CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 30: Combination of Three Rotation Axes in 3D

In the previous lecture, we reached a milestone in the course by completing the discussion on two-dimensional point groups and plane groups. In the present lecture, we begin the discussion on the extension of these concepts to the third dimension. In doing so, the two-dimensional point groups are extended to three-dimensional point groups, and the plane groups are extended to what are known as space groups. We first focus on three-dimensional point groups.

One important observation is that all the two-dimensional point groups discussed earlier can be directly extended to three-dimensional point groups. Since there are ten two-dimensional point groups, this immediately gives rise to ten three-dimensional point groups. This can be understood through a simple example. Consider the two-dimensional point group $2mm$. In this group, there are two mirror lines, and at the intersection of the two orthogonal mirrors, there exists a twofold rotation axis, which gives rise to the notation $2mm$. Now, imagine introducing a third axis perpendicular to this point group. In three dimensions, the two-dimensional rotation axis remains, while the two mirrors become mirror planes. One may visualize one mirror plane and a second mirror plane perpendicular to the first. Denoting these planes as M_1 and M_2, the rotation axis lies along the line of intersection of the two mirror planes. This construction represents a straightforward extension of the two-dimensional $2mm$ group into three dimensions.

Thus, the ten three-dimensional point groups obtained in this manner are simply extensions of the two-dimensional point groups. However, three dimensions introduce an additional feature that does not exist in two dimensions. In two dimensions, rotation axes cannot intersect, whereas in three dimensions, the intersection of rotation axes becomes possible.

To illustrate this, consider a rotation axis denoted as axis A, with a rotation of angle α about this axis. Let there be another rotation axis, denoted as axis B, oriented at some angle with respect to axis A, with a rotation of angle β about it. We now ask the following question: what is the result of performing a rotation of α about axis A, followed by a rotation of β about axis B? In other words, what symmetry operation results from this combination?

Consider an asymmetric motif. After a rotation of α about axis A, the motif moves from its original position, motif 1, to a new position, motif 2. Next, a rotation of β about axis B moves motif 2 to another position, motif 3. Thus, motif 1 transforms to motif 2 under A_α, and motif 2 transforms to motif 3 under B_β. We now seek a single symmetry operation that directly transforms motif 1 to motif 3.

Since both operations are rotations about axes A and B, there is no change in handedness, and therefore neither inversion nor reflection can occur. The only remaining possibility is another rotation. We therefore introduce a third rotation axis, denoted as axis C, with a rotation angle γ, such that a rotation of γ about axis C takes motif 1 directly to motif 3. Hence, the combined operation of A_α followed by B_β is equivalent to C_γ.

In three dimensions, the rotation axes A, B, and C are oriented at specific angles relative to one another. Let the angle between axes C and B be denoted by a, the angle between axes A and C by b, and the angle between axes A and B by c. We therefore have three rotation angles α, β, and γ about axes A, B, and C, respectively, and three interaxial angles a, b, and c between the axes themselves. Our objective is to determine relationships among these angles. Through such relationships, we can identify the possible combinations of crystallographic rotation axes, noting that the axes A, B, and C must correspond to the allowed crystallographic rotation axes.

Before deriving a general solution, we consider a specific example using matrices. Recall the rotation matrices in Cartesian coordinates x, y, and z. A rotation about the x-axis by an angle θ is represented by the matrix

$$R_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}.$$

Similarly, a rotation about the y-axis by an angle θ is given by

$$R_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix},$$

and a rotation about the z-axis by an angle θ is

$$R_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

These matrices were derived in an earlier lecture.

Now consider the case in which there is a twofold rotation axis about the x-axis and a twofold rotation axis about the y-axis. This corresponds to setting $\theta = \pi$ for both rotations, that is, a 180° rotation about each axis. The combined operation is $R_x(\pi)$ followed by $R_y(\pi)$, and we seek the resulting rotation.

Substituting $\theta = \pi$ into $R_y(\theta)$ gives

$$R_y(\pi) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Similarly, substituting $\theta = \pi$ into $R_x(\theta)$ gives

$$R_x(\pi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Multiplying these matrices yields

$$R_y(\pi) * R_x(\pi) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

This resulting matrix corresponds exactly to $R_z(\pi)$, which represents a 180° rotation about the z-axis.

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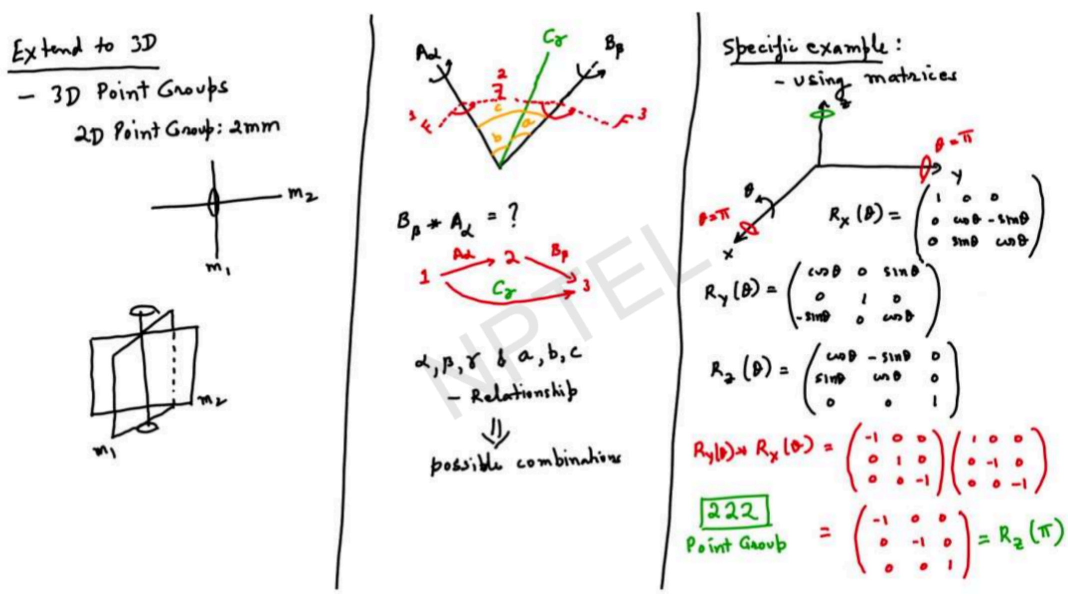

This result implies that if two twofold rotation axes are perpendicular to each other, the combined effect of 180° rotations about these axes is a 180° rotation about a third axis perpendicular to both. Consequently, when combining twofold rotation axes, all three axes must be mutually perpendicular. This leads to the three-dimensional point group

222 in which the three twofold rotation axes are orthogonal to one another. In this specific case, $\alpha = \beta = \gamma = 180^{\circ}$, and $a = b = c = 90^{\circ}$.

While all possible combinations can be determined using matrix methods, it is more instructive to seek a general solution. For this purpose, we turn to geometry rather than matrix multiplication. Our goal is to find a general relationship between the rotation angles α, β, and γ and the interaxial angles a, b, and c.

To achieve this, imagine that the three rotation axes A_{α}, B_{β}, and C_{γ} intersect at a single point, which is the center of a sphere of unit radius. Each axis intersects the surface of the sphere at a point, denoted as poles A, B, and C. Before proceeding further, we briefly digress to recall some properties of spherical geometry.

Consider a sphere and a circle drawn on its surface such that the circle has the largest possible radius. This occurs when the plane of the circle passes through the center of the sphere, for example, the equatorial plane. Such circles are known as great circles. There are infinitely many great circles on the surface of a sphere.

Given two points P and Q on the surface of a sphere, the shortest distance between them is not a straight line, but rather the arc of the great circle passing through both points. If the sphere has unit radius, this distance is equal to the angle subtended at the center of the sphere by points P and Q. Let this angle be denoted by α, so that the distance $PQ = \alpha$.

Now consider a line drawn from the center of the sphere perpendicular to the plane of the great circle containing arc PQ. This perpendicular intersects the surface of the sphere at a point, which we denote as A. If this perpendicular is treated as a rotation axis, then a rotation of angle α about this axis moves point P to point Q. The point A is therefore called the pole of the great circle containing arc PQ.

Now consider three poles A, B, and C on the surface of a unit sphere, corresponding to rotation axes OA, OB, and OC, respectively, where O denotes the center of the sphere. The shortest distances between these poles lie along arcs of great circles. Let the distance between poles B and C be denoted by a, the distance between A and C by b, and the distance between A and B by c. Since the sphere has unit radius, these distances can be treated as angular measures.

The arcs connecting A, B, and C form a spherical triangle. At each vertex of this triangle, there is an interior angle. Let the interior angles at vertices A, B, and C be denoted by A, B, and C, respectively. Thus, there are six angles in total: the side lengths a, b, and c, and the interior angles A, B, and C. These angles are related by the spherical cosine rule.

One useful form of the cosine rule for a spherical triangle is

$$\cos a = \frac{\cos A + \cos B \cos C}{\sin B \sin C},$$

with analogous expressions obtained by symmetry:

$$\cos b = \frac{\cos B + \cos C \cos A}{\sin C \sin A},$$

$$\cos c = \frac{\cos C + \cos A \cos B}{\sin A \sin B}.$$

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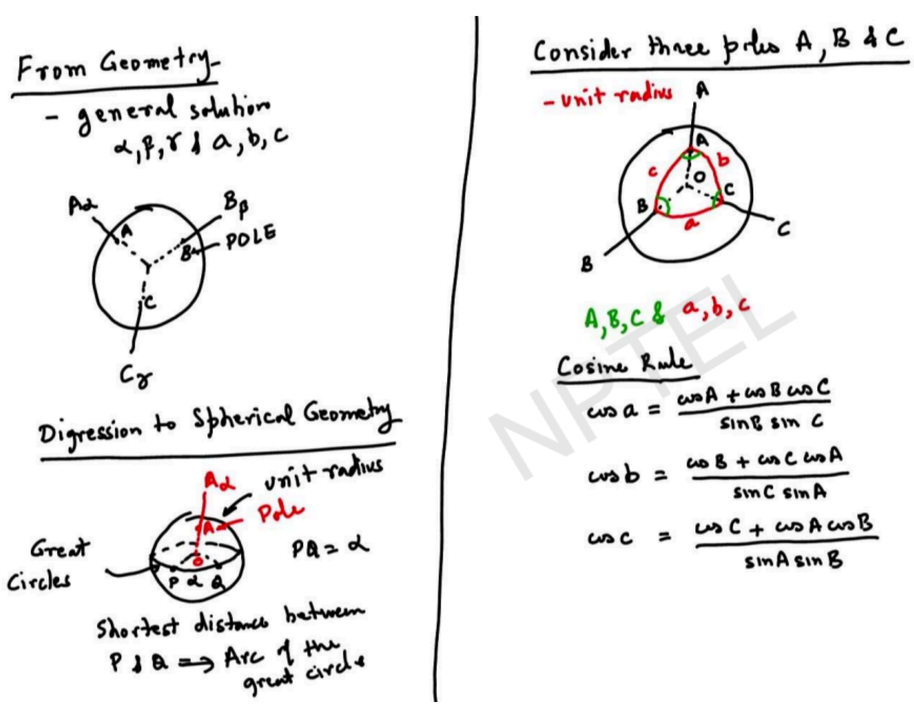

These relations provide the geometric framework required to determine the general relationship between the rotation angles α, β, and γ and the angular positions of the rotation axes a, b, and c when three rotation axes intersect at a point.

Thank you.