COMPUTATION OF INTERFACIAL ANGLES, INTERZONAL ANGLES, AND CLINOGRAPHIC PROJECTION BY MATRIX METHODS

W. L. Bond,

Bell Telephone Laboratories, Murray Hill, New Jersey.

ABSTRACT

A way of setting up the general crystallographic axes a, b, c on unit orthogonal axes x, y, z is used to afford a matrix method of computing interfacial angles and zonal angles. It also affords a method of making clinographic projections.

Introduction

The problems of crystal geometry are mainly problems of relations between directions in space. The "direction" of a crystal face is most conveniently characterized by the direction of a line perpendicular to the face, this line being called the normal of the face. It is often very helpful to restrict this normal to unit length, in which case it is called a unit normal. A unit normal, then, is a line having both length and direction and hence fits the definition of a vector. In specifying a group of vectors we may state their lengths and directions very conveniently in terms of a set of three non-coplanar vectors which intersect at a point called the origin. We shall always call these three vectors the base vectors to avoid confusing them with the other vectors. Let us assume that we have base vectors a, b, and c of length a, b, and c units, respectively, and wish to specify a vector V in terms of a, b, and c. We imagine moving V about in space, without changing its direction, until the tail end of V is at the origin. We now find that we can reach the head end of V by taking V_1 steps of length a along a, then taking V_2 steps of length b parallel to b and finally V_3 steps of length c parallel to c, see Fig. 1. These three numbers V_1 , V_2 , and V_3 are the components of the vectors V on the abc basis. We shall denote this fact by means of the equation:

$$(\mathbf{V})_a = \begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix}_a$$

where the subscripts a remind us that these components are stated on the a b c basis which we shall henceforth call the a basis.

On another system with base vectors d e f the components of V will be quite different. Let us say that on this system, which we shall call the d basis, the components are V_1' , V_2' , and V_3' ; that is:

$$(\boldsymbol{V})_d = \begin{pmatrix} V_1' \\ V_2' \\ V_3' \end{pmatrix}_d.$$

If we know the relationship between the a and d bases, we can compute the components of any vector V on one basis given its components on the other. This relationship between bases is most conveniently given in

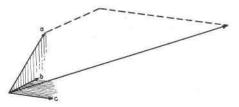


Fig. 1. Illustration of the vector $\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}_a$.

terms of a matrix, i.e., a rectangular array of numbers (the numbers being the components of one basis on the other). As an illustration of a matrix, and also of a special kind of "multiplication" known as matrix multiplication, we multiply the vector

$$(V)_a = \begin{pmatrix} 1\\2\\3 \end{pmatrix} \text{ by the matrix } m = \begin{pmatrix} 4 & 5 & 6\\7 & 8 & 9\\10 & 11 & 12 \end{pmatrix}$$

$$m(V)_a = \begin{pmatrix} 4 & 5 & 6\\7 & 8 & 9\\10 & 11 & 12 \end{pmatrix} \begin{pmatrix} 1\\2\\3 \end{pmatrix} = \begin{pmatrix} 4 \times 1 + 5 \times 2 + 6 \times 3\\7 \times 1 + 8 \times 2 + 9 \times 3\\10 \times 1 + 11 \times 2 + 12 \times 3 \end{pmatrix} = \begin{pmatrix} 32\\50\\68 \end{pmatrix}$$

which is a new vector. It is seen that the resultant components are found by summing products in a systematic way, namely, the first resulting component is the sum of the terms of the first row of the matrix multiplied in turn by the components of the vector, the second is the sum of the terms of the second row of the matrix multiplied in turn by the components of the vector, and similarly for the last component. After a little practice this kind of "multiplication" becomes purely mechanical. In terms of this kind of multiplication we now give the equation that allows us to compute the components on one basis given the components on the other basis and given the matrix connecting the bases:

$$(\mathbf{V})_d = M(\mathbf{V})_a. \tag{1}$$

As an example, we write the matrix that gives the relationship between a simple set of vectors x, y, z (all of unit length and mutually perpendicular) and the set of vectors a b c taken as the axes of a triclinic crystal,

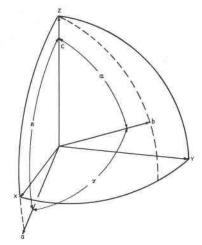


Fig. 2. Triclinic system as related to x system.

b being equal to unity. If we take c as lying along z and let a lie in the plane of x and z (see Fig. 2)* we get the matrix:

$$M = \begin{pmatrix} a \sin \beta & v_1 & 0 \\ 0 & v_2 & 0 \\ a \cos \beta & \cos \alpha & c \end{pmatrix}$$
 (2)

where α , β and γ are the triclinic angles of the crystal and where

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

and

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

Here β is taken as the obtuse angle of the regular triclinic axes. In this matrix, M, the columns are the components of the vectors a, b and c on the x basis, that is:

$$(a)_x = \begin{pmatrix} a \sin \beta \\ 0 \\ a \cos \beta \end{pmatrix}_x, \quad (b)_x = \begin{pmatrix} v_1 \\ v_2 \\ \cos \alpha \end{pmatrix}_x \text{ and } (c)_x = \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix}_x.$$

* The x basis is convenient not only in performing certain crystallographic computations, as will be shown below, but also as a basis to which to refer the vectors and tensors involved in the expression of elastic and electric properties of crystals.

As an illustration of the use of equation (1) we will compute the components on the x basis of a vector

$$(V)_a = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}_a.$$

By matrix multiplication we see that:

$$(V)_x = \begin{pmatrix} a \sin \beta & v_1 & 0 \\ 0 & v_2 & 0 \\ a \cos \beta & \cos \alpha & c \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} a \sin \beta \\ 0 \\ a \cos \beta + c \end{pmatrix}_x.$$

To solve the inverse problem, namely, given $(V)_x$ to find $(V)_a$ we use the reciprocal matrix M^{-1} , the columns of which are the components of x y and z on a b and c, respectively.

$$M^{-1} = \begin{pmatrix} \frac{1}{a \sin \beta} & \frac{-v_1}{a v_2 \sin \beta} & 0\\ 0 & 1/v_2 & 0\\ -\frac{\cot \beta}{c} & \frac{v_1 \cot \beta - \cos \alpha}{v_2 c} & 1/c \end{pmatrix}$$
(3)

we may easily verify that $M^{-1}\begin{pmatrix} a \sin \beta \\ 0 \\ a \cos \beta + c \end{pmatrix}_x = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}_a$.

We need one more variant of these matrices, namely the transposed matrix \overline{M} . It is merely the matrix re-written so that the columns appear as rows and the rows as columns. For example, the transposed M^{-1} matrix is:

$$\overline{M}^{-1} = \begin{bmatrix}
\frac{1}{a \sin \beta} & 0 & \frac{-\cot \beta}{c} \\
\frac{-v_1}{av_2 \sin \beta} & 1/v_2 & \frac{v_1 \cot \beta - \cos \alpha}{v_2 c} \\
0 & 0 & 1/c
\end{bmatrix}$$
(4)

This can be read "M bar reciprocal."

Vectors themselves can be regarded as one-column three-row, or one-row three column, matrices. Indeed they have implicitly been so regarded while we subjected them to matrix multiplication. Thus as a special case of the transposed matrix we have the transposed vector, for instance $(\overline{V})_x = (V_1, V_2, V_3)_x$.

On the x basis some equations become quite simple. For example, the cosine of the angle between two unit vectors $(V)_x$ and $(W)_x$ is given by matrix multiplication as:

$$\cos \epsilon_w^{\ v} = (\overline{V})_x(W)_x \tag{5}$$

which is the matrix notation for the familiar vector definition of scalar product. To illustrate we take the two unit vectors

$$(V)_x = \begin{pmatrix} 1/2 \\ \sqrt{3}/2 \\ 0 \end{pmatrix} \text{ and } (W)_x = \begin{pmatrix} 0 \\ -1/2 \\ \sqrt{3}/2 \end{pmatrix}.$$

$$\cos \epsilon_{w^v} = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right)_x \begin{pmatrix} 0 \\ -1/2 \\ \sqrt{3}/2 \end{pmatrix}_x = \frac{1}{2} \times 0 - \frac{1}{2} \times \frac{\sqrt{3}}{2} + 0 \times \frac{\sqrt{3}}{2},$$

$$\cos \epsilon_{w^v} = \frac{-\sqrt{3}}{4}, \text{ whence } \epsilon_{w^v} = 115^{\circ}40'.$$

In the order to utilize equation (5), if the vectors on the x basis are not of unit length, we must make them so. We can do this by dividing each vector by its length. The length of a vector is the square root of the sum of the squares of its components on the x basis. This process we shall call "normalizing."* It will be symbolized by the superscript n after a vector. For example, the vector

$$V = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}_x$$

normalizes to

$$(V)_{x^{n}} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}_{x} \frac{1}{\sqrt{1+2^{2}+3^{2}}} = \begin{pmatrix} 1/\sqrt{14} \\ 2/\sqrt{14} \\ 3/\sqrt{14} \end{pmatrix}_{x}.$$

The case of triclinic crystals being the most complicated case in crystallography, we should expect the matrices for simpler crystal systems to be simpler than the matrix M, as indeed they are. If we put $\alpha = \gamma = 90^{\circ}$ we meet the conditions of the monoclinic system. Equations (2) and (3) give the respective forms for the monoclinic system:

$$M_m = \begin{pmatrix} a \sin \beta & 0 & 0 \\ 0 & 1 & 0 \\ a \cos \beta & 0 & c \end{pmatrix}. \tag{6}$$

$$M_m^{-1} = \begin{bmatrix} \frac{1}{a \sin \beta} & 0 & 0 \\ 0 & 1 & 0 \\ \frac{-\cot \beta}{a} & 0 & 1/c \end{bmatrix}$$
 (7)

^{*} Normal is used in two senses. As first used, a line normal to a plane is perpendicular to it. When we normalize it we reduce it to a "Norm," namely unit length.

If we put $\beta = 90^{\circ}$ we find the forms for the orthorhombic system:

$$M_0 = \begin{pmatrix} a & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & c \end{pmatrix}. \tag{8}$$

$$M_0^{-1} = \begin{pmatrix} 1/a & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1/c \end{pmatrix}. \tag{9}$$

If, in equations (2) and (3) we put a=b=1, $\alpha=\beta=90^{\circ}$ and $\gamma=120^{\circ}$, we find the form for the hexagonal system:

$$M_h = \begin{pmatrix} 1 & -1/2 & 0 \\ 0 & \sqrt{3}/2 & 0 \\ 0 & 0 & c \end{pmatrix} . \tag{10}$$

$$M_{h}^{-1} = \begin{pmatrix} 1 & 1/\sqrt{3} & 0\\ 0 & 2/\sqrt{3} & 0\\ 0 & 0 & 1/c \end{pmatrix} . \tag{11}$$

For completeness we give the matrices for the little used rhombohedral or trigonal system:

$$M_r = \begin{pmatrix} 3/2 & -3/2 & 0\\ \sqrt{3}/2 & \sqrt{3}/2 & -\sqrt{3}\\ c & c & c \end{pmatrix}. \tag{12}$$

$$M_r^{-1} = \frac{1}{3} \begin{pmatrix} 1 & 1/\sqrt{3} & 1/c \\ -1 & 1/\sqrt{3} & 1/c \\ 0 & -2/\sqrt{3} & 1/c \end{pmatrix}$$
 (13)

where c (the same c as that in the hexagonal system) is given in terms of the rhombohedral angle α by

$$c = \frac{\sqrt{1\cdot 5 + 3\cos\alpha}}{1 - \cos\alpha}.$$
 (14)

In equations (8) and (9) we put a=1 to obtain the forms for the tetragonal system:

$$M_t = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & c \end{pmatrix} . \tag{15}$$

$$M_{t}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1/c \end{pmatrix}. \tag{16}$$

Finally, we put c=1 to obtain the matrix for the isometric system:

$$M_{i} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = M_{i}^{-1}. \tag{17}$$

In the following, general rules will be stated in terms of the matrix M, it being understood that the appropriate subscript will be supplied according to the system of the crystal being studied.

A great aid to understanding crystal problems is the concept of a vector basis reciprocal to the a basis. We shall call this the A basis. Its base vectors are A, B and C. On the x basis the components of A are the three terms of the first column of \overline{M}^{-1} , of B are the terms of the second column, and of C are those of the last column. A is perpendicular to B and C, B to C and A, C to A and B. Given a vector $(V)_A$ on the A basis we can find its component on the x basis by means of the equation

$$(\mathbf{V})_x = \overline{M}^{-1}(\mathbf{V})_A. \tag{18}$$

THE DIRECTION OF FACE NORMALS AND INTERFACIAL ANGLES

A crystal face with Miller indices $(h \ k \ l)_a$ on the a basis has a normal with components on the A basis of:

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix}_A$$
.

If we wish to convert this to the x basis we apply equation (18). This shows us how to compute the angle between any two faces, say $(h \ k \ l)$ and $(h' \ k' \ l')$ for we may write them as vectors

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix}_A$$
 and $\begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}_A$

on the A basis, then convert these normals to components on the x basis, normalize them, and multiply them together as in equation (5) to give the cosine of the angle between the plane normals, this being the angle crystallographers call the angle between planes. As an example we take rhodonite, and compute the angle between two faces. Here a=1.0728 b=1, and c=0.6213, $\alpha=103^{\circ}$ 18', $\beta=108^{\circ}$ 44', and $\gamma=81^{\circ}$ 39'. Whence $v_1=0.07533$ and $v_2=0.97026$ so that

$$\overline{M}^{-1} = \begin{pmatrix} .98428 & 0 & .54585 \\ -.07642 & 1.0306 & .32915 \\ 0 & 0 & 1.6095 \end{pmatrix},$$

The angle between the planes $(\overline{2}21)$ and $(\overline{2}21)$ is the angle between their normals $N_{\overline{2}21}$ and $N_{\overline{2}21}$.

$$N_{\overline{2}21} = \overline{M}^{-1} \begin{pmatrix} -2\\2\\1 \end{pmatrix} = \begin{pmatrix} -1.4227\\2.5432\\1.6095 \end{pmatrix}_{x}, N_{\overline{2}21}^{n} = \begin{pmatrix} -.42737\\.76396\\.48349 \end{pmatrix}_{x}$$

$$N_{\overline{2}21} = \overline{M}^{-1} \begin{pmatrix} -2\\-2\\1 \end{pmatrix} = \begin{pmatrix} -1.4227\\-1.5792\\1.6095 \end{pmatrix}_{x}, N_{\overline{2}21} = \begin{pmatrix} -.55360\\-.59231\\+.60637 \end{pmatrix}_{x}$$

$$\cos(\overline{2}21) \wedge (\overline{2}\overline{2}1) = (-.42737, .76396, .48349) \begin{pmatrix} -.53360\\-.59231\\+.60367 \end{pmatrix}$$

$$= .22804 - .45250 + .29188 = .06742$$

$$(\overline{2}21) \wedge (\overline{2}\overline{2}1) = 86°8'.$$

whence

DIRECTION OF EDGES

The zone symbol* derived from the indices of a pair of planes can be interpreted as the components, on the a basis, of a vector parallel to both planes. (It can also be interpreted as the indices, on the reciprocal basis, of a plane perpendicular to both of the original planes.) To find the components on the x basis we have only to multiply the zone symbol by the appropriate M matrix.

Angles Between Edges

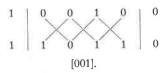
To find the cosine of the angle between two edges we first "cross multiply" to obtain the two zone symbols of the edges. These are considered as vectors on the a basis and their components on the x basis are computed. These vectors are converted into unit vectors and their scalar product found. Rhodonite will again be used as an example: find the angle between the edge formed by (100) and ($\overline{221}$) and the edge formed by (100) and (110). The zone symbol of (100) and ($\overline{221}$) is:

^{*} It will be recalled that the zone symbol [uvw] for the planes $(h \ k \ l)$ and $(h_1 \ k_1 \ l_1)$ is given by cross-multiplication according to the scheme $u=kl_1-lk_1, v=lh_1-hl_1, w=hk_1-hk_1$.

Hence the edge between (100) and $(\overline{221})$ is parallel to the vector

$$\begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix}_a$$
.

The zone symbol of (100) and (110) is



Since the edge between (221) and (100) is:

$$(E_{100}^{221})_a = \begin{pmatrix} 0\\1\\2 \end{pmatrix}$$
, we have $(E_{100}^{221})_x = M(E_{100}^{221})_a$

$$= \begin{pmatrix} 1.0161 & .07533 & 0\\0 & .97026 & 0\\-.34460 & -.23005 & .6213 \end{pmatrix} \begin{pmatrix} 0\\1\\2 \end{pmatrix}_a = \begin{pmatrix} .07533\\.97026\\1.0125 \end{pmatrix}_x$$

which gives the unit vector:

$$E' = \begin{pmatrix} .05364 \\ .69087 \\ .72095 \end{pmatrix}_x.$$

Similarly

$$E_{110}^{100} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_{a} = \begin{pmatrix} 0 \\ 0 \\ .6213 \end{pmatrix}_{x}$$

which becomes the unit vector

$$E^{\prime\prime} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Finally

$$\cos E_{100}^{\overline{221}} \wedge E_{110}^{100} = (001) \begin{pmatrix} .05364 \\ .69087 \\ .72095 \end{pmatrix} = .72095,$$

or the angle is 43°52'.

CLINOGRAPHIC PROJECTION BY MATRIX COMPUTATION

An edge direction $(E)_x$ can be projected onto the plane of the clinographic projection by multiplying by the matrix:

$$K = \begin{pmatrix} \frac{-1}{\sqrt{10}} & \frac{3}{\sqrt{10}} & 0\\ \frac{-3}{\sqrt{370}} & \frac{-1}{\sqrt{370}} & \frac{6}{\sqrt{37}} \end{pmatrix}.$$
 (19)*

Good enough for practical use is the approximation (with reversed sign):

$$K' = \begin{pmatrix} 6 & -18 & 0 \\ 3 & 1 & -19 \end{pmatrix}. \tag{20}$$

In drawing crystals of the hexagonal system it is customary to turn the crystal 30° further clockwise than for other systems. This changes the clinographic matrix. It can be conveniently taken as

$$K_H = \begin{pmatrix} 758 & -963 & 0\\ 110.7 & 52.7 & -1000 \ c \end{pmatrix}. \tag{21}$$

If D is the two dimensional vector giving the direction of the projection of an edge we have:

$$D = K(E)_x. (22)$$

But $(E)_x = M(E)_a$ where

$$D = KM(E)_a. (23)$$

As an example we again take rhodonite

$$K'M = \begin{pmatrix} 6 & -18 & 0 \\ 3 & 1 & -19 \end{pmatrix} \begin{pmatrix} 1.016 & .0753 & 0 \\ 0 & .970 & 0 \\ -.345 & -.230 & .621 \end{pmatrix}$$
$$= \begin{pmatrix} 6.70 & -17.01 & 0 \\ 10.60 & 5.57 & 11.80 \end{pmatrix}.$$

Whence, the edge, for instance, between $(\overline{221})$ and (100) which is

$$E_{100}^{\overline{2}21} = \begin{pmatrix} 0\\1\\2 \end{pmatrix}$$

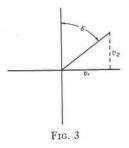
is projected as

$$KM = \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 6.70 & -17.01 & 0 \\ 10.60 & 5.57 & 11.8 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix} = \begin{pmatrix} -17.01 \\ 29.2 \end{pmatrix}.$$

Hence, in Fig. 3, we would lay out 17.01 units to the left of the origin and 29.2 units up. The edge projection is parallel to this line. It may be

^{*} Here the bottom row (18/ $\sqrt{370}$, 6/ $\sqrt{370}$, 1/ $\sqrt{37}$) has been omitted from the complete matrix K. The complete matrix is convenient for the computation of stereoscopic pairs of drawings of objects viewed from the clinographic angle. This subject will be presented in a later paper.

more convenient to compute angles from the vertical in terms of the tangents. As $\tan \delta = D_1/D_2$, see Fig. 3, if D_1/D_2 is positive S is measured



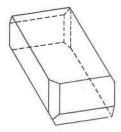


Fig. 3a. Rhodonite as drawn from matrix calculations.

clockwise from the vertical, counterclockwise if D_1/D_2 is negative. Slide rule computations are entirely satisfactory.

SUMMARY

- (1) A vector $(V)_a$ on the a basis becomes $(V)_x = M(V)_a$ on the x basis.
- (2) A vector can be normalized by dividing it by the square root of the sum of the squares of its components on the x basis.
- (3) The cosine of the angle S between two unit vectors $(V)_x$ and $(W)_x$ is $\cos S = (\overline{V})_x(W)_x$.
 - (4) The vector $\begin{pmatrix} h \\ k \\ l \end{pmatrix}_A$ is perpendicular to the plane (hkl) and hence this

plane has a normal on the x basis of:

$$(N_{hkl})_x = \overline{M}^{-1} \begin{pmatrix} h \\ k \\ l \end{pmatrix}_A.$$

(5) The zone symbol [mnp], derived from any two faces of the zone

by cross multiplication of the face indices, is a vector $\begin{pmatrix} m \\ n \\ p \end{pmatrix}_a$. It becomes on the x basis:

$$(V)_x = M \begin{pmatrix} m \\ n \\ p \end{pmatrix}_a.$$

(6) A clinographic projection of a crystal may be made by multiplying the matrix KM by the zone symbols of the crystal face pairs.