \mu_n \left( \frac{kT}{e} \right) = (6000)(0.0259)$$

or

$$D_n = 155.4 \text{ cm}^2/\text{s}$$

Then

$$J_{diff} = \frac{-(1.6 \times 10^{-19})(155.4)(5 \times 10^{16})}{(0.1 \times 10^{-4})} \exp\left(\frac{-x}{L}\right)$$

or

$$J_{diff} = -1.243 \times 10^5 \exp\left(\frac{-x}{L}\right) \text{ A/cm}^2$$

(b)

$$0 = J_{drift} + J_{diff}$$

Now

$$J_{drift} = e\mu_n n E$$

$$= (1.6 \times 10^{-19})(6000)(5 \times 10^{16}) \left[ \exp\left(\frac{-x}{L}\right) \right] E$$

or

$$J_{drift} = (48) \left[ \exp\left(\frac{-x}{L}\right) \right] E$$

We have

$$J_{drift} = -J_{diff}$$

so

$$(48) \left[ \exp\left(\frac{-x}{L}\right) \right] E = 1.243 \times 10^5 \exp\left(\frac{-x}{L}\right)$$

which yields

$$E = 2.59 \times 10^3 \text{ V/cm}$$

# Key takeaways (Lecture #13)

- Drift current:

$$J_{drift} = J_{n\,drift} + J_{p\,drift}$$

$$J_{drift} = q \mu_n n \xi + q \mu_p p \xi = (q \mu_n n + q \mu_p p) \xi$$

- Diffusion current:

$$J_{n\,diff} = -q\varphi_n = q D_n \frac{dn}{dx} \quad J_{p\,diff} = q\varphi_p = -q D_p \frac{dp}{dx}$$

- Einstein Relation:

$$D_n = \frac{k_B T}{q} \mu_n \quad D_p = \frac{k_B T}{q} \mu_p$$