Chapter 2
Crystal Lattices and Reciprocal Lattices

Abstract In this chapter, the basic unit vectors in real space and the basic unit vectors in reciprocal space, as well as their reciprocal relationships, are described. The commonly used Bravais lattices are summarized. The direction, plane, and interplanar spacing in a real space lattice are defined. The wavevectors, momentum change, Bragg condition, Miller indices, and reciprocal lattice vectors used in wave diffraction are defined. The reason one needs the reciprocal space to determine structure is explained.

2.1 Crystal Lattices in Real Space

The atoms in a crystal can be mathematically represented as points in a three-dimensional (3D) real space lattice. If these lattice points are arranged in a periodic fashion, then one can define real space unit vectors **a**, **b**, and **c** and the angles α, β, and γ. See Fig. 2.1.

2.1.1 Basic Vectors and the Translational Vector

In diffraction experiments using crystalline samples, atoms are arranged in a highly ordered fashion with specific periodic positions and symmetry. For example, in Fig. 2.2 we sketch a building block (shaded volume) of a three-dimensional (3D) crystalline solid with a cubic symmetry in the x-, y-, and z- axes from $-\infty$ to ∞. The distance between the two nearest-neighbor atoms in the x direction is the basic vector **a**, the distance between the two nearest-neighbor atoms in the y direction is the basic vector **b**, and the distance between the two nearest-neighbor atoms in the z direction is the basic vector **c**. For a simple cubic lattice, the angles α, β, and γ are 90 degrees. All atoms are equivalent when they follow the periodicity. For a reference or origin located at any of these atoms, the crystal is exactly the same. This invariance can be described by a translational vector **T** defined as

$$\mathbf{T} = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}, \tag{2.1}$$

where n_1, n_2, and n_3 are integers.

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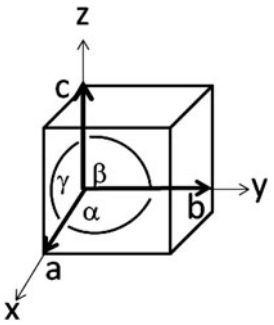

Fig. 2.1 A unit cell with three basic vectors **a**, **b**, and **c**. The angles between a pair of vectors are α, β, and γ

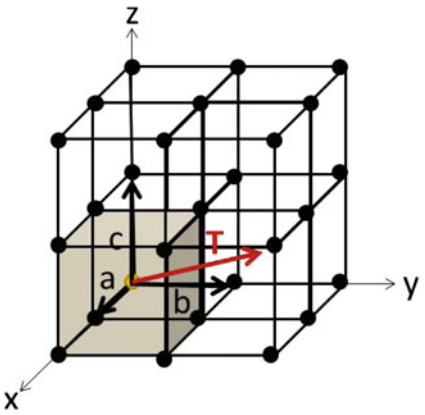

Fig. 2.2 A three-dimensional cubic lattice with basic vectors **a**, **b**, and **c**. **T** is the translational vector

This means that if a crystal is translated by a translational vector joining any two atoms, for example **T**, the crystal looks exactly the same as it does before the translation. Any lattice point in a crystal can be reached through the lattice translation operation or the crystal translational vector **T**. This crystal translational vector **T** connects any two lattice points in the crystal. See Fig. 2.2. For example, the lattice point located at the end of vector **T** can be reached by the translational vector $\mathbf{T} = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$ where $n_1 = 2$, $n_2 = 2$, and $n_3 = 1$. All lattice points can be reached by combinations of n_1, n_2, and n_3.

2.1.2 Bravais Lattices

The example of a simple cubic lattice described previously and sketched in Fig. 2.3a is just one of three Bravais-lattice types in a cubic-lattice system. The other two types are face-centered cubic (FCC) and body-centered cubic (BCC). See Figs. 2.3b and 2.3c. This cubic lattice system is one of seven lattice systems. The remaining six are hexagonal (see Fig. 2.3d), triclinic, trigonal, monoclinic (two Bravais types), orthorhombic (four Bravais types), and tetragonal (two Bravais types) systems. These

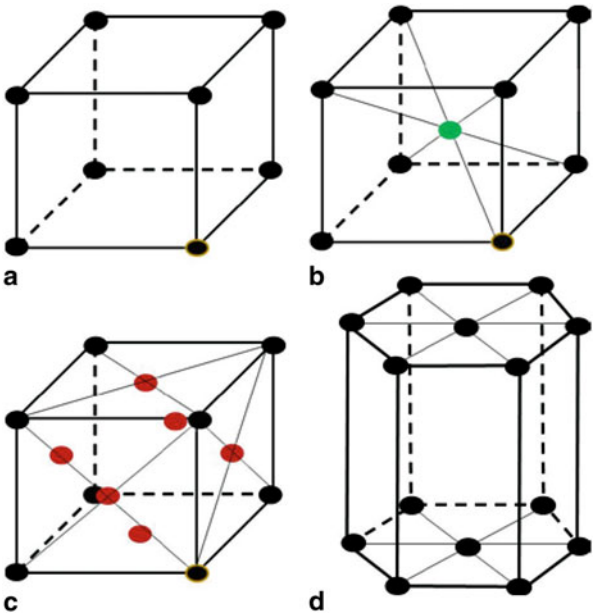

Fig. 2.3 Examples of Bravais lattices. **a** Simple cubic. **b** Body-centered cubic. **c** Face-centered cubic. **d** Hexagonal

seven systems have a total of 14 Bravais lattice types in three dimensions. These seven systems have different lengths of a, b, and c, and different angles of α, β, and γ (Kittel 1986). See Table 2.1 for the 14 Bravais lattices under the seven crystal systems. All lattice points in a Bravais lattice are equivalent.

2.1.3 Non-Bravais Lattices

There is a second kind of lattice called non-Bravais lattice, where some lattice points are non-equivalent. This non-Bravais lattice can be treated as a lattice with a basis. The basis contains a group of atoms identical in composition, arrangement, and orientation. The basis is stationed near each site of a Bravais lattice. The non-Bravais lattice can be treated as a combination of more than one interpenetrating Bravais with a fixed relative orientation to each other. Take body-centered cubic (BCC) as an example. One can treat a BCC structure, such as the one shown in Fig. 2.4b, as a simple cubic lattice (Fig. 2.4a) with a basis of two identical atoms attached to every lattice point of a simple cubic. The positions of these two atoms are the first atom at the lattice point 0, 0, and 0 of a basis and the second atom at position $^1/_2$ **a**, $^1/_2$ **b**, and $^1/_2$ **c** from the lattice point at 0, 0, and 0. Another example is an FCC lattice shown in Fig. 2.4d where the basis consists of two identical atoms with one atom at the lattice point 0, 0, and 0 and the other atom at 0 **a**, $^1/_2$ **b**, and $^1/_2$ **c** from the lattice point at 0, 0, and 0. See Fig. 2.4c. If one attaches a basis on each simple cubic lattice, an FCC lattice can be produced. See Fig. 2.4d.

Table 2.1 The 14 Bravais lattices under seven crystal systems

System	Conventional cell axes and angles	Number of lattices
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^o$	3
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^o, \gamma = 120^o$	1
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	1
Trigonal	$a = b = c$ $\alpha = \beta = \gamma < 120^o, \neq 90^o$	1
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^o \neq \beta$	2
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^o$	2
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^o$	4

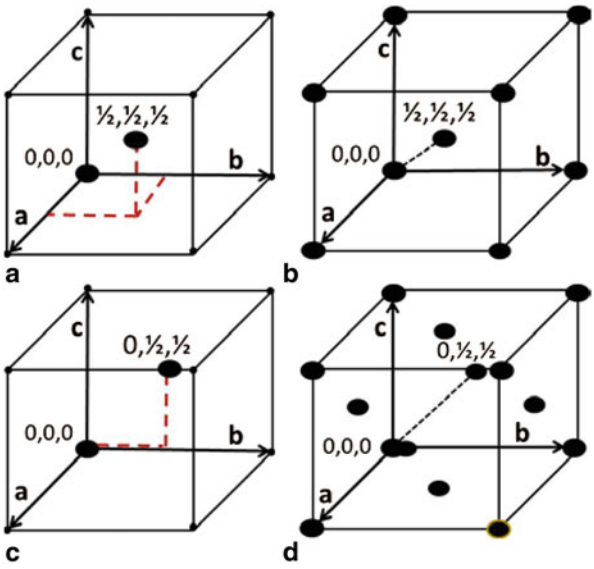

Fig. 2.4 A basis vector in a non-Bravais lattice. **a** Two identical atoms in a cubic cell with their positions labeled. **b** A basic vector (*dashed line*) connects two atoms in a body-centered cubic. **c** Two identical atoms in a cubic cell with their positions labeled. **d** A basic vector (*dashed line*) connects two atoms in a face-centered cubic

The elemental composition of two atoms in a basis can vary, but their arrangement and orientation remain the same. An example of a two-element lattice is CsCl. It can be treated as a simple cubic lattice with a basis that has one Cs^+ ion at 0, 0, and 0 and one Cl^- ion at $^1/_2$ **a**, $^1/_2$ **b**, and $^1/_2$ **c** from the lattice point at 0, 0, and 0. Another example of a different composition but the same arrangement and orientation is NaCl. It can be treated as having alternate Na^+ and Cl^- ions at the lattice points of a simple cubic. In this case for each ion on a lattice point, there are six nearest neighbors of oppositely charged ions. A different view is that NaCl can be thought of as the interweaving of an FCC lattice of Na^+ ions and an FCC lattice of Cl^- ions. In this case, the basis consists of one Cl^- ion at 0, 0, and 0 and one Na^+ at $^1/_2$ **a**, $^1/_2$ **b**, and $^1/_2$ **c** from the lattice point at 0, 0, and 0.

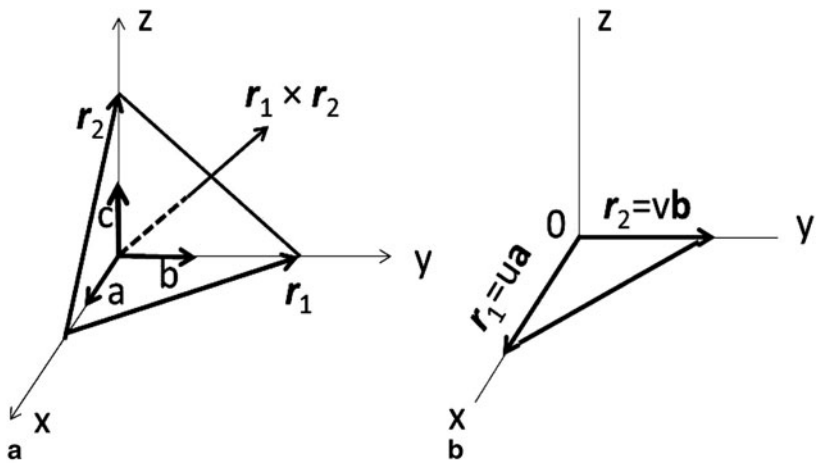

Fig. 2.5 **a** Two vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are in a plane, and the cross product of the two vectors shows the direction. **b** An example of an xy plane with its plane direction along the z direction

2.1.4 Primitive and Nonprimitive Cells

The volume of a cube with basic vectors **a**, **b**, and **c** as sides is a unit cell of a lattice. If the unit cell has the smallest possible volume, it is a primitive cell that contains one atom per unit cell. Sometimes it is convenient to use a nonprimitive cell that has a larger volume, but exhibits the lattice symmetry more clearly. The nonprimitive cell is an integral multiple of the primitive cell. For example, the FCC lattice has four lattice points per conventional cell, and the BCC lattice has two lattice points per conventional cell.

2.1.5 Plane and Direction in a Real Space Lattice

A lattice plane can be defined by passing through three noncollinear lattice points. The orientation of a plane is a vector perpendicular to the plane. For example, $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the two vectors shown in Fig. 2.5a. Each vector connects two lattice points. A cross product of these two vectors (Christman 1988) is

$$\boldsymbol{r}_1 \times \boldsymbol{r}_2 = \mathrm{xyz}\left[\frac{\mathbf{b}\times\mathbf{c}}{\mathrm{x}} + \frac{\mathbf{c}\times\mathbf{a}}{\mathrm{y}} + \frac{\mathbf{a}\times\mathbf{b}}{\mathrm{z}}\right]. \tag{2.2}$$

This cross product of $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ is perpendicular to the plane, consisting of $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ using the right-hand rule as indicated in Fig. 2.5a. An example is given in Fig. 2.5b. Assuming a cubic lattice with $\boldsymbol{r}_1 = \mathrm{u}\ \mathbf{a}$ and $\boldsymbol{r}_2 = \mathrm{v}\ \mathbf{b}$, then a plane consisting of $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ is in the xy-plane. The direction of this plane is $\boldsymbol{r}_1 \times \boldsymbol{r}_2 = \mathrm{u}\ \mathbf{a} \times \mathrm{v}\ \mathbf{b} = \mathrm{u}\ \mathrm{v}\ \mathbf{c}$ which is along the z-direction.

2.1.6 Alternative Way to Define Plane Direction

First we choose a lattice point 0 as a reference and then choose the lattice vector joining a point away from the reference and along the line in a direction $\mathbf{T} = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$. The direction of a plane is the integral triplet $[n_1 n_2 n_3]$. The direction is enclosed by a square bracket [ ]. Remove a common factor if n_1, n_2, and n_3 have one, and then reduce the triplet to the smallest integer with the same relative ratios. For example, if we choose 0 as the reference and a lattice point at $1\mathbf{a}$, $1\mathbf{b}$, and $1\mathbf{c}$, then $\mathbf{T} = 1\mathbf{a} + 1\mathbf{b} + 1\mathbf{c}$. The direction is [111]. If we choose a lattice point 0 as a reference and a lattice point $1\mathbf{c}$ along the z-axis, then $\mathbf{T} = 0\mathbf{a} + 0\mathbf{b} + 1\mathbf{c}$. The direction is [001], or in the +z-axis. If the third lattice point is chosen at $-1\mathbf{c}$, then the direction is $[00\bar{1}]$, which is along the −z-axis.

2.1.7 Plane Orientation and Interplanar Spacing Using Miller Indices

The orientation of a plane can be specified by Miller indices *hkl* enclosed by parentheses ( ), (*hkl*). This is obtained by three intercepts on x-, y-, and z-axes in terms of lattice constants a, b, and c, i.e. (x/a, y/b, z/c). Take the reciprocals of these three numbers, (a/x, b/y, c/z). Reduce them to the three smallest integers by multiplying a common factor n (na/x, nb/y, nc/z) and enclose these three integers in parentheses to give (*hkl*). For example, a plane intercepts the x-, y-, and z-axes at ∞, ∞, and 1, respectively. Then the reciprocals of ∞, ∞, and 1 are 0, 0, and 1, respectively. The Miller indices for this plane are (001). See Fig. 2.6a. If a plane intercepts the negative side of the z-axis at −1c, with infinity at the y- and z-axes, then the Miller indices are labeled by placing a minus sign over the number like this: $(00\bar{1})$. See Fig. 2.6b.

Figure 2.6c–f illustrate examples (002), (110), (011), and (111), respectively. If a unit cell has a certain rotational symmetry, and through a rotation, one plane can be equivalent to a nonparallel plane, then all these rotationally obtained planes can be represented by the same Miller indices with curly brackets, {*hkl*}. For example, a cubic unit cell (100) can be rotated 90° using the x-, y-, or z-axis as the rotational axis to obtain (010) and (001). The $(\bar{1}00), (0\bar{1}0), (00\bar{1})$ planes are parallel to (100), (010), and (001), respectively. These six planes can be labeled as {100} with curly brackets. In other words, the indices {*hkl*} represent all planes equivalent to the plane (*hkl*) through rotational symmetry. For {111} through rotational symmetry, there are four planes (111), $(\bar{1}11), (1\bar{1}1)$, and $(11\bar{1})$. The $(\bar{1}\bar{1}\bar{1}), (1\bar{1}\bar{1}), (\bar{1}1\bar{1})$, and $(\bar{1}\bar{1}1)$ planes are parallel to (111), $(\bar{1}11), (1\bar{1}1)$, and $(11\bar{1})$, respectively.

As can be seen from this explanation of how to define Miller indices by reducing intercepts to the three smallest integers, all parallel and equivalent planes are labeled by the same Miller indices. For example, triplet intercepts such as x, y, z; $2x$, $2y$, $2z$; and $3x$, $3y$, $3z$, can be labeled by the same (111) family of planes because the reciprocals of intercepts 2, 2, 2 and 3, 3, 3 give $^1/_2$, $^1/_2$, $^1/_2$ and $^1/_3$, $^1/_3$, $^1/_3$,

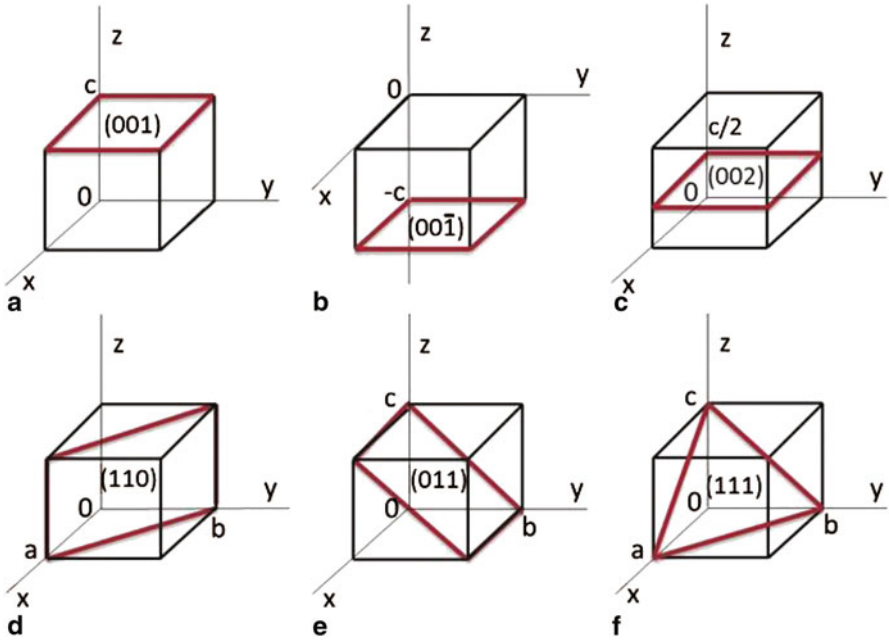

Fig. 2.6 Various planes in a cubic lattice. **a** The (001) plane. **b** (00$\bar{1}$) plane. **c** (002) plane. **d** (110) plane. **e** (011) plane. **f** (111) plane

respectively. Reducing these fractional numbers to the smallest three integers having the same ratio, one obtains the (111) index plane. This concept of a family of planes is important because most diffraction experiments involve the scattering of waves from a family of equivalent planes, not just one single plane.

For a cubic system, it can be shown that the vector [*hkl*] is normal to the planes defined by the Miller indices {*hkl*}.

2.1.8 Interplanar Spacing Between the Same Miller Index Planes and the Angle Between Different Miller Index Planes

2.1.8.1 Cubic Lattices

The interplanar spacing d_{hkl} between planes of the same {*hkl*} family is the shortest perpendicular distance between these (*hkl*) planes. The shaded plane (*hkl*) shown in Fig. 2.7 is in a Cartesian coordinate system and makes intercepts with the three axes at *x*, *y*, and *z*. The arrow indicates the normal direction of the plane. The angles between the x-, y-, and z-axes to the normal are α', β', and γ', respectively. Assume that there is another plane parallel to and behind the plane shown, and it is passing the origin of the Cartesian coordinates. The d_{hkl} is the perpendicular distance from

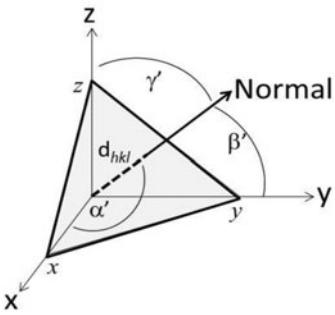

Fig. 2.7 Interplanar spacing d_{hkl} is the perpendicular distance between parallel planes

the origin along the normal direction to the plane or the dashed line. From Fig. 2.7, one illustrates

$$d_{hkl} = x\cos\alpha' = y\cos\beta' = z\cos\gamma'. \tag{2.3}$$

Using the directional cosines relationship

$$\cos^2\alpha' + \cos^2\beta' + \cos^2\gamma' = 1, \tag{2.4}$$

one obtains

$$d_{hkl} = \frac{1}{\sqrt{\frac{1}{x^2} + \frac{1}{y^2} + \frac{1}{z^2}}}. \tag{2.5}$$

Recall the common factor n and $h = na/x$, $k = nb/y$, and $l = nc/z$. By substituting x, y, and z into the previous equation, one gets

$$d_{hkl} = \frac{n}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}}. \tag{2.6}$$

For a simple cubic cell where the cube edges are $a = b = c$, and the right angles are $\alpha = \beta = \gamma = 90°$, the previous formula reduces to

$$d_{hkl} = \frac{na}{\sqrt{h^2 + k^2 + l^2}}. \tag{2.7}$$

For example, in a simple cubic cell, the d_{hkl} for (001) planes is $d_{001} = a$, and the d_{hkl} for (002) planes $d_{002} = a/2$.

The angle θ_p between planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ is

$$\cos\theta_p = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)}\sqrt{(h_2^2 + k_2^2 + l_2^2)}}. \tag{2.8}$$

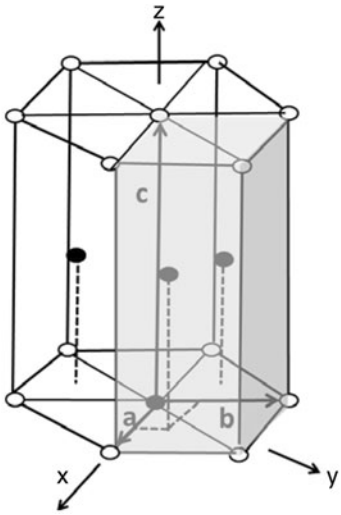

Fig. 2.8 A hexagonal close-packed structure where the angle between basic vectors **a** and **b** is 120°

2.1.8.2 Hexagonal Close Packed Lattice

Some of our reflection high-energy electron diffraction RHEED pole figure examples presented later have a hexagonal lattice, such as Ru and Mg. Here, we also describe the real-space and reciprocal-space lattices of a hexagonal structure.

The primitive vectors **a** and **b**, shown in Fig. 2.8, have an angle of 120° between them in the basal plane and **c** is perpendicular to the basal plane. The unit vector lengths and the angle between unit vectors are $a = b \neq c$, $\alpha = \beta = 90°$, and $\gamma = 120°$.

$$\begin{aligned}
\mathbf{a} &= a\hat{x}, \\
\mathbf{b} &= a\left\{-\sin(30°)\,\hat{x} + \cos(30°)\,\hat{y}\right\} = \frac{1}{2}a\left(-\hat{x} + \sqrt{3}\hat{y}\right), \text{and} \\
\mathbf{c} &= c\hat{z},
\end{aligned} \tag{2.9}$$

where

$$\frac{c}{a} = \sqrt{\frac{8}{3}}.$$

The distance d_{hkl} between a family of planes (hkl) is

$$\frac{1}{d_{hkl}^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}. \tag{2.10}$$

The angle θ_p between planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ is

$$\cos\theta_p = \frac{4}{3a^2}\left[h_1h_2 + k_1k_2 + \frac{1}{2}(h_1k_2 + h_2k_1) + \frac{3a^2}{4c^2}l_1l_2\right] d_{h_1k_1l_1}\, d_{h_2k_2l_2}. \tag{2.11}$$

For similar crystallographic formulas associated with other systems such as trigonal (or rhombohedral), tetragonal, orthorhombic, monoclinic, and triclinic structures, Jackson has a complete description (Jackson 1991).

If one prefers to index a plane using $(hkil)$ where $i = -(h + k)$, then the angle between two directions, $[h_1k_1i_1l_1]$ and $[h_2k_2i_2l_2]$, was derived by Frank (1965) as

$$\cos\alpha = \frac{h_1h_2 + k_1k_2 + i_1i_2 + \lambda^2 l_1l_2}{\left(h_1^2 + k_1^2 + i_1^2 + \lambda^2 l_1^2\right)^{1/2}\left(h_2^2 + k_2^2 + i_2^2 + \lambda^2 l_2^2\right)^{1/2}}, \tag{2.12}$$

where

$$\lambda^2 = \frac{2}{3}\left(\frac{c}{a}\right)^2.$$

2.2 Reciprocal Lattices

2.2.1 Why Reciprocal Space?

To determine a real space lattice structure, the most popular experimental technique is some form of diffraction. Methods include x-ray, electron, atom, and neutron diffraction. The particles in these techniques have dual properties and behave as matter waves through the de Broglie relationship, $\lambda = h/p$, where λ is wavelength, h is Planck's constant ($= 6.63 \times 10^{-34}$ J · s), and p is the magnitude of momentum. The propagation of a wave is described by the advancement of a wave front. Assuming a plane wave propagation, the wavevector $\mathbf{k}_{in}$ is perpendicular to the plane wave front. The relationship between $\mathbf{p}$ and $\mathbf{k}$ is $\mathbf{p} = [h/(2\pi)]\,\mathbf{k}$. From the de Broglie relationship ($\lambda = h/p$ and $\mathbf{p} = [h/(2\pi)]\,\mathbf{k}$), one obtains $|\mathbf{k}| = 2\pi/\lambda$. Note that the wavevector $\mathbf{k}_{in}$ has a unit of inverse length. It is convenient to define a reciprocal space lattice in the momentum space that is related to the real space lattice. The symmetry of a real space lattice and the symmetry of its reciprocal space lattice is related. The unit vectors in the reciprocal space lattice have a reciprocal relationship with the unit vectors in the real space lattice. Here we give a simple description of the relationship. A more detailed discussion of the problem will be presented in Chap. 3.

We have introduced real-space lattice points, basic unit vectors, the direction of a real-space plane, and interplanar spacing d_{hkl}. Reciprocal space also consists of reciprocal lattice points and reciprocal vectors. We can relate real space and reciprocal space using geometry in an actual diffraction experiment.

The diffraction of a wave involves an incoming wavevector $\mathbf{k}_{in}$ and a scattered wavevector $\mathbf{k}_{out}$. The direction of $\mathbf{k}_{out}$ differs from the direction of $\mathbf{k}_{in}$ (except in the forward scattering case where $\mathbf{k}_{out} = \mathbf{k}_{in}$). The difference in direction is the scattering angle 2θ. See Fig. 2.9a. If the scattering is elastic then $|\mathbf{k}_{out}| = |\mathbf{k}_{in}| = |\mathbf{k}| = k$. We consider specular scattering, $\theta_{in} = \theta_{out} = \theta$. See Fig. 2.9b. The change in wavevectors or the momentum transfer is defined as $\mathbf{K} = \mathbf{k}_{out} - \mathbf{k}_{in}$. Applying trigonometry as shown in Fig. 2.9, one obtains

$$\sin\theta = \frac{|\mathbf{K}/2|}{|\mathbf{k}_{in}|}, \tag{2.13}$$

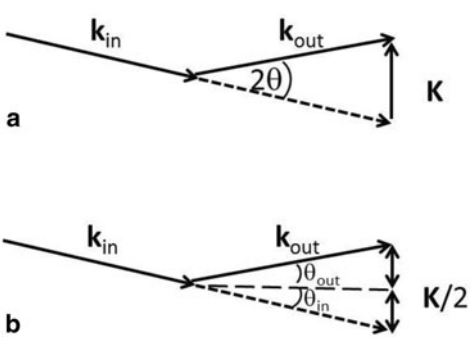

Fig. 2.9 Wave scattering from a sample. **a** The scattering angle is 2θ, and the outgoing wavevector $\mathbf{k}_{out}$ has a momentum change $\mathbf{K}$, relative to the incoming wavevector $\mathbf{k}_{in}$. **b** Specular scattering where $\theta_{out} = \theta_{in} = \theta$

or

$$|\mathbf{K}| = 2\,|\mathbf{k}_{in}|\sin\theta. \tag{2.14}$$

Using $k = 2\pi/\lambda$, one obtains

$$|\mathbf{K}| = \frac{4\pi\sin\theta}{\lambda}. \tag{2.15}$$

In a scattering experiment, one knows the wavelength λ and can measure the scattering angle 2θ, and then the magnitude of $\mathbf{K}$ change can be obtained from Eq. (2.15).

2.2.2 Bragg Condition

We will see that this change of momentum $\mathbf{K}$ is related to interplanar spacing d_{hkl} in a real-space crystal. Figure 2.10 illustrates this. The incoming wavevector $\mathbf{k}_{in}$ is incident on the first plane (plane 1) with an angle θ_{in}, and it is scattered as ray 1. The outgoing wavevector $\mathbf{k}_{out}$ is scattered specularly with $\theta_{out} = \theta_{in}$. The same wave scattering from the second plane is ray 2. The interplanar spacing d_{hkl} is the perpendicular distance between the first and second planes or a to b. The path length of ray 2 travels more than that of ray 1. The path length difference is

$$cb + bd = d_{hkl}\sin\theta + d_{hkl}\sin\theta = 2d_{hkl}\sin\theta. \tag{2.16}$$

If this path-length difference is an integer number n of wavelength λ, then a constructed interference occurs to give the maximum intensity. This is Bragg's law.

$$2d_{hkl}\sin\theta_B = n\lambda. \tag{2.17}$$

Combining Eqs. (2.15) and (2.17), we obtain the reciprocal relationship between the change of wavevectors $\mathbf{K_B}$ and the interplanar spacing d_{hkl} at the Bragg condition,

$$|\mathbf{K}_B| = \frac{2\pi n}{d_{hkl}}. \tag{2.18}$$

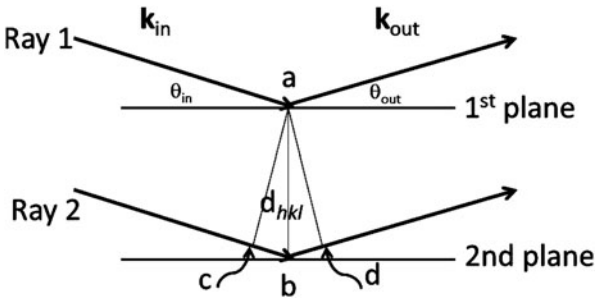

Fig. 2.10 Bragg scattering from two parallel planes. $\theta_{out} = \theta_{in} = \theta$ for specular diffraction. Wave 2 travels $2d_{hkl}\sin\theta$ further than wave 1

Later, in Sect. 2.2.4, we will show that $d_{hkl} = \frac{2\pi}{|\mathbf{G}(hkl)|}$, where $\mathbf{G}(hkl)$ is a reciprocal lattice vector. At Bragg condition, a constructive interference occurs, and this momentum change $\mathbf{K}_B$ is equal to a vector $\mathbf{G}(hkl)$ in the reciprocal space (Williams and Carter 1996),

$$\mathbf{K}_B = \mathbf{G}(hkl). \tag{2.19}$$

2.2.3 Reciprocal Space Basic Vectors and their Relationship to Real Space Basic Vectors

In general, a diffraction experiment involves a 3D sample. The previous derivation is for one dimension. In the following, the real space and reciprocal space relationship in terms of vectors in three dimensions will be derived. We have defined the position vector of a lattice point in a 3D crystal in real space by

$$\boldsymbol{r}_n = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}, \tag{2.20}$$

where n_1, n_2, and n_3 are integers and **a**, **b**, and **c** are real space unit vectors.

In Fig. 2.11, we sketched one unit cell in real space with basic vectors **a**, **b**, and **c**. Similarly, we can also define a reciprocal lattice vector $\mathbf{G}(hkl)$

$$\mathbf{G}(hkl) = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*, \tag{2.21}$$

where h, k, and l are the Miller indices of a crystal plane (hkl) and $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$ are reciprocal unit vectors.

Mathematically, one can show that $\mathbf{G}(hkl) \bullet \boldsymbol{r}_n$ is always an integer,

$$\mathbf{G}\,(hkl) \bullet \boldsymbol{r}_n = \text{integer}. \tag{2.22}$$

Or

$$\left(h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*\right) \bullet (n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}) = \text{integer}. \tag{2.23}$$

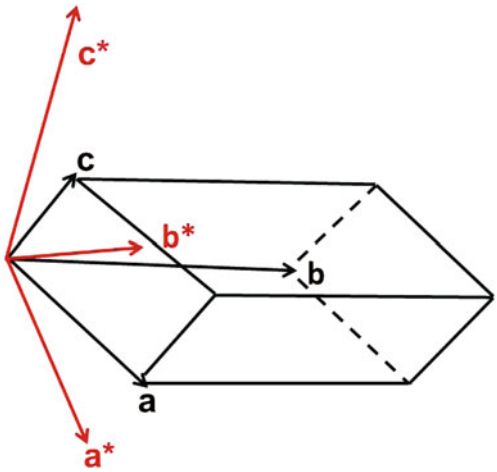

Fig. 2.11 Reciprocal basic vectors $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$ and their relationship to the real-space basic vectors **a**, **b**, and **c**

From vector algebra, when the previous equation is satisfied, one obtains the reciprocal lattice vectors

$$\mathbf{a}^* = 2\pi\frac{\mathbf{b}\times\mathbf{c}}{\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})}, \mathbf{b}^* = 2\pi\frac{\mathbf{c}\times\mathbf{a}}{\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})}, \mathbf{c}^* = 2\pi\frac{\mathbf{a}\times\mathbf{b}}{\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})}, \tag{2.24}$$

Where $\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c})$ is the volume V of a unit cell in real space. See Fig. 2.11. The previous relationships can be rewritten as

$$\mathbf{a}^* = 2\pi\frac{\mathbf{b}\times\mathbf{c}}{\mathrm{V}}, \mathbf{b}^* = 2\pi\frac{\mathbf{c}\times\mathbf{a}}{\mathrm{V}}, \mathbf{c}^* = 2\pi\frac{\mathbf{a}\times\mathbf{b}}{\mathrm{V}}. \tag{2.25}$$

This means vector $\mathbf{a}^*$ is the cross product of **b** and **c** or $\mathbf{a}^*$ is perpendicular to the plane consisting of **b** and **c**. Using the right-hand rule, one obtains $\mathbf{a}^*$, shown in Fig. 2.11. Similarly, $\mathbf{b}^*$ is obtained from the cross product of **c** and **a**, and $\mathbf{c}^*$ is obtained from the cross product of **a** and **b**. Vectors **a**, **b**, and **c** are related to $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$ as

$$\mathbf{a}^*\cdot\mathbf{b} = \mathbf{a}^*\cdot\mathbf{c} = \mathbf{b}^*\cdot\mathbf{a} = \mathbf{b}^*\cdot\mathbf{c} = \mathbf{c}^*\cdot\mathbf{a} = \mathbf{c}^*\cdot\mathbf{b} = 0, \tag{2.26}$$

and

$$\mathbf{a}^*\cdot\mathbf{a} = \mathbf{b}^*\cdot\mathbf{b} = \mathbf{c}^*\cdot\mathbf{c} = 2\pi. \tag{2.27}$$

The magnitude of $\mathbf{a}^*$ is inversely proportional to the magnitude of **a**. The same relationship is true for $\mathbf{b}^*$ and $\mathbf{c}^*$. This means the size of a reciprocal lattice unit cell is inversely proportional to the size of the real space unit cell.

One can obtain the reciprocal unit vectors $\mathbf{a}^*$, $\mathbf{b}^*$, and $\mathbf{c}^*$ from **a**, **b**, and **c** in the previous relationships. A reciprocal lattice can be generated by $\mathbf{G}(hkl) = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$, where h, k, and l are integers.

We illustrate the relationship between the reciprocal unit vectors and the real space unit vectors in a two-dimensional lattice shown in Fig. 2.12. A two-dimensional real

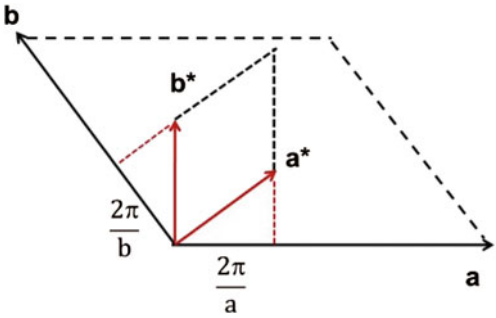

Fig. 2.12 Relationship between real-space basic vectors **a** and **b** and reciprocal-space basic vectors $\mathbf{a}^*$ and $\mathbf{b}^*$

space unit mesh consists of unit vectors **a** and **b** that are parallel to the page. The $\mathbf{a}^*$ is perpendicular to **b**, and the $\mathbf{b}^*$ is perpendicular to **a**. Also, the length of $\mathbf{a}^*$ projected on **a** is $2\pi/a$ and is the inverse of the length of **a**. Also, $\mathbf{b}^*$ and **b** are related in a similar way.

For example, if one has the (001) plane in real space, the reciprocal lattice direction in the reciprocal space can be determined as $\mathbf{G}(hkl) = \mathbf{G}(001) = \mathbf{c}^*$ since $h = 0$, $k = 0$, and $l = 1$. This means $\mathbf{G}(001)$ is perpendicular to **a** and **b** (because of the cross product of $\mathbf{a} \times \mathbf{b}$) and its magnitude is inversely proportional to the magnitude of **c**.

2.2.4 *Reciprocal Lattice Vector and its Relationship to Interplanar Spacing*

We can further examine the direction and magnitude of the reciprocal lattice vector $\mathbf{G}(hkl)$ for a general case. The (hkl) plane is defined as a plane intercepting the **a**, **b**, and **c** axes at a/h, b/k, and c/l, respectively. The plane ABC shown in Fig. 2.13 represents the (hkl) plane. The vectors **AB** and **AC** equal $\mathbf{b}/k - \mathbf{a}/h$ and $\mathbf{c}/l - \mathbf{a}/h$, respectively. The cross product **AB** × **AC** is a vector $\mathbf{G}(hkl)$ perpendicular to the (hkl) plane or parallel to the normal of the (hkl) plane.

$$\mathbf{G}(hkl) = \mathbf{AB} \times \mathbf{AC} = hkl\left[\frac{\mathbf{b} \times \mathbf{c}}{h} + \frac{\mathbf{c} \times \mathbf{a}}{k} + \frac{\mathbf{a} \times \mathbf{b}}{l}\right]. \tag{2.28}$$

The unit vector

$$\mathbf{n} = \frac{\mathbf{G}(hkl)}{|\mathbf{G}(hkl)|}. \tag{2.29}$$

To obtain the shortest distance d_{hkl} between a family of (hkl) planes, that is, the distance from point O to the (hkl) plane, one can take the dot product of **OA** or any vector in the (hkl) plane and **n**.

$$d_{hkl} = \frac{\mathbf{a}}{h} \cdot \mathbf{n} = \frac{\mathbf{a}}{h} \cdot \frac{\mathbf{G}(hkl)}{|\mathbf{G}(hkl)|} = \frac{\mathbf{a}}{h} \cdot \frac{(h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*)}{|\mathbf{G}(hkl)|} = \frac{2\pi}{|\mathbf{G}(hkl)|}. \tag{2.30}$$

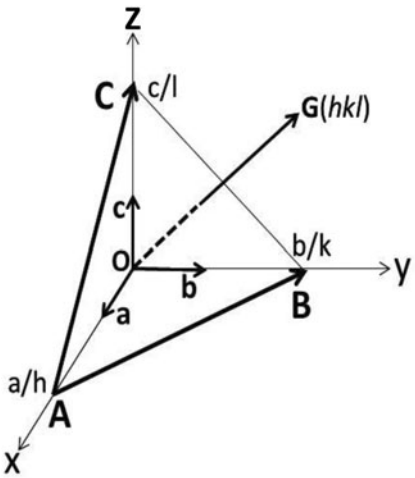

Fig. 2.13 Reciprocal lattice vector **G**(*hkl*) is perpendicular to the (*hkl*) plane consisting of vectors **AB** and **AC** with interception a/*h*, b/*k*, and c/*l* on x-, y-, and z-axes

For example, to find out the value of d_{001}, one first calculates

$$|\mathbf{G}(001)| = \left|0\mathbf{a}^* + 0\mathbf{b}^* + 1\mathbf{c}^*\right| = \left|1\mathbf{c}^*\right|, \tag{2.31}$$

and then

$$d_{001} = \frac{2}{\mathbf{G}(001)} = \frac{2}{|\mathbf{c}^*|} = \frac{2\pi}{\left|\frac{2\pi}{\mathbf{c}}\right|} = |\mathbf{c}| = \mathrm{c}. \tag{2.32}$$

2.2.5 *Reciprocal Lattice Vector and Interplanar Spacing Applied to a Hexagonal Lattice*

Using the primitive vectors **a**, **b**, and **c** in Eq. (2.9) for real space and substituting these vectors in the definition of reciprocal primitive vectors (**a***, **b***, and **c***) in Eq. (2.24), one can obtain the primitive vectors in the reciprocal space for a hexagonal lattice.

$$\begin{aligned}
\mathbf{a}^* &= \left(\frac{2\pi}{\mathrm{a}}\right)\frac{\sqrt{3}\hat{\mathrm{x}} + \hat{\mathrm{y}}}{\sqrt{3}}, \\
\mathbf{b}^* &= \left(\frac{2\pi}{\mathrm{a}}\right)\frac{2\hat{\mathrm{y}}}{\sqrt{3}}, \\
\mathbf{c}^* &= \left(\frac{2\pi}{\mathrm{c}}\right)\hat{\mathrm{z}}.
\end{aligned} \tag{2.33}$$

Substitute **a***, **b***, and **c*** into the reciprocal lattice vector **G**(*hkl*) for a hexagonal lattice, and one obtains

$$\mathbf{G}(hkl) = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* = 2\pi\left(\frac{h}{\mathrm{a}}\hat{\mathrm{x}} + \frac{h+2k}{\mathrm{a}\sqrt{3}}\hat{\mathrm{y}} + \frac{l}{\mathrm{c}}\hat{\mathrm{z}}\right). \tag{2.34}$$

Substituting Eq. (2.34) in Eq. (2.30), the spacing d_{hkl} between the family of planes with Miller indices (hkl) is

$$\frac{1}{d_{hkl}^2} = \frac{|\mathbf{G}(hkl)|^2}{4\pi^2} = \frac{h^2}{a^2} + \frac{h^2 + 4hk + 4k^2}{3a^2} + \frac{l^2}{c^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}. \tag{2.35}$$

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