Mani Naidu

Engineering Physics

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ALWAYS LEARNING

ENGINEERING PHYSICS Volume 1

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ENGINEERING PHYSICS Volume 1



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Chennai • Delhi

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Appendix A

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Preface

The contents of *Engineering Physics Volume 1* have been designed to cater the needs of B.Tech. students at the freshman level in engineering colleges. The book follows a simple narrative style with emphasis on clarity. The concepts are treated rigorously to help students gain a deep-seated understanding of the key elements intrinsic to the subject. To this end, a list of important formulae, solved problems, multiple-choice questions and review questions have been included at the end of most chapters. These pedagogical elements would prepare the student-reader to face both internal tests and term-end examinations with ease.

Engineering Physics Volume 1 deals with the physics of substances that are of practical utility. It covers topics on crystal physics, properties of matter and thermal physics, quantum physics, acoustics and ultrasonics, photonics and fiber optics.

We hope this book will be beneficial to both students and teachers of physics who handle the subject in engineering colleges. Comments, feedback and suggestions for the improvement of this book are welcome. Any error that may have crept into the book inadvertently may kindly be brought to our notice or to that of the publisher.

S. Mani Naidu

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About the Author

Born in 1957, Dr Sreerama Mani Naidu was awarded a master's degree in Engineering Physics by the S.V.U. College of Engineering, Tirupati, in 1982. Beginning his career as a young Research Assistant at the Regional Engineering College, Trichy, Tamil Nadu, he did extensive research in the field of non-destructive testing of materials, a field that continues to be alluring to the present day. In 1986, he returned as a full-time research scholar to S.V.U. College of Engineering, Tirupati, and earned his Ph.D. for his significant research work on X-ray crystal and molecular structure determination.

An exemplar academician, many of Dr Naidu's research papers have been published in international journals of repute. He is currently an Associate Professor of Physics at Sree Vidyanikethan Engineering College, A. Rangampet, Tirupati. This page is intentionally left blank.

Road Map to the Syllabus

UNIT I CRYSTAL PHYSICS

Lattice – Unit cell – Bravais lattice – Lattice planes – Miller indices – d spacing in cubic lattice – Calculation of number of atoms per unit cell – Atomic radius – Coordination number – Packing factor for SC, BCC, FCC and HCP structures – Diamond and graphite structures (qualitative treatment) – Crystal growth techniques – solution, melt (Bridgman and Czochralski) and vapour growth techniques (qualitative).

Refer Chapter 1

UNIT II PROPERTIES OF MATTER AND THERMAL PHYSICS

Elasticity – Hooke's law – Relationship between three modulii of elasticity (qualitative) – stress-strain diagram – Poisson's ratio – Factors affecting elasticity – Bending moment – Depression of a cantilever – Young's modulus by uniform bending – I-shaped girders.

Modes of heat transfer – thermal conductivity – Newton's law of cooling – Linear heat flow – Lee's disc method – Radial heat flow – Rubber tube method – conduction through compound media (series and parallel).

Refer Chapter 2

UNIT III QUANTUM PHYSICS

Black body radiation – Planck's theory (derivation) – Deduction of Wien's displacement law and Rayleigh – Jeans' Law from Planck's theory – Compton effect. Theory and experimental verification – Properties of Matter waves – G.P Thomson experiment – Schrödinger's wave equation – Time independent and time dependent equations – Physical significance of wave function – Particle in a one dimensional box – Electron microscope – Scanning electron microscope – Transmission electron microscope.

Refer Chapter 3

UNIT IV ACOUSTICS AND ULTRASONICS

Classification of Sound – decibel – Weber-Fechner law – Sabine's formula – derivation using growth and decay method – Absorption Coefficient and its determination – factors affecting acoustics of buildings and their remedies.

XVi Road Map to the Syllabus

Production of ultrasonics by magnetostriction and piezoelectric methods – acoustic grating – Non Destructive Testing – pulse echo system through transmission and reflection modes – A, B and C – scan displays, Medical applications – Sonogram.

Refer Chapter 4

UNIT V PHOTONICS AND FIBRE OPTICS

Spontaneous and stimulated emission – Population inversion – Einstein's A and B coefficients – derivation – Types of lasers – Nd:YAG, CO₂, Semiconductor lasers (homojunction and heterojunction) – Industrial and Medical Applications.

Principle and propagation of light in optical fibres – Numerical aperture and Acceptance angle – Types of optical fibres (material, refractive index, mode) – attenuation, dispersion, bending – Fibre Optical Communication system (Block diagram) – Active and passive fibre sensors – Endoscope.

Refer Chapter 5



CHAPTER

Crystal Physics

1.1 Introduction

Matter exists in three different states; they are gaseous, liquid and solid states. In gaseous and liquid states, the atoms or molecules of the substance move from one place to other, and there is no fixed position of atoms in the substance. In solids, the positions of the atoms or molecules are fixed and may or may not be present periodically at regular intervals of distance. If the atoms or molecules in a solid are periodical at regular intervals of distances in three-dimensional space, then that solid is known as crystalline solid. If the atoms or molecules do not have such a periodicity in a solid, then that solid is known as amorphous solid. When the periodicity of atoms or molecules is extended throughout the solid, then the solid is known as single crystalline solid. If the periodicity of atoms or molecules is extended throughout the solid, then the solid is known as single crystalline solid. If the study of geometric form and other physical properties of crystalline solids by using X-rays, electron beams and neutron beams constitute the science of crystallography.

Distinction between crystalline and amorphous solids

Crystalline Solids	Amorphous Solids		
1. The atoms or molecules of the crystalline solids are periodic in space.	1. The atoms or molecules of the amorphous solids are not periodic in space.		
2. Some crystalline solids are anisotropic i.e., the magnitude of physical properties [such as refractive index, electrical conductivity, thermal conductivity, etc.,] are different along different directions of the crystal.	2. Amorphous solids are isotropic i.e., the magnitude of the physical properties are same along all directions of the solid.		

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3. Crystalline solids have sharp melting points.	3. Amorphous solids do not posses sharp melting points.
 Breaks are observed in the cooling curve of a crystalline solid. 	4. Breaks are not observed in the cooling curve.
 A crystal breaks along certain crystallographic planes. 	5. When an amorphous solid breaks, the broken surface is irregular because it has no crystal planes.

1.2 Space Lattice (or) Crystal Lattice

In a solid crystalline material, the atoms or molecules are arranged regularly and periodically in three dimensions. To explain crystal symmetries easily, it is convenient to represent an atom or a group of atoms that repeats in three dimensions in the crystal as a unit. If each such unit of atoms or atom in a crystal is replaced by a point in space, then the resultant points in space are called space lattice. Each point in space is called a lattice point and each unit of atoms or atom is called basis or pattern. A space lattice represents the geometrical pattern of crystal in which the surroundings of each lattice point is the same.

If the surroundings of each lattice point is same or if the atom or all the atoms at lattice points are identical, then such a lattice is called Bravais lattice. On the other hand, if the atom or the atoms at lattice points are not same, then it is said to be a non-Bravais lattice. Figure 1.1 shows a two-dimensional lattice.

Figure 1.1 Two-dimensional lattice



To represent translational vectors or basis vectors, consider a co-ordinate system with its origin at the lattice point 'O'. Let $\overrightarrow{OA} = 2\vec{a}$ and $\overrightarrow{AB} = \vec{b}$, such that $\overrightarrow{OB} = 2\vec{a} + \vec{b}$. where \vec{a} and \vec{b} are called translational or basis vectors along X and Y directions. The position vector \vec{R} of any lattice point can be represented as $\vec{R} = n_1\vec{a} + n_2\vec{b}$. where n_1 and n_2 are integers, their values depend on the position vector of a point can be expressed as $\vec{R} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$, where \vec{a} , \vec{b} and \vec{c} are the translational or basis vectors along X.

1.3 Unit Cell and Lattice Parameters

Unit cells for most of the crystals are parallelopipeds or cubes having three sets of parallel faces. A unit cell is the basic structural unit or building block of the crystal. A unit cell is defined as the smallest parallelopiped volume in the crystal, which on repetition along the crystallographic axes gives the actual crystal structure or the smallest geometric figure, which on repetition in three-dimensional space, gives the actual crystal structure called a unit cell. The choice of a unit cell is not unique but it can be constructed in a number of ways; Fig. 1.2 shows different ways of representing unit cells in a two-dimensional lattice. A unit cell can be represented as ABCD or A'B'C'D' or A''B''C''D'', etc.

To define the lattice parameters, first we define crystallographic axes. These axes are obtained by the intersection of the three non-coplanar faces of the unit cell. The angle between these faces or crystallographic axes are known as interfacial or interaxial angles. The angles between the axes Y and Z is α , between Z and X is β and between X and Y is γ . The translational vectors or primitives a, b, c of a unit cell along X, Y, Z axes and interaxial angles α , β , γ are called cell parameters. These cell parameters are shown in Fig. 1.3.

The cell parameters determine the actual size and shape of the unit cell. A unit cell can be primitive or non-primitive depending on the number of lattice point/s in it. A primitive unit cell contains only one lattice point. If a unit cell contains more than one lattice point, then it is called non-primitive or multiple cells. For example, BCC and FCC are non-primitive unit cells.

Figure 1.2 Unit cells in crystal lattice



Figure 1.3 Unit cell parameters



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1.4 Crystal Systems and Bravais Lattices

For representing the type of distribution of lattice points in space, seven different co-ordinate systems are required. These co-ordinate systems are called crystal systems. The crystal systems are named on the basis of geometrical shape and symmetry. The seven crystal systems are: (1) Cubic (2) Tetragonal (3) Orthorhombic (4) Monoclinic (5) Triclinic (6) Rhombohedral (or Trigonal) and (7) Hexagonal. Space lattices are classified according to their symmetry. In 1948, Bravais showed that 14 lattices are sufficient to describe all crystals. These 14 lattices are known as Bravais lattices and are classified into 7 crystal systems based on cell parameters. The Bravais lattices are categorized as primitive lattice (P); body-centred lattice (I); face-centred lattice (F) and base-centred lattice (C). These seven crystal systems and Bravais lattices are described below.

1. Cubic crystal system: In this crystal system, all the unit cell edge lengths are equal and are at right angles to one another i.e., a = b = c and $\alpha = \beta = \gamma = 90^{\circ}$. In cubic system, there are three Bravais lattices; they are simple (primitive); body-centred and face-centred. These are shown in Fig. 1.4 Examples for cubic system are Au, Cu, Ag, NaCl, diamond, etc.



In simple cubic lattice, lattice points or atoms are present at the corners of the cube. In bodycentred cube, atoms are present at the corners and one atom is completely present at the centre of the cube. In the case of face-centred cube, atoms are present at corners and at the centres of all faces of cube.

2. Tetragonal crystal system: In this crystal system, two lengths of the unit cell edges are equal whereas the third length is different. The three edges are perpendicular to one another i.e., $a = b \neq c$ and $\alpha = \beta = \gamma = 90^{\circ}$. In tetragonal system, there are two Bravais lattices; they are simple and body-centred. These are shown in Fig. 1.5. Examples for tetragonal crystal systems are TiO₂, SnO₂, etc.

Figure 1.5 Tetragonal crystal system



3. Orthorhombic crystal system: In this crystal system, unit cell edge lengths are different and they are perpendicular to one another i.e., $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90^{\circ}$. There are four Bravais lattices in this system. They are simple, face centred, body centred and base centred. These are shown in Fig. 1.6. Examples for orthorhombic crystal system are BaSO₄, K₂SO₄, SnSO₄, etc.

Figure 1.6 Orthorhombic crystal system



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4. Monoclinic crystal system: In this crystal system, the unit cell edge lengths are different. Two unit cell edges are not perpendicular, but they are perpendicular to the third edge i.e., $a \neq b \neq c$; $\alpha = \gamma = 90^{\circ} \neq \beta$. This crystal system has two Bravais lattices; they are simple and base centred. These are shown in Fig. 1.7. Examples for Monoclinic crystal system are CaSO₄.2H₂O (gypsum), Na₃AlF₆ (cryolite), etc.

Figure 1.7 Monoclinic crystal system



5. Triclinic crystal system: In this crystal system, the unit cell edge lengths are different and are not perpendicular i.e., $a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma \neq 90^{\circ}$ and all the angles are different. This crystal exists in primitive cell only. This is shown in Fig. 1.8. Examples for triclinic crystal system are K₂Cr₂O₇, CuSO₄. 5H₂O, etc.

Figure 1.8 Triclinic crystal system



6. Rhombohedral [Trigonal] crystal system: In this crystal system, all the lengths of unit cell edges are equal. The angles between the axes are equal but other than 90° i.e., a = b = c and $\alpha = \beta = \gamma \neq$ 90°. The Bravais lattice is simple only as shown in Fig. 1.9. Examples for Rhombohedral crystal system are As, Bi, Sb, etc.

Figure 1.9 Rhombohedral crystal system



7. Hexagonal crystal system: In this crystal system, two sides of the unit cell edge lengths are equal and the angle between these edges is 120°. These two edges are perpendicular to the third edge, and not equal in length i.e., $a = b \neq c$ and $\alpha = \beta = 90^{\circ}$; $\gamma = 120^{\circ}$. The Bravais lattice is primitive only. This is shown in Fig. 1.10. The atoms in this crystal system are arranged in the form of a hexagonal close pack.

Figure 1.10 Hexagonal crystal system



The 14 Bravais lattices of 7 crystal systems are shown in the table below.

SI. No	Crystal System	Types of Bravais Lattices	No. of Bravais Lattices	Relation between Lengths and Angles
1	Cubic	P, I, F	3	
2	Tetragonal	P, I	2	$\mathbf{a} = \mathbf{b} \neq \mathbf{c}$ $\alpha = \beta = \gamma = 90^{\circ}$
3	Orthorhombic	P, I, F, C	4	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^{\circ}$
4	Monoclinic	P, C	2	$a \neq b \neq c$ $\alpha = \gamma = 90^{\circ} \neq \beta$
5	Triclinic	Ρ	1	$ \begin{array}{l} \mathbf{a} \neq \mathbf{b} \neq \mathbf{c} \\ \alpha \neq \beta \neq \gamma \end{array} $
6	Rhombohedral (Trigonal)	Р	1	a = b = c $\alpha = \beta = \gamma \neq 90^{\circ}$
7	Hexagonal	Ρ	1	$a = b \neq c$ $\alpha = \beta = 90^{\circ}$ $\gamma = 120^{\circ}$

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1.5 Crystal Planes, Directions and Miller Indices

Crystal planes are defined as some imaginary planes inside a crystal in which large concentration of atoms are present. Inside the crystal, there exists certain directions along which large concentration of atoms exists. These directions are called crystal directions. Figure 1.11 shows a two-dimensional lattice with different orientations of crystal planes.





Crystal planes and directions can be represented by a set of three small integers called Miller indices [because Miller derived a method of representing crystal planes]. These integers are represented in general as h, k and l. If these integers are enclosed in round brackets as (hkl), then it represents a plane. On the other hand, if they are enclosed in square brackets as [hkl], then it represents crystal direction perpendicular to the above-said plane. Next, we will see the way of obtaining Miller indices for a plane.

(i) As shown in Fig. 1.12, take a lattice point as origin '0' of crystallographic axes X, Y and Z in a space lattice. The unit cell translational distances or lattice constants along X, Y and Z directions are *a*, *b* and *c*, respectively. Let a crystal plane ABC intersect these three axes at 2*a*, 3*b* and *c*. In general, the intercepts can be represented as *pa*, *qb*, and *rc*.

Figure 1.12 Miller indices for a plane ABC



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(ii) Divide these intercepts with lattice points translational distances along the axes to obtain intercepts of the plane in terms of multiples of unit cell translational lengths.

i.e.,
$$\frac{2a}{a}, \frac{3b}{b}, \frac{c}{c}$$

2, 3, 1
eneral $\frac{pa}{a}, \frac{qb}{b}, \frac{rc}{c}$

in g

(iii) Take the reciprocals of these multiples, they are $\frac{1}{2}, \frac{1}{3}, \frac{1}{1}$; in general $\frac{1}{p}, \frac{1}{q}, \frac{1}{r}$

- (iv) Clear these fractions [by multiplying with LCM] to smallest integers having the same ratio as the fractions, enclose these integers in brackets.
 - $\frac{1}{2} \times 6, \frac{1}{3} \times 6, \frac{1}{1} \times 6$ 3 2 6

Represent some important crystal planes and directions in a Figure 1.13 cubic crystal







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in general $\frac{pqr}{p}, \frac{pqr}{q}, \frac{pqr}{r}$

Miller indices of the plane ABC is (326). In general, indices of a plane are represented as (hkl) = (qr pr pq)

or $\frac{1}{p}: \frac{1}{q}: \frac{1}{r} = b: k: l$

Miller indices may be defined as a set of three small integers obtained by clearing the reciprocals of the three intercepts [in terms of multiples of unit cell edges] made by a plane on crystallographic axes. Fig 1.13 shows some important crystal planes and direction in a cubic crystal.

Now, we will see the important features of Miller indices:

- (i) Miller indices represent a set of equidistant parallel planes.
- (ii) If the Miller indices of a plane represent some multiples of Miller indices of another plane, then these planes are parallel. For example (844) and (422) or (211) are parallel planes.
- (iii) If (hkl) are the Miller indices of a plane, then the plane divides the lattice constant 'a' along X-axis into h equal parts, 'b' along Y-axis into k equal parts and 'c' along Z-axis into l equal parts.
- (iv) If a plane is parallel to one of the crystallographic axes, then the plane intersects that axis at infinity and the Miller indices along that direction is zero.
- (v) If a plane cuts an axis on the negative side of the origin, then the corresponding index is negative and is indicated by placing a minus sign above the index. For example, if the plane cuts on negative Y-axis, then Miller indices of the plane is (*bkl*).
- (vi) When Miller indices are enclosed in curly brackets, $\{bkl\}$, they refer to planes which in the crystal are equivalent even though their Miller indices may differ. For example in a cubic lattice, all cube faces are equivalent, they are (100), (010), (001), (100), (010), (001); these planes are represented as $\{100\}$. Similarly, a full set of equivalent directions in a crystal is represented by a symbol < bkl >. For example, the eight body diagonals of a cube [111], $[1\overline{1}\overline{1}], [1\overline{1}\overline{1}], [1\overline{1}\overline{1}], [1\overline{1}\overline{1}], [1\overline{1}\overline{1}], [1\overline{1}\overline{1}], [1\overline{1}\overline{1}]$ are designated as <111>.

1.6 Distance of Separation Between Successive hkl Planes

The separation between successive parallel planes in rectangular axes crystal system can be extracted easily. Let us consider a rectangular [cartesian] coordinate system with origin '0' at one of the lattice points. Let (*bkl*) be the Miller indices of a plane ABC, which makes intercepts OA, OB and OC on X, Y and Z axes, respectively as shown Fig 1.14. A normal to this plane from the origin passes through a point N in the plane ABC, such that $ON = d_1$. This normal makes α', β' , and γ' angles with X, Y and Z-axes, respectively. Since the plane segments 'a' into 'b' equal parts, b into k equal parts and c into l equal parts, then the intercepts OA, OB and OC are such that:

Figure 1.14 Orthorhombic crystal



where *a*, *b*, *c* are the unit cell edge lengths along X, Y and Z-axes, respectively. From Fig. 1.14

$$\cos \alpha' = \frac{d_1}{OA}, \ \cos \beta' = \frac{d_1}{OB} \qquad \text{and} \qquad \cos \gamma' = \frac{d_1}{OC}$$
 (1.2)

Let the coordinates of N be x, y and z along X, Y and Z axes, then:

$$(ON)^{2} = d_{1}^{2} = x^{2} + y^{2} + z^{2}$$
(1.3)

Also from Fig. 1.14:

$$\cos \alpha' = \frac{x}{d_1}, \ \cos \beta' = \frac{y}{d_1}, \ \cos \gamma' = \frac{z}{d_1}$$
(1.4)

Substitute Equation (1.4) in (1.3) gives:

$$d_1^2 = d_1^2 \cos^2 \alpha' + d_1^2 \cos^2 \beta' + d_1^2 \cos^2 \gamma'$$

= $d_1^2 [\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma']$

(or)
$$\cos^2 \alpha' + \cos^2 \beta' + \cos^2 \gamma' = 1$$
 (1.5)

Substitute Equation (1.2) in (1.5) gives:

$$\frac{d_1^2}{(OA)^2} + \frac{d_1^2}{(OB)^2} + \frac{d_1^2}{(OC)^2} = 1$$
(1.6)

Again substitute Equation (1.1) in (1.6)

$$\frac{d_1^2 b^2}{a^2} + \frac{d_1^2 k^2}{b^2} + \frac{d_1^2 l^2}{c^2} = 1 \qquad \text{(or)} \qquad d_1^2 \left[\frac{b^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \right] = 1$$

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$$d_1 = \frac{1}{\sqrt{\frac{b^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$
(1.7)

Let $\left(\frac{b}{2} \frac{k}{2} \frac{l}{2}\right)$ be the Miller indices of the next plane A' B' C', this plane makes intercepts OA', OB'

and OC' on X, Y and Z axes, respectively. A normal from the origin to this plane passes through a point N', so that $ON' = d_2$. As the extension of d_1 is d_2 , it makes same angles α' , β' and γ' with X, Y and Z-axes, respectively. Since the plane segments 'a' into h/2 equal parts, b into k/2 equal parts and c into l/2 equal parts, then the intercepts OA', OB' and OC' are such that:

$$OA' = \frac{a}{\binom{b}{2}} = \frac{2a}{b}, OB' = \frac{b}{\binom{b}{2}} = \frac{2b}{k} \quad \text{and} \quad OC' = \frac{c}{\binom{l}{2}} = \frac{2c}{l}$$
(1.1')

From Fig. 1.14,

$$\cos \alpha' = \frac{d_2}{(OA')}, \ \cos \beta' = \frac{d_2}{(OB')} \qquad \text{and} \qquad \cos \gamma' = \frac{d_2}{(OC')}$$
(1.2')

Let the coordinates of N' are x', y' and z' along X, Y and Z-axes, respectively.

$$\left(\mathrm{ON}'\right)^2 = d_2^2 = x'^2 + y'^2 + z'^2 \tag{1.3'}$$

Also from Fig 1.14:

$$\cos \alpha' = \frac{x'}{d_2}, \ \cos \beta' = \frac{y'}{d_2}$$
 and $\cos \gamma' = \frac{z'}{d_2}$ (1.4')

Substitute Equation (1.4') in (1.3') gives:

$$d_{2}^{2} = d_{2}^{2} \cos^{2} \alpha' + d_{2}^{2} \cos^{2} \beta' + d_{2}^{2} \cos^{2} \gamma'$$

= $d_{2}^{2} \left[\cos^{2} \alpha' + \cos^{2} \beta' + \cos^{2} \gamma' \right]$
(or) $\cos^{2} \alpha' + \cos^{2} \beta' + \cos^{2} \gamma' = 1$ (1.5')

Substitute Equation (1.2') in (1.5') gives:

$$\frac{d_2^2}{\left(\text{OA}'\right)^2} + \frac{d_2^2}{\left(\text{OB}'\right)^2} + \frac{d_2^2}{\left(\text{OC}'\right)^2} = 1$$
(1.6')

Again substitute Equation (1.1') in (1.6') gives:

$$\frac{d_{2}^{2}b^{2}}{(2a)^{2}} + \frac{d_{2}^{2}k^{2}}{(2b)^{2}} + \frac{d_{2}^{2}l^{2}}{(2c)^{2}} = 1 \quad \text{(or)} \quad d_{2}^{2} \left[\frac{b^{2}}{(2a)^{2}} + \frac{k^{2}}{(2b)^{2}} + \frac{l^{2}}{(2c)^{2}} \right] = 1$$
(or)
$$d_{2} = \frac{1}{\sqrt{\frac{b^{2}}{(2a)^{2}} + \frac{k^{2}}{(2b)^{2}} + \frac{l^{2}}{(2c)^{2}}}} \quad \text{(or)} \quad d_{2} = \frac{2}{\sqrt{\frac{b^{2}}{a^{2}} + \frac{k^{2}}{b^{2}} + \frac{l^{2}}{c^{2}}}} \quad (1.7')$$

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Let the separation between the planes ABC and A'B'C' is 'd'.

$$\therefore d = d_2 - d_1 = \frac{1}{\sqrt{\frac{b^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}$$
(1.8)

Using Equation (1.8), we can determine the interplanar separation in orthorhombic crystals. For tetragonal crystal $a = b \neq c$, substitute these values in Equation (1.8), we have:

$$d = \frac{1}{\sqrt{\frac{b^2}{a^2} + \frac{k^2}{a^2} + \frac{l^2}{c^2}}} = \frac{1}{\sqrt{\frac{b^2 + k^2}{a^2} + \frac{l^2}{c^2}}}$$
(1.9)

For cubic crystals: a = b = c, substitute these values in Equation (1.8), we have:

$$d = \frac{1}{\sqrt{\frac{b^2}{a^2} + \frac{k^2}{a^2} + \frac{l^2}{a^2}}} \quad \text{(or)} \quad d = \frac{a}{\sqrt{b^2 + k^2 + l^2}} \quad (1.10)$$

The calculation of interplanar spacing for other crystal systems is complicated, so we will not discuss them.

1.7 Structure and Packing Fractions of Simple Cubic [SC] Structure

The unit cell edge lengths of this structure along the crystallographic axes and interaxial angles are equal [i.e., a = b = c and $\alpha = \beta = \gamma = 90^{\circ}$]. Atoms are present only at the corners of this unit cell. A corner atom is shared by eight unit cells, so that the contribution of a corner atom to a unit cell is 1/8. The cube has eight corners, hence the contribution of eight corner atoms to a unit cell or the number of atoms per unit cell $= \frac{1}{8} \times 8 = 1$. Let 'r' be the radius of an atom. The surfaces of the atoms touch along the cube edges. So, the distance between the centres of two neighbouring atoms or the nearest neighbour distance (2r) is equal to the lattice constant 'a'. In simple cubic cell, the number of nearest neighbour atoms to an atom or co-ordination number is six. Since atoms are present at a distance of 'a' along $\pm X$, $\pm Y$ and $\pm Z$ directions. The number of nearest equidistant neighbouring atoms to an atom in the structure is called co-ordination number. Figure 1.15 shows the simple cubic structure. Next, we find the fraction of the unit cell volume occupied by the atoms. The simple cubic structure contains only one atom per unit cell.

The volume occupied by atoms in the unit cell $(v) = 1 \times \frac{4}{3} \pi r^3$ and

The volume of unit cell $(V) = a^3$. Hence, the packing factor or density of packing in the unit cell (PF)

$$= \frac{v}{V} = \frac{\frac{4}{3}\pi r^3}{a^3} = \frac{4}{3}\frac{\pi r^3}{(2r)^3} = \frac{\pi}{6} = 0.52 \text{ or } 52\%$$