

CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 31: Combination of Three Rotation Axes in 3D - I

Continuing from the previous lecture, we consider the construction in which three rotation axes pass through the center of a sphere. Let us now focus on two rotation axes, denoted as A_α and B_β . For clarity, the sphere itself will not be drawn, as it would clutter the figure. One may imagine that the plane on which the construction is drawn represents a portion of the surface of the sphere.

Consider pole A , which is the point where rotation axis A intersects the surface of the sphere. Similarly, consider a second rotation axis passing through the center of the sphere and intersecting the surface at point B , which we again refer to as a pole. About pole A there is a rotation of angle α , and about pole B there is a rotation of angle β .

The poles A and B , lying on the surface of the sphere, can be joined by a great circle, which represents the shortest distance between them. Now consider the following construction. Through point A , draw another great circle that makes an angle of $\alpha/2$ with the great circle AB . Let this great circle be denoted as AX , with the angle between AX and AB equal to $\alpha/2$. If we now rotate this great circle AX by an angle α about the axis A , it moves to a new position, which we denote as AX' .

A similar construction is carried out at pole B . Through point B , draw another great circle that makes an angle of $\beta/2$ with the great circle AB , and denote this great circle as BY . The angle between BY and AB is therefore $\beta/2$. Rotating this great circle by an angle β about the axis B moves it to a new position, denoted as BY' .

From the construction, it is clear that since a rotation of β has been applied about the B axis, and the original angle was $\beta/2$, the corresponding angle on the opposite side must

also be $\beta/2$. Similarly, the angle between the great circles AX' and AB is $\alpha/2$. Let the intersection of the great circles AX' and BY be denoted by point C , and the intersection of AX and BY' be denoted by point C' .

Now consider the spherical triangles ABC and ABC' . These two triangles share a common side AB , and the angles adjacent to this side are equal, namely $\alpha/2$ at A and $\beta/2$ at B for both triangles. Thus, we have a side included between two equal angles in each case. By analogy with Euclidean geometry, the two spherical triangles ABC and ABC' are congruent. Consequently, the remaining sides and angles of the two triangles are also equal.

An important implication of this construction concerns the motion of point C . The point C moves to C' under a rotation of α about axis A , and subsequently, under a rotation of β about axis B , the point C' moves back to C . In other words, the combined operation A_α followed by B_β leaves point C invariant. Since invariant points are of particular importance in point symmetry, this implies that point C corresponds to the location of a rotation axis. Therefore, the combined operation $B_\beta * A_\alpha$ gives rise to a third rotation axis whose pole is at C . Let this third rotation axis correspond to a rotation of angle γ .

At this stage, we have identified three rotation angles α , β , and γ . While α and β are given, the value of γ is not yet known, and will be determined through further analysis. Next, consider the motion of pole A under the combined operation $B_\beta * A_\alpha$. A rotation of α about axis A leaves pole A invariant. However, a subsequent rotation of β about axis B moves the entire great circle AB to a new position, thereby moving pole A to a new location, denoted as A' . The points A' and C can then be joined by a great circle.

Now consider the spherical triangles ABC and $A'BC$. The side AB is equal to the side $A'B$, since the latter is obtained by rotating the former about axis B . The included angle at B is $\beta/2$ in both triangles, and the triangles share a common side BC . Thus, the triangles ABC and $A'BC$ are congruent. As a result, the sides AC and $A'C$ are equal, and the corresponding angles are equal. In particular, the angle at A is $\alpha/2$.

Focusing now on the angles at pole C , the angles $\angle ACB$ and $\angle A'CB$ are equal. Since C corresponds to a rotation axis, and pole A moves to pole A' under the combined operation $B_{\beta} * A_{\alpha}$, the same transformation can be represented as a single rotation of angle γ about axis C . Hence, each of the angles at C must be equal to $\gamma/2$.

We now concentrate solely on the spherical triangle ABC . The interior angles of this triangle are $\alpha/2$, $\beta/2$, and $\gamma/2$. The angular distances between the poles correspond to the angles between the rotation axes: let the distance between A and B be denoted by c , between A and C by b , and between B and C by a . These distances are precisely the angles between the rotation axes A , B , and C .

We now apply the spherical cosine rule to triangle ABC . In this notation, the interior angles are $A = \alpha/2$, $B = \beta/2$, and $C = \gamma/2$, while the side lengths are a , b , and c . The cosine rule then gives

$$\cos a = \frac{\cos A + \cos B \cos C}{\sin B \sin C} = \frac{\cos(\alpha/2) + \cos(\beta/2) \cos(\gamma/2)}{\sin(\beta/2) \sin(\gamma/2)},$$

$$\cos b = \frac{\cos B + \cos C \cos A}{\sin C \sin A} = \frac{\cos(\beta/2) + \cos(\gamma/2) \cos(\alpha/2)}{\sin(\gamma/2) \sin(\alpha/2)},$$

and

$$\cos c = \frac{\cos C + \cos A \cos B}{\sin A \sin B} = \frac{\cos(\gamma/2) + \cos(\alpha/2) \cos(\beta/2)}{\sin(\alpha/2) \sin(\beta/2)}.$$

Thus, we obtain a complete set of relationships between the interaxial angles a , b , c and the rotation angles α , β , and γ .

Before concluding the lecture, let us apply these relations to a specific case discussed earlier, namely the combination of three twofold rotation axes, corresponding to the point group 222. In this case, we have rotations of π about each axis, so that

$$\alpha = \beta = \gamma = \pi.$$

Substituting these values into the cosine-rule expressions, all terms in the numerators vanish, while the denominators evaluate to unity. Hence,

$$\cos A = \cos B = \cos C = 0,$$

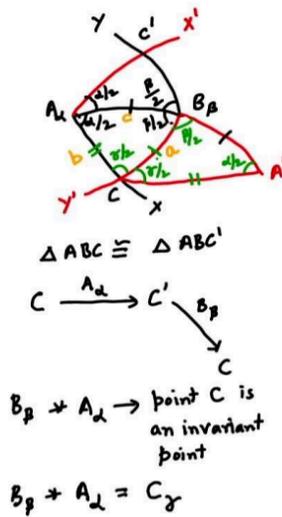
which implies

$$A = B = C = \pi/2.$$

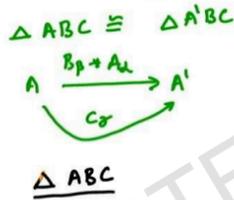
This result is identical to that obtained earlier using matrix multiplication: when three twofold rotation axes meet at a point, they must be mutually perpendicular. This is the only possible combination for three twofold rotation axes.

We now conclude this lecture. Before proceeding to the next lecture, it is instructive to consider other possible combinations of rotational symmetries. For example, one may ask what happens when a threefold axis combines with two twofold axes, or when a twofold, a threefold, and a fourfold axis are combined. One may also ask whether certain combinations are forbidden. All such results can be obtained directly from the three equations derived above. It is therefore recommended that you attempt these exercises before moving on to the next lecture, where several of these possibilities will be discussed and a complete list of allowed combinations of rotation axes will be presented. Thank you.

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Focus on pole A:
 $B_p * A_d \rightarrow$ pole A moves to A'



Cosine Rule

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

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

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

$$\cos a = \frac{\cos \frac{a}{2} + \cos \frac{b}{2} \cos \frac{c}{2}}{\sin \frac{b}{2} \sin \frac{c}{2}}$$

$$\cos b = \frac{\cos \frac{b}{2} + \cos \frac{c}{2} \cos \frac{a}{2}}{\sin \frac{c}{2} \sin \frac{a}{2}}$$

$$\cos c = \frac{\cos \frac{c}{2} + \cos \frac{a}{2} \cos \frac{b}{2}}{\sin \frac{a}{2} \sin \frac{b}{2}}$$

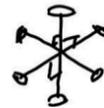
Example: 222

A_π, B_π, C_π

$$a = b = c = \pi$$

$$\cos a = \cos b = \cos c = 0$$

$$\Rightarrow a = b = c = \frac{\pi}{2}$$



\rightarrow SAME RESULT AS OBTAINED FROM MATRIX MULTIPLICATION