TRANSFORMATION OF AXES

W. L. Bond,
Bell Telephone Laboratories,
Murray Hill, New Jersey.

In choosing axes for a crystal often the first selection is later found to be unsatisfactory and a new set must be chosen. For example, the first chosen cell may turn out to be larger than necessary and simplification will follow adoption of the smaller cell. In dealing with the most general crystal system—the triclinic—it becomes obvious that the crystal axes **a b c** are not the axes of immediate reference. *X*-ray measurements determine d_{001} for example, not c, and the relation between d_{001} and c is not simple. An optical goniometer measures the angle between normals to the faces (001) and (100) which is not β nor related simply to β. Both these types of measurements are related simply to a set of axes which are perpendicular to the cell faces—the so called reciprocal cell axes. We find that, in dealing with triclinic crystals we must have two systems of axes, the direct system and the reciprocal system. This dual axial system is a great convenience in computations for all crystal systems. Hence we seek ways of converting information gathered and expressed in one system into its proper expression in another system.

On a set of axes, **a, b, c** called the a basis we define a new set **a′, b′, c′** called the a' basis by means of the vector expressions:

$$\left.\begin{aligned}\mathbf{a}' &= \Phi_{11}\mathbf{a}+\Phi_{21}\mathbf{b}+\Phi_{31}\mathbf{c}\\ \mathbf{b}' &= \Phi_{12}\mathbf{a}+\Phi_{22}\mathbf{b}+\Phi_{32}\mathbf{c}\\ \mathbf{c}' &= \Phi_{13}\mathbf{a}+\Phi_{23}\mathbf{b}+\Phi_{33}\mathbf{c}\end{aligned}\right\}. \tag{1}$$

A vector **V** can be written on the a' basis as

$$(\mathbf{V})_{a'} = V_1'\mathbf{a}'+V_2'\mathbf{b}'+V_3'\mathbf{c}'. \tag{2}$$

We can convert this back to the a basis by substituting for **a′, b′** and **c′** their equivalents on the a basis (eq. (1)):

$$\begin{aligned}(\mathbf{V})_a = {} & V_1'(\Phi_{11}\mathbf{a}+\Phi_{21}\mathbf{b}+\Phi_{31}\mathbf{c})\\ & +V_2'(\Phi_{12}\mathbf{a}+\Phi_{22}\mathbf{b}+\Phi_{32}\mathbf{c})\\ & +V_3'(\Phi_{13}\mathbf{a}+\Phi_{23}\mathbf{b}+\Phi_{33}\mathbf{c})\end{aligned}$$

which can be rearranged as:

$$\begin{aligned}(\mathbf{V})_a = {} & (\Phi_{11}V_1'+\Phi_{12}V_2'+\Phi_{13}V_3')\mathbf{a}\\ & +(\Phi_{21}V_1'+\Phi_{22}V_2'+\Phi_{23}V_3')\mathbf{b}\\ & +(\Phi_{31}V_1'+\Phi_{32}V_2'+\Phi_{33}V_3')\mathbf{c}\end{aligned} \tag{3}$$

Let us adopt a short hand notation. The vector $(\mathbf{V})_{a'} = V_1'\mathbf{a}'+V_2'\mathbf{b}'+V_3'\mathbf{c}'$ will be written

$\begin{pmatrix} V_1' \\ V_2' \\ V_3' \end{pmatrix}_{a'}$. In this notation $(\mathbf{V})_a = \begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix}_a$. But by eq. (3) this is

$$\begin{pmatrix} \Phi_{11}V_1' + \Phi_{12}V_2' + \Phi_{13}B_3' \\ \Phi_{21}V_1' + \Phi_{22}V_2' + \Phi_{23}V_3' \\ \Phi_{31}V_1' + \Phi_{32}V_2' + \Phi_{33}V_3' \end{pmatrix}_a .$$

The last array can be obtained by a purely mechanical manipulation of the arrays $\Phi = \begin{pmatrix} \Phi_{11}\Phi_{12}\Phi_{13} \\ \Phi_{21}\Phi_{22}\Phi_{23} \\ \Phi_{31}\Phi_{32}\Phi_{33} \end{pmatrix}$ and $(\mathbf{V})_{a'} = \begin{pmatrix} V_1' \\ V_2' \\ V_3' \end{pmatrix}_{a'}$. We write

$$(\mathbf{V})_a = \Phi(\mathbf{V})_{a'} \tag{4}$$

which is equivalent to:

$$\begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix}_a = \begin{pmatrix} \Phi_{11}\Phi_{12}\Phi_{13} \\ \Phi_{21}\Phi_{22}\Phi_{23} \\ \Phi_{31}\Phi_{32}\Phi_{33} \end{pmatrix} \begin{pmatrix} V_1' \\ V_2' \\ V_3' \end{pmatrix}_{a'} = \begin{pmatrix} \Phi_{11}V_1' + \Phi_{12}V_2' + \Phi_{13}V_3' \\ \Phi_{21}V_1' + \Phi_{22}V_2' + \Phi_{23}V_3' \\ \Phi_{31}V_1' + \Phi_{32}V_2' + \Phi_{33}V_3' \end{pmatrix}_a . \tag{4'}$$

The first term of the resultant vector is formed by the first row of the prefactor (Φ in this case) and the first column of the post factor ($\mathbf{V}'$, which has but one column, in this case). This first term of the resultant vector is the sum of the products taken in order. Likewise the second term of the resultant is formed from the second row of the prefactor and the first column of the post factor, similarly for the third term of the resultant, as can be seen by studying eq. (4'). If the post factor had more than one column we could consider each column as a separate vector, and get a resultant with the same number of columns as has the post factor. This manipulation is "matrix multiplication." It is merely a mechanical method of handling equations.

As an example we take:

$$\mathbf{a}' = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}_a , \mathbf{b}' = \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix}_a , \mathbf{c}' = \begin{pmatrix} 0 \\ -1/2 \\ 1/2 \end{pmatrix}_a$$

what does a vector $\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}_{a'}$ become on the a basis? By eq. (4)

$$(\mathbf{V})_a = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & -1/2 \\ 0 & 1/2 & 1/2 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}_{a'} = \begin{pmatrix} 1 \\ -1/2 \\ 5/2 \end{pmatrix}_a .$$

We now examine the converse case, that is, convert a given $(\mathbf{V})_a$ to the a' basis. We imagine a matrix Φ^{-1} such that multiplying equation (4) through by Φ^{-1} as a prefactor we get $\Phi^{-1}(\mathbf{V})_a = \Phi^{-1}\Phi(\mathbf{V})_{a'} = (\mathbf{V})_{a'}$. Our problem now is to find such a matrix. We can solve eq. (1) by determinants and find $\mathbf{a}, \mathbf{b}, \mathbf{c}$, in terms of $\mathbf{a}', \mathbf{b}'$, and $\mathbf{c}'$. In terms of the new functions of the Φ_{ij}'s we could now go through the previous analysis and

reach the answer. The actions necessary to solve this problem by determinants can be made into a mechanical manipulation.

By the determinant of a square matrix Φ we mean the same array of values but considered as a determinant instead of as a matrix, it is commonly written $|\Phi|$; when we mean the value of the determinant rather than the array we will use Δ, By the $(_{ij})$ minor of the determinant we mean the determinant left after striking out the ith row and jth column. For example the (21) minor of $|\Phi|$ is:

$$\Delta_{ij}=\begin{vmatrix}\Phi_{12} & \Phi_{13}\\ \Phi_{32} & \Phi_{33}\end{vmatrix}.$$

A determinant of but four terms can be immediately evaluated as the major diagonal product less the other diagonal product:

$$\Delta_{21}=\begin{vmatrix}\Phi_{12} & \Phi_{13}\\ \Phi_{32} & \Phi_{33}\end{vmatrix}=\Phi_{12}\Phi_{33}-\Phi_{32}\Phi_{13}.$$

The 9 term determinant can be evaluated in terms of the minors of any row or column. For example to develop the determinant of Φ in terms of the minors of the first row:

$$\Delta=\Phi_{11}\Delta_{11}-\Phi_{12}\Delta_{12}+\Phi_{13}\Delta_{13}.$$

The expression for development in terms of any other row or column is obvious, except for the matter of signs. The signs must be taken from the scheme $\begin{vmatrix}+&-&+\\ -&+&-\\ +&-&+\end{vmatrix}$ which gives to each ij minor the sign $(-1)^{i+j}$.

We define the "transposed" matrix $\bar{\Phi}$ which is merely Φ with columns written as rows and rows as columns.*

$$\bar{\Phi}=\begin{pmatrix}\Phi_{11}\Phi_{21}\Phi_{31}\\ \Phi_{12}\Phi_{22}\Phi_{32}\\ \Phi_{13}\Phi_{23}\Phi_{33}\end{pmatrix}. \tag{5}$$

If Δ is the value of the determinant of Φ in these terms we have:

$$\overline{(\Phi^{-1})}=\frac{1}{\Delta}\begin{pmatrix}\Delta_{11}(-1)^{1+1} & \Delta_{12}(-1)^{1+2} & \Delta_{13}(-1)^{1+1}\\ \Delta_{21}(-1)^{1+2} & \Delta_{22}(-1)^{2+2} & \Delta_{23}(-1)^{2+2}\\ \Delta_{31}(-1)^{1+3} & \Delta_{32}(-1)^{3+2} & \Delta_{33}(-1)^{3+3}\end{pmatrix}.$$

Since $\overline{(\Phi^{-1})}=(\bar{\Phi})^{-1}$ we can omit the parentheses and immediately write Φ^{-1} from (5). As an example, for $\Phi=\begin{pmatrix}1 & 0 & 0\\ 0 & 1/2 & -1/2\\ 0 & 1/2 & 1/2\end{pmatrix}$. $\Delta=1/2$ (Δ is the relative cell size. If Δ is negative one system is right handed, the other left handed.)

* This transposed matrix is identical to Barker's matrix:

$$uvw/u'v'w'/u''v''w''=\begin{pmatrix}u & v & w\\ u' & v' & w'\\ u'' & v'' & u''\end{pmatrix}$$

$$\bar{\Phi}^{-1}=2\begin{pmatrix}1/2 & 0 & 0\\ 0 & 1/2 & -1/2\\ 0 & 1/2 & 1/2\end{pmatrix}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & -1\\ 0 & 1 & 1\end{pmatrix} \text{ or } \Phi^{-1}=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 1\\ 0 & -1 & 1\end{pmatrix}.$$

In terms of our new matrix Φ^{-1} we now write

$$(\mathbf{V})_{a'}=\Phi^{-1}(\mathbf{V})_a. \tag{6}$$

Now Φ^{-1} is so related to Φ that $\Phi\Phi^{-1}=\Phi^{-1}\Phi=I$, where I is a matrix with ones on the major diagonal and zeros everywhere else:

$$I=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}.$$

In multiplying one square matrix by another we can consider the second one as three single column matrices (vectors) and multiply them out to give three vectors (single column matrices) which are written side by side in proper order. This array is then considered to be the resultant matrix. Trial proves that $VI=IV=V$ hence we can consider eq. (6) as derived from eq. (4) by multiplying eq. (4) through by the prefactor Φ^{-1}.

It is a fact that only square matrices have reciprocals and that not every square matrix has a reciprocal.

As an example of the use of a reciprocal matrix we solve for the components of $\begin{pmatrix}1\\ -1/2\\ 5/2\end{pmatrix}_a$ when written on the a' basis. By eq. (6);

$$(\mathbf{V})_{a'}=\Phi^{-1}(\mathbf{V})_a=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 1\\ 0 & -1 & 1\end{pmatrix}\begin{pmatrix}1\\ -1/2\\ 5/2\end{pmatrix}_a=\begin{pmatrix}1\\ 2\\ 3\end{pmatrix}_{a'}.$$

We notice in this equation that the three columns of Φ^{-1} are the components of **a, b,** and **c** respectively on the a' basis. If we call $(\mathbf{V})_a$ the "combined vector," since it is multiplied by the matrix prefactor Φ^{-1}, and $(\mathbf{V})_{a'}$ the "uncombined vector," since it is multiplied by no matrix prefactor; we can write this observation in the form of the following transformation theorem which is a useful memory aid for vector transformation equations.

Transformation Theorem.

In a vector transformation equation the three columns of the matrix prefactor are the components of the three base vectors of the "combined vector" on the reference system of the "uncombined vector."

Applying this memory aid to Eq. (4), that is to the converse relation $(\mathbf{V})_a=\Phi(\mathbf{V})_{a'}$ we would say that the three columns of Φ are the three components of the a' base vectors on the a basis. This is actually the case.

Vector Products: By definition the vector product of two vectors **r** and **s** is a vector, perpendicular to both **r** and **s** and of length $rs \sin(\mathbf{rs})$. It is

apparent that it is the area of a parallelogram defined by $\mathbf{r}$ and $\mathbf{s}$, hence its vector nature. It is an absolute quantity, independent of the basis on which it is expressed. From its definition we see that $\mathbf{r}\times\mathbf{s}=-\mathbf{s}\times\mathbf{r}$ and that $\mathbf{r}\times\mathbf{r}=0$. The cross $\times$ earmarks this product as a vector product to distinguish it from other kinds of products.

If we express both $\mathbf{r}$ and $\mathbf{s}$ on the a basis, then write the vector product, $\mathbf{r}\times\mathbf{s}$ we have:

$$\mathbf{s}=s_1\mathbf{a}+s_2\mathbf{b}+s_3\mathbf{c}$$
$$\mathbf{r}=r_1\mathbf{a}+r_2\mathbf{b}+r_3\mathbf{c}$$
$$\mathbf{r}\times\mathbf{s}=(r_2s_3-r_3s_2)\mathbf{b}\times\mathbf{c}+(r_3s_1-r_1s_3)\mathbf{c}\times\mathbf{a}+(r_1s_2-r_2s_1)\mathbf{a}\times\mathbf{b}.$$

This is in terms of three new vectors, each of which is perpendicular to a pair of the original set. We define these new ones as $u\mathbf{A}=\mathbf{b}\times\mathbf{c}$, $u\mathbf{B}=\mathbf{c}\times\mathbf{a}$, $u\mathbf{C}=\mathbf{a}\times\mathbf{b}$. We call this new set the A basis and say that it is a set reciprocal to the set a.

In terms of these new base vectors we may write a vector product mechanically by writing each vector twice in one column, striking out the top and bottom member and "cross multiplying" as:

$$(\mathbf{r})_a\times(\mathbf{s})_a=\begin{array}{cc} r_1 & s_1 \\ \hline r_2 & s_2 \\ r_3 & s_3 \\ r_1 & s_1 \\ r_2 & s_2 \\ \hline r_3 & s_3 \end{array}=u\begin{bmatrix} r_2s_3-r_3s_2 \\ r_3s_1-r_1s_3 \\ r_1s_2-r_2s_1 \end{bmatrix}_A. \tag{7}$$

Since A is perpendicular to $\mathbf{b}$ and $\mathbf{c}$, and $\mathbf{B}$ is perpendicular to $\mathbf{c}$ and $\mathbf{a}$, then $\mathbf{c}$ is perpendicular to $\mathbf{A}$ and $\mathbf{B}$. Similarly $\mathbf{a}$ is perpendicular to $\mathbf{B}$ and $\mathbf{C}$, and $\mathbf{b}$ to $\mathbf{C}$ and $\mathbf{A}$. Hence, if the $\mathbf{A}$ basis is reciprocal to the a basis, then the a basis can be made reciprocal to the A basis and the reciprocity is mutual. We can hence form vector products of two vectors written on the A basis and get an answer written on the a basis but involving an as yet undetermined scalar constant U'.

Plane Normals: A plane (hkl) has axial intercepts $\mathbf{a}/h$, $\mathbf{b}/k$, $\mathbf{c}/l$. A vector $(-\mathbf{a}/h+\mathbf{b}/k)\times(-\mathbf{a}/h+\mathbf{c}/l)$ is perpendicular to this plane. Expanding the cross product we have:

$$\mathbf{N}_{hkl}=\frac{\mathbf{b}\times\mathbf{c}}{kl}+\frac{\mathbf{c}\times\mathbf{a}}{lh}+\frac{\mathbf{a}\times\mathbf{b}}{hk}.$$

If we multiply through by the scalar hkl/u and substitute $\mathbf{A}$ for $l/u\mathbf{b}\times\mathbf{c}$, $\mathbf{B}$ for $l/u\mathbf{c}\times\mathbf{a}$, $\mathbf{C}$ for $l/u\mathbf{a}\times\mathbf{b}$ we have, as a normal to the plane (hkl)

$$\mathbf{N}_{hkl}=\begin{pmatrix} h \\ k \\ l \end{pmatrix}_A. \tag{8}$$

That is, a line from the origin to the point $\begin{pmatrix} h \\ k \\ l \end{pmatrix}_A$ is perpendicular to the plane (hkl).

Scalar Products: By definition, the scalar product $\mathbf{r}\cdot\mathbf{s}$ of two vectors $\mathbf{r}$ and $\mathbf{s}$ is a scalar of magnitude $rs\cos(\mathbf{rs})$. It is an absolute quantity, independent of the basis on which it is written. It is the length of one of the vectors multiplied by the component of the other vector on the first. It is earmarked by the dot to distinguish it from the vector product.

The Scalar Triple Product: Combining the definition of vector product and scalar product we have the scalar triple product of three vector **r, s,** and **t** as $\mathbf{r}\times\mathbf{s}\cdot\mathbf{t}$. (The cross product is to be taken first.) It is easily seen to be the volume of the parallelepiped defined by **r, s** and **t**. It is also an absolute quantity, independent of the basis on which it is written.

The scalar product can be formed rather simply by mixing the bases, since **A** is perpendicular to **b** and **c** it has no component on them similarly for **B** and **C**, hence we find:

$$\mathbf{r}=r_1\mathbf{a}+r_2\mathbf{b}+r_3\mathbf{c}$$
$$\mathbf{S}=S_1\mathbf{A}+S_2\mathbf{B}+S_3\mathbf{C}$$
$$\mathbf{r}\cdot\mathbf{S}=r_1S_1\mathbf{a}\cdot\mathbf{A}+r_2S_2\mathbf{b}\cdot\mathbf{B}+r_3S_3\mathbf{c}\cdot\mathbf{C}$$

substituting $\frac{\mathbf{b}\times\mathbf{c}}{u}$ for $\mathbf{A}$, $\frac{\mathbf{c}\times\mathbf{a}}{u}$ for $\mathbf{B}$ and $\frac{\mathbf{a}\times\mathbf{b}}{u}$ for $\mathbf{C}$ we have:

$$\mathbf{r}\cdot\mathbf{S}=(r_1S_1+r_2S_2+r_3S_3)\ \frac{\mathbf{a}\cdot\mathbf{b}\times\mathbf{c}}{u}\ .$$

Hence if we take u equal to the volume of the unit cell:

$$u=\mathbf{a}\times\mathbf{b}\cdot\mathbf{c}\cdots \tag{9}$$

We can simplify the expression of the scalar product to any one of the following:

$$\begin{aligned}(\mathbf{r})_a\cdot(\mathbf{S})_A&=(\mathbf{R})_A\cdot(\mathbf{s})_a=r_1S_1+r_2S_2+r_3S_3,\ \text{a scalar}\\&=R_1s_1+R_2s_2+R_3s_3\\&=(\bar{\mathbf{R}})_A(\mathbf{s})_a=(\bar{\mathbf{s}})_a(\mathbf{R})_A=(\bar{\mathbf{r}})_a(\mathbf{S})_A=(\bar{\mathbf{S}})_A(\mathbf{r})_a.\end{aligned} \tag{10}$$

If the a basis has a reciprocal basis A, the a' basis must have a reciprocal basis A′. The scalar product of two vectors is an absolute quantity, independent of the basis of expression. Hence $(\bar{\mathbf{S}})_A(\mathbf{r})_a-(\bar{\mathbf{S}})_A\Phi(\mathbf{r})_{a'}$ since $(\mathbf{V})_a=\Phi(\mathbf{V})_{a'}$.

Here $(\bar{\mathbf{S}})_A\Phi$ must equal $(\bar{\mathbf{S}})_{A'}$ whence

$$(\mathbf{V})_{A'}=\bar{\Phi}(\mathrm{V})_A. \tag{11}$$

Conversely

$$(\mathbf{V})_A=\bar{\Phi}^{-1}(\mathbf{V})_{A'}. \tag{11'}$$

We see then that the columns of $\bar{\Phi}$ are the A base vectors expressed on the A' basis and that the columns of $\bar{\Phi}^{-1}$ are the A' base vectors expressed on the A basis.

Transformation of Plane Indices: By eq. 8, a plane of indices (hkl) has a normal $\begin{pmatrix} h \\ k \\ l \end{pmatrix}_A$ and conversely, a line $\begin{pmatrix} h \\ k \\ l \end{pmatrix}_A$ defines a plane (hkl). Hence by eq. (11) a transformation from the basis a to the basis a' by means of $(\mathbf{V})_a = \Phi(\mathbf{V})_{a'}$ implies a transformation from indices (hkl) to $(h'k'l')$ where

$$(h'k'l') = (hkl)\Phi. \tag{12}$$

For example, using the previous value of Φ, a plane $(111)_a$ becomes, on the a' basis:

$$(hkl)_{a'} = (111)_a \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & -1/2 \\ 0 & 1/2 & 1/2 \end{pmatrix} = (110)_{a'} .$$

Zonal Relations: Since the plane (hkl) has a normal $\mathbf{N} = \begin{pmatrix} h \\ k \\ l \end{pmatrix}_A$ and the plane $(h'k'l')$ has a normal $\mathbf{N}' = \begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_A$ the line that is common to both planes is perpendicular to both normals. It is given by the vector product $\mathbf{N} \times \mathbf{N}'$. Since cross multipying of two vectors in the reciprocal system gives the resultant vector in the direct system, we see that the vector $\mathbf{Z} = \begin{pmatrix} kl' - k'l \\ lh' - l'h \\ hk' - h'k \end{pmatrix}_a$ lies in both planes and is hence their intersection. $\mathbf{Z}$ is called the zone axis. It is generally given as a *zone symbol* $[uvw]$ in square brackets and if u, v, w have a common factor it is divided out. It is emphasized that the zone symbol gives the components on the a basis of a line parallel to all planes belonging to that zone.

Any plane $(h''k''l'')$ belonging to the zone Z has its normal perpendicular to the vector Z. Hence the scalar product must vanish, and by eq. (10) we have the zonal equation:

$$(uvw)_a \begin{pmatrix} h \\ k \\ l \end{pmatrix}_A = uh + vk + wl = 0 . \tag{13}$$

Rectangular Axes: We now introduce a special set of rectangular axes, **xyz**. They are of unit length, mutually perpendicular and chosen so that **z** lies along **c** and **x** lies in the plane of **a** and **c**. We have a transformation which changes vectors from one basis to the other as:

$$(\mathbf{V})_x = \mathrm{m}(\mathbf{V})_a \tag{14}$$

and conversely

$$(\mathbf{V})_a = \mathrm{m}^{-1}(\mathbf{V})_x \tag{14'}$$

where by the transformation theorem:

$$\mathrm{m}=\begin{vmatrix} a\sin\beta & \mathrm{v}_1 b & 0 \\ 0 & \mathrm{v}_2 b & 0 \\ a\cos\beta & b\cos\alpha & c \end{vmatrix}, \qquad \mathrm{m}^{-1}=\begin{vmatrix} \dfrac{1}{a\sin\beta} & \dfrac{-\mathrm{v}_1}{a\mathrm{v}_2\sin\beta} & 0 \\ 0 & 1/(\mathrm{v}_2 b) & 0 \\ \dfrac{-1}{c\tan\beta} & \dfrac{\mathrm{v}_1\cot\beta-\cos\alpha}{\mathrm{v}_2 c} & 1/c \end{vmatrix}.$$

Here we do not assume that b is necessarily unity. If we are interested in x-ray problems we use the true translations a_0, b_0, c_0 as in eq. (18″). If we are interested only in interfacial angles, etc., we can use the axial ratio values with $b=1$ in which case m becomes M. Since **x**, **y** and **z** are mutually perpendicular and of unit length the volume of this cell is unity and the x basis is self reciprocal. Since the columns of m are the components of **a**, **b** and **c** on the x basis, we can write the scalar product of **a** and **b** as: $\mathbf{a}\cdot\mathbf{b}=ab\cos\gamma=ab\,\mathrm{v}_1\sin\beta+\mathrm{ab}\cos\alpha\cos\beta$

whence

$$v_1=\frac{\cos\gamma-\cos\alpha\cos\beta}{\sin\beta}$$

as $v_1^2b^2+v_2^2b^2+b^2\cos^2\alpha=\mathrm{b}^2$ we find that:

$$v_2=\frac{\sqrt{1+2\cos\alpha\cos\beta\cos\gamma-(\cos^2\alpha+\cos^2\beta+\cos^2\gamma)}}{\sin\beta}. \tag{15}$$

As

$$\begin{aligned} &(\mathbf{V})_{a'}=\Phi^{-1}(\mathbf{V})_a \quad \text{and} \quad (\mathbf{V})_a=\mathrm{m}^{-1}(\mathbf{V})_x \quad \text{then} \\ &(\mathbf{V})_{a'}=\Phi^{-1}\mathrm{m}^{-1}(\mathbf{V})_x \quad \text{and conversely} \\ &(\mathbf{V})_x=\mathrm{m}\Phi(\mathbf{V})_{a'}. \end{aligned} \tag{16}$$

Derivation of New Crystallographic Data: On the a' basis, $\mathbf{a}'=\begin{pmatrix}1\\0\\0\end{pmatrix}_{a'}$, whence we can compute its components on the x basis by (16). Its true length is the square root of the sum of the squares of its components on the x basis. Similarly we compute $\mathbf{b}'$ and $\mathbf{c}'$ and can then find a new axial ratio $a':b':c'$.

Having computed $(\mathbf{a}')_x$ and $(\mathbf{b}')_x$ we normalize* them and take their scalar product. This is $\cos\gamma'$. Similarly for α' and β'.

As an example we consider a monoclinic crystal for which $a:b:c=1.6:1:1.5$, $\beta=95°$. This was found to be body centered when indexed on this cell. A transformation $\phi=\begin{pmatrix}1&0&0\\0&1&0\\-1&0&1\end{pmatrix}$ is used to give a base centered cell. We wish to find the new $a:b:c$ ratio and the new β angle. Since

* Normalizing is reducing a vector to unit length by dividing each component by the true length of the vector.

$$\mathrm{M}=\begin{pmatrix} 1.5939 & 0 & 0 \\ 0 & 1 & 0 \\ -.1395 & 0 & 1.5 \end{pmatrix}, (\mathbf{a}')_{\mathbf{x}}=\mathrm{M}\Phi\begin{pmatrix}1\\0\\0\end{pmatrix}=\begin{pmatrix}1.5939\\0\\-1.6395\end{pmatrix}_{\mathbf{x}},$$

$$(\mathbf{b}')_{\mathbf{x}}=\mathrm{m}\Phi\begin{pmatrix}0\\1\\0\end{pmatrix}=\begin{pmatrix}0\\1\\0\end{pmatrix}_{\mathbf{x}}, (\mathbf{c}')_{\mathbf{x}}=\mathrm{m}\Phi\begin{pmatrix}0\\0\\1\end{pmatrix}=\begin{pmatrix}0\\0\\1.5\end{pmatrix}.$$

This new a axis has a length $a'=\sqrt{1.5939^2+1.6395^2}=2.2866$, while $b'=1.00$ and $c'=1.500$. Hence $a:b:c=2.2866:1:1.500$. Also since $(a')_{\mathbf{x}}$ and $(c')_{\mathbf{x}}$ normalize to

$$\begin{pmatrix}.69706\\0\\-.71700\end{pmatrix}_{\mathbf{x}} \text{ and } \begin{pmatrix}0\\0\\1\end{pmatrix} \text{ respectively } \mathbf{a}\cdot\mathbf{c}=-.717, =\cos\beta', \text{ whence } \beta'=135°49'.$$

Just as the transformation from the a basis to the a' basis by means of $(\mathbf{V})_{a'}=\Phi^{-1}(\mathbf{V})_a$ leads to the transformation from the A basis to the A' basis by means of $(\mathbf{V})_{A'}=\bar{\Phi}(\mathbf{V})_A$ so the transformation from the a basis to the x basis by means of $(\mathbf{V})_{\mathbf{x}}=\mathrm{m}(\mathbf{V})_a$ leads to the transformation from the A basis to the x basis by means of:

$$(\mathbf{V})_{\mathbf{x}}=\bar{\mathrm{m}}^{-1}(\mathbf{V})_A \tag{17}$$

(because the x basis is self reciprocal). We can now write an equation relating the A basis directly to the a basis by combining (14) and (17):

$$(\mathbf{V})_a=\mathrm{m}^{-1}\bar{\mathrm{m}}^{-1}(\mathbf{V})_A \tag{18}$$

and conversely:

$$(\mathbf{V})_A=\bar{\mathrm{m}}\mathrm{m}(\mathbf{V})_a. \tag{18'}$$

On expanding (18') we find:

$$(\mathbf{V})_{A0}=\begin{pmatrix} a_0^2 & a_0b_0\cos\gamma & a_0c_0\cos\beta \\ a_0b_0\cos\gamma & b_0^2 & b_0c_0\cos\alpha \\ a_0c_0\cos\beta & b_0c_0\cos\alpha & c_0^2 \end{pmatrix}(\mathbf{V})_a. \tag{18''}$$

Here we have used the true translation vectors $\mathbf{a}_0$, $\mathbf{b}_0$, $\mathbf{c}_0$ in order to derive the standard equations (21) and (22). The subscript zero of A_0 indicates the fact that this basis is reciprocal to the a_0 basis instead of the a basis. Actually just as $\mathbf{a}_0$ is $\mathbf{b}_0$ times as long as is $\mathbf{a}$ so A_0 is $1/b_0$ times as long as is $\mathbf{A}$. If the axial angles of the reciprocal system are α^*, β^* and γ^* an expression similar to eq. (18') must hold.

$$(\mathrm{V})_a=\begin{pmatrix} \mathrm{A}_0^2 & \mathrm{A}_0\mathrm{B}_0\cos\gamma^* & \mathrm{A}_0\mathrm{C}_0\cos\beta^* \\ \mathrm{A}_0\mathrm{B}_0\cos\gamma^* & \mathrm{B}_0^2 & \mathrm{B}_0\mathrm{C}_0\cos\alpha^* \\ \mathrm{A}_0\mathrm{C}_0\cos\beta^* & \mathrm{B}_0\mathrm{C}_0\cos\alpha^* & \mathrm{C}_0^2 \end{pmatrix}(\mathrm{V})_{\mathrm{A}}. \tag{19}$$

Hence the 3×3 matrix in equation (18'') must be identical to the reciprocal of the 3×3 matrix in eq. (19). This reciprocal is:

$$u=\frac{1}{V_2^2 \sin^2\gamma^*}\begin{vmatrix} \frac{1}{A_0^2}\sin^2\alpha^* & \frac{1}{A_0B_0}(\cos\alpha^*\cos\beta^*-\cos\gamma^*) & \frac{1}{A_0C_0}(\cos\gamma^*\cos\alpha^*-\cos\beta^*) \\ \frac{1}{A_0B_0}(\cos\alpha^*\cos\beta^*-\cos\gamma^*) & \frac{1}{B_0^2}\sin^2\beta^* & \frac{1}{B_0C_0}(\cos\beta^*\cos\gamma^*-\cos\alpha^*) \\ \frac{1}{A_0C_0}(\cos\gamma^*\cos\alpha^*-\cos\beta^*) & \frac{1}{B_0C_0}(\cos\beta^*\cos\gamma^*-\cos\alpha^*) & \frac{1}{C_0^2}\sin^2\gamma^* \end{vmatrix}$$

where $$V_2=\frac{\sqrt{1+2\cos\alpha^*\cos\beta^*\cos\gamma^*-(\cos^2\alpha^*+\cos^2\beta^*+\cos^2\gamma^*)}}{\sin\gamma^*}. \tag{20}$$

Equating corresponding major diagonal terms of (18″) and u:

$$\left.\begin{aligned} a_0^2&=\frac{\sin^2\alpha^*}{V_2^2A_0^2} \\ b_0^2&=\frac{\sin^2\beta^*}{V_2^2B_0^2} \\ c_0^2&=\frac{\sin^2\gamma^*}{V_2^2C_0^2}. \end{aligned}\right\} \tag{21}$$

Equating the other corresponding terms and making use of eqs. (21) we obtain

$$\left.\begin{aligned} \cos\alpha&=\frac{\cos\beta^*\cos\gamma^*-\cos\alpha^*}{\sin\beta^*\sin\gamma^*} \\ \cos\beta&=\frac{\cos\gamma^*\cos\alpha^*-\cos\beta^*}{\sin\gamma^*\sin\alpha^*} \\ \cos\gamma&=\frac{\cos\alpha^*\cos\beta^*-\cos\gamma^*}{\sin\alpha^*\sin\beta^*} \end{aligned}\right\}. \tag{22}$$

If the unstarred terms become starred and the starred terms lose their stars the resulting equations are also true.

The Reciprocal Lattice: The volume of the tetrahedron defined by the vectors $\mathbf{a}/h$, $\mathbf{b}/k$, $\mathbf{c}/l$ is alternatively:

$$\text{Vol}=\frac{1}{6}\,\frac{\mathbf{a}}{h}\times\frac{\mathbf{b}}{k}\cdot\frac{\mathbf{c}}{l} \quad\text{and}\quad \text{Vol}=\frac{1}{6}\,d_{hkl}\times\left(\frac{\mathbf{a}}{h}-\frac{\mathbf{b}}{k}\right)\cdot\left(\frac{\mathbf{a}}{h}-\frac{\mathbf{c}}{l}\right)$$

where $\mathbf{d}_{hkl}$ is the perpendicular from the origin to the plane (hkl). Equating these values of the volume and simplifying we have:

$$\mathbf{d}_{hkl}\cdot\begin{pmatrix}\mathrm{h}\\ \mathrm{k}\\ \mathrm{l}\end{pmatrix}_{A_0}=1. \tag{23}$$

Since d_{hkl} and $\begin{pmatrix}h\\ k\\ l\end{pmatrix}_{A_0}$ are both perpendicular to the plane (hkl) we may write their absolute values:

$$\left|\frac{1}{d_{hkl}}\right|=\left|\begin{pmatrix}h\\ k\\ l\end{pmatrix}_{A_0}\right|. \tag{24}$$

Hence we see that the space lattice formed from the base vectors $\mathbf{A}_0$, $\mathbf{B}_0$ and $\mathbf{C}_0$ by giving h, k and l all integral values is not only a three dimensional plot of the normals of all planes (hkl) but is also a three dimensional plot of the reciprocals of distances between atomic planes. It is called a reciprocal lattice.

Since the absolute value of $\mathrm{m}=\begin{pmatrix}h\\k\\l\end{pmatrix}_{A_0}$ is the square root of the sum of the squares of its components on the x basis and this, by Eq. (17) is: $\bar{\mathrm{m}}^{-1}\begin{pmatrix}h\\k\\l\end{pmatrix}$ we can use the $\bar{\mathrm{m}}^{-1}$ matrix as a means of computing interplanar spacings. This is especially convenient for triclinic crystals.

Formally.
$$\frac{1}{d_{hkl}}=\sqrt{\mathrm{D}_1^2+\mathrm{D}_2^2+\mathrm{D}_3^2} \tag{25}$$

where
$$\begin{pmatrix}\mathrm{D}_1\\\mathrm{D}_2\\\mathrm{D}_3\end{pmatrix}=\bar{\mathrm{m}}^{-1}\begin{pmatrix}h\\k\\l\end{pmatrix}. \tag{26}$$

By means of the transformation theorem we can set up the $\bar{\mathrm{m}}^{-1}$ matrix in terms of reciprocal cell constants. By Eq. (17), the columns of $\bar{\mathrm{m}}^{-1}$ must be the vectors $\mathbf{A}_0$, $\mathbf{B}_0$, $\mathbf{C}_0$, on the x basis. Hence
$$\mathrm{m}^{-1}=\begin{pmatrix}\mathrm{A}_0\sin\gamma^* & 0 & \mathrm{C}_0\mathrm{V}_1\\ \mathrm{A}_0\cos\gamma^* & \mathrm{B}_0 & \mathrm{C}_0\cos\alpha^*\\ 0 & 0 & \mathrm{C}_0\mathrm{V}_2\end{pmatrix} \tag{27}$$

where
$$\mathrm{V}_1=\frac{\cos\beta^*-\cos\alpha^*\cos\gamma^*}{\sin\gamma^*} \tag{28}$$

and V_2 is given by Eq. (20).
Applying the above we see that, indeed
$$\mathrm{A}_0=\frac{1}{d_{100}},\qquad \mathrm{B}_0=\frac{1}{d_{010}},\qquad \mathrm{C}_0=\frac{1}{d_{001}}.$$

Hence we can evaluate the constants of (27) by x-ray measurements alone since:
$$\cos\alpha^*=\frac{d_{010}d_{001}}{2}\left(\frac{1}{d_{011}^2}-\frac{1}{d_{010}^2}-\frac{1}{d_{001}^2}\right)=\frac{-d_{010}d_{001}}{2}\left(\frac{1}{d_{01\bar{1}}^2}-\frac{1}{d_{010}^2}-\frac{1}{d_{001}^2}\right),$$
$$\cos\beta^*=\frac{d_{001}d_{100}}{2}\left(\frac{1}{d_{101}^2}-\frac{1}{d_{100}^2}-\frac{1}{d_{001}^2}\right)=\frac{-d_{001}d_{100}}{2}\left(\frac{1}{d_{10\bar{1}}^2}-\frac{1}{d_{100}^2}-\frac{1}{d_{001}^2}\right)$$
and finally
$$\cos\gamma^*=\frac{d_{100}d_{010}}{2}\left(\frac{1}{d_{110}^2}-\frac{1}{d_{100}^2}-\frac{1}{d_{010}^2}\right)=\frac{-d_{100}d_{010}}{2}\left(\frac{1}{d_{1\bar{1}0}^2}-\frac{1}{d_{100}^2}-\frac{1}{d_{010}^2}\right). \tag{29}$$

As an example let us assume that

$$d_{110}=5.000, \qquad d_{010}=6.667, \qquad d_{001}=4.000$$

$$d_{011}=3.091, \qquad d_{101}=2.889, \qquad d_{110}=4.178.$$

From this data, Eqs. (29) give $\alpha^*=74°49'$, $\beta^*=80°2'$, $\gamma^*=85°1'$. Also $V_1=0.1510$, $V_2=0.9532$. So that:

$$\bar{m}^{-1}=\begin{pmatrix} .1992 & 0 & .0378 \\ .0174 & .1500 & .0655 \\ 0 & 0 & .2383 \end{pmatrix}.$$

From this matrix we can compute the d spacing and vector normal of any plane. Let us do this for the plane $(12\bar{3})$.

Here
$$D=\bar{m}^{-1}\begin{pmatrix} 1 \\ 2 \\ -3 \end{pmatrix}=\begin{pmatrix} .0858 \\ .1209 \\ -.7149 \end{pmatrix}.$$

So that

$$\frac{1}{d_{12\bar{3}}}=\sqrt{.0858^2+.1209^2+.7149^2}=.7301$$

whence $d_{123}=1.370$. Finally the unit normal of the plane $(12\bar{3})$ is

$$1.370\begin{pmatrix} .0858 \\ .1209 \\ -.7149 \end{pmatrix}=\begin{pmatrix} .1175 \\ .1655 \\ -.9792 \end{pmatrix},$$

that is, the factor that normalizes the vector perpendicular of the face (hkl) on the x basis is d_{hkl}.

Summary

1. $(\mathbf{V})_a=\Phi(\mathbf{V})_{a'}$ transforms vectors $(\mathbf{V})_{a'}$ on the a' basis to the proper expression on the a basis. Here the columns of Φ are the a' base vectors expressed on the a basis.

2. $(\mathbf{V})_{a'}=\Phi^{-1}(\mathbf{V})_a$ transforms $\mathbf{V}$ from the a basis to the a' basis, the columns of Φ^{-1} are the a base vectors written on the a' basis.

3. The vector product of two vectors $\mathbf{r}$ and $\mathbf{s}$ written in the same system is expressed on the reciprocal system as

$$u\begin{pmatrix} r_2s_3-r_3s_2 \\ r_3s_1-r_1s_3 \\ r_1s_2-r_2s_1 \end{pmatrix}_A$$

where u is the volume of the direct space unit cell.

4. The scalar product of two vectors $\mathbf{r}$ and $\mathbf{s}$ one of which is expressed on the direct system, the other on the reciprocal system is: $r_1s_1+r_2s_2+r_3s_3$.

5. A plane (hkl) has a normal $\begin{Bmatrix} h \\ k \\ l \end{Bmatrix}_A$ and this vector is of length $\frac{1}{d_{hkl}}$ where d_{hkl} is the distance of this plane from the origin. Hence it is the distance between such planes.

6. The vector product of the normals of two planes (hkl) and $(h'k'l')$ is a vector parallel to the line of intersection of the two planes. It is called the zone axis. The vector, written in transposed form is the zone symbol.

7. The vector product of two vectors formed from zone symbols is a vector in reciprocal space and hence represents a plane in direct space.