Diffractometer Geometry: Problems 1 and 2

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Equipment Overview

A piece of mechanical equipment consists of two independent stacks of rotary stages. All rotational axes coincide ideally at a single point of intersection, at which the object to be examined is mounted.

Reference Frame

We define a right-handed coordinate system with basis vectors assigned as follows:

$$\begin{aligned}
\hat{x} &= \text{longitudinal (toward equipment, our line of sight)} \\
\hat{y} &= \text{lateral (to our left)} \\
\hat{z} &= \text{vertical (normal to the floor, pointing upward)}
\end{aligned}$$

This satisfies the right-hand rule: $\hat{x} \times \hat{y} = \hat{z}$.

Equipment Description

The equipment consists of two independent stacks of rotary stages. In the default orientation (all angles at 0°), the stacks are described as follows.

Stack 1 — Detector Stack

- **S1-1**: rotation axis in the vertical direction ($+\hat{z}$). Sign of rotation consistent with the coordinate system (right-hand rule about $+\hat{z}$).
- **S1-2**: sits on S1-1. Rotation axis in the lateral direction ($+\hat{y}$). Positive rotation takes $+\hat{x}$ toward $+\hat{z}$. The detector is mounted on a radial arm on S1-2, directed toward the point of intersection.

Stack 2 — Sample Stack

- **S2-1**: rotation axis in the vertical direction ($+\hat{z}$). Axis is colinear with S1-1; the two stages are mechanically independent. Sign of rotation consistent with the coordinate system.
- **S2-2**: sits on S2-1. Rotation axis in the lateral direction ($+\hat{y}$). Same sign of rotation as S1-2.
- **S2-3**: sits on S2-2. Rotation axis in the longitudinal direction ($+\hat{x}$). Sign of rotation consistent with the coordinate system (right-hand rule about $+\hat{x}$).
- **S2-4**: sits on S2-3. Rotation axis in the vertical direction ($+\hat{z}$). Sign of rotation consistent with the coordinate system.

Problem 1

Basis Vector Assignment

We assign basis vectors to the reference frame as follows:

$$\begin{aligned}\hat{x} &= \text{longitudinal}\\ \hat{y} &= \text{lateral}\\ \hat{z} &= \text{vertical}\end{aligned}$$

Right-handedness is confirmed by $\hat{x} \times \hat{y} = \hat{z}$.

Stage Orientations and Sign of Rotation

The sign of rotation follows the right-hand rule: the thumb points along the positive axis vector and the fingers curl in the direction of positive rotation.

Stack 1 — Detector Stack

Stage	Physical Axis	Axis Vector	Positive Rotation
S1-1	vertical	$+\hat{z}$	CCW viewed from $+\hat{z}$
S1-2	lateral	$+\hat{y}$	$+\hat{x}$ toward $+\hat{z}$

The detector is mounted on a radial arm on S1-2, directed inward toward the sample point.

Stack 2 — Sample Stack

Stage	Physical Axis	Axis Vector	Positive Rotation
S2-1	vertical	$+\hat{z}$	CCW viewed from $+\hat{z}$
S2-2	lateral	$+\hat{y}$	$+\hat{x}$ toward $+\hat{z}$
S2-3	longitudinal	$+\hat{x}$	$+\hat{y}$ toward $+\hat{z}$
S2-4	vertical	$+\hat{z}$	CCW viewed from $+\hat{z}$

S2-1 and S1-1 share the same axis of rotation but are mechanically independent.

Computing the Orientation Matrix U

Step 1 — Define the lab frame. The lab frame is fixed with basis $\{\hat{x}, \hat{y}, \hat{z}\}$ as assigned above.

Step 2 — Rotation matrix for each stage. Each stage i with unit rotation axis $\hat{n}_i$ and rotation angle θ_i contributes a rotation matrix $\mathbf{R}_i(\theta_i)$ via the Rodrigues formula:

$$\mathbf{R}_i(\theta_i) = \mathbf{I}\cos\theta_i + (1-\cos\theta_i)\,(\hat{n}_i \otimes \hat{n}_i) + \sin\theta_i\,[\hat{n}_i]_\times \tag{1}$$

where $[\hat{n}]_\times$ is the skew-symmetric cross-product matrix:

$$[\hat{n}]_\times = \begin{pmatrix} 0 & -n_z & n_y \\ n_z & 0 & -n_x \\ -n_y & n_x & 0 \end{pmatrix} \tag{2}$$

Step 3 — Compose the sample stack rotations. The total rotation applied to the sample is the ordered product of stage matrices, from outermost (floor) to innermost (top):

$$\mathbf{R}_{\text{sample}} = \mathbf{R}_{\text{S2-1}}(\theta_1)\,\mathbf{R}_{\text{S2-2}}(\theta_2)\,\mathbf{R}_{\text{S2-3}}(\theta_3)\,\mathbf{R}_{\text{S2-4}}(\theta_4) \tag{3}$$

The order is significant: each stage rotates everything mounted above it.

Step 4 — Define U. The orientation matrix $\mathbf{U}$ maps a reference vector $\mathbf{h}$ expressed in the crystal (sample) frame to its direction in the lab frame:

$$\mathbf{h}_{\text{lab}} = \mathbf{R}_{\text{sample}}\,\mathbf{U}\,\mathbf{h}_{\text{crystal}} \tag{4}$$

Given two non-parallel reference vectors measured at known stage angles, $\mathbf{U}$ is determined by:

$$\mathbf{U} = \mathbf{R}_{\text{sample}}^{-1}\,\mathbf{M}_{\text{lab}}\,\mathbf{M}_{\text{crystal}}^{-1} \tag{5}$$

where the columns of $\mathbf{M}_{\text{lab}}$ and $\mathbf{M}_{\text{crystal}}$ are the reference vectors in the lab and crystal frames respectively, with the third column taken as the cross product of the first two to complete the basis.

Problem 2

Are Different Basis Assignments Possible?

Yes. The assignment of $\{\hat{x}, \hat{y}, \hat{z}\}$ to the three physical directions was a choice, not a necessity. Any right-handed assignment is valid. For three physical directions there are **6 possible right-handed assignments**:

Assignment	$\hat{x}$	$\hat{y}$	$\hat{z}$
1 (chosen)	longitudinal	lateral	vertical
2	lateral	vertical	longitudinal
3	vertical	longitudinal	lateral
4	lateral	longitudinal	vertical
5	longitudinal	vertical	lateral
6	vertical	lateral	longitudinal

Assignments 1–3 are cyclic (even) permutations of (longitudinal, lateral, vertical); assignments 4–6 are anti-cyclic (odd) permutations. Both sets are right-handed.

Stage Axis Vectors Under Each Assignment

The physical rotation axes are unchanged; only their coordinate expression varies.

Stage	Physical Axis	A1	A2	A3	A4	A5	A6
S1-1	vertical	$+\hat{z}$	$+\hat{x}$	$+\hat{y}$	$+\hat{z}$	$+\hat{y}$	$+\hat{x}$
S1-2	lateral	$+\hat{y}$	$+\hat{z}$	$+\hat{x}$	$+\hat{x}$	$+\hat{z}$	$+\hat{y}$
S2-1	vertical	$+\hat{z}$	$+\hat{x}$	$+\hat{y}$	$+\hat{z}$	$+\hat{y}$	$+\hat{x}$
S2-2	lateral	$+\hat{y}$	$+\hat{z}$	$+\hat{x}$	$+\hat{x}$	$+\hat{z}$	$+\hat{y}$
S2-3	longitudinal	$+\hat{x}$	$+\hat{y}$	$+\hat{z}$	$+\hat{y}$	$+\hat{x}$	$+\hat{z}$
S2-4	vertical	$+\hat{z}$	$+\hat{x}$	$+\hat{y}$	$+\hat{z}$	$+\hat{y}$	$+\hat{x}$

Effect on U

The matrix $\mathbf{U}$ does not change physically — it encodes the same geometric relationship regardless of basis choice. What changes is its numerical representation.

Let $\mathbf{P}$ be the 3×3 orthogonal permutation matrix that transforms coordinates from one basis assignment to another, satisfying $\mathbf{P}^{-1} = \mathbf{P}^{\top}$. Then the orientation matrix under the new assignment is:

$$\mathbf{U}' = \mathbf{P}\,\mathbf{U}\,\mathbf{P}^{\top} \tag{6}$$

This is a similarity transformation, which preserves:

- The eigenvalues of $\mathbf{U}$ (same rotation angles),

- $\det(\mathbf{U}') = \det(\mathbf{U}) = +1$ (proper rotation),
- The physical meaning of the orientation.

Only the numerical entries of $\mathbf{U}$ differ between assignments. The choice of basis is purely a convention.