

# Solid State Physics.

→ Crystallography

Unit-II.

→ Free electron theory

Solid

↓  
Crystal

↓  
Non crystal / Amorphous

↓  
Single polycrystal

Solid → The atoms ~~or~~ and molecules in solids are attached to one another with strong forces of attraction. The solid maintains a definite volume and shape.

Solid state physics

The solid state physics is the branch of physics deals with physical properties of solids, particularly crystals including the behaviour of e<sup>-</sup>s in this solid.

Characteristics of solid on the basis of structure.

The solids may be broadly classified as —

### ① Crystalline / Crystal

### ② Non-crystal (amorphous)

- Crystal :- The crystalline state of solids is characterised by regular or periodic arrangement of atoms of all molecules.

The crystalline solid may be subdivided into:-

- i) single crystal      ii) polycrystal.

### ① Single crystal

The crystalline state of solids is characterised by regular or periodic arrangement of atoms of all molecules.

The crystalline solid may be subdivided into-

### ① Single crystal

### ② Polycrystal

- Single Crystal → In single crystal the periodicity of atoms extends throughout the material.  
e.g. diamond, quartz, mica etc.

- Polycrystal → A polycrystalline material is a collection of a number of small crystallites with random orientation separated by well defined boundaries. The small crystallites are known as grains and the boundaries as grain boundaries.

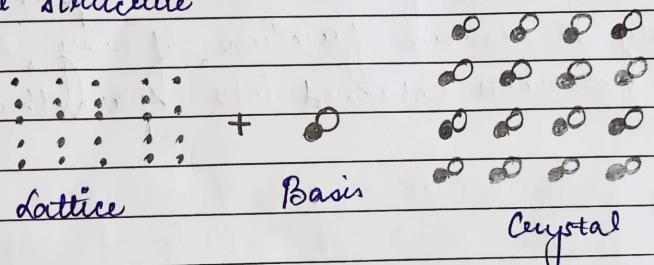
- Non crystalline / Amorphous : The non crystalline or amorphous solid are characterized by the completely random arrangement of atoms & molecules.  
e.g. glass.

Lattice: The lattice has been defined as an array of imaginary points which are so arranged in space that each point has identical surroundings.

### Bases

An atom or group of atoms must be placed on each lattice point in a regular fashion will give crystal structure such an atom or group of atom is called the basis.

thus, a lattice combined with a basis generates the crystal structure



Unit Cell: The unit cell is defined as the smallest unit of the lattice which on continuous repetition generates the complete lattice.

It is of two types:-

(i) Primitive → If a unit cell contain a single atom is called a primitive unit cell. Eg. simple cubic (SC) lattice.

(ii) Non primitive :- If a unit cell contain more than one atom is known as non primitive unit cell. Eg. BCC structure; FCC structure.

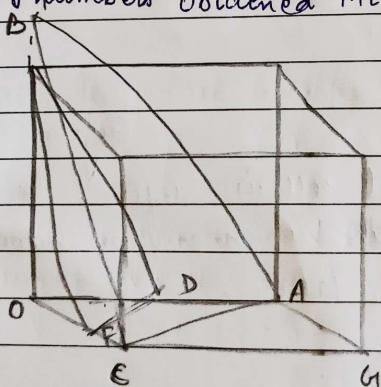
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# Miller Indices: The scheme to represent the orientation of planes in a lattice was first introduced by Miller. A British crystallographer. The indices of the planes are therefore known as Miller indices.

The steps involved to determine the Miller indices of a plane are as follows:-

(i) Find the intercepts of the plane on the crystallographic axis.

(ii) Take reciprocals of these intercepts.  
Simply to remove fraction, if any, and enclosed the numbers obtained into parenthesis



Consider a plane A, B, C having Intercept 1, 2, 1 with the crystallographic axis A, B and C respectively of a cubic lattice.

(i) Intercept : 1 2 1  
(ii) Reciprocals : 1 1 1

(iii) Simplification : 1 1 2

Hence, the mirror miller indices of the plane is written as  $(2, 1, 2)$

The Miller indices of a plane in general are written as  $\frac{1}{a}, \frac{1}{b}, \frac{1}{c}$  or  $(h k l)$

Type I :-

In a crystal, a plane cuts intercepts of  $2a, 3b,$   
 $6c$  along the three crystallographic axis  
determining the Miller indices of the plane.

Sop:- Intercepts :  $2a$        ~~$6b$~~        $6c$

Division by unit :  $2$        $3$        $6$   
unit translation

Reciprocal :  $\frac{1}{2}$        $\frac{1}{3}$        $\frac{1}{6}$

Simplification : -  $3$        $2$        $1$

The required Miller indices of the plane are  
 $(3 2 1)$

Type II

Determine the Miller indices of the plane which is parallel to x axis and cut intercepts ~~to~~ 2 and  $\frac{1}{2}$ , respectively along y and z axis

Sop:- Intercepts :  $0$        $2b$        $c/2$

Division by unit :  $0$        $2$        $\frac{1}{2}$

unit translation

Reciprocal :  $0$        $\frac{1}{2}$        $2$

Simplification :  $0$        $1$        $4$

The required Miller indices of the plane are  
 $(0 1 4)$

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### Type III.

Q. An orthorhombic crystal whose primitive translation are  $a = 1.21 \text{ \AA}$ ;  $b = 1.84 \text{ \AA}$  and  $c = 1.97 \text{ \AA}$  respectively. If a plane with Miller indices  $(2, 3, 1)$  cuts an intercept of  $1.2 \text{ \AA}$  along the  $x$ -axis, find the length of intercepts along  $y$  and  $z$  axis.

I	Intercepts : $p_a$	$q_b$	$r_c$	Rough
II	Division by unit translation : $p^{-1}$	$q^{-1}$	$r^{-1}$	
III	Reciprocal : $p^{-1}$	$q^{-1}$	$r^{-1}$	
IV	Simplification : $-h$	$k$	$l$	

$$p^{-1} : q^{-1} : r^{-1} = h : k : l = 2 : 3 : -1$$

$$\frac{p}{p} : q : r = \frac{1}{2} : \frac{1}{3} : -1$$

The ratio of actual lengths of the intercepts are

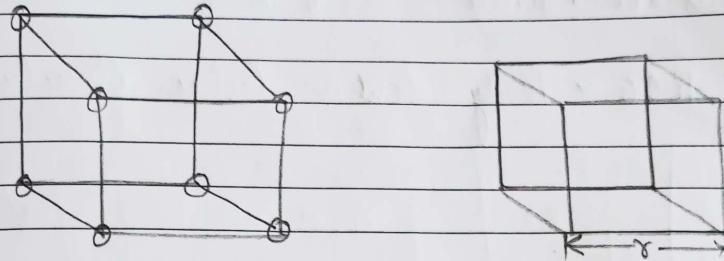
$$l_1 : l_2 : l_3 = p_a : q_b : r_c, \frac{1.21}{2} : \frac{1.84}{3} : -1.97$$

Since  $l_1$  is given as  $1.21 \text{ \AA}$  we therefore multiply the right R.H.S by 2 so that  $l_1 : l_2 : l_3 =$

$$1.21 : \frac{3.68}{3} : -3.94$$

$$l_2 = 1.23 \text{ \AA}, l_3 = -3.94 \text{ \AA}$$

### ① simple cubic (sc)



In simple cubic structure 8 atoms occupy 8 corners of the cube. So, the effective number of atoms contained within a unit cell is  $(8 \times 1/8) = 1$

The relation between the radius ( $r$ ) of the atoms with lattice parameter ( $a$ ) is  $r = a/2$ .

The volume actually occupied by an atom within a unit cell  $= \frac{4}{3} \pi r^3$

$$= \frac{2}{3} \pi \times \frac{a^3}{8}$$

$$V = \frac{\pi a^3}{6}$$

Volume of the unit cell = volume of the cube

$$V = a^3$$

The atomic packing factor is defined as the volume occupied by the atom within a unit cell.

Atomic packing factor (APF) =  $\frac{V}{V}$

$$f = \frac{\frac{\pi a^3}{6}}{a^3}$$

$$f = \frac{\pi}{6} \quad f = 0.520852\%$$

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E.g. polonium exhibit this structure at room temperature. This signifies that this structure is not stable.

(ii) BCC  $\rightarrow$  Body Centre Cubic Structure



$$\begin{aligned} (4r)^2 &= (\sqrt{2}a)^2 + a^2 \\ 16a^2 &= 2a^2 + a^2 \\ 16a^2 &= 3a^2 \\ 4r &= \sqrt{3}a \\ \Rightarrow r &= \frac{\sqrt{3}}{4}a \end{aligned}$$

In BCC structure 8 atoms occupy 8 corners of the cube and one atom is at the Body center position. So, the effective number of atoms within the unit cell.

$$8 \times \frac{1}{8} + 1 = 2 \rightarrow \text{Overall no. of atoms in cube}$$

The relation b/w the radius of the atoms and lattice parameters ( $a$ ) is given by :-

$$\boxed{r = \frac{\sqrt{3}}{4}a}$$

The volume occupied by the atoms within a unit cell,

$$V = 2 \times \frac{4}{3} \pi r^3$$

$$= \frac{2}{3} \times \frac{4}{3} \pi \left( \frac{\sqrt{3}a}{4} \right)^3$$

$$= \frac{2}{3} \times \frac{4}{3} \pi \times \frac{3\sqrt{3}}{4 \times 4^2} a^3$$

$$= \frac{2\sqrt{3}}{8} \pi a^3$$

Volume of the unit cell.  $A.P.F = \frac{V'}{V} = \frac{\sqrt{3}}{8} \pi a^3$

$$= 0.68 \text{ or } 68\%$$

### Face center cubic Structure (FCC)

In FCC structure 8 atoms occupy 8 corners of the cube of atom at each face. So, the effective number of atoms within a unit cell.  $\frac{8 \times 1}{8} + \frac{3 \times 1}{2} = 1 + 3 = 4$

The relation b/w the radius ( $r$ ) of the atoms & lattice parameter ( $a$ ) is given by :-

$$(4r)^2 = a^2 + a^2$$

$$= 2a^2$$

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

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

Volume occupied by the atoms within the unit cell

$$V = 4 \times \frac{4}{3} \pi r^3$$

$$= \frac{4 \times 4}{3} \pi \times \frac{2\sqrt{2}}{4 \times 3} a^3$$

$$V = \frac{\pi \times 2\sqrt{2}}{4 \times 3} a^3$$

$$V = \frac{\sqrt{2} \pi a^3}{6}$$

Volume of the unit cell

$$\text{APF} = \frac{V'}{V} = \frac{\frac{\sqrt{2}}{6} \pi a^3}{a^3} = 0.0760876\%$$

Q. The atomic radius of simple cubic lattice is  
a or  $\frac{a}{2}$

### # Inner planar spacing

Consider three mutually perpendicular coordinate axis  $Ox, Oy, Oz$  and assume that a plane ( $HKL$ ) parallel to the plane passing through the origin makes intercepts  $a/m, b/k, c/l$  respectively on the three axis at  $A, B, C$  respectively as shown in the figure.

Let  $OP (=d)$ , interplanar spacing be normal to the plane drawn from the origin & respectively makes angle  $\alpha, \beta, \gamma$  with the three axis. Therefore  $OA = a/m, OB = b/k, OC = c/l$  from triangle  $OPA$ ,  $\cos \alpha = \frac{OP}{OA} = \frac{d}{a/m}$

$$\cos^2 \alpha = \frac{d^2}{a^2/m^2} \quad \cos^2 \beta = \frac{d^2}{b^2/k^2} \quad \cos^2 \gamma = \frac{d^2}{c^2/l^2}$$

Now making use of the direction cosine which state that  $\cos^2 \alpha + \cos^2 \beta + \cos^2 \gamma = 1$

[P.T.O]

Q. Define and derive expression for linear, planar, and volume density of a crystal.

Ans.

Linear density : The linear density of a crystal is the number of atoms per unit length along a specific crystallography direction.

The linear density can be calculated using the following formula

$$f_L = \frac{N}{L} \text{ where } f_L \text{ is the linear density i.e. the number of atoms per unit length.}$$

N : Number of atoms in the unit cell

L : length of the unit cell

Planar Density : The planar density of a crystal is the number of atoms per unit area on a specific crystallography plane.

$$f_P = \frac{N}{A}$$

$f_P$  : Planar density

N : Number of atoms per unit cell

A : Area of the unit cell

Volume Density : The volume density of a crystal is the number of atoms per unit volume. The volume density can be calculated as

$$f_V = \frac{N}{V}$$

Q. What are the lattice parameters and discuss the seven types of crystal systems on the basis of lattice.

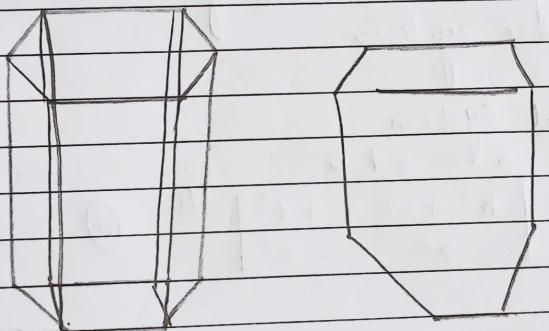
Am. Lattice parameters: The lattice parameter are the parameters which are used to describe the length along three crystallography axis. In three dimensional space it is described as lattice parameters  ~~$a = b = c$~~   $a \neq b \neq c$ . All the seven crystal system of three dimensional space are listed below

S. No.	Crystal system	Lattice parameters	Corresponding Angles
1.	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$
2.	Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
3.	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
4.	Rhombohedral/Tetragonal	$a = b = c$	<del><math>\alpha &gt; \beta = \gamma \neq 90^\circ</math></del>
5.	Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ \quad \gamma = 120^\circ$
6.	Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90^\circ \neq \beta$
7.	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$

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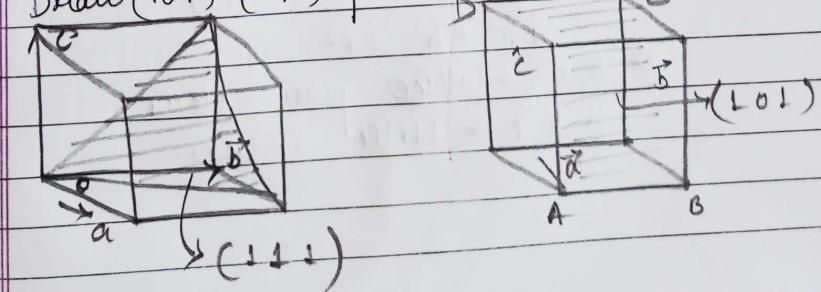
### In two dimension lattice

S.No.	Crystal System	Lattice parameters	Corresponding Angles.
1.	Oblique	$a \neq b$	$\gamma \neq 90^\circ$
2.	Rectangular	$a \neq b$	$\gamma = 90^\circ$
3.	Square	$a = b$	$\gamma = 90^\circ$
4.	Hexagonal	$a = b$	$\gamma = 120^\circ$



Q. What are the essential requirements for laser action.  
 optical medium, pumping, active Medium  
 resonator, source

Q. Draw (101) (111) planes in a cubic unit cell



[P.T.O]

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$$\frac{d^2}{(a/m)^2} + \frac{d^2}{(b/k)^2} + \frac{d^2}{(c/l)^2} = 1$$

$$d^2 \left[ \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right] = 1$$

$$d = \left[ \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right]^{1/2} \quad \text{--- (i)}$$

This is the general formula and is applicable to the primitive lattice of orthorhombic, tetragonal, and cubic system.

(i) Tetragonal System

$$a = b \neq c$$

$$d = \left[ \frac{h^2 + k^2 + l^2}{a^2} \right]^{1/2} \quad \text{--- (ii)}$$

(ii) Cubic System

$$a = b = c$$

$$d = \left[ \frac{h^2 + k^2 + l^2}{a^2} \right]^{1/2}$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad \text{--- (iii)}$$

$a, b, c \rightarrow$  lattice parameters  
 $h, k, l \rightarrow$  Miller Indices