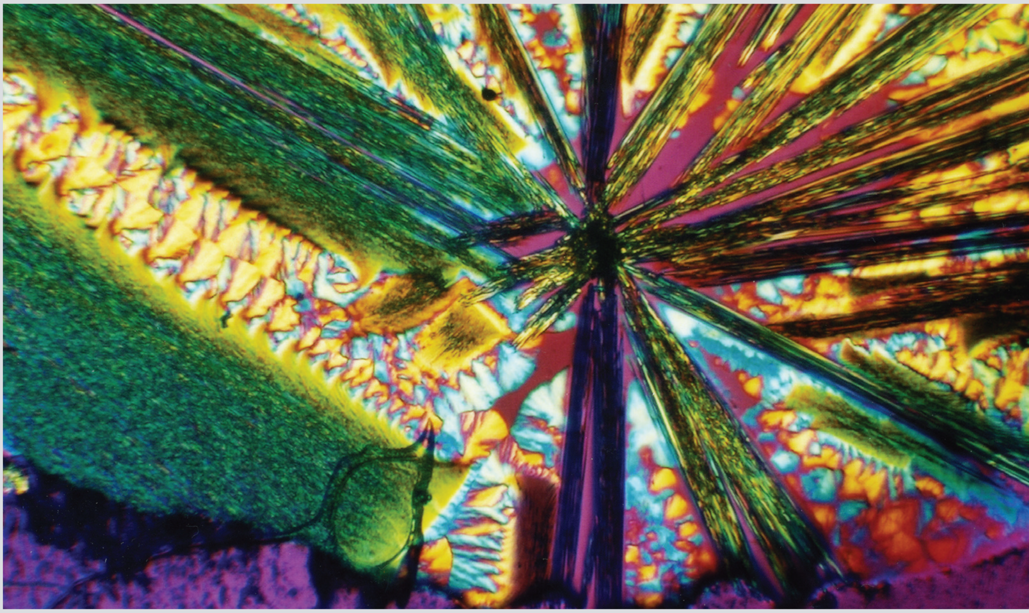
Second Edition

Crystallography and Crystal Defects



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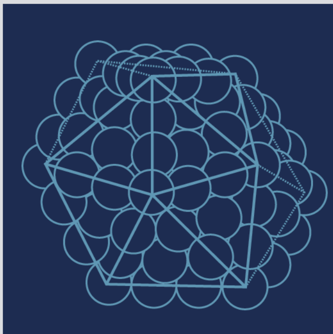

Crystallography and Crystal Defects

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ANTHONY KELLY and KEVIN M. KNOWLES

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WILEY

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Preface to the Second Edition

This fully revised and updated edition has been prepared by a very active worker in the field, who has used previous editions extensively both in teaching and in research, together with one of the original authors. Since the first edition, written in the late 1960s, understanding of crystal defects such as dislocations, stacking faults, twin, grain and interphase boundaries and of their effect on the mechanical and electrical properties of materials has grown enormously and has been accompanied by a total change in style of the way in which both research and teaching are carried out through the use of the fast digital computer. This edition takes account of this change.

It provides a fully updated account of basic crystallography and of structural imperfections in materials, while ensuring that it remains accessible to both undergraduate and postgraduate students and to others wishing to have a basic understanding of crystallography and why this subject is important when dealing with real (i.e. imperfect) materials.

This edition has discussions of a number of new topics not covered in previous editions such as piezoelectricity, groups, subgroups and supergroups, liquid crystals, incommensurate materials and the structure of foamed and amorphous materials, and martensitic transformations in nickel–titanium shape memory alloys and zirconia ceramics. The topic of quasicrystalline materials, covered briefly in the revised edition published in 2000, has been rewritten and linked to discussions of icosahedral packing and the understanding of topologically close-packed structures.

Constructions involving the stereographic projection have been moved to an appendix. It is now usual to produce stereographic projections via proprietary software packages. Accounts of three-dimensional coordinate geometry and spherical trigonometry have been rewritten using vector algebra, matrix algebra and quaternions. Such algebra is also amenable to the use of spreadsheets.

Tables of data and references in previous editions have been meticulously checked and updated. Numbered references are listed in full at the end of each chapter, together with suggestions for further reading. The problems at the end of each chapter have been reviewed and updated. Brief solutions to these are given after the appendices. More detailed worked solutions are available on the password protected Wiley Web page accompanying this book at http://booksupport.wiley.com. Lists of websites and computer software packages relevant to the topics we have covered here are given in a new appendix.

The authors are extremely grateful to those who have helped to foster our interest in crystallography. AK would like to thank in particular the late Geoffrey Groves, co-author of the first edition, as well as Patricia Kidd, co-author of the revised edition published in 2000; KMK would like to thank the late David Smith, his DPhil supervisor at Oxford, and also a former PhD student of AK.

We are both grateful to James Elliott for his great help with preparing diagrams of polymer crystals and to other colleagues from both of our departments at Cambridge and at Churchill College, Cambridge for their advice and encouragement.

In attempting to strike a balance between general background knowledge, specialist research knowledge and succinctness of description, we have inevitably had to make compromises in every chapter; each could have been a separate volume. We hope the reader whose understanding of crystallography and crystal defects goes well beyond what we have described here will nevertheless find parts where we have enriched his or her knowledge. Finally, we hope that all readers will enjoy reading this book as much as we have enjoyed both its writing and its revision.

Anthony Kelly
Kevin M. Knowles

Part I

Perfect Crystals

1

Lattice Geometry

1.1 The Unit Cell

Crystals are solid materials in which the atoms are regularly arranged with respect to one another. This regularity of arrangement can be described in terms of symmetry elements; these elements determine the symmetry of the physical properties of a crystal. For example, the symmetry elements show in which directions the electrical resistance of a crystal will be the same. Many naturally occurring crystals, such as halite (sodium chloride), quartz (silica) and calcite (calcium carbonate), have very well-developed external faces. These faces show regular arrangements at a macroscopic level, which indicate the regular arrangements of the atoms at an atomic level. Historically, such crystals are of great importance because the laws of crystal symmetry were deduced from measurements of the interfacial angles in them; measurements were first carried out in the seventeenth century. Even today, the study of such crystals still possesses some heuristic advantages in learning about symmetry.

Nowadays the atomic pattern within a crystal can be studied directly by techniques such as high-resolution transmission electron microscopy. This atomic pattern is the fundamental pattern described by the symmetry elements and we shall begin with it.

In a crystal of graphite the carbon atoms are joined together in sheets. These sheets are only loosely bound to one another by van der Waals forces. A single sheet of such atoms provides an example of a two-dimensional crystal; indeed, recent research has shown that such sheets can actually be isolated and their properties examined. These single sheets are now termed 'graphene'. The arrangement of the atoms within a sheet of graphene is shown in Figure 1.1a. In this representation of the atomic pattern, the centre of each atom is represented by a small dot, and lines joining adjacent dots represent bonds between atoms. All of the atoms in this sheet are identical. Each atom possesses three nearest neighbours.

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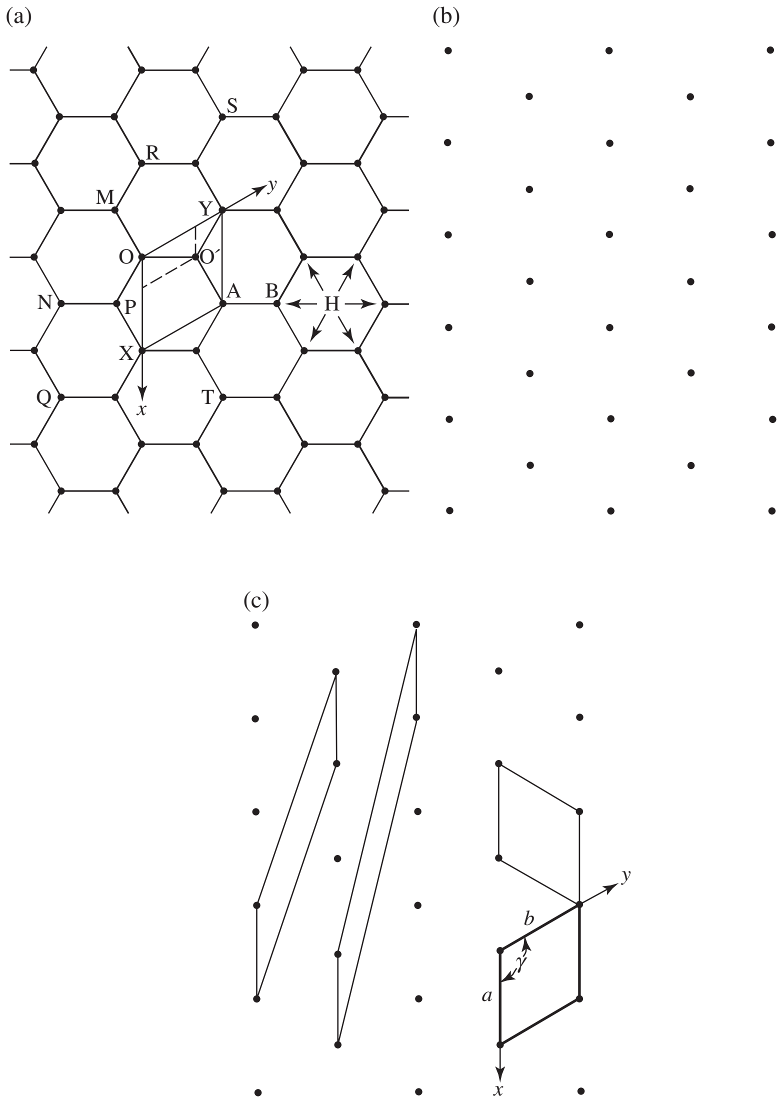

Figure 1.1

We describe this by saying that the coordination number is 3. In this case the coordination number is the same for all the atoms. It is the same for the two atoms marked A and B. However, atoms A and B have different environments: the orientation of the neighbours is different at A and B. Atoms in a similar situation to those at A are found at N and Q; there is a similar situation to B at M and at P.

It is obvious that we can describe the whole arrangement of atoms and interatomic bonds shown in Figure 1.1a by choosing a small unit such as OXAY, describing the arrangement of the atoms and bonds within it, then moving the unit so that it occupies the position NQXO and repeating the description and then moving it to ROYS and so on, until we have filled all space with identical units and described the whole pattern. If the repetition of the unit is understood to occur automatically, then to describe the crystal we need only describe the arrangement of the atoms and interatomic bonds within one unit. The unit chosen we would call the 'unit parallelogram' in two dimensions (in three dimensions, the 'unit cell'). In choosing the unit we always choose a parallelogram in two dimensions or a parallelepiped in three dimensions. The reason for this will become clear later.

Having chosen the unit, we describe the positions of the atoms inside it by choosing an origin O and taking axes Ox and Oy parallel to the sides, so that the angle between Ox and Oy is $\geq 90°$. We state the lengths of the sides a and b, taking a equal to the distance OX and b equal to the distance OY (Figure 1.1a), and we give the angle γ between Ox and Oy. In this case $a = b = 2.45$ Å[1] (at 25 °C) and $\gamma = 120°$. To describe the positions of the atoms within the unit parallelogram, we note that there is one at each corner and one wholly inside the cell. The atoms at O, X, A, Y all have identical surroundings.[2]

In describing the positions of the atoms we take the sides of the parallelogram, a and b, as units of length. Then the coordinates of the atom at O are (0, 0); those at X (1, 0); those at Y (0, 1); and those at A (1, 1). The coordinates of the atom at O′ are obtained by drawing lines through O′ parallel to the axes Ox and Oy. The coordinates of O′ are therefore $\left(\frac{1}{3}, \frac{2}{3}\right)$. To describe the contents fully inside the unit parallelogram – that is, to describe the positions of the atoms – we need only give the coordinates of the atom at the origin, (0, 0), and those of the atom at O′. The reason is that the atoms at X, A and Y have identical surroundings to those at O and an atom such as O, X, A or Y is shared between the four cells meeting at these points. The number of atoms contained within the area OXAY is two. O′ is within the area, giving one atom. O, Y, A, X provide four atoms each shared between four unit cells, giving an additional $4 \times \frac{1}{4} = 1$. A second way of arriving at the same result is to move the origin of the unit cell slightly away from the centre of the atom at O so that the coordinate of the O atom is $(\varepsilon_1, \varepsilon_2)$ and the coordinate of the O′ atom is $\left(\frac{1}{3} + \varepsilon_1, \frac{2}{3} + \varepsilon_2\right)$, where $0 < \varepsilon_1$, $\varepsilon_2 << 1$. Under these circumstances the centres of the atoms at X, A and Y lie outside the unit cell, so that the atom count within the unit cell is simply two. We note that the minimum number of atoms which a unit parallelogram could contain in a sheet of graphene is two, since the atoms at O and O′ have different environments.

To describe the atomic positions in Figure 1.1a we chose OXAY as one unit parallelogram. We could equally well have chosen OXTA. The choice of a particular unit parallelogram or unit cell is arbitrary, subject to the constraint that the unit cell tessellates, that is it repeats periodically, in this case in two dimensions. Therefore, NQPM is not a permissible choice – although NQPM is a parallelogram, it cannot be repeated to produce the graphene structure because P and M have environments which differ from those at N and Q.

The corners of the unit cell OXAY in Figure 1.1a all possess identical surroundings. We could choose and mark on the diagram all points with surroundings identical to those at O, X, A and so on. Such points are N, Q, R, S and so on. The array of all such points with surroundings identical to those of a given point we call the mesh or net in two dimensions (a lattice in three dimensions). Each of the points is called a lattice point.

---

[1] 1 Å = 10^{-10} m.

[2] In choosing a unit parallelogram or a unit cell, the crystal is always considered to be infinitely large. The pattern in Figure 1.1a must then be thought of as extending to infinity. The fact that O, X, A and Y in a finite crystal are at slightly different positions with respect to the boundary of the pattern can then be neglected.

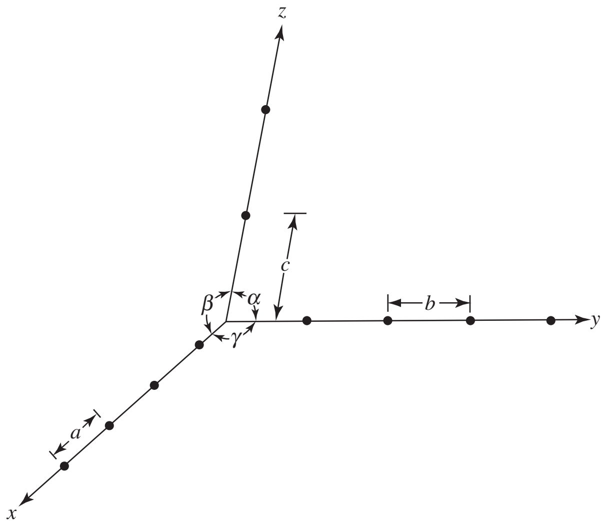

Figure 1.2

A formal definition of the lattice is as follows: *A lattice is a set of points in space such that the surroundings of one point are identical with those of all the others. The type of symmetry described by the lattice is referred to as translational symmetry.* The lattice of the graphene crystal structure drawn in Figure 1.1a is shown in Figure 1.1b. It consists of a set of points with identical surroundings. Just a set of points: no atoms are involved. Various primitive unit cells are marked in Figure 1.1c. A primitive unit cell is defined as a unit parallelogram which contains just one lattice point. The conventional unit cell for graphene corresponding to OXAY in Figure 1.1a is outlined in Figure 1.1c in heavy lines and the corresponding x- and y-axes are marked.

In general, the conventional primitive unit cell of a two-dimensional net which shows no obvious symmetry is taken with its sides as short and as nearly equal as possible, with γ, the angle between the x- and y-axes, taken to be obtuse, if it is not equal to 90°. However, the symmetry of the pattern must always be taken into account. The net shown in Figure 1.1b is very symmetric and in this case we can take the sides to be equal, so that $a = b$ and $\gamma = 120°$.

Comparisons of Figures 1.1a and b emphasize that the choice of the origin for the lattice is arbitrary. If we had chosen O′ in Figure 1.1a as the origin instead of O and then marked all corresponding points in Figure 1.1a, we would have obtained the identical lattice with only a change of origin. The lattice then represents an essential element of the translational symmetry of the crystal however we choose the origin.

In three dimensions the definition of the lattice is the same as in two dimensions. The unit cell is now the parallelepiped containing just one lattice point. The origin is taken at a corner of the unit cell. The sides of the unit parallelepiped are taken as the axes of the crystal, x, y, z, using a right-handed notation. The angles α, β, γ between the axes are called the axial angles (see Figure 1.2). The smallest separations of the lattice points along the x-, y- and z-axes are denoted by a, b, c respectively and called the lattice parameters.

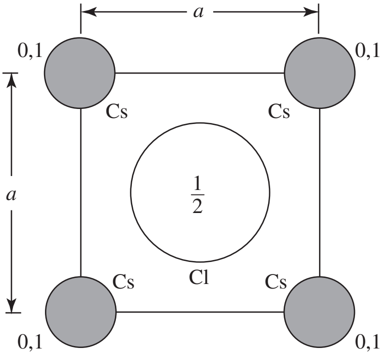

Figure 1.3 The numbers give the elevations of the centres of the atoms, along the *z*-axis, taking the lattice parameter *c* as the unit of length

Inspection of the drawing of the arrangement of the ions in a crystal of caesium chloride, CsCl, in Figure 3.17 shows that the lattice is an array of points such that $a = b = c$, $\alpha = \beta = \gamma = 90°$, so that the unit cell is a cube. There is one caesium ion and one chlorine ion associated with each lattice point. If we take the origin at the centre of a caesium ion, then there is one caesium ion in the unit cell with coordinates (0, 0, 0) and one chlorine ion with coordinates $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$. A projection along the *z*-axis is shown in Figure 1.3. It must be remembered that the caesium ions at the corners of the unit cell project on top of one another; thus ions at elevations 0 and 1 are superimposed, as indicated in Figure 1.3. Since translational symmetry dictates that if there is an ion at $(x, y, 0)$, there must be an ion with exactly the same environment at $(x, y, 1)$, the ions at elevation 1 along the *z*-axis can be omitted by convention. It is also standard practice when drawing projections of crystal structures not to indicate the elevations of atoms or ions if they are 0.

It is apparent from this drawing of the crystal structure of caesium chloride that the coordination number for each caesium ion and each chlorine ion is eight, each ion having eight of the other kind of ion as neighbours. The separation of these nearest neighbours, *d*, is easily seen to be given by:

$$d = \left[\left(\frac{a}{2}\right)^2 + \left(\frac{b}{2}\right)^2 + \left(\frac{c}{2}\right)^2\right]^{1/2} = \frac{\sqrt{3}a}{2} \tag{1.1}$$

since $a = b = c$.

The number of units of the formula CsCl per unit cell is clearly 1.

1.2 Lattice Planes and Directions

A rectangular mesh of a hypothetical two-dimensional crystal with mesh parameters *a* and *b* of very different magnitude is shown in Figure 1.4. Note that the parallel mesh lines OB, O′B′, O″B″ and so on all form part of a set and that the spacing of all lines in the set is quite

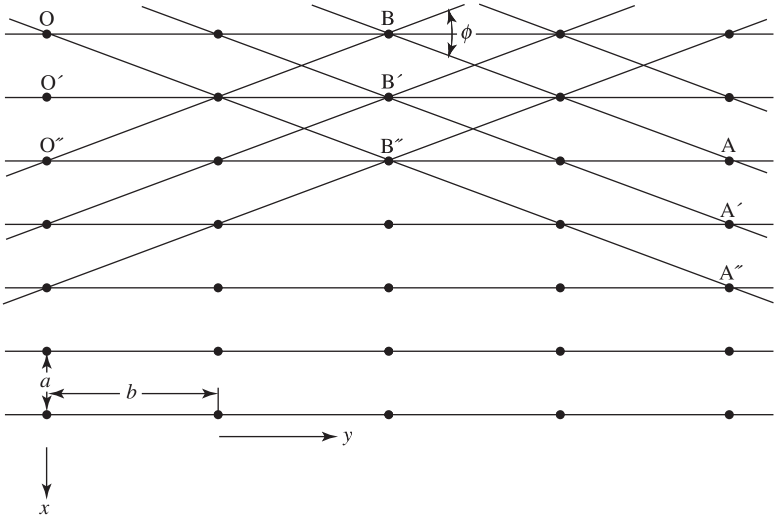

Figure 1.4

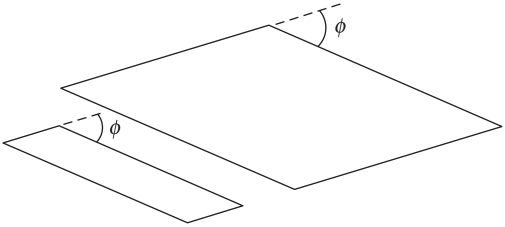

Figure 1.5

regular; this is similar for the set of lines parallel to AB: A′B′, A″B″ and so on The spacing of each of these sets is determined only by **a** and **b** (and the angle between **a** and **b,** which in this example is 90°). Also, the angle between these two sets depends only on the *ratio* of *a* to *b,* where *a* and *b* are the magnitudes of **a** and **b** respectively. If external faces of the crystal formed parallel to O″B and to AB, the angle between these faces would be uniquely related to the ratio *a* : *b*. Furthermore, this angle would be independent of how large these faces were (see Figure 1.5). This was recognized by early crystallographers, who deduced the existence of the lattice structure of crystals from the observation of the constancy of angles between corresponding faces. This law of constancy of angle states: *In all crystals of the same substance the angle between corresponding faces has a constant value.*

The analogy between lines in a mesh and planes in a crystal lattice is very close. Crystal faces form parallel to lattice planes and important lattice planes contain a high density of lattice points. Lattice planes form an infinite regularly spaced set which collectively passes through all points of the lattice. The spacing of the members of the set is determined only by the lattice parameters and axial angles, and the angles between various lattice planes are determined only by the axial angles and the ratios of the lattice parameters to one another.

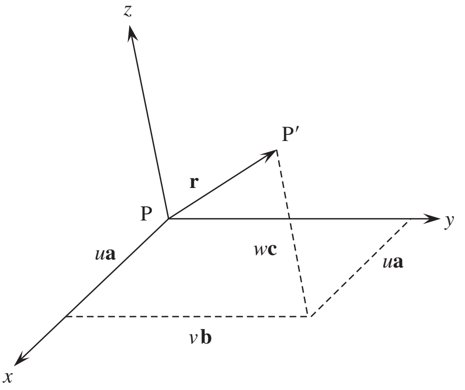

Figure 1.6

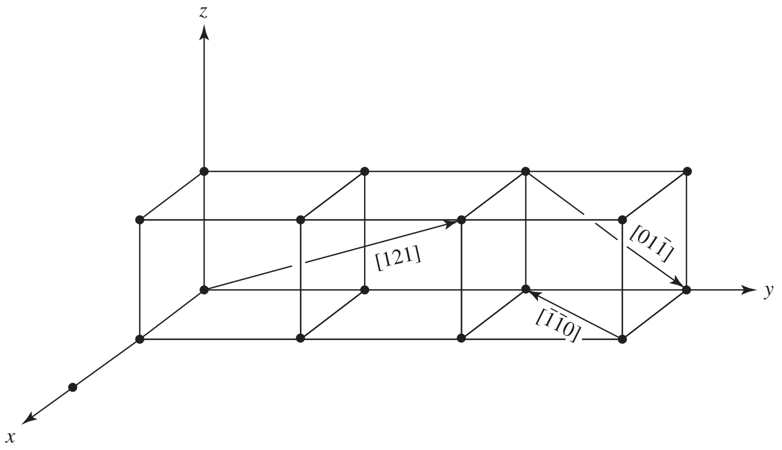

Figure 1.7

Prior to establishing a methodology for designating a set of lattice planes, it is expedient to consider how directions in a crystal are specified. A direction is simply a line in the crystal. Select any two points on the line, say P and P′. Choose one as the origin, say P (Figure 1.6). Write the vector **r** between the two points in terms of translations along the *x*-, *y*- and *z*-axes so that:

$$\mathbf{r} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c} \tag{1.2}$$

where **a**, **b** and **c** are vectors along the *x*-, *y*- and *z*-axes, respectively, and have magnitudes equal to the lattice parameters (Figure 1.6). The direction is then denoted as [*uvw*] – always cleared of fractions and reduced to its lowest terms. The triplet of numbers indicating a direction is always enclosed in square brackets. Some examples are given in Figure 1.7. Negative values of *u*, *v*, and *w* are indicated in this figure by a bar over the appropriate index.

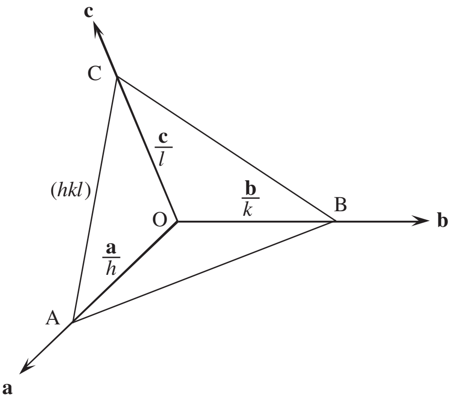

Figure 1.8

If u, v and w are integers and the origin P is chosen at a lattice point, then P′ is also a lattice point and the line PP′ produced is a row of lattice points. Such a line is called a *rational* line, just as a plane of lattice points is called a rational plane.

We designate a set of lattice planes as follows (see Figure 1.8). Let one member of the set meet the chosen axes, x, y, z, at distances from the origin of A, B and C respectively. We can choose the origin to be a lattice point. Vectors **a**, **b** and **c** then define the distances between adjacent lattice points along the x-, y- and z-axes, respectively. The Miller indices (hkl) of the set of lattice planes are then defined in terms of the intercepts A, B and C so that the length OA = a/h, where a is the magnitude of **a**; likewise, OB = b/k and OC = c/l.

Thus, for example, the plane marked Y in Figure 1.9 makes intercepts on the axes of infinity, 2b and infinity, respectively. Taking the reciprocals of these intercepts gives $h = 0$, $k = \frac{1}{2}$ and $l = 0$. Clearing the fractions gives $h = 0$, $k = 1$ and $l = 0$. Hence, the set of lattice planes parallel to Y is designated (010). The triplet of numbers describing the Miller index is always enclosed in round brackets. Similarly, the plane marked P in Figure 1.9 has intercepts 1a, 2b and $\frac{1}{3}c$. Therefore, taking the reciprocals of these intercepts, $h = 1$, $k = \frac{1}{2}$ and $l = 3$. Clearing the fractions, we have (216) as the Miller indices. The indices of a number of other planes are shown in Figure 1.9. Negative values of the intercepts are indicated in the Miller index notation by a bar over the appropriate index (see the examples in Figure 1.9).

The reason for using Miller indices to index crystal planes is that they greatly simplify certain crystal calculations. Furthermore, with a reasonable choice of unit cell, small values of the indices (hkl) belong to widely spaced planes containing a large areal density of lattice points. Well-developed crystals are usually bounded by such planes, so that it is found experimentally that prominent crystal faces have intercepts on the axes which when expressed as multiples of a, b and c have ratios to one another that are small rational numbers.[3]

---

[3] Formally, the *law of rational indices* states that all planes which can occur as faces of crystals have intercepts on the axes which, when expressed as multiples of certain unit lengths along the axes (themselves proportional to a, b, c), have ratios that are small rational numbers. A rational number can always be written as p/q, where p and q are integers.

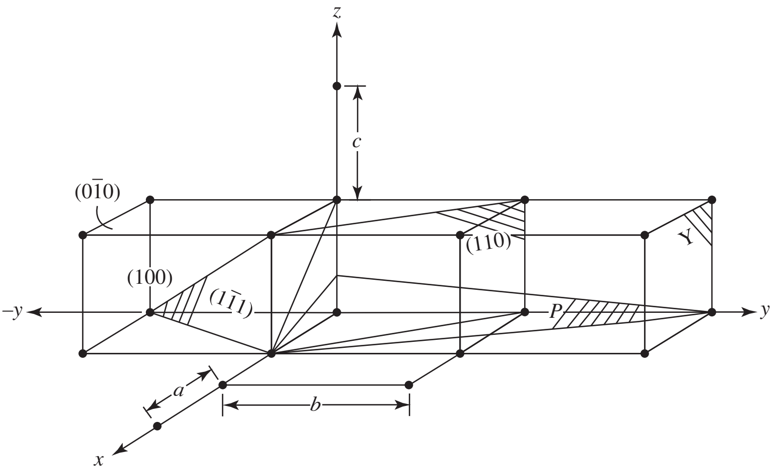

Figure 1.9

1.3 The Weiss Zone Law

This law expresses the mathematical condition for a vector [*uvw*] to lie in a plane (*hkl*). This condition can be determined through elementary vector considerations. Consider the plane (*hkl*) in Figure 1.10 with the normal to the plane $\overrightarrow{\mathrm{OP}}$.

A general vector, **r**, lying in (*hkl*) can be expressed as a linear combination of any two vectors lying in this plane, such as $\overrightarrow{\mathrm{AB}}$ and $\overrightarrow{\mathrm{AC}}$. That is:

$$\mathbf{r} = \lambda\overrightarrow{\mathrm{AB}} + \mu\overrightarrow{\mathrm{AC}} \tag{1.3}$$

for suitable λ and μ. Hence, expressing $\overrightarrow{\mathrm{AB}}$ and $\overrightarrow{\mathrm{AC}}$ in terms of **a**, **b** and **c**, it follows that:

$$\mathbf{r} = \lambda\left(\frac{\mathbf{b}}{k} - \frac{\mathbf{a}}{h}\right) + \mu\left(\frac{\mathbf{c}}{l} - \frac{\mathbf{a}}{h}\right) = -\frac{(\lambda+\mu)}{h}\mathbf{a} + \frac{\lambda}{k}\mathbf{b} + \frac{\mu}{l}\mathbf{c} \tag{1.4}$$

If we reexpress this as $\mathbf{r} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$ – a general vector [*uvw*] lying in (*hkl*) – it follows that:

$$u = -\frac{(\lambda+\mu)}{h}, \qquad v = \frac{\lambda}{k}, \qquad w = \frac{\mu}{l} \tag{1.5}$$

and so:

$$hu + kv + lw = 0 \tag{1.6}$$

which is the condition for a vector [*uvw*] to lie in the plane (*hkl*): the **Weiss zone law**. It is evident from this derivation that it is valid for arbitrary orientations of the *x*-, *y*- and *z*-axes with respect to one another.

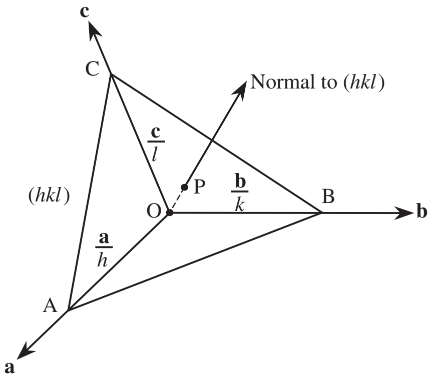

Figure 1.10

Frequently a number of important crystal lattice planes all lie in the same zone; that is, they intersect one another in parallel lines. For instance, in Figure 1.9 the planes (100), (0$\bar{1}$0) and (110) are all parallel to the direction [001]. They would be said to lie in the zone [001], since [001] is a common direction lying in all of them. The normals to all of these planes are perpendicular to [001]. This is not an accident – the normals are constrained to be perpendicular to [001] by the Weiss zone law.

To see why, we can make use of elementary vector algebra relationships discussed in Appendix 1, Section A1.1. Consider the plane (*hkl*) shown in Figure 1.10. The vector normal to this plane, **n**, must be parallel to the cross product $\overrightarrow{\mathrm{AB}}\times\overrightarrow{\mathrm{AC}}$. Hence:

$$\mathbf{n}\parallel\left(\frac{\mathbf{b}}{k}-\frac{\mathbf{a}}{h}\right)\times\left(\frac{\mathbf{c}}{l}-\frac{\mathbf{a}}{h}\right),\ \text{i.e.,}\quad \mathbf{n}\parallel\left(\frac{\mathbf{b}\times\mathbf{c}}{kl}-\frac{\mathbf{b}\times\mathbf{a}}{hk}-\frac{\mathbf{a}\times\mathbf{c}}{hl}\right) \tag{1.7}$$

and so after some straightforward mathematical manipulation, making use of the identities

$$\mathbf{a}\times\mathbf{b}=-\mathbf{b}\times\mathbf{a}\ \text{and}\ \mathbf{c}\times\mathbf{a}=-\mathbf{a}\times\mathbf{c},$$

it is apparent that **n** is parallel to the vector $h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$. That is:

$$\mathbf{n}=\xi(h\mathbf{a}^*+k\mathbf{b}^*+l\mathbf{c}^*) \tag{1.8}$$

for a constant of proportionality, ξ. The vectors **a***, **b*** and **c*** in Equation 1.8 are termed *reciprocal lattice vectors*, defined through w equations:

$$\mathbf{a}^*=\frac{\mathbf{b}\times\mathbf{c}}{\mathbf{a}.[\mathbf{b}\times\mathbf{c}]},\qquad \mathbf{b}^*=\frac{\mathbf{c}\times\mathbf{a}}{\mathbf{a}.[\mathbf{b}\times\mathbf{c}]},\qquad \mathbf{c}^*=\frac{\mathbf{a}\times\mathbf{b}}{\mathbf{a}.[\mathbf{b}\times\mathbf{c}]} \tag{1.9}$$

If the normal to the (*hkl*) set of planes is simply taken to be the vector

$$\mathbf{n}=h\mathbf{a}^*+k\mathbf{b}^*+l\mathbf{c}^* \tag{1.10}$$

the magnitude of **n** is inversely proportional to the spacing of the *hkl* planes; that is, it is inversely proportional to the distance OP in Figure 1.10 (Section A1.2), irrespective of the orientations of the x-, y- and z-axes with respect to one another.

Furthermore, it is evident that the scalar product of a normal to a set of planes, **n**, with a vector $\mathbf{r} = [uvw]$ lying on one of these planes must be zero. That is, $\mathbf{r}.\mathbf{n} = 0$. Writing out this dot product explicitly, we obtain the result:

$$hu + kv + lw = 0$$

which is the Weiss zone law. This demonstrates that the Weiss zone law is a scalar product between two vectors, one of which lies in one of a set of planes and the other of which is normal to the set of planes.

Given the indices of any two planes, say $(h_1k_1l_1)$ and $(h_2k_2l_2)$, the indices of the zone $[uvw]$ in which they lie are found by solving the simultaneous equations:

$$h_1u + k_1v + l_1w = 0 \tag{1.11}$$

$$h_2u + k_2v + l_2w = 0 \tag{1.12}$$

Since it is only the ratios $u : v : w$ which are of interest, these equations can be solved to give:

$$\begin{aligned} u &= k_1l_2 - k_2l_1 \\ v &= l_1h_2 - l_2h_1 \\ w &= h_1k_2 - h_2k_1 \end{aligned} \tag{1.13}$$

There are other methods of producing the same result. For example, we could write down the directions in the form:

$$\begin{array}{cccccc} h_1 & k_1 & l_1 & h_1 & k_1 & l_1 \\ h_2 & k_2 & l_2 & h_2 & k_2 & l_2 \end{array}$$

We then cross out the first and the last columns and evaluate the 2 × 2 determinants from (i) the second and third columns, (ii) the third and fourth columns and (iii) the fourth and fifth columns:

$$\begin{array}{ccccccccc} \cancel{h_1} & k_1 & & l_1 & & h_1 & & k_1 & \cancel{l_1} \\ & & \times & & \times & & \times & & \\ \cancel{h_2} & k_2 & & l_2 & & h_2 & & k_2 & \cancel{l_2} \end{array} \tag{1.14}$$

Therefore, we find $[uvw] = [k_1l_2 - k_2l_1,\ l_1h_2 - l_2h_1,\ h_1k_2 - h_2k_1]$. A third method is to evaluate the determinant

$$\begin{vmatrix} \mathbf{a} & \mathbf{b} & \mathbf{c} \\ h_1 & k_1 & l_1 \\ h_2 & k_2 & l_2 \end{vmatrix} \tag{1.15}$$

to determine $[uvw]$. The result is $[uvw] = (k_1l_2 - k_2l_1)\,\mathbf{a} + (l_1h_2 - l_2h_1)\,\mathbf{b} + (h_1k_2 - h_2k_1)\,\mathbf{c}$.

Thus, for example, supposing $(h_1k_1l_1) = (112)$ and $(h_2k_2l_2) = (\bar{1}43)$, we would have:

$$\begin{array}{ccccccccccc} \cancel{1} & 1 & & 2 & & 1 & & 1 & \cancel{2} \\ & & \times & & \times & & \times & & \\ \cancel{\bar{1}} & 4 & & 3 & & \bar{1} & & 4 & \cancel{3} \end{array}$$

and so $[uvw] = [-5, -5, 5] \equiv [1\,1\,\bar{1}]$. Likewise, given two directions $[u_1v_1w_1]$ and $[u_2v_2w_2]$, we can obtain the plane (hkl) containing these two directions by solving the simultaneous equations:

$$hu_1 + kv_1 + lw_1 = 0 \tag{1.16}$$

$$hu_2 + kv_2 + lw_2 = 0 \tag{1.17}$$

Using a similar method to the one used to produce Equation 1.14, we draw up the three 2 × 2 determinants as follows:

$$\begin{array}{ccccccccc} \cancel{u_1} & v_1 & & w_1 & & u_1 & & v_1 & \cancel{w_1} \\ & & \times & & \times & & \times & & \\ \cancel{u_2} & v_2 & & w_2 & & u_2 & & v_2 & \cancel{w_2} \end{array} \tag{1.18}$$

to find that $(hkl) = (v_1w_2 - v_2w_1, w_1u_2 - w_2u_1, u_1v_2 - u_2v_1)$. The method equivalent to Equation 1.15 is to evaluate the determinant:

$$\begin{vmatrix} \mathbf{a}^* & \mathbf{b}^* & \mathbf{c}^* \\ u_1 & v_1 & w_1 \\ u_2 & v_2 & w_2 \end{vmatrix} \tag{1.19}$$

It is also evident from Equations 1.11 and 1.12, the conditions for two planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ to lie in the same zone $[uvw]$, that by multiplying Equation 1.11 by a number m and Equation 1.12 by a number n and adding them, we have:

$$(mh_1 + nh_2)u + (mk_1 + nk_2)v + (ml_1 + nl_2)w = 0 \tag{1.20}$$

Therefore the plane $(mh_1 + nh_2, mk_1 + nk_2, ml_1 + nl_2)$ also lies in $[uvw]$. In other words, the indices formed by taking linear combinations of the indices of two planes in a given zone provide the indices of a further plane in that same zone. In general m and n can be positive or negative. If, however, m and n are both positive, then the normal to the plane under consideration must lie between the normals of $(h_1k_1l_1)$ and $(h_2k_2l_2)$: we will revisit this result in Section 2.2.

1.4 Symmetry Elements

The symmetrical arrangement of atoms in crystals is described formally in terms of elements of symmetry. The symmetry arises because an atom or group of atoms is repeated in a regular way to form a pattern. Any operation of repetition can be described in terms of one of the following three different types of pure symmetry element or symmetry operator.