

# A Journey into Reciprocal Space

A crystallographer's perspective

**A M Glazer**



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*Physics Department, University of Oxford and Physics Department,  
University of Warwick and Jesus College Oxford*

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ISBN 978-1-6817-4621-0 (ebook)

ISBN 978-1-6817-4620-3 (print)

ISBN 978-1-6817-4623-4 (mobi)

DOI 10.1088/978-1-6817-4621-0

Version: 20171001

IOP Concise Physics

ISSN 2053-2571 (online)

ISSN 2054-7307 (print)

A Morgan & Claypool publication as part of IOP Concise Physics

Published by Morgan & Claypool Publishers, 1210 Fifth Avenue, Suite 250, San Rafael, CA, 94901, USA

IOP Publishing, Temple Circus, Temple Way, Bristol BS1 6HG, UK

*Dedicated to all those undergraduates who have had to suffer  
my tutorials for the last 40 years!*



# Contents

<b>Preface</b>	<b>x</b>
<b>Acknowledgements</b>	<b>xi</b>
<b>Author biography</b>	<b>xii</b>
<b>1 Direct space</b>	<b>1-1</b>
1.1 What are crystals?	1-1
1.2 Miller indices	1-2
1.3 Point symmetry	1-4
1.4 Point groups	1-11
1.5 Translational symmetry	1-13
1.6 Crystal structures	1-25
1.7 Space groups	1-33
References	1-37
<b>2 The reciprocal lattice</b>	<b>2-1</b>
Brief history	2-1
2.1 Definition	2-2
2.2 Construction	2-3
2.3 Geometrical calculations	2-6
References	2-10
<b>3 Diffraction</b>	<b>3-1</b>
3.1 Laue equations	3-1
3.2 Bragg's Law	3-2
3.3 The Ewald sphere	3-6
3.4 Lost in reciprocal space?	3-6
3.5 Intensity	3-16
3.6 Fourier transformation	3-19
3.7 Convolution theorem	3-20
3.8 Two simple 'Rules'	3-25
3.9 Lattice diffraction	3-26
3.10 Structure factors	3-28
3.11 Form factors	3-29
3.12 Anomalous dispersion	3-31

3.13	Intensity calculations	3-38
3.14	Solution of crystal structures	3-42
3.15	Fourier synthesis	3-44
3.16	The Patterson method	3-48
3.17	Charge flipping	3-50
3.18	The Rietveld method	3-52
3.19	Total scattering analysis	3-54
3.20	Aperiodic crystals	3-55
3.21	Disordered crystals	3-60
	References	3-61
<b>4</b>	<b>Dynamical diffraction</b>	<b>4-1</b>
4.1	Multiple scattering	4-1
4.2	Renninger effect	4-2
4.3	Two-beam approximation in electron diffraction	4-3
4.4	Pendellösung or thickness fringes	4-8
	References	4-10
<b>5</b>	<b>Waves in a periodic medium</b>	<b>5-1</b>
5.1	Waves in space	5-1
5.2	Periodic boundary conditions	5-2
5.3	Bloch's theorem	5-4
5.4	Brillouin zones	5-5
5.5	Wigner–Seitz cell	5-7
5.6	Higher-order Brillouin zones	5-10
5.7	Density of states	5-12
	References	5-14
<b>6</b>	<b>Thermal and electronic properties</b>	<b>6-1</b>
6.1	Specific heat capacity of solids	6-1
6.2	Einstein model	6-2
6.3	Debye model	6-3
6.4	Vibrations of atoms	6-9
6.5	Lattice dynamics	6-21
6.6	Heat conduction	6-23
6.7	Interaction with radiation	6-27

6.8	Free electrons in a metal	6-33
6.9	Nearly free electrons	6-35
6.10	Metal or insulator?	6-38
	References	6-42
<b>Appendix</b>	<b>Wigner–Seitz constructions</b>	<b>A-1</b>

# Preface

The concept of reciprocal space is over 100 years old, and has been made particular use of by crystallographers in order to understand the patterns of spots when x-rays are diffracted by crystals. However, it has a much more general use, especially in the physics of the solid state. In order to understand what it is, how to construct it and how to make use of it, it is first necessary to start with the so-called real or direct space and then show how reciprocal space is related to it. Real space describes the objects we see around us, especially with regards to crystals, their physical shapes and symmetries and the arrangements of atoms within: the so-called crystal structure. Reciprocal space on the other hand deals with the crystals as seen through their diffraction images. Indeed, crystallographers are accustomed to working backwards from the diffraction images to the crystal structures, which we call crystal structure solution. In solid state physics, one usually works the other way, starting with reciprocal space to explain various solid-state properties, such as thermal and electrical phenomena.

In this book, I start with the crystallographer's point of view of real and reciprocal space and then proceed to develop this in a form suitable for physics applications. Note that while for the crystallographer reciprocal space is a handy means of dealing with diffraction, for the solid-state physicist it is thought of as a way to describe the formation and motion of waves, in which case the physicist thinks of reciprocal space in terms of momentum or wave-vector  $\mathbf{k}$ -space. This is because, for periodic structures, a characteristic of normal crystals, elementary quantum excitations, e.g. phonons and electrons, can be described both as particles and waves. The treatment given here, will be by necessity brief, but I would hope that this will suffice to lead the reader to build upon the concepts described. I have tried to write this book in a suitable form for both undergraduate and graduate students of what today we call 'condensed matter physics'.

# Acknowledgements

I was fortunate to learn all about crystallography from two great scientists, Kathleen Lonsdale, my PhD supervisor, and Helen D Megaw at the Cavendish Laboratory, Cambridge, who introduced me to the world of perovskites. Although I had started out as a chemist, I soon appreciated from them the value of condensed matter physics and how it related to crystallography. Thus, when I was appointed to the Clarendon Laboratory, Oxford in 1976 I was in a good position to teach undergraduates and graduates about the solid state, sometimes from a unique point of view. The topics described in this book owe much to hours of discussions, sometimes quite heated, with many of my tutees at Jesus College Oxford. There is nothing like teaching students to make one realize how little one really understands about a subject, and how to relearn something that you thought was already done and dusted. Despite retirement, I continue to learn.

# Author biography

## A M Glazer

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Mike Glazer is Emeritus Professor of Physics at the University of Oxford and Jesus College Oxford, and Visiting Professor at the University of Warwick. From 2014 to 2017 he was also Vice-President of the International Union of Crystallography. His PhD research between 1965 and 1968 was under the supervision of Kathleen Lonsdale at University College London, working on the crystallography of organic mixed crystals. In 1968–1969, he was a Fellow at Harvard University, and then from 1969 to 1976 he was at the Cavendish Laboratory, Cambridge. In 1976, he was appointed Lecturer in Physics at the Clarendon Laboratory Oxford and as an Official Fellow and Tutor at Jesus College Oxford. Mike Glazer's research has mainly been in understanding the relationship between physical properties of crystals and their structures. He is perhaps best known for his classification system for tilted octahedra in perovskites. He is also one of the co-founders of Oxford Cryosystems Ltd, which supplies the world market in low-temperature apparatus for crystallographers.

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## Chapter 1

### Direct space

*'Je ne te parlerai que cristaux'*

L Pasteur, in a letter to Charles Chappuis from Strasbourg (July, 1850)

In order to set out on our journey, we shall first have to follow Pasteur and talk about crystals in terms of *Direct* (or *Real*) *Space*. Once this is understood, we can then advance to the next leg of the journey that takes us into *Reciprocal Space* itself, the principal aim of this book. This discussion will centre mainly around crystalline materials from the point of view of their symmetries. There are many books (e.g. [1–5]) and web pages that explain these ideas more fully than I shall be able to do here.

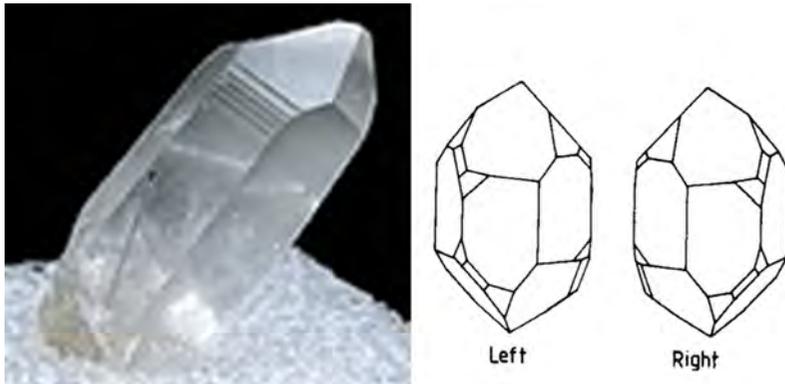
#### 1.1 What are crystals?

Crystals (from the Greek κρυσταλλος, meaning ‘rock crystal’ but also ‘ice’ from κρυσ, ‘icy cold, frost’) have been known about for centuries as minerals that have naturally-occurring flat faces bearing some sort of symmetry relationship to each other. Probably the most well-known mineral crystal is that of quartz, especially in its clear form called rock crystal (figure 1.1).

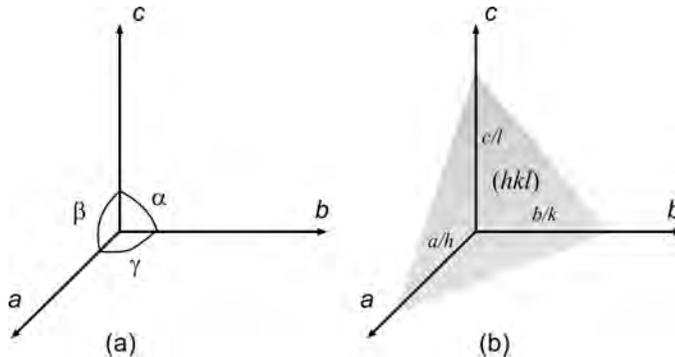
Quartz, chemical formula  $\text{SiO}_2$ , grows naturally as elongated prisms with large faces arranged around a 3-fold axis of symmetry, together with inclined faces top and bottom. This particular mineral exists in two crystalline habits that are mirror images of each other, a symmetry property known as *chirality* (see [6] for an interesting discussion of the errors made in the literature describing quartz).

**Definition.** *Crystal habit is the formal name for the shape of a crystal. Some examples of crystal habit are acicular (needle-like), prismatic (elongated prisms) and stellate (star-shaped). There are many others.*

**Definition.** *Crystal morphology is a term that describes the crystal in terms of its habit, defect nature and polymorphism (where a substance can crystallize in different forms, e.g. diamond and graphite).*



**Figure 1.1.** On the left an example of a natural crystal of quartz (rock crystal). On the right morphological drawings of left and right-handed habits of quartz crystals.

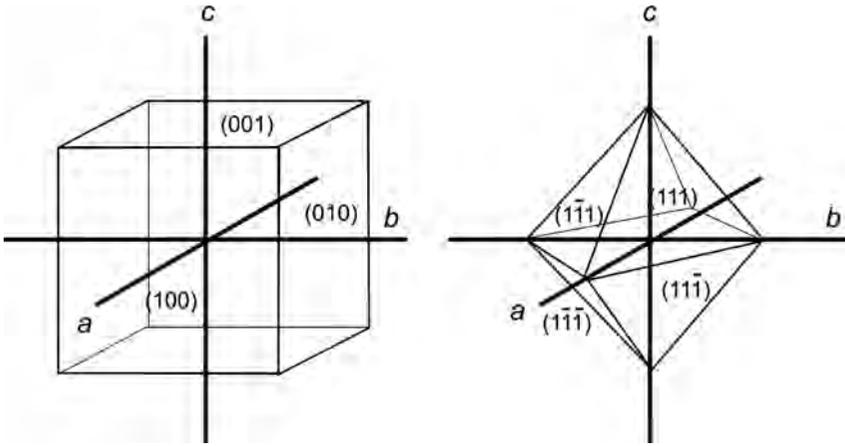


**Figure 1.2.** Miller indices. (a) Right-hand convention for choice of axes. (b) Definition of a plane.

## 1.2 Miller indices

In order to be able to characterize the different crystal habits, it is necessary to introduce a system whereby each of the crystal faces can be assigned a label. The most commonly used system was introduced in 1839 by the British mineralogist William Hallows Miller. To explain this, we first need to adopt a convention for naming axes and angles in a crystal.

Figure 1.2(a) shows the right-hand screw convention for the choice of axes  $a$ ,  $b$  and  $c$  and for interaxial angles  $\alpha$ ,  $\beta$  and  $\gamma$ . Note that these axes can be any length in general and the angles need not be  $90^\circ$ , depending on the crystal symmetry. In figure 1.2(b), a plane (in grey) intersects the three axes to make intercepts at  $a/h$ ,  $b/k$  and  $c/l$ . The plane is then indexed as  $(hkl)$ . According to the Law of Rational Indices found by René Just Häuy in the 19th century, the indices should be integers, although there are in fact a few rare cases, such as in the mineral calaverite,  $\text{AuTe}_2$ , where some faces could only be indexed on irrational indices.



**Figure 1.3.** Miller indices for the faces of a cube and an octahedron. Only the front faces are marked in this figure.

**Notation.** *Miller indices are written in parentheses like this  $(hkl)$ .*

So, a face that is perpendicular to the  $a$  axis and is parallel to  $b$  and to  $c$  has the plane symbol  $(100)$ , as it cuts off unit intercept along  $a$  and infinite intercept along  $b$  and  $c$  (figure 1.3). Similarly, the faces of an octahedron, once the axes have been assigned, have indices  $(111)$ ,  $(1\bar{1}1)$ ,  $(1\bar{1}\bar{1})$ ,  $(11\bar{1})$ , ..... as each face cuts off unit intercept on all three axes.

**Notation.** *Negative indices are marked with a bar above the number. In my experience, this is said 'bar 1' in the United Kingdom, while Americans usually say '1 bar'! Not sure what the rest of the world says.*

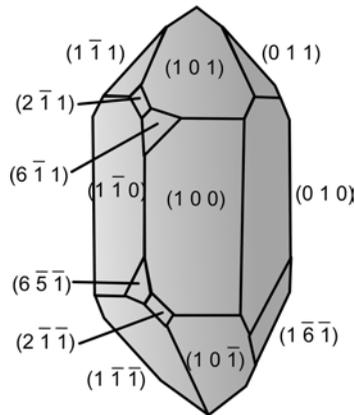
**Definition.** *The complete set of indexed faces with a particular set of Miller indices related by symmetry is called a form and is denoted  $\{hkl\}$ . Thus, an octahedron has the form  $\{111\}$ .*

Returning to our old friend, quartz (figure 1.4), the habit is complicated and the indices of the faces appear to be unrelated to each other. This arises because of a peculiarity in crystals with so-called hexagonal/trigonal symmetry, i.e., those that contain a single 6-fold or 3-fold axis of symmetry. In this case, the Miller index is best extended to four indices  $(hkil)$ , in other words using four axes rather than three. The  $c$ -axis is along the 6- or 3-fold axis, while the other three are perpendicular to  $c$  and are  $120^\circ$  from each other. The following rule applies

$$h + k + i = 0. \tag{1.1}$$

So, for example, if we consider the  $(101)$  face it can be alternatively written as  $(10\bar{1}1)$ . Then permuting the first three indices we get the  $\{10\bar{1}1\}$  form:

$$(10\bar{1}1) (\bar{1}011) (0\bar{1}11) (01\bar{1}1) (1\bar{1}01) (\bar{1}101) \tag{1.2}$$



**Figure 1.4.** Sketch of a quartz crystal showing indices  $(hkl)$  for the visible faces.

which, when referred back to the 3-axis symbol, becomes

$$(101) (\bar{1}01) (0\bar{1}1) (011) (1\bar{1}1) (\bar{1}11) \quad (1.3)$$

You can now see why it is in figure 1.4 that the three faces  $(101)$ ,  $(011)$ ,  $(1\bar{1}1)$  are related about the vertical axis (the three remaining faces of the form are hidden behind the diagram).

In the same way, we see that the two faces marked  $(6\bar{1}1)$  and  $(6\bar{5}\bar{1})$  (in 4-axis symbols  $(6\bar{1}\bar{5}1)$  and  $(6\bar{5}\bar{1}\bar{1})$ ) are related. as far as the first two indices are concerned, with only the last index being of opposite sign.

### 1.3 Point symmetry

*Tidiness is a virtue, symmetry is often a constituent of beauty...*

Winston Churchill

Let us now look at what sort of symmetry operators are needed to describe the symmetry of a crystal.

**Definition.** *Point symmetry operators are those that describe symmetry operations that act through a point in space.*

In crystallographic symmetry we shall need three types of point symmetry operator: proper rotations, inversions and rotoinversions (or roto reflections).

#### Proper rotations

A proper rotation is one that rotates a position vector through an angle about an axis that passes through a defined point. Repeated rotation finally brings the

**Table 1.1.** Crystallographic rotations.

Symbol	Operation	Element	Matrix
1( $E$ )	Identity	–	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
2( $C_2$ )	2-fold rotation	Axis	$\begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{bmatrix}$
3( $C_3$ )	3-fold rotation	Axis	$\begin{bmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{bmatrix}$
4( $C_4$ )	4-fold rotation	Axis	$\begin{bmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
6( $C_6$ )	6-fold rotation	Axis	$\begin{bmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$

position vector back to its starting position. Table 1.1 shows the rotations (here, about the  $c$ -axis) used to describe crystallographic symmetry.

Notice that the only rotations considered are 2, 3, 4 and 6-fold (I have also included operation 1, the trivial identity operation in this table). The symbols are given in two common notations: the International system, described originally by the French mineralogist Charles-Victor Mauguin and the German crystallographer Carl Hermann, and the Schoenflies system (in parentheses). These days, it is the International Notation that is used in crystallography, while subjects such as spectroscopy tend to use the Schoenflies system. The table also gives matrices  $R$  that carry out the operation

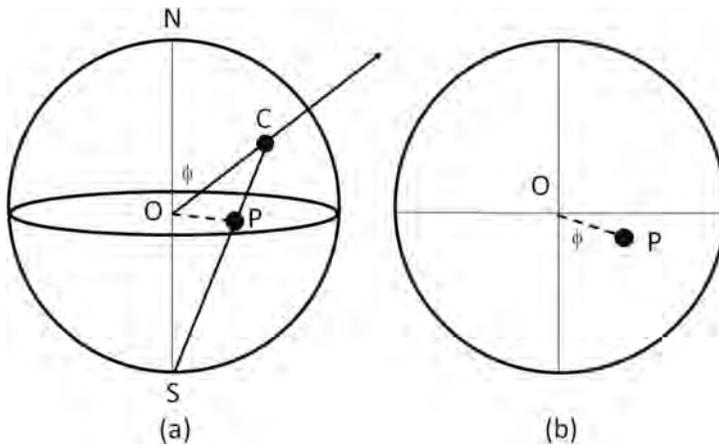
$$R\mathbf{r} = \mathbf{r}'. \quad (1.4)$$

Thus, with rotation axes along  $c$  the rotation operations have the following mappings of points:

$$\begin{aligned} 2: (x, y, z) &\rightarrow (\bar{x}, \bar{y}, z) \\ 3: (x, y, z) &\rightarrow (\bar{y}, x - y, z) \\ 4: (x, y, z) &\rightarrow (\bar{y}, x, z) \\ 6: (x, y, z) &\rightarrow (x - y, x, z). \end{aligned} \quad (1.5)$$

**Note.** The axis of rotation is an example of what is termed a symmetry element, which in the examples given in the table has been chosen to lie along the  $c$ -axis of the crystal.

A useful way to represent the effect of applying symmetry operations is by making use of the stereographic projection. This is a way of representing points on a



**Figure 1.5.** The stereographic projection. (a) Construction of a pole (b) resulting projection onto a plane.

sphere by projecting onto a plane, much in the way a map of the world is often represented viewed down onto the North Pole. Imagine (figure 1.5(a)) that there is a point C on the surface of a sphere. Now draw a line SC: this intersects the horizontal plane perpendicular to NS at the point P. N and S can be thought of as the north and south poles, respectively. Figure 1.5(b) shows the projection plane viewed from above where the point P is plotted. The distance OP in this projection is a measure of the angle  $\phi$  measured from the north pole ( $90^\circ$ -latitude in cartography) and the point P is called a pole.

Figure 1.6 shows how the effects of symmetry operations are conventionally shown in stereographic projections. The upper four diagrams are for the proper rotations. Consider first the diagram for the rotation operation 2. The small circle with the plus sign next to it represents any object in space (not necessarily a circle!). I shall call this the ‘object’ and its position in the diagram a general position. The plus sign indicates that it is on the northern hemisphere (you may prefer to think of it as being above the plane of the paper towards you). In each case start with the object near the bottom. The 2-fold operation about the axis perpendicular to the stereographic projection, i.e., along NS, rotates this through  $180^\circ$  to the general position near the top. We see that the resulting object remains in the northern hemisphere as marked by the plus sign. The black symbol at the centre of the stereographic projection, looking somewhat like a rugby football, denotes the 2-fold axis.

**Note.** *It is conventional to apply rotation operations anticlockwise about the chosen axis.*

Note also, that if the 2-fold rotation is applied again, the object returns to its starting position, i.e.,

$$2^2 = 1 \quad \text{or} \quad C_2^2 = E \quad (1.6)$$

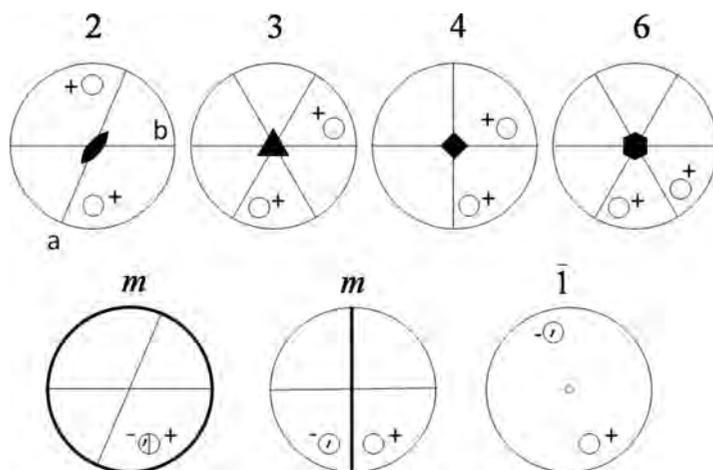


Figure 1.6. Stereographic projections showing rotations and inversion operations.

The next three diagrams show the effect of rotations 3, 4 and 6. By studying these diagrams (or by multiplying out the matrices in table 1.1) we can find interesting relationships such as the following:

$$\begin{aligned} 6^5 &= 6^{-1} \\ 6^4 &= 3^2 = 3^{-1} \\ 6^3 &= 2 \end{aligned} \tag{1.7}$$

Figure 1.7 shows a few examples of rotational symmetry in some everyday objects. It is a good exercise to see how many examples of rotation symmetry you can find during a walk through your neighbourhood.

### Reflections and inversions

Symmetry operations that are classed as inversions are given in table 1.2.

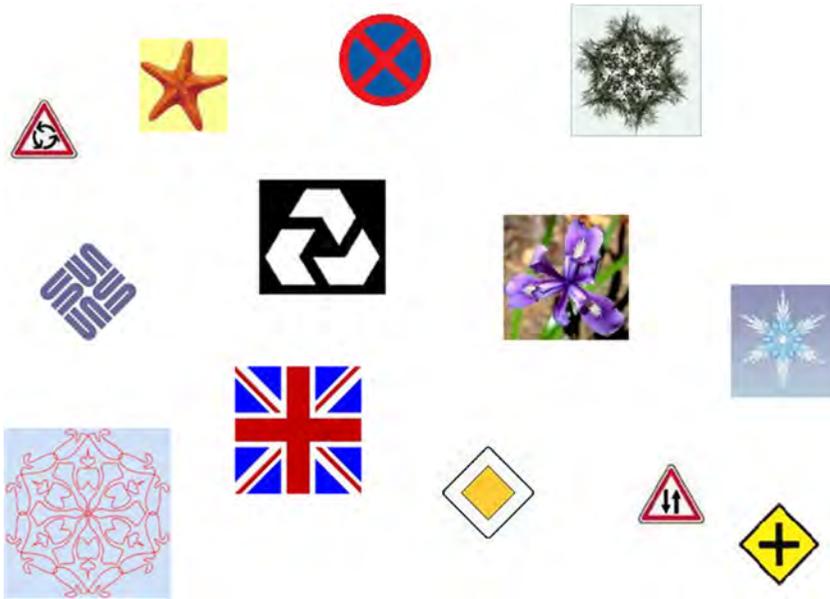
The operation of reflection is one that reflects every point in an object as if through a mirror. For a mirror plane perpendicular to the  $c$ -axis

$$m: (x, y, z) \rightarrow (x, y, \bar{z}) \tag{1.8}$$

Figure 1.8 also shows some examples of reflections. An important effect of the reflection operation is to convert left-handed objects into right-handed objects, such as in the relationship between the two quartz crystals in figure 1.1.

It is not possible to transform a left-handed object into a right-handed object by using a rotation, and vice versa. Actually, in mathematical terms, this statement is not quite true, provided that we are allowed to change dimensionality: we first transform the description of a three-dimensional chiral object into four dimensions, rotate it and then collapse back into three dimensions! Oh the joys of mathematics!

The bottom line of figure 1.6 shows the stereographic projections for the inversion operations. The first two diagrams are different views of the same type of operation, namely the reflection or mirror operation. In the first stereographic projection, a



**Figure 1.7.** Some examples of everyday objects showing rotational symmetry. Reprinted from [7] with permission of Elsevier.

**Table 1.2.** Reflections and inversions.

Symbol	Operation	Element	Matrix
$m(\sigma)$	Reflection	Mirror plane	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$
$\bar{I}(i)$	Inversion	Inversion centre	$\begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$

mirror plane is located on the plane perpendicular to the  $c$ -axis: this is signified by the thick black line round the perimeter. The effect of this is to reflect the object from the northern to the southern hemisphere (or from above to behind the plane of projection). As this places the reflected object directly beneath the original object in this projection, this is indicated by splitting the object symbol by a vertical line. The minus sign now indicates that the reflected object is below the plane of projection and the comma indicates a change of chirality or hand. The second stereographic projection shows the reflection operation this time with the mirror plane, indicated by the thick line, perpendicular to the  $b$ -axis.

The third diagram shows the inversion operation:

$$\bar{I}: (x, y, z) \rightarrow (\bar{x}, \bar{y}, \bar{z}) \quad (1.9)$$



Figure 1.8. Examples of reflection symmetry in everyday objects.

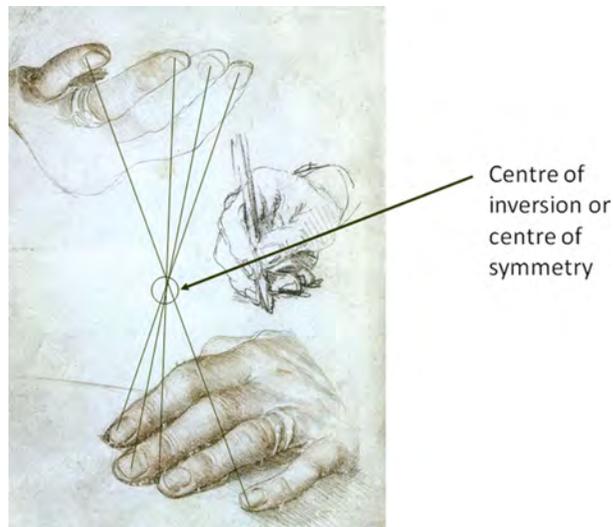


Figure 1.9. Drawing of left and right hands of Erasmus of Rotterdam by Holbein (1523). Lines have been added to indicate the inversion relationship. Reprinted from [7] with permission of Elsevier.

This operation is nicely illustrated by a drawing by Holbein of the hands of Erasmus of Rotterdam (figure 1.9). The relationship between the two hands as drawn shows that each point on one hand is (more or less) related to an equivalent point on the other hand, as indicated by the added lines, and these lines all pass through a point

known as the *centre of inversion*, sometimes called the *centre of symmetry*. Any object that contains a centre of symmetry is said to be *centrosymmetric*. Some scientists use the terms *centric* and *acentric*, but this is incorrect, for these terms are used in crystallography to refer to intensity distributions in the diffraction patterns. Note, that just like with reflections, inversion also changes the chirality of an object.

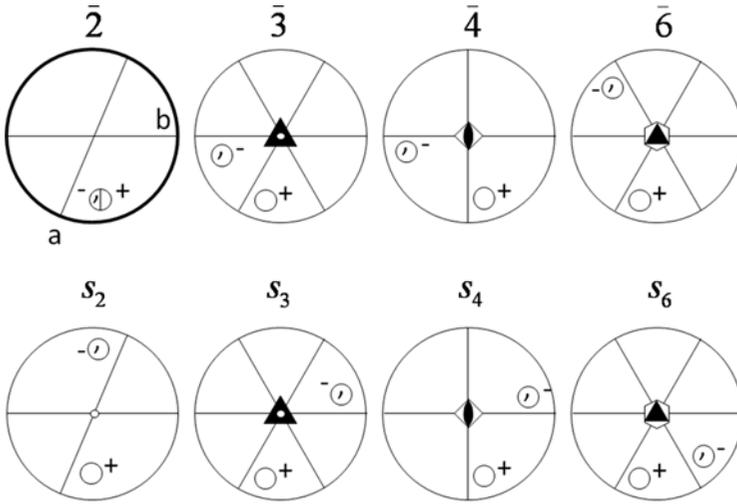
### Rotoinversions and roto reflections

The final types of point symmetry operations that we need to discuss are slightly more complicated than the others. The complication arises because of the different ways in which the International and Schoenflies systems define these operations. These operations are a combination of a rotation and an inversion (International system) or a rotation and a reflection (Schoenflies system).

Table 1.3 lists these operations and figure 1.10 shows the stereographic projections.

**Table 1.3.** Crystallographic rotoinversions and roto reflections.

Symbol	Operation	Element	Matrix
$\bar{2}$	Rotoinversion	Point	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$
$S_2$	Rotoreflexion	Point	$\begin{bmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$
$\bar{3}$	Rotoinversion	Point	$\begin{bmatrix} 0 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$
$S_3$	Rotoreflexion	Point	$\begin{bmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$
$\bar{4}$	Rotoinversion	Point	$\begin{bmatrix} 0 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$
$S_4$	Rotoreflexion	Point	$\begin{bmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$
$\bar{6}$	Rotoinversion	Point	$\begin{bmatrix} \bar{1} & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$
$S_6$	Rotoreflexion	Point	$\begin{bmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{bmatrix}$



**Figure 1.10.** Stereographic projections for rotoinversions operations (top) and roto reflections operations (bottom).

The following mappings then follow for the International system:

$$\begin{aligned}
 \bar{2}: (x, y, z) &\rightarrow (x, y, \bar{z}) = m: (x, y, z) \\
 \bar{3}: (x, y, z) &\rightarrow (y, \bar{x} + y, \bar{z}) \\
 \bar{4}: (x, y, z) &\rightarrow (y, \bar{x}, \bar{z}) \\
 \bar{6}: (x, y, z) &\rightarrow (\bar{x} + y, \bar{y}, \bar{z})
 \end{aligned}
 \tag{1.10}$$

We see from this several relationships. First of all, the International  $\bar{2}$  operation is in fact equivalent to a reflection while the Schoenflies  $S_2$  operation is equivalent to an inversion. More confusingly, perhaps, we find the following:

$$\begin{aligned}
 \bar{3} &= S_6^5 = S_6^{-1} \\
 \bar{4} &= S_4^3 = S_4^{-1} \\
 \bar{6} &= S_3^5 = S_3^{-1} \\
 S_3 &= \bar{6}^5 = \bar{6}^{-1} \\
 S_6 &= \bar{3}^5 = \bar{3}^{-1}
 \end{aligned}
 \tag{1.11}$$

So, for these types of operations there is a possible confusion between 3-fold and 6-fold roto-operations depending on which system one uses. Beware!

## 1.4 Point groups

Suppose the symmetry of a crystal can be described by a 2-fold rotation, and at the same time by a reflection perpendicular to the 2-fold axis. Taking the 2-fold axis to lie along the  $c$ -axis, and using the matrices in tables 1.1 and 1.2 we find the following relationships.

$$\begin{aligned}
 2.2 &= 1 \\
 m.m &= 1 \\
 2.m &= \bar{1} \\
 \bar{1}.\bar{1} &= 1
 \end{aligned}
 \tag{1.12}$$

This shows that the combination of the 2-fold and perpendicular reflection operation generates a centre of inversion. Therefore, in this case we have four symmetry operations  $\{1, 2, m, \bar{1}\}$ . We now show that these operations together form a group, as defined in mathematics by the following four criteria.

1. The following multiplication table of operations can be written

	1	2	$m$	$\bar{1}$
1	1	2	$m$	$\bar{1}$
2	2	1	$\bar{1}$	$m$
$m$	$m$	$\bar{1}$	1	2
$\bar{1}$	$\bar{1}$	$m$	2	1

showing that the effect of each operation on another always generates another that is one of the four, and so these operations form a closed set. Because this particular matrix is symmetric, this is known as an Abelian group (not all groups are Abelian though).

2. There is an identify operation 1.
3. There is an inverse operation given by  $XX^{-1} = 1$ . In this case, each operation is its own inverse.

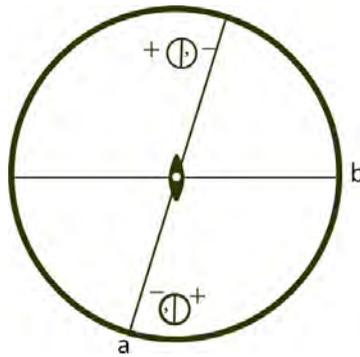
$$\begin{aligned}
 1.1 &= 1 \\
 2.2 &= 1 \\
 m.m &= 1 \\
 \bar{1}.\bar{1} &= 1
 \end{aligned}
 \tag{1.13}$$

4. Associativity is true. For example

$$2.(m.\bar{1}) = (2.m).\bar{1} \tag{1.14}$$

Figure 1.11 shows a stereographic projection for this group including the symmetry elements. We see from this that this group contains 4 operations, 4 elements and generates 4 general positions and is therefore a group of order 4.

**Definition.** *The order of a group is given by the number of operations that it contains.*



**Figure 1.11.** Stereographic projection for the point group  $2/m(C_{2h})$ .

This group is given the symbol  $2/m$ , the  $/$  indicating that the 2-fold axis is perpendicular to the mirror plane, in the International notation. The Schoenflies symbol is  $C_{2h}$ : C stands for cyclic and the subscript 2 is for the 2-fold axis and h for a horizontal mirror plane.

**Note.** *If we use all the possible rotations, inversions and rotoinversion operations relevant to crystal symmetry to form groups it is found that in three dimensions there are 32 distinct point groups, sometimes called the 32 geometric crystal classes. These are listed in table 1.4.*

## 1.5 Translational symmetry

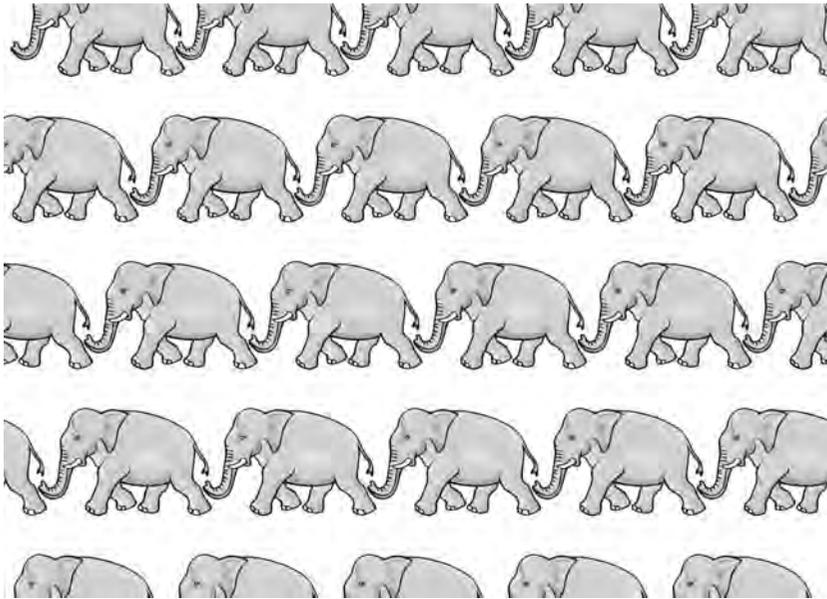
So far, our discussion on symmetry has been with respect to macroscopic objects such as the crystals we might see around us. We shall now turn our attention to the internal structure of a crystal and how we can describe the arrangements of atoms that make up this structure. The point symmetries will still be relevant at the microscopic scale of atoms and molecules in the crystal. However, before looking at atomic arrangements, we shall first have to introduce a form of symmetry that is characteristic of ideal crystalline materials, *translational symmetry*.

**Definition.** *Translational symmetry is the symmetry that is exhibited by a collection of equivalent objects repeated regularly throughout space.*

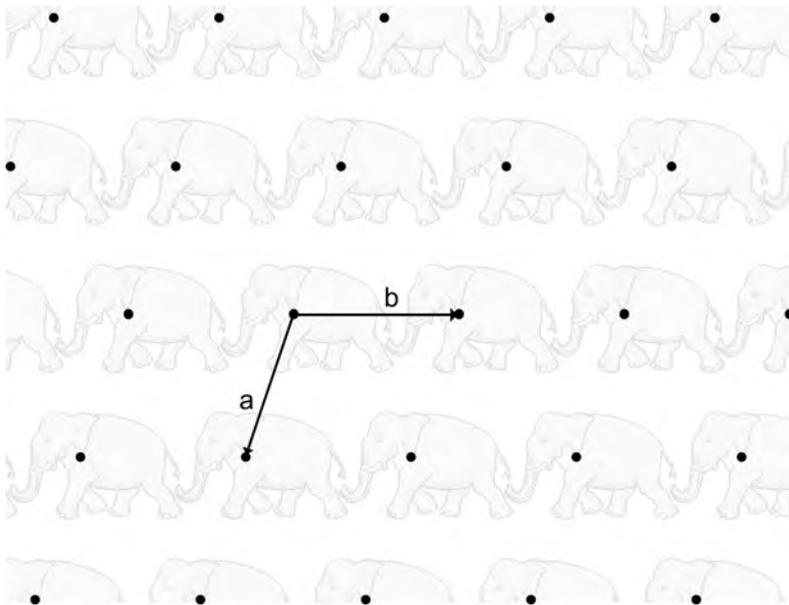
Figure 1.12 shows a picture of a herd of elephants in a regularly repeating pattern that can be described by translational symmetry. Each elephant is at a fixed distance from its neighbour in each direction in space.

### Lattices

Suppose now we replace each of the elephants in figure 1.12 by a point, for instance placed at the tip of each tusk. Now remove the elephants (figure 1.13). The result is a



**Figure 1.12.** A herd of elephants illustrating translational symmetry.



**Figure 1.13.** Lattice describing translational symmetry of figure 1.12.

repeating pattern of points. Now I have to emphasize something here that I have seen many students (and working scientists for that matter) become confused about. Do not mistake the points in this figure for atoms. These are mathematical, infinitesimal points and the only reason I have drawn them with a finite diameter

is so that you can see them. Mathematically we can treat the points as a series of repeating delta functions. This then leads to an important definition.

**Definition.** *A lattice is a regular repeating array of points (not atoms!).*

Here is my ‘Government Health Warning’. Unfortunately, you will see in many textbooks a reference to the word ‘lattice’ when they actually mean arrays of atoms, not points. So, for instance if we had a repeating pattern of single atoms it would look just like figure 1.13, but in fact this would not be a lattice but a crystal structure (more of this below). In the figure, I have left traces of the original elephants so that you can see where the lattice points have been set. A lattice is a mathematical device that acts as a template to tell us how to position atoms and molecules in space: as such a lattice has no physical existence. A powerful microscope would not show us a lattice but a crystal structure instead. Similarly, when a textbook mentions, for example, the diamond lattice or the copper lattice, they almost certainly should have said the diamond crystal structure and the copper crystal structure. Diamond has pairs of carbon atoms repeating throughout space and copper has single copper atoms repeating throughout space, and so they look quite different. On the other hand, they have the same lattice type, apart from an overall change in dimensions: both have all-face-centred lattices (see below). Please resist using the term ‘lattice structures’ which you will often see in books: it is an old term and these days it is best avoided as it can create a confusion between lattice and structure. You may think that I am being a bit ‘picky’, but misunderstandings of this sort can have practical consequences. I recall many years ago, a student who wasted a year’s computing resources on an erroneous electronic band structure calculation because he had not understood the difference between lattice and structure.

In figure 1.13 the lattice is shown as a two-dimensional array, but of course in three dimensions there will be repeating lattice points above and below this plane. Now, two arbitrarily chosen axes,  $a$  and  $b$ , have been marked, with an origin arbitrarily chosen on one of the lattice points (we can assume that there is a  $c$ -axis pointing out of the plane of points). Once the axes and origin have been chosen, all lattice points can be reached by the so-called *primitive* translation vector  $\mathbf{t}_n$

$$\mathbf{t}_n = n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c} \quad (1.15)$$

where  $n_1$ ,  $n_2$  and  $n_3$  are integers. Therefore, it is the primitive translation vector that defines the lattice.

### Unit cells

Having defined the lattice, we can make good use of the periodicity it exhibits. Consider figure 1.14, where the same lattice is shown, but this time with two regions outlined in black. These regions are called unit cells.

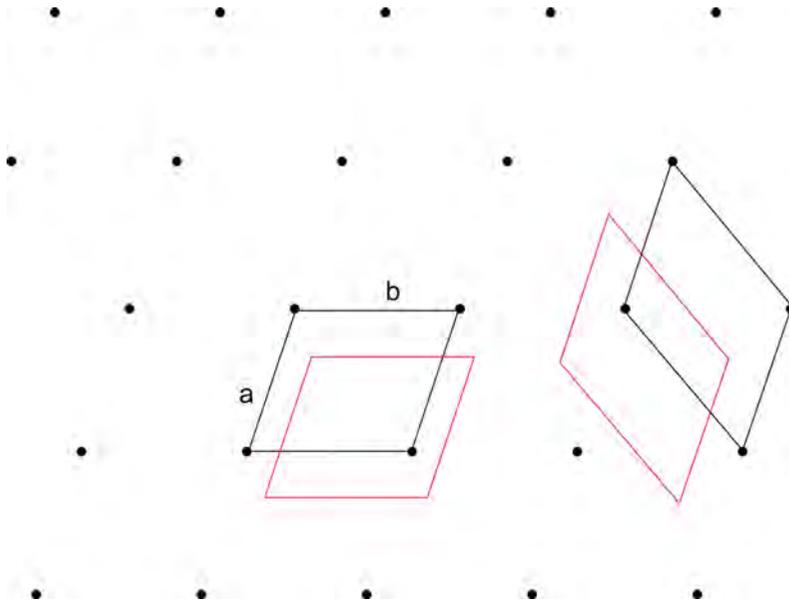
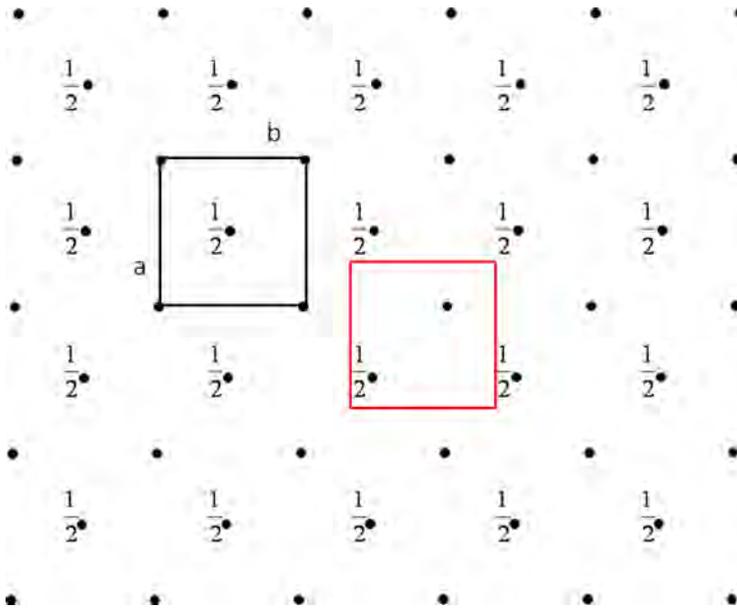


Figure 1.14. A primitive lattice showing primitive unit cells.

**Definition.** *A unit cell is a region of space which when repeated by primitive translational symmetry fills all space. It can in principle be of any shape, although crystallographers always use a parallepiped shape to describe the unit cell.*

So, the importance of defining a unit cell is that we need only consider the unit cell alone (used in describing crystal structures where we add atoms and molecules into each unit cell) and then allow the primitive translation operator to repeat it. In other words, it is not necessary to write down all the coordinates of the lattice points or atoms in the whole crystal. That after all is the point of symmetry: it enables us to specify just a few things and then allow symmetry operators to generate everything else.

In this lattice two examples of unit cell are drawn, but a moment's thought should convince you that in fact we could define an infinite number of different unit cells. Furthermore, these unit cells both have the same volume (in three dimensions). How do we know this? Simply count the number of lattice points per unit cell and we shall find that it is the same for both unit cells drawn. Now here is a little trick. Often you will see that to count the number of lattice points per unit cell books will often try to partition the lattice points between neighbouring unit cells, as if there were fractions of a lattice point (I don't know how to make a fraction of a point!). So, in the figure we might take a lattice point at each corner of the unit cell and then say that each point is shared between neighbouring unit cells. But there is a much easier way to do the counting. Simply move the origin of the unit cell, as the origin is in fact arbitrary: if we move one unit cell then all the others must move with it and so still fill all space.



**Figure 1.15.** Body-centred (*I*) unit cell and lattice. The points marked  $\frac{1}{2}$  lie on a plane through  $c/2$  above the unmarked points.

Here, the displaced unit cells are in red and then it is easy to see that each contains just one lattice point. These unit cells must therefore have the same volume, like all other possible unit cells that contain just one lattice point.

**Definition.** *Unit cells that contain one lattice point are called primitive unit cells and the lattice described by them is called a primitive lattice. Primitive lattices are designated by the letter *P*.*

While in any lattice one can define an infinite variety of primitive unit cells, it is often useful to define so-called *centred* unit cells. In figure 1.15, the unmarked points form a lattice at height 0, while the points marked  $\frac{1}{2}$  are those on the plane above at a distance  $c/2$ . The next plane repeats the plane at height  $c$  and so on. Also shown is an example of a unit cell with a lattice point at the origin, at coordinate position  $(0, 0, 0)$  and another point in the centre of the unit cell at  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . These coordinates are given as fractions of the unit cell edges  $a$ ,  $b$  and  $c$ . Displacing the unit cell (marked in red) immediately shows that this centred unit cell contains two lattice points. Because this unit cell has a lattice point at its centre it is called a *body-centred unit cell* and the lattice is a body-centred lattice. This type of lattice is conventionally given the symbol *I*. Figure 1.16 shows other types of centering together with their conventional symbols and fractional coordinates of the lattice points. The *C*-face centred unit cell can equally be described as *A* or *B*-centering simply by changing the labels for the axes.