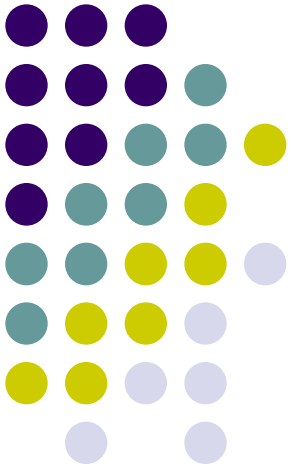
Engineering Physics:

Physics of Materials: Crystal Structure



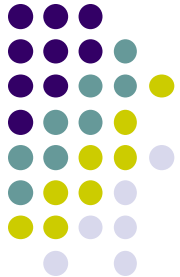
Dr. Anurag Srivastava

Web address: https://profanurag.in

Email: profanurag@gmail.com

Visit me: Room-110, Block-E, IIITM Campus

Crystallographic Directions and Planes



- **Crystal planes** are defined as some imaginary planes inside a crystal in which large concentration of atoms are present. Inside the crystal, there exists certain directions along which large concentration of atoms exists. These directions are called **crystal directions**.

- Indices of crystallographic points, directions, and planes are given in terms of the lattice constants of the unit cell. For points and directions, you can consider the indices to be coefficients of the lattice constants.

Bracket Conventions

- In crystallography there are conventions as to how the indices of planes and directions are written. When referring to a specific plane, "round" brackets are used:

  (*hkl*)

- When referring to a set of planes related by symmetry, then "curly" brackets are used:

  {*hkl*}

- These might be the (100) type planes in a cubic system, which are (100), (010), (001), (100),(010) and (001) . These planes all "look" the same and are related to each other by the symmetry elements present in a cube, hence their different indices depend only on the way the unit cell axes are defined. That is why it is useful to consider the equivalent (010) set of planes.

Bracket Conventions

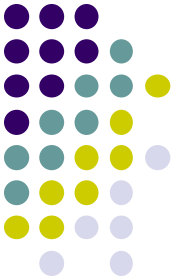
- Directions in the crystal can be labeled in a similar way. These are effectively vectors written in terms of multiples of the lattice vectors **a**, **b**, and **c**. They are written with "square" brackets:

  [*UVW*]

- A number of crystallographic directions can also be symmetrically equivalent, in which case a set of directions are written with "triangular" brackets:

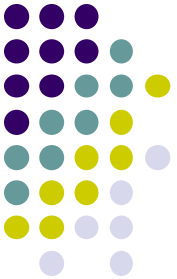
  <*UVW*>

Crystallographic Directions



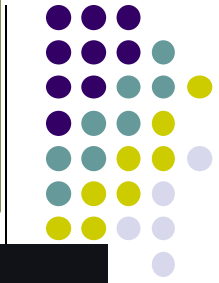
- Crystallographic directions and planes are a system of notation used in crystallography to describe the geometric features within a crystal lattice.
- This system, primarily consisting of Miller indices, is essential for discussing and comparing crystal structures and for understanding how material properties, such as mechanical and electrical behavior, vary with orientation

Crystallographic Directions



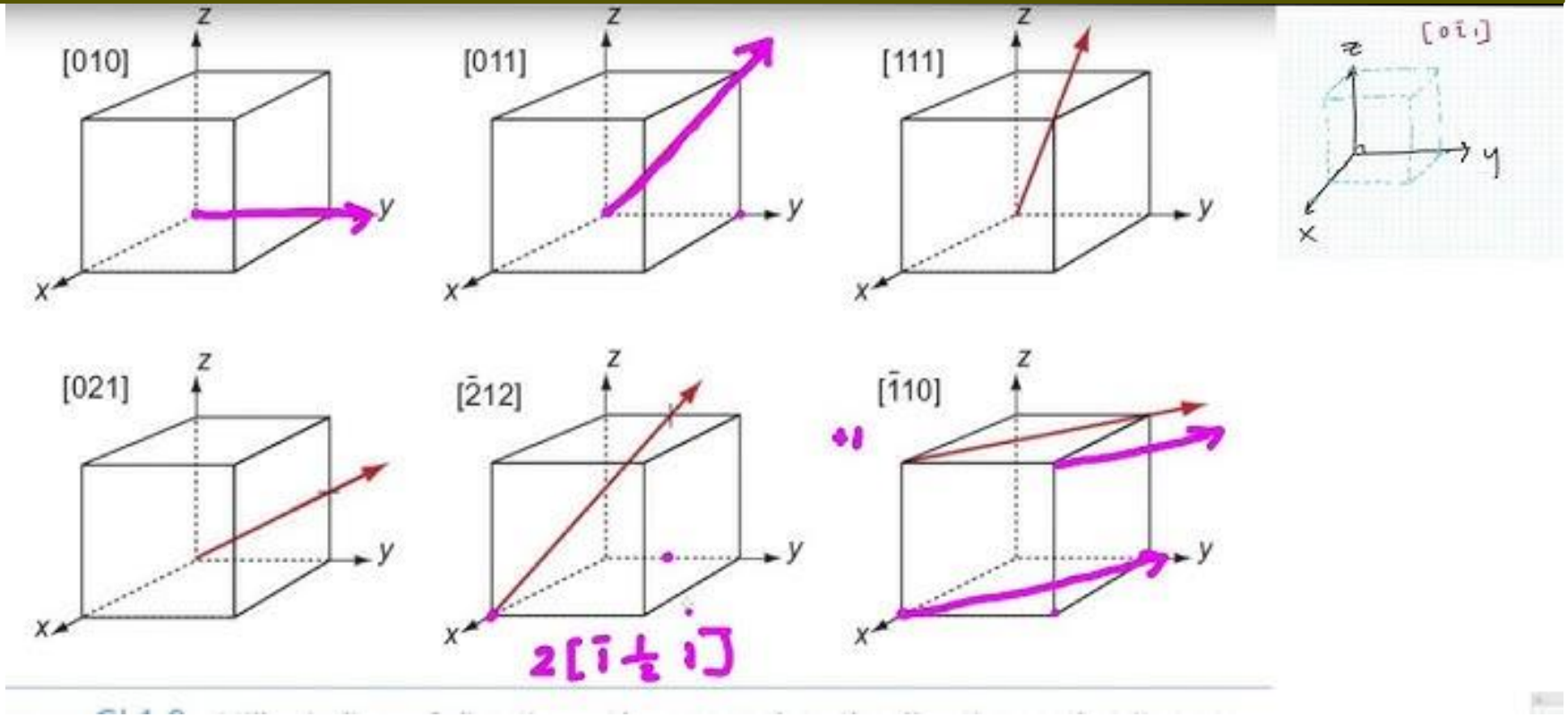
A crystallographic direction is a vector that represents a line connecting two points in a crystal lattice. The indices for a direction are designated by three integers enclosed in square brackets, such as [uvw]

Steps to Determine Crystallographic Directions

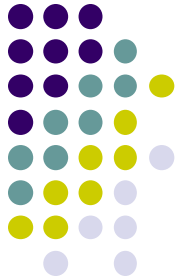


1. **Establish an origin and coordinate axes** at one corner of the unit cell.
2. **Position the vector** to pass through the origin. If necessary, the vector can be translated to start at the origin as long as it remains parallel to its original orientation.
3. **Determine the length of the vector projection** on each of the three axes (x, y, and z) in terms of the lattice parameters (a, b, and c).
4. **Reduce the numbers** to the smallest possible integers by multiplying or dividing them by a common factor.
5. **Enclose the integers** in square brackets $[uvw]$ without commas. A negative number is denoted by a bar over the index, for example, $[\bar{1}10]$.
6. A **family of directions** that are symmetrically equivalent is denoted by angle brackets, such as $< 100 >$.

Crystallographic Directions



Crystallographic Plance (Miller indices)



Crystallographic planes are identified by a set of three integers called Miller indices, designated as (hkl). These indices are based on the intercepts the plane makes with the crystal axes.

Miller indices

A Miller index is a series of co-prime integers that are inversely proportional to the intercepts of the crystal face or crystallographic planes with the edges of the unit cell.

It describes the orientation of a plane in the 3-D lattice with respect to the axes.

The general form of the Miller index is (h, k, l) where h, k, and l are integers related to the unit cell along the a, b, c crystal axes.

Steps to determine Miller indices

1. **Check the origin.** If the plane passes through the chosen origin, translate the plane or select a new origin in an adjacent unit cell.

2. **Find the intercepts.** Determine the points where the plane intersects the x, y, and z axes. These intercepts are measured in terms of the unit cell dimensions. If a plane is parallel to an axis, its intercept is considered to be at infinity (∞).

3. **Take the reciprocals.** Take the reciprocal of each intercept value. The reciprocal of an infinite intercept is 0.

4. **Clear fractions.** Multiply the set of reciprocals by a common factor to convert them to the smallest possible integers.

5. **Enclose in parentheses.** The final integer indices are enclosed in parentheses (hkl) without commas. A negative index is written with a bar over the number, like ($\bar{1}11$).

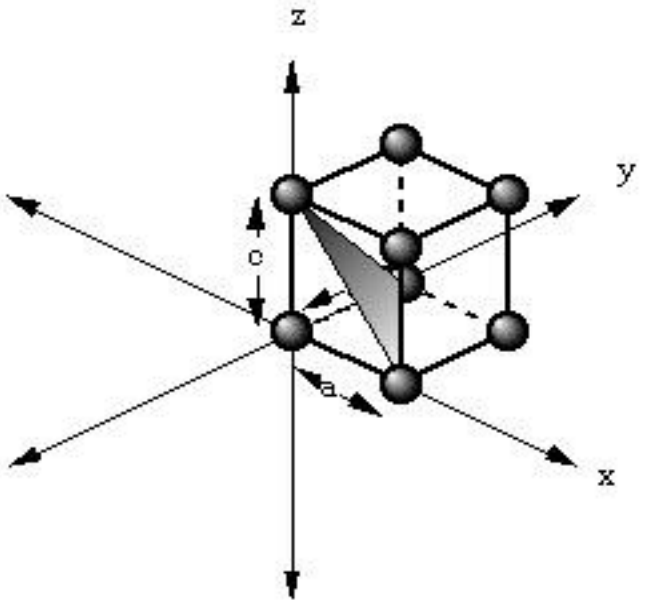
6. A **family of planes** is designated by curly braces, such as $\{100\}$. In cubic systems, a plane (hkl) is perpendicular to the direction [hkl].

Miller Indices

Rules for determining Miller Indices:

1. Determine the intercepts of the face along the crystallographic axes, *in terms of unit cell dimensions.*
2. Take the reciprocals
3. Clear fractions
4. Reduce to lowest terms

An example of the (111) plane (h=1, k=1, l=1) is shown on the right.



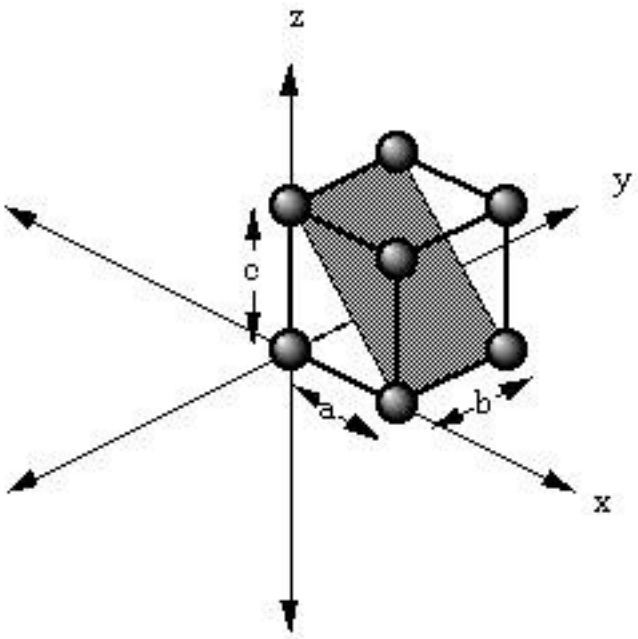
	a	b	c
intercept length	1	1	1
reciprocal	$\frac{1}{1}$	$\frac{1}{1}$	$\frac{1}{1}$
cleared fraction	1	1	1

Miller indice (111)

Another example:

Rules for determining Miller Indices:

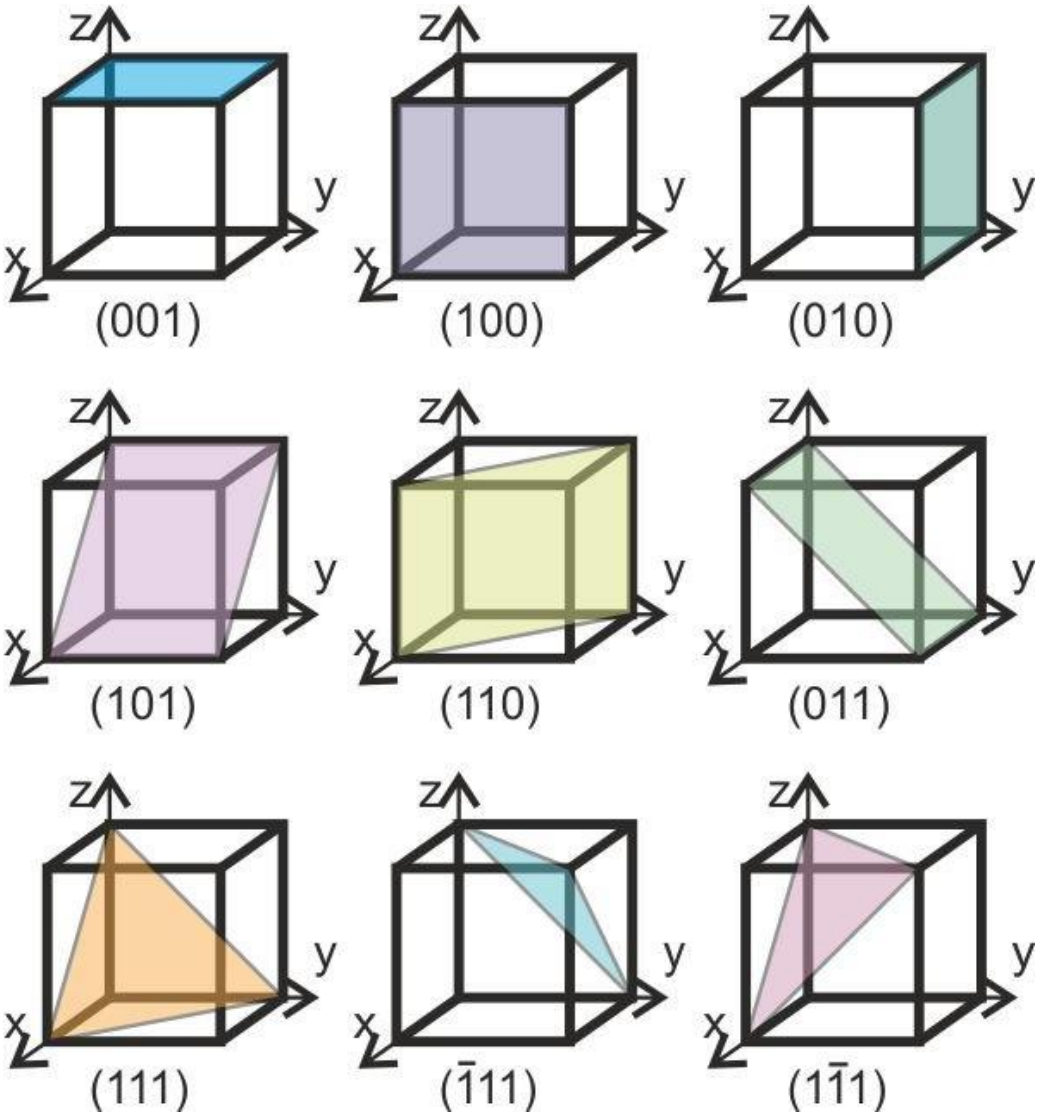
1. **Determine the intercepts of the face along the crystallographic axes, *in terms of unit cell dimensions.***
2. **Take the reciprocals**
3. **Clear fractions**
4. **Reduce to lowest terms**



	a	b	c
intercept length	1	∞	1
reciprocal	$\frac{1}{1}$	$\frac{1}{\infty}$	$\frac{1}{1}$
cleared fraction	1	0	1

Miller indice (101)

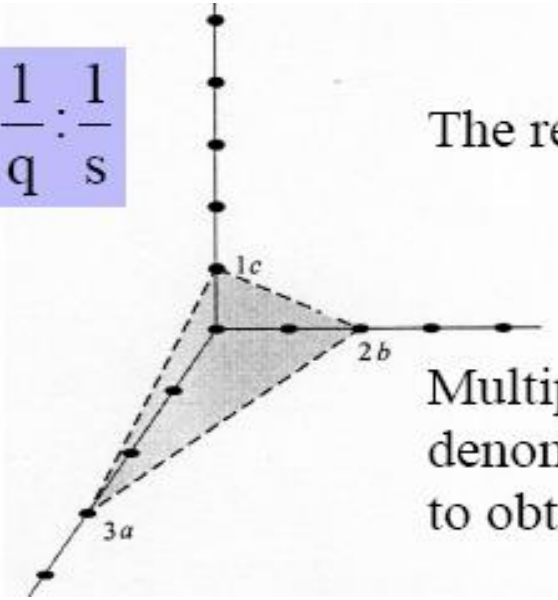
Miller Indices: Examples



Crystal Planes and Miller Indices

Real crystals are not infinitely large. They have surfaces. Crystal surfaces are often related to different lattice planes. Lattice planes are characterized with **Miller indices (hkl)**, which are a set of integers with no common factors, inversely proportional to the intercepts of the crystal plane along the crystal axes:

$$h : k : l = \frac{1}{p} : \frac{1}{q} : \frac{1}{s}$$



$p = 3,\ q = 2,\ s = 1$

The reciprocals of the intercepts are

$$\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{1}\right)$$

Multiply the smallest common denominator, which is 6 in this case, to obtain

$$(hkl) = (2,3,6)$$

Parallel lattice planes have same Miller indices and are entirely equivalent to each other.

Where does a protein crystallographer see the Miller indices?

- Common crystal faces are parallel to lattice planes
- Each diffraction spot can be regarded as a X-ray beam reflected from a lattice plane, and therefore has a unique Miller index.

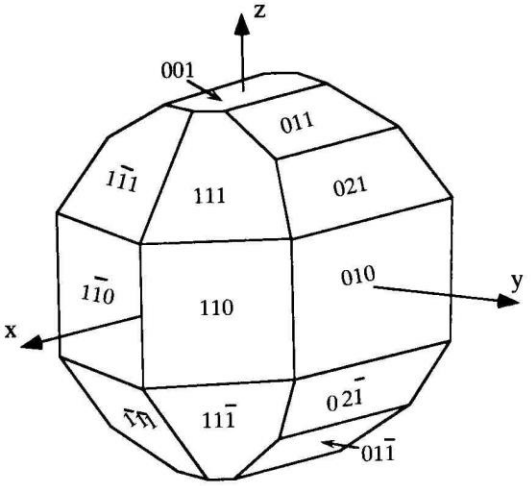
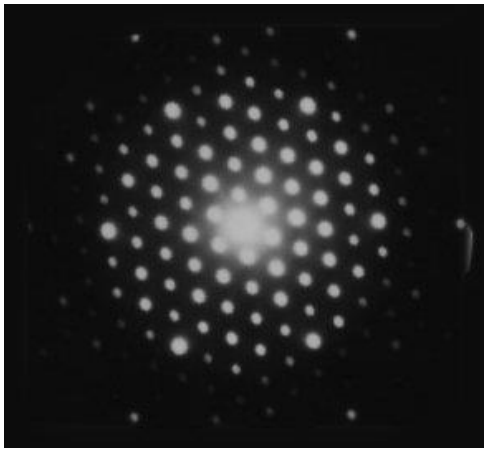
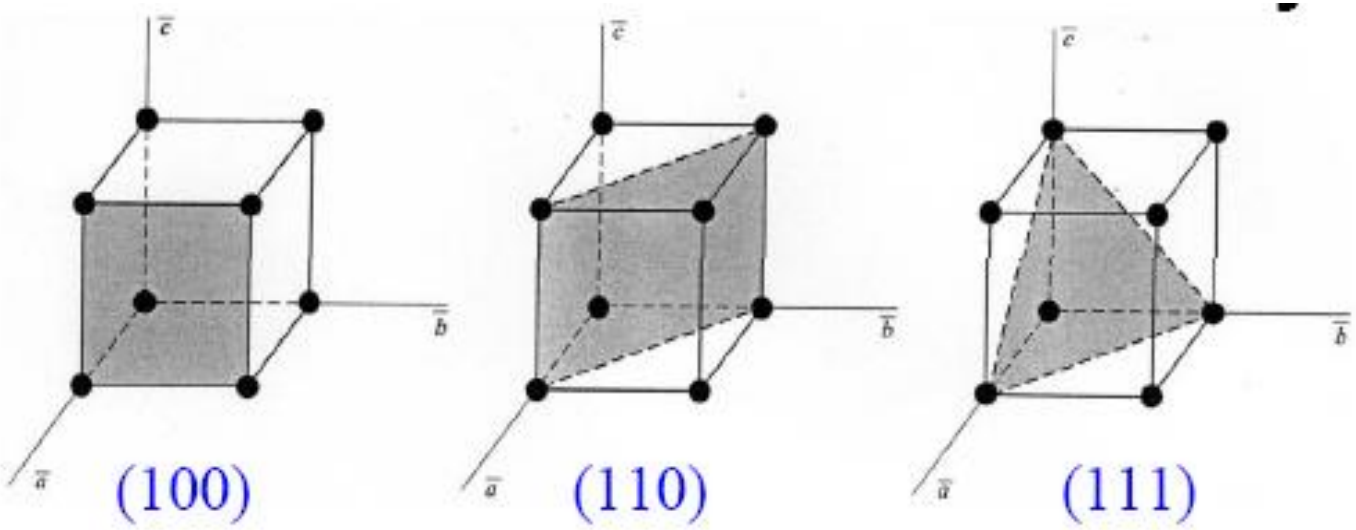


Figure 3.7. A crystal showing several faces.

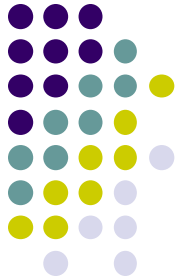


Common Lattice Planes in Cubic Crystals



1. When planes are parallel to certain axes, the corresponding intercepts will be ∞ and thus the reciprocals will be zeros.
2. If a plane passes through the origin, we would obtain infinity as one or more of the Miller indices. However, we can avoid the use of infinity by translating the origin to another equivalent lattice point since the location of the origin is entirely arbitrary.
3. Each face plane of the sc structure is entirely equivalent. These planes are grouped together and referred to as the **{100}** set of planes.
4. The distance between parallel lattice planes and the concentrations of atoms in specific planes are important parameters.

Symmetry



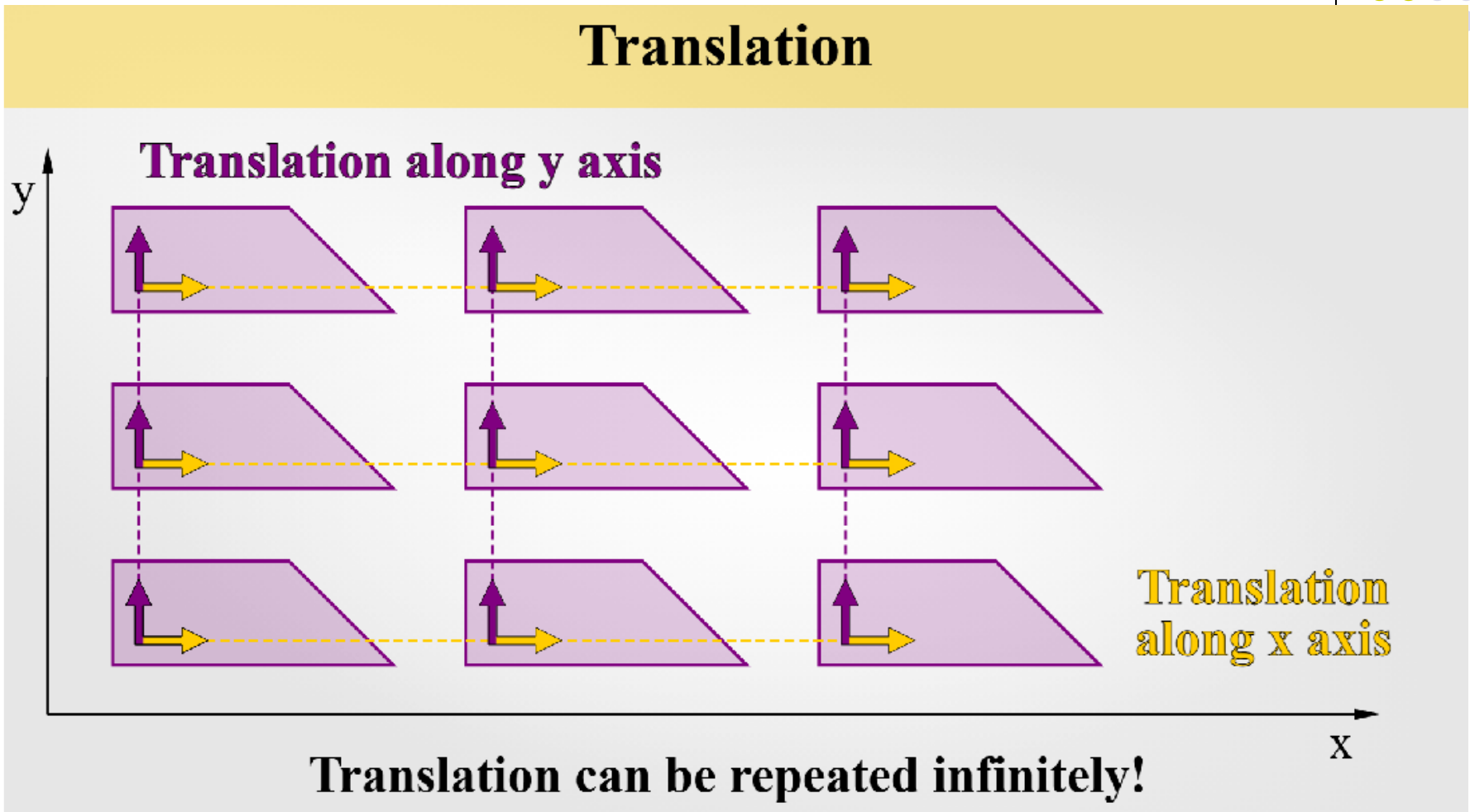
A state in which parts on opposite sides of a plane, line, or point display arrangements that are related to one another via a symmetry operation such as translation, rotation, reflection or inversion.

Application of the symmetry operators leaves the entire crystal unchanged.

Symmetry Elements:
Translation

The first point is repeated at equal distances along a line by a translation uT, where T is the translation vector and u is an integer

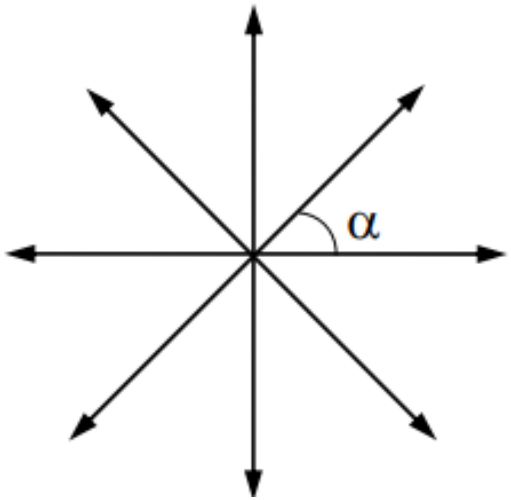
Symmetry Elements:
Translation



Symmetry Elements:
Translation

moves all the points in the asymmetric unit the same distance in the same direction. This has no effect on the handedness of figures in the plane. There are no invariant points (points that map onto themselves) under a translation.

Symmetry Elements:
Rotation



A rotation can be applied on the translation vector T in all directions, clock or anti-clock wise, through equal angles α, Because of the regular pattern, the translation between these two points will be some multiple of T (pT)

Symmetry Elements:
Rotation

turns all the points in the asymmetric unit around one axis, the center of rotation. A rotation does not change the handedness of figures. The center of rotation is the only invariant point (point that maps onto itself).

Symmetry Elements:
Rotation

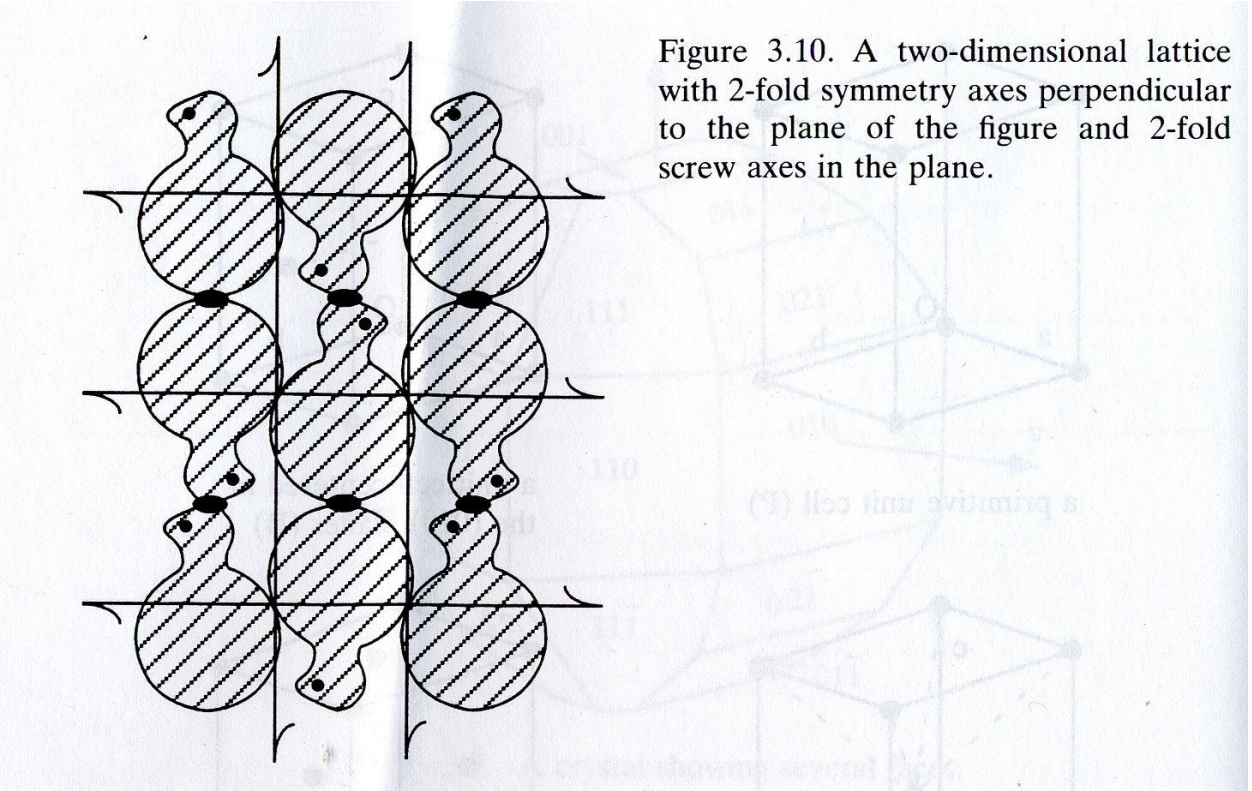


Figure 3.10. A two-dimensional lattice with 2-fold symmetry axes perpendicular to the plane of the figure and 2-fold screw axes in the plane.

Symmetry Elements: Rotation

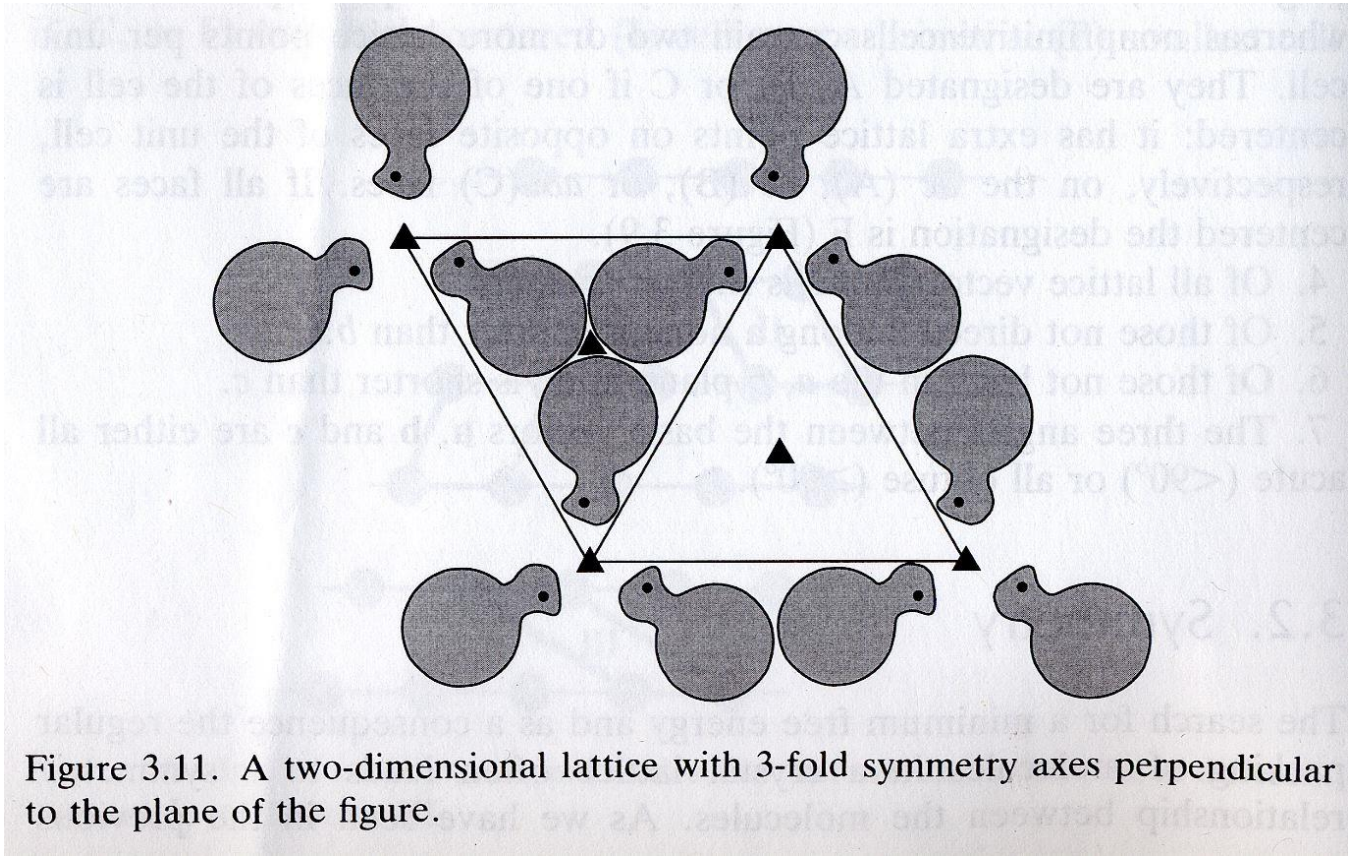
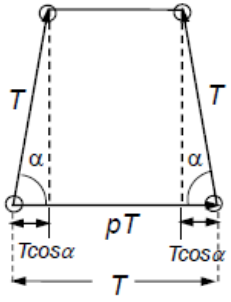


Figure 3.11. A two-dimensional lattice with 3-fold symmetry axes perpendicular to the plane of the figure.

Symmetry operations

Rotation

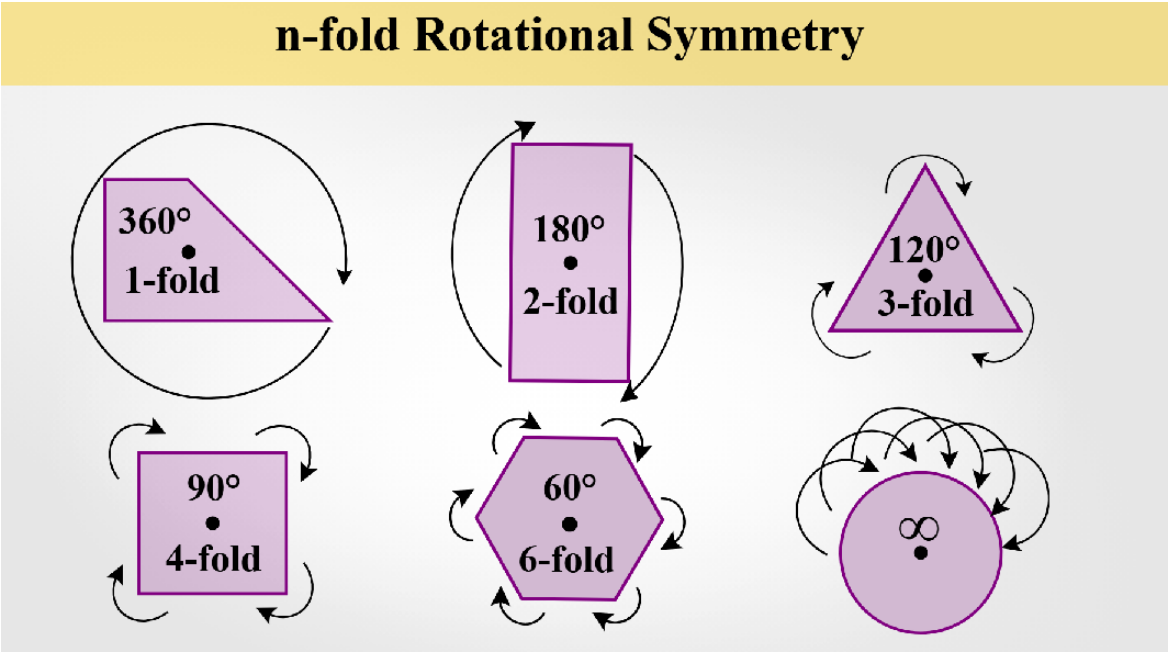


$$T = T\cos\alpha + pT + T\cos\alpha = pT + 2T\cos\alpha$$

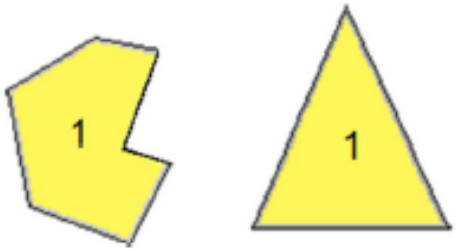
$$\cos\alpha = (1 - p)/2$$

p	α°	n-fold	Symbol
0	60	6	⬢
1	90	4	■
2	120	3	▲
3	180	2	⬮
-1	0/360	1	

An n-fold rotation symmetry means rotation through an angle of $2\pi/n$ will repeat the object or motif n times in a full 360^o rotation. n =1 means no symmetry.

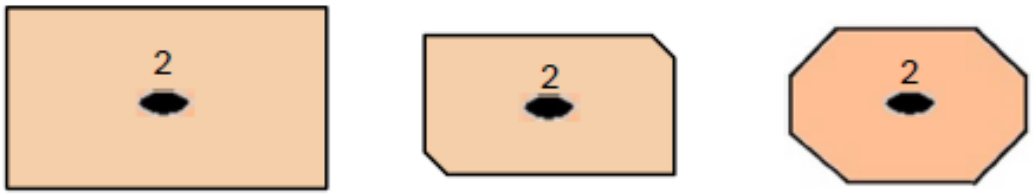


Rotation



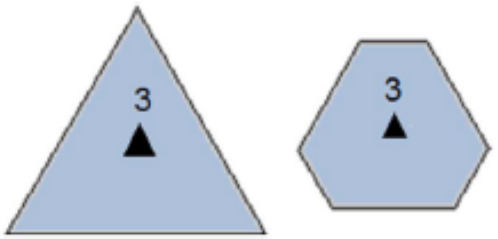
1-Fold Rotation Axis - An object that requires rotation of a full 360º to repeat itself has no rotational symmetry.

2-fold Rotation Axis - If an object appears identical after a rotation of 180º, that is twice in a 360º rotation, then it is said to have a 2-fold ($2\pi/180$) rotation symmetry

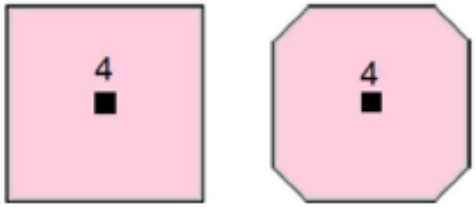


Rotation

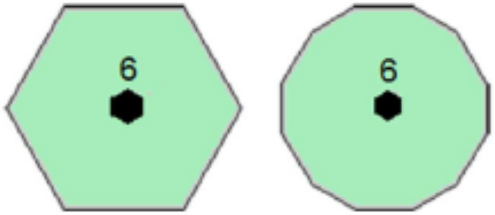
Similarly we have 3, 4 and 6-fold rotational symmetry



3 fold – 2π/120



4 fold – 2π/90



6 fold – 2π/60

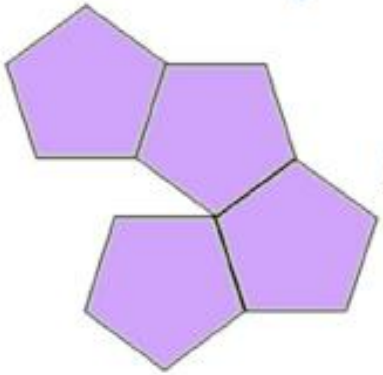
Rotation

Is it possible to have 5, 7 or 8-fold rotation symmetry?

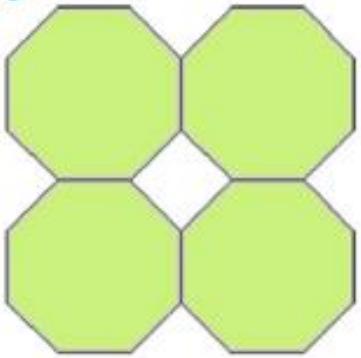
Objects with 5, 7 and 8 or higher order symmetry do exist in nature, e.g. star fish (5-fold), flowers with 5 or 8-fold symmetry.



However, these are not possible in crystallography as they cannot fill the space completely

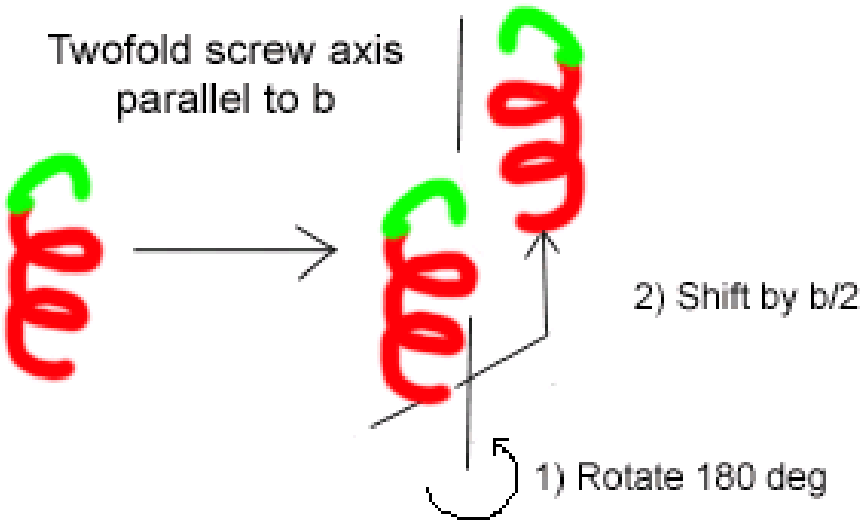


5 fold



8 fold

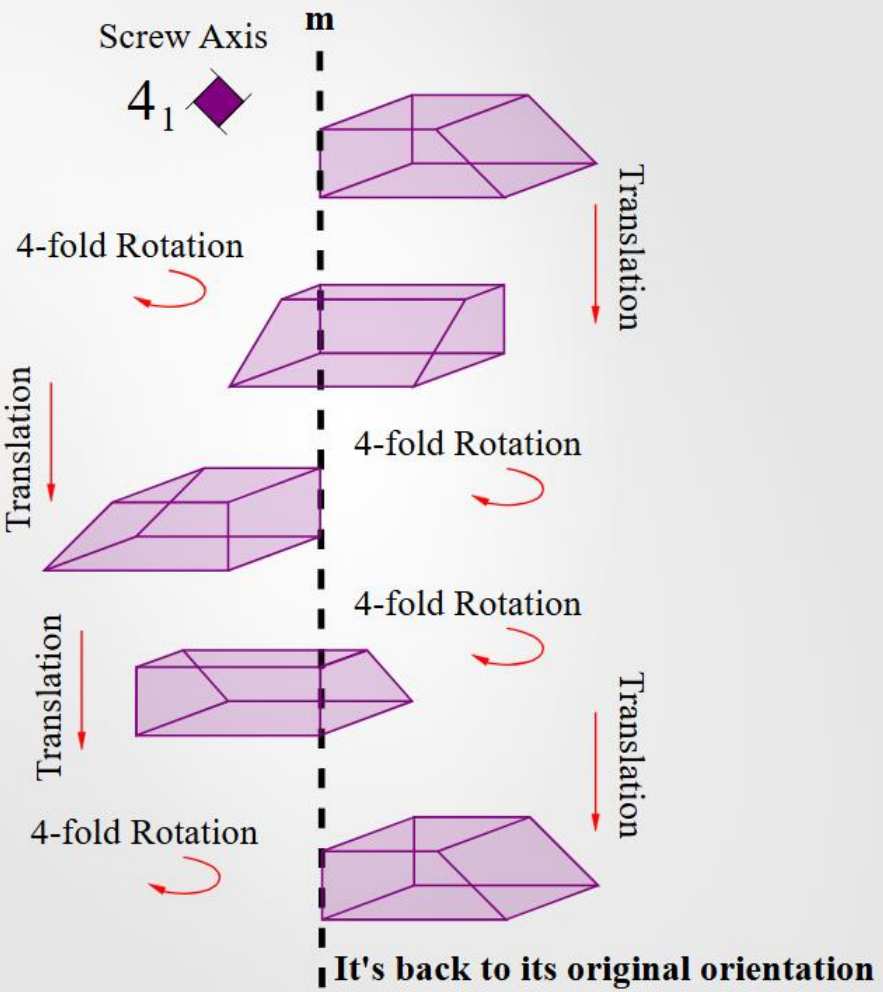
Symmetry Elements
Screw axes (rotation + translation)



rotation about the axis of symmetry by 360°/n, followed by a translation parallel to the axis by r/n of the unit cell length in that direction. (r < n)

Screw

Screw = Translation + Rotation



Symmetry Elements
Screw axes (rotation + translation)

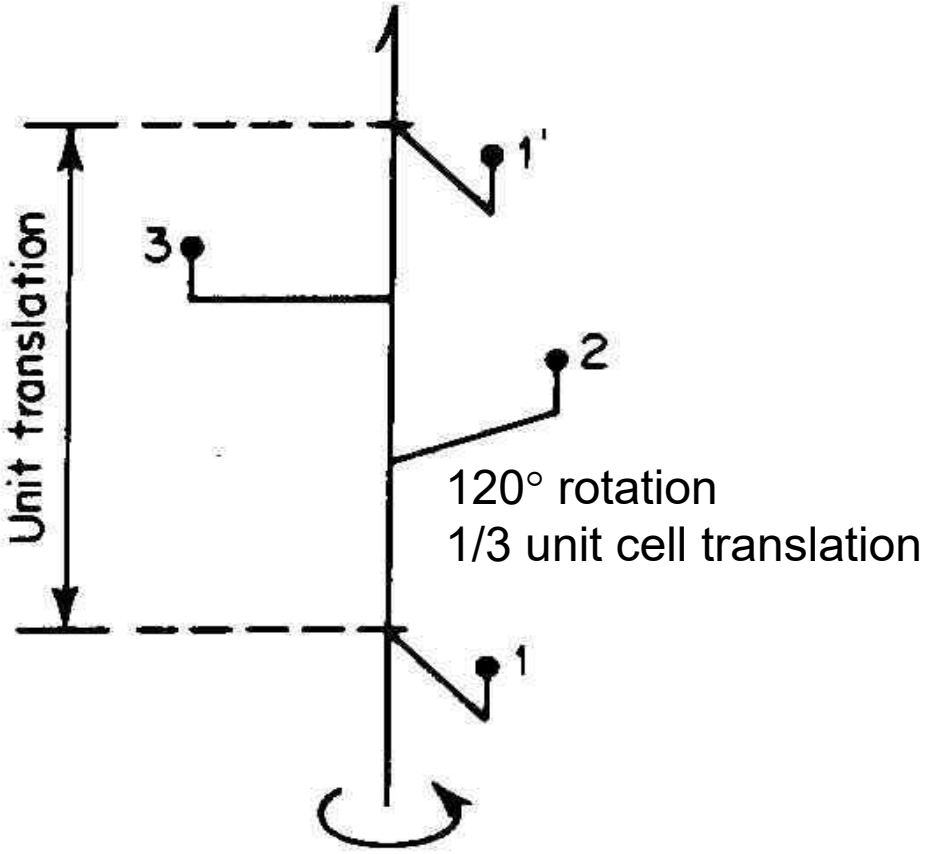


Figure 3.20. Screw axis 3_1.

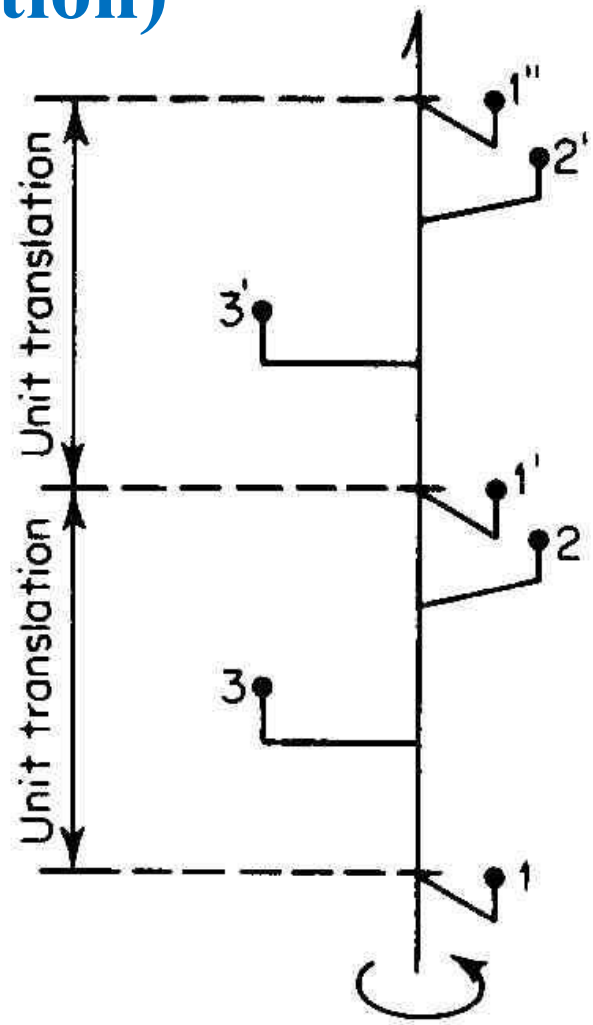


Figure 3.21. Screw axis 3_2.

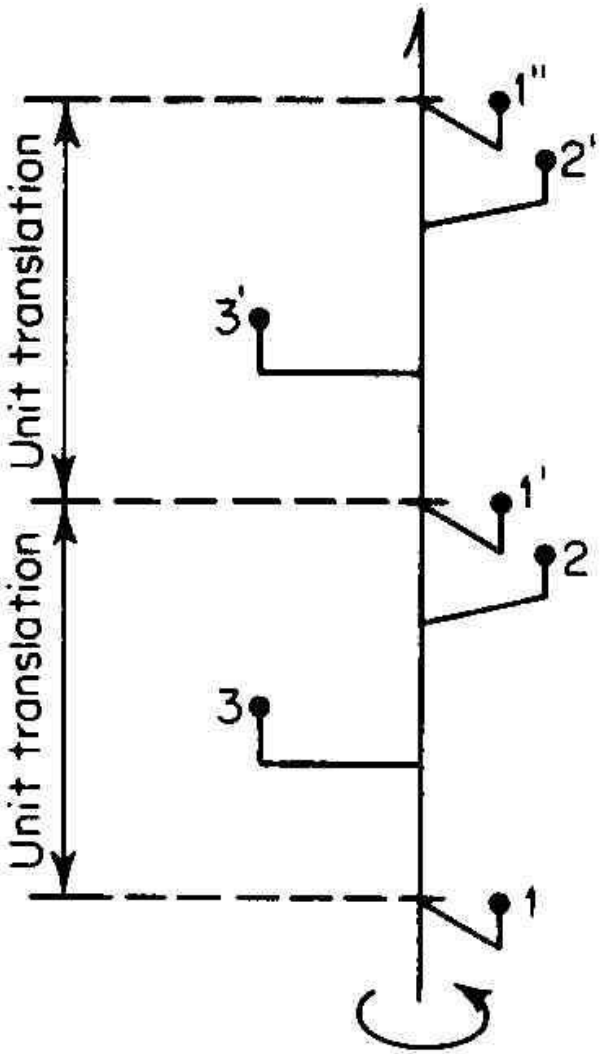
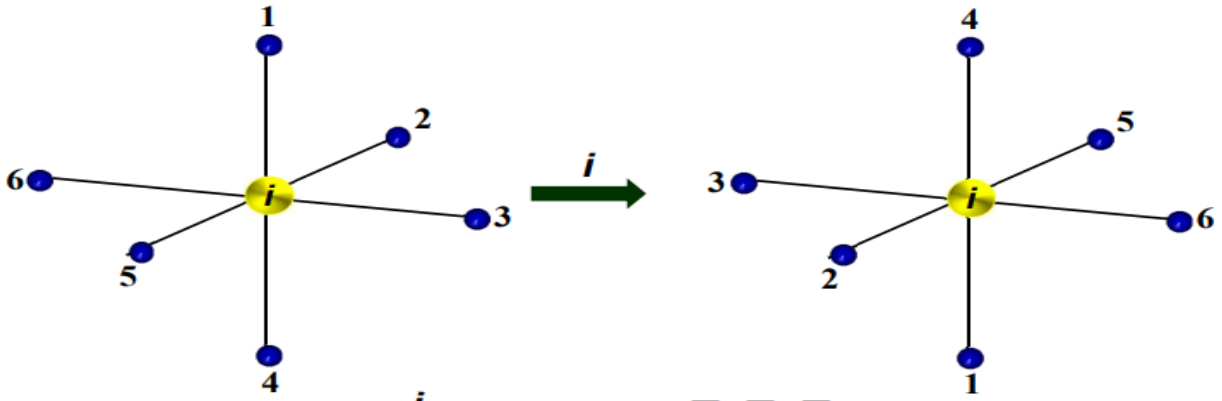


Figure 3.21. Screw axis 3_2.

Symmetry Elements

Inversion symmetry

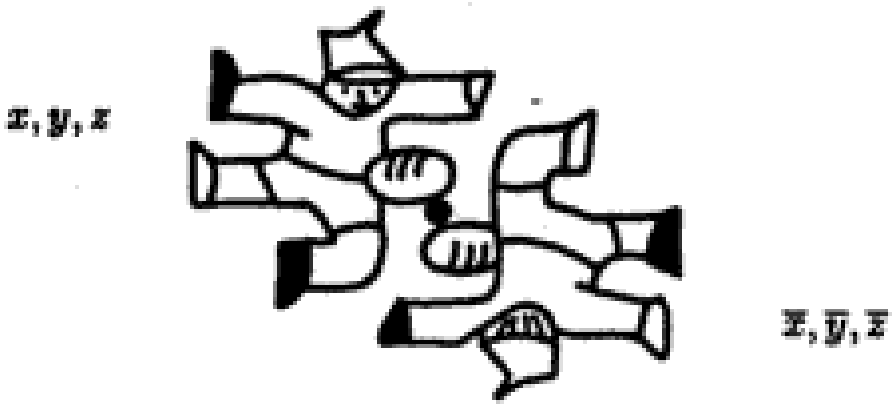


$xyz \xrightarrow{i} -x\ -y\ -z\ (\ \bar{x}\ \bar{y}\ \bar{z})$

In this operation, every part of the object is reflected through an inversion center called center of symmetry which is denoted as i. The object is reproduced inverted from its original position.

Symmetry Elements

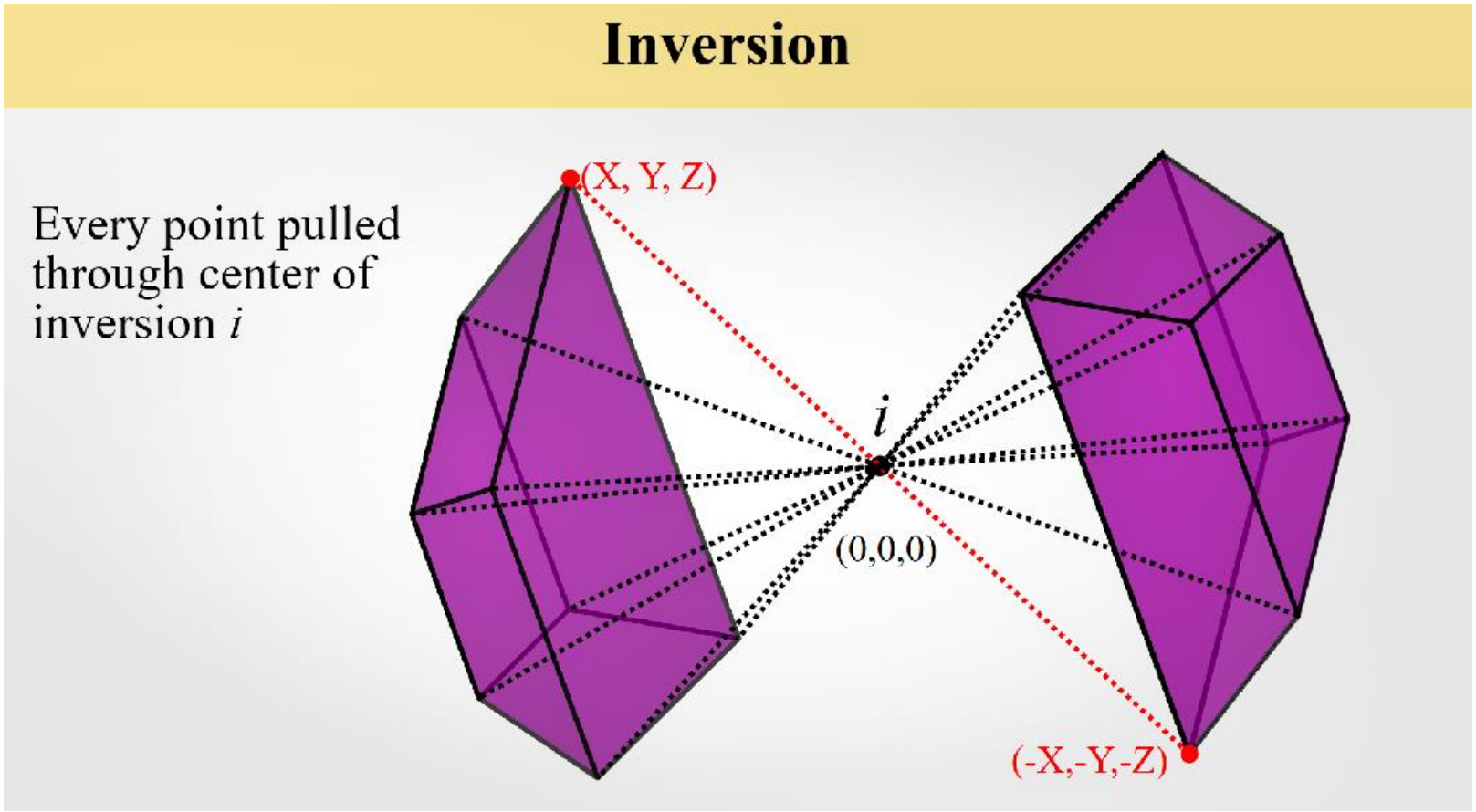
Inversion, or center of symmetry



every point on one side of a center of symmetry has a similar point at an equal distance on the opposite side of the center of symmetry.

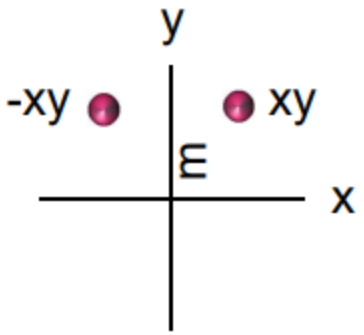
Symmetry Elements

Inversion, or center of symmetry



Symmetry Elements

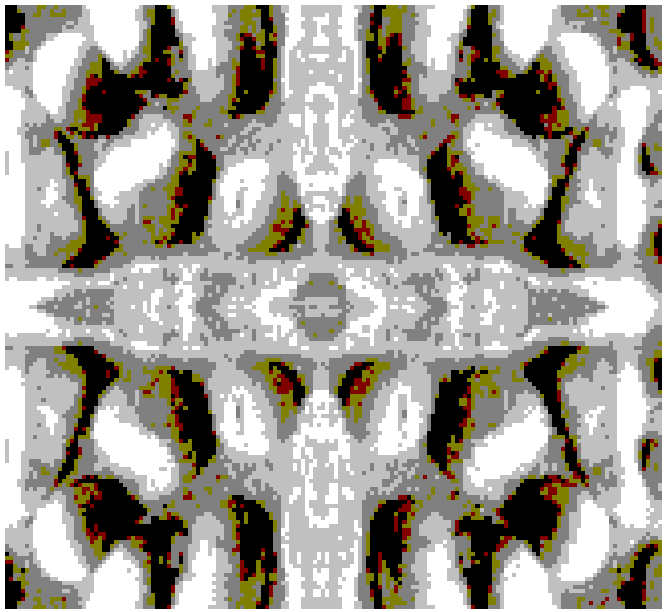
Reflection or Mirror symmetry



An object with a reflection symmetry will be a mirror image of itself across a plane called mirror plane (m).

Symmetry Elements

Reflection or Mirror symmetry

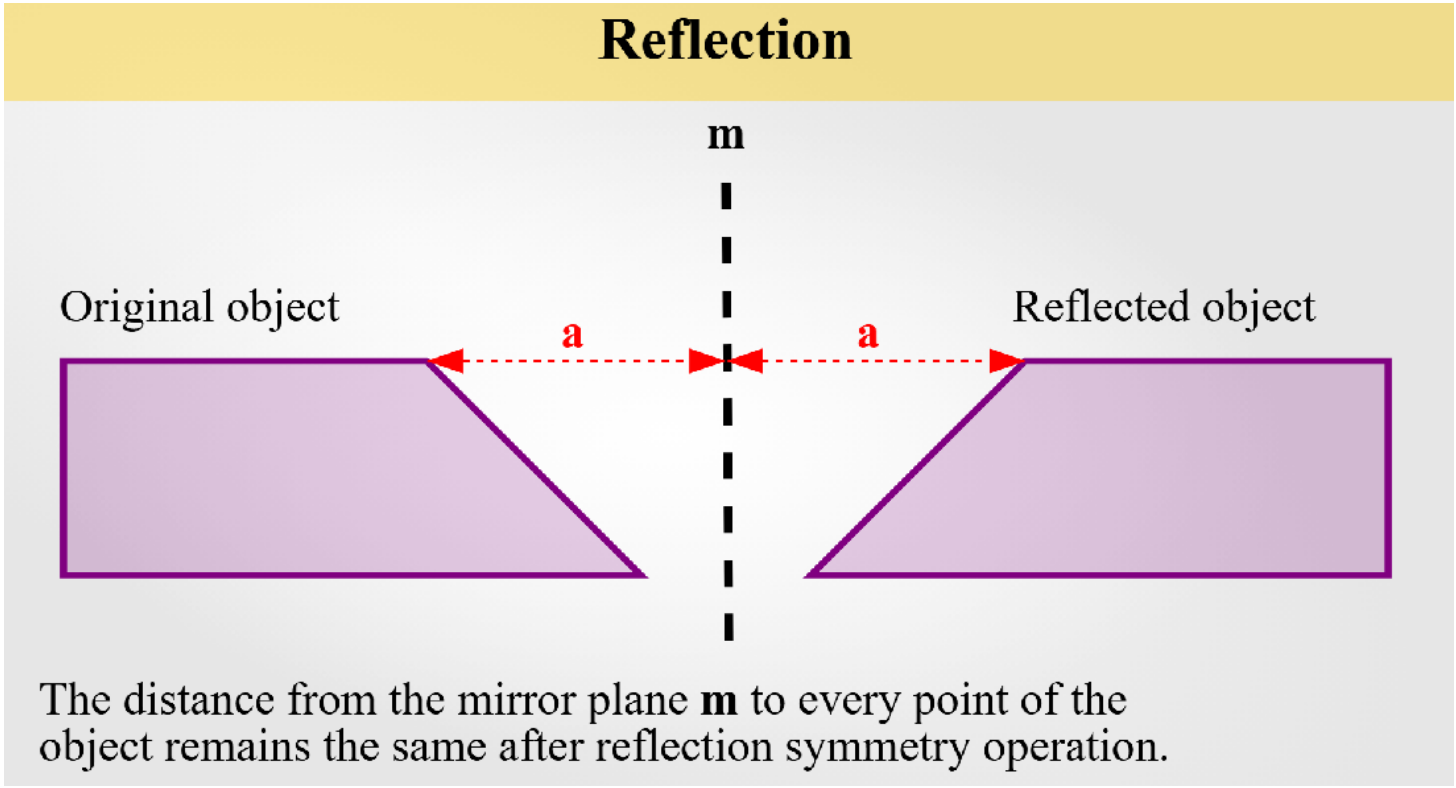


flips all points in the asymmetric unit over a line, which is called the mirror, and thereby changes the handedness of any figures in the asymmetric unit.

The points along the mirror line are all invariant points (points that map onto themselves) under a reflection.

Symmetry Elements

Reflection or Mirror symmetry



Symmetry elements: mirror plane and inversion center

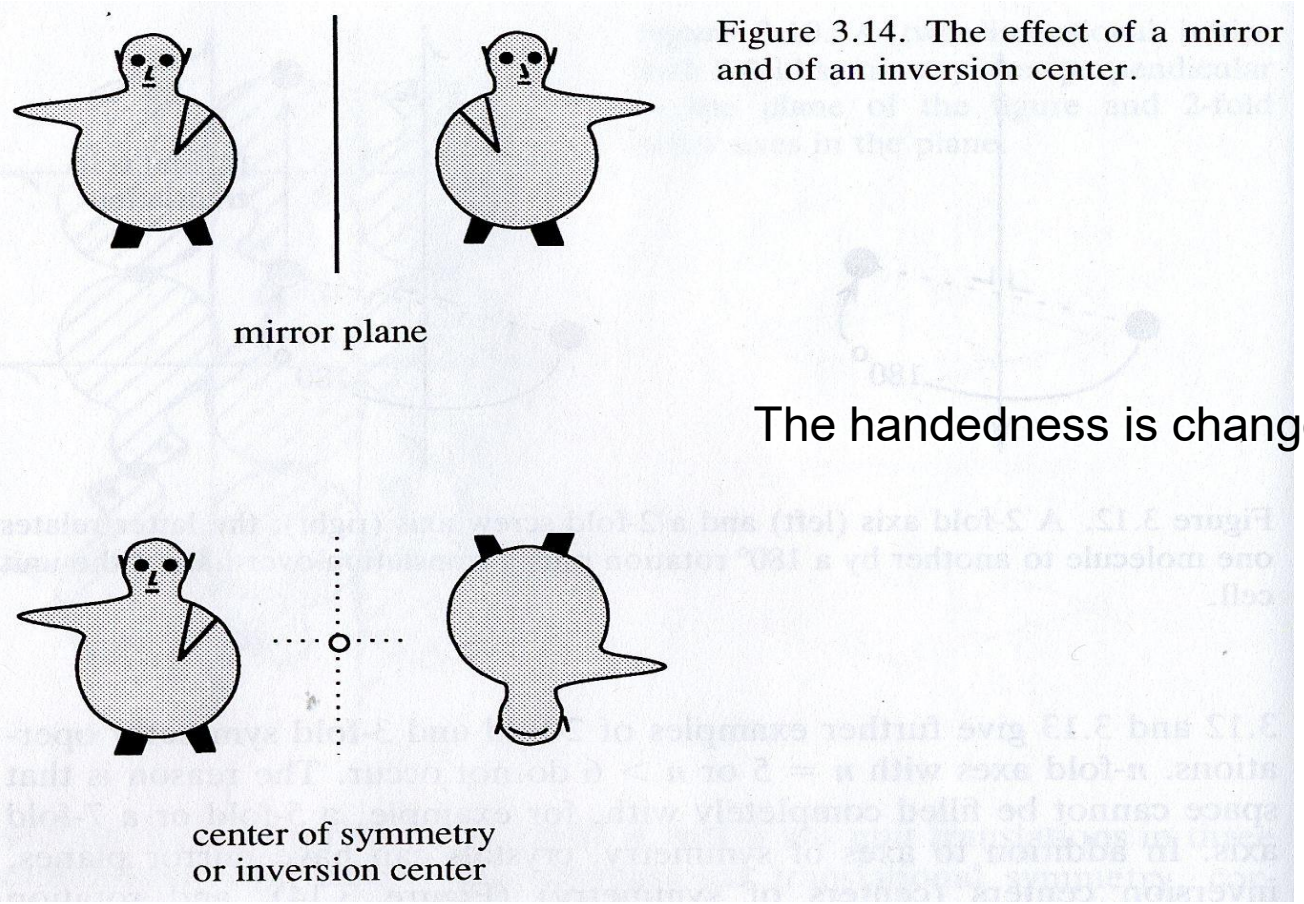


Figure 3.14. The effect of a mirror and of an inversion center.

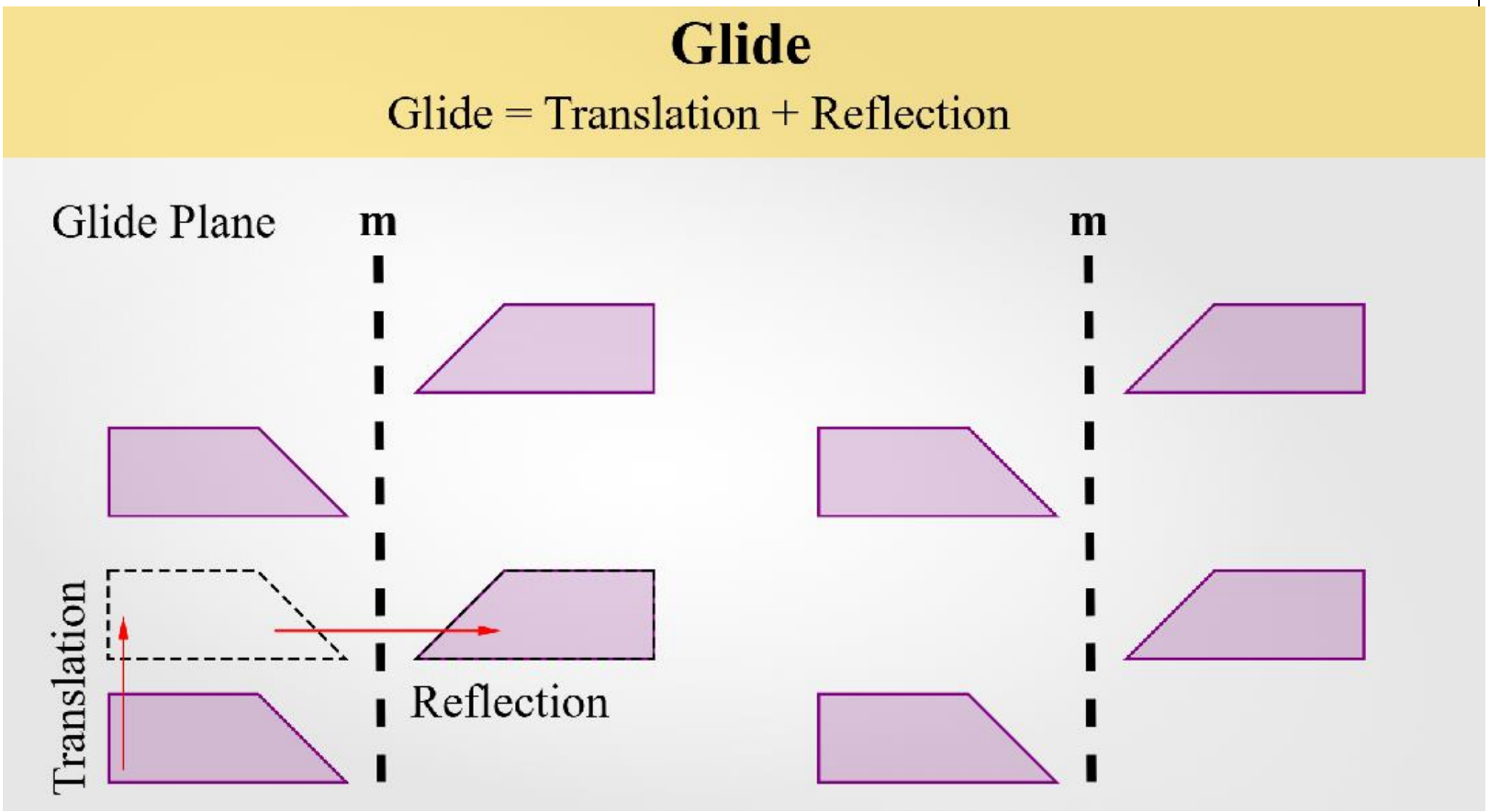
The handedness is changed.

Symmetry Elements
Glide reflection (mirror plane + translation)

reflects the asymmetric unit across a mirror and then translates parallel to the mirror. A glide plane changes the handedness of figures in the asymmetric unit. There are no invariant points (points that map onto themselves) under a glide reflection.

Symmetry Elements

Glide reflection (mirror plane + translation)



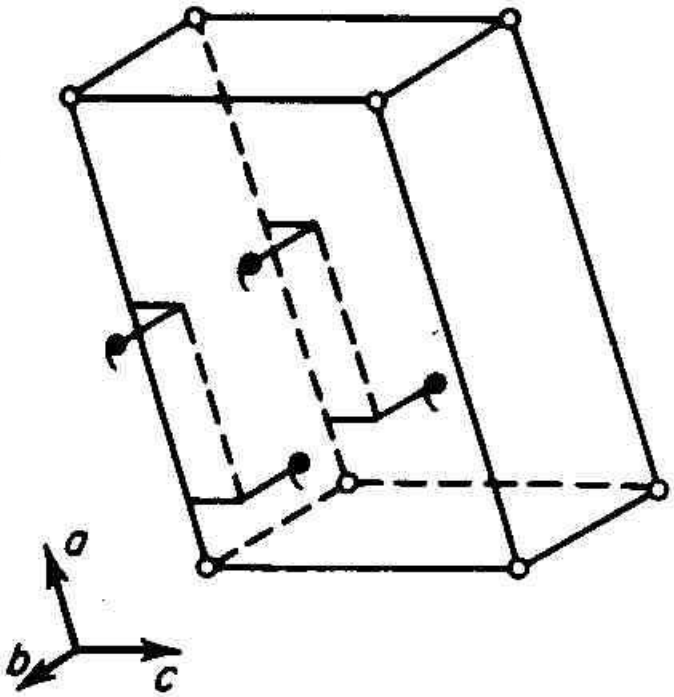
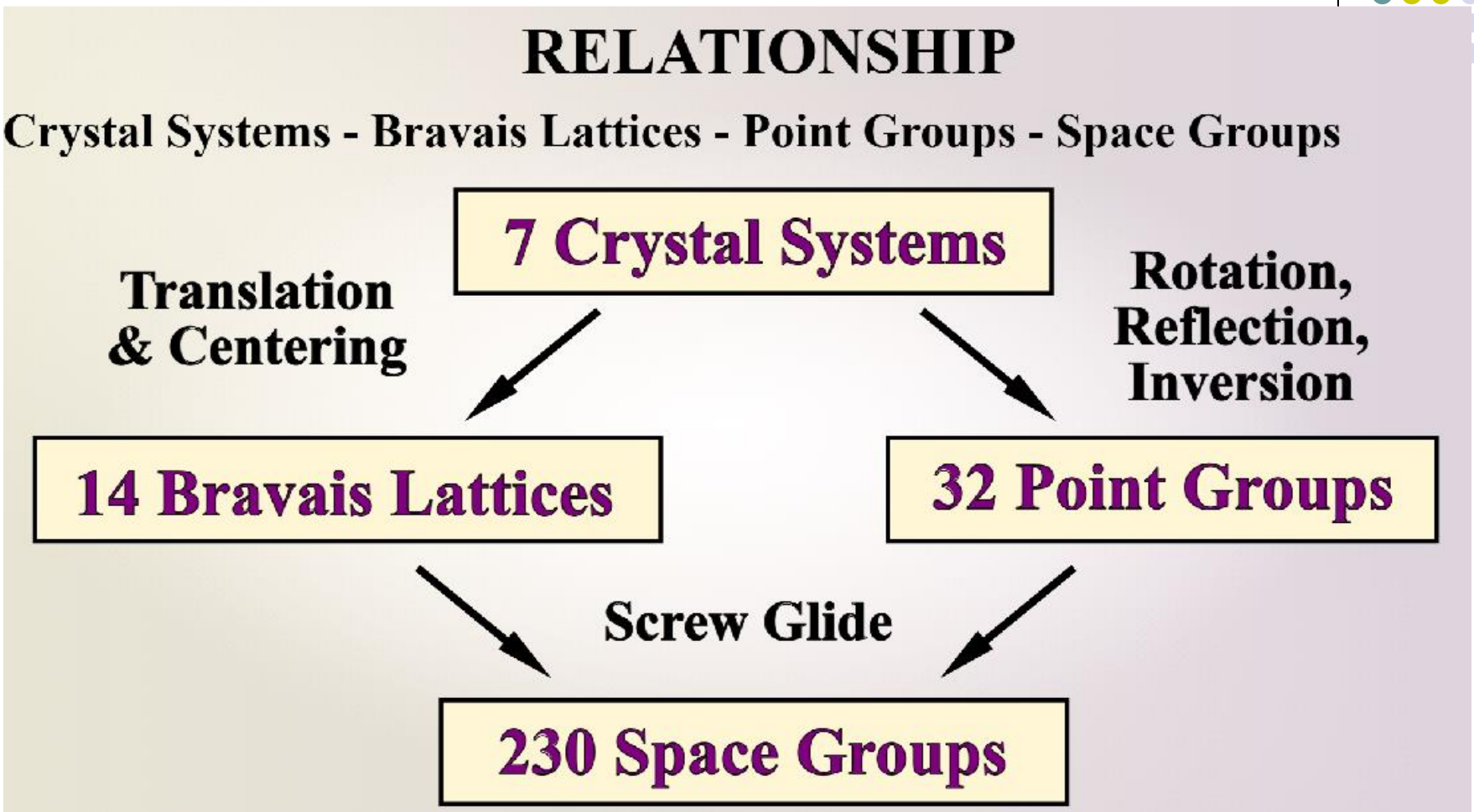


Figure 3.22. Glide plane *a*.

Table 3.1. Graphic Symbols for Symmetry Elements[a]

Symmetry axis or symmetry point	Graphic symbol	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol
Symmetry axes normal to the plane of projection (three dimensions) and symmetry points in the plane of the figure (two dimensions)			
Identity	None	None	1
Twofold rotation axis Twofold rotation point (two dimensions)		None	2
Twofold screw axis: "2 sub 1"		$\frac{1}{2}$	2_1
Threefold rotation axis Threefold rotation point (two dimensions)		None	3
Threefold screw axis: "3 sub 1"		$\frac{1}{3}$	3_1
Three fold screw axis: "3 sub 2"		$\frac{2}{3}$	3_2
Fourfold rotation axis Fourfold rotation point (two dimensions)		None	4
Fourfold screw axis: "4 sub 1"		$\frac{1}{4}$	4_1
Fourfold screw axis: "4 sub 2"		$\frac{1}{2}$	4_2
Fourfold screw axis: "4 sub 3"		$\frac{3}{4}$	4_3
Sixfold rotation axis Sixfold rotation point (two dimensions)		None	6

(continued)


RELATIONSHIP
Crystal Systems - Bravais Lattices - Point Groups - Space Groups
7 Crystal Systems
Translation & Centering
Rotation, Reflection, Inversion
14 Bravais Lattices
32 Point Groups
Screw Glide
230 Space Groups

Point and Space groups

Symmetry operations generate a variety of arrangements of lattice points in three dimensions. There are **32** unique ways in which lattice points can be arranged in space. These non-translation elements are called ***point-groups***.

A large number of 3D structures are generated when translations [linear translation, translation + reflection (glide plane) and translation + rotation (screw axis)] are applied to the point groups. There are **230** unique shapes which can be generated this way. These are called ***space groups***.