M.Sc. - (III - Sem)

Condensed Matter Physics

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* PHYSICS *

UNIT - I

Crystalline solids:

Those solids in which atoms and molecules are arranged internally in a definite or regular manner and posses a definite geometrical shape throughout the crystal structure.

Examples: Mica, Quartz, sugar, Copper sulphate etc.

Characteristics of crystalline solids:

1. These type of solids have "long range order".
2. These solids have flat surfaces.
3. These solids are "Anisotropic".

It means that in crystalline solids physical properties like electrical and thermal conductivity, compressibility, shape etc are different along different directions.

4. Bonds b/w atom/molecules have equal strength.

5. They have sharp melting point.

Reason: It is because when the melting point is attained on heating these solids all the bonds breaks altogether causing a sudden change in the state of the solid i.e from solid to liquid.

6. On crystallisation, these solids have minimum energies and hence are more stable.

→ Amorphous Solids:

Those solids in which the atoms and molecules are arranged internally in an indefinite or irregular manner and so that, they do not passes a definite external geometrical shape throughout the crystal structure.

Examples: Glass, rubber, elemental form of sulphur etc.

Characteristics of amorphous solids:

1. These solids have "short range order"
2. These solids do not have flat surfaces.
3. These solids are "Isotropic" i.e opposite of "Anisotropic"
4. The bonds b/w atoms and molecules are of unequal strength

5. They do not have sharp melting point.

Semicrystalline solids:

These are also called "Polycrystalline solids" & may be defined as,

- A solid which have many crystallites grown together to form an interlacking mass (like rocks) which are seperated by well defined boundries and orient randomly (in all arbitory directions).

Characterstics of semi-crystalline solids:

1. They are "isotropic" in nature
2. They can be grown as a single crystal under suitable specific conditions.
3. The surface is random.

Examples: Rocks, sand, metals, salts etc.

Notes:

1. The branch of science under the shadow of which the crystals and their structure is studied is called "crystallogsaphy" or "crystal physics"
2. In crystalline solids following result holds,

$$\boxed{f + c = e + 2}$$

Where, f = faces of crystalline solids
c = The number of angles.

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Where, f = faces of crystalline solids
c = The number of angles.

e = edges of crystalline solids.

3. Crystalline solids have reticulate structure, which means the constituent particles of solids are arranged in a periodic manner in 3D {space}.

4. Amorphous solids do not have a reticulate structure.

→ **Crystals:**

It may be defined as a solid composed of atoms or other microscopic particles arranged in an orderly repetitive manner.

Crystals are also the purest available solids but, it does not mean that they do not have any impurity.

→ **Types of crystals:**

There are following types of crystals {reference in Pradeep fundamental XIIth}.

1. **Single crystals:**

The crystal in which the pattern of constituent particles (periodicity) continues throughout the peice of crystal. These crystals can vary from a fraction of centimeter to few centimeters.

2. **Monocrystals:**

These actually are very small sized single crystals which

are not visible through the naked eyes. They usually have dimensions $\approx 5 \times 10^{-8}$ m.

3. **Polycrystals:**

A polycrystal is basically a collection of some monocrystals together such that the faces of the monocrystals are joined together.

Examples: Ceramic, Y_2O_3, BaO and $Cu(II)O_2$.

4. **Liquid crystal:**

These are fluid substances (more like of liquids) having "long range order" and by nature are mainly organic compounds which on heating do not directly convert into liquids (liquid phase). These are widely used in making LCDs.

Example: Alkyl carbophenyl and Chalestral ester.

→ **Crystallisation:**

It is a process by which the crystals are basically obtained.

Example: Crystals of rock salt (NaCl) are obtained from evaporating sea water.

→ **Crystal lattice:**

It may be defined as "A geomatrical array (arran-

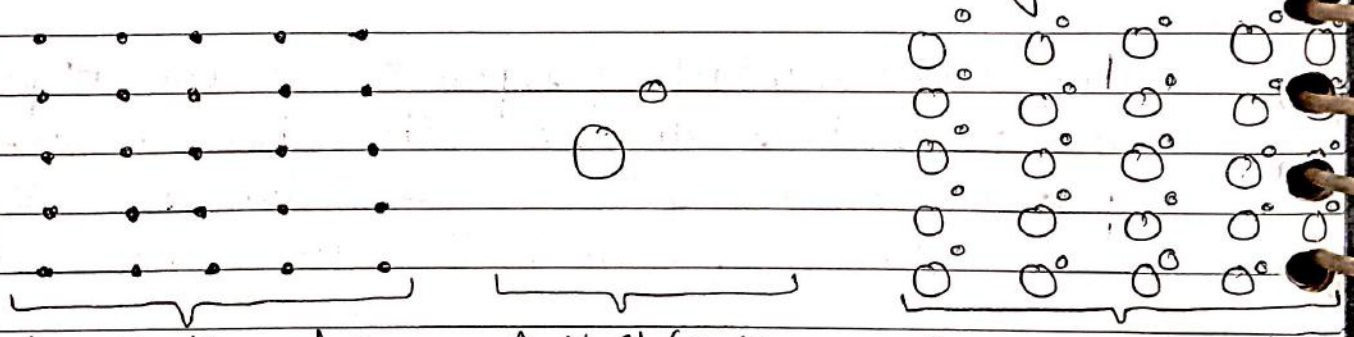
gement) of imaginary points in space where when atoms or molecules of a solid are placed becomes a uniform or regular pattern called the "crystal structure".

In simple words, a collection of imaginary points in a 3D (space) is called a "crystal lattice" and these imaginary points are called "lattice points".

But when these imaginary points gets occupied or captured by constituents of a crystal the resulting arrangement is called "crystal structure".

Important notation:

Lattice + basis → Arrangement of atoms OR crystal structure



A collection of some imaginary points i.e lattice | A NaCl (rock Salt) molecule i.e a basis | Crystal lattice of NaCl i.e Crystal Structure.

→ Lattice is 3D, 2D or 1D arrangement of points or site where constituent particles of crystals are to be placed.

→ Basis is that constituent particle which is placed on lattice points in a lattice to obtain a desired crystal structure.

Note :

1. Each and every point in the lattice is called a lattice point (or lattice sites.)

2. In some books (like M. A. Wahab) following types of lattices are also discussed.

"In 1848, Bravais introduced the concept of space lattice (or crystal lattice).

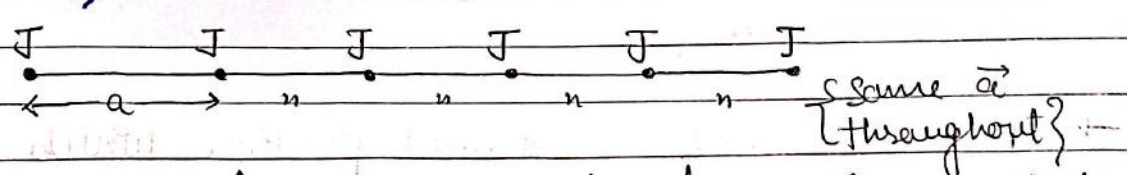
In order to understand the concept of space lattice let us first understand the following term.

→ Translation vectors :—

The vectors which propogate or can be produced in a certain direction to obtain a regular pattern periodically (after a certain time interval regularly) are called the translation vectors.

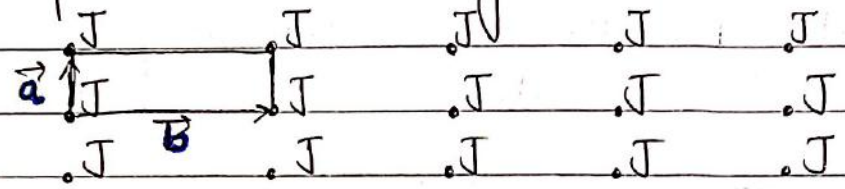
A/c to Bravais the following type of lattices are possible.

- When a vector is produced along only one direction at a time it gives us a linear arrangement, shown below,



This type of arrangement of imaginary points is called "linear lattice or rectilinear lattice".

- When two translation vectors (from same reference point) are produced along two directions gives us the plane like arrangement shown below,



This is regarded as a planar lattice

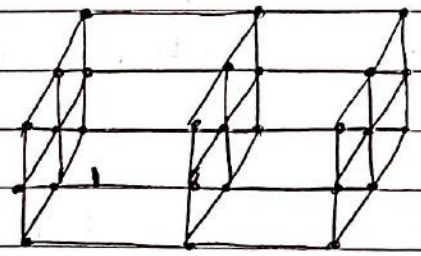
It should always be remembered that the array is not a lattice of points (T_s) instead it is called a lattice array of (T_s')

The length of any other translation vector from the reference point is given as,

$$T = n_1\vec{a} + n_2\vec{b}$$

{Where n_1 and n_2 are the integers & $\vec{a}$ & $\vec{b}$ are the translation vectors}.

- When three vectors are produced (from a same reference point) along three directions they give us the space like arrangement as shown below.



→ This is a space lattice or crystal lattice and has symmetry all over.

The location of any other point (lattice point) or the length of translation vectors other than $\vec{a}$, $\vec{b}$ & $\vec{c}$ is given as,

$$\boxed{T = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}}$$

Where, n_1, n_2 and n_3 are the arbitary integers.

→ **Bravais lattice :**

A lattice in which all lattice points are occupied with identical constituent particles of a crystal is generally refered as Bravais lattice

→ **Direct lattice :**

It is a unique type of lattice which may be defined as "An arrangement of a single atom or molecule repeated along all the directions i.e crystal structure made of a single constituent particle".

It may also be regarded about the direct lattice that "A lattice made or obtained by a primitive unit cell and has same basis for the lattice throughout the crystal structure is called "Direct lattice".

It therefore concludes that each crystal lattice in a crystal structure contains a number of direct lattice.

Also, the configuration of a direct lattice is described by the orientation (revolution/rotation/spining) of different constituent particles.

→ **Bravais lattice in two dimensions: Plane lattice :**

The lattice in a plane (or 2D) are generally called as "Bravais lattice in 2D" or plane lattice.

If an oblique lattice is modified in terms of a, b and ϕ the shape of the lattice will be changed (i.e unit cell will be modified independently). Such modified lattices are known as "Special lattice".

× Ques: How to obtain special lattice?

Ans: We have three variables by which we can change or modify an oblique lattice.
If the length along two directions is taken i.e a, b there are two possibilities,

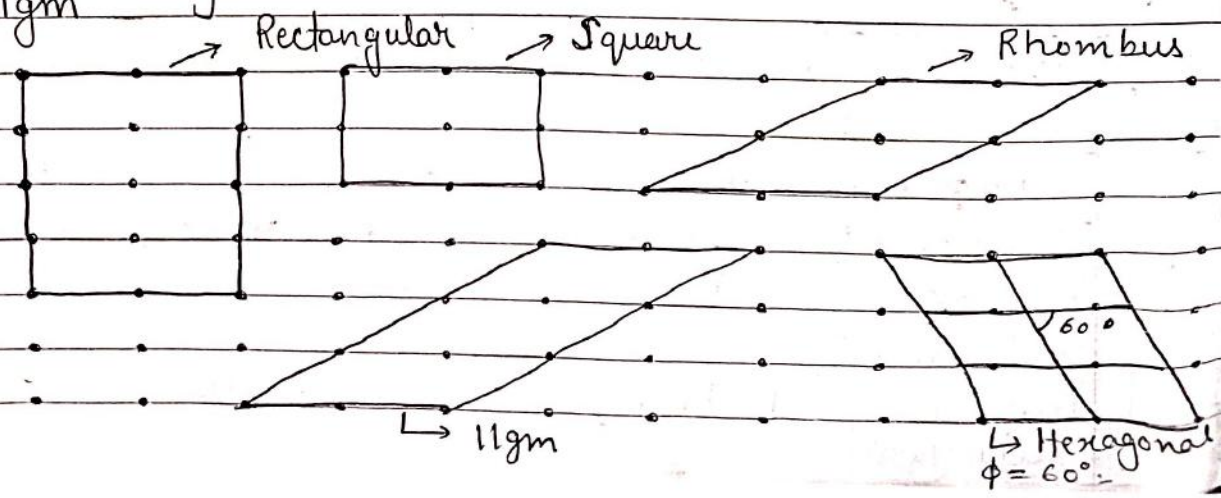
(i) $a = b$ (ii) $a \neq b$

Further, the angle between two vectors a & b i.e ϕ can provide more options as it could take various values from which common is $\phi = 90°$.

A suitable combination of a, b & ϕ makes a unique or special lattice which are in general listed as

1. Square
2. Rectangle
3. Rhombus
4. ||gm

These are the shapes of lattices named by us as "special lattice". The lattice shapes are shown below.



There may be more than one unit cell if we have to choose from a lot of possible ones in a plane (discused earlier in W-F unit cell).

Note :

1. Generally those unit cells are chosen which have higher symmetry.
2. It is not necessary that the chosen cell have to be primitive
3. An equilateral triangle can not be used as the basis of lattice because of,
When it will be represented to fill a plane the orientation (movement along axis) invalue a change in addition to its translation.

Types of brausais lattice in 2D.

There are five plane lattice formed in 2D. These are as follows

1. General lattice i.e oblique {only one}
2. Special lattice i.e shown in table {four}

	Serial Number	Lattice Type	Conventional unit cell	Axes and angles	Points group symmetry about lattice pt.
General lattice	1.	Oblique	Parallelogram	$a \neq b$, $\phi = 90°$	2
Special lattice	2.	Square	Square	$a = b$, $\phi = 90°$	4 mm
	3.	Hexagonal	60° Rhombus	$a = b$, $\phi = 120°$	6 mm
	4.	Primitive rectangular	Rectangle	$a \neq b$, $\phi = 90°$	2 mm
	5.	Centred rectangular	Rectangle	$a \neq b$ $\phi = 90°$	2 mm

→ **Invariance of oblique lattice:**

Invariance mean a property in which a substance does not change its state or property and remains conserved or constant i.e substance do not vary.

Oblique lattice are invariant only for rotation at an angle of $2\pi/n$ where $n = 1$ and 2.

If we apply some suitable restrictions on the a, b & ϕ lattice parameters oblique lattice is invariant for rotation at $2\pi/n$ where $n = 3, 4, 6$ or those of mirror reflection.

→ **Bravais lattice in 3D or space lattice:**

Just like Bravais lattice in two dimensions Bravais lattice in 3D were obtained by restricting lattice translations a, b & c and the angles α, β and γ between them.

There are fourteen types of lattices possible in 3D. These are divided as,

1. Triclinic which is general.
2. The other thirteen like,

   Monoclinic
   Orthorhombic
   tetragonal
   trigonal
   Hexagonal
   Cubic

   } which are special.

Symbols – P – Primitive (lattice pt. are at the corners of unit cell only)
C – Side or Base centred (lattice points are at corners & at 2 face centres)
I – Body centred (lattice points are at corners and at body centre)
F – Face centred (lattice points are at corners and at six face centres).

Crystal Systems	Restrictions on Conventional Cell; axes & angles	Associated lattice		Characteristic Symmetry elements	To be specified		
		Num.	Symbol		Axes	Angle	Total
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	1	P	None	a, b, c	α, β, γ	6
Monoclinic	$a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \beta$	2	P, C	1 two fold rotation axis or m ($\equiv \bar{2}$)	a, b, c	γ	4
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	4	P, C, F, I	3 two fold rotation axis or m (mutually ⊥)	a, b, c	—	3
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	2	P, I	1 four fold rotation axis or m ($\equiv \bar{4}$)	a, c	—	2
Trigonal (Rhombohedral)	$a = b = c$ $\alpha = \beta = \gamma < 120^\circ$	1	P	1 three fold rotation axis or m ($\equiv \bar{3}$)	a	α	2
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	1	P	1 Six fold rotation axis or m ($\equiv \bar{6}$)	a, c	—	2
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	3	P or Sc I or bcc F or fcc	4 three fold rotations axis or m ($\equiv \bar{3}$) (⊥ to cube diagonal)	a	—	1

Note:
1. The diagrams of these 14 crystal structures in 3D are made & explained in closed packed structures later.
2. Bravais was a "French" crystallographer who proposed these 2D and 3D crystal structures in 19th Century.

→ Indices (not from exam pt. of veiw):

Before understanding Indices let us go through the following basic terms,

1. **Rational** : The geometrical features of a crystal represented by lattice points.

2. **Rational point** : The lattice point (site) w.r.t another lattice point inside crystal structure.

3. **Rational line** : A row of rational points or lattice points in plane or space.

4. **Rational plane** : A plane obtained by lattice points

5. **Miller Indices** : It is a conventional notation which is used to describe the lattice pt, directions and planes.

Note : Other feature (not listed above) are are irrational in crystal structure.

Site Indices : In general the position of lattice pts relative to a chosen origin are,

$x = ma$, $y = nb$ and $z = pc$ {Where x, y, z are axis}

If a cubic lattice of unit length translations (i.e $a = b = c = 1$) is taken then,

$(x, y, z) \equiv (m, n, p)$ {i.e axis are represent by numbers or integers}

These numbers are then termed as "Site indices" and are written as $[[m, n, p]]$

Example, If $x = -2a$, $y = 1b$, $z = -3c$ Then,
The site indicis are $[[\bar{2}, 1, \bar{3}]]$
Where "bar" represents -ve sign.

Indices of direction:

It may be described as "Three smallest integers that determine the position of the site nearest to the origion on the given direction (i.e x, y, z)".
Therefare, the site indices are at the same time the indices of direction.

families of directions: These may be defined as similar or even idential indices in a crystal system. (When indices are equal or same these are called equivalent direc^n)

In general equivalent directions are represented as $\langle hkl \rangle$.
Example, In a cubic system $\langle 100 \rangle$ comprises of $[100], [\bar{1}00], [010], [0\bar{1}0], [001]$ & $[00\bar{1}]$, lattice sites

Indices of lattice plane: Lattice planes are the assembly of a number of equidistant ||el planes passing through the lattice points. From simple geometrical concepts the eq^n of this (the lines inside plane or space representation) line (shown in fig) is given as,

$$\frac{x}{a} + \frac{y}{b} = 1 \quad \text{for 2D or plane}$$

$$\frac{x}{a} + \frac{y}{b} + \frac{z}{c} = 1 \quad \text{for 3D or Space}$$