2

Lattices, planes and directions

- *How does a crystal lattice differ from a crystal structure?*
- *What is a primitive unit cell?*
- *What are Miller-Bravais indices used for?*

The development of the idea of a lattice was among the earliest mathematical explorations in crystallography. Crystal structures and crystal lattices are different, although these terms are frequently (and incorrectly) used as synonyms. A crystal **structure** is built of **atoms**. A crystal **lattice** is an infinite pattern of **points**, each of which must have the same surroundings in the same orientation. A lattice is a mathematical concept.

All crystal structures can be built up from a lattice by placing an atom or a group of atoms at each lattice point. The crystal structure of a simple metal and that of a complex protein may both be described in terms of the same lattice, but whereas the number of atoms allocated to each lattice point is often just one for a simple metallic crystal, it may easily be thousands for a protein crystal.

2.1 Two-dimensional lattices

In two dimensions, if any lattice point is chosen as the origin, the position of any other lattice point is defined by the vector $\mathbf{P}(uv)$:

$$\mathbf{P}(uv) = u\mathbf{a} + v\mathbf{b} \qquad (2.1)$$

where the vectors **a** and **b** define a parallelogram and u and v are integers. The parallelogram is the **unit cell** of the lattice, with sides of length a and b. The coordinates of the lattice points are indexed as u, v, (Figure 2.1). Standard crystallographic terminology writes negative values as $\bar{u}$ and $\bar{v}$, (pronounced u bar and v bar). To agree with the convention for crystal systems given in Table 1.1, it is usual to label the angle between the lattice vectors, γ. The **lattice parameters** are the lengths of the axial vectors and the angle between them, a, b and γ. The choice of the vectors **a** and **b**, which are called the **basis vectors** of the lattice, is completely arbitrary, and any number of unit cells can be constructed. However, for crystallographic purposes it is most convenient to choose as small a unit cell as possible and one that reveals the symmetry of the lattice.

Despite the multiplicity of possible unit cells, only five unique two-dimensional or **plane lattices**

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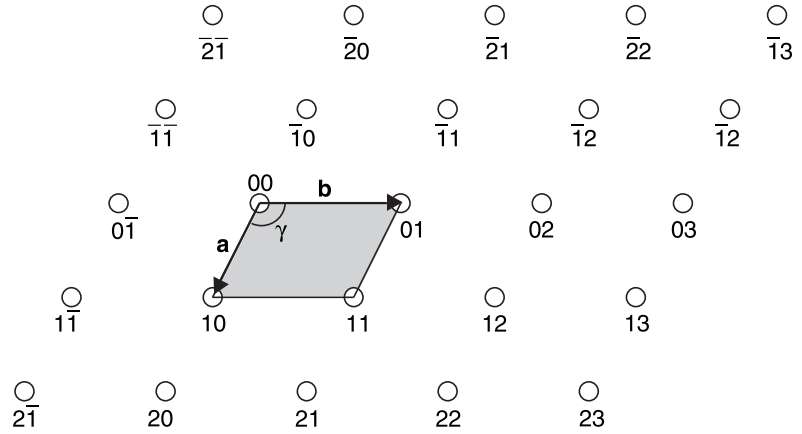


Figure 2.1 Part of an infinite lattice: the numbers are the indices, *u*, *v*, of each lattice point. The unit cell is shaded. Note that the points are exaggerated in size and do not represent atoms

are possible, (Figure 2.2). Those unit cells that contain only one lattice point are called **primitive** cells, and are labelled *p*. They are normally drawn with a lattice point at each cell corner, but it is easy to see that the unit cell contains just one lattice point by mentally displacing the unit cell outline slightly. There are four primitive plane lattices, oblique, (*mp*), (Figure 2.2a), rectangular, (*op*),

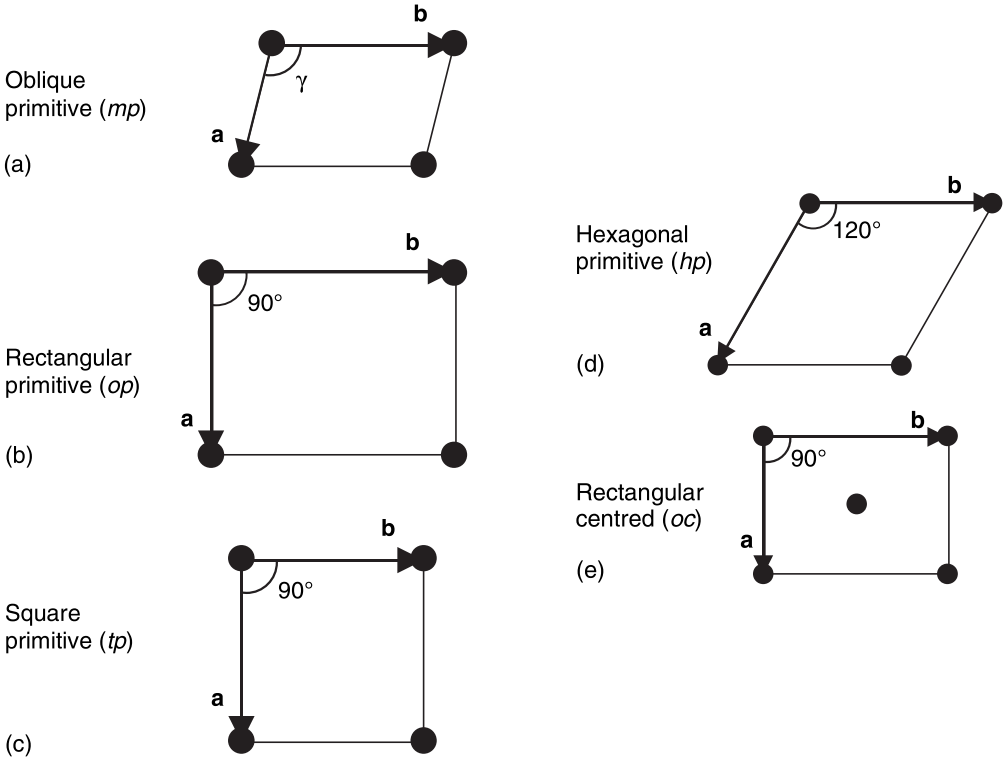


Figure 2.2 The unit cells of the five plane lattices: (a) oblique, (*mp*); (b) rectangular, (*op*); (c) square, (*tp*); (d) hexagonal, (*hp*); (e) rectangular centred, (*oc*)

(Figure 2.2b), square, (*tp*), (Figure 2.2c), and hexagonal, (*hp*), (Figure 2.2d).

The fifth plane lattice contains one lattice point at each corner and one in the unit cell centre. Such unit cells are called **centred** cells, and are labelled *c*. In this particular case, as the lattice is rectangular it is designated *oc*, (Figure 2.2e). The unit cell contains two lattice points, as can be verified by displacing the unit cell outline slightly. It is easily seen that this lattice could also be drawn as a primitive lattice, (Figure 2.3). This latter lattice, known as a rhombic (*rp*) lattice, has the two basis vectors of equal length, and an interaxial angle, γ, different from 90°. In terms of the basis vectors of the centred *oc* cell, **a** and **b**, the basis vectors of the rhombic *rp* cell, $\mathbf{a}'$ and $\mathbf{b}'$ are:

$$\mathbf{a}' = \tfrac{1}{2}(\mathbf{a} + \mathbf{b}); \quad \mathbf{b}' = \tfrac{1}{2}(-\mathbf{a} + \mathbf{b})$$

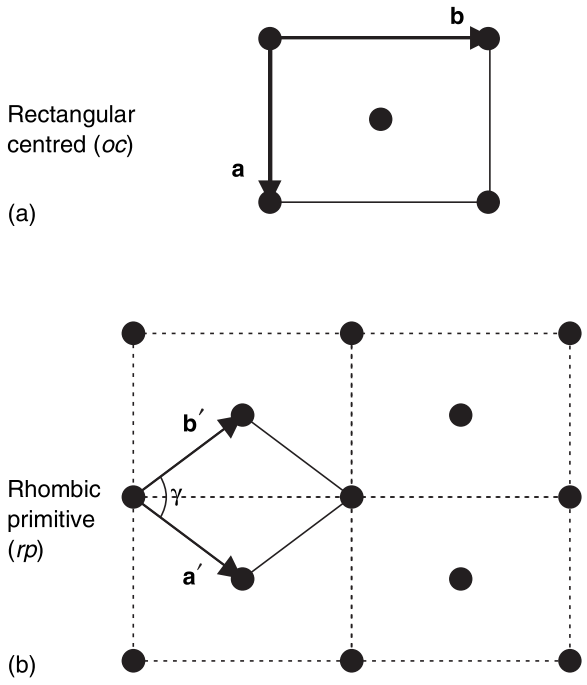


Figure 2.3 The relationship between the rectangular (*oc*) lattice (a) and (b) the equivalent rhombic primitive (*rp*) designation of the same lattice

Table 2.1 The five plane lattices

Crystal system (Lattice type)	Lattice symbol	Lattice parameters
Oblique	*mp*	$a \neq b$, $\gamma \neq 90°$
Rectangular primitive	*op*	$a \neq b$, $\gamma = 90°$
Rectangular centred	*oc*	$a \neq b$, $\gamma = 90°$
	rp	$a' = b'$, $\gamma \neq 90°$
Square	*tp*	$a = b$, $\gamma = 90°$
Hexagonal	*hp*	$a = b$, $\gamma = 120°$

Note that this is a vector equation and the terms are to be added vectorially (see Appendix 1). The five plane lattices are summarised in Table 2.1.

Although the lattice points in any primitive cell can be indexed in accordance with equation (2.1), using integer values of *u* and *v*, this is not possible with the *oc*-lattice. For example, taking the basis vectors as the unit cell sides, the coordinates of the two lattice points in the unit cell are 0, 0 and ½, ½. For crystallographic purposes it is better to choose a basis that reflects the symmetry of the lattice rather than stick to the rigid definition given by equation (2.1). Because of this, lattices in crystallography are defined in terms of **conventional crystallographic bases** (and hence **conventional crystallographic unit cells**). In this formalism, the definition of equation (2.1) is relaxed, so that the coefficients of each vector, *u*, *v*, must be either **integral** or **rational**. (A rational number is a number that can be written as a/b where both *a* and *b* are integers.) The oc lattice makes use of this definition, as the rectangular nature of the lattice is of prime importance. Remember though, that the *oc* and *rp* definitions are simply alternative descriptions of the same array of points. The lattice remains unique. It is simply necessary to use the description that makes things easiest.

It is an axiomatic principle of crystallography that a lattice cannot take on the symmetry of a regular pentagon. It is easy to see this. Suppose

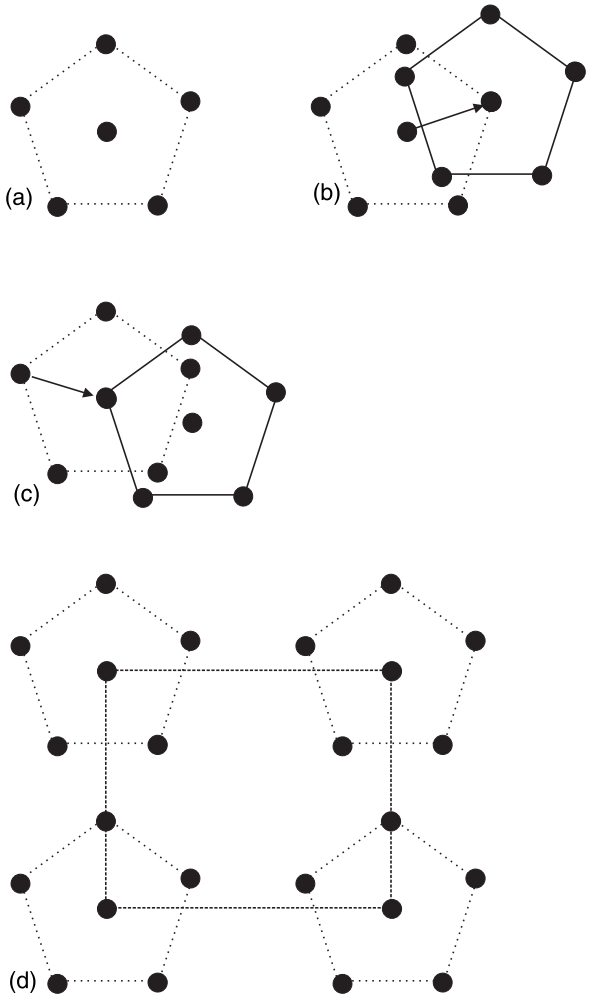


Figure 2.4 Lattices with pentagonal symmetry cannot form: (a) a fragment of a 'lattice' with pentagonal symmetry; (b, c) displacement of the fragment by a lattice vector does not extend the lattice; (d) fragments with pentagonal symmetry can be part of a pattern by placing each on a lattice point

that a lattice fragment is drawn in which a lattice point is surrounded by five others arranged at the vertices of a regular pentagon, (Figure 2.4a). Now each point in a lattice must have the exactly the same surroundings as any other lattice point. Displacement of the fragment by a lattice vector (Figure 2.4b,c) will show that some points are seen to be closer than others, which means that the construction is not a lattice. However, the fragment can form part of a pattern by placing the fragment itself upon each point of a lattice, in this case an *op* lattice (Figure 2.4d).

2.2 Unit cells

The unit cells described above are conventional crystallographic unit cells. However, the method of unit cell construction described is not unique. Other shapes can be found that will fill the space and reproduce the lattice. Although these are not often used in crystallography, they are encountered in other areas of science. The commonest of these is the **Wigner-Seitz** cell.

This cell is constructed by drawing a line from each lattice point to its nearest neighbours, (Figure 2.5a). A second set of lines is then drawn normal to the first, through the midpoints, (Figure 2.5b). The polygon so defined, (Figure 2.5c), is called the **Dirichlet region** or the Wigner-Seitz cell. Because of the method of construction, a Wigner-Seitz cell will always be primitive. Three-dimensional equivalents are described in Section 2.5.

2.3 The reciprocal lattice in two dimensions

Many of the physical properties of crystals, as well as the geometry of the three-dimensional patterns of radiation diffracted by crystals, (see Chapter 6) are most easily described by using the **reciprocal lattice**. The two-dimensional (plane) lattices, sometimes called the **direct lattices**, are said to occupy **real space**, and the reciprocal lattice occupies **reciprocal space**. The concept of the reciprocal lattice is straightforward. (Remember, the reciprocal lattice is simply another lattice.) It is defined in terms of two basis vectors labelled **a*** and **b***.

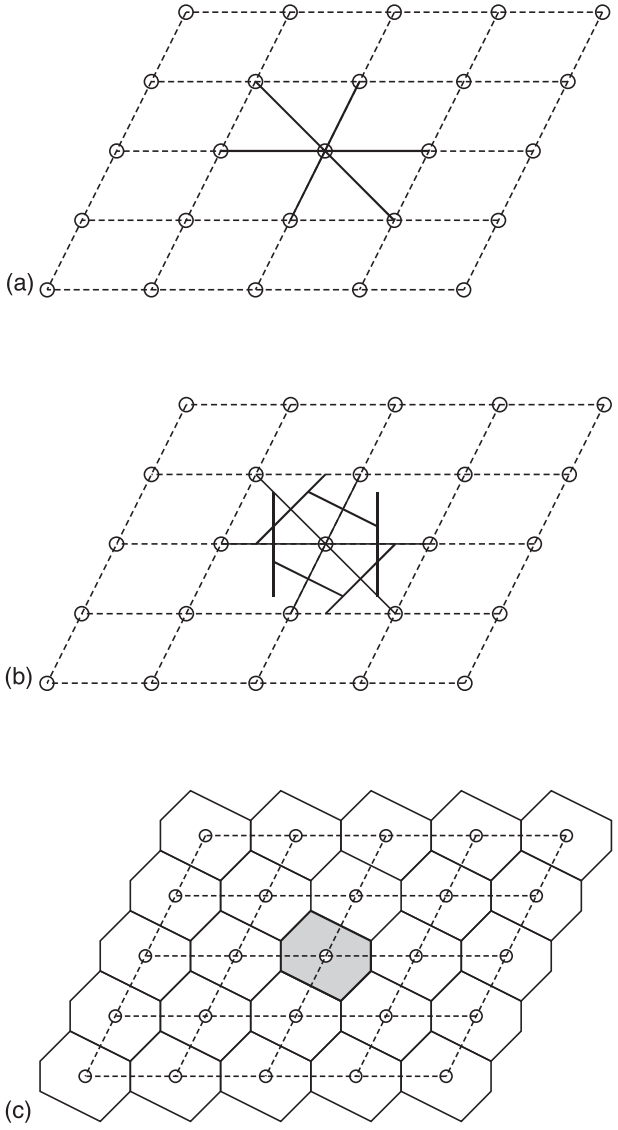


Figure 2.5 The construction of a Wigner-Seitz cell or Dirichlet region: (a) draw a line from each lattice point to its nearest neighbours; (b) draw a set of lines normal to the first, through their mid-points; (c) the polygon formed, (shaded) is the cell required

The direction of these vectors is perpendicular to the end faces of the direct lattice unit cell. The lengths of the basis vectors of the reciprocal lattice are the inverse of the perpendicular distance from the lattice origin to the end faces of the direct lattice unit cell. For the square and rectangular plane lattices, this is simply the inverse of the lattice spacing:

$$a^* = 1/a, \quad b^* = 1/b$$

For the oblique and hexagonal plane lattices, these are given by:

$$a^* = 1/d_{10}, \quad b^* = 1/d_{01}$$

where the perpendicular distances between the rows of lattice points is labelled d_{10} and d_{01}.

The construction of a reciprocal plane lattice is simple and is illustrated for the oblique plane (*mp*) lattice. Draw the plane lattice and mark the unit cell (Figure 2.6a). Draw lines perpendicular to the two sides of the unit cell. These lines give the axial directions of the reciprocal lattice basis vectors, (Figure 2.6b). Determine the perpendicular distances from the origin of the direct lattice to the end faces of the unit cell, d_{10} and d_{01} (Figure 2.6c). The inverse of these distances, $1/d_{10}$ and $1/d_{01}$, are the reciprocal lattice axial lengths, a^* and b^*.

$$1/d_{10} = a^*$$
$$1/d_{01} = b^*$$

Mark the lattice points at the appropriate reciprocal distances, and complete the lattice, (Figure 2.6d). Note that in this case, as in all real and reciprocal lattice pairs, the vector joining the origin of the reciprocal lattice to a lattice point *hk* is perpendicular to the (*hk*) planes in the real lattice and of length $1/d_{hk}$, (Figure 2.6e).

It will be seen that the angle between the reciprocal axes, **a*** and **b***, is $(180 - \gamma) = \gamma*$, when the angle between the direct axes, **a** and **b**, is γ. It is thus simple to construct the reciprocal lattice by drawing **a*** and **c*** at an angle of $(180 - \gamma)$ and marking out the lattice with the appropriate spacing a^* and b^*.

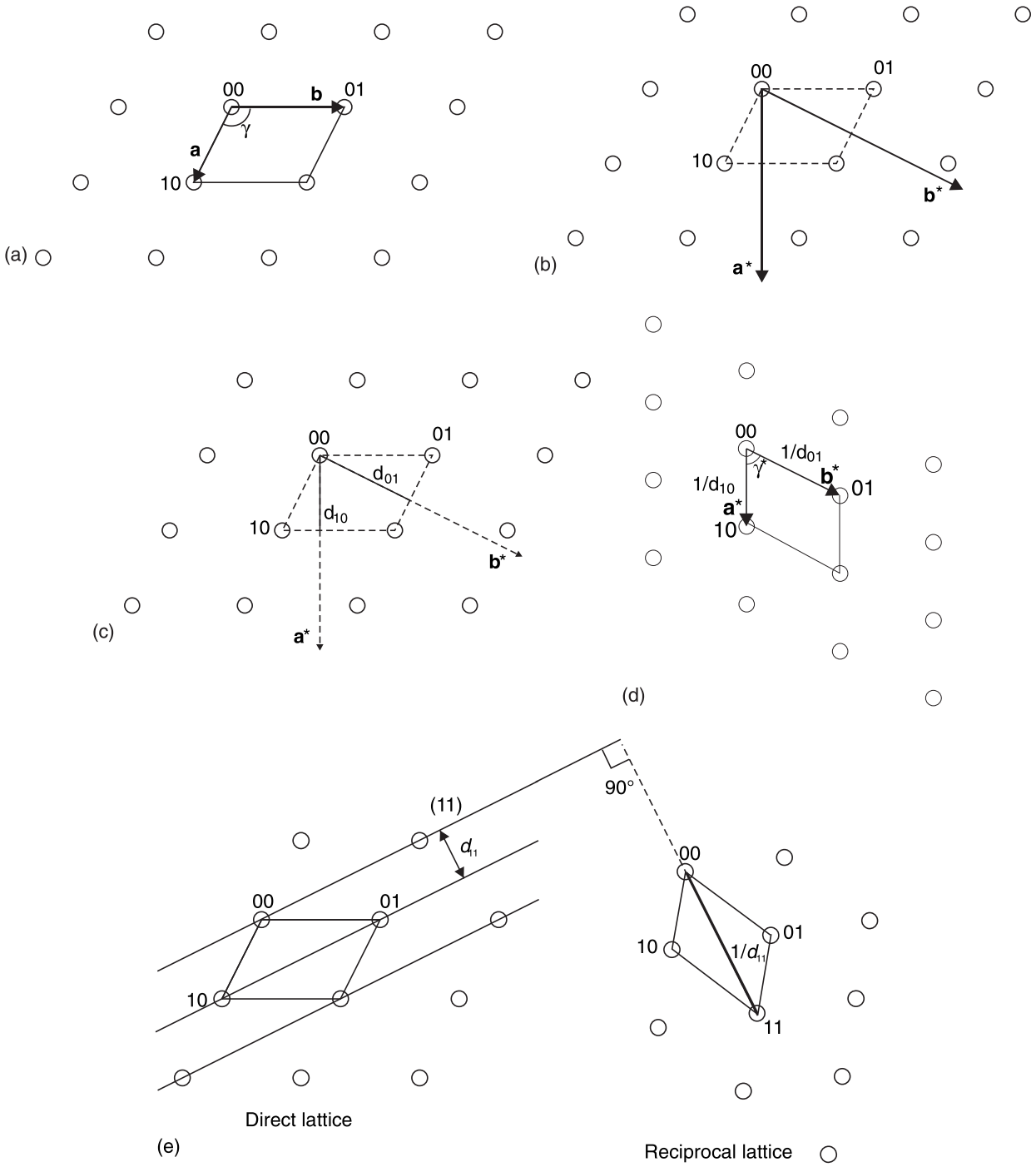


Figure 2.6 The construction of a reciprocal lattice: (a) draw the plane lattice and mark the unit cell; (b) draw lines perpendicular to the two sides of the unit cell to give the axial directions of the reciprocal lattice basis vectors; (c) determine the perpendicular distances from the origin of the direct lattice to the end faces of the unit cell, d_{10} and d_{01}, and take the inverse of these distances, $1/d_{10}$ and $1/d_{01}$, as the reciprocal lattice axial lengths, a^* and b^*; (d) mark the lattice points at the appropriate reciprocal distances, and complete the lattice; (e) the vector joining the origin of the reciprocal lattice to a lattice point hk is perpendicular to the (hk) planes in the real lattice and of length $1/d_{hk}$

Sometimes it can be advantageous to construct the reciprocal lattice of the centred rectangular *oc*-lattice using the primitive unit cell. In this way it will be found that the primitive reciprocal lattice so formed can also be described as a centred rectangular lattice. This is a general feature of reciprocal lattices. Each direct lattice generates a reciprocal lattice of the same type, i.e. $mp \rightarrow mp$, $oc \rightarrow oc$, etc. In addition, the reciprocal lattice of a reciprocal lattice is the direct lattice.

A construction in reciprocal space identical to that used to delineate the Wigner-Seitz cell in direct space gives a cell known as the first **Brillouin zone**, (Figure 2.7). The first Brillouin zone of a lattice is thus a primitive cell.

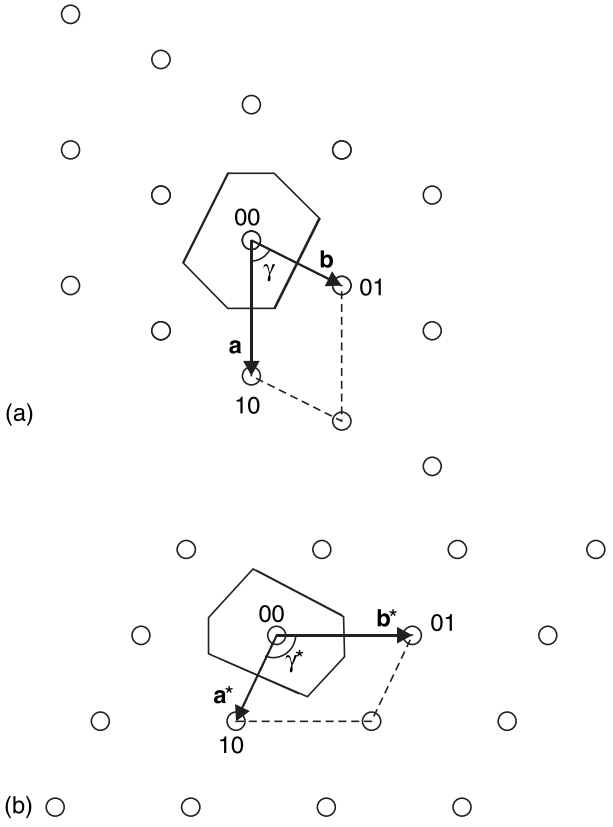


Figure 2.7 The first Brillouin zone of a reciprocal lattice: (a) the real lattice and Wigner-Seitz cell; (b) the reciprocal lattice and first Brillouin zone. The zone is constructed by drawing the perpendicular bisectors of the lines connecting the origin, 00, to the nearest neighbouring lattice points, in an identical fashion to that used to obtain the Wigner-Seitz cell in real space

2.4 Three-dimensional lattices

Three-dimensional lattices use the same nomenclature as the two-dimensional lattice described above. If any lattice point is chosen as the origin, the position of any other lattice point is defined by the vector $\mathbf{P}(uvw)$:

$$\mathbf{P}(uvw) = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

where **a**, **b**, and **c** are the basis vectors, and u, v and w are positive or negative integers or rational numbers. As before, there are any number of ways of choosing **a**, **b** and **c**, and crystallographic convention is to choose vectors that are small and reveal the underlying symmetry of the lattice. The parallelepiped formed by the three basis vectors **a**, **b** and **c**, defines the unit cell of the lattice, with edges of length a, b, and c. The numerical values of the unit cell edges and the angles between them are collectively called the lattice parameters of the unit cell. It follows from the above description that the unit cell is not unique and is chosen for convenience and to reveal the underlying symmetry of the crystal.

There are only 14 possible three-dimensional lattices, called **Bravais** lattices (Figure 2.8). Bravais lattices are sometimes called direct lattices. Bravais lattices are defined in terms of conventional crystallographic bases and cells, (see Section 2.1). The rules for selecting the preferred lattice are determined by the symmetry of the lattice, (see Chapters 3, 4 for information on symmetry). In brief, the *main conditions* are:

(i) The three basis vectors define a right-handed coordinate system, that is, **a** (or x)

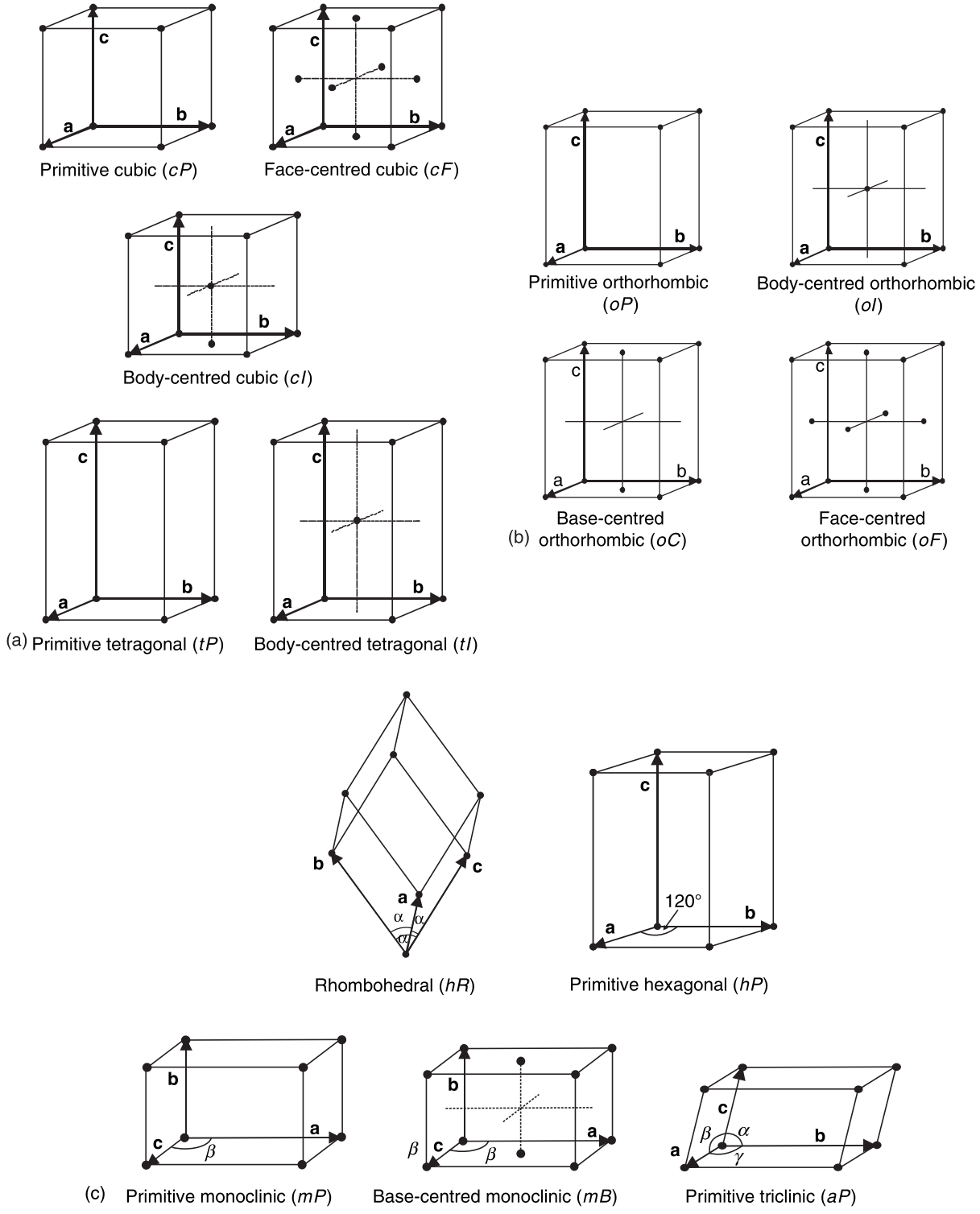


Figure 2.8 The 14 Bravais lattices. Note that the lattice points are exaggerated in size and are not atoms. The monoclinic lattices have been drawn with the **b**-axis vertical, to emphasise that it is normal to the plane containing the **a**- and **c**-axes

points out of the page, **b** (or y) points to the right and **c** (or z) is vertical.

(ii) The **a**, **b** and **c** basis vectors for a cubic lattice are parallel to the three four-fold symmetry axes.

(iii) The basis vector **c** for the hexagonal lattice lies parallel to the unique six-fold symmetry axis; **a** and **b** are along two-fold symmetry axes perpendicular to **c** and at 120° to each other.

(iv) The basis vector **c** for the tetragonal lattice is taken along the unique four-fold symmetry axis; **a** and **c** lie along two-fold symmetry axes perpendicular to each other and **c**.

(v) The basis vectors **a**, **b** and **c** for an orthorhombic crystal lie along three mutually perpendicular two-fold symmetry axes.

(vi) The unique symmetry direction in monoclinic lattices is conventionally labelled **b**; **a** and **c** lie in the lattice net perpendicular to **b** and include an oblique angle.

(vii) A rhombohedral lattice is described in two ways. If described in terms of a hexagonal lattice, **c** lies along the three-fold symmetry axis, with **a** and **c** chosen as for the hexagonal system. In terms of rhombohedral axes, **a**, **b** and **c** are the shortest non-coplanar lattice vectors symmetrically equivalent with respect to the three-fold axis.

(viii) A triclinic cell is chosen as primitive.

The smallest unit cell possible for any of the lattices, the one that contains just one lattice point, is the primitive unit cell. A primitive unit cell, usually drawn with a lattice point at each corner, is labelled *P*. All other lattice unit cells contain more than one lattice point. A unit cell with a lattice point at each corner and one at the centre of the unit cell, (thus containing two lattice points in total), is called a **body-centred** unit cell, and labelled *I*. A unit cell with a lattice point in the middle of each face, thus containing four lattice points, is called a **face-centred** unit cell, and labelled *F*. A unit cell that has just one of the faces of the unit cell centred, thus containing two lattice points, is labelled ***A*-face-centred**, *A*, if the centred faces cut the **a**-axis, ***B*-face-centred**, *B*, if the centred faces cut the **b**-axis and ***C*-face-centred**, *C*, if the centred faces cut the **c**-axis. The 14 Bravais lattices are summarised in Table 2.2. Note that all of the non-primitive Bravais lattices can be described in terms of alternative primitive unit cells.

The rhombohedral primitive lattice is often described in terms of a hexagonal lattice, but the lattice points can also be indexed in terms of a cubic face-centred lattice in the unique case in which the rhombohedral angle α_r is exactly equal to 60°, (also see Section 4.5).

As in two-dimensions, a lattice with a three-dimensional unit cell derived from regular pentagons, such as an icosahedron, cannot be constructed.

2.5 Alternative unit cells

As outlined above, a number of alternative unit cells can be described for any lattice. The most widely used is the Wigner-Seitz cell, constructed in three dimensions in an analogous way to that described in Section 2.2. The Wigner-Seitz cell of a body-centred cubic Bravais *I* lattice is drawn in Figure 2.9a,b. It has the form of a truncated octahedron, centred upon any lattice point, with the square faces lying on the cube faces of the Bravais lattice unit cell. The Wigner-Seitz cell of a face-centred cubic Bravais *F* lattice is drawn in Figure 2.9c,d. The polyhedron is a regular

Table 2.2 Bravais lattices

Crystal system	Lattice symbol	Lattice parameters
Triclinic	*aP*	$a \neq b \neq c$, $\alpha \neq 90°$, $\beta \neq 90°$, $\gamma \neq 90°$;
Monoclinic primitive	*mP*	$a \neq b \neq c$, $\alpha = 90°$, $\beta \neq 90°$, $\gamma = 90°$;
Monoclinic centred	*mC*	
Orthorhombic primitive	*oP*	$a \neq b \neq c$, $\alpha = \beta = \gamma = 90°$
Orthorhombic *C*-face-centred	*oC*	
Orthorhombic body-centred	*oI*	
Orthorhombic face-centred	*oF*	
Tetragonal primitive	*tP*	$a = b \neq c$, $\alpha = \beta = \gamma = 90°$
Tetragonal body-centred	*tI*	
Trigonal (Rhombohedral)	*hR*	$a = b = c$, $\alpha = \beta = \gamma$ (primitive cell); $a' = b' \neq c'$, $\alpha' = \beta' = 90°$, $\gamma' = 120°$ (hexagonal cell)
Hexagonal primitive	*hP*	$a = b \neq c$, $\alpha = \beta = 90°$, $\gamma = 120°$
Cubic primitive	*cP*	$a = b = c$, $\alpha = \beta = \gamma = 90°$
Cubic body-centred	*cI*	
Cubic face-centred	*cF*	

rhombic dodecahedron. Note that it is displaced by ½ **a** with respect to the crystallographic cell, and is centred upon the lattice point marked * in Figure 2.9c. The lattice points labelled A, B, C help to make the relationship between the two cells clearer. Recall that a Wigner-Seitz cell is always primitive. Other unit cells are sometimes of use when crystal structures are discussed, (see Chapter 7).

2.6 The reciprocal lattice in three dimensions

As with the two-dimensional lattices, the three-dimensional (Bravais) lattices, the direct lattices, are said to occupy real space, and the reciprocal lattices occupy reciprocal space. Similarly, a reciprocal lattice is simply a lattice. It is defined in terms of three basis vectors **a***, **b*** and **c***. The direction of these vectors is perpendicular to the end faces of the direct lattice unit cell. This means that a direct axis will be perpendicular to a reciprocal axis if they have different labels, that is, **a** is perpendicular to **b*** and **c***. The reciprocal lattice axes are parallel to the direct lattice axes for cubic, tetragonal and orthorhombic direct lattices, that is, **a** is parallel to **a***, **b** is parallel to **b*** and **c** is parallel to **c***.

A direct lattice of a particular type, (triclinic, monoclinic, orthorhombic, etc.), will give a reciprocal lattice cell of the same type, (triclinic, monoclinic, orthorhombic, etc.). The reciprocal lattice of the cubic *F* direct lattice is a cubic *I* lattice and

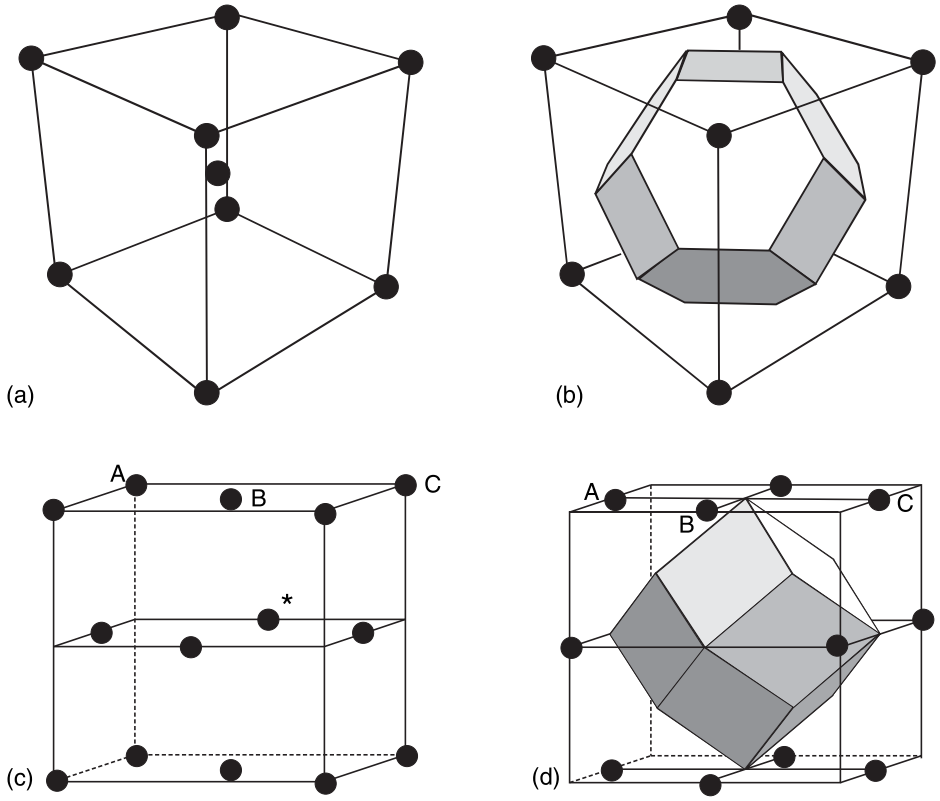


Figure 2.9 Wigner-Seitz cells: (a) the body-centred cubic lattice; (b) the Wigner-Seitz cell of (a); (c) the face-centred cubic lattice; (d) the Wigner-Seitz cell of (c). The face-centred cubic lattice point marked * forms the central lattice point in the Wigner-Seitz cell

the reciprocal lattice of the cubic I lattice is a cubic F lattice.

The reciprocal lattice of a reciprocal lattice is the direct lattice.

The lengths of the basis vectors of the reciprocal lattice, a^*, b^* and c^*, are the inverse of the perpendicular distance from the lattice origin to the end faces of the direct lattice unit cell, d_{100}, d_{010} and d_{001}, that is:

$$a^* = 1/d_{100},\ b^* = 1/d_{010},\ c^* = 1/d_{001}$$

For cubic, tetragonal and orthorhombic lattices, these are equivalent to:

$$a^* = 1/a,\ b^* = 1/b,\ c^* = 1/c$$

The construction of a three-dimensional reciprocal lattice is similar to that for a plane lattice, although more complex in that the third dimension is less easy to portray. The construction of the reciprocal lattice of a P monoclinic lattice is described in Figure 2.10. The direct lattice has a lozenge-shaped unit cell, with the **b**-axis normal to the **a**- and **c**-axes, (Figure 2.10a). To construct the sheet containing the **a*** and **c*** axes, draw the direct lattice unit cell projected down **b**, and draw normals to the end faces of the unit cell, (Figure 2.10b). These give the directions of the reciprocal lattice **a*** and **c*** axes. The reciprocals of the perpendicular distances from the origin to the faces of the unit cell give the axial lengths, (Figure 2.10c). These allow the reciprocal lattice plane to be drawn, (Figure 2.10d).

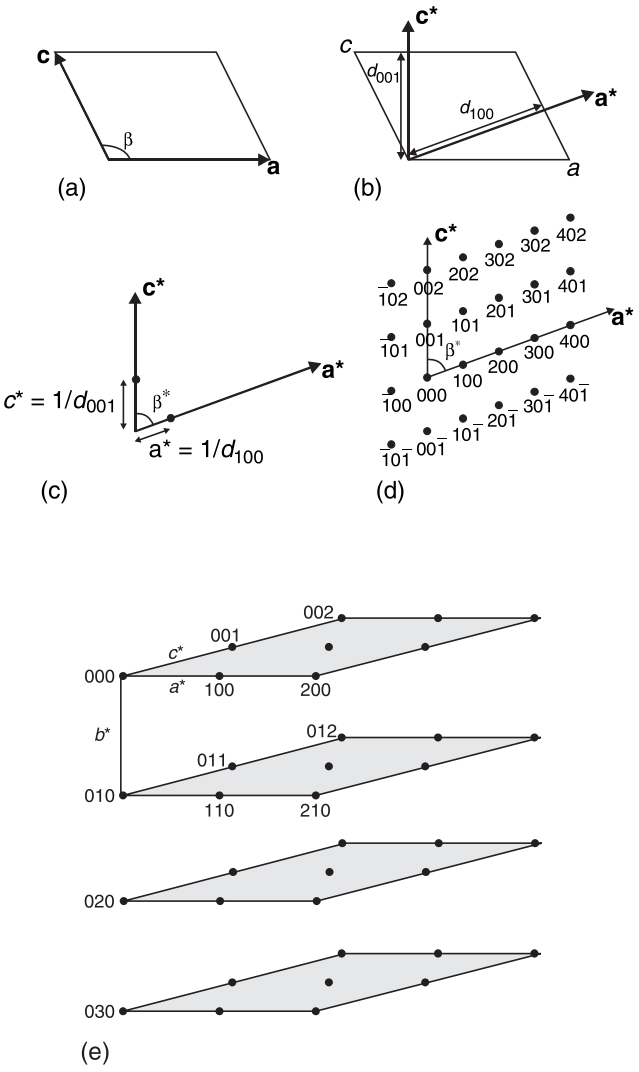


Figure 2.10 The construction of a reciprocal lattice: (a) the **a**–**c** section of the unit cell in a monoclinic (*mP*) direct lattice; (b) reciprocal lattice axes lie perpendicular to the end faces of the direct cell; (c) reciprocal lattice points are spaced $a^* = 1/d_{010}$ and $c^* = 1/d_{001}$; (d) the lattice plane is completed by extending the lattice; (e) the reciprocal lattice is completed by adding layers above and below the first plane

The b-axis is normal to **a** and **c**, and so the **b*** axis is parallel to **b** and normal to the section containing **a*** and **c***, drawn. The length of the **b*** axis is equal to $1/b$. The reciprocal lattice layer containing the 010 point is then identical to Figure 2.10d, but is stacked a distance of **b*** vertically below it, and the layer containing the $0\bar{1}0$ point is vertically above it, (Figure 2.10e). Other layers then follow in the same way.

For some purposes, it is convenient to multiply the length of the reciprocal axes by a constant. Thus, physics texts frequently use a reciprocal lattice spacing 2π times that given above, that is:

$$a^* = 2\pi/d_{100},\ b^* = 2\pi/d_{010},\ c^* = 2\pi/d_{001}.$$

Crystallographers often use a reciprocal lattice scale multiplied by λ, the wavelength of the radiation used to obtain a diffraction pattern, so that:

$$a^* = \lambda/d_{100},\ b^* = \lambda/d_{010},\ c^* = \lambda/d_{001}.$$

As with two-dimensional lattices, the procedure required to construct the (primitive) Wigner-Seitz cell in the direct lattice yields a cell called the first Brillouin zone when applied to the reciprocal lattice. The lattice that is reciprocal to a real space face-centred cubic *F* lattice is a body-centred cubic *I* lattice. The (primitive) Wigner-Seitz cell of the cubic body-centred *I* lattice, (Figure 2.9a), a truncated octahedron, (Figure 2.9b), is therefore identical in shape to the (primitive) first Brillouin zone of a face-centred cubic *F* lattice. In the same way, the lattice that is reciprocal to a real space body-centred cubic *I* lattice is a face-centred cubic *F* lattice. The Wigner-Seitz cell of the real space face-centred cubic *F* lattice, (Figure 2.9c), a regular rhombic dodecahedron, (Figure 2.9d), is identical in shape to the first Brillouin zone of a body-centred centred cubic *I* lattice, (Table 2.3).

Table 2.3 Reciprocal and real space cells

Lattice	Direct lattice	Reciprocal lattice
plane	oblique *mp*: Wigner-Seitz cell Figure 2.7a	oblique *mp*: 1st Brillouin zone Figure 2.7b
cubic 3-d	*F* lattice: Wigner-Seitz cell is a rhombic dodecahedron, Figure 2.9d.	*I* lattice: 1st Brillouin zone is a truncated octahedron, Figure 2.9b
	I lattice: Wigner-Seitz cell is a truncated octahedron, Figure 2.9b	*F* lattice: 1st Brillouin zone is a rhombic dodecahedron, Figure 2.9d

2.7 Lattice planes and Miller indices

As described in Chapter 1, the facets of a well-formed crystal or internal planes through a crystal structure are specified in terms of **Miller Indices**, h, k and l, written in round brackets, (hkl). The same terminology is used to specify planes in a lattice.

Miller indices, (hkl), represent not just one plane, but the set of all identical parallel lattice planes. The values of h, k and l are the reciprocals of the fractions of a unit cell edge, a, b and c respectively, intersected by an appropriate plane. This means that a set of planes that lie parallel to a unit cell edge is given the index 0 (zero) regardless of the lattice geometry. Thus a set of planes that pass across the ends of the unit cells, cutting the **a**-axis at a position 1 a, and parallel to the **b**- and **c**-axes of the unit cell has Miller indices (100), (Figure 2.11a,b). The same principles apply to the other planes shown. The set of planes that lies parallel to the **a**- and **c**-axes, and intersecting the end of each unit cell at a position 1 b have Miller indices (010), (Figure 2.11c,d). The set of planes that lies parallel to the **a**- and **b**-axes, and intersecting the end of each unit cell at a position 1 c have Miller indices (001), (Figure 2.11e,f). Planes cutting both the **a**-axis and **b**-axis at 1 a and 1 b will be (110) planes, (Figure 2.11 g,h), and planes cutting the **a**-, **b**- and **c**-axes at 1 a, 1 b and 1 c will be (111). Remember that the Miller indices refer to a family of planes, not just one. For example, Figure 2.12 shows part of the set of (122) planes, which cut the unit cell edges at 1 a, ½ b and ½ c.

The Miller indices for lattice planes can be determined using a simple method. For generality, take a triclinic lattice, and imagine a set of planes parallel to the **c**-axis, intersecting parallel sheets of lattice points as drawn in Figure 2.13. The Miller indices of this set of planes are determined by travelling along the axes in turn and counting the number of spaces between planes encountered on passing from one lattice point to the next. Thus, in Figure 2.13, three spaces are crossed on going from one lattice point to another along the **a**-direction, so that h is 3. In travelling along the **b**-direction, two spaces are encountered in going from one lattice point to another, so that the value of k is 2. As the planes are supposed to be parallel to the **c**-axis, the value of l is 0. The planes have Miller indices (320). For non-zero values of l, repeat the sketch so as to include **a**- and **c**- or **b**- and **c**-, and repeat the procedure.

The planes described in Figures 2.11, 2.12 and 2.13 are crossed in travelling along positive directions of the axes. Some planes may intersect one of the axes in a positive direction and the other in a negative direction. Negative intersections are written with a negative sign over the index, $\bar{h}$, (pronounced h bar), $\bar{k}$, (pronounced k

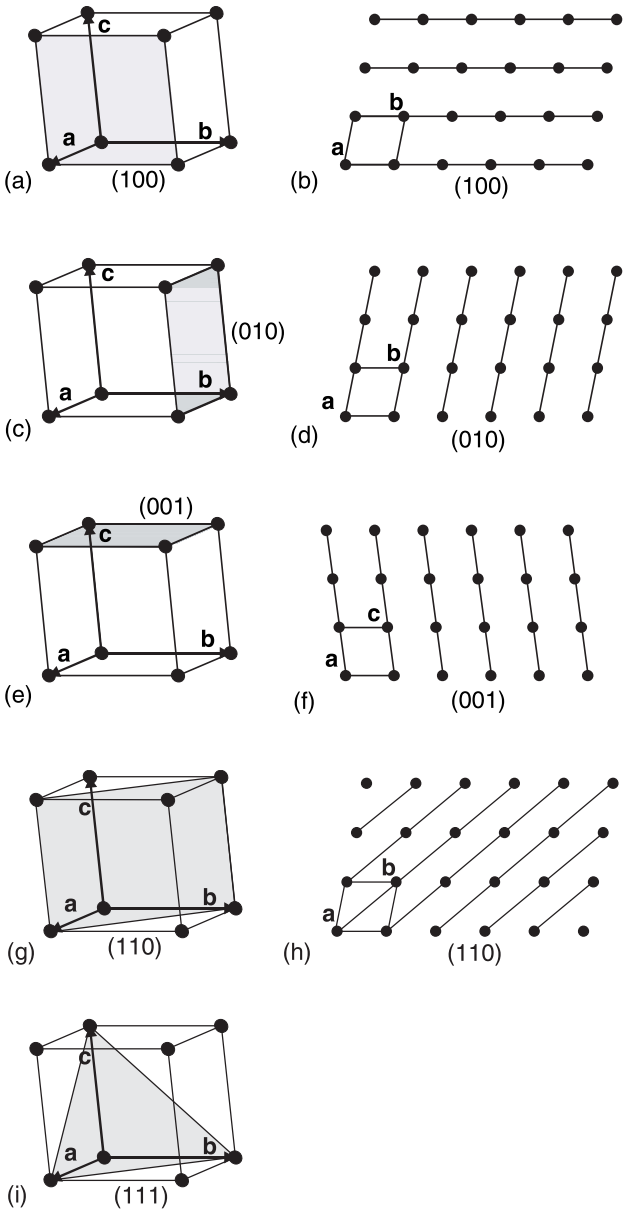


Figure 2.11 Miller indices of lattice planes: (a, b) (100); (c, d) (010); (e, f) (001), (g, h) (110); (i) (111)

bar) and $\bar{l}$, (pronounced l bar). For example, there are four planes related to (110), three of which involve travelling in a negative axial direction in order to count the spaces between the planes encountered, (Figure 2.14). The plane shown as a dotted line in Figure 2.14a cuts the **a**-axis at $+1a$ and the **b**-axis at $+1b$, and the planes have

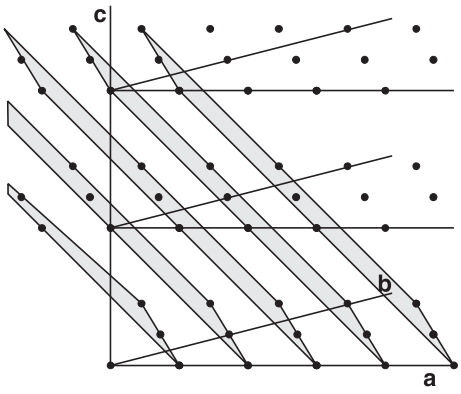


Figure 2.12 Part of the set of (122) lattice planes

Miller indices (110). The plane shown as a dotted line in Figure 2.14b cuts the **a**-axis at $-1a$ and the **b**-axis at $+1b$, and the planes have Miller indices ($\bar{1}$10), (pronounced one bar, one, zero). The plane shown as a dotted line in Figure 2.14c cuts the **a**-axis at $+1a$ and the **b**-axis at $-1b$, and the planes have Miller indices (1$\bar{1}$0), (pronounced one, one bar, zero). Finally the plane shown as a dotted line in Figure 2.14d cuts the **a**-axis in $-1a$ and the **b**-axis in $-1b$, so the planes have Miller indices ($\bar{1}\bar{1}$0), (pronounced one bar, one bar, zero). Note that a ($\bar{1}\,\bar{1}\,0$) plane is identical to a (110) plane, as the position of the axes is arbitrary; they can be placed anywhere on the diagram.

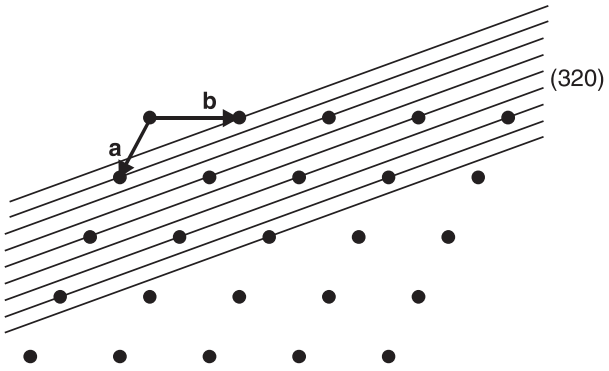


Figure 2.13 Determination of Miller indices: count the spaces crossed on passing along each cell edge, to give (320)

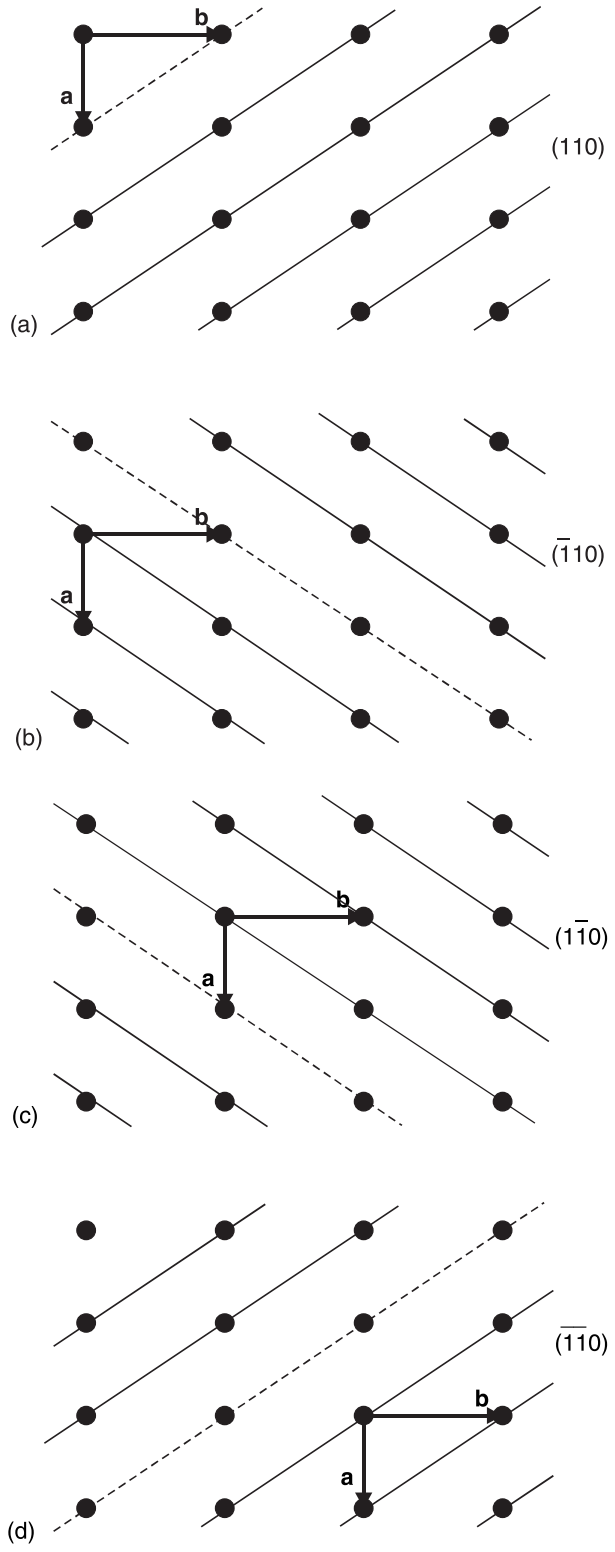


Figure 2.14 Negative Miller indices: (a) (110); (b) $(\bar{1}10)$; (c) $(1\bar{1}0)$; (d) $(\bar{1}\bar{1}0)$

Similarly, planes with Miller indices $(1\bar{1}0)$ are identical to $(\bar{1}10)$ planes.

In the three-dimensional direct and reciprocal lattice pairs, the vector joining the origin of the reciprocal lattice to a lattice point *hkl* is perpendicular to the (*hkl*) planes in the real lattice and of length $1/d_{hkl}$. An alternative method of constructing the reciprocal lattice is thus to draw the normals to the relevant (*hkl*) planes on the direct lattice and plot the reciprocal lattice points along lines parallel to these normals at separations of $1/d_{hkl}$. This method is often advantageous when constructing the reciprocal lattices for all of the face- or body-centred direct lattices. The same is true for the planar direct and reciprocal lattice pairs. The vector joining the origin of the reciprocal lattice to a lattice point *hk* is perpendicular to the (*hk*) planes in the real lattice and of length $1/d_{hk}$.

In lattices of high symmetry, there are always some sets of (hkl) planes that are identical from the point of view of symmetry. For example, in a cubic lattice, the (100), (010) and (001) planes are identical in every way. Similarly, in a tetragonal lattice, (110) and $(\bar{1}10)$ planes are identical. Curly brackets, {hkl}, designate these related planes. Thus, in the cubic system, the symbol {100} represents the three sets of planes (100), (010), and (001), the symbol {110} represents the six sets of planes (110), (101), (011), $(\bar{1}10)$, $(\bar{1}01)$, and $(0\bar{1}1)$, and the symbol {111} represents the four sets (111), $(11\bar{1})$, $(1\bar{1}1)$ and $(\bar{1}11)$.

2.8 Hexagonal lattices and Miller-Bravais indices

The Miller indices of planes in hexagonal lattices can be ambiguous. For example, three sets of planes lying parallel to the **c**-axis, which is imagined to be perpendicular to the plane of the diagram, are shown in (Figure 2.15). These planes have Miller indices A, (110), B, $(1\bar{2}0)$ and C, $(\bar{2}10)$. Although these Miller indices seem to refer

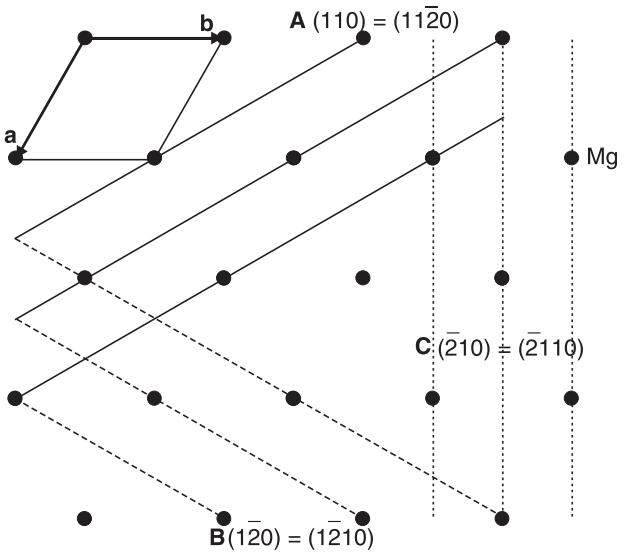


Figure 2.15 Miller-Bravais indices in hexagonal lattices. The three sets of identical planes marked have different Miller indices but similar Miller-Bravais indices

to different types of plane, clearly the three planes are identical, and all are equivalent to the planes through the 'long' diagonal of the unit cell. In order to eliminate this confusion, four indices, (*hkil*), are often used to specify planes in a hexagonal crystal. These are called **Miller-Bravais indices** and are only used in the hexagonal system. The index i is given by:

$$h + k + i = 0, \text{ or } i = -(h + k)$$

In reality this third index is not needed, as it is simply derived from the known values of h and k. However, it does help to bring out the relationship between the planes. Using four indices, the planes are A, (11$\bar{2}$0), B, (1$\bar{2}$10) and C, ($\bar{2}$110). Because it is a redundant index, the value of i is sometimes replaced by a dot, to give indices (*hk.l*). This nomenclature emphasises that the hexagonal system is under discussion without actually including a value for i.

2.9 Miller indices and planes in crystals

In most lattices, and all primitive lattices, there are no planes parallel to (100) with a smaller spacing than the (100) planes, because lattice planes must pass through sheets of lattice points or nodes, (see Figure 2.11). The same can be said of (010), (001), (110) and other planes. However, such planes can be described in crystals, and are significant. These can be characterised in the same way as lattice planes. For example, the fluorite structure, described in Chapter 1, has alternating planes of Ca and F atoms running perpendicular to the **a**-, **b**- and **c**-axes, (see Figure 1.12). Taking the (100) planes as an example, these lie through the end faces of each unit cell and are perpendicular to the **b**- and **c**-axes, (Figure 2.16a). They contain only Ca atoms. A similar plane, also containing only Ca atoms runs through the middle

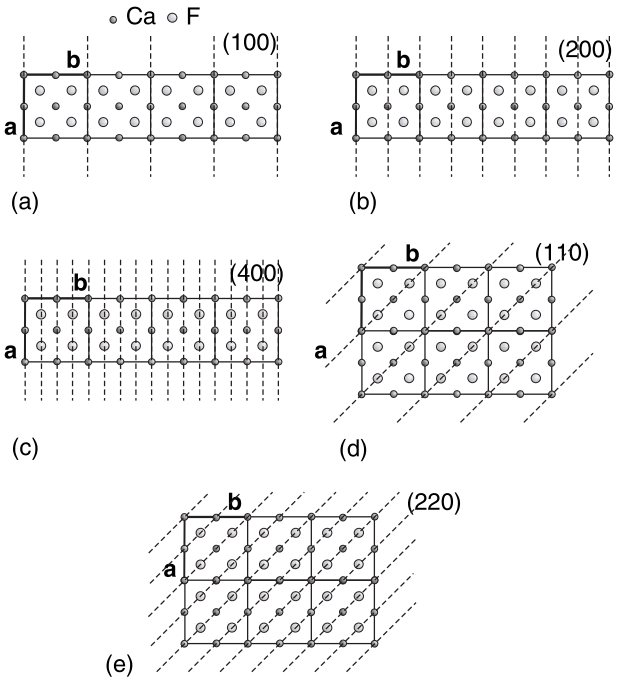


Figure 2.16 Planes in a crystal: (a) (100); (b), (200); (c) (400); (d) (110); (e) (220). The crystal structure is that of fluorite, CaF_2

of the cell. Using the construction described earlier, (Figure 2.13), these can be indexed as (200), as two interplanar spaces are crossed in moving one lattice parameter distance, (Figure 2.16b). Thus all the set of (200) planes contain only Ca atoms. The set of parallel planes with half the spacing of the (200) set will be indexed as (400), as four spaces are crossed in moving one lattice parameter distance. However, these planes are not all identical, as some contain only F atoms and others only Ca atoms, (Figure 2.16c). The Miller indices of (110), (Figure 2.16d) and (220), (Figure 2.16e) planes can be determined in the same way, by counting the spaces crossed in moving along one unit cell length in each direction. The atomic composition of both sets of planes is the same.

Any general set of planes parallel to the **b**- and **c**-axes, and so only cutting the **a** cell edge is written (*h*00). Any general set of planes plane parallel to the **a**- and **c**-axes, and so only cutting the **b** cell-edge has indices (0*k*0) and any general plane parallel to the **a**- and **b**-axes, and so cutting the **c** cell-edge has indices (00*l*). Planes that cut two edges and parallel to a third are described by indices (*hk*0), (0*kl*) or (*h*0*l*). Planes that are at an angle to all three axes have indices (*hkl*). Negative intersections and symmetrically equivalent planes are defined using the same terminology as described in Section 2.7, above.

2.10 Directions

The response of a crystal to an external stimulus such as a tensile stress, electric field, and so on, is frequently dependent upon the direction of the applied stimulus. It is therefore important to be able to specify directions in crystals in an unambiguous fashion. Directions are written generally as [*uvw*] and are enclosed in square brackets. Note that the symbol [*uvw*] includes all parallel directions, just as (*hkl*) specifies a set of parallel planes.

The three indices *u*, *v*, and *w* define the coordinates of a point within the lattice. The index *u* gives the coordinates in terms of the lattice repeat *a* along the **a**-axis, the index *v* gives the coordinates in terms of the lattice repeat *b* along the **b**-axis and the index *w* gives the coordinates in terms of the lattice repeat *c* along the **c**-axis. The direction [*uvw*] is simply the vector pointing from the origin to the lattice point with coordinates *u*, *v*, *w*. The direction [230], with $u = 2$ and $v = 3$, is drawn in Figure 2.17a. Remember, though, that, any parallel direction shares the symbol [*uvw*], because the origin of the coordinate system is not fixed and can always be moved to the starting point of the vector, (Figure 2.17b). (A North wind is always a North wind, regardless of where you stand.)

The direction [100] is parallel to the **a**-axis, the direction [010] is parallel to the **b**-axis and [001] is parallel to the **c**-axis. The direction [111] lies along the body diagonal of the unit cell. Negative values of u, v and w are written $\bar{u}$, (pronounced

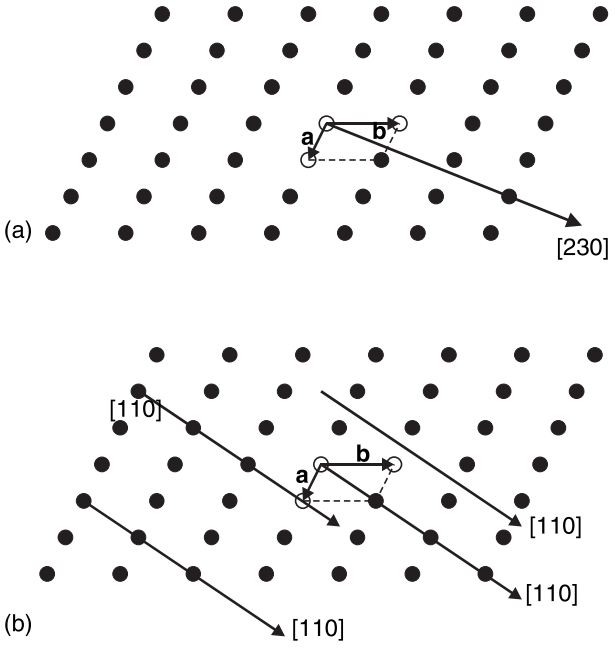


Figure 2.17 Directions in a lattice: (a) [230]; (b) [110]

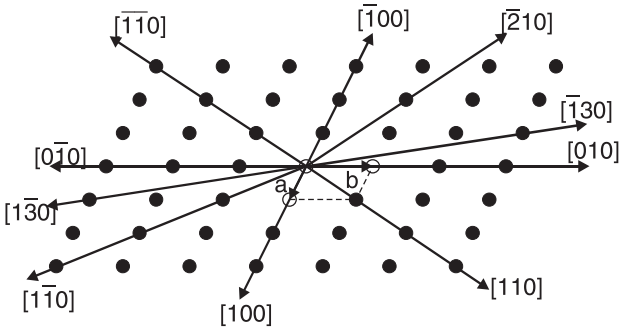


Figure 2.18 Directions in a lattice

u bar), $\bar{v}$, (pronounced v bar) and $\bar{w}$, (pronounced w bar). Further examples of directions in a lattice are illustrated in Figure 2.18. Because directions are vectors, $[uvw]$ is not identical to $[\bar{u}\,\bar{v}\,\bar{w}]$, in the same way that the direction 'North' is not the same as the direction 'South'.

Directions in a crystal are specified in the same way. In these instances the integers u, v, w are applied to the unit cell vectors, **a**-, **b**- and **c**-. As with Miller indices, it is sometimes convenient to group together all directions that are identical by virtue of the symmetry of the structure. These are represented by the notation $\langle$uvw$\rangle$. In a cubic crystal the symbol $\langle 100\rangle$ represents the six directions [100], [$\bar{1}$00], [010], [0$\bar{1}$0], [001], [00$\bar{1}$].

A **zone** is a set of planes, all of which are parallel to a single direction. A group of planes which intersect along a common line therefore forms a zone. The direction that is parallel to the planes, which is the same as the line of intersection, is called the **zone axis**. The zone axis [uvw] is perpendicular to the plane (uvw) in cubic crystals but *not* in crystals of other symmetry.

It is sometimes important to specify a vector with a definite length. In such cases the vector, **R**, is written by specifying the end coordinates, u, v w, with respect to an origin at 0, 0, 0. Should the vector be greater or less than the specified length, it is prefixed by the appropriate scalar multiplier,

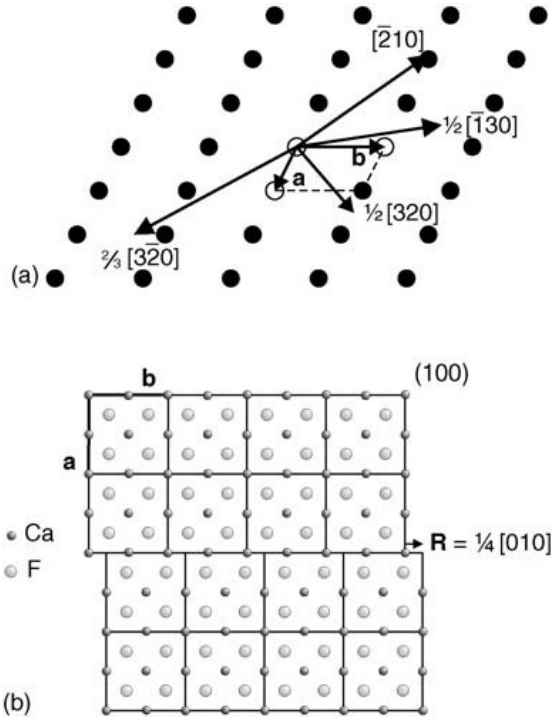


Figure 2.19 Vectors: (a) vectors in a lattice; (b) the displacement of part of a crystal of fluorite, CaF_2, by a vector, $\mathbf{R} = \frac{1}{4}$ [010] with respect to the other half

(see Appendix 1), in accordance with normal vector arithmetic, (Figure 2.19a).

Crystals often contain planar boundaries which separate two parts of a crystal that are not in perfect register. Vectors are used to define the displacement of one part with respect to the other. For example, a fault involving the displacement of one part of a crystal of fluorite, CaF_2, by ¼ of the unit cell edge, i.e. $\mathbf{R} = \frac{1}{4}$ [010] with respect to the other part[1], is drawn in (Figure 2.19b).

As with Miller indices, directions in hexagonal crystals are sometimes specified in terms of a

[1]In cubic crystals, a vector such as that describing the boundary drawn in Figure 2.19b is frequently denoted as ¼ **a** [010]. Similarly, a vector ⅔[3$\bar{1}$0] may be written as ⅔ **a** [3$\bar{1}$0]. This notation is confusing, and is best avoided.

four-index system, $[u'v'tw']$ called **Weber indices**. The conversion of a three-index set to a four-index set is given by the following rules.

$$[uvw] \rightarrow [u'v'tw']$$
$$u' = n(2u - v)/3$$
$$v' = n(2v - u)/3$$
$$t = -(u' + v')$$
$$w' = nw$$

In these equations, n is a factor *sometimes* needed to make the new indices into smallest integers. Thus the direction [00l] always transforms to [000l]. The three equivalent directions in the basal (0001) plane of a hexagonal crystal structure such as magnesium, (Figure 2.20), are obtained by using the above transformations. The correspondence is:

$$[100] = [2\bar{1}\bar{1}0]$$
$$[010] = [\bar{1}2\bar{1}0]$$
$$[\bar{1}\bar{1}0] = [\bar{1}\bar{1}20]$$

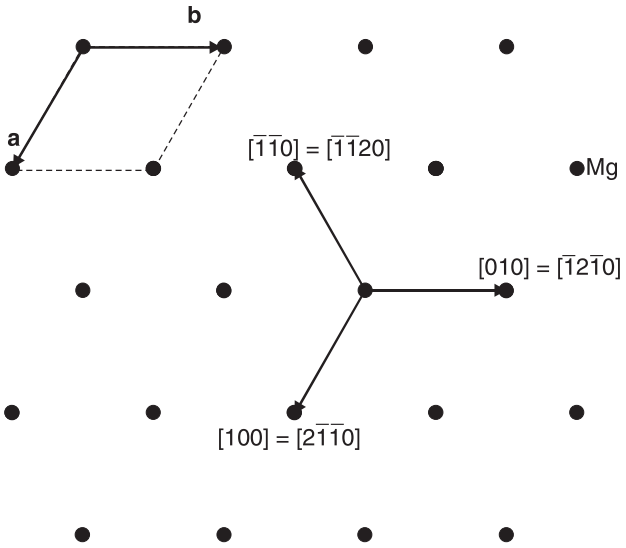


Figure 2.20 Directions in a hexagonal lattice

The relationship between directions and planes depends upon the symmetry of the crystal. In cubic crystals, (and *only* cubic crystals), the direction $[hkl]$ is normal to the plane (hkl).

2.11 Lattice geometry

The most important metrical properties of lattices and crystals for everyday crystallography are given below. These are expressed most compactly using vector notation, but are given here 'in longhand', without derivation, as a set of useful tools.

The volume of the reciprocal unit cell, V* is given by:

$$V^* = 1/V$$

where V is the volume of the direct unit cell.
The direction $[uvw]$ lies in the plane (hkl) when:

$$hu + kv + lw = 0$$

The intersection of two planes, $(h_1k_1l_1)$ and $(h_2k_2l_2)$ is the direction $[uvw]$, where:

$$u = k_1l_2 - k_2l_1$$
$$v = h_2l_1 - h_1l_2$$
$$w = h_1k_2 - h_2k_1$$

Three planes, $(h_1k_1l_1)$, $(h_2k_2l_2)$ and $(h_3k_3l_3)$ form a zone when:

$$h_1(k_2l_3 - l_2k_3) - k_1(h_2l_3 - l_2h_3) + l_1(h_2k_3 - k_2h_3) = 0$$

The plane $(h_3k_3l_3)$ belongs to the same zone as $(h_1k_1l_1)$ and $(h_2k_2l_2)$ when:

$$h_3 = mh_1 \pm nh_2; k_3 = mk_1 \pm nk_2; l_3 = ml_1 \pm ml_2$$

where m and n are integers.

Table 2.4 Interplanar spacing d_{hkl}

System	$1/(d_{hkl})^2$
cubic	$[h^2 + k^2 + l^2]/a^2$
tetragonal	$[(h^2 + k^2)/a^2] + [l^2/c^2]$
orthorhombic	$[h^2/a^2] + [k^2/b^2] + [l^2/c^2]$
monoclinic	$[h^2/a^2 \sin^2\beta] + [k^2/b^2] + [l^2/c^2 \sin^2\beta] - [(2hl\cos\beta)/(ac\ \sin^2\beta)]$
triclinic*	$[1/V^2]\ \{[S_{11}h^2] + [S_{22}k^2] + [S_{33}l^2] + [2S_{12}hk] + [2S_{23}kl] + [2S_{13}hl]\}$
hexagonal	$[4/3][(h^2 + hk + k^2)/a^2] + [l^2/c^2]$
rhombohedral	$\{[(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + hl)(\cos^2\alpha - \cos\alpha)]/[a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)]\}$

* V = unit cell volume.

$S_{11} = b^2c^2\sin^2\alpha \quad S_{22} = a^2c^2\sin^2\beta \quad S_{33} = a^2b^2\sin^2\gamma$

$S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma) \quad S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$

$S_{13} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$

The three directions $[u_1v_1w_1]$, $[u_2v_2w_2]$ and $[u_3v_3w_3]$ lie in one plane when

$$u_1(v_2w_3 - w_2v_3) - v_1(u_2w_3 - w_2u_3) + w_1(u_2v_3 - v_2u_3) = 0$$

Two directions $[u_1v_1w_1]$ and $[u_2v_2w_2]$ lie in a single plane (hkl) when:

$$h = v_1w_2 - v_2w_1$$
$$k = u_2w_1 - u_1w_2$$
$$l = u_1v_2 - u_2v_1$$

Table 2.5 Unit cell volume, V

System	V
Cubic	a^3
tetragonal	a^2c
orthorhombic	abc
monoclinic	$abc\ \sin\beta$
triclinic	$abc\sqrt{(1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma)}$
hexagonal	$\left[\sqrt{(3)}/2\right][a^2c] \approx 0.866a^2c$
rhombohedral	$a^3\sqrt{(1 - 3\cos^2\alpha + 2\cos^3\alpha)}$

The reciprocal lattice vector

$$\mathbf{r} = u\mathbf{a}^* + v\mathbf{b}^* + w\mathbf{c}^*$$

lies perpendicular to the direct lattice planes (uvw), and the direct lattice vector

$$\mathbf{R} = h\mathbf{a} + k\mathbf{b} + l\mathbf{c}$$

lies perpendicular to the reciprocal lattice planes (hkl).

Answers to introductory questions

How does a crystal lattice differ from a crystal structure?

Crystal structures and crystal lattices are different, although these terms are frequently (and incorrectly) used as synonyms. A crystal structure is built of atoms. A crystal lattice is an infinite pattern of points, each of which must have the same surroundings in the same orienta-

Table 2.6 Interplanar angle φ

System	$\cos\varphi$
cubic	$[h_1h_2 + k_1k_2 + l_1l_2]/\{[h_1^2 + k_1^2 + l_1^2][h_2^2 + k_2^2 + l_2^2]\}^{1/2}$
tetragonal	$\dfrac{\dfrac{h_1h_2 + k_1k_2}{a^2} + \dfrac{l_1l_2}{c^2}}{\left[\left(\dfrac{h_1^2 + k_1^2}{a^2} + \dfrac{l_1^2}{c^2}\right)\left(\dfrac{h_2^2 + k_2^2}{a^2} + \dfrac{l_2^2}{c^2}\right)\right]^{1/2}}$
orthorhombic	$\dfrac{\dfrac{h_1h_2}{a^2} + \dfrac{k_1k_2}{b^2} + \dfrac{l_1l_2}{c^2}}{\left[\left(\dfrac{h_1^2}{a^2} + \dfrac{k_1^2}{b^2} + \dfrac{l_1^2}{c^2}\right)\left(\dfrac{h_2^2}{a^2} + \dfrac{k_2^2}{b^2} + \dfrac{l_2^2}{c^2}\right)\right]^{1/2}}$
monoclinic*	$d_1d_2\left(\dfrac{h_1h_2}{a^2\sin^2\beta} + \dfrac{k_1k_2}{b^2} + \dfrac{l_1l_2}{c^2\sin^2\beta} - \dfrac{(l_1h_2 + l_2h_1)\cos\beta}{ac\sin^2\beta}\right)$
triclinic*	$\dfrac{d_1d_2}{V^2}[S_{11}h_1h_2 + S_{22}k_1k_2 + S_{33}l_1l_2 + S_{23}(k_1l_2 + k_2l_1) + S_{13}(l_1h_2 + l_2h_1) + S_{12}(h_1k_2 + h_2k_1)]$
hexagonal	$\dfrac{h_1h_2 + k_1k_2 + \frac{1}{2}(h_1k_2 + h_2k_1) + \dfrac{3a^2l_1l_2}{4c^2}}{\left[\left(h_1^2 + k_1^2 + h_1k_1 + \dfrac{3a^2l_1^2}{4c^2}\right)\left(h_2^2 + k_2^2 + h_2k_2 + \dfrac{3a^2l_2^2}{4c^2}\right)\right]^{1/2}}$
rhombohedral*	$\dfrac{d_1d_2\{(h_1h_2 + k_1k_2 + l_1l_2)\sin^2\alpha + [h_1(k_2 + l_2) + k_1(h_2 + l_2) + l_1(h_2 + k_2)\cos\alpha(\cos\alpha - 1)]\}}{a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)}$

* V = unit cell volume, d_1 is the interplanar spacing of $(h_1k_1l_1)$ and d_2 is the interplanar spacing of $(h_2k_2l_2)$ and

$S_{11} = b^2c^2\sin^2\alpha \quad S_{22} = a^2c^2\sin^2\beta \quad S_{33} = a^2b^2\sin^2\gamma$

$S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma) \quad S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$

$S_{13} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$

tion. A lattice is a mathematical concept. There are only 5 different two-dimensional (planar) lattices and 14 different three-dimensional (Bravais) lattices.

All crystal structures can be built up from the Bravais lattices by placing an atom or a group of atoms at each lattice point. The crystal structure of a simple metal and that of a complex protein may both be described in terms of the same lattice, but whereas the number of atoms allocated to each lattice point is often just one for a simple metallic crystal, it may easily be thousands for a protein crystal.

What is a primitive unit cell?

A primitive unit cell is a lattice unit cell that contains only one lattice point. The four primitive plane lattice unit cells are labelled *p*: oblique, (*mp*), rectangular, (*op*), square, (*tp*) and hexagonal, (*hp*). They are normally drawn with a lattice

point at each cell corner, but it is easy to see that the unit cell contains just one lattice point by mentally displacing the unit cell outline slightly. There are five primitive Bravais lattices, labelled *P*: triclinic, (*aP*), monoclinic primitive, (*mP*), tetragonal primitive, (*tP*), hexagonal primitive, (*hP*) and cubic primitive, (*cP*). In addition the trigonal lattice, when referred to rhombohedral axes, has a primitive unit cell, although the lattice is labelled *hR*.

What are Miller-Bravais indices used for?

The facets of a well-formed crystal or internal planes through a crystal structure are specified in terms of Miller Indices, *h*, *k* and *l*, written in round brackets, (*hkl*). Miller indices, (*hkl*), represent not just one plane, but the set of all identical parallel planes.

The Miller indices of planes in crystals with a hexagonal unit cell can be ambiguous. In order to eliminate this confusion, four indices, (*hkil*), are often used to specify planes in a hexagonal crystal. These are called Miller-Bravais indices and are only used in the hexagonal system. The index *i* is given by:

$$h + k + i = 0, \text{or } i = -(h + k)$$

In reality this third index is not needed, as it is simply derived from the known values of *h* and *k*. However, it does help to bring out relationships between planes that are not obvious when using just three indices. Because it is a redundant index, the value of *i* is sometimes replaced by a dot, to give indices (*hk.l*). This nomenclature emphasises that the hexagonal system is under discussion without actually including a value for *i*.

Problems and exercises

Quick quiz

1 A lattice is:
(a) A crystal structure
(b) An ordered array of points
(c) A unit cell

2 The basis vectors in a lattice define:
(a) The crystal structure
(b) The atom positions
(c) The unit cell

3 The number of different two-dimensional plane lattices is:
(a) 5
(b) 6
(c) 7

4 A rectangular primitive plane lattice has lattice parameters:
(a) $a \neq b$, $\gamma = 90^\circ$
(b) $a = b$, $\gamma = 90^\circ$
(c) $a \neq b$, $\gamma \neq 90^\circ$

5 The number of Bravais lattices is:
(a) 12
(b) 13
(c) 14

6 An orthorhombic body centred Bravais lattice has lattice parameters:
(a) a, b, c, $\alpha = \beta = \gamma = 90^\circ$
(b) $a(=b)$, c, $\alpha = \beta = \gamma = 90^\circ$
(c) $a(=b)$, c, $\alpha = \beta = 90^\circ, \gamma = 120^\circ$

7 A face centred (F) lattice unit cell contains:
(a) One lattice point
(b) Two lattice points
(c) Four lattice points

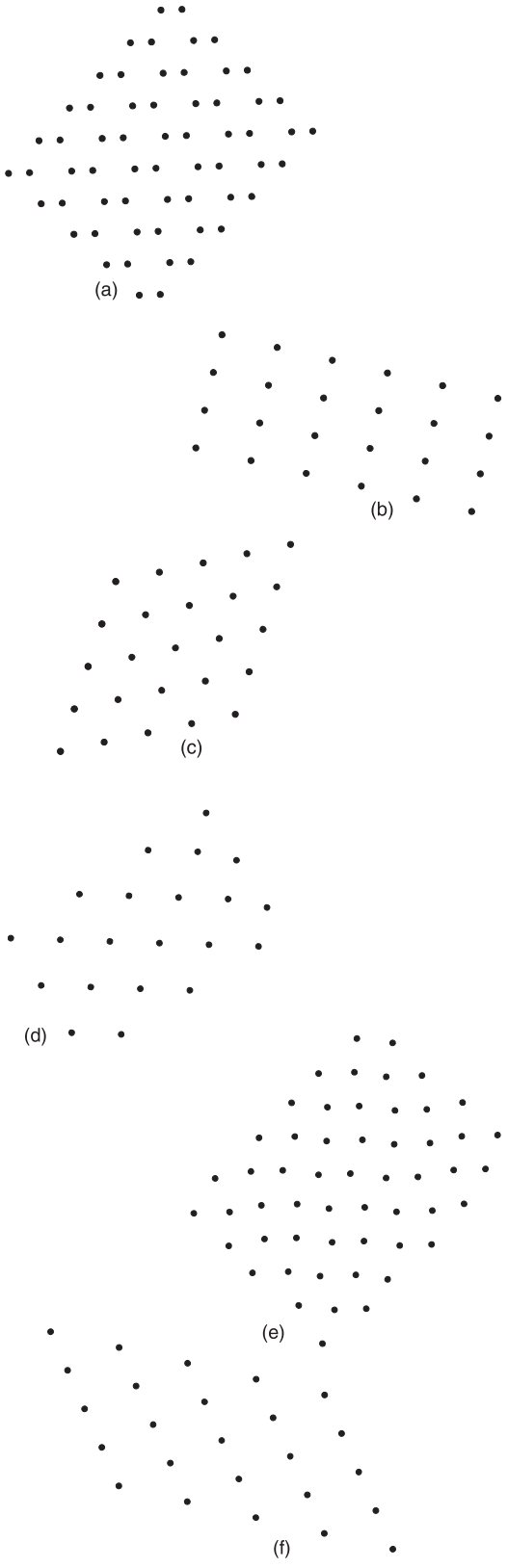
8 A unit cell with a lattice point at each corner and one at the centre of the cell is labelled:
(a) B
(b) C
(c) I

9 The notation [uvw] means:
(a) A single direction in a crystal
(b) A set of parallel directions in a crystal
(c) A direction perpendicular to a plane (uvw)

10 The notation {hkl} represents:
(a) A set of directions that are identical by virtue of the symmetry of the crystal
(b) A set of planes that are identical by virtue of the symmetry of the crystal
(c) Both a set of planes or directions that are identical by virtue of the symmetry of the crystal

Calculations and Questions

2.1 Several patterns of points are shown in the figure below. Assuming these to be infinite in extent, which of them are plane lattices? For those that are lattices, name the lattice type.



2.2 Draw the plane direct and reciprocal lattice for:

(a) an oblique lattice with parameters $a = 8$ nm, $b = 12$ nm, $\gamma = 110°$

(b) a rectangular centred lattice with parameters $a = 10$ nm, $b = 14$ nm

(c) the rectangular lattice in (b) drawn as a primitive lattice

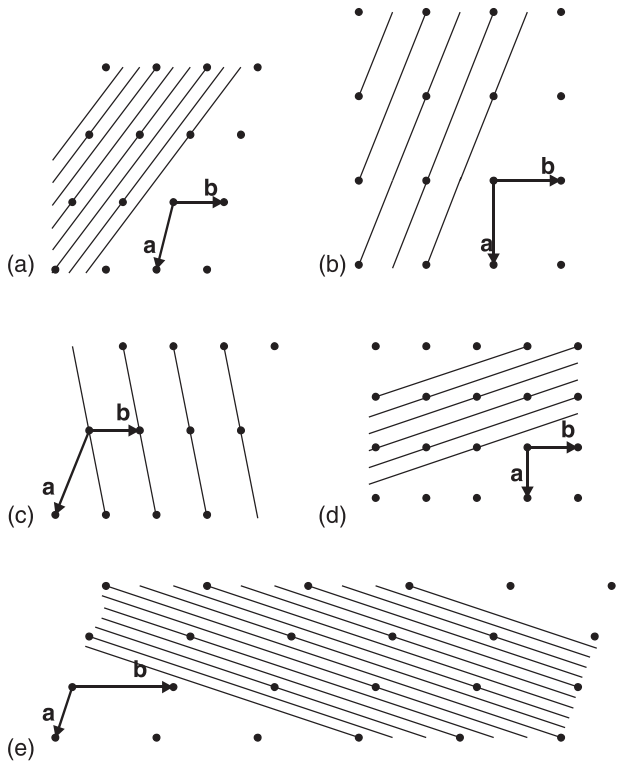
Confirm that the reciprocal lattices in (b) and (c) are identical and rectangular centred.

2.3 Sketch the direct and reciprocal lattice for

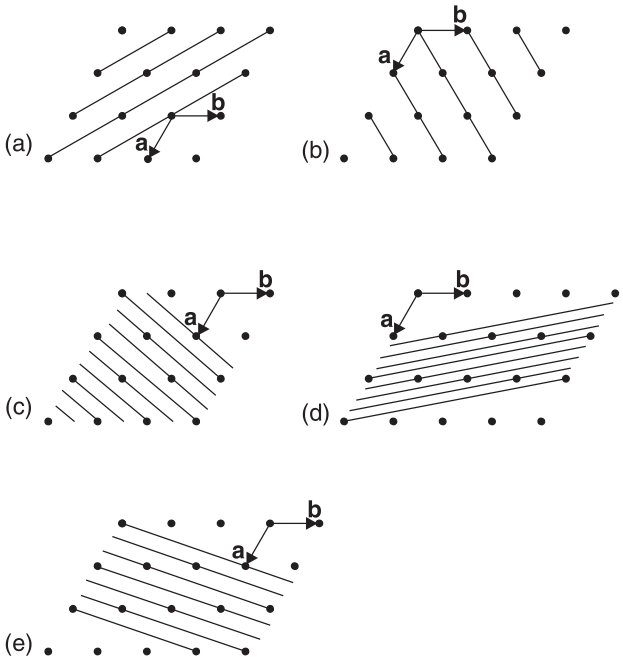
(a) a primitive monoclinic Bravais lattice with $a = 15$ nm, $b = 6$ nm, $c = 9$ nm, $\beta = 105°$

(b) a primitive tetragonal Bravais lattice with $a = 7$ nm, $c = 4$ nm

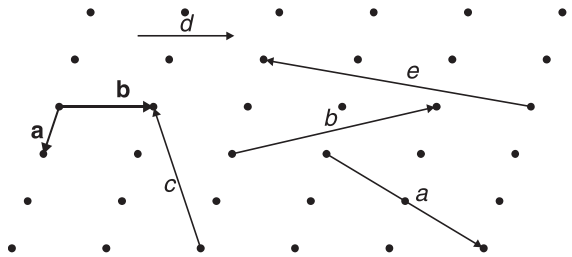
2.4 Index the lattice planes drawn in the figure below. The **c**-axis in all lattices is normal to the plane of the page and hence the index l is 0 in all cases.



2.5 Index the lattice planes drawn in the figure below using Miller – Bravais ($hkil$) and Miller indices (hkl). The lattice is hexagonal with the **c**-axis is normal to the plane of the page and hence the index l is 0 in all cases.



2.6 Give the indices of the directions marked on the figure below. In all cases the axis not shown is perpendicular to the plane of the paper and hence the index w is 0 in all cases.



2.7 Along what direction $[uvw]$ do the following pairs of planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ intersect? (a) (110), (1$\bar{1}$0); (b) ($\bar{2}$10), (011); (c) (111), (100); (d) (212), (1$\bar{2}$1).

2.8 Calculate the interplanar spacing, d_{hkl}, for: (a) (111), cubic, $a = 0.365\,\text{nm}$; (b) (210), tetragonal, $a = 0.475\,\text{nm}$, $c = 0.235\,\text{nm}$; (c) (321) orthorhombic, $a = 1.204\,\text{nm}$, $b = 0.821\,\text{nm}$, $c = 0.652\,\text{nm}$; (d) (222), monoclinic, $a = 0.981\,\text{nm}$, $b = 0.365\,\text{nm}$, $c = 0.869\,\text{nm}$, $\beta = 127.5^\circ$; (e) (121), hexagonal, $a = 0.693\,\text{nm}$, $c = 1.347\,\text{nm}$.