CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

Prof. Sandeep Sangal

IIT Kanpur

Lecture 33: Stereographic Projection: Stereograms of Point Groups

In this lecture, I am going to examine a method of representing three-dimensional point symmetries using what is known as stereographic projection. In stereographic projection, axes, motifs, and symmetry elements are represented on the surface of a sphere.

Consider the surface of a sphere, and let us introduce a coordinate system. The sphere is bisected into two equal halves by a circle passing through its center. This circle may be referred to as the equatorial circle, as it forms the equator of the sphere. The x and y axes lie in the plane of this equatorial circle, while the z-axis is normal to the equatorial circle.

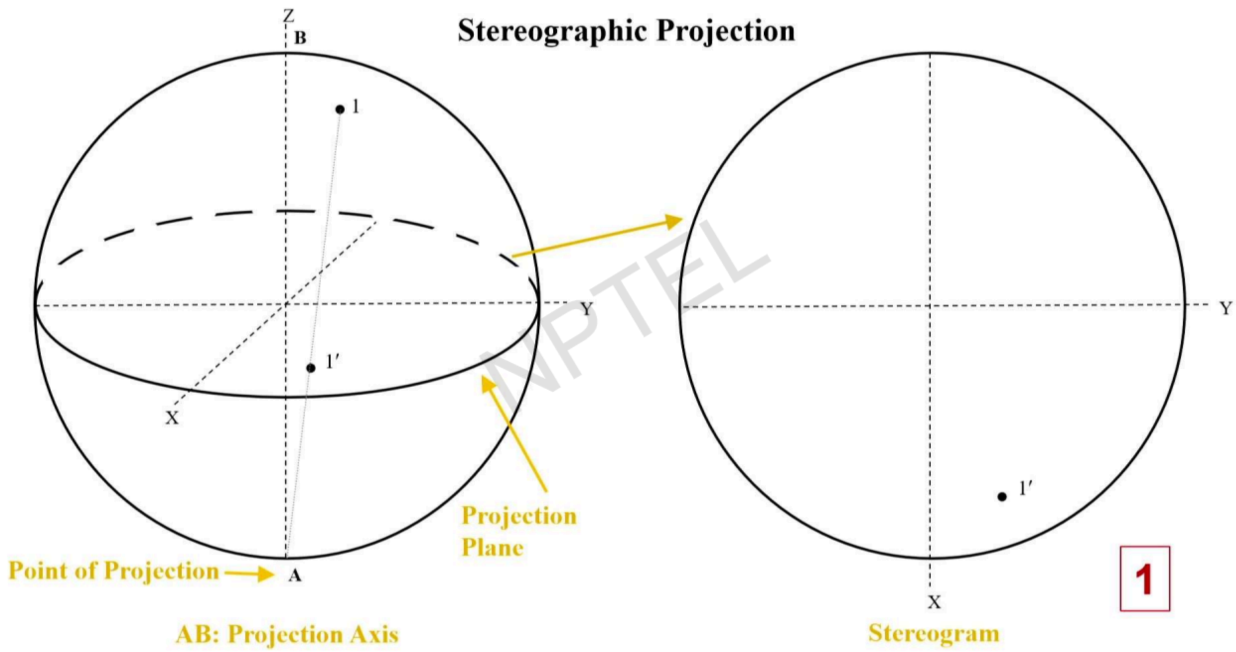
The z axis may also be labeled as the axis AB, where AB is referred to as the projection axis, and the equatorial plane is referred to as the projection plane. All features on the sphere are ultimately projected onto this two-dimensional projection plane.

Let us assume that there is a point labeled 1 on the surface of the sphere. Recalling the earlier discussion on combining rotation axes, the rotation axis was taken to pass through the center of the sphere and intersect the surface at a point, which is referred to as a pole. This pole may represent either a motif or a rotation axis.

To project this pole onto the projection plane, we use point A as the point of projection. A straight line is drawn from the point of projection A to point 1. This line intersects the projection plane at a point, which we denote as $1'$. The point $1'$ therefore represents the projection of pole 1 onto the two-dimensional plane. Once projected, the projection plane may be conceptually removed from the sphere and represented independently. Such a diagram is referred to as a stereogram, and all symmetry elements will be represented using this construction.

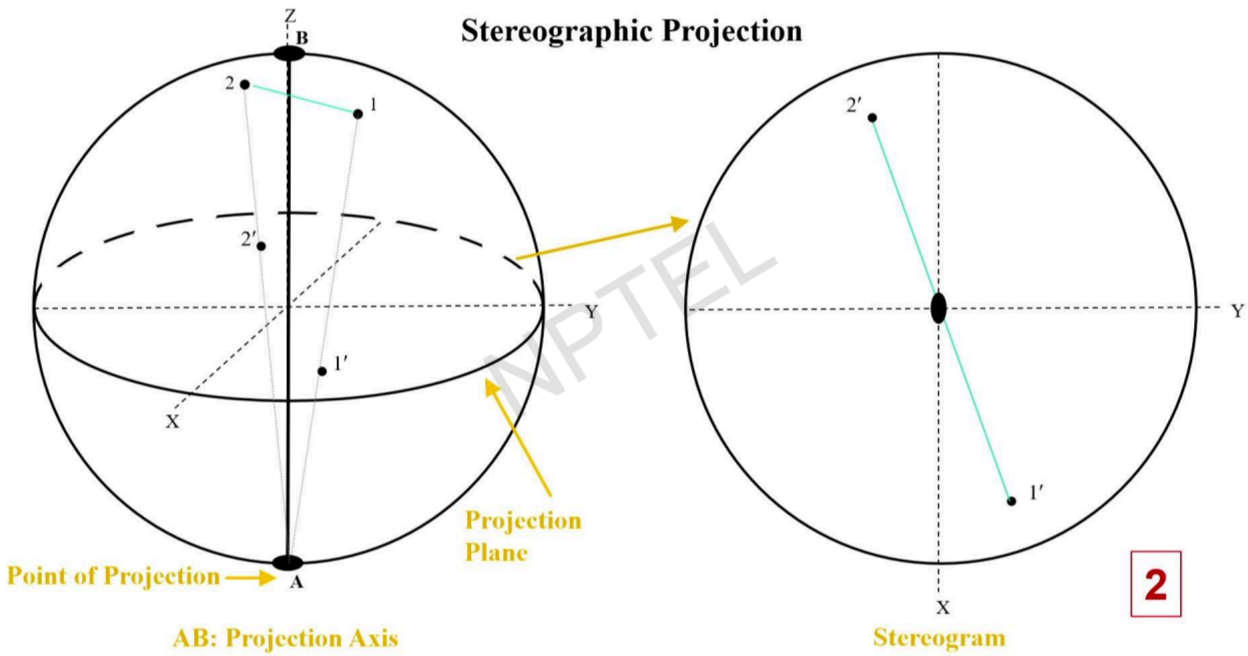
If the point 1' corresponds to a pole lying in the upper hemisphere, it is represented as a filled or dark circle. This configuration corresponds to symmetry 1, or the absence of symmetry.

(Refer Slide Time: 03:42)



Now consider the case where there is a twofold rotation axis along the projection axis AB. The twofold rotation axis rotates pole 1 by 180°, producing another pole on the surface of the sphere, labeled as pole 2. Pole 2 is projected onto the projection plane using the same point of projection A by drawing a straight line from A to 2. This line intersects the projection plane at a point denoted as 2'. Thus, pole 1 is transformed into pole 2 by a rotation of 180°, and the corresponding stereogram contains the points 1' and 2'. The line joining 1' and 2' may be drawn only for reference and is not essential. The twofold rotation axis itself is projected to the center of the stereogram. This representation therefore corresponds to symmetry 2, indicating the presence of a twofold rotation axis.

(Refer Slide Time: 05:38)



By extension, higher-order rotation axes may also be represented. A threefold rotation axis will generate three poles and hence three points in the stereogram. Similarly, fourfold and sixfold rotation axes will generate four and six points, respectively, with the sixfold case corresponding to rotations of 60°.

Next, let us introduce an additional symmetry element in the form of a mirror plane. In this case, the projection plane itself also serves as the mirror plane. The poles 1 and 2, which lie in the upper hemisphere, will be reflected across the mirror plane into the lower hemisphere, producing poles 3 and 4.

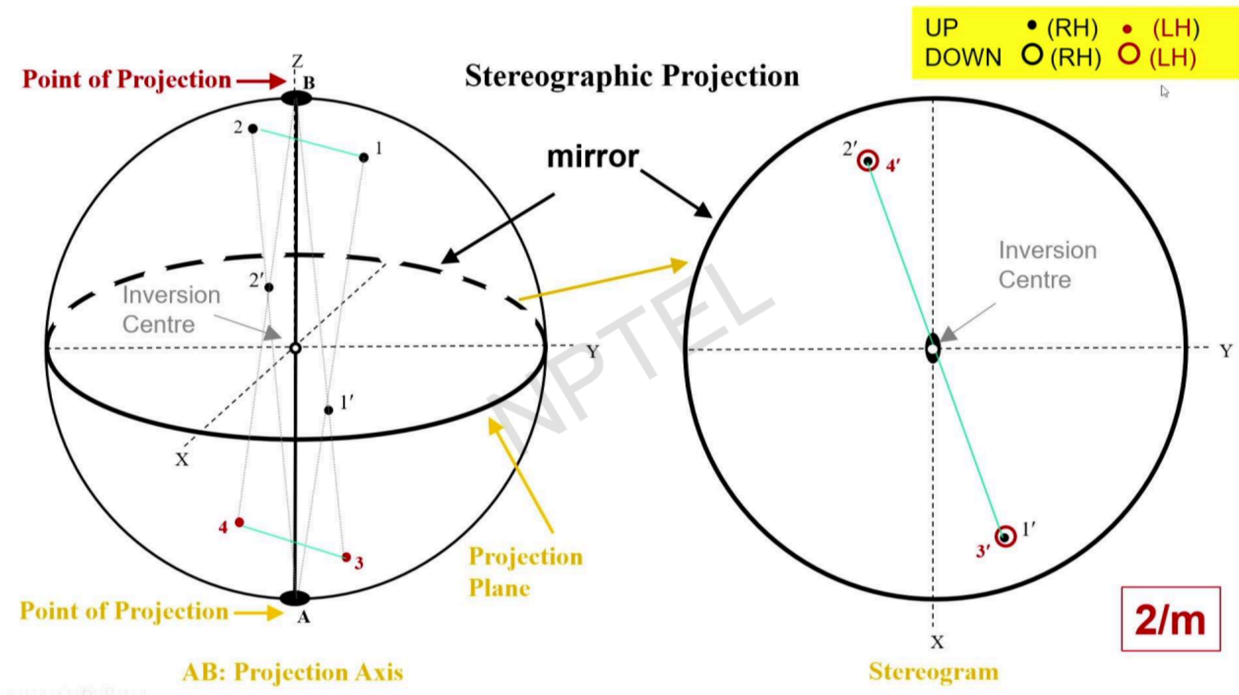
These poles must also be projected onto the projection plane. If one attempts to project poles 3 and 4 using point A as the point of projection, the projection lines extend outside the equatorial circle. Although the projection plane may be considered infinite, this approach becomes increasingly unsatisfactory as a pole approaches the point of projection A, since its projection would move arbitrarily far away on the plane.

To resolve this, poles lying in the lower hemisphere are projected using point B as the point of projection. Lines drawn from point B to poles 3 and 4 intersect the projection plane within the equatorial circle. An important observation is that, for reflections, the projected points of the reflected poles coincide with the projected points of the original poles. Thus, the projections of poles 3 and 4 coincide with 1' and 2', respectively.

These projections are represented using open circles, indicating that they originate from the lower hemisphere. Additionally, the boundary circle of the stereogram is drawn as a thick or dark line to indicate the presence of a mirror plane. In the stereogram, 1' is reflected to 3', and 2' is reflected to 4'.

It is also useful to note that pole 1 may be related to pole 4 through an inversion operation. The inversion center is located at the center of the sphere, and its projection corresponds to the center of the stereogram. Minor inconsistencies in numbering may be ignored, as the essential symmetry relationships remain unchanged.

(Refer Slide Time: 10:33)



This particular point group is represented as $2/m$. The oblique line indicates that the mirror plane is perpendicular to the twofold rotation axis. In the stereogram, open circles are shown in red to indicate a change in handedness. For clarity, black symbols may be interpreted as right-handed, while red symbols represent left-handed configurations.

The legend used is as follows: filled circles correspond to poles in the upper hemisphere, open circles correspond to poles in the lower hemisphere, black indicates right-handedness, and red indicates left-handedness.

Now consider another configuration (222). Starting again with point group 2, which contains only a single twofold rotation axis at the center, imagine that an additional twofold rotation axis is introduced along the y axis. This additional axis rotates poles 1 and 2 by 180° about the y axis, producing two new poles in the lower hemisphere. These poles are projected onto the projection plane using point B as the point of projection.

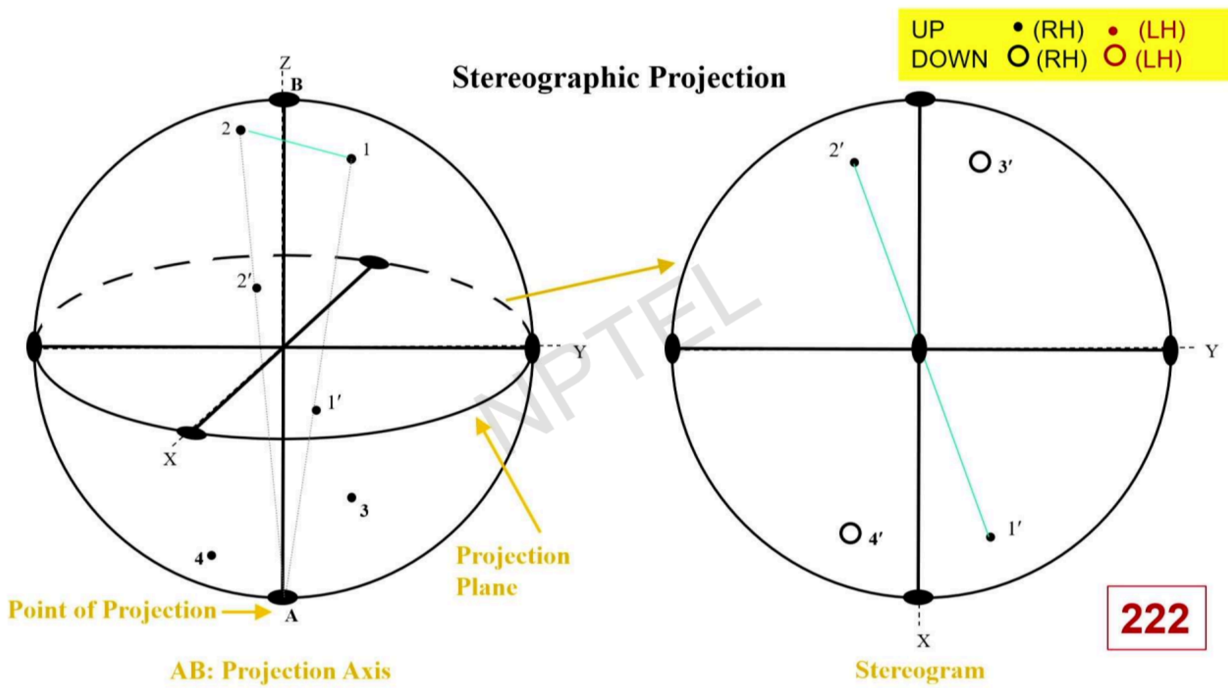
It is important to recall that if two mutually perpendicular twofold rotation axes are present, a third twofold rotation axis must also exist, oriented at 90° to the other two. This represents a combination of three rotation axes. The consistency of this configuration can be verified by examining how the poles transform under successive rotations. The additional twofold rotation axis rotates the poles in a manner that preserves the overall symmetry of the system.

On the stereogram, the points or poles 3 and 4 are reflected and are represented by open circles. On the stereogram, the other twofold rotation axes are also projected, and they appear in this manner. Thus, there is a twofold rotation axis along the x axis, another twofold rotation axis along the y axis, and a twofold rotation axis at the center, which is perpendicular to the plane and also perpendicular to the twofold axes along x and y.

If we examine only the stereogram, point $1'$ can be taken to point $3'$ by the twofold rotation axis along y, while point $1'$ can be taken to point $4'$ by the twofold rotation axis along x. Further, points $1'$, $2'$, $3'$, and $4'$ all coincide with themselves under the action of the central twofold rotation axis. The point group formed in this case is therefore the point group 222.

At this stage, we no longer need to draw three-dimensional constructions on the surface of the sphere. From this point onward, all symmetry operations can be represented directly on the stereogram.

(Refer Slide Time: 13:07)

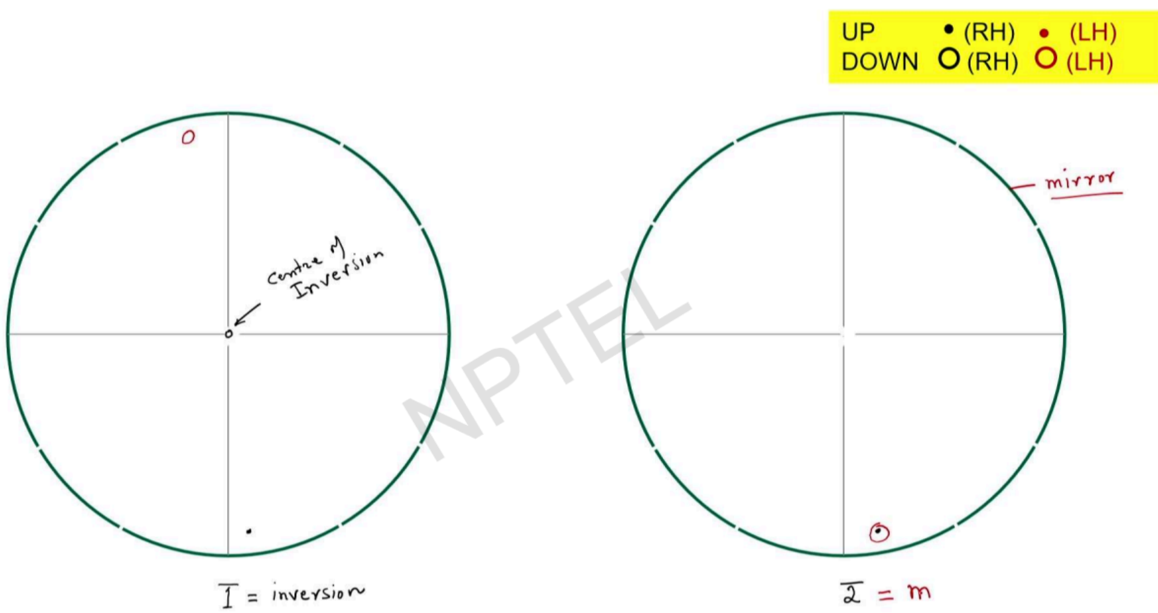


Let us now consider a two-dimensional plane in which we wish to represent a rotoinversion axis $\bar{1}$. We begin with a point located in the upper hemisphere, denoted as an "up" position. Recall from the previous lecture that a onefold rotoinversion corresponds to a rotation of 360° followed by inversion. A rotation of 360° returns the point to its original position, after which inversion takes place. As a result, the point moves to the lower hemisphere and is represented by an open circle. A change in color is used to indicate the change in handedness, signifying a transition from a right-handed to a left-handed object.

If we examine this operation more carefully, a onefold rotoinversion is equivalent to the presence of an inversion center at the center of the sphere. In the stereogram, this inversion center is represented by a small circle at the center of the diagram. Therefore, instead of referring to this symmetry as a onefold rotoinversion axis, it may simply be described as pure inversion symmetry.

Next, consider the twofold rotoinversion axis, denoted as $\bar{2}$. Once again, we begin with a point in the upper hemisphere. This point is rotated by 180°, bringing it to the opposite position on the stereogram, and is then inverted. After inversion, the point returns to a position directly below the original point, with a corresponding change in handedness. The symmetry represented by $\bar{2}$ can also be interpreted differently. If the operation is viewed as a mirror reflection with the mirror plane coinciding with the projection plane, the point in the upper hemisphere reflects into the lower hemisphere, and both points project to the same position. Hence, $\bar{2}$ is equivalent to the mirror point group m ($\bar{2} = m$).

(Refer Slide Time: 16:14)



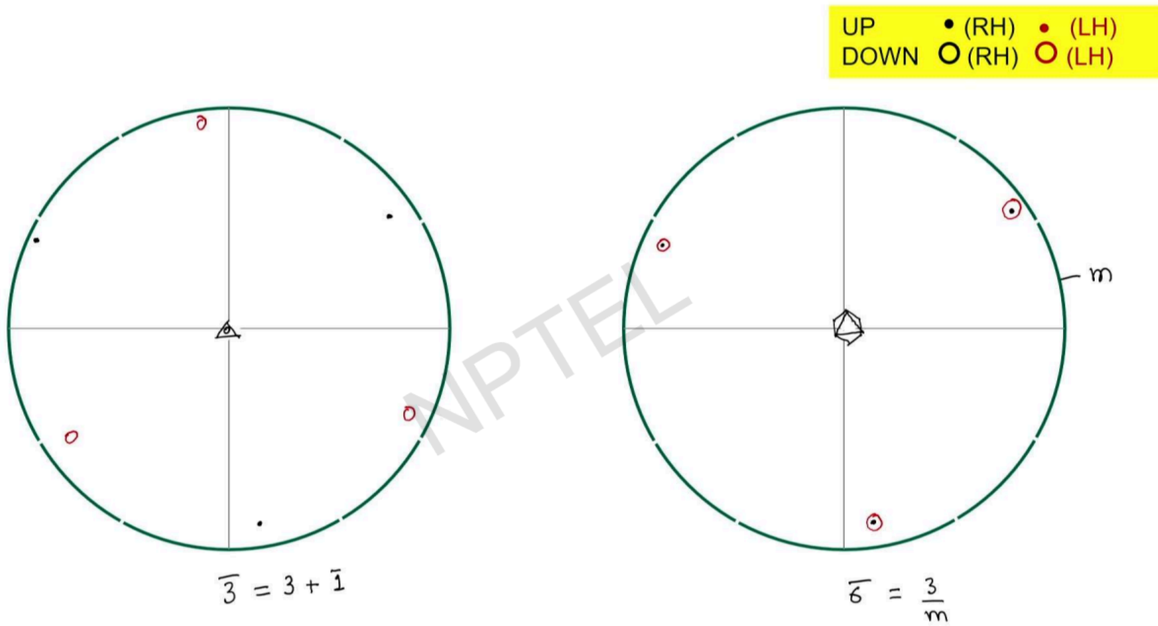
Now consider the threefold rotoinversion axis, $\bar{3}$. We begin with a point in the upper hemisphere and rotate it by 120°. After this rotation, inversion is applied, moving the point to the lower hemisphere with a change in handedness. Starting from this new point, another rotation of 120° is applied, followed by inversion, returning the point to the upper hemisphere. This sequence is repeated: a further rotation of 120° followed by inversion moves the point back to the lower hemisphere, and one final rotation and inversion returns the point to its original position. Once the starting point is reached, the pattern repeats, indicating that the diagram is complete.

From this stereogram, it is evident that there exists a proper threefold rotation axis. In addition, there is an inversion center, as all points, both black and red can be brought into self-coincidence through inversion, with the handedness changing appropriately. For example, a point in the lower hemisphere moves to the upper hemisphere upon inversion, with the correct change in handedness. This inversion center is represented by a small circle at the center of the stereogram. Thus, the $\overline{3}$ roto-inversion axis can be decomposed into a combination of a threefold rotation axis and an inversion center.

Next, let us consider the sixfold rotoinversion axis, $\overline{6}$. As before, we begin with a point in the upper hemisphere and apply a rotation of 60°, followed by inversion, which moves the point to the lower hemisphere. From the lower hemisphere, another rotation of 60° followed by inversion brings the point back to the upper hemisphere. Repeating this sequence of rotation and inversion successively generates all points of the pattern. After completing six such operations, the point returns to its original position, indicating that the stereogram is complete.

Inspection of this diagram reveals the presence of a mirror plane. The points in the upper and lower hemispheres are related by reflection in the projection plane, and this mirror plane brings all points into self-coincidence. Graphically, a sixfold rotoinversion is represented by a hexagon indicating the sixfold component. However, it is also evident that a threefold rotation symmetry is present. Consequently, the graphical notation for $\overline{6}$ consists of a hexagon with an inscribed triangle. From this diagram, it is clear that $\overline{6}$ can be represented by the point group $3/m$, since a threefold rotation axis combined with a mirror plane perpendicular to it produces the same stereogram.

(Refer Slide Time: 22:24)

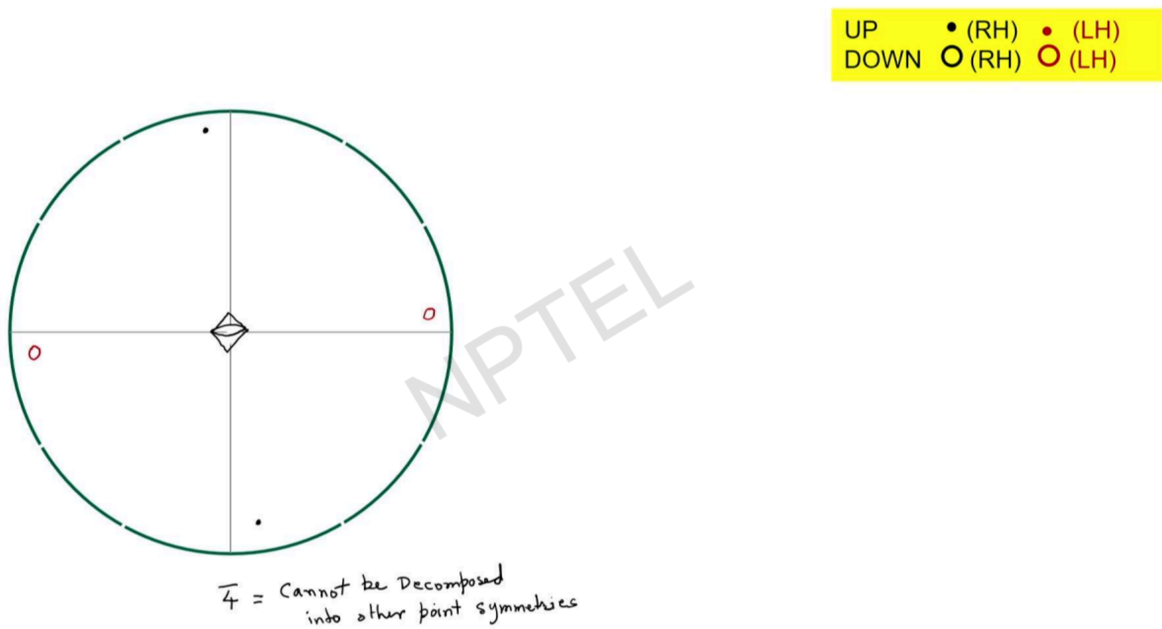


Up to this point, all rotoinversion axes have been shown to be representable in terms of other point symmetries, such as inversion, rotation, mirror symmetry, or combinations thereof. We now consider the remaining case, the fourfold rotoinversion axis, $\bar{4}$.

To construct $\bar{4}$, we begin with a point in the upper hemisphere and apply a rotation of 90°, followed by inversion, which moves the point to the lower hemisphere with a change in handedness. From this position, another rotation of 90° followed by inversion brings the point back to the upper hemisphere. Repeating this sequence of rotation and inversion ultimately returns the point to its starting position, completing the diagram.

This stereogram exhibits an additional twofold rotation symmetry at the center. Specifically, a rotation of 180° brings the entire pattern into self-coincidence. To represent this symmetry graphically, a square is used to denote the fourfold component, with a twofold symbol inscribed inside the square to indicate the additional twofold rotation. The significant feature of this pattern is that it cannot be decomposed into other point symmetries. In this case, $\bar{4}$ is a unique rotoinversion axis among the crystallographic symmetries and must be treated differently from the other rotoinversion axes.

(Refer Slide Time: 24:48)



Thank you.