CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 18: Matrix Representations of Reflection Operation

This lecture focuses on representing reflection symmetry using matrices. We begin by considering the reflection matrix. First, imagine a mirror plane and draw the coordinate axes. The x and y axes lie in the mirror plane, while the z axis is normal to it. Take any point (x, y, z) and reflect it through the horizontal mirror plane; it will be mapped below the mirror or below the xy-plane. The reflected point becomes $(x, y, -z)$, where the negative z coordinate is indicated using a bar notation.

If the mirror is the xy-plane, the reflection operation is denoted by σ_{xy}, indicating that the mirror lies in the xy-plane. The corresponding matrix is

$$\sigma_{xy} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$$

Multiplying this matrix by the column vector (x, y, z) gives $(x, y, -z)$, exactly as expected.

If the mirror instead lies in the yz-plane, then the x-axis is normal to the mirror. The matrix for σ_{yz} becomes

$$\sigma_{yz} = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Similarly, if the mirror lies in the xz-plane, meaning the y-axis is normal to the mirror, the matrix becomes

$$\sigma_{xz} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

We now consider a more general mirror. Draw the x-axis, y-axis, and the z-axis normal to the xy-plane. Suppose the mirror makes an angle α with the x-axis. When a point (x, y) is reflected across this mirror, it moves to (x', y'). To determine the reflection matrix, we proceed as follows. First, rotate the coordinate system by $-\alpha$ so that the mirror coincides with the xz-plane, making the y-axis normal to the mirror. This rotation is represented by $R_z(-\alpha)$. Next, apply the reflection σ_{xz}, and finally rotate back by $+\alpha$ using $R_z(\alpha)$. The complete operation is therefore

$$R = R_z(\alpha)\,\sigma_{xz}\,R_z(-\alpha).$$

Write the matrices explicitly. The rotation $R_z(\alpha)$ is $\begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$. The reflection σ_{xz} is $\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$. For $R_z(-\alpha)$ substitute $-\alpha$ into the rotation formula, giving $\begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$.

$$R = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Multiply the last two matrices first. Multiplying $R_z(-\alpha)$ by σ_{xz} yields a matrix whose first row becomes $(\cos\alpha, \sin\alpha, 0)$ and second row becomes $(\sin\alpha, -\cos\alpha, 0)$, with the third row unchanged as $(0, 0, 1)$. Copy $R_z(\alpha)$ next to it and perform the final multiplication. For the first element of the resulting matrix, multiply the first row of the left matrix with the first column of the right matrix: $cos\alpha cos\alpha - sin\alpha sin\alpha = cos^2\alpha - sin^2\alpha = cos2\alpha$. Similarly, the first row and second column produce $sin2\alpha$, while the first row and third column produce 0. Continuing the multiplication for the second row yields $(sin2\alpha, - cos2\alpha, 0)$, and the third row remains $(0, 0, 1)$.

Thus, the reflection matrix for the general mirror is $\begin{pmatrix} \cos 2\alpha & \sin 2\alpha & 0 \\ \sin 2\alpha & -\cos 2\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$. Multiplying this matrix by (x, y, z) gives the reflected point (x', y', z) because the mirror lies in the plane containing x' and y' while leaving z unchanged.

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos 2\alpha & \sin 2\alpha & 0 \\ \sin 2\alpha & -\cos 2\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

In subsequent lectures, combinations of mirror operations, and combinations of mirrors with rotations, will be used to derive all two-dimensional point groups.

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