

CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 19: Combination of Two Mirrors

In this lecture, we will first consider the combination of two mirrors. Earlier, we examined two mirrors that were perpendicular to each other, but now we will look at how two mirrors can be combined when they meet at an arbitrary angle. Let us assume that one mirror lies in the xz plane, and another mirror intersects it at the origin, making an angle α . Let this second mirror be M_2 . We want to determine the resulting symmetry operation when the reflection σ_1 is followed by the reflection σ_2 .

$$\sigma_2 * \sigma_1 = A_{2\alpha}$$

In the previous lecture, we constructed the reflection matrices for mirrors M_1 and M_2 . For mirror M_2 , the reflection matrix is

$$\begin{bmatrix} \cos(2\alpha) & \sin(2\alpha) & 0 \\ \sin(2\alpha) & -\cos(2\alpha) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

and for mirror M_1 , the reflection σ_1 is represented by

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Here, σ_1 corresponds to a mirror in the xz plane with its normal along the y axis. Thus, the second row of the matrix carries a -1 on the diagonal, while the remaining diagonal elements are 1.

Multiplying these two matrices gives the resulting matrix

$$\begin{bmatrix} \cos(2\alpha) & -\sin(2\alpha) & 0 \\ \sin(2\alpha) & \cos(2\alpha) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

To understand this matrix, compare it with the standard rotation matrix

$$\begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

which represents a rotation about the z axis. Clearly, the resulting matrix corresponds to a rotation through an angle 2α about the z axis. Therefore, the combination of σ_1 followed by σ_2 results in a rotation $A_{2\alpha}$ at the origin.

This matrix method can also be understood geometrically. Consider two mirrors, M_1 in the xz plane and M_2 inclined at an angle α . Place an asymmetric motif and identify one point on it that makes an angle β with the origin. Reflection through mirror M_1 maps this motif to a new position with reversed handedness. Let this be motif 2, with the same angle β . This is the action of σ_1 .

Next, motif 2 reflects through mirror M_2 , producing motif 3, whose handedness is again reversed and therefore matches the handedness of motif 1. Since motifs 1 and 3 have the same handedness, the transformation from motif 1 to motif 3 must be a rotation.

To determine the rotation angle, note that the angle between motif 2 and mirror M_2 is $\alpha - \beta$, and after reflection this angle is preserved. Therefore, the total angular change required to map motif 1 to motif 3 is

$$\beta + \beta + (\alpha - \beta) + (\alpha - \beta)$$

which simplifies to 2α . This matches the result obtained through the matrix method, confirming that the combined effect of the two reflections is a rotation $A_{2\alpha}$.

Now let us move further and consider whether α can take any arbitrary value. Since we are dealing with rotational symmetry in a crystallographic context, only crystallographic rotations are allowed. Therefore, not all values of α are permissible, and restrictions must be placed on α accordingly, because only certain rotational symmetries are allowed in crystals.

If a rotation axis generates a rotation of $2\pi/n$ for an n -fold rotation, then n is restricted to the crystallographic values 1, 2, 3, 4, and 6. Consequently, the combined action of the two mirrors must satisfy the condition that

$$n \cdot 2\alpha = 2\pi$$

This immediately gives

$$\alpha = \frac{\pi}{n}$$

Thus, the angle α between the two mirrors is restricted by the allowed values of n . Listing these explicitly, for $n = 1, 2, 3, 4,$ and 6 , we obtain the corresponding values of α : for $n = 1$, $\alpha = \pi$; for $n = 2$, $\alpha = \pi/2$; for $n = 3$, $\alpha = \pi/3$; for $n = 4$, $\alpha = \pi/4$; and for $n = 6$, $\alpha = \pi/6$. These correspond to angles of $180^\circ, 90^\circ, 60^\circ, 45^\circ,$ and 30° respectively. These are the only possible angles between the two mirrors M_1 and M_2 .

We have previously seen a special case of this result: when a two-fold rotational symmetry is combined with a mirror, an additional mirror appears at 90° . Conversely, if two mirrors M_1 and M_2 are placed at 90° , a two-fold rotational symmetry necessarily appears at their intersection, corresponding to the case $n = 2$. More generally, if a reflection operation σ_1 is followed by a rotation of angle α , the resulting operation is another reflection σ_2 whose mirror lies at an angle of $\alpha/2$ with respect to the first mirror.

This can be shown through matrix multiplication. The rotation matrix for an angle α is

$$A(\alpha) = \begin{bmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

and if we place the mirror M_1 and introduce a two-fold rotational symmetry as indicated schematically in the figure, one can verify that the new mirror M_2 lies at an angle of $\alpha/2$.

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Combination of two mirrors

$\sigma_2 \circ \sigma_1 = A_{2d}$

$$\begin{pmatrix} \cos 2d & \sin 2d & 0 \\ \sin 2d & -\cos 2d & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos 2d & -\sin 2d & 0 \\ \sin 2d & \cos 2d & 0 \\ 0 & 0 & 1 \end{pmatrix} = R_z(2d)$$

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

1 Rotation \rightarrow 3

Total angle of rotation
 $= \beta + \beta + (\alpha - \beta) + (\alpha - \beta)$
 $= 2\alpha$

Not all α values allowed

- Only crystallographic rotations allowed
- rotation axis, $A_{\frac{2\pi}{n}}$ (n-fold)

$n = 1, 2, 3, 4 \text{ and } 6$

$n \times 2d = 2\pi$
 $\Rightarrow \boxed{\alpha = \pi/n}$

n	1	2	3	4	6
α	π	$\frac{\pi}{2}$	$\frac{\pi}{3}$	$\frac{\pi}{4}$	$\frac{\pi}{6}$
	180°	90°	60°	45°	30°

Conversely

$A_\alpha \circ \sigma_1$

$\rightarrow \sigma_2$ at an angle of $\alpha/2$

Before proceeding to derive all the two-dimensional point groups, it is useful to recall a few properties of rotation and reflection matrices. For a rotation matrix $A(\alpha)$, the determinant is always + 1, consistent with our assumption of a right-handed coordinate system. Moreover, the inverse of a rotation matrix equals its transpose, so that

$$A(\alpha)^{-1}A(\alpha) = A(\alpha)^T A(\alpha) = I$$

In contrast, the determinant of any reflection matrix is - 1

And a reflection matrix is equal to its own inverse, meaning

$$\sigma^{-1}\sigma = I$$

These properties are straightforward but important when working with symmetry operations.

With these preliminaries complete, we are now ready to construct all the possible two-dimensional point groups, which we will begin developing in the next lecture.

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Properties of rotation/reflection matrices (Right Handed Coord. System)

* A_d : $\text{Det}(A_d) = +1$
 $A_d^{-1} = A_d^T$
 $A_d^{-1} \cdot A_d = A_d^T \cdot A_d = \text{Identity Matrix}$

* σ : $\text{Det}(\sigma) = -1$
 $\sigma^{-1} = \sigma$
 $\Rightarrow \sigma^{-1} \cdot \sigma = \text{Identity Matrix}$

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