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B.Sc (PS)Chemistry, Sem VI

Solid State Physics

Reciprocal Lattice and Brillouin Zone

19<sup>th</sup> March 2020

### 2.5 PROPERTIES OF RECIPROCAL LATTICE

1. Each point in a reciprocal lattice corresponds to particular set of parallel planes of the direct lattice.
2. The distance of a reciprocal lattice point from an arbitrarily fixed origin is inversely proportional to the interplanar spacing of the corresponding parallel planes of the direct lattice.
3. The volume of a unit cell of the reciprocal lattice is inversely proportional to the volume of the corresponding unit cell of the direct lattice.
4. The unit cell of the reciprocal lattice need not be a parallelepiped. It is customary to deal with Wigner-Seitz cell of the reciprocal lattice which constitutes the Brillouin zone.
5. The direct lattice is the reciprocal lattice to its own reciprocal lattice. Simple cubic lattice is self-reciprocal whereas *bcc* and *fcc* lattices are reciprocal to each other.

### 2.6 BRAGG'S LAW IN RECIPROCAL LATTICE

The Bragg's diffraction condition obtained earlier by considering reflection from parallel lattice planes can be used to express geometrical relationship between the vectors in the reciprocal lattice. Consider a reciprocal lattice as shown in Fig. 2.12. Starting from the point A (not necessarily a reciprocal lattice point), draw a vector  $\vec{AO}$  of length  $1/\lambda$  in the direction of the incident x-ray beam which terminates at the origin O of the reciprocal lattice. Taking A as the centre, draw a sphere of radius AO which may intersect some point B of the reciprocal lattice.

Let the coordinates of point B be  $(h', k', l')$  which may have a highest common factor  $n$ , i.e., the coordinates are of the type  $(nh, nk, nl)$ , where  $h, k$  and  $l$  do not have a common factor other than unity. Apparently, vector  $\vec{OB}$  is the reciprocal vector. It must, therefore, be normal to the plane  $(h'k'l')$  or  $(hkl)$  and should have length equal to  $1/d_{h'k'l'}$  or  $n/d_{hkl}$ . Thus,

$$|\vec{OB}| = n/d_{hkl} \quad (2.26)$$

It follows from the geometry of Fig. 2.12. that one such plane is the plane AE. If  $\angle EAO = \theta$  is the angle between the incident ray and the normal, then from  $\triangle AOB$ , we have

$$OB = 2 OE = 2 OA \sin\theta = (2 \sin\theta)/\lambda \quad (2.27)$$

From Eqs. (2.26) and (2.27), we get

$$(2 \sin\theta)/\lambda = n/d_{hkl}$$

$$2d_{hkl} \sin\theta = n\lambda$$

or  
 which is the Bragg's law,  $n$  being the order of reflection. Thus we notice that if the coordinates of a reciprocal point,  $(nh, nk, nl)$ , contain a common factor  $n$ , then it represents  $n$ th order reflection from the planes  $(hkl)$ . It is also evident from the above geometrical construction that the Bragg's condition will be satisfied for a given wavelength  $\lambda$  provided the surface of radius  $1/\lambda$  drawn about the point A intersects a point of the reciprocal lattice. Such a construction is called *Ewald construction*.

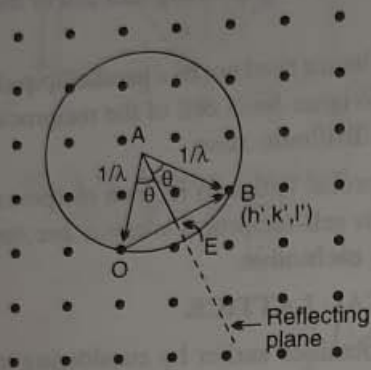


Fig. 2.12. Ewald construction in the reciprocal lattice.

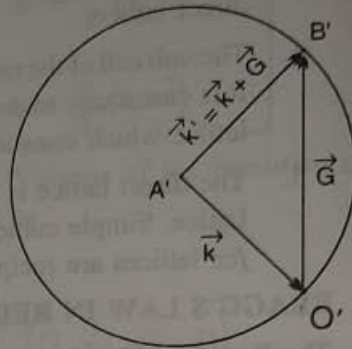


Fig. 2.13. Magnified Ewald construction relating reciprocal lattice vector to the wave vectors of the incident and reflected radiation.

The Bragg's law itself takes a different form in the reciprocal lattice.

To obtain the modified form of the Bragg's law, we redraw the vectors  $\vec{AO}$ ,  $\vec{OB}$  and  $\vec{AB}$  such that each is magnified by a constant factor of  $2\pi$ . Let the new vectors be  $\vec{A'O'}$ ,  $\vec{O'B'}$  and  $\vec{A'B'}$  respectively as shown in Fig. 2.13. Since

$$A'O' = 2\pi (AO) = 2\pi/\lambda,$$

we can represent the wave vector  $\mathbf{k}$  by the vector  $\vec{A'O'}$ . The vector  $\vec{O'B'}$  is the reciprocal vector and is written as  $\mathbf{G}$ . Thus according to vector algebra,  $\vec{A'B'}$  must be equal to  $(\mathbf{k} + \mathbf{G})$ . For diffraction to occur, the point B' must be on the sphere, i.e.,

$$|\vec{A'B'}| = |\vec{A'O'}|$$

$$(\mathbf{k} + \mathbf{G})^2 = k^2$$

$$k^2 + 2\mathbf{k} \cdot \mathbf{G} + G^2 = k^2$$

$$2\mathbf{k} \cdot \mathbf{G} + G^2 = 0$$

$$(2.28)$$

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This is the vector form of Bragg's law and is used in the construction of the Brillouin zones.

The vector  $\vec{A'B'}$  represents the direction of reflected or scattered beam. Denoting it by  $\mathbf{k}'$ , we get

$$\mathbf{k}' = \mathbf{k} + \mathbf{G}$$

which gives

$$k'^2 = k^2 \quad (2.29)$$

and

$$\mathbf{k}' - \mathbf{k} = \Delta\mathbf{k} = \mathbf{G} \quad (2.30)$$

This indicates that the scattering does not change the magnitude of wave vector  $\mathbf{k}$ ; only its direction is changed. Also, the scattered wave differs from the incident wave by a reciprocal lattice vector  $\mathbf{G}$ .

## 2.7 BRILLOUIN ZONES

It has been indicated in the Ewald construction that all the  $\mathbf{k}$ -values for which the reciprocal lattice points intersect the Ewald sphere are Bragg reflected. A *Brillouin zone* is the locus of all those  $\mathbf{k}$ -values in the reciprocal lattice which are Bragg reflected. We construct the Brillouin zones for a simple square lattice of side  $a$ . The primitive translation vectors of this lattice are

$$\mathbf{a} = a\hat{\mathbf{i}}; \quad \mathbf{b} = a\hat{\mathbf{j}}$$

The corresponding translation vectors of the reciprocal lattice are

$$\mathbf{a}^* = (2\pi/a)\hat{\mathbf{i}}; \quad \mathbf{b}^* = (2\pi/a)\hat{\mathbf{j}}$$

Therefore, the reciprocal lattice vector is written as

$$\mathbf{G} = (2\pi/a)(h\hat{\mathbf{i}} + k\hat{\mathbf{j}})$$

where  $h$  and  $k$  are integers. The wave vector  $\mathbf{k}$  can be expressed as

$$\mathbf{k} = k_x\hat{\mathbf{i}} + k_y\hat{\mathbf{j}}$$

From the Bragg's condition (2.28), we have

$$2\mathbf{k} \cdot \mathbf{G} + G^2 = 0$$

$$\text{or } \frac{4\pi}{a} [(k_x\hat{\mathbf{i}} + k_y\hat{\mathbf{j}}) \cdot (h\hat{\mathbf{i}} + k\hat{\mathbf{j}})] + \frac{4\pi^2}{a^2} (h^2 + k^2) = 0$$

$$\text{or } hk_x + kk_y = -(\pi/a)(h^2 + k^2) \quad (2.31)$$

The  $\mathbf{k}$ -values which are Bragg reflected are obtained by considering all possible combinations of  $h$  and  $k$ .

For  $h = \pm 1$  and  $k = 0$ ,  $k_x = \pm\pi/a$  and  $k_y$  is arbitrary;

Also, for  $h = 0$  and  $k = \pm 1$ ,  $k_y = \pm\pi/a$  and  $k_x$  is arbitrary.

These four lines, i.e.,  $k_x = \pm\pi/a$  and  $k_y = \pm\pi/a$ , are plotted in Fig. 2.14. Taking origin as shown, all the  $k$ -vectors originating from it and terminating on these lines will produce Bragg reflection. The square bounded by these four lines is called the *first Brillouin zone*. Thus the first zone of a square lattice of side  $a$  is a square of side  $2\pi/a$ . In addition to this set of lines, some other sets of lines are also possible which satisfy (2.31). For example, for  $h = \pm 1$  and  $k = \pm 1$ , the condition (2.31) gives the following set of four lines,

$$\pm k_x \pm k_y = 2\pi/a$$

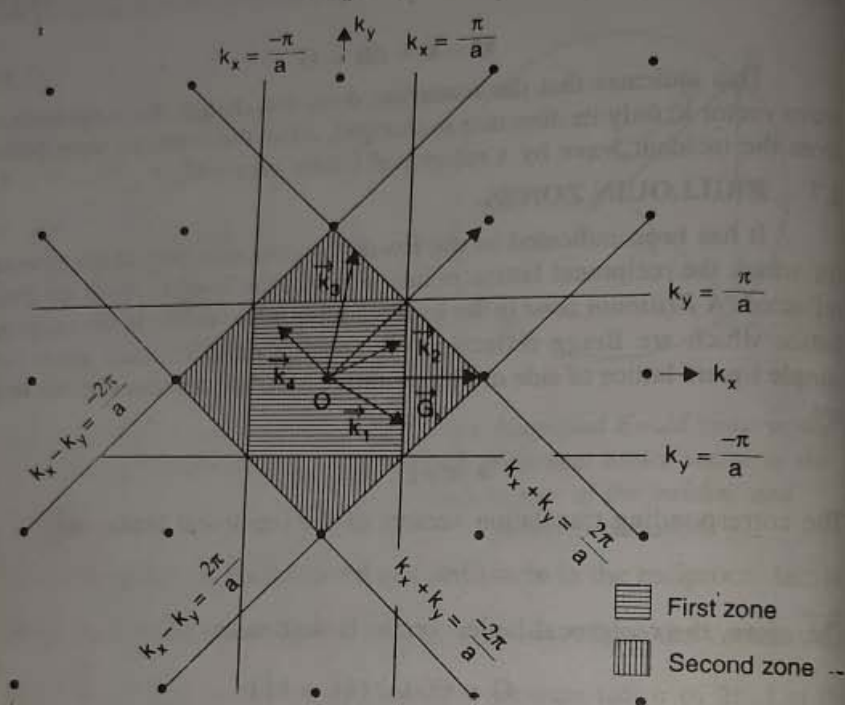


Fig. 2.14. Brillouin zones of a square lattice in its reciprocal lattice. The vectors  $k_1$ ,  $k_2$  and  $k_3$  are Bragg reflected whereas  $k_4$  is not. The vectors  $k_1$  and  $k_2$  have the same reciprocal lattice vector  $G_1$ , while  $G_2$  is the reciprocal vectors of  $k_3$ .

These lines are also plotted in Fig. 2.14. The additional area bounded by these four lines is the *second Brillouin zone*. Similarly the other zones can be constructed. The boundaries of the Brillouin zones represent the loci of  $k$ -values that are Bragg reflected and hence may be considered as the reflecting planes. The boundaries of the first zone represent the reflecting planes for the first order reflection, those of the second zone represent the reflecting planes for the second order reflection, and so on. A  $k$ -vector that does not terminate at a zone boundary cannot produce Bragg reflection. Thus the Brillouin zone pattern can be employed to determine the x-ray diffraction pattern of a crystal and vice versa.

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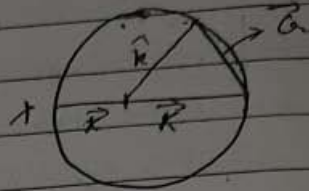
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Fig  
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4 locus of all these points where diffracted beam & reciprocal lattice point intersect on circle / or sphere it is known as Ewald sphere / sphere of Reflection

$$|K| = |K'| = \frac{2\pi}{\lambda}$$



$$\vec{K}' = \vec{K} + \vec{G}$$

$$K'^2 = (\vec{K} + \vec{G})^2$$

$$K'^2 = K^2 + G^2 + 2\vec{K} \cdot \vec{G}$$

$$\boxed{G^2 + 2\vec{K} \cdot \vec{G} = 0}$$

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### Atomic and geometrical factor

The different directions of the diffracted beam obtained according to Bragg's law are governed entirely by geometry & size of unit cell and therefore these directions are not affected by the arrangement of atoms associated with each lattice point.

However the complexity of atomic structure within unit cell do effect the intensity of diffracted beam. The intensity of diffracted beam primarily depends upon <sup>atomic</sup> scattering factor and position of each atom in unit cell.

## Atomic Scattering

Since the  $e^-$  are the only component of atom that scatter  $x$ -rays significantly, the  $x$ -rays scattered from one part of atom interfere with those scattered from other part at all angles of scattering.

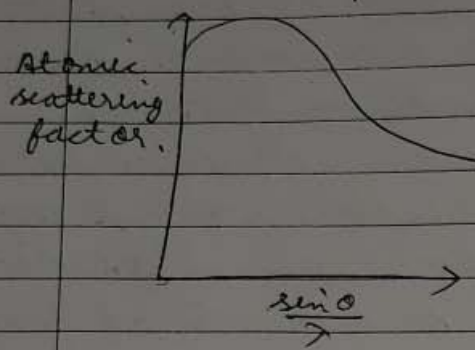
And at  $\theta = 0$  or  $360^\circ$  all atoms scatter in phase. Since, the  $e^-$  are distributed throughout the atomic volume, the diffracted beams are obtained as a result of combination of scattered waves from  $e^-$ 's of all atoms in unit cell. Hence process involves two distinct combin contributions.

1. Scattering from  $e^-$  in same atom i.e. (atomic scattering factor / atomic form factor) denoted by  $f$
2. The summation of this scattering from all atoms in unit cell i.e. (geometrical scattering factor  $F$ )

The Atomic scattering factor is a measure of efficiency of an atom in scattering  $x$ -rays and it is defined as ratio of amplitude scattered by actual  $e^-$  distribution in an atom to that scattered by  $1e^-$  localised at point.

Therefore if atoms are assumed to be points only, then atomic scattering factor will be equal to no of  $e^-$  present.

The Atomic scattering factor of an atom falls off with increasing scattering angle or more precisely with increasing value of  $\frac{\sin \theta}{\lambda}$



In order to know <sup>the</sup> intensity of a ray beam scattered by 1 unit cell in particular direction where there is diffraction maximum. It is necessary to sum the waves that arise due to all atoms in unit cell.

Mathematically, this involves adding the wave of same wavelength with diff. amplitude & phase. The intensity of scattered beam is then obtained by squaring resultant amplitude.

If the position of atoms in unit cell are denoted by  $x, y, z$ , the resultant amplitude can be expressed as  
for a given  $hkl$  reflection

$$F(hkl) = \sum_{i=1}^N f_i \exp [2\pi i (hx_i + ky_i + lz_i)] \quad \text{--- (1)}$$

$$F(hkl) = \sum_{i=1}^N f_i \cos 2\pi (hx_i + ky_i + lz_i) + j(\sin) \sum_{i=1}^N f_i \sin 2\pi (hx_i + ky_i + lz_i) \quad (2)$$

But intensity of diffracted beam is given by square of amplitude so

$$I \propto |F(hkl)|^2 \quad (3)$$

expression of intensity of diffracted beam

$$|F(hkl)|^2 = \left[ \sum_{i=1}^N f_i \cos 2\pi (hx_i + ky_i + lz_i) \right]^2 + \left[ \sum_{i=1}^N f_i \sin 2\pi (hx_i + ky_i + lz_i) \right]^2 \quad (4)$$

Consider an example of bcc structure. Consider the position of atoms at  $(0, 0, 0)$  &  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ .

So  $x_1 = y_1 = z_1 = 0$  &  $x_2 = y_2 = z_2 = \frac{1}{2}$

So

$$|F|^2 = f^2 \left( \cos 2\pi \cdot 0 + \cos 2\pi \left( \frac{h}{2} + \frac{k}{2} + \frac{l}{2} \right) \right)^2$$

$$+ f^2 \left( \sin 2\pi \cdot 0 + \sin 2\pi \left( \frac{h}{2} + \frac{k}{2} + \frac{l}{2} \right) \right)^2 \quad (5)$$

or

$$|F|^2 = f^2 \left[ (1 + \cos \pi (h+k+l))^2 + \sin^2 \pi (h+k+l) \right]$$

from eq (5), it can be seen that

$F = 2f$  &  $I = 4f^2$ , when  $h+k+l = \text{even integer}$   
 $F = 0$  &  $I = 0$ , when  $h+k+l = \text{odd integer}$ .

Metals sodium has bcc structure & it is always noted for diffraction <sup>spectrum</sup> pattern of sodium that lines corresponding to

$$F(hkl) = \sum_{i=1}^N f_i \cos 2\pi (hx_i + ky_i + lz_i) + j(\text{units}) \sum_{i=1}^N f_i \sin 2\pi (hx_i + ky_i + lz_i) \quad (2)$$

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So

$$|F|^2 = f_i^2 (\cos 2\pi \cdot 0 + \cos 2\pi (\frac{h}{2} + \frac{k}{2} + \frac{l}{2}))^2$$

$$+ f_i^2 (\sin 2\pi \cdot 0 + \sin 2\pi (\frac{h}{2} + \frac{k}{2} + \frac{l}{2}))^2 \quad (5)$$

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Metals sodium has bcc structure & it is always noted for diffraction <sup>spectrum</sup> pattern of sodium that lines corresponding to

(100), (300), (111), (221) etc are missing from spectrum while lines corresponding (200) (110) (220) <sup>planes</sup> are present in spectrum.

The absence of lines can be understood by considering that the beam from these planes are out of phase by  $\pi$  and hence not contributing. However the other planes are contributing in diffracted beam.

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Elementary lattice dynamics  
lattice vibrations

The elastic vibration of the atom in a solid are influenced or are due to thermal / heat energy which is provided to solid. The heat energy increases the internal energy of solid and is manifested mainly as:

- 1. Increase in vibration of atom about their mean position usually called lattice vibration and increasing the K.E of free e<sup>-</sup>. Lattice vibration can be thought of as series of superimposed sound / strain waves / lattice waves with a frequency spectrum determined by elastic properties of crystal and quanta of elastic wave of energy is called phonons (In analogy with photon). All the concepts such as wave particle duality which apply to photon apply equally on phonon. Similar to photons, phonons are bosons and are

## (i) Simple Cubic Crystals

The effective number of atoms in a unit cell of simple cubic structure is one. Assuming that it lies at the origin, the structure factor given by Eq. (2.45) comes out to be unity. The diffraction amplitude, from Eq. (2.44), becomes

$$F(h'k'l) = f$$

Thus all the diffraction lines predicted by the Bragg's law would appear in the diffraction pattern provided the value of  $f$  is large enough to produce peaks of observable intensity.

## (ii) Body-Centred Cubic Crystals

The effective number of atoms in a *bcc* unit cell is two; one occupies a corner position and the other occupies the centre of the cube. If the coordinates of corner atom be arbitrarily taken as (0,0,0), then the coordinates of the other atom become  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . Since both the atoms are identical, Eq. (2.44) gives the value of  $F$  as

$$\begin{aligned} F(h'k'l) &= f \sum_j e^{2\pi i(u_j h' + v_j k' + w_j l')} \\ &= f [1 + e^{i\pi(h' + k' + l')}] \end{aligned} \quad (2.47)$$

The expression within the square brackets represents the structure factor for *bcc* crystal. Here it has been assumed that only one of the eight corners of the cube is occupied and has the coordinates (0,0,0). The validity of this assumption can be verified by considering all the corner positions and using the fact that the contribution of each corner atom is  $1/8$ . This yields the same structure factor as included in Eq. (2.47).

We also find from Eq. (2.47) that the structure factor becomes zero for odd values of  $(h' + k' + l')$ , since  $e^{i\pi n}$  equals  $-1$  if  $n$  is odd. For even values of  $(h' + k' + l')$ ,  $F(h'k'l)$  equals  $2f$  and, from Eq. (2.46), the intensity becomes proportional to  $4f^2$ . Thus in a *bcc* structure, reflections like (100), (111), (210), etc. are missing, whereas the diffraction lines corresponding to (110), (200), (222), etc. reflections are present. It is to be noted that the presence or absence of a reflection is considered only in terms of the first order reflection. This is because the Miller indices of the planes  $(h'k'l')$  used in Eq. (2.43) may have a common factor  $n$ ; thus we determine reflections from the planes  $(nh nk nl)$ . As described earlier, the appropriate Bragg's law applicable to such a case is

$$2d_{h'k'l'} \sin\theta = \lambda \quad (2.48)$$

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$$\begin{aligned} F(h'k'l) &= f \sum_j e^{2\pi i(u_j h' + v_j k' + w_j l')} \\ &= f [1 + e^{i\pi(h' + k' + l')}] \end{aligned} \quad (2.47)$$

The expression within the square brackets represents the structure factor for *bcc* crystal. Here it has been assumed that only one of the eight corners of the cube is occupied and has the coordinates  $(0,0,0)$ . The validity of this assumption can be verified by considering all the corner positions and using the fact that the contribution of each corner atom is  $1/8$ . This yields the same structure factor as included in Eq. (2.47).

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$$2d_{h'k'l'} \sin\theta = \lambda \quad (2.48)$$

$(h'k'l')$  planes have a path difference of  $\lambda$  or the phase difference of  $2\pi$ . Thus considering reflections from (100) planes as shown in Fig. 2.19a, we find that the waves reflected from the top and bottom surfaces of the cube differ in phase by  $2\pi$ . Since in *bcc* crystals, there exists a central plane which is exactly identical to the (100) planes, a wave reflected from this plane must have a phase difference of  $\pi$  relative to its neighbouring (100) planes. Thus the diffracted beams from a regular (100) plane and a body centre plane interfere destructively in pairs causing absence of (100) reflection. Similarly, by using Eq. (2.48), it can be shown that the first order reflections from any two neighbouring (200) planes must differ in phase by  $2\pi$  radians and hence undergo constructive interference causing the occurrence of these reflections in *bcc* crystals. The presence of second order reflections from (100) planes can be shown by using Eq. (2.1) The second order reflection from two neighbouring (100) planes has a phase difference of  $4\pi$  radians, which means that the reflection from the middle plane would differ from the reflections from top and bottom planes by a phase difference of  $2\pi$ . The situation is exactly identical to that shown in Fig. 2.19b, thus indicating that the second order reflection from (100) planes is present. As described earlier, it overlaps with the first order reflection from (200) planes.

### (iii) Face-Centred Cubic Crystal

An *fcc* unit cell has four identical atoms. One of these atoms is contributed by corners and may arbitrarily be assigned coordinates (0,0,0), whereas the other three are contributed by face centres and have the coordinates  $(\frac{1}{2}, 0, \frac{1}{2})$ ,  $(\frac{1}{2}, \frac{1}{2}, 0)$  and  $(0, \frac{1}{2}, \frac{1}{2})$ . From Eq. (2.39), the diffraction amplitude becomes

$$F(h'k'l') = f [1 + e^{\pi i(h'+l')} + e^{\pi i(h'+k')} + e^{\pi i(k'+l')}]$$

where the expression within the square brackets is the structure factor for *fcc* crystals. It is obvious that the structure factor is non-zero only if  $h$ ,  $k$  and  $l$  are all even or all odd and has a value equal to 4. Thus the diffraction amplitude becomes  $4f$  and the intensity becomes proportional to  $16f^2$ . The structure factor vanishes for all other odd-even combinations of  $h$ ,  $k$  and  $l$ . Hence reflections of the type (111), (200), (220), etc. are present, whereas those of the type (100), (110), (211), etc. are absent for an *fcc* crystal.

The conclusions drawn above regarding allowed reflections for *sc*, *bcc* and *fcc* crystals are summarized in Table 2.1 and are called extinction rules. The extinction rules for *dc* structure are also included.

TABLE 2.1 Extinction rules for cubic crystals.

| Crystal | Reflections allowed for   |
|---------|---|
| SC      | all possible values of $h, k$ and $l$   |
| BCC     | even values of $(h + k + l)$  |
| FCC     | all odd or all even values of $h, k$ and $l$  |
| DC      | all odd $h, k$ and $l$ , or all even $h, k$ and $l$ with $(h + k + l)$ divisible by 4 |

The ratios of  $(h^2 + k^2 + l^2)$  values for allowed reflections from cubic crystals as obtained from the extinction rules are given as follows :

$$\text{SC} : 1 : 2 : 3 : 4 : 5 : 6 : 8 \dots$$

$$\text{BCC} : 2 : 4 : 6 : 8 : 10 : 12 : 14 \dots$$

$$\text{or } 1 : 2 : 3 : 4 : 5 : 6 : 7 : \dots$$

$$\text{FCC} : 3 : 4 : 8 : 11 : 12 : 16 : 19 \dots$$

$$\text{DC} : 3 : 8 : 11 : 16 : 19 \dots$$

A comparison of these ratios with the observed ratios of  $\sin^2\theta$  values is made to identify the cubic crystal structures.

## SOLVED EXAMPLES

**Example 2.1.** An x-ray beam of wavelength  $0.71\text{\AA}$  is diffracted by a cubic KCl crystal of density  $1.99 \times 10^3 \text{ kg m}^{-3}$ . Calculate the interplanar spacing for (200) planes and the glancing angle for the second order reflection from these planes. The molecular weight of KCl is 74.6 amu and the Avogadro's number is  $6.023 \times 10^{26} \text{ kg}^{-1} \text{ mole}^{-1}$ .

**Solution.** For cubic crystals, we have

$$a^3 = \frac{n' M}{N \rho}$$

where  $a$  is the lattice constant,  $n'$  is the number of molecules in a unit cell,  $M$  is the molecular weight,  $N$  is the Avogadro's number and  $\rho$  is the density.

KCl has the same structure as NaCl

$$n' = 4$$

$$\therefore a^3 = \frac{4 \times 74.6}{6.023 \times 10^{26} \times 1.99 \times 10^3} = 0.249 \times 10^{-27} \text{ m}^3$$

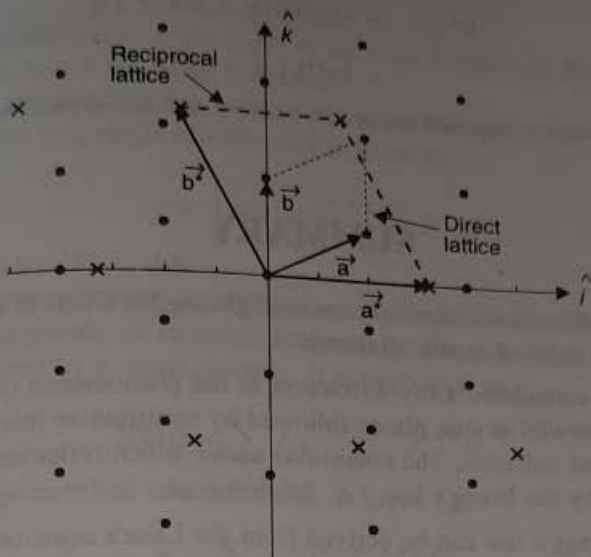


Fig. 2.20. Two-dimensional direct and reciprocal lattices.

**Example 2.4.** The primitive translation vectors of a two-dimensional lattice are

$$\mathbf{a} = 2\hat{i} + \hat{j}, \quad \mathbf{b} = 2\hat{j}$$

Determine the primitive translation vectors of its reciprocal lattice.

**Solution.** We assume that the third translation vector  $\mathbf{c}$  of the given lattice lies along the  $z$ -axis and is of unit magnitude, i.e.,

$$\mathbf{c} = \hat{k}$$

From Eqs. (2.18), the reciprocal lattice vectors are given by

$$\mathbf{a}^* = 2\pi \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}}, \quad \mathbf{b}^* = 2\pi \frac{\mathbf{c} \times \mathbf{a}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}}$$

It is obvious that vectors  $\mathbf{a}^*$  and  $\mathbf{b}^*$  lie in the plane of  $\mathbf{a}$  and  $\mathbf{b}$ .

$$\begin{aligned} \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) &= (2\hat{i} + \hat{j}) \cdot (2\hat{j} \times \hat{k}) \\ &= 2(2\hat{i} + \hat{j}) \cdot \hat{k} \\ &= 2(2 + 0) = 4 \end{aligned}$$

$$\mathbf{a}^* = (2\pi/4) (2\hat{j} \times \hat{k}) = \pi\hat{i}$$

$$\begin{aligned} \mathbf{b}^* &= (2\pi/4) [\hat{\mathbf{k}} \times (2\hat{\mathbf{i}} + \hat{\mathbf{j}})] \\ &= (\pi/2) [-\hat{\mathbf{i}} + 2\hat{\mathbf{j}}] \end{aligned}$$

$\mathbf{a}^*$  and  $\mathbf{b}^*$  are the required reciprocal vectors and are shown in Fig. 2.20.

## SUMMARY

1. A crystal acts as a three-dimensional grating for x-rays of wavelength of the order of atomic diameter.
2. Bragg considered x-ray diffraction as the phenomenon of reflection from parallel atomic planes followed by constructive interference of reflected radiation. The conditions under which reflection occurs is given by the Bragg's law, i.e.,  $2d \sin\theta = n\lambda$
3. The Bragg's law can be derived from the Laue's equations given as  $\mathbf{a} \cdot \mathbf{N} = nh\lambda$ ,  $\mathbf{b} \cdot \mathbf{N} = nk\lambda$ ,  $\mathbf{c} \cdot \mathbf{N} = nl\lambda$
4. X-ray diffraction is utilized to determine the structure of solids and for the study of x-ray spectroscopy. The position of diffraction lines determines the space lattice and their intensity determines the basis.
5. Every direct lattice in real space is associated with a reciprocal lattice.

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