NANO106 Handout 6 - Determining Symmetry Matrices

Shyue Ping Ong
University of California, San Diego
9500 Gilman Drive, Mail Code 0448, La Jolla, CA 92093-0448

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1 Introduction

This document outlines how you determine crystal summary matrices. Two fairly complicated examples are provided to demonstrate the procedure in addition to the lecture slides.

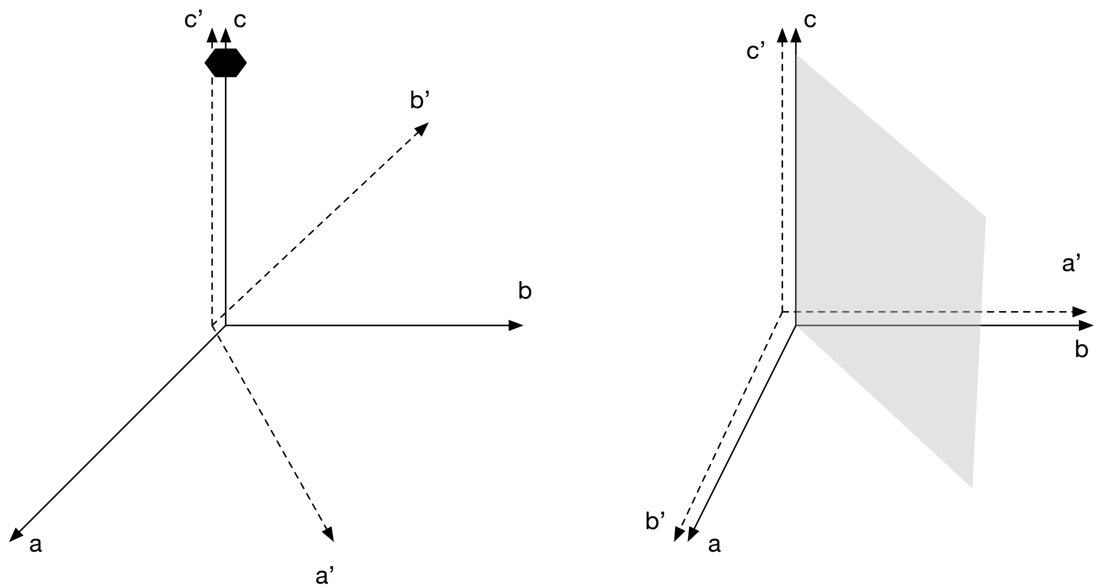
Let us first outline the general procedure.

1. Find an appropriate crystal system for the symmetry operation. This is typically indicated. Otherwise, you should use the more convenient lattice compatible with that symmetry. E.g., for 4-fold or 6-fold rotations, you use a tetragonal or hexagonal cell.
2. Align the crystal to the appropriate symmetry positions. Sometimes this is also specifically spelled out.
3. "Inspect" how your crystal axes transform under the symmetry operation, i.e., just imagine performing the operation on the crystal axes.
4. Express the new lattice vectors in terms of your old lattice vectors.
5. Determine the transformation matrix C that relates your new lattice vectors to your old ones.
6. The transpose of the transformation matrix is your crystal symmetry matrix.

2 Example 1: Six-fold rotation in hexagonal crystal

Consider the symmetry operation as shown in Figure (i) above. Let us now follow the steps. Steps 1 and 2 are already done.

Step 3: Figure (i) shows the effect of the symmetry operation on the lattice vectors.



(i) Six-fold rotation about c-axis in hexagonal crystal (e.g., like the ones in the 6 or 6mm point group)

(ii) Diagonal vertical mirror plane in tetragonal crystal (e.g., like the ones in the 4mm point group)

Figure 1: Symmetry operations on crystal axes

Step 4: The new lattice vectors can be expressed in terms of the old lattice vectors as:

$$\mathbf{a}' = \mathbf{a} + \mathbf{b}$$

$$\mathbf{b}' = -\mathbf{a}$$

$$\mathbf{c}' = \mathbf{c}$$

Step 5: We may express the above relationships as the following matrix operation.

$$\begin{pmatrix} \mathbf{a}' \\ \mathbf{b}' \\ \mathbf{c}' \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix}$$

Step 6: Taking the transpose of the transformation matrix, we have the rotation matrix as:

$$D(6) = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

3 Example 2: Diagonal vertical mirror plane in tetragonal crystal

Consider the symmetry operation as shown in Figure (ii) above. Let us now follow the steps. Steps 1 and 2 are already done.

Step 3: Figure (ii) shows the effect of the symmetry operation on the lattice vectors.

Step 4: The new lattice vectors can be expressed in terms of the old lattice vectors as:

$$\mathbf{a}' = \mathbf{b}$$

$$\mathbf{b}' = \mathbf{a}$$

$$\mathbf{c}' = \mathbf{c}$$

Step 5: We may express the above relationships as the following matrix operation.

$$\begin{pmatrix} \mathbf{a}' \\ \mathbf{b}' \\ \mathbf{c}' \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{pmatrix}$$

Step 6: Taking the transpose of the transformation matrix, we have the rotation matrix as:

$$D(m_diagonal) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$