

CoE 211 ELECTRONIC DEVICE PHYSICS

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Chapter One

The Crystal Structure of Solids

Chapter objectives

- Introduce the crystalline structure of solids and describe the concept of a unit cell,
- Discuss the simple cubic, body-centered cubic, and face-centered cubic crystalline structures. Also, give an idea about diamond and zincblende lattice structures in semiconductors.
- Review various atomic bonding.

1.1 Introduction

- Solid: It refers to one of the four fundamental states of matter. The other states are liquid, gas, and plasma.
- Crystal of solid: It is the collection of atoms, molecules or ions into a single solid entity.



Figure: Crystal solid: Quartz.



Figure: Crystal solid: Silicon.

1.2 Semiconductor Materials

- Conductivity of semiconductor lies between that of conductors and of insulators.
- Semiconductor materials are elemental or compounds.
 -) Elemental is composed of single species of atoms, such as Si and Ge.
 -) Compound can be formed from an element in group III and an element in group V,
 - Binary compound: GaAs, GaP,
 - Ternary compound: e.g., $\text{Al}_x\text{Ga}_{1-x}\text{As}$, where $0 \leq x \leq 1$ is the fraction of the element's atomic concentration.
 - Quaternary compound: e.g., $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y}$, $0 \leq x \leq 1$ and $0 \leq y \leq 1$.
- Compound semiconductors offer better characteristics (optical feature, higher frequency, higher power) than the elementals.

III	IV	V
5 B Boron	6 C Carbon	
13 Al Aluminum	14 Si Silicon	15 P Phosphorus
31 Ga Gallium	32 Ge Germanium	33 As Arsenic
49 In Indium		51 Sb Antimony

(a)

Elemental semiconductors	
Si	Silicon
Ge	Germanium
Compound semiconductors	
AlP	Aluminum phosphide
AlAs	Aluminum arsenide
GaP	Gallium phosphide
GaAs	Gallium arsenide
InP	Indium phosphide

(b)

Figure: (a) Portion of the periodic table. (b) A list of some semiconductor materials.

1.3 Types of Solids

Based on the spatial arrangement of atoms in the crystal, solids are broadly classified into

- 1 **Crystalline:** Atoms are arranged in a regular and repeated manner.
- 2 **Amorphous:** Atoms do not exhibit any long-range pattern or structure. e.g., amorphous Si thin-film is a switch in Liquid Crystal Displays (LCDs).
- 3 **Polycrystalline:** Small sections of the materials have common patterns that differ from the other sections. e.g., polycrystalline Si gates are used in Metal Oxide-Semiconductor Field-Effect Transistors (MOSFETs).

Electrical properties of crystalline are much better than Amorphous and Polycrystalline.

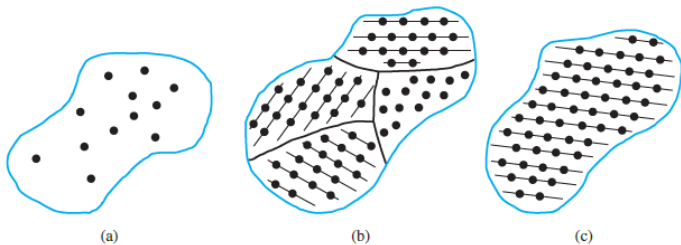


Figure: Classification of solids according to their atomic arrangement: (a) amorphous, (b) polycrystalline, (c) crystalline.

1.4 Crystalline Structure

- **Unit cell:** A small portion of the crystal that could be used to reproduce the whole crystal. Unit cell is NOT necessarily unique and NOT necessarily *primitive*.
- **Lattice:** Spatial array of dots that is used to represent atoms.
- **Lattice constant:** A length that describes the unit cell and measured in Å, angstroms. Note $1\text{Å} = 10^{-8}\text{ cm}$.
- **Primitive unit cell:** It corresponds to the minimum volume that covers a single lattice point.

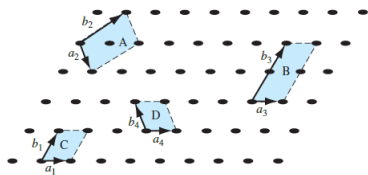


Figure: Sample two-dimensional lattice: Various possible unit cells.

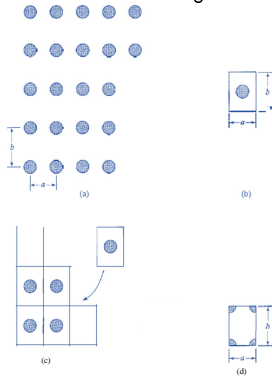
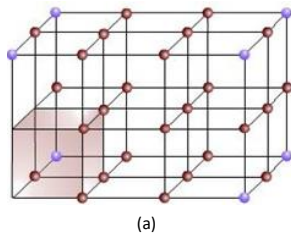


Figure: (a) Sample two-dimensional lattice. (b) Unit cell corresponding to the part (a) lattice. (c) Reproduction of the original lattice. (d) Alternative unit cell.

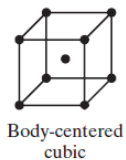
1.4.1 Three-Dimensional Lattices

Common shapes of 3d unit cells are

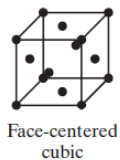
- 1 Simple cubic: It has an atom located at each corner.
- 2 Body-centered cubic (BCC): It has an additional atom at the center of the cube.
- 3 Face-centered cubic (FCC): It has additional atoms on each face plane.



(b)



(c)



(d)

Figure: Common 3d lattices: (b) Simple cubic, (b) body-centered cubic, and (c) face-centered cubic.

1.4.1 Three-Dimensional Lattices (cont.)

- Knowing crystal structure determines the volume density of atoms.

$$\text{Volume density} = \frac{\text{no. atoms per unit cell}}{V_{\text{unit cell}}}. \quad (1)$$

-) $V_{\text{unit cell}}$ is the volume of unit cell.

- BCC lattice: It has one atom per lattice point. The unit cell has one atom at the center and $\frac{1}{8}$ at each corner. Then,

$$\text{Atoms per unit cell} = 1 + 8 \times \frac{1}{8} = 2.$$

-) e.g., for a lattice constant $a = 5 \text{ \AA}$, the volume density is

$$\text{Volume density} = \frac{2}{a^3} = \frac{2}{(5 \times 10^{-8})^3} = 1.6 \times 10^{22} \text{ atoms/cm}^3.$$

- FCC lattice: It has one atom per lattice point. The unit cell has $\frac{1}{2}$ atom at each face and $\frac{1}{8}$ at each corner. Then,

$$\text{Atoms per unit cell} = 8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4.$$

-) For a lattice constant $a = 5 \text{ \AA}$, the volume density is

$$\text{Volume density} = \frac{4}{a^3} = \frac{4}{(5 \times 10^{-8})^3} = 3.2 \times 10^{22} \text{ atoms/cm}^3.$$

1.4.2 Packing Factor (PF)

- PF is the ratio of the particles volume in a certain unit cell to the unit cell volume.

$$\text{PF} = \frac{N_p V_p}{V_{\text{unit cell}}} . \quad (2)$$

-) N_p is the number of particles.
-) V_p is the volume of ONE particle.
- In (2), consider all the particles have the same size and they have the sphere shape. Recall $V_{\text{sphere}} = \frac{4}{3}\pi r^3$, where r is the radius of the sphere.
- PF is < 1 . Higher values for PF means dense packing and more stable crystal structure.

1.4.2 Packing Factor (PF) (cont.)

Example 1.1: Determine PF for BCC and FCC structures. Assume the nearest neighbors atoms in these lattices are in touch. Comment on the obtained values.

1.5 Crystalline Structure for Semiconductor

- The elements of group IV, such as Si and Ge are crystallized in **diamond cubic structure**.
 -) The diamond cubic structure can be obtained from the FCC lattice with an extra atom placed at $(\frac{a}{4}\hat{x} + \frac{a}{4}\hat{y} + \frac{a}{4}\hat{z})$ from each corner point.
 -) The diamond cubic structure has 8 atoms per unit cell. There are 4 atoms inside the unit cell.
- Most III-V semiconductors such as GaAs are crystallized in **zincblende structure**. It is identical to the diamond structure except Ga occupies the 4 atoms inside the unit cell and As occupies the remaining.

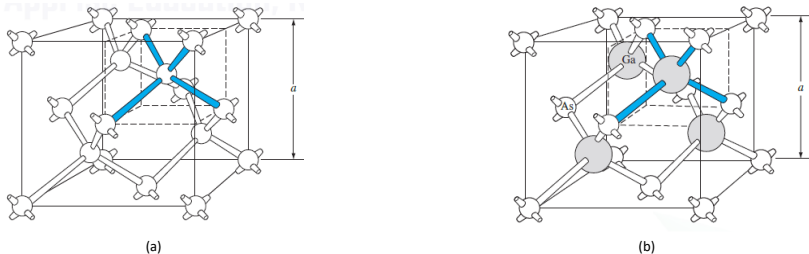


Figure: (a) Diamond cubic structure, (b) zincblende structure for GaAs. The solid lines represent the *tetrahedral* chemical bonds.

1.6 Atomic Bonding

The chemical bonds among atoms would determine the crystal structure of a solid.

- **Ionic Bond:** It occurs when an electron transfers from one atom to another.

-) e.g., The Sodium Chloride (NaCl) structure has FCC lattice with two ions (1 Na^+ and 1 Cl^-) associated with each corner point. There are 8 ions (4 Na^+ and 4 Cl^-) per unit cell.

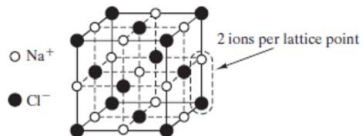


Figure: NaCl crystal structure.

- **Covalent Bond:** It shares valence electrons between two adjacent atoms. e.g., the diamond cubic structure for Si.
- **Metallic Bond:** In BCC and FCC structures, atoms of the metals reside at the lattice points and their valence electrons are shared by any large group of adjacent atoms.

-) e.g., copper has FCC structure and each atom has 14 nearest neighbors with each atom sharing many valence electrons.

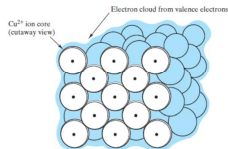


Figure: Metallic bond for copper.

- **Van der Waals Bond:** It is a weak bond that occurs when the effective center of positive charges in the nucleus is not the same as that of the negative charge of the surrounded electrons. This leads to a small electric dipole that can interact with the dipoles of other atoms. There is no electron sharing in this bond.

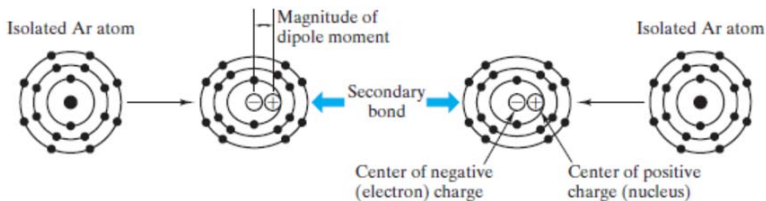


Figure: Van der Waals bond in Argon (Ar).

End of Chapter One