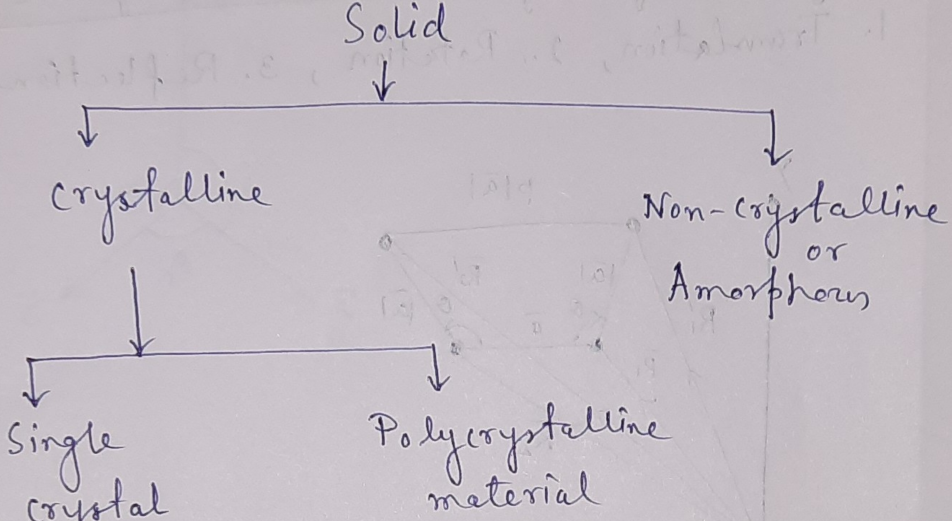
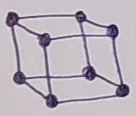
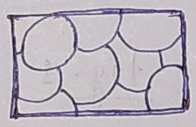
Study Material – Sem. 5 – C12T

– Crystal Structure – Dr. T. Kar

– Class 1 :–





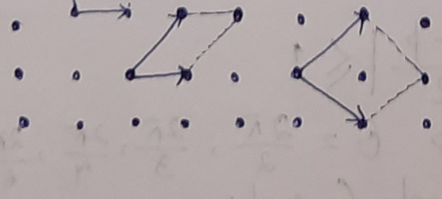


- **Crystal Translational Vectors**

$$\overrightarrow{T} = n_1 \bar{a} + n_2 \bar{b} + n_3 \bar{c}$$

$$\vec{r}\,' = \vec{r} + \overrightarrow{T}$$

- **Unit Cell**



(i) Primitive unit cell

(ii) Non-primitive unit cell

• Lattice & Basis

Lattice + Basis = Crystal Structure

• Symmetry operation in 2D crystal

1. Translation, 2. Rotation, 3. Reflection

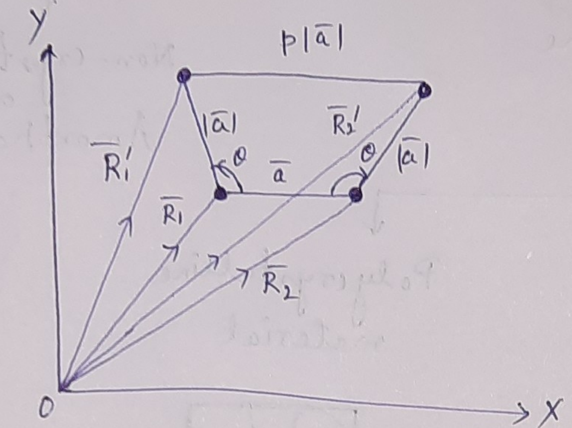


Fig. 1

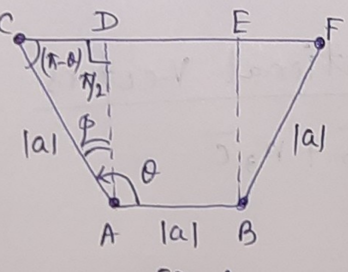


Fig. 2

$DE = AB = |\bar{a}|$

$CD = ?$

$\pi - \theta + \pi/2 + \phi = \pi$

$\therefore \phi = \theta - \pi/2$

$\therefore CD = |\bar{a}| \sin(\theta - \pi/2)$

$\therefore p|\bar{a}| = |\bar{a}| + 2|\bar{a}| \sin(\theta - \pi/2)$

or, $p = 1 - 2\cos\theta$

$\therefore |\cos\theta| = \left|\frac{1-p}{2}\right| \leq 1$

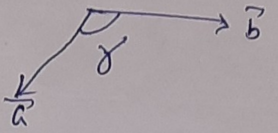
$p = 3, 2, 1, 0, -1 \Rightarrow \theta = \frac{2\pi}{2}, \frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}, \frac{2\pi}{1}$

$\Rightarrow n = 1, 2, 3, 4$ and 6 only.

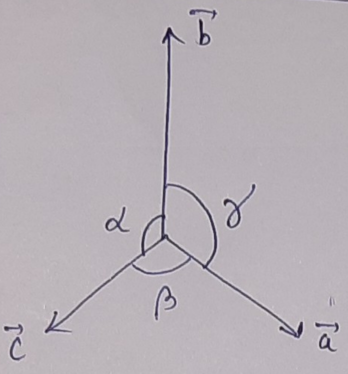
2D Bravais Lattice

point group →

Space group →



3D Bravais lattice



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ELEMENTS OF CRYSTAL STRUCTURE

The solid state of matter can be put into two broad categories on the basis of their structure : the crystalline or non-crystalline (or amorphous). The distinction between the two does not, however, depend on their external appearance or macroscopic form ; instead, they are distinguished from one another primarily by the degree of order exhibited by the arrangement of the fundamental particles—atoms, molecules or ions comprising them. In crystalline solids, the atoms or the molecules or ions (which may be compared with 'building blocks') are stacked in a regular manner, just like the soldiers do on the parade ground, thus forming a three-dimensional pattern which may be obtained by a three-dimensional repetition of a building block or 'pattern unit'. When the regularity of the pattern extends throughout a certain piece of solid, then it can be treated for many purposes a 'single crystal' and would be so called. However, most of the solids of technical interest, such as metals, ceramics, ionic salts, are not single crystals, but often consist of a large number of small crystal sections (grains) of various shapes and sizes packed to one another in a quite irregular way along the interfaces called the grain boundaries. In such materials the regularity or periodicity is interrupted at the grain boundaries though the structure may be more stable. These materials are called polycrystalline. The size of grain in which the structure is periodic may vary from submicroscopic (several Angstroms) upwards and when it becomes comparable to the size of pattern unit, one can no longer speak of crystals, since the essential feature of a crystal is its periodicity of structure. One then speaks of amorphous substances.

Most solid matter is crystalline *i.e.* nature favours the crystalline state of solids. This is because the energy of the ordered atomic arrangement is lower than that of an irregular packing of atoms. However when the atoms are not given an opportunity to arrange themselves properly, *e.g.*, the temperature of a liquid is dropped abruptly arresting the motion of atoms before they can rearrange themselves, the amorphous material may be formed. We shall presently deal with the structure of perfect (ideal) or nearly perfect crystals. These studies form the basis for studying the influence of imperfections and impurities in an otherwise perfectly periodic crystal, as we shall see in a later chapter.

Crystal Translational Vectors

Let us consider an ideal crystal. As has been indicated, it is composed of atoms or groups of atoms arranged in a regular pattern so that the atomic arrangement at one location looks exactly the same in all respects as the arrangement at a corresponding location somewhere else. In the language of crystals, we say that in such a crystal there exists some smallest group of atoms (called the pattern-unit) that repeats itself exactly in all directions in the crystal by means of the translation operation **T** defined as

$$\mathbf{T}=n_1\mathbf{a}+n_2\mathbf{b}+n_3\mathbf{c}, \qquad \text{...(1)}$$

where n_1, n_2, n_3 are arbitrary integers and **a**, **b**, **c** are vectors defined as the fundamental translation vectors. Moreover, see that the application of this operation (1) to any point **r** (measured from some arbitrary origin) results in a point **r**′ :

$$\mathbf{r}'=\mathbf{r}+\mathbf{T}=\mathbf{r}+n_1\mathbf{a}+n_2\mathbf{b}+n_3\mathbf{c}, \qquad \text{...(2)}$$

which is identical in all respects to the original point **r**, and thus satisfies the essential feature of a perfect crystal. This is not possible for an imperfect crystal : there **r**′ is not identical to **r** for any arbitrary choice of n_1, n_2, n_3 and the vectors **a**, **b**, **c** are not translational vectors. Thus in order for an assembly of atoms to be defined as crystal structure, it must be possible to find three translation vectors **a**, **b**, **c** which satisfy (2) such that **r**′ is identical to **r**. In other words, we can say that if no **a**, **b**, **c** exist according to the above prescription, the assembly cannot be classified to be a crystal. These translation vectors **a**, **b**, **c** are often called as crystal axes, or basis vectors.

Now, with reference to a given crystal there may be many ways of choosing these translation vectors. Fig. 1 (representing, for simplicity, the part of a two-dimensional crystal with only two fundamental translation vectors **a** and **b**) illustrates two such choices; here $\mathbf{a}_1$, $\mathbf{b}_1$ and $\mathbf{a}_2$, $\mathbf{b}_2$ are translation vectors. However, $\mathbf{a}_1$ and $\mathbf{b}_1$

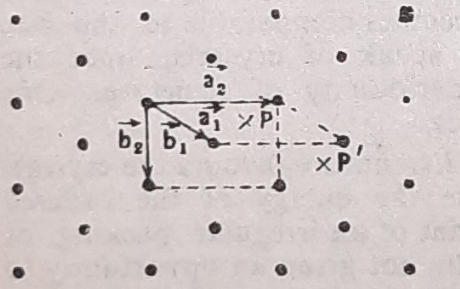

Fig. 1. Primitive ($\mathbf{a}_1$, $\mathbf{b}_1$) and non-primitive ($\mathbf{a}_2$, $\mathbf{b}_2$) translation vectors of a lattice.

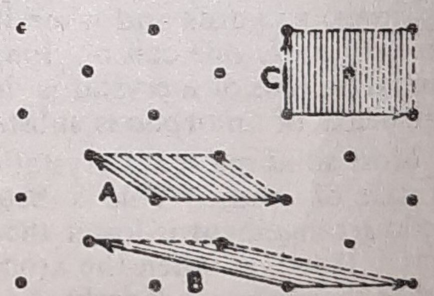

Fig. 2. Possible primitive and non-primitive cells of a lattice. Other cells are also possible.

are such that every identical point in the crystal can be reached by an application of the translation operation

$$\mathbf{T}=\mathbf{a}_1n_1+\mathbf{b}_1n_2$$

with some combination of n_1 and n_2. For example, we can get P' from **P** by using the operation $\mathbf{T}=0.\mathbf{a}_1+1.\mathbf{b}_1$ and can write

$$\mathbf{P}'=\mathbf{P}+0.\mathbf{a}_1+1.\mathbf{b}_1.$$

Such translation vectors are called the primitive translation vectors. On the other hand, the vectors $\mathbf{a}_2$ and $\mathbf{b}_2$ cannot do it. When we try to do it using $\mathbf{a}_2$ and $\mathbf{b}_2$ we get

$$\mathbf{P}'=\mathbf{P}+\tfrac{1}{2}\mathbf{a}_2+\tfrac{1}{2}\mathbf{b}_2.$$

But this involves non-integer coefficients of $\mathbf{a}_2$ and $\mathbf{b}_2$ and thus is not in accord with the periodicity of the crystal. Such axes are called the non-primitive translation vectors. For the description of the crystal structure either type of the translation vectors may be used. Usually, one which is orthogonal is convenient, specially for calculating purposes. Further, they must be shortest in length. Keeping these factors in mind, the vectors $\mathbf{a}_2$ and $\mathbf{b}_2$ are regarded as convenient for the description of the lattice shown in fig. 1.

Unit Cell

Now, consider the parallelograms or the rectangles based on the translation vectors as shown in fig. 2. These are defined as the unit cells of the crystal. To understand the importance of the unit cells, let us consider only one of them. It is apparent that under the action of the translation operation (1) for some combination of n's, it is carried into a region which is exactly identical to the original region and under the action of the various possible translation operations, it reproduces the entire crystal. Thus, in a way it serves as a 'unit' in terms of which the crystral can be considered to be constructed and is so called. We can suitably compare it with the building block of a wall. It must also be clear that to know the properties of a crystal, it is only sufficient to know the properties of a unit cell of the crystal.

Since with reference to a given crystal there exists a number of possible unit cells (see fig. 2), the next thing which must be considered is which one to choose as a conventional unit cell. In fact, the choice of a conventional unit cell is a matter of convenience. Usually, a cell with shortest possible size (area $\mathbf{a}\times\mathbf{b}$ in two-dimensions and volume $\mathbf{a}.\mathbf{b}\times\mathbf{c}$ in three-dimensions) and sides is chosen as a convenient unit cell. In this respect the parallelogram *A* in fig. 2 is taken as convenient and conventional unit cell for the concerned lattice. We see that this cell contains lattice points (to be defined in the next section) only at the corners. Since a lattice point is shared by four unit cells which touch there, we can say that $\frac{1}{4}$ of a lattice point is associated with this cell and thus there is a lattice density of one point associated with this cell. But this is the character of what is known a primitive unit cell. Thus, the convenient unit cell is minimum area-primitive cell with shortest possible sides. Sometimes it is, however, more convenient to use a cell of larger area and thus containing more than one lattice point. The rectangle *C* shown in fig. 2 is one such cell, for example. The cells of this type are known as the non-primitive unit cells. The most important reason for choosing a non-primitive unit cell is that it satisfies the symmetry elements better. This point will be illustrated at the appropriate discussion.

Lattice and Basis

A lattice is a regular periodic arrangement of points in space that looks a net-like structure. The environment about any particular point is in every way the same as that about any other point. All the points are connected, as we would expect, by the translation operation **T** defined as

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

In other words, the lattice can be thought of as generated by the translation operation **T** ; for, if one point and a set of translation vectors are chosen, then the application of **T** with all possible values of n's will do it of course. It is now essential to distinguish a lattice from the crystal structure : a lattice is a mathematical concept whereas the crystal structure is a physical picture, and it is formed by associating identically with every lattice point a structural or a building unit. This structural unit is called the basis. The basis consists of an atom or a group of atoms[1,2] and in an ideal crystal it is identical in composition, arrangement and orientation. The distinction between the crystal and the lattice is illustrated in fig. 3 and the logical relation is

lattice + basis = crystal structure

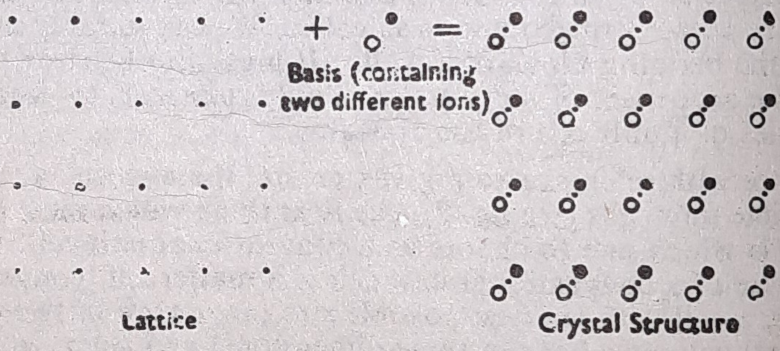

Fig. 3. Distinction between a lattice and crystal structure.

The crystal structure is thus specified characteristically by the type of the lattice associated with it, which in turn requires the fundamental translation vectors and their relations with each other to be specified. These relations emerge from the consideration of the symmetry operations of the crystal structures. We now discuss them. For simplicity we shall discuss them for a two-dimensional

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[1] The basis generally contains several atoms or molecules, upto perhaps 100 in inorganic crystals and 10^5 in protein crystals. In ionic crystals it is composed of two distinct types of ions.

[2] The number of atoms in the basis gives the number of atoms in primitive cell as there it a density of one lattice point per primitive cell.

crystal. The discussion shall apply fairly completely to three-dimensional crystals.

Symmetry Operatios for a Two-Dimensional Crystal

A symmetry operation is one which leaves the crystal environment invariant. We have already seen that the translations fulfil this requirement, but these are not the only type of symmetry operations. Rotation about an axis, reflection in a plane and inversion about a point and combination of these are the other symmetry operations. These operations, however, form a distinct class—called the point symmetry operations and apply to all objects whereas the translations apply only to lattices. We now understand the meaning of the various symmetry operations. Since we are limiting our discussion to two-dimensions, we will consider only rotational and reflection point symmetry operations (as these are the only point operations in two dimensions) and the translations. We shall remember that in two-dimensions an axis of rotation is a point and a plane of reflection is a line.

Translations. The translation symmetry is the manifestation of the order of crystalline solids. According to it, if we are at **r** and then translate the crystal by an amount **T** defined by (1), then the new environment arround **r** appears identical to the old.

Rotations. A body is said to possess the rotational symmetry about an axis if the rotation of the body about this axis by some angle θ leaves the body invariant, that is, if after rotation the body appears as it did prior to rotation. In order for the body to be truly invariant by the rotation, there must be an integral number of such rotations in one complete revolution of the body. Thus, the rotational angle θ must be an integral submultiple of 2π ; that is, θ must be equal to $(2\pi/n)$ with n an integer. The integer n is called the multiplicity of the rotation axis. The regular polygons are examples of the bodies having rotational symmetry : with n sides, a polygon have an n-fold rotation axis. A rotation axis is designated by the symbol n.

Since our concern here is with lattices and crystal structures, we must now discuss the rotational symmetry as applied to them. Suppose, then the point **r** of a lattice is a rotation axis ; then every point $\mathbf{r}'=\mathbf{r}+\mathbf{T}$ must also be a rotation axis in order to satisfy the translational symmetry. This requirement has the important result that certain rotations are not compatible with the translation operation. That is, for certain rotations $\mathbf{T}\neq n_1\mathbf{a}+n_2\mathbf{b}+n_3\mathbf{c}$ in a lattice. In fact, only 1-, 2-, 3-, 4- and 6-fold rotations axes can exist in a lattice. We now set out to prove this restriction.

With reference to fig. 4 suppose that $\mathbf{R}_1$ and $\mathbf{R}_2$ are two vectors drawn to the two closest lattice points. Letting these points are in the direction of the primitive translation vector **a** (taken in fig. along the x-axis), $|\mathbf{a}|=|\mathbf{R}_1-\mathbf{R}_2|$ is the minimum separation distance between lattice points in that direction. Now assume that a line perpendicular to the page and passing through the lattice point defined by $\mathbf{R}_1$ is an n-fold axis of rotation. Since all lattice points are equivalent, there must also be a similar axis through the tip of $\mathbf{R}_2$. Taking then $\theta=2\pi/n$, consider a counter-clockwise rotation θ of $\mathbf{a}$ about $\mathbf{R}_1$: it produces a new lattice vector $\mathbf{R}_1'$. Similarly, a clockwise rotation by the same angle θ of $\mathbf{a}$ about $\mathbf{R}_2$ produces a new lattice vector $\mathbf{R}_2'$. The tips of these vectors $\mathbf{R}_1'$ and $\mathbf{R}_2'$ are the new lattice points ; as such, $\mathbf{R}_1'-\mathbf{R}_2'$ must also be a lattice vector. From the fig. 4 we see that $\mathbf{R}_1'-\mathbf{R}_2'$ is parallel to the x-axis and we must therefore have $\mathbf{R}_1'-\mathbf{R}_2'$ to be equal to some integral multiple of $\mathbf{a}$ *i.e.* we must have

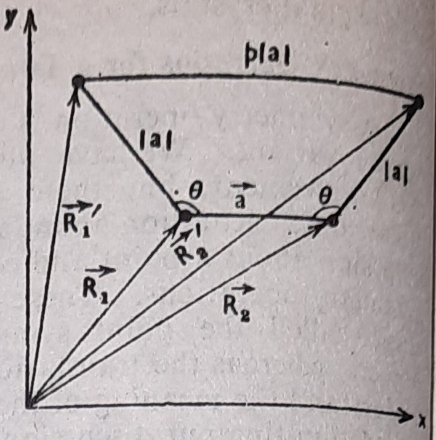

Fig. 4. Geometry used in proving that only 1-, 2-, 3-, 4- and 6-fold rotation axes can exist in a lattice.

$$|\mathbf{R}_1'-\mathbf{R}_2'| = |pa| \text{ ; } p \text{ an integer.}$$

If it is not, then $\mathbf{R}_1'-\mathbf{R}_2'$ is not a translation vector of the lattice and the array is not periodic.

Now, with the aid of figure 4, it is a simple matter to write

$$|pa| = |a| + 2|a| \sin\left(\theta - \frac{\pi}{2}\right)$$

$$= |a| (1-2\cos\theta)$$

$$\therefore \quad p = 1-2\cos\theta \qquad \text{...(3)}$$

or

$$|\cos\theta| = \left|\frac{1-p}{2}\right| \leqslant 1$$

This equation can be satisfied only for $p=3, 2, 1, 0, -1$. Consequently,

$$\theta = \frac{2\pi}{2}, \frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}, \frac{2\pi}{1},$$

giving $n=1, 2, 3, 4$ and 6 only.

We thus see that a crystal can have only 1-, 2-, 3-, 4-, and 6-fold axes of rotation. It is thus interesting to note that, for example, a crystal cannot have five-fold* rotation axis. In other words, translational symmetry is not compatible with five fold

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*To prove exclusively that a five-fold symmetry is impossible in a lattice, prove that equation (3) is not satisfied for $\theta=2\pi/5$.

axis of symmetry. Fig. 5 makes this convincing physically: here we see that a connected array of pentagons does not fill all the space. The array itself has a five-fold symmetry about point *A*, but there exists no set of vectors that satisfies the translation operation and thus the array cannot be classified as a lattice. In other words, the array has 5-fold rotational axis but not the translational symmetry. Similarly, other rotations, like 7-fold can be excluded.

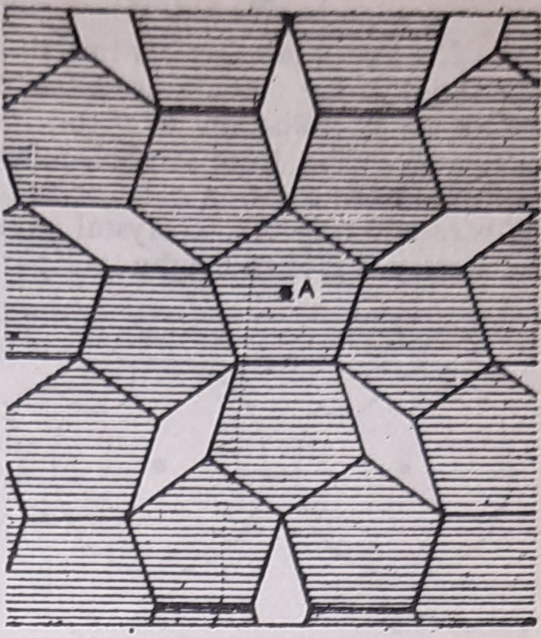


Fig. 5. Demonstration that a five-fold axis cannot exist in a lattice.

Reflections. A body is said to possess the reflection symmetry if a plane can be drawn in the body dividing it into two exactly similar parts, so that one half is the reflection of the other half. In other words, according to this symmetry one half of the body when reflected in the above plane reproduces the other half. The plane is known as the reflection plane (or line) and is designated by *m*. The notched wheel, for example, shown in fig. 6 has a reflection plane through the centre of the notch.

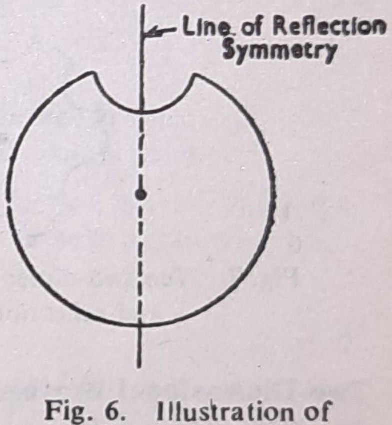


Fig. 6. Illustration of reflection symmetry about-dotted line.

Concerning ourselves with lattices and crystal structures, we next consider the combinations of the reflections with allowed rotations. Since these two operations are the only point operations in two dimensions, such combinations will determine the total symmetry types of lattices about a point. In fact, the total symmetry of space about a point is determined by a collection of symmetry elements at that point. For instance, symmetry of a cube about its centre is described by collecting all the symmetry elements there. The group of such a set of symmetry operations at a point is called a 'point group.' Now, since there are two possible point groups associated with a rotation axis (with or without reflection symmetry), there are therefore a total of ten possible point groups permissible in two-dimensional crystal. These are designated as under:

1, 1m, 2, 2mm, 3, 3m, 4, 4mm, 6, 6mm.

The first symbol refers to the rotations about a point : thus the point group 6 contains 6-fold rotations. The second symbol refers to a reflection line (or lines) parallel to the rotation axis (or axes). The third symbol refers to the reflection lines perpendicular to the rotation axis (or axes). These ten point groups are illustrated in fig. 7. A crystal having any particular point-group symmetry is said to belong to a particular 'crystal class'.

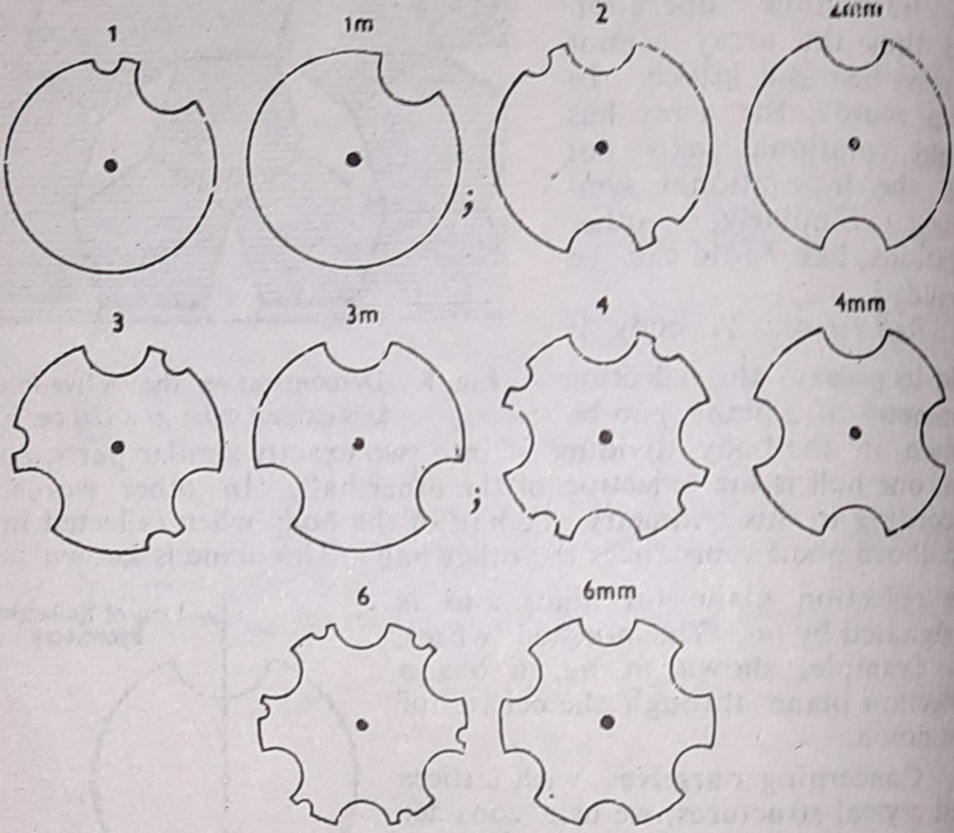


Fig. 7. Ten two-dimensional point groups consisting of rotation and reflection operations illustrated by means of notched wheels.

Two-Dimensional Bravais Lattices

We now have means of classifying two-dimensional lattices. The point groups 1 and 2 obviously require a general lattice such as one shown in fig. 9 (*a*)—called an oblique lattice. It has no restrictions on the length of **a** and **b** and on the angle between them. It is easily seen that it is left invariant under rotations of 2π and π about any lattice point. The point group 4 requires a square lattice shown in fig. 9 (b). In this lattice **a**=**b** and the angle between them is 90°. The point groups 3 and 6 require a hexagonal lattice shown in fig. 9 (*c*). This lattice has **a**=**b** and the angle between **a** and **b** is 120°. Thus, the pure rotations predict only three distinct two-dimensional lattices.

We now consider the reflection symmetry. We note that it is imperative for the square and hexagonal lattices to possess the reflection symmetry : there are two sets of reflection planes. But the oblique lattices in general do not have this symmetry. When they do, it is a little more significant : two additional lattice types result, as we see below.

Let us consider an oblique lattice, as illustrated in fig. 8 with primitive translation vectors **a** and **b**. We wish to find out what relations between **a** and **b** result when we impose reflection symmetry on this lattice. With reference to a cartesian co-ordinate system (x, y), we begin with

$$\mathbf{a}=a_x\mathbf{i},$$
$$\mathbf{b}=b_x\mathbf{i}+b_y\mathbf{j}.$$

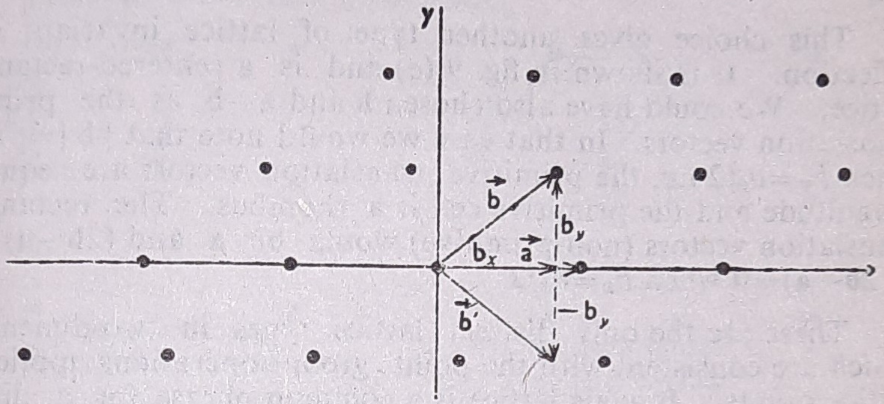


Fig. 8. Illustrating that the lattice will have reflection symmetry about x-axis only when the vector b' lies on a lattice point.

Let us assume that the x-axis is a reflection line. The reflection of the lattice in this line then produces new vectors **a**′, **b**′ :

$$\mathbf{a}'=a_x\mathbf{i},$$
$$\mathbf{b}'=b_x\mathbf{i}-b_y\mathbf{j}. \qquad \text{...(4)}$$

If the lattice is invariant under the reflection operation, then **a**′ and **b**′ must also be the lattice vectors, *i.e.* they must be of the form $n_1\mathbf{a}+n_2\mathbf{b}$, where n_1 and n_2 are integers.

Since **a**′ is evidently so ($\mathbf{a}'=\mathbf{a}$), let us therefore set

$$\mathbf{b}'=n_1\mathbf{a}+n_2\mathbf{b}=n_1a_x\mathbf{i}+n_2\,(b_x\mathbf{i}+b_y\mathbf{j}). \qquad \text{.. (5)}$$

Equating coefficients of **i** and **j** in equations (4) and (5), we get

$$b_x=n_1a_x+n_2b_x \quad \text{and} \quad -b_y=n_2b_y$$
$$\text{or} \quad n_2=-1.$$

Therefore

$$b_x=\frac{n_1a_x}{2} \qquad \text{...(6)}$$

and b_y is arbitrary. One possibility of choosing **b** is then given by $n_1=0$. We have

$$b_x=0\ ;\ b_y=\text{arbitrary}$$

so that

$$\mathbf{b}=b\mathbf{j}$$

and

$$\mathbf{a}=a\mathbf{i}$$

The resulting lattice is a primitive rectangular lattice (since $\mathbf{a}.\mathbf{b}=0$, $\therefore\ \phi=90°$). This is shown in fig. 9 (*d*).

Another possibility of choosing **a** and **b** is given by $n_1=1$, We have

$$b_x=\frac{a_x}{2} \quad \text{or} \quad 2b_x=a_x : b_y=\text{arbitrary}$$

so that

$$\mathbf{b}=\tfrac{1}{2}a\mathbf{i}+b_y\mathbf{j}$$

and

$$\mathbf{a}=a\mathbf{i}.$$

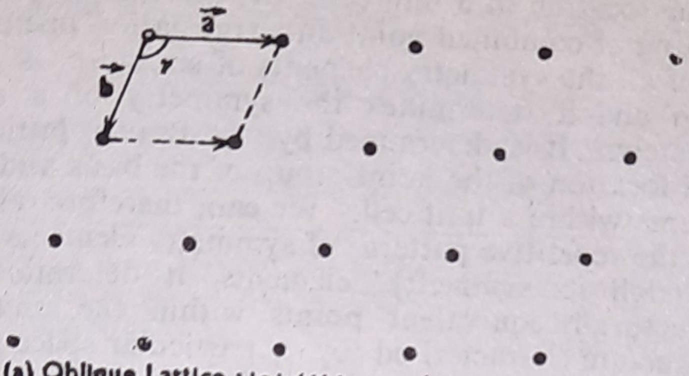
This choice gives another type of lattice invariant under reflection. It is shown in fig. 9 (e) and is a centered-rectangular lattice. We could have also chosen **b** and **a**−**b** as the primitive translation vectors. In that case we would note that $|\mathbf{b}|=|\mathbf{a}-\mathbf{b}|$ when $b_x=a_x/2$ *i.e.* the primitive translation vectors are equal in magnitude and the primitive cell is a rhombus. The rectangular translation vectors (non-primitive) would be **a** and (2**b**−**a**) since $\mathbf{a}.(2\mathbf{b}-\mathbf{a})=0$ when $b_x=a_x/2$.

These are the only distinct lattice types in two-dimensions which are consistent with the point group operations applied to lattice points. Bravais lattice is a common phrase for a distinct lattice type : we say that there are five Bravais lattices in two-dimensions. These are summarised in the table no. 1 with their characteristic symmetry elements.

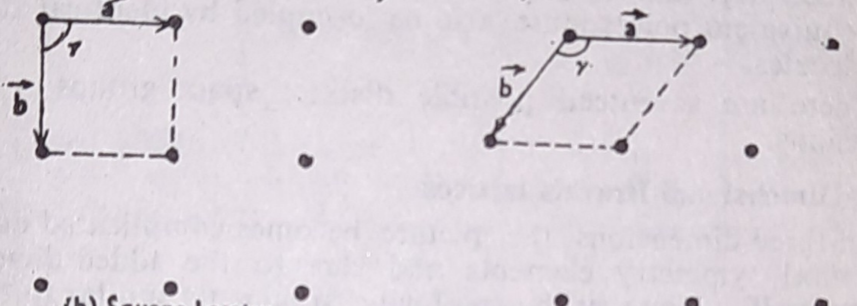
TABLE No. 1

Lattice	Conventional unit cell	Axes of conventional unit cell	Point-group symmetry of lattice about lattice points
Oblique	Parallelogram	$a\neq b,\ \gamma\neq 90°$	1, 2
Rectangular primitive	Rectangle	$a\neq b,\ \gamma=90°$	1m, 2mm
Rectangular centered	Rectangle	$a\neq b,\ \gamma=90°$	1m, 2mm
Square	Square	$a=b,\ \gamma=90°$	4, 4 mm
Hexagonal	60° rhombus	$a=b,\ \gamma=120°$	6, 6mm, 3, 3m

Another means of classification is by crystal system. The primitive and centered-rectangular lattices are regarded as belonging to a single rectangular crystal system. There are thus four crystal systems in two-dimensions—oblique, rectangular, square, and hexagonal. This classification is of more wide use in three-dimensional lattices.

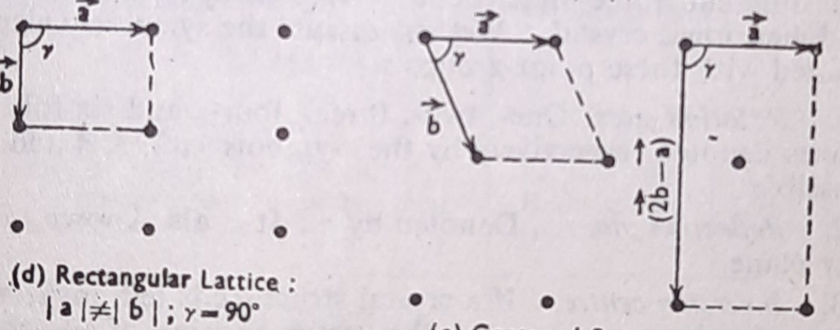


(a) Oblique Lattice ; $|a| \neq |b|$; γ = arbitrary



(b) Square Lattice : $|a| = |b|$; $\gamma = 90^\circ$

(c) Hexagonal Lattice : $|a| = |b|$; $\gamma = 120^\circ$



(d) Rectangular Lattice : $|a| \neq |b|$; $\gamma = 90^\circ$

(e) Centered Rectangular Lattice : (primitive cell $a| \neq |b|$; $\gamma \neq 90^\circ$ but $|b| = |a-b)$ (non-primitive cell $a| \neq |b|$; $\gamma = 90^\circ$)

Fig. 9. Five two-dimensional Bravais lattices: One [*i.e.*, (*a*)] is general lattice and the remaining four are special, resulting from this general lattice as a result of the restrictions placed on the length and orientation of its translation vectors **a**, **b** by the symmetry operations.

Now, since a crystal structure is formed by associating with every lattice point a unit assembly or basis of atoms, the actual crystal structure may not have the same point-group as does its lattice ; it may have lower point symmetry. For example, it is possible for a crystal with a square lattice to have only the operations 4 without having all the operations 4 mm. In fact, in order to specify the symmetry of a crystal structure completely, we must consider two additional aspects : (*i*) there may be point symmetries at more than one location in a unit cell. (*ii*) there exist symmetry elements consisting of combined point and translation operations. The collection of all the symmetry elements of structure is called the 'space group' and it determines the symmetry of a crystal structure completely. It is determined by the Bravais lattice and by the type and location of the point-group of the basis and other symmetry elements within a unit cell. We can, therefore, also say that it specifies the repetitive pattern of symmetry elements of the structure. Through its symmetry elements, it determines the positions of structurally equivalent points within the unit cell. For a crystal structure characterised by a particular space group, it is necessary that if any one point in the cell is occupied, all other equivalent points must also be occupied by identical atoms or molecules.

There are seventeen possible distinct space groups in two-dimensions.

Three-Dimensional Bravais lattices

In three dimensions the picture becomes complicated due to additional symmetry elements and due to the added dimensionality itself. However, by employing arguments similar to those used in two-dimensional crystals, it is possible to show that there are 32 different three-dimensional point-groups permissible in a three-dimensional crystal. We first discuss the symmetry elements associated with these point-groups :

1. *Rotation axes.* One-, two-, three-, four-, and six-fold rotation axes denoted respectively by the symbols 1, 2, 3, 4 and 6 are permissible.

2. *Reflection plane.* Denoted by m. It is also known as the mirror plane.

3. *Inversion centre.* If a crystal structure is left invariant by the operation $\mathbf{r} \rightarrow -\mathbf{r}$, where $\mathbf{r}$ is the vector position of an arbitrary point in the crystal referred to a lattice point, it is said to possess a centre of inversion. This symmetry element implies that for each point located at $\mathbf{r}$ relative to a lattice point there exists an identical point at $-\mathbf{r}$. An inversion centre is denoted by $\bar{1}$.

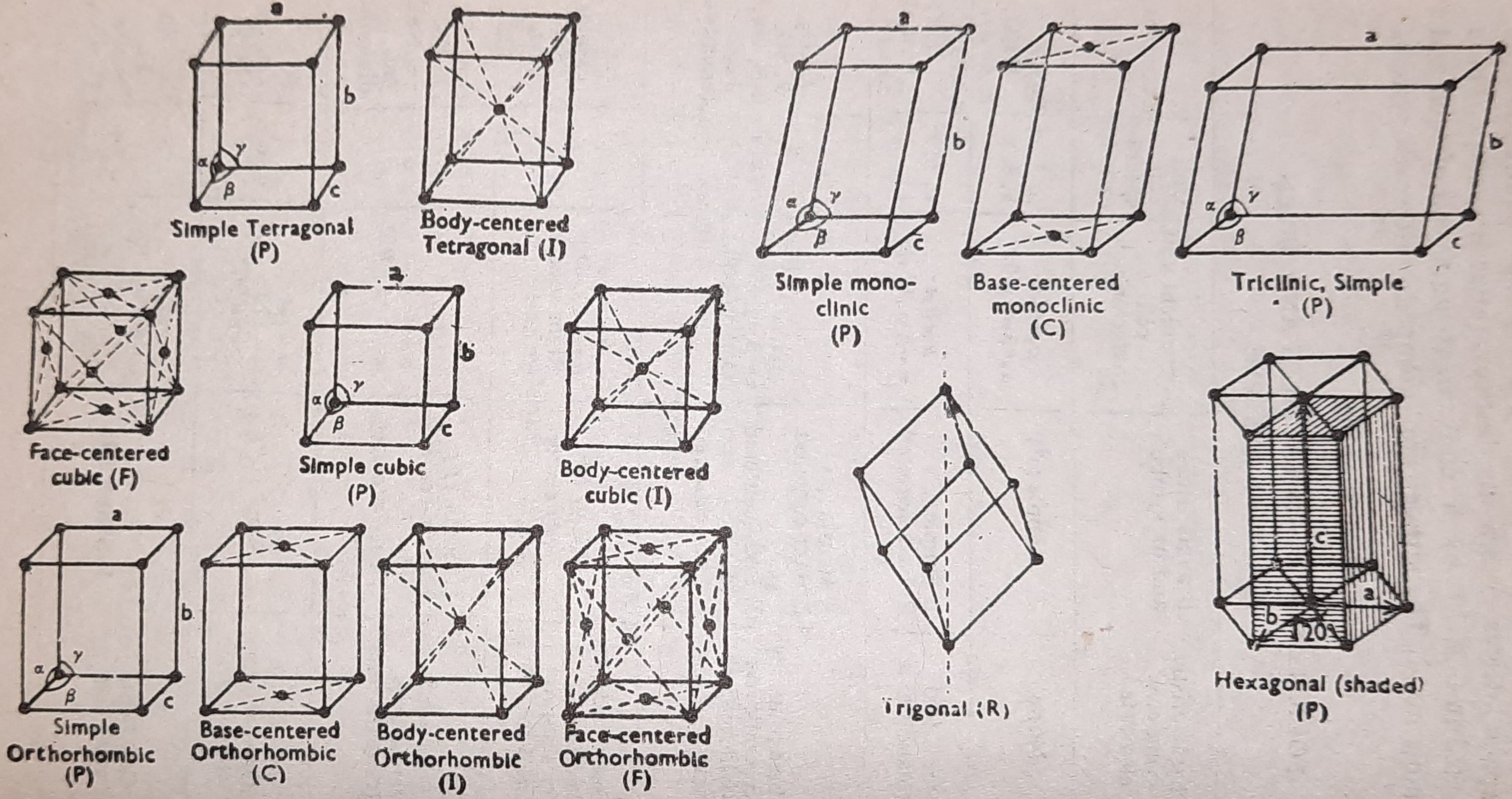
4. *Rotation inversion axes.* If a crystal structure is left invariant by a rotation followed by an inversion about a lattice point through which rotation axis passes, it is said to possess a rotation inversion axis. This operation is also known as an improper rotation and the corresponding axis as an improper axis. Crystals can possess one-, two-, there-, four-, and six-fold rotation-inversion axes denoted by the symbols $\bar{1}$, $\bar{2}$ $(\equiv m)$, $\bar{3}$, $\bar{4}$, $\bar{6}$ $(\equiv 3$ plus normal reflection plane).

The thirty-two permitted crystal point groups require fourteen different space lattices or Bravais lattices (after Bravais). These are illustrated in figs. 10 by a convenient unit cell of each and listed in table no. 2. The lattices are grouped into seven systems

TABLE NO. 2

FOURTEEN BRAVAIS LATTICES AND SEVEN CRYSTAL SYSTEMS

Systems	Characteristic symmetry elements	Bravais lattice and its symbol	Convenient unit cell characteristics	Unit cell specification	Examples
Triclinc	None	1. Simple (*P*)	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90°$	$a, b, c;$ α, β, γ	$CuSO_4 \cdot 5H_2O$, $K_2Cr_2O_7$
Monoclinic	One 2-fold rotation axis	1. Simple (*P*) 2 Base centered (*C*)	$a \neq b \neq c$ $\alpha = \beta = 90° \neq \gamma$	$a, b, c;$ γ	$CaSO_4 \cdot 2H_2O$ (gypsum) borax
Orthorhombic	Three mutually perpendicular 2-fold rotation axes	1. simple (*P*) 2. Base centered (*C*) 3. Body-centered (*I*) 4. Face-centered (*F*)	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$ (Orthorhomb)	a, b, c	KNO_3, K_2SO_4, α-S, Ga, Fe_3C (cementite)
Tetragonal	One 4 fold axis and two 2-fold axes normal to the 4-fold axis	1. Simple (*P*) 2. Body centered (*I*)	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$ Right square (prism)	a, c	β-Sn (white) TiO_2 SnO_2
Cubic	Four 3-fold rotation axes (cube diagonals)	1. Simple (*P*) 2. Body-centered (*I*) 3. Face-centered (*F*)	$a = b = c$ $\alpha = \beta = \gamma = 90°$	a	Au, Ag Cu Fe, NaCl, ZnS, diamond
Hexagonal	One 6-fold rotation axis	1. Simple (*P*)	$a = b \neq c$ $\alpha = 120°$ $\beta = \gamma = 90°$	a, c	SiO_2, Zn, Cd NiAs
Trigonal	One 3-fold rotation axis	1. Simple (*R*)	$a = b = c$ $\alpha = \beta = \gamma \neq 90°$ but $<$ 120° (Right Prism)	$a ; \alpha$	As, Sb, Bi, calcite ($CaCO_3$)



Simple Terragonal (P)

Body-centered Tetragonal (I)

Simple mono-clinic (P)

Base-centered monoclinic (C)

Triclinic, Simple (P)

Face-centered cubic (F)

Simple cubic (P)

Body-centered cubic (I)

Trigonal (R)

Hexagonal (shaded) (P)

Simple Orthorhombic (P)

Base-centered Orthorhombic (C)

Body-centered Orthorhombic (I)

Face-centered Orthorhombic (F)

Fig. 10. The fourteen Bravais or space lattices illustrated by conventional (=convenient) unit cells which are not always primitive cells The figure for hexagonal system also shows the relation of the primitive cell with the prism of hexagonal symmetry which is the conventional cell.

according to certain specifications about the lengths of edges and angles between them of a convenient unit cell. It might appear at first sight that there should be other possible Bravais lattices ; for example, one might suggest in the tetragonal system the possibility of a face-centred type. However, such a lattice would, upon choosing a different set of axes, be identical with the body-centered tetragonal lattice in which the side of the base of the unit cell is $1/\sqrt{2}$ times what it is for the original lattice. Other examples may be considered similarly.

There are 230 distinct space groups in three-dimensions.