Mechanical Engineering

Material Science

Comprehensive Theory

with **Solved Examples** and **Practice Questions**

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Material Science

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Chapter 2

Crystal Structure

2.1 INTRODUCTION

Properties exhibited by any material is dependent upon the arrangement of atoms in the lattice i.e. the regularity with which the atoms are arranged with respect to one another, the type of bond between the atoms, crystal structure and so on.

Materials are generally classified as

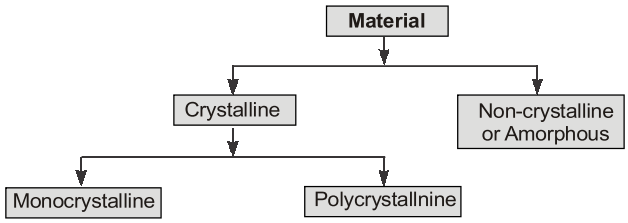


Figure 2.1

- **Crystalline Material** is one in which atoms are arranged in repetitive or periodic array over large atomic distances. Crystalline materials are further classified in Monocrystalline and Polycrystalline materials. e.g. Metals.
- **Monocrystalline Material** or single crystals are the materials in which same atomic order is extended in the entire specimen. On the other hand Polycrystalline solids are the materials which are composed of small crystals or grains having different crystallographic orientations.
- **Noncrystalline Material** does not possess a systematic and regular arrangement of atoms. They are also called as amorphous or supercooled liquids as their crystal structure resembles liquid. These materials possess relatively complex atomic or molecular structure and become ordered with great difficulty e.g. inorganic glass, ceramics.

2.1.1 Unit Cell

Crystalline structures are build up by small group of atoms which are repeated in the entire material. These repeat entities are called as unit cells.

When describing crystalline structures, atoms are represented as solid spheres having well defined diameters. This is known as Atomic hard sphere model.

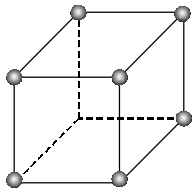


Figure 2.2

2.1.2 Lattice

Lattice is a three dimensional array of points in which each point is identically spaced and located with respect to each other. In other words, unit cell when repeated in three directions will generate the entire lattice.

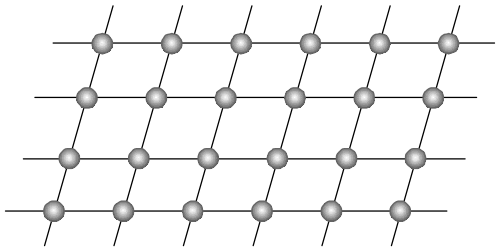


Figure 2.3

2.1.3 Bravais Lattices

In order to define a unit cell, six parameters are required namely *a*, *b*, *c*, α, β and γ. The magnitude of vectors *a*, *b* and *c* are called lattice parameters.

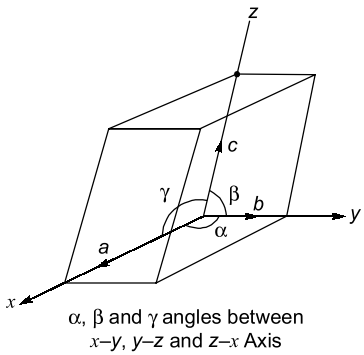
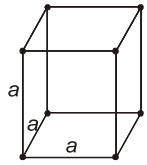
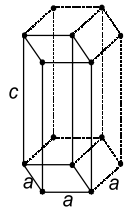
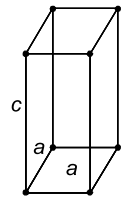
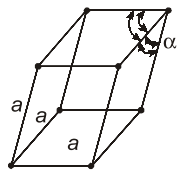
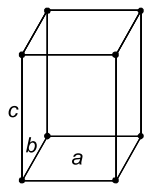
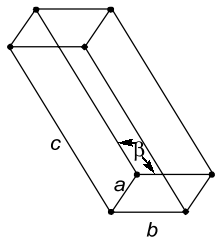
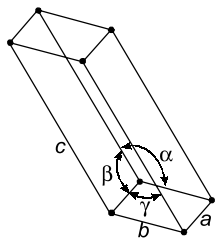


Figure 2.4

There are 14 ways in which atoms or molecules can be arranged in a three dimensional pattern, in such a way that every atom has exactly identical surroundings. These fourteen different arrangements are called as Bravais Lattices.

Crystal system	Lattice parameters	Inter axial Angles Relationship	Unit Cell Geometry
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	

Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	
Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

In some of crystal systems like Cubic, Tetragonal, Monoclinic and Orthorhombic more than one type of lattice arrangement exists. In general, there are four types of lattice arrangements namely.

1. **Simple or Primitive unit cell:** In this type the atoms are present only at the corners of the unit cell.
2. **Non Primitive unit cell or centered unit cell:** In this type the atoms are present at corners and also at some other position in the unit cell. They can be Face Centered, Body Centered and End Centered unit cell.

Face Centered unit cell: In this type the atoms are present at the corner and at center each face of the unit cell.

Body Centered unit cell: In this type the atoms are present at the corners and the body center of the unit cell.

End face-centered or Base Centered: In this type apart from corner atoms two extra atoms are present at the centre of any two opposite faces of unit cell.

2.2 Coordination Number and Atomic Packing Factor

Atoms in the lattice are not separate entities but they are strongly bonded with each other. Moreover, the type of arrangement of the nearest neighbours around an atom is different in different structures. This arrangement is called as coordination and the number of nearest neighbours is called coordination number.

Closeness of these atoms is measured by the packing factor. Packing factor is defined as the ratio of the volume occupied by the atoms in a unit cell to the volume of unit cell.

$$\text{Packing Factor} = \frac{\text{Volume occupied by the atoms in a unit cell}}{\text{Volume of unit cell}}$$

2.3 Space Lattice

Simple Cubic Lattice:

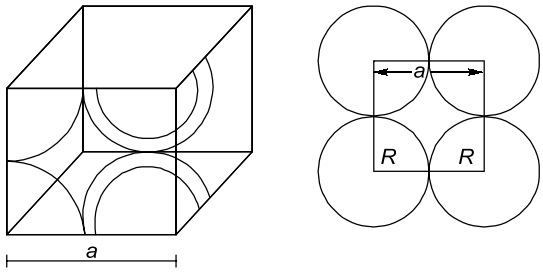


Fig. 2.5: Simple Cubic

There are eight corners and hence number of corner atoms is 8.

$\therefore$ The total number of atoms per unit cell is

$$\frac{1}{8} \times 8 = 1$$

From figure, Edge of cube = a and $a = 2R$ (from figure)

Volume occupied by atoms = Number of atoms × Volume of one atom

$$= 1 \times \frac{4}{3}\pi R^3$$

Volume of unit cell = $a^3 = (2R)^3$

$$\therefore \quad \text{Packing Factor} = \frac{\text{Volume occupied by atoms}}{\text{Volume of unit cell}} = \frac{1 \times \frac{4}{3}\pi R^3}{(2R)^3} = \frac{\pi}{6} = 0.52$$

This shows that only 52% of space is occupied in simple cubic structure.

Coordination number of SCC lattice is 6.

2.4 Face Centered Cubic Lattice

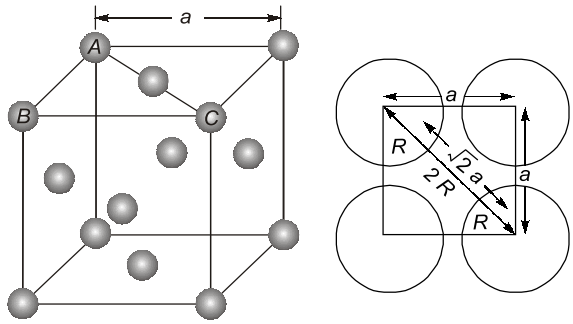


Figure 2.6

There are eight corners and hence number of corner atoms is 8.

The number of atoms at the centre of face = 6

∴ The number of atoms per unit cell is

$$\left(\frac{1}{8}\times 8\right)+\left(\frac{1}{2}\times 6\right) = 4$$

Volume occupied by atoms = Number of atoms × Volume of one atom

$$= 4\times\frac{4}{3}\pi R^3$$

Volume of unit cell $= a^3$

From the figure, $\sqrt{2}\,a = 4\,R$

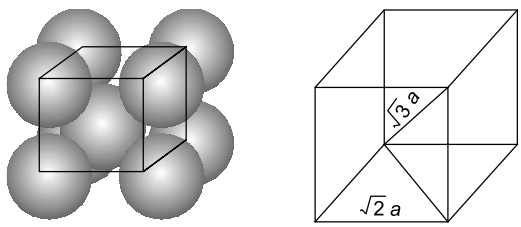
∴ Volume of unit cell $= a^3 = \left(\frac{4R}{\sqrt{2}}\right)^3$

$$\text{Packing Factor} = \frac{\text{Volume occupied by atoms}}{\text{Volume of unit cells}} = \frac{\frac{16}{3}\pi R^3}{\left(\frac{4R}{\sqrt{2}}\right)^3} = 0.74$$

74% of the space is occupied.

2.5 Body Centered Cubic Lattice

In a BCC lattice each atom is bonded closely to the neighbouring atom along the body diagonal. There are 8 corners and hence number of corner atoms is 8.



(a) (b)

Figure 2.7

The number of atoms at the body center = 1

∴ The total number of atoms per unit cell is

$$\left(\frac{1}{8}\times 8\right)+1 = 2$$

Volume occupied by atoms = No. of atoms × Volume of one atom = $2\times\frac{4}{3}\pi R^3$

Volume of unit cell = a^3

From the figure, $\sqrt{3}a = 4R$

∴ Volume of unit cell = $\left(\frac{4R}{\sqrt{3}}\right)^3$

$$\text{Packing Factor} = \frac{\text{Volume occupied by atoms}}{\text{Volume of unit cells}} = \frac{\frac{8}{3}\pi R^3}{\left(\frac{4R}{\sqrt{3}}\right)^3} = \frac{\sqrt{3}\pi}{8} = 0.68$$

The packing factor in BCC lattice is lesser than FCC but greater than SCC lattice. Coordination number of BCC lattice is 12.

Density of unit cell:

$$\rho = \frac{M}{V}$$

M = Mass of unit cell

V = Volume of unit cell

M = Mass of one atom × no. of atoms

$$m = \frac{\text{Atomic weight}}{\text{Avogadro's No. } (6.023\times 10^{23})} = \frac{M_0}{N_A}$$

$$\rho = \frac{n\times m}{V} = \frac{n\times M_0}{V\times N_A}$$

2.6 Mechanism of Crystallization

(i) Transition from liquid to the solid state takes place by nuclei formation and growth. Atoms in the material have both kinetic energy and potential energy.

(ii) Kinetic energy is related to the speed at which the atom molecules and it is a function of temperature. It is because at a higher temperature, diffusion phenomena will be predominate which is caused by higher kinetic energy of atoms.

(iii) Potential energy is related to the distance between atoms. Kinetic energy of atoms in the liquid as well as solid phase is same but there is a significance difference in the potential energy.

(iv) If there is an alloy with eutectoid composition or there is a pure material, mechanism of crystallization is called skin forming at boundary of the liquid metal since the temperature is low, solid will nucleate.

(v) The solidification front will move towards the centre and there will be symmetric crystal growth from the surface towards centre.

(vi) If mushy zone appears in the alloy nucleation will takes place not only on the surface but in the liquid region as well. In this case there will be multi directional crystal growth called dendrite formation.

(vii) If the cooling rate of the liquid metal are slow, nucleation will take place at smaller number of places which produces grain structure. if the cooling rates are very high, nucleation will takes place at large number of places, which produces fine grain structure.

Objective Brain Teasers

Q.1 The material property which depends only on the basic crystal structure is
(a) Fatigue strength
(b) Work hardening
(c) Fracture strength
(d) Elastic constant

Q.2 For a Rhombohedral space lattice, which one of the following is correct?
(a) $\alpha = \beta = \gamma = 90°$
(b) $\alpha = \beta = \gamma \neq 90°$
(c) $\alpha = \gamma = 90° \neq \beta$
(d) $\alpha \neq \beta \neq \gamma \neq 90°$

Q.3 Which one of the following pairs is not correctly matched?

	Space Lattice		Relation between Atomic radius r and Edge element a
(a)	Simple cubic structure	:	$a^2 = 4r^2$
(b)	Body-centred cubic structure	:	$3a^2 = 16r^2$
(c)	Triclinic	:	$2a^2 = 3r^2$
(d)	Face-centred cubic structure	:	$a^2 = 8r^2$

Q.4 Match **List-I** (Crystal Structure) with **List-II** (Example) and select the correct answer using the codes given below the Lists:

List-I
A. Simple Cubic
B. Body-centered Cubic
C. Face-centered Cubic
D. Hexagonal Close Packed

List-II
1. Zinc
2. Copper
3. Alpha iron at room temperature
4. Manganese

Codes:

	A	B	C	D
(a)	4	3	1	2
(b)	4	3	2	1
(c)	3	4	2	1
(d)	3	4	1	2

Q.5 Match **List-I** (Element) with **List-II** (Crystal Structure) and select the correct answer using the code given below the Lists :

List-I		List-II
A. Alpha Iron		1. Hexagonal closed packed
B. Copper		2. Body-centred cubic
C. Zinc		3. Amorphous
D. Glass		4. Face-centred cubic

Codes:

	A	B	C	D
(a)	2	3	1	4
(b)	1	4	2	3
(c)	2	4	1	3
(d)	1	3	2	4

Q.6 In the atomic hard-sphere model of the crystal structure of Copper, what is the edge length of unit cell?
(a) 2 x Atomic radius
(b) $(4/\sqrt{3})$ x Atomic radius
(c) $(2\sqrt{2})$ x Atomic radius
(d) J2 x Atomic radius

Q.7 The coordination number for FCC crystal structure is
(a) 4 (b) 8
(c) 12 (d) 16

ANSWERS

1. (d) 2. (b) 3. (c) 4. (b) 5. (c)
6. (c) 7. (c)

Hints & Explanation

1. (d)

Property dependent on basic crystal structure	Property dependent on crystal imperfection
Density	Electrical conductivity
Specific heat	Yield stress
Coefficient of thermal expansion	Creep
Melting point	Fracture strength
Elastic constant	Semiconductivity
Hardness and ductility	Work hardening
	Fatigue strength

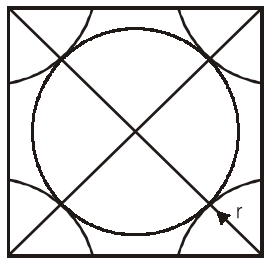
4. (b)

No of lattice point = $1+\frac{1}{4}\times 1=2$;

area a^2 $\therefore$ planner density $2/a^2$

6. (c)

Cu – F.C.C Structure



$4r = \sqrt{2}\,a$

$a = \frac{4r}{\sqrt{2}} = 2\sqrt{2r}$

Edge length of unit all = $(2\sqrt{2})$ x Atomic radius.

Student's Assignments

Q.1 What are space lattice, unit cell and lattice parameters? Explain.

Q.2 If the atomic radius of aluminium is 0.143 nm, calculate volume of its unit cell.

Q.3 Calculate the radius of iridium atom, having an FCC crystal structure, a density of 22.4 g/cc and atomic weight of 192.2 g/mol.

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