Conversion of Orientation Matrices

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Orientation Matirx

Definition and Applying

This section describes how to apply the orientation matrices. It includes their definitions and justifications for the way in which they are used. The key, is to remember that the components of a vector refer to its representation (or frame). The vector is not actually rotated, only the representation in different frames will change. In this viewpoint, the rotation matrix associated with a grain is just a new coordinate system used to describe the same direction. The lab or sample frame is the base orientation, and it is described by three orthonormal vectors, $\hat{x}$, $\hat{y}$, and $\hat{z}$. which are

$$\hat{x} = \hat{x}_L = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \hat{y} = \hat{y}_L = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \text{ and } \hat{z} = \hat{z}_L = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{1}$$

Likewise, orientation A is described by three perpendicular unit vectors $\hat{H}_A$, $\hat{K}_A$, and $\hat{L}_A$ which point in the direction of $(hkl) = (100)$, (010), and (001) for the A orientation.

Consider the orientation matrix A which is defined as,

$$\mathsf{A} = \begin{pmatrix} H_{xA} & H_{yA} & H_{zA} \\ K_{xA} & K_{yA} & K_{zA} \\ L_{xA} & L_{yA} & L_{zA} \end{pmatrix}. \tag{2}$$

Where $\hat{H}_A = H_{xA}\hat{x} + H_{yA}\hat{y} + H_{zA}\hat{z}$ is a vector in the direction of the H axis for frame A, and there are two similar equation for $\hat{K}_A$ and $\hat{L}_A$. To understand how to use these matrices to transform between coordinate systems, consider the general vector $\vec{V}$. Note that $\vec{V}$ is just a vector; it has only one direction, although its representation may vary from frame to frame. The components of $\vec{V}$ in the lab frame are:

$$\begin{array}{rcll} \vec{V} \cdot \hat{x}_L & = & V_{Lx} & \text{component along } \hat{x} \text{ direction} \\ \vec{V} \cdot \hat{y}_L & = & V_{Ly} & \text{component along } \hat{y} \text{ direction} \\ \vec{V} \cdot \hat{z}_L & = & V_{Lz} & \text{component along } \hat{z} \text{ direction.} \end{array} \tag{3}$$

Similarly in frame A, the components of $\vec{V}$ are:

$$\begin{array}{rcll} \vec{V} \cdot \hat{H}_A & = & V_{AH} & \text{component along } \hat{H}_A \text{ direction} \\ \vec{V} \cdot \hat{K}_A & = & V_{AK} & \text{component along } \hat{K}_A \text{ direction} \\ \vec{V} \cdot \hat{L}_A & = & V_{AL} & \text{component along } \hat{L}_A \text{ direction.} \end{array} \tag{4}$$

This can be written more compactly using matrix notation as,

$$\mathsf{A}\vec{V}_L = \begin{pmatrix} H_{xA} & H_{yA} & H_{zA} \\ K_{xA} & K_{yA} & K_{zA} \\ L_{xA} & L_{yA} & L_{zA} \end{pmatrix} \times \begin{pmatrix} V_{Ax} \\ V_{Ay} \\ V_{Az} \end{pmatrix} = \begin{pmatrix} \vec{H}_A \cdot \vec{V}_L \\ \vec{K}_A \cdot \vec{V}_L \\ \vec{L}_A \cdot \vec{V}_L \end{pmatrix} = \begin{pmatrix} V_{AH} \\ V_{AK} \\ V_{AL} \end{pmatrix} = \vec{V}_A \tag{5}$$

where the subscripts L and A indicate that components refer to the lab and A frames respectively. $\vec{V} = V_{Lx}\hat{x} + V_{Ly}\hat{y} + V_{Lz}\hat{z} = V_{AH}\hat{H}_A + V_{AK}\hat{K}_A + V_{AL}\hat{L}_A$. In the above equation, the matrix A

transforms from (xyz) in the lab frame to (hkl) in frame A, the matrix $\mathsf{A}^{-1}(=\mathsf{A}^{\mathsf{T}})$ can transform in the other direction, from (hkl) in frame A to (xyz) in the lab frame.

$$\mathsf{A}^{-1} \times \begin{pmatrix} h \\ k \\ l \end{pmatrix} = \begin{pmatrix} H_{xA} & K_{xA} & L_{xA} \\ H_{yA} & K_{yA} & L_{yA} \\ H_{zA} & K_{zA} & L_{zA} \end{pmatrix} \times \begin{pmatrix} h \\ k \\ l \end{pmatrix} = \begin{pmatrix} hH_{xA} + kK_{xA} + lL_{xA} \\ hH_{yA} + kK_{yA} + lL_{yA} \\ hH_{zA} + kK_{zA} + lL_{zA} \end{pmatrix} \tag{6}$$

The first component of this vector is simply the amount in the $\hat{x}$ direction which is $\hat{x}\cdot(h\hat{H}+k\hat{K}+l\hat{L})$, and likewise $\hat{y}\cdot(h\hat{H}+k\hat{K}+l\hat{L})$ in the $\hat{y}$ direction and $\hat{z}\cdot(h\hat{H}+k\hat{K}+l\hat{L})$ in the $\hat{z}$ direction.

Equation (5) defines a transform from the lab frame to frame A as, $\mathsf{A}\vec{V}_L = \vec{A}$. Likewise there will be a similar transform for another grain B.

$$\begin{array}{lll} \mathsf{A}\vec{V}_L = \vec{V}_A & \text{or} & \mathsf{A}^{-1}\vec{V}_A = \vec{V}_L \ \text{ and} \\ \mathsf{B}\vec{V}_L = \vec{V}_B & \text{or} & \mathsf{B}^{-1}\vec{V}_B = \vec{V}_L \end{array} \tag{7}$$

Equating $\vec{V}_L$ for the two grains give the transform from grain A to B,

$$\mathsf{B}\mathsf{A}^{-1}\vec{V}_A = \vec{V}_L. \tag{8}$$

Cubic Symmetry Operations

For cubic materials, it is necessary to deal with the ambiguity arising from the 24 indistinguishable orientations that a cubic grain may assume. The cubic symmetry operations may be described by a set of 24 proper rotations $\{\mathsf{S}^i\}$. These correspond to 4-fold $(\pm 90^\circ, 180^\circ)$ rotations about the $\{100, 010, 001\}$, 3-fold $(\pm 120^\circ)$ rotations about the $\{111, \bar{1}11, 1\bar{1}1, 1\bar{1}\bar{1}\}$, 2-fold (180°) rotations about the $\{011, 101, \bar{1}01, 0\bar{1}1, 110, 1\bar{1}0\}$, and the identity matrix. In a simple unrotated frame, the S^i take on the simple forms expected for these rotations, *i.e.*, a 90° rotation about $\hat{z}$ is

$$\mathsf{S} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

As an example pre-multiply A by this S,

$$\mathsf{SA} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \times \begin{pmatrix} H_{xA} & H_{yA} & H_{zA} \\ K_{xA} & K_{yA} & K_{zA} \\ L_{xA} & L_{yA} & L_{zA} \end{pmatrix} = \begin{pmatrix} K_{xA} & K_{yA} & K_{zA} \\ -H_{xA} & -H_{yA} & -H_{zA} \\ L_{xA} & L_{yA} & L_{zA} \end{pmatrix} \equiv \begin{pmatrix} \hat{K}_A \\ -\hat{H}_A \\ \hat{L}_A \end{pmatrix}.$$

Which can be restated as the simple relation

$$\mathsf{S} \times \mathsf{A} = \mathsf{S} \times \begin{pmatrix} \hat{H}_A \\ \hat{K}_A \\ \hat{L}_A \end{pmatrix} = \begin{pmatrix} \hat{K}_A \\ -\hat{H}_A \\ \hat{L}_A \end{pmatrix}.$$

This is just a 90° rotation about the $\hat{L}_A$ axis. Since we see that pre-multiplying A (or B) by S^i gives the transformed A^i. Starting with equation (8) we can substitute any of the cubic symmetry equivalent A^i for A to get

$$\begin{array}{rcl} \mathsf{B}(\mathsf{A}^i)^{-1}\vec{V}_A & = & \vec{V}_L \\ \mathsf{B}(\mathsf{S}^i\mathsf{A})^{-1}\vec{V}_A & = & \vec{V}_L \\ (\mathsf{B}\mathsf{A}^{-1}\mathsf{S}^i)\vec{V}_A & = & \vec{V}_L \end{array} \tag{9}$$

Where we have made use of the fact that the set of operators $\{\mathsf{S}^i\}$ is closed, so $\{\mathsf{S}^i\}$ contains an inverse for each of its elements. The criterion for choosing the appropriate i is to minimize the total rotation angle between frames A and B. This is simply done because the total rotation angle θ is obtained from

$$\mathrm{Tr}(\mathsf{B}\mathsf{A}^{-1}\mathsf{S}^i) = 1 + 2\cos(\theta). \tag{10}$$

Then choose the i that maximizes $\mathrm{Tr}(\mathsf{B}\mathsf{A}^{-1}\mathsf{S}^i)$.

Lines in Data File

In each line of the "save ori" file as of February 11, 2005, the first 3 values are the X, Y, and Z positions of the voxel in the beam line coordinate system (defined below). The next 9 values describe the orientation matrix (*i.e.* the matrices A, B, ...). If columns 4-12 are $c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8, c_9$, then the matrix A is

$$\mathsf{A} = \begin{pmatrix} H_{xA} & H_{yA} & H_{zA} \\ K_{xA} & K_{yA} & K_{zA} \\ L_{xA} & L_{yA} & L_{zA} \end{pmatrix} = \begin{pmatrix} c_1 & c_2 & c_3 \\ c_4 & c_5 & c_6 \\ c_7 & c_8 & c_9 \end{pmatrix}. \tag{11}$$

The next 3 values, columns 13-15, contain the direction of the Rodrigues vector, and the final column contains the total rotation angle.

Beam Line and Sample Coordinates

The last issue has to do with describing how this fits in with the beam line and sample coordinate systems. In the data file the first three columns are X, Y, Z. These refer to the beam line coordinates ($\hat{Z}$ along x-rays, $\hat{Y}$ up, and $\hat{X}$ out the door). The PM500 sample translation stage frame is in (X H F) coordinates, where $\hat{X}$ is out the door, $\hat{F}$ is down away from the telescope, and $\hat{H}$ is up and down stream at 45°). $F = (Z - Y)/\sqrt{2}$, and $H = (Z + Y)/\sqrt{2}$. The sample frame (referred to as the lab frame above) is just the PM500 frame rotated about the X axis, so that $\hat{y} = -\hat{H}$ and $\hat{z} = -\hat{F}$.

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -\sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}} \\ 0 & \sqrt{\frac{1}{2}} & -\sqrt{\frac{1}{2}} \end{pmatrix} \begin{pmatrix} \hat{X} \\ \hat{Y} \\ \hat{Z} \end{pmatrix} = \begin{pmatrix} \hat{X} \\ -\sqrt{\frac{1}{2}}\hat{Y} - \sqrt{\frac{1}{2}}\hat{Z} \\ +\sqrt{\frac{1}{2}}\hat{Y} - \sqrt{\frac{1}{2}}\hat{Z} \end{pmatrix} = \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix}. \tag{12}$$

where $(\hat{x}\hat{y}\hat{z})$ is the coordinate system used by the orientation matrices above, and referred to as the sample or lab frame. In the lab frame, $\hat{z}$ is the outward pointing surface normal of the sample, $\hat{x}$ is out the door, and $\hat{y}$ points upstream and down at 45°.

It is important to keep the sample and beam line coordinate systems straight when obtaining crystallographic information about a grain boundary. The boundary normal will be in the beam line system $(\hat{X}\hat{Y}\hat{Z})$, since it is derived from the voxel positions. However the identification of the hkl of a surface will be in the sample frame $(\hat{x}\hat{y}\hat{z})$, since that is the system used by the orientation matrices. So use equation (12) to convert to the same frame before comparing directions.

The 24 Cubic Symmetry operations

These are the 24 proper rotations, and so contain no mirror planes, for the full 48 cubic symmetry operations, simply include -1 times each of this matrices.

$$\mathsf{S}^1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ Identitymatrix}$$

$$\mathsf{S}^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \quad 90^\circ \text{ rotation about the } \quad (1,0,0)$$

$$\mathsf{S}^3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad 180^\circ \text{ rotation about the } \quad (1,0,0)$$

$$\mathsf{S}^4 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad 90^\circ \text{ rotation about the } \quad (-1,0,0)$$

$$\mathsf{S}^5 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad 90^\circ \text{ rotation about the } \quad (0,1,0)$$

$$\mathsf{S}^6 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad 180^\circ \text{ rotation about the } \quad (0,1,0)$$

$$\mathsf{S}^7 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad 90^\circ \text{ rotation about the } \quad (0,-1,0)$$

$$\mathsf{S}^8 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad 90^\circ \text{ rotation about the } \quad (0,0,1)$$

$$\mathsf{S}^9 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad 180^\circ \text{ rotation about the } \quad (0,0,1)$$

$$\mathsf{S}^{10} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad 90^\circ \text{ rotation about the } \quad (0,0,-1)$$

$$\mathsf{S}^{11} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \quad 120^\circ \text{ rotation about the } \quad (1,1,1)$$

$$\mathsf{S}^{12} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad 120^\circ \text{ rotation about the } \quad (-1,-1,-1)$$

$$\mathsf{S}^{13} = \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad 120^\circ \text{ rotation about the } \quad (-1,1,1)$$

$$\mathsf{S}^{14} = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix} \quad 120^\circ \text{ rotation about the } \quad (1,-1,-1)$$

$$\mathsf{S}^{15} = \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \quad 120^\circ \text{ rotation about the } \quad (1,-1,1)$$

$$\mathsf{S}^{16} = \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix} \quad 120^\circ \text{ rotation about the } \quad (-1,1,-1)$$

$$\mathsf{S}^{17} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix} \quad 120^\circ \text{ rotation about the } \quad (-1,-1,1)$$

$$\mathsf{S}^{18} = \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \quad 120^\circ \text{ rotation about the } \quad (1,1,-1)$$

$$\mathsf{S}^{19} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad 180^\circ \text{ rotation about the } \quad (1,0,1)$$

$$\mathsf{S}^{20} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad 180^\circ \text{ rotation about the } \quad (0,1,1)$$

$$\mathsf{S}^{21} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \quad 180^\circ \text{ rotation about the } \quad (-1,0,1)$$

$$\mathsf{S}^{22} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \quad 180^\circ \text{ rotation about the } \quad (0,-1,1)$$

$$\mathsf{S}^{23} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad 180^\circ \text{ rotation about the } \quad (1,1,0)$$

$$\mathsf{S}^{24} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad 180^\circ \text{ rotation about the } \quad (1,1,0)$$