UNIT 3 RECIPROCAL LATTICE SPACE

Structure

3.1 Introduction
3.2 Construction of Reciprocal Lattice
3.3 Mathematical Treatment of Reciprocal Lattice
3.4 Reciprocal Lattices of Special Crystal Structures
3.5 The Brillouin Zone
3.6 Summary
3.7 Terminal Questions
3.8 Solutions and Answers

3.1 INTRODUCTION

You are now familiar with the geometrical arrangement of atoms in a crystal. In Unit 2 you must have noted that the geometrical configuration and inter-atomic distances were defined in three-dimensional real space where conventional units of measurement apply. Is there another way to express the same periodic arrangement of atoms in a crystal? The answer to this question is in the affermative; we can also express the same arrangement in what is called **reciprocal space**. The measurements in reciprocal space are in the reciprocal units of length (m^{-1}, m^{-2}, m^{-3}). The arrangement of points in the reciprocal space representing a crystal is called **reciprocal lattice.** This representation comes very handy in interpreting the results of experiments involving *X*-ray diffraction for determination of crystal structure. You will learn the details in Unit 4. Moreover, the concept of reciprocal lattice also simplifies the representation of parallel crystal planes.

In Sec. 3.2 you will learn to construct a reciprocal lattice for a given direct lattice. The mathematical treatment of this construction is discussed in Sec. 3.3. You will learn to build the reciprocal lattices of sc, fcc and bcc crystals in Sec. 3.4. Similar to the Wigner-Seitz primitive unit cell, we use the concept of Brillouin zone to define the primitive unit cell in reciprocal space. It is extremely important in the theoretical analysis of electronic structures of solids characterized by periodic potential. You will learn about the Brillouin zone in Sec. 3.5.

Objectives

After studying this unit, you should be able to:

- represent different crystal planes as vectors in reciprocal space;
- obtain reciprocal lattice for a given direct lattice;
- determine the reciprocal lattices of sc, fcc and bcc crystals; and
- construct the Brillouin zones in reciprocal lattice space.

3.2 CONSTRUCTION OF RECIPROCAL LATTICE

While studying Miller indices in Unit 2, you may have noticed that all the crystal planes parallel to each other are equivalent. This is because infinite translational symmetry in a crystal makes one plane indistinguishable from any other parallel plane. We can represent them by the same set of Miller indices. In the reciprocal lattice, we represent each family of parallel planes by a single point.

Let us now learn to construct a reciprocal lattice. Refer to Fig. 3.1. It shows a single family of infinite, parallel and equidistant planes. Let the interplanar distance be d_{hkl}.

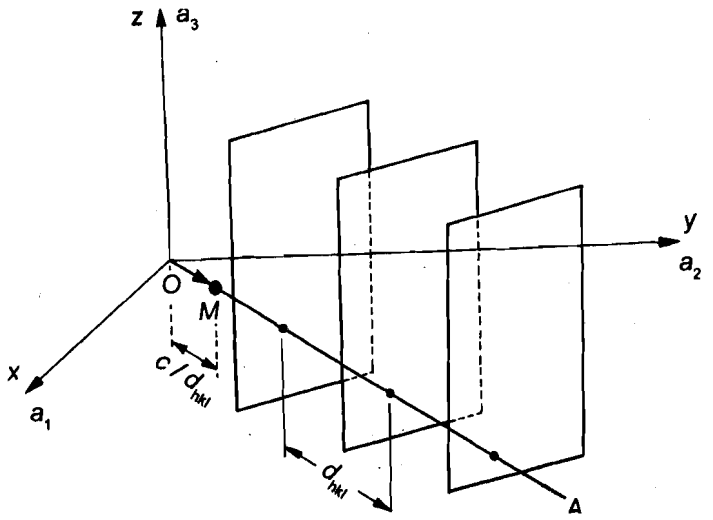

Fig. 3.1: Reciprocal lattice point of a family of parallel equidistant planes

Let us choose origin of coordinate axes at any arbitrary lattice point O, say and draw a common normal OA to these planes from it. Then the point M on this normal which is located at a distance inversely proportional to the interplanar spacing from the origin defines the reciprocal lattice point. It means that

$$OM = \frac{c}{d_{hkl}}, \tag{3.1}$$

where c is a dimensionless constant of proportionality. Note here that the whole family of parallel lattice planes has been represented by a single point (M) and the dimensions of OM are reciprocal of length. The vector joining point O and M is called a **reciprocal lattice vector** (RLV) for these planes.

If we consider the special case of family of planes defined by Miller indices (010) in orthogonal lattice space as shown in Fig.3.2a, the reciprocal lattice point M will be situated at a distance $\frac{c}{d_{010}}$ on y-axis (Fig.3.2b)

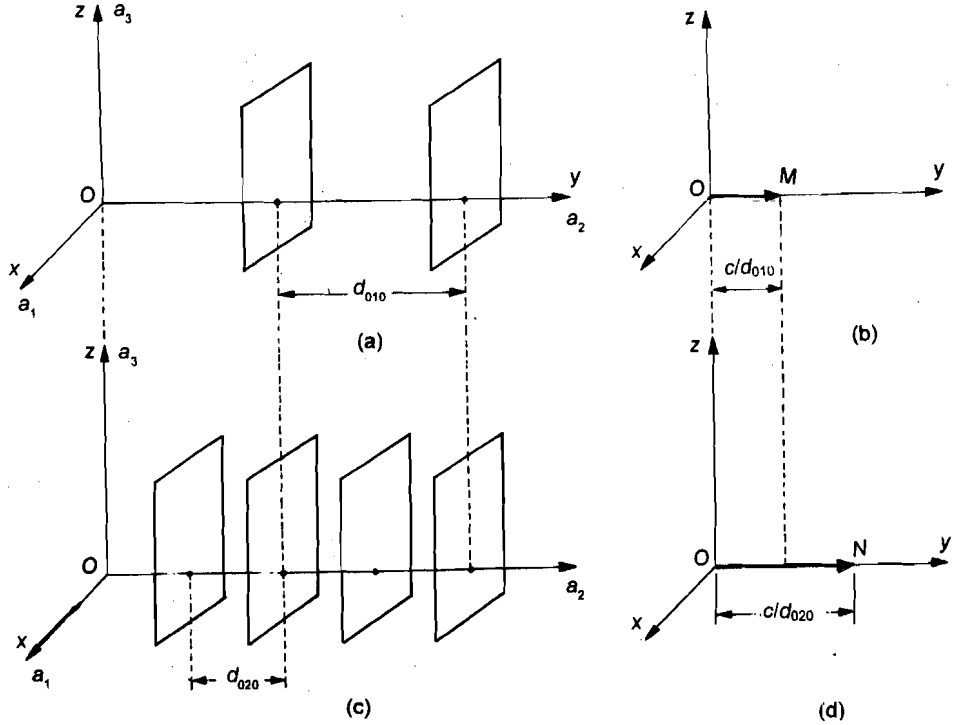

Fig.3.2: a) Family of (010) planes in direct lattice; b) reciprocal lattice point corresponding to (010) planes; c) family of (020) planes in direct lattice; and d) reciprocal lattice point corresponding to (020) planes

Next, if we consider a family of (020) planes as shown in Fig. 3.2c, the interplanar distance will be d_{020}, which is half the interplanar distance of (010) case. In this case, the reciprocal lattice point (N) will be situated on the y-axis but at a distance $\frac{c}{d_{020}}$, which is twice OM (Fig. 3.2d).

In this way, the set of planes (010), (020), (030), ... will result in a linear array of reciprocal lattice points along y-axis. Similarly, if we consider the planes with other Miller indices, it will result in, reciprocal lattice points arranged in three-dimensions giving rise to a 3-D reciprocal lattice (Fig.3.3).

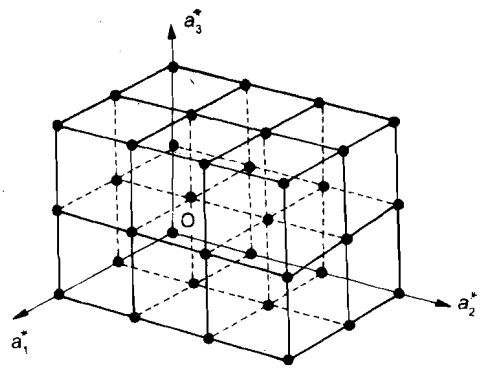

Fig.3.3: Reciprocal lattice in 3-D

Let us now consider one example to construct a reciprocal lattice vector.

Example 1: Construct a reciprocal lattice vector for the plane shown in Fig.3.4.

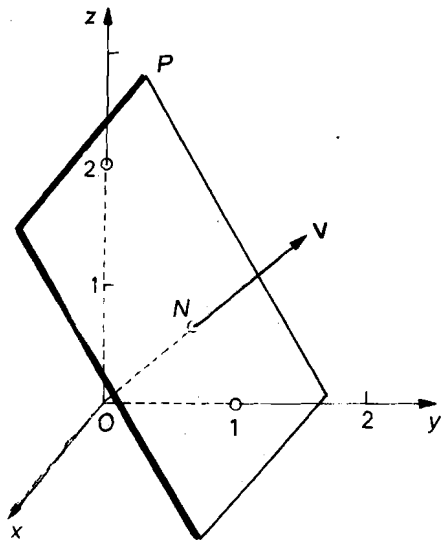

Fig. 3.4: A plane with Miller indices (021)

Plane P intersects x, y and z-axes at ∞, 1 and 2 respectively. Hence its Miller indices are (021).

The direction of reciprocal lattice vector **V** is along the normal drawn from O to plane P. i.e. along ON.

The interplanar distance $ON = d_{021} = \frac{a}{\sqrt{(0)^2 + (2)^2 + (1)^2}} = \frac{a}{\sqrt{5}}$.

Interplanar distance d_{hkl} is given by $\frac{a}{\sqrt{h^2 + k^2 + l^2}}$

The length of reciprocal lattice vector

$$V \propto \frac{1}{d_{021}}\left[i.e.\frac{\sqrt{5}}{a}\right] \text{ (say)} = \frac{c\sqrt{5}}{a}.$$

Hence **V** is in the direction *ON*, normal to plane *P* and its magnitude is $\frac{c\sqrt{5}}{a}$.

From the above example, we may now conclude that *the reciprocal vector is in a direction perpendicular to the plane it represents and its length is proportional to the reciprocal of interplanar distance*. The choice of the proportionality constant *c* is dependent on the application as will be discussed later.

In general, a reciprocal lattice vector is defined as

$$\mathbf{V} = \hat{\mathbf{n}}\frac{c}{d_{hkl}}, \tag{3.2}$$

where $\hat{\mathbf{n}}$ is the unit vector normal to (*hkl*) planes. **V** can also be represented by $\hat{\mathbf{V}}_{\mathbf{hkl}}$.

Let us now discuss the general procedure used to construct a reciprocal lattice. Refer to Fig.3.5. Let $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ be the unit vectors of a crystal in direct lattice space which

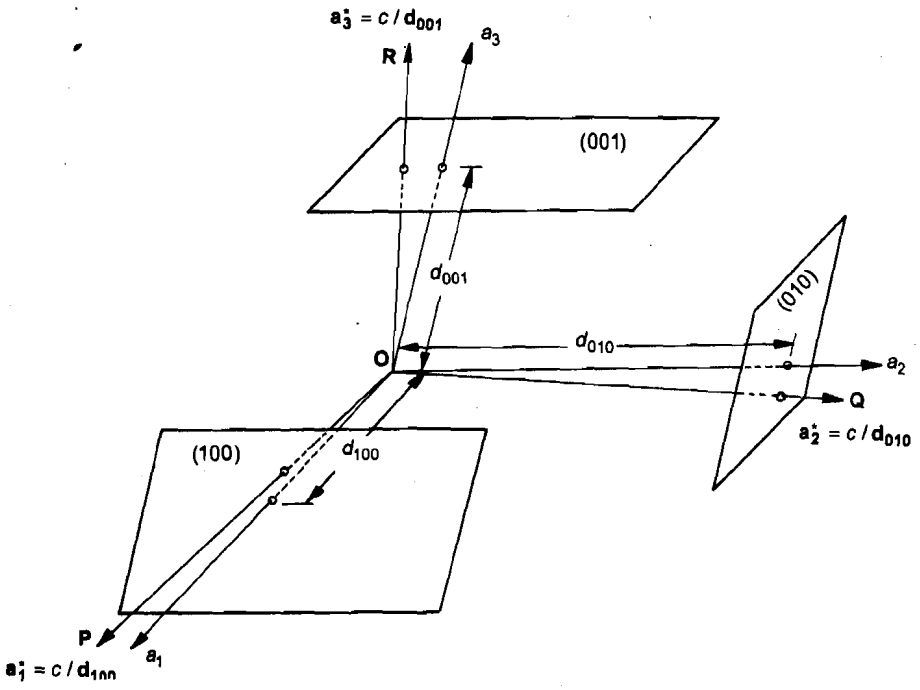

Fig 3.5: Construction of 3-D reciprocal lattice

may or may not be orthogonal. Note that the planes (100), (010) and (001) are parallel to a_2a_3-, a_1a_3- and a_1a_2-planes respectively and intersect a_1, a_2, a_3 axes at respective unit lengths. **OP**, **OQ** and **OR** are the three vectors perpendicular to these three planes. Hence effectively **OP** represents the family of planes (100) and length $OP = \frac{c}{d_{100}}$, where d_{100} denotes interplanar distance for (100) family. Similarly **OQ** and **OR** represent (010) and (001) planes with respective lengths of $\frac{c}{d_{010}}$ and $\frac{c}{d_{001}}$. So the vectors **OP**, **OQ** and **OR** represent the principal axes in the reciprocal lattice

space and are denoted by $\mathbf{a}_1^*, \mathbf{a}_2^*$ and $\mathbf{a}_3^*$ $\left(\text{or } \mathbf{d}_{100}^*, \mathbf{d}_{010}^* \text{ and } \mathbf{d}_{001}^*\right)$, respectively.

For the (200) plane, the reciprocal lattice vector will be $\mathbf{d}_{200}^*$ in the direction of **OP** but with twice the length.

In this way, we can represent every reciprocal lattice vector by a point in reciprocal space with distance between the point and the origin (in reciprocal lattice space) equal to $\frac{c}{d_{hkl}}$ and direction perpendicular to the corresponding planes in direct space. It is given by

$$\mathbf{d}_{hkl}^* = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^* \text{ (if } c = 1). \qquad (3.3)$$

This essentially means that we can reach any reciprocal lattice point through translation along reciprocal lattice axes $\mathbf{a}_1^*, \mathbf{a}_2^*$ and $\mathbf{a}_3^*$ by h, k and l units, respectively. You will note that we have obtained this result from the geometrical considerations only. We would like you to attempt an SAQ now.

SAQ 1

Spend 5 min.

Obtain the principal reciprocal lattice vectors and reciprocal points for (100), (110), (010), (210) families of planes in the 2-D crystal lattice shown in Fig. 3.6.

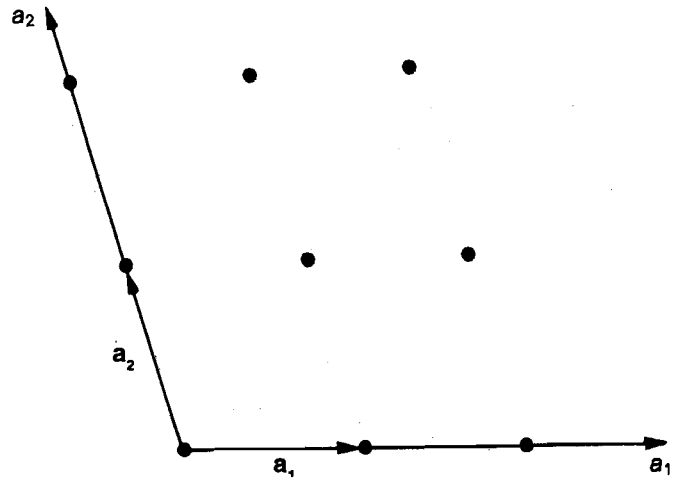

Fig. 3.6: 2-D crystal lattice

Having discussed how to construct reciprocal lattice in 2-D, let us now consider the 3-D case. Fig. 3.7 shows a unit cell characterizing a monoclinic crystal. Here, $a_1 \neq a_2 \neq a_3$ and $\alpha = \beta = 90° \neq \gamma$. Note that $\mathbf{a}_1^*$ is perpendicular to a_2a_3-plane, $\mathbf{a}_2^*$ is perpendicular to a_1a_3-plane and $\mathbf{a}_3^*$ is perpendicular to a_1a_2-plane. This implies that $\mathbf{a}_1$ is perpendicular to both $\mathbf{a}_2^*$ and $\mathbf{a}_3^*$. Similarly, we can say that $\mathbf{a}_2$ is perpendicular to $\mathbf{a}_1^*$ and $\mathbf{a}_3^*$ and $\mathbf{a}_3$, is perpendicular to $\mathbf{a}_1^*$ and $\mathbf{a}_2^*$. That is, there is complete reciprocity between the direct and reciprocal vectors. These conditions are mathematically expressed as:

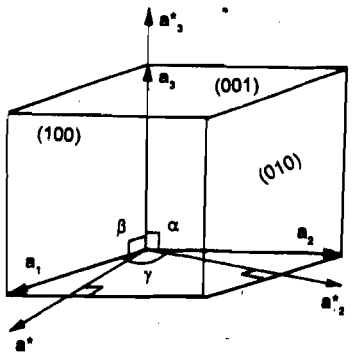

Fig.3.7: Monoclinic lattice with reciprocal lattice vectors

$$\left.\begin{aligned} &\mathbf{a}_1^* \cdot \mathbf{a}_2 = \mathbf{a}_1^* \cdot \mathbf{a}_3 = \mathbf{a}_2^* \cdot \mathbf{a}_1 = \mathbf{a}_2^* \cdot \mathbf{a}_3 = \mathbf{a}_3^* \cdot \mathbf{a}_1 = \mathbf{a}_3^* \cdot \mathbf{a}_2 = 0, \\ &\text{and} \\ &\mathbf{a}_1^* \cdot \mathbf{a}_1 = \mathbf{a}_2^* \cdot \mathbf{a}_2 = \mathbf{a}_3^* \cdot \mathbf{a}_3 = 1. \end{aligned}\right\} \qquad (3.4)$$

You will learn to apply these relations in the following sections.

3.3 MATHEMATICAL TREATMENT OF RECIPROCAL LATTICE

In this section, we shall obtain some more relations between direct and reciprocal lattices. Let us consider a parallelepiped to represent a cell in the direct lattice as

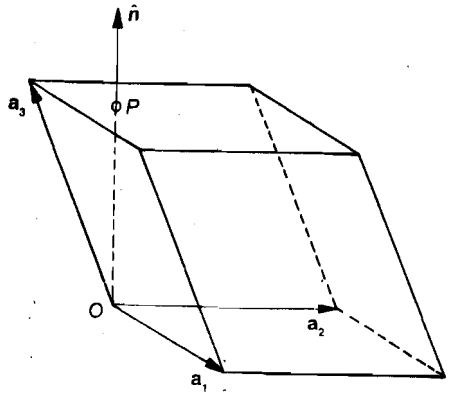

Fig.3.8: Volume of a unit cell

From Unit 1of PHE-04 course you will recall that the area of a parallelogram defined by vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ is equal to their cross product i.e. $\mathbf{a}_1 \times \mathbf{a}_2$ and the volume of parallelepiped defined by vectors $\mathbf{a}_1, \mathbf{a}_2$ and $\mathbf{a}_3$ is equal to their scalar tripe product, i.e. $(\mathbf{a}_1 \times \mathbf{a}_2).\mathbf{a}_3$. This can also be written as $(\mathbf{a}_2 \times \mathbf{a}_3) . \mathbf{a}_1$ and $(\mathbf{a}_3 \times \mathbf{a}_1) . \mathbf{a}_2$.

shown in Fig. 3.8. We know that the volume of the parallelepiped is equal to the product of the area of the base and its height *OP*. By refering to the Fig.3.8, you will note that the height of the cell is equal to the interplanar distance d_{001}. Hence we can write,

$$d_{001} = \frac{\text{Volume of the cell}}{\text{Area of the base of the cell}} = \frac{(\mathbf{a}_1 \times \mathbf{a}_2).\mathbf{a}_3}{\mathbf{a}_1 \times \mathbf{a}_2} \qquad (3.5)$$

and

$$\mathbf{d}^*_{001} = \frac{\hat{\mathbf{n}}}{|\mathbf{d}_{001}|} = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{(\mathbf{a}_1 \times \mathbf{a}_2).\mathbf{a}_3}, \qquad (3.6)$$

where $\hat{\mathbf{n}}$ is the unit vector in the direction of **OP**. Here we have taken $c = 1$. By definition, the reciprocal lattice vector $\mathbf{a}^*_3$ is perpendicular to the a_1a_2-plane and its length is inversely proportional to d_{001}. Hence we can write,

$$\mathbf{a}^*_3 = \mathbf{d}^*_{001} = \frac{\hat{\mathbf{n}}}{|\mathbf{d}_{001}|} = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{(\mathbf{a}_1 \times \mathbf{a}_2).\mathbf{a}_3}. \qquad (3.7)$$

Following the same steps, you can convince yourself that

$$\mathbf{a}^*_1 = \mathbf{d}^*_{100} = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{(\mathbf{a}_2 \times \mathbf{a}_3).\mathbf{a}_1} \qquad (3.8)$$

and

$$\mathbf{a}^*_2 = \mathbf{d}^*_{010} = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{(\mathbf{a}_3 \times \mathbf{a}_1).\mathbf{a}_2}. \qquad (3.9)$$

To ensure that you have understood the concepts discussed above, we would like you to solve the following SAQ.

SAQ 2

Spend 5 min.

An arbitrary plane with Miller indices (*hkl*) is shown in Fig. 3.9. It is denoted in reciprocal lattice space as $\mathbf{d}^*_{hkl} = h\mathbf{a}^*_1 + k\mathbf{a}^*_2 + l\mathbf{a}^*_3$. Prove that $\mathbf{d}^*_{hkl}$ is perpendicular to the family of planes (*hkl*) in the direct lattice space.

Hint: It is enough to prove that reciprocal lattice vector is normal to any two non-linear vectors in (*hkl*) plane.

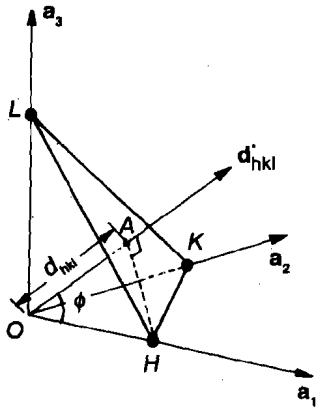

Fig.3.9: Reciprocal lattice vector of (*hkl*) plane

Having proved that the vector $\mathbf{d}^*_{hkl}$ is perpendicular to the plane (*hkl*), let us calculate its magnitude. To accomplish this, we first note that the unit vector along $\mathbf{d}^*_{hkl}$ can be written as

$$\hat{\mathbf{n}} = \frac{h\mathbf{a}^*_1 + k\mathbf{a}^*_2 + l\mathbf{a}^*_3}{\left|\mathbf{d}^*_{hkl}\right|}. \qquad (3.10)$$

In Fig.3.9 the distance OA is the interplanar spacing in real space, d_{hkl}. Since $\mathbf{d}^*_{hkl}$ is normal to the (*hkl*) plane, it is perpendicular to all the vectors within the plane. Hence it is perpendicular to HA. If the angle between OA and OH is ϕ then

$$d_{hkl} = OA = OH\cos\phi. \qquad (3.11)$$

But OH is intercept of the plane (*hkl*) on the a_1-axis. So, by definition of Miller indices, its magnitude is

$$d_{hkl} = \frac{|\mathbf{a}_1|}{h}\cos\phi. \qquad (3.12)$$

Since reciprocal lattice vector $\mathbf{d}^*_{hkl}$ is along OA, with unit vector $\hat{\mathbf{n}}$, d_{hkl} can be expressed as

$$d_{hkl} = \frac{\mathbf{a}_1}{h}.\ \hat{\mathbf{n}}. \qquad (3.13)$$

Substituting for $\hat{\mathbf{n}}$ from Eq. (3.10), we obtain

$$d_{hkl} = \frac{\mathbf{a}_1}{h}.\frac{h\mathbf{a}^*_1 + k\mathbf{a}^*_2 + l\mathbf{a}^*_3}{\left|\mathbf{d}^*_{hkl}\right|}$$

$$= \frac{h\mathbf{a}_1.\mathbf{a}^*_1 + k\mathbf{a}_1.\mathbf{a}^*_2 + l\mathbf{a}_1.\mathbf{a}^*_3}{h\left|\mathbf{d}^*_{hkl}\right|}. \qquad (3.14)$$

From Eq. (3.4), you will recall that $\mathbf{a}_1.\mathbf{a}^*_2 = \mathbf{a}_1.\mathbf{a}^*_3 = 0$. Then Eq. (3.14) simplifies to

$$d_{hkl} = \frac{h(1)}{h\left|\mathbf{d}^*_{hkl}\right|} = \frac{1}{\left|\mathbf{d}^*_{hkl}\right|}, \qquad (3.15)$$

or

$$\left|\mathbf{d}^*_{hkl}\right| = \frac{1}{d_{hkl}}. \qquad (3.16)$$

In words, this result may be interpreted as *the reciprocal lattice vector is perpendicular to the family of planes it represents in real space and its length is reciprocal of the interplanar distance in the real space*. This conclusion is consistent with that obtained on the basis of the geometrical construction.

You must have noted the similarity between the direct and reciprocal lattice vectors: In direct lattice, any lattice point can be reached by a translation $p\mathbf{a}_1 + q\mathbf{a}_2 + r\mathbf{a}_3$. The definition of the reciprocal vector viz. $h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$ makes it trivial that the points in the reciprocal space generate a three-dimensional lattice very similar to that in the real space. Consequently, the points defined in reciprocal lattice possess the same symmetry operations (rotation, reflection, translation and inversion) as in the direct lattice and hence we get triclinic, monoclinic, orthorhombic, triagonal, hexagonal, tetragonal and cubic lattices in the reciprocal space also.

Can you define the reciprocal of a reciprocal lattice? If your answer is direct lattice, you are logical and correct.

It may be noted here that in the above discussion, we have considered the constant of proportionality c as unity. However, in general it can take different values depending on given physical situation/system. In solid state theory, value of c is taken as 2π. (This is chosen to have conformity with the solution of Schrödinger equation for periodic potential in solids.)

3.4 RECIPROCAL LATTICES OF SPECIAL CRYSTAL STRUCTURES

Let us now use the concepts developed above to obtain the reciprocal lattices of some special crystal structures. For simplicity, we first consider a simple cubic structure.

Simple Cubic Structure

From Sec. 2.4 of the preceding unit, you would recall that the primitive lattice vectors of simple cubic structure in real space are characterized by

$$a_1 = a_2 = a_3 = a \text{ and } \alpha = \beta = \gamma = 90°$$

As the basis vectors are perpendicular to each other, from Eq (2.4) you will recall that

$$\mathbf{a}_1 = a\hat{\mathbf{i}}$$
$$\mathbf{a}_2 = a\hat{\mathbf{j}}$$
$$\mathbf{a}_3 = a\hat{\mathbf{k}}.$$

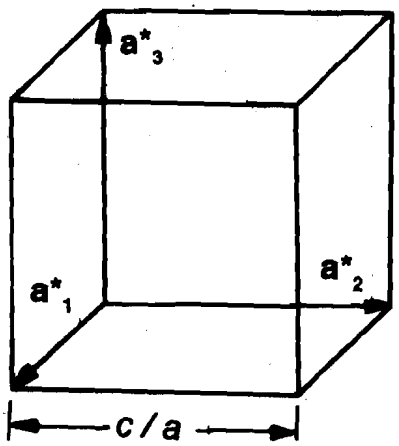

Fig. 3.10: Reciprocal lattice of simple cube

Using these relations in Eq. (3.8), we find that the reciprocal lattice vectors of basis are

$$\mathbf{a}_1^* = c\frac{\mathbf{a}_2 \times \mathbf{a}_3}{(\mathbf{a}_2 \times \mathbf{a}_3).\mathbf{a}_1} = c\frac{a\hat{\mathbf{j}} \times a\hat{\mathbf{k}}}{(a\hat{\mathbf{j}} \times a\hat{\mathbf{k}}).a\hat{\mathbf{i}}} = c\frac{a^2\hat{\mathbf{i}}}{a^3(\hat{\mathbf{i}}.\hat{\mathbf{i}})} = c\frac{\hat{\mathbf{i}}}{a}. \qquad (3.17)$$

Similarly from Eqs. (3.9) and (3.7), you will find that

$$\mathbf{a}_2^* = c\frac{\hat{\mathbf{j}}}{a} \qquad (3.18)$$

and

$$\mathbf{a}_3^* = c\frac{\hat{\mathbf{k}}}{a}. \qquad (3.19)$$

What conclusions can be drawn from these results? All three reciprocal lattice vectors are of equal length c/a and are mutually perpendicular. This is shown in Fig. 3.10.

Having obtained the reciprocal lattice vectors for sc system, let us now consider an fcc structure.

Face-Centred Cubic Structure

For an fcc crystal shown in Fig.3.11, primitive lattice vectors are defined by Eq. (2.11):

$$\mathbf{a}_1 = \frac{a}{2}\left(\hat{\mathbf{j}} + \hat{\mathbf{k}}\right),$$

$$\mathbf{a}_2 = \frac{a}{2}\left(\hat{\mathbf{k}} + \hat{\mathbf{i}}\right)$$

and

$$\mathbf{a}_3 = \frac{a}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}}\right).$$

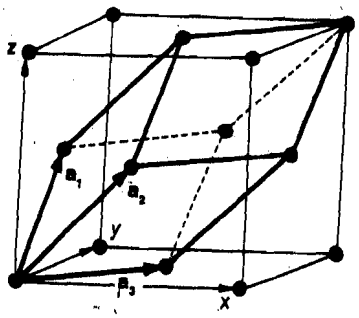

Fig.3.11: Primitive cell in fcc lattice

To determine the reciprocal lattice vectors for an fcc lattice structure, we first calculate the volume of the primitive unit cell in direct space defined by these vectors:

$$\text{Volume of cell, } V_f = \left(\mathbf{a}_1 \times \mathbf{a}_2\right).\mathbf{a}_3 \tag{3.20}$$

$$= \left\{\left[\frac{a}{2}\left(\hat{\mathbf{j}} + \hat{\mathbf{k}}\right)\right] \times \left[\frac{a}{2}\left(\hat{\mathbf{k}} + \hat{\mathbf{i}}\right)\right]\right\}.\left[\frac{a}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)\right] \tag{3.21}$$

$$= \frac{a^3}{8}\left[\hat{\mathbf{j}} \times \hat{\mathbf{k}} + \hat{\mathbf{j}} \times \hat{\mathbf{i}} + \hat{\mathbf{k}} \times \hat{\mathbf{k}} + \hat{\mathbf{k}} \times \hat{\mathbf{i}}\right].\left[\hat{\mathbf{i}} + \hat{\mathbf{j}}\right]$$

$$= \frac{a^3}{8}\left[\mathbf{i} - \hat{\mathbf{k}} + \mathbf{0} + \mathbf{j}\right].\left[\hat{\mathbf{i}} + \hat{\mathbf{j}}\right]$$

$$= \frac{a^3}{8}(1+1)$$

$$= \frac{a^3}{4}. \tag{3.22}$$

The reciprocal lattice vector

$$\mathbf{a}_1^* = c\frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_f} = c\frac{\left[\frac{a}{2}\left(\hat{\mathbf{k}} + \hat{\mathbf{i}}\right)\right] \times \left[\frac{a}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)\right]}{\frac{a^3}{4}} \tag{3.23}$$

$$= \frac{c}{a}\left(\hat{\mathbf{k}} \times \hat{\mathbf{i}} + \hat{\mathbf{k}} \times \hat{\mathbf{j}} + \hat{\mathbf{i}} \times \hat{\mathbf{i}} + \hat{\mathbf{i}} \times \hat{\mathbf{j}}\right)$$

$$= \frac{c}{a}\left(\hat{\mathbf{j}} - \hat{\mathbf{i}} + 0 + \hat{\mathbf{k}}\right)$$

$$= \frac{c}{a}\left(-\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right). \tag{3.24}$$

Similarly, it can be shown that

$$\mathbf{a}_2^* = \frac{c}{a}\left(\hat{\mathbf{i}} - \hat{\mathbf{j}} + \hat{\mathbf{k}}\right) \tag{3.25}$$

and

$$\mathbf{a}_3^* = \frac{c}{a}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right). \tag{3.26}$$

If value of c is set equal to 2, Eqs. (3.24)-(3.26) are just the primitive lattice vectors of a bcc lattice defined by Eq. (2.10). Hence the reciprocal lattice of a face-centred cubic lattice is a body-centred cubic structure.

We can extend this argument to the other crystal systems as well. Since direct and reciprocal lattices exhibit the same symmetry operations, they belong to the same crystal system, i.e. reciprocal lattices for monoclinic, triclinic... and cubic lattice are also monoclinic, triclinic, ... cubic, respectively. However the two lattices may have different Bravais structures within the same crystal system.

Now you should answer the following SAQ.

Spend 5 min.

SAQ 3

Prove that the reciprocal lattice of bcc is an fcc structure.

3.5 THE BRILLOUIN ZONE

In Unit 2 you have learnt that the primitive unit cell in the direct crystal lattice has the smallest volume. Now you may ask: What is the primitive cell in reciprocal lattice? The answer to this question is: It is the Wigner-Seitz cell in the reciprocal lattice and is called the **first Brillouin zone** (FBZ). It is of very special importance in understanding the electronic structure using band theory of solids. You will learn about it in Unit 10, Block-3 of this course. The first Brillouin zone has the smallest volume. It is obtained by planes that are perpendicular bisectors of the reciprocal lattice vectors.

In the following, this is illustrated for a simple case of 2-D rectangular reciprocal lattice (Fig.3.12). Point O is chosen as the origin. To construct the first Brillouin zone we follow the following steps:

- Join the nearest neighbouring reciprocal lattice points with origin $\left(\mathbf{a}_1^*, \mathbf{a}_2^*, -\mathbf{a}_1^* \text{ and } -\mathbf{a}_2^*\right)$.
- Draw perpendicular bisectors PQ, QR, RS and SP of $\mathbf{a}_2^*, \mathbf{a}_1^*, -\mathbf{a}_2^*$ and $-\mathbf{a}_1^*$ respectively.
- The area enclosed by these bisectors viz. $PQRS$ is the first Brillouin zone for the given rectangular reciprocal lattice in 2-D.

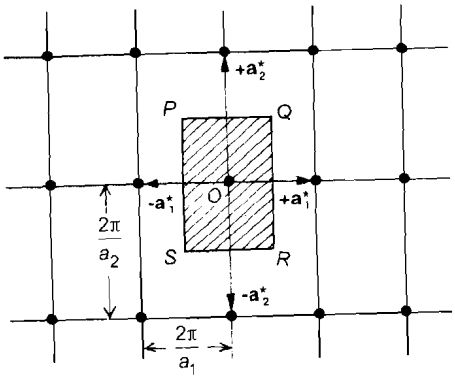

Fig.3.12: The FBZ of a rectangular reciprocal lattice

Before you proceed further, we would like you to draw first Brillouin zones for some other geometries.

SAQ 4

Spend 10 min.

Draw the first Brillouin zone for

(a) 2-D oblique reciprocal lattice
(b) 3-D simple cubic reciprocal lattice.

While solving this SAQ, you must have noted that the first Brillouin zone for a 2-D oblique lattice has hexagonal shape, whereas for 3-D sc lattice, the first Brillouin zone is also a cube with sides $\frac{2\pi}{a}$.

For a 3-D cubic reciprocal lattice, the reciprocal lattice vectors as given by Eqs. (3.17) – (3.19) with c equated to 2π are $\mathbf{a}_1^* = \frac{2\pi}{a}\hat{\mathbf{i}}$, $\mathbf{a}_2^* = \frac{2\pi}{a}\hat{\mathbf{j}}$ and $\mathbf{a}_3^* = \frac{2\pi}{a}\hat{\mathbf{k}}$. The boundaries of the first Brillouin zone are therefore the planes normal to the 6 reciprocal lattice vectors $\pm\mathbf{a}_1^*, \pm\mathbf{a}_2^*$ and $\pm\mathbf{a}_3^*$ at their mid-points;

$$\pm\frac{2\pi}{2a}\mathbf{a}_1^* = \pm\frac{\pi}{a}\hat{\mathbf{i}},$$

$$\pm\frac{2\pi}{2a}\mathbf{a}_2^* = \pm\frac{\pi}{a}\hat{\mathbf{j}},$$

and

$$\pm\frac{2\pi}{2a}\mathbf{a}_3^* = \pm\frac{\pi}{a}\hat{\mathbf{k}}. \qquad (3.27)$$

These 6 planes enclose a cube with edges $2\pi/a$.

You can construct the first Brillouin zone of a bcc lattice following the steps listed above. The reciprocal lattice vectors in this case are:

$$\mathbf{a}_1^* = \frac{2\pi}{a}\left(\hat{\mathbf{j}} + \hat{\mathbf{k}}\right),$$

$$\mathbf{a}_2^* = \frac{2\pi}{a}\left(\hat{\mathbf{k}} + \hat{\mathbf{i}}\right),$$

and

$$\mathbf{a}_3^* = \frac{2\pi}{a}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}}\right). \tag{3.28}$$

The reciprocal vector $\mathbf{V} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$

$$= \frac{2\pi}{a}\left[(k+l)\hat{\mathbf{i}} + (h+l)\hat{\mathbf{j}} + (h+k)\hat{\mathbf{k}}\right]. \tag{3.29}$$

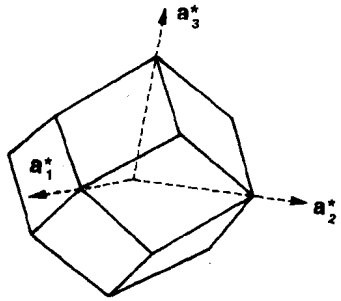

Fig.3.13: FBZ of a bcc lattice

The shortest 12 non-zero reciprocal vectors are $\frac{2\pi}{a}\left(\pm\hat{\mathbf{i}} \pm \hat{\mathbf{j}}\right)$; $\frac{2\pi}{a}\left(\pm\hat{\mathbf{j}} \pm \hat{\mathbf{k}}\right)$ and $\frac{2\pi}{a}\left(\pm\hat{\mathbf{i}} \pm \hat{\mathbf{k}}\right)$. The region enclosed by the perpendicular bisector planes of these 12 vectors is the first Brillouin zone which has the shape of a 12–faced solid called rhombic dodecahedron (Fig. 3.13).

After learning about the construction of Brillouin zone, you may like to solve the following SAQ.

Spend 5 min.

SAQ 5

Determine the first Brillouin zone for fcc lattice.

Let us now summarize the highlights of this unit.

3.6 SUMMARY

- With every crystal structure two types of lattices can be associated: a **direct crystal lattice** in real space and a **reciprocal lattice** in reciprocal space.
- **The reciprocal and direct lattice vectors are related as**:

$$\mathbf{a}_1^* = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{(\mathbf{a}_2 \times \mathbf{a}_3).\mathbf{a}_1},\ \mathbf{a}_2^* = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{(\mathbf{a}_3 \times \mathbf{a}_1).\mathbf{a}_2} \text{ and } \mathbf{a}_3^* = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{(\mathbf{a}_1 \times \mathbf{a}_2).\mathbf{a}_3}$$

  where $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are the primitive vectors of the direct lattice and $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ are the reciprocal lattice vectors.

- The reciprocal lattice of sc lattice is also a sc structure.
- The reciprocal lattice of fcc is bcc and vice versa.
- The first Brillioun zone is the primitive cell of reciprocal lattice. It can be constructed similar to the Wigner-Seitz cell in the direct lattice.

3.7 TERMINAL QUESTIONS

Spend 25 min.

1. The primitive translation vectors of a lattice are

$$\mathbf{a}_1 = 2\hat{\mathbf{i}} + \hat{\mathbf{j}},\ \mathbf{a}_2 = 2\hat{\mathbf{j}} \text{ and } \mathbf{a}_3 = \hat{\mathbf{k}}.$$

   Determine the primitive translation vectors in reciprocal lattice.

2. The primitive translation vectors of a hexagonal direct lattice are

$$\mathbf{a}_1 = \frac{a}{2}\hat{\mathbf{i}} + \frac{1}{16}a\hat{\mathbf{j}},\ \mathbf{a}_2 = -\frac{a}{2}\hat{\mathbf{i}} + \frac{1}{16}a\hat{\mathbf{j}} \text{ and } \mathbf{a}_3 = c\hat{\mathbf{k}}.$$

Calculate i) the volume of the primitive cell and ii) the primitive translation vectors of a reciprocal lattice.

3. The bcc structure has lattice constant of 3.5Å. Determine the boundaries of the first Brillouin zone.

4. Prove that volume of a unit cell in a reciprocal lattice is inversely proportional to that of direct lattice by taking example of simple cubic lattice.

3.8 SOLUTIONS AND ANSWERS

Self-Assessment Questions

1. The principal reciprocal lattice vectors $\mathbf{a}_1^*$, $\mathbf{a}_2^*$ and the reciprocal lattice points for (100), (110), (010) and (210) planes are indicated in Fig.3.14

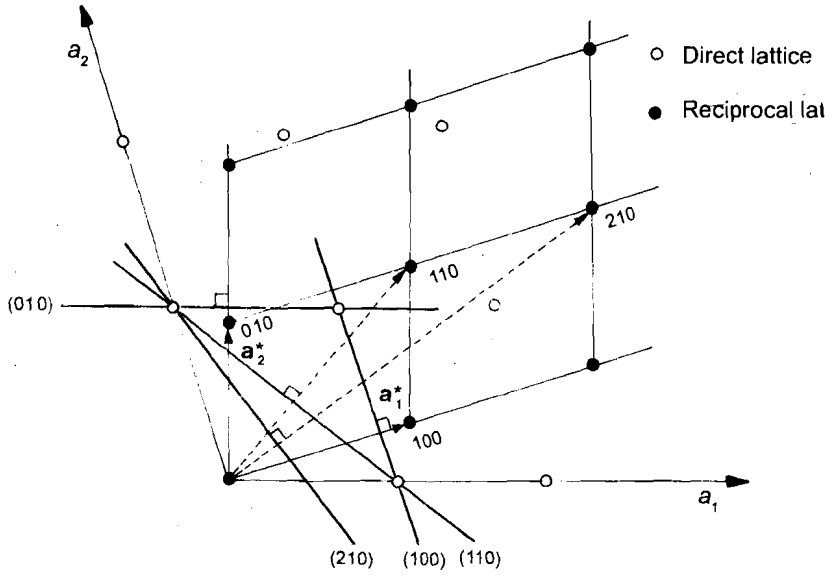

Fig.3.14: Representation of crystal planes in reciprocal space

2. As shown in Fig. 3.15, the plane with Miller indices (*hkl*) cuts the crystal axes a_1, a_2, and a_3 at $\frac{|\mathbf{a}_1|}{h}, \frac{|\mathbf{a}_2|}{k}$ and $\frac{|\mathbf{a}_3|}{l}$ respectively. To prove that $\mathbf{d}_{hkl}^*$ is perpendicular to this plane, we take its dot product with two non-linear vectors in the plane and see if the result is zero. Vectors **HK** and **KL** lie in plane (*hkl*).

Since

$$\mathbf{HK} = \frac{\mathbf{a}_1}{h} - \frac{\mathbf{a}_2}{k},$$

$$\mathbf{d}_{hkl}^* \cdot \mathbf{HK} = \left(h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*\right)\cdot\left(\frac{\mathbf{a}_1}{h} - \frac{\mathbf{a}_2}{k}\right)$$

$$= \mathbf{a}_1^* \cdot \mathbf{a}_1 - \mathbf{a}_2^* \cdot \mathbf{a}_2$$

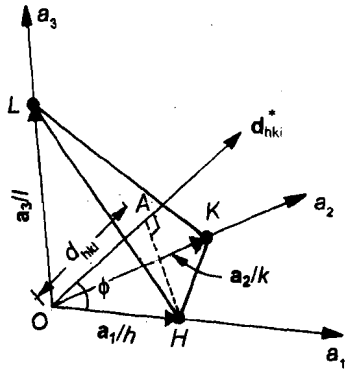

Fig.3.15: RLV of (*hkl*) planes

It can be easily shown using Eq. (3.4) that both these dot products are equal to 1. Hence $\mathbf{d}_{hkl}^* \cdot \mathbf{HK} = 0$.

Similarly ,

$$\mathbf{KL} = \frac{\mathbf{a}_2}{k} - \frac{\mathbf{a}_3}{l}$$

and

$$\mathbf{d}^*_{\mathbf{hkl}} \cdot \mathbf{KL} = \left(h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*\right).\left(\frac{\mathbf{a}_2}{k} - \frac{\mathbf{a}_3}{l}\right)$$

$$= 0$$

As vector $\mathbf{d}^*_{\mathbf{hkl}}$ is perpendicular to two non-linear vectors in a plane, it is perpendicular to the entire plane containing these vectors. Hence $\mathbf{d}^*_{\mathbf{hkl}}$ is perpendicular to the family of planes represent by (*hkl*) indices.

3. The basis vectors of bcc lattice are defined in Eq. (2.10) as

$$\mathbf{a}_1 = \frac{a}{2}\left(-\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right),$$

$$\mathbf{a}_2 = \frac{a}{2}\left(\hat{\mathbf{i}} - \hat{\mathbf{j}} + \hat{\mathbf{k}}\right),$$

and

$$\mathbf{a}_3 = \frac{a}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right).$$

Hence the volume of primitive cell

$$V_b = \left(\mathbf{a}_1 \times \mathbf{a}_2\right).\mathbf{a}_3$$

$$= \left\{\left[\frac{a}{2}\left(-\hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{k}}\right)\right] \times \left[\frac{a}{2}\left(\hat{\mathbf{i}} - \hat{\mathbf{j}} + \hat{\mathbf{k}}\right)\right]\right\}.\left[\frac{a}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right)\right]$$

$$= \frac{a^3}{8}\left[-\hat{\mathbf{i}}\times\hat{\mathbf{i}} + \hat{\mathbf{i}}\times\hat{\mathbf{j}} - \hat{\mathbf{i}}\times\hat{\mathbf{k}} + \hat{\mathbf{j}}\times\hat{\mathbf{i}} - \hat{\mathbf{j}}\times\hat{\mathbf{j}} + \hat{\mathbf{j}}\times\hat{\mathbf{k}} + \hat{\mathbf{k}}\times\hat{\mathbf{i}} - \hat{\mathbf{k}}\times\hat{\mathbf{j}} + \hat{\mathbf{k}}\times\hat{\mathbf{k}}\right].\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right.$$

$$= \frac{a^3}{8}\left[0 + \hat{\mathbf{k}} + \hat{\mathbf{j}} - \hat{\mathbf{k}} + 0 + \hat{\mathbf{i}} + \hat{\mathbf{j}} + \hat{\mathbf{i}} + 0\right].\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right)$$

$$= \frac{a^3}{8}\left[2\hat{\mathbf{i}} + 2\hat{\mathbf{j}}\right].\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right)$$

$$= \frac{a^3}{2}.$$

The reciprocal lattice vectors are given by

$$\mathbf{a}_1^* = c\frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_b}$$

$$= c\frac{\left[\frac{a}{2}\left(\hat{\mathbf{i}} - \hat{\mathbf{j}} + \hat{\mathbf{k}}\right)\right] \times \left[\frac{a}{2}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}} - \hat{\mathbf{k}}\right)\right]}{\frac{a^3}{2}}$$

$$V_b = \frac{c}{2a}\left[\hat{\mathbf{i}}\times\hat{\mathbf{i}}+\hat{\mathbf{i}}\times\hat{\mathbf{j}}-\hat{\mathbf{i}}\times\hat{\mathbf{k}}-\hat{\mathbf{j}}\times\hat{\mathbf{i}}-\hat{\mathbf{j}}\times\hat{\mathbf{j}}+\hat{\mathbf{j}}\times\hat{\mathbf{k}}+\hat{\mathbf{k}}\times\hat{\mathbf{i}}+\hat{\mathbf{k}}\times\hat{\mathbf{j}}-\hat{\mathbf{k}}\times\hat{\mathbf{k}}\right]$$

$$= \frac{c}{2a}\left[0+\hat{\mathbf{k}}+\hat{\mathbf{j}}+\hat{\mathbf{k}}+0+\hat{\mathbf{i}}+\hat{\mathbf{j}}-\hat{\mathbf{i}}+0\right]$$

$$= \frac{c}{2a}\left[2\hat{\mathbf{j}}+2\hat{\mathbf{k}}\right]$$

$$= \frac{c}{a}\left(\hat{\mathbf{j}}+\hat{\mathbf{k}}\right)$$

Similarly

$$\mathbf{a}_2^* = \frac{c}{a}\left(\hat{\mathbf{i}}+\hat{\mathbf{k}}\right),$$

$$\mathbf{a}_3^* = \frac{c}{a}\left(\hat{\mathbf{i}}+\hat{\mathbf{j}}\right).$$

With $c = 2$, these reciprocal vector depict the primitive basis vectors in fcc lattice.

4. The first Brillouin zone of (a) 2-D oblique reciprocal lattice is shown in Fig.3.16a. (b) 3-D simple cubic reciprocal lattice in shown in Fig.3.16b.

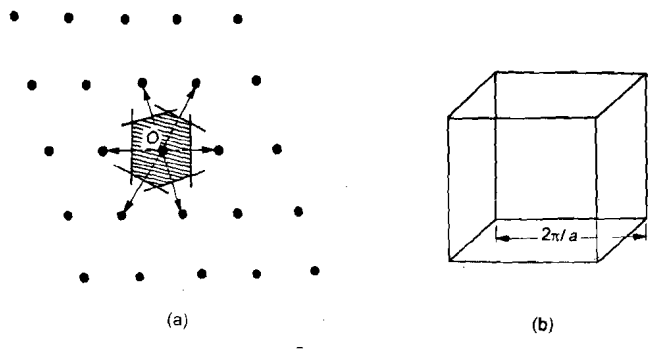

Fig.3.16: a) FBZ of 2-D oblique reciprocal lattice; and b) FBZ of 3-D sc reciprocal lattice

5. The first Brillouin zone of an fcc lattice may be found with its reciprocal lattice vectors defined by Eq. (3.24)-(3.26) such that the reciprocal lattice vector becomes

$$\mathbf{G} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*.$$

with $c = 2\pi$, we get

$$\mathbf{G} = \frac{2\pi}{a}\left[(-h+k+l)\hat{\mathbf{i}} + (h-k+l)\hat{\mathbf{j}} + (h+k-l)\hat{\mathbf{k}}\right].$$

The shortest 8 non-zero reciprocal lattice vectors G are : $\frac{2\pi}{a}(\pm\mathbf{i}\pm\mathbf{j}\pm\mathbf{k})$. The boundaries of the first Brillouin zone are determined by the perpendicular bisector planes to the above 8 vectors. However, the corners of the octahedron obtained in this manner are truncated by the planes which are normal bisectors to the next neighbouring 6 reciprocal lattice vectors.

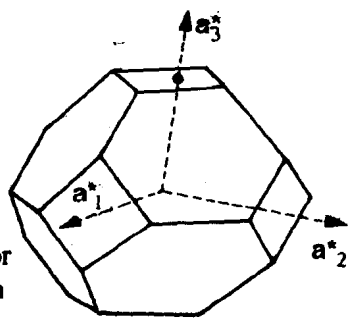

Fig.3.17: FBZ of a fcc reciprocal lattice

The first Brillouin zone has the shape of the truncated octahedron as shown in Fig.3.17.

Terminal Questions

1. The volume of reciprocal unit cell is given by

$$V_{uc} = (\mathbf{a}_1 \times \mathbf{a}_2).\mathbf{a}_3$$

$$= \left[(2\hat{\mathbf{i}} + \hat{\mathbf{j}}) \times (2\hat{\mathbf{j}})\right].\hat{\mathbf{k}}$$

$$= [4\hat{\mathbf{k}} - 0].\hat{\mathbf{k}}$$

$$= 4.$$

The reciprocal lattice vectors are

$$\mathbf{a}_1^* = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{4} = \frac{2\hat{\mathbf{j}} \times \hat{\mathbf{k}}}{4} = \frac{2\hat{\mathbf{i}}}{4} = \frac{\hat{\mathbf{i}}}{2},$$

$$\mathbf{a}_2^* = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{4} = \frac{\hat{\mathbf{k}} \times (2\hat{\mathbf{i}} + \hat{\mathbf{j}})}{4} = \frac{2\hat{\mathbf{j}} - \hat{\mathbf{i}}}{4},$$

and

$$\mathbf{a}_3^* = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{4} = \frac{(2\hat{\mathbf{i}} + \hat{\mathbf{j}}) \times 2\hat{\mathbf{j}}}{4} = \frac{4\hat{\mathbf{k}}}{4} = \hat{\mathbf{k}}.$$

2. (i) Volume of primitive cell

$$V_h = (\mathbf{a}_1 \times \mathbf{a}_2).\mathbf{a}_3$$

$$= \left[\left(\frac{a}{2}\hat{\mathbf{i}} + \frac{a}{16}\hat{\mathbf{j}}\right) \times \left(-\frac{a}{2}\hat{\mathbf{i}} + \frac{a}{16}\hat{\mathbf{j}}\right)\right].\left(c\hat{\mathbf{k}}\right)$$

$$= \begin{vmatrix} \frac{a}{2} & \frac{a}{16} & 0 \\ -\frac{a}{2} & \frac{a}{16} & 0 \\ 0 & 0 & c \end{vmatrix}$$

$$= \frac{a}{2}\left(\frac{ac}{16}\right) + \frac{a}{16}\left(\frac{ac}{2}\right) = \frac{a^2c}{16}.$$

(ii) The primitive reciprocal lattice vectors are

$$\mathbf{a}_1^* = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_h} = \frac{\left(-\frac{a}{2}\hat{\mathbf{i}} + \frac{a}{16}\hat{\mathbf{j}}\right) \times \left(c\hat{\mathbf{k}}\right)}{V_h}$$

$$= \frac{\frac{ac}{2}\hat{\mathbf{j}} + \frac{ac}{16}\hat{\mathbf{i}}}{V_h} = \frac{16}{a^2c}\left[\frac{ac}{16}\hat{\mathbf{i}} + \frac{ac}{2}\hat{\mathbf{j}}\right]$$

$$= \frac{\hat{\mathbf{i}}}{a} + \frac{8}{a}\hat{\mathbf{j}}.$$

$$\mathbf{a}_2^* = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{V_h} = \frac{\left(c\hat{\mathbf{k}}\right) \times \left(\frac{a}{2}\hat{\mathbf{i}} + \frac{a}{16}\hat{\mathbf{j}}\right)}{V_h}$$

$$= \frac{\frac{ac}{2}\hat{\mathbf{j}} - \frac{ac}{16}\hat{\mathbf{i}}}{V_h} = \frac{16}{a^2 c}\left[-\frac{ac}{16}\hat{\mathbf{i}} + \frac{ac}{2}\hat{\mathbf{j}}\right] = \frac{-\hat{\mathbf{i}}}{a} + \frac{8}{a}\hat{\mathbf{j}}\,.$$

$$\mathbf{a}_3^* = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{V_h} = \frac{\left(\frac{a}{2}\hat{\mathbf{i}} + \frac{a}{16}\hat{\mathbf{j}}\right) \times \left(-\frac{a}{2}\hat{\mathbf{i}} + \frac{a}{16}\hat{\mathbf{j}}\right)}{V_h}$$

$$= \frac{\frac{a^2}{32}\hat{\mathbf{k}} + \frac{a^2}{32}\hat{\mathbf{k}}}{V_h} = \frac{16}{a^2 c}\left[\frac{a^2}{16}\hat{\mathbf{k}}\right] = \frac{\hat{\mathbf{k}}}{c}\,.$$

3. The first Brillouin zone of bcc lattice is constructed by bisecting planes to reciprocal lattice vectors $\frac{2\pi}{a}\left(\pm\hat{\mathbf{i}} \pm \hat{\mathbf{j}}\right); \frac{2\pi}{a}\left(\pm\hat{\mathbf{j}} \pm \hat{\mathbf{k}}\right)$ and $\frac{2\pi}{a}\left(\pm\hat{\mathbf{i}} \pm \hat{\mathbf{k}}\right)$. Hence the boundaries of the FBZ will be $\frac{1}{2}\frac{2\pi}{a}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}}\right) = \frac{\pi}{3.5}\left(\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)$ Å^{-1} and similarly $\frac{\pi}{3.5}\left(\hat{\mathbf{i}} - \hat{\mathbf{j}}\right)$ Å^{-1}; $\frac{\pi}{3.5}\left(-\hat{\mathbf{i}} + \hat{\mathbf{j}}\right)\text{Å}^{-1}$ ...., $\frac{\pi}{3.5}\left(-\hat{\mathbf{i}} - \hat{\mathbf{k}}\right)\text{Å}^{-1}$. These 12 points define the boundary of FBZ of given crystal lattice.

4. The unit cell of simple cubic system in direct lattice has edge length of a. The volume of this cell is therefore a^3. In reciprocal lattice, the unit cell edge length is $\frac{2\pi}{a}$ as given in Eq. (3.27). Hence, the volume of this cell is $\left(\frac{2\pi}{a}\right)^3 = \frac{8\pi^3}{a^3}$ which is inversely proportional to a^3, the volume of unit cell in direct lattice.