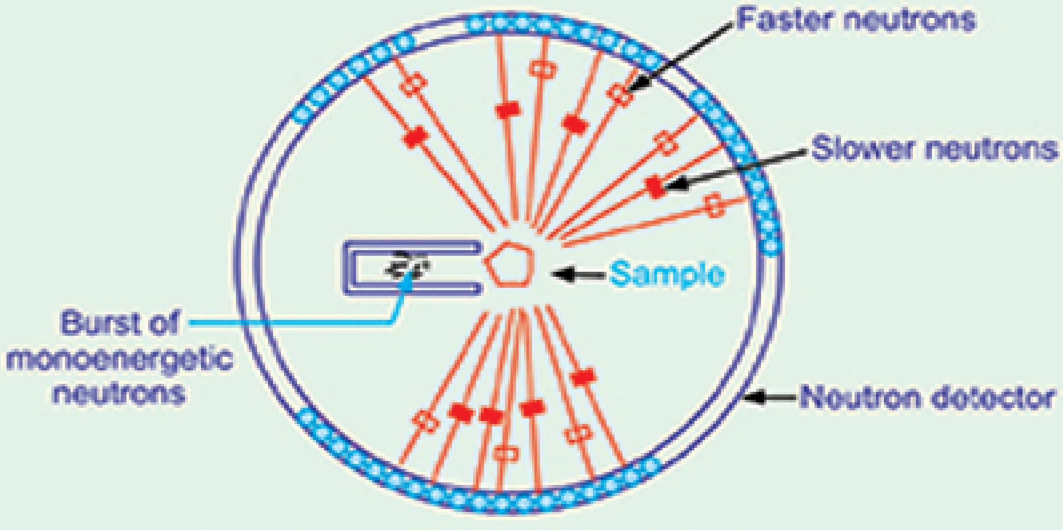
Shivaji University - B.Sc. Part-III
Semester-VI

SOLID STATE PHYSICS

(PHYSICS : PAPER-XVI)



Neutron Diffraction Apparatus

Dr. M. G. PATIL
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Dr. R. H. PATIL
S. V. MALGAONKAR

NIRALI PRAKASHAN
ADVANCEMENT OF KNOWLEDGE

A TEXT BOOK OF

PHYSICS

Solid State Physics

(Paper - XVI)

FOR

B.Sc. Part - III : Semester - VI

As Per New Revised Syllabus of Shivaji University, Kolhapur, June 2015

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PREFACE

This book is primarily intended for B.Sc. - III students of Semester - VI course of Shivaji University, Kolhapur. The book is strictly written according to new syllabus prescribed by Shivaji University, Kolhapur from June 2015.

It is our great pleasure to present this book to the students and respected teachers in proper time. The subject matter is presented in lucid and simple language. The book covers all the chapters according to the syllabus. The material is presented in comprehensive way and sequence of articles in each chapter helps the student to understand the subject. Different diagrams are given in the book to understand the basic principles. The solved numerical examples, multiple choice type questions, short answer type questions and long answer type questions are given at the end of each chapter. Some numerical problems are also given for self study.

We are heartly thankful to Principal Abhaykumar Salunkhe, President, Mrs. Shubhangi Gavade, the Secretary and Dr. Ashok Karande, Joint Secretary, Swami Vivekanand Shikshan Sanstha, Kolhapur, Dr. Arvind Burangale, Secretary, Rayat Shikshan Sanstha, Satara, Dr. H. B. Patil, Principal, Vivekanand College, Kolhapur. Dr. Milind Hujare, Principal. D.K.A.S.C. College Ichalkaranji, Dr. S. V. Kakatkar and Dr. V. C. Mahajan, Vivekanand College, Kolhapur, who inspired us to write this book.

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We are thankful to Nirali Prakashan, Pune for making us a part of their team of Authors. We thank Mr. **Dineshbhai Furia** and **Mr. Jignesh Furia** for publishing this book.

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We hope that this book will be found useful to the students and teachers. We will appreciate any suggestions for the improvement of the book.

– Authors

SYLLABUS

Unit - I **(11)**

Crystal Structure

Crystalline and non-crystalline solids, Space lattice, Basis and crystal structure, Unit cell – Primitive and non-primitive, Bravais lattices – Space groups and crystal structures, Symmetry elements of cubic system, Miller indices, Relation between lattice constant, Interplaner spacing and Miller indices, Simple crystal structures – Cubic (SC, BCC, FCC) and hexagonal close packed (HCP) (with respect to coordination number, Atomic radius, Atoms per unit cell, Packing fraction).

Unit - II **(11)**

X-Ray Diffraction by Crystals :

Reciprocal lattice, Properties of reciprocal lattice, Bragg's law in reciprocal lattice (Ewald's construction), Powder method of X-ray diffraction and analysis of cubic crystal structure.

Unit - III **(11)**

Lattice Vibrations :

Elastic vibrations of linear one-dimensional monoatomic lattice, Expression for frequency and dispersion curve, Elastic vibrations of linear one dimensional diatomic lattice – optical and acoustical excitations in ionic crystals, Experimental determination of dispersion relations.

Unit - IV **(12)**

1. Free Electron Theory of Metals and Band Theory of Solids :

Sommerfield's free electron model for electrical conductivity of metals, Fermi-Dirac distribution, Origin of energy bands - Valence band, Conduction band, Band gap energy, Distinction between metals, semiconductors and insulators, Hall effect – Hall voltage and Hall coefficient.

2. Solid State Device :

Timer (IC 555) - Block diagram, Function of each block, Pin configuration, Applications – Astable, Monostable, Bistable multivibrator.

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1. Crystal Structure **1.1 – 1.34**

Unit II

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5. Solid State Device **5.1 – 5.18**

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UNIT-I

1

CHAPTER

CRYSTAL STRUCTURE

SYLLABUS

Crystalline and non-crystalline solids, Space lattice, Basis and crystal structure, Unit cell – Primitive and non-primitive, Bravais lattices – Space groups and crystal structures, Symmetry elements of cubic system, Miller indices, Relation between lattice constant, Interplaner spacing and Miller indices, Simple crystal structures – Cubic (SC, BCC, FCC) and hexagonal close packed (HCP) (with respect to coordination number, Atomic radius, Atoms per unit cell, Packing fraction).

1.1 INTRODUCTION

The matter is usually regarded to exist in solid state or fluid state. Fluid state is further divided into gaseous and liquid state. All the materials are composed of atoms and molecules. The solid state of matter can be put into two categories on the basis of their structure i.e. crystalline solid and non-crystalline solid (amorphous). They are distinguished from one another primarily by the degree of order exhibited by the arrangement of the fundamental particles – atoms, molecules or ions comprising them.

Crystallography is the study of the solid in the form of crystals. The discovery of X-rays gives the powerful and precise tool for study of the internal arrangement of atoms in the crystal. Once the internal arrangement of atoms in the crystal is known, their physical properties can be studied.

1.2 CRYSTALLINE AND NON-CRYSTALLINE SOLID

In crystalline solid, the atoms or the molecules or ions are stacked in a regular (or periodic) manner, thus forming a three dimensional pattern. Smallest group of atoms called pattern unit or building block, which repeat itself in all directions to form a crystal.

When the regularity of the pattern extends throughout a certain piece of solid, then it is called single crystal. However, most of the solids are not single crystals, but often consist of a large number of small single crystal sections (grains) of various shapes and sizes packed to one another along the interfaces called the grain boundaries. In such materials the regularity or periodicity is interrupted at the grain boundaries, these materials are called polycrystalline.

When the size of grain becomes comparable to the size of pattern unit, the periodicity structure is completely disturbed, then the material is said to be in an amorphous state.

Distinction between Crystalline and Non-crystalline Solid :

Crystalline solid	Amorphous solid
1. Regular arrangement of particles or atoms.	1. Random arrangement of particles or atoms.
2. They have different physical properties (thermal, electrical) in different directions, i.e. they are anisotropic.	2. They have same physical properties in all directions i.e. they are isotropic.
3. The cooling curve for them has breaks because of crystallization.	3. The cooling curve is smooth.
4. The melting point is very sharp.	4. The melting point is not sharp.
5. Due to slow growth process, the constituent particles take definite position, where the potential energy of the configuration is minimum during growth. A long range order exists in crystalline solid.	5. Due to the quick growth process or phase change, the atoms do not have sufficient time to obtain the configuration of minimum energy. Therefore, short range order occurs in amorphous solid. e.g. glass, plastics, etc.

The crystals are formed when a substance changes from one state to another state i.e. in phase transformation. A change from the liquid phase to solid crystallization and a change from gaseous phase to the solid crystallization occur by sublimation. Once the crystal is formed, the atoms or molecules (building blocks) are bonded by chemical bonds like covalent bond, ionic bond, metallic bond and Van der Waal's bonds, etc. The crystals are bounded by perfectly flat faces and have sharp and straight edges. Crystal exhibits certain symmetries. Now-a-days X-rays, electron beam, neutron beam provide a tool for studying the internal structure of crystal. The study of the geometric form and other physical properties of crystalline solid by using X-ray diffraction, electron diffraction or neutron diffraction is called science of crystallography.

Different features of crystals :

1. Faces : The crystals are bounded by number of perfectly flat surfaces. These surfaces are called as faces. The face of the crystal may be like (cubes, alum) or unlike (galena).

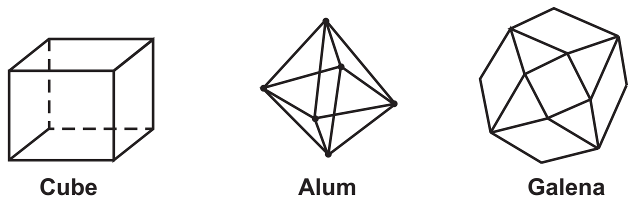


Fig. 1.1

2. Form : All the faces corresponding to a crystal are said to constitute a form. The crystal that consist of all like faces is termed to have a simple form, while the crystal having two or more simple forms is called to have a combination form.

3. Edges and interfacial angles : The intersection of two adjacent faces form the edges of crystal. The angle between any two faces of crystal is termed as the interfacial angle. The relation between plane faces (f), straight edges (e) and interfacial angle (c) is given by

$$f + c = e + z$$

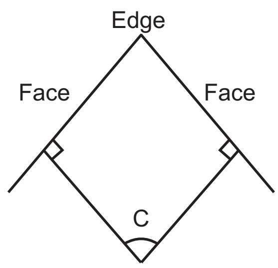


Fig. 1.2

1.3 SPACE LATTICE

Crystals are made up of regular and periodic three dimensional pattern of atoms in space. From geometrical point of view every atom is repetition of some arbitrarily chosen 'motif' atom of the mass. When a motif is repeated systematically in three dimensions, it results in a pattern called space lattice. Thus space lattice is defined as the periodic array of points in space such that the environment about each point is the same. In other words, a lattice is a periodic arrangement of points in space. The environment about any other point is in every way the same as that about any other point. All the points are connected by the translation operation T which is defined as $\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$, where n_1, n_2 and n_3 are arbitrary integers and $\vec{a}$, $\vec{b}$ and $\vec{c}$ are fundamental translation vectors.

If the array of points form a plane, it is two dimensional lattice and if the array of point repeats in three dimensions, it is three dimensional space lattice or simply space lattice.

(a) Two dimensional lattice **(b) Two dimensional collection of points (not lattice)**

Fig. 1.3

In Fig. 1.3 (a) and (b), array of point in two dimensions are shown. In Fig. 1.3 (a) we observe that the environment about any point is same but in Fig. 1.3 (b) it is not the same.

1.4 BASIS AND CRYSTAL STRUCTURE

Since a point being an infinitesimal spot in space, is imaginary, a lattice of point is an imaginary concept because a point is a dimensionless quantity. A lattice is a mathematical concept whereas the crystal structure is a physical structure. Crystal is formed by associating identically with every lattice point, a structural or building unit. This structural unit is called the basis or pattern. This basis consists of an atom or group of atoms. When the basis is repeated with correct periodicity in all direction it gives the actual crystal structure. (The lattice points may or may not be the atom sites.)

The logical relation between crystal and lattice is

$$\text{Lattice} + \text{Basis} = \text{Crystal structure}$$

The distinction between crystal and lattice is illustrated in Fig. 1.4.

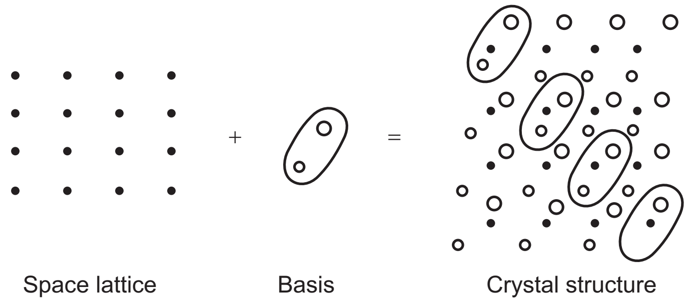


Fig. 1.4 : Crystal structure and basis

Thus crystal structure is specified characteristically by the type of the lattice associated with it.

1.5 UNIT CELL – PRIMITIVE AND NON-PRIMITIVE

An ideal crystal is constructed by a regular repetition in space of identical structural unit or building blocks usually termed as unit cell of the crystal. Thus unit cell of the crystal is the fundamental unit, like a brick (which may consist of a group of atoms, molecules or ions) which repeat at regular interval in three dimensions to form a crystalline solid.

For the very simplest of the monoatomic crystals, the building block is a single atom, but in most crystals the building block contains several atoms or molecules.

It is usually to choose as a unit cell, a parallelopiped formed by lattice points only at their corners. If unit cell contains only one lattice point, it is called primitive (simple) cell. On the other hand if a unit cell contains more than one lattice point, it is called non-primitive or multiple cell.

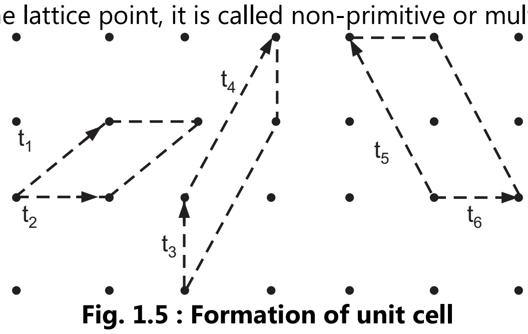


Fig. 1.5 : Formation of unit cell

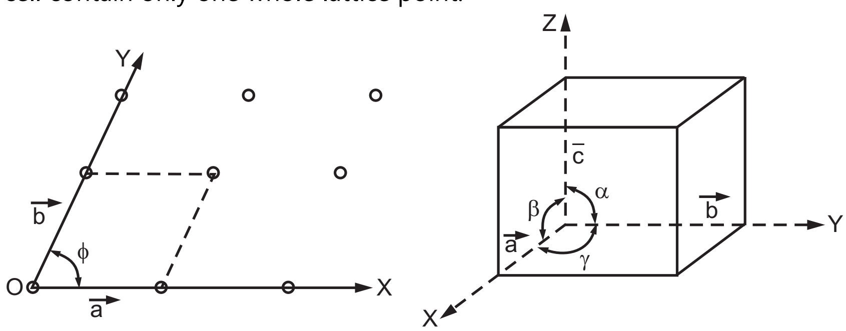
In Fig. 1.5, if pairs of translation such as t_1t_2 or t_3t_4 are chosen, they are said to definite a primitive cell because it contain only one lattice point (or atom). If translation like t_5, t_6 are chosen, the unit cell contain more than one lattice point and it is non-primitive cell.

Number of lattice points per unit cell :

In two dimensional space lattice, each unit cell is considered as a parallelogram which has a representative lattice point at its each corner. Each corner lattice point is common to four similar unit cells and its contribution to a particular cell is $\frac{1}{4}$. Since there are four corners to unit cell, the total number of lattice points per unit cell will be $\frac{1}{4} \times 4 = 1$. Such cell is called the primitive cell.

In three dimensional space, an elementary rectangular parallelopiped (mutually non-coplaner translation) represents a most general unit cell. A rectangular parallelopiped has a lattice point at its corner. Also each corner is common to eight similar unit cells. Therefore its contribution to a particular cell is $\frac{1}{8}$. There are eight corners to the unit cell. Therefore total number of lattice points per unit cell is $\frac{1}{8} \times 8 = 1$.

Thus both in two dimension and three dimension space lattice, each cell contain only one whole lattice point.



(a) Two dimensional space lattice unit cell **(b) Three dimensional space lattice unit cell**

Fig. 1.6 : Lattice parameters

The unit cell is defined by the length of edges and the angles between them are called lattice parameters. In two dimensional space lattice, unit cell [Fig. 1.6 (a)] is represented by the vectors $\vec{a}$ and $\vec{b}$ and angle ϕ between them. In three dimension space lattice, unit cell [Fig. 1.6 (b)] is represented by vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ as length of edges (sides) which are called crystallographic axes and the α, β and γ as the angles between corresponding crystal axes. The volume of unit cell is $V = \left|(\vec{a} \times \vec{b})\cdot \vec{c}\right|$.

1.6 SYMMETRY ELEMENTS OF CUBIC SYSTEM

A symmetry operation (geometrical operation) is a transformation performed on the body (crystal) which leaves it unchanged or invariant i.e. if a body attain its initial configuration even after performing operation on it then the body is said to possess a symmetry corresponding to that operation. In other words, if the environment of crystal (or cubic system) remain unchanged after performing symmetry operation on it then the crystal (cubic system) is said to possess a symmetry corresponding to that operation.

There are four types of symmetry elements for cubic system i.e. there are four principal means for repeating motif in space.

I. Translation :

Translation by an amount T keep the crystal environment invariant.

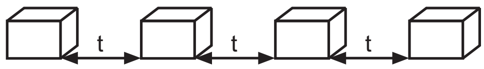


Fig. 1.7

II. Rotational axis of symmetry (n-fold axis of symmetry) :

A crystal is said to possess rotational symmetry about an axis if the rotation of the crystal about this axis by some angle θ leaves the crystal invariant.

A cube is said to possess n fold rotation axis of symmetry if rotation through $\left(\frac{360}{n}\right)$ about an axis brings the cube into self coincidence (congruent position), where the integer n is called the multiplicity of the rotation axis. n can have only the value 1 (single fold axis), 2 (diad axis), 3 (triad axis), 4 (tetrad axis) or 6 (hexad axis) i.e. only five rotation axis in all.

1. If n = 1, the cube must be rotated through 360^o to achieve congruence. Such axis is called identity axis and every crystal possesses an infinite number of such axes.

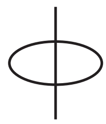


Fig. 1.8

2. If n = 2, the cube must be rotated through 180^o to achieve congruence and the axis is called diad axis (⬬), each passing through the middle point of a pair of opposite parallel edges. Since there are twelve edges in the cube, pair will be six i.e. six axes of two fold symmetry.

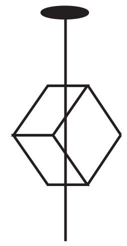


Fig. 1.9

3. If n = 3, the corresponding angle of rotation is 120^o and the axis is called triad axis (▲), about each diagonal of the cube i.e. four axes of three fold symmetry.

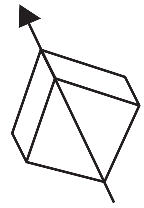


Fig. 1.10

4. If n = 4, the angle of rotation is 90^o and the axis of rotation is called tetrad axis (◆), one normal to each three pairs of parallel faces of cube i.e. three axis of four fold symmetry.

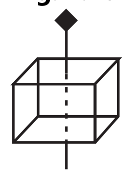


Fig. 1.11

5. If n = 6, the angle of rotation is 60^o and the axis of rotation is called hexad axis (⬣).

Crystals do not show five fold or any other symmetry axis higher than six, because the crystal is not just a solid body, but identical atomic or molecular arrangement is periodic in three dimensions. Crystal has translation periodicity and identical repetition of a unit can take place only when we consider 1, 2, 3, 4 and 6 fold axes. Thus the pentagon lattice is not possible. Pentagon cannot be made to meet at a point, being a constant angle to one another.

Thus cube has 6 diad axes, 4 triad axes and 3 tetrad axes, the total rotational axis of symmetry for cube are 13.

III. Plane of symmetry (m) : Reflection planes or Mirror planes :

A plane can be drawn in the crystal which contains the centre of the crystal. Thus one half of the crystal is the reflection of the other half. Then the crystal is said to have a plane of symmetry. Thus if a crystal is cut along the plane and put it on a mirror, then the image will produce the other half of the crystal. Such a plane is known as plane of symmetry or symmetry plane and is represented by m.

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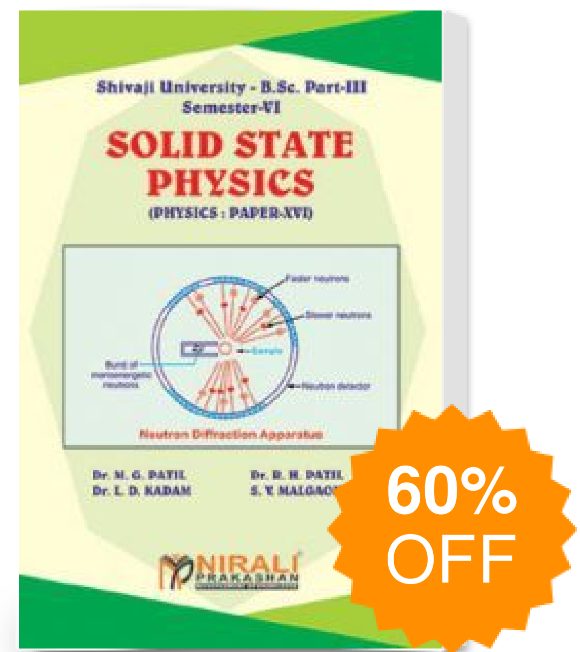

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