

A METHOD FOR CONSTRUCTING AND INTERPRETING MATRIX REPRESENTATIONS OF SPACE-GROUP OPERATIONS*

MONTE B. BOISEN, JR. AND G. V. GIBBS

Department of Geological Sciences, Virginia Polytechnic Institute and State University,
Blacksburg, Virginia 24061 U.S.A.

ABSTRACT

A systematic method is presented for constructing the matrix representation of a space-group operation given its geometric description and conversely for finding the geometric description of the space-group operation given its matrix representation.

SOMMAIRE

Une méthode systématique permet, étant donné la description géométrique d'une opération de symétrie d'un groupe spatial, d'en construire la représentation matricielle et, réciproquement, de déduire la description géométrique de la représentation matricielle.

(Traduit par la Rédaction)

INTRODUCTION

A series of rules has been presented by Wondratschek & Neubüser (1967) that allows the determination of the geometrical nature of a space-group operation from its matrix representation. By taking advantage of reasoning founded on an understanding of elementary space-group theory (Buerger 1963, Bloss 1971), we have simplified the method by avoiding the large number of rules used in methods like that presented by Wondratschek & Neubüser (1967) and summarized by Bradley & Cracknell (1972).

PRELIMINARIES

To formulate a matrix representation of a space-group operation, a well-defined basis for the vector space on which the matrix will operate is required. To simplify the discussion, we choose the unit-cell edge vectors $\{a, b, c\}$ that outline the conventional unit cell (Table

2.2.1, *International Tables*, Vol. I) as a basis for the vector space. Then a general vector $r = xa$

+ $yb + zc$ can be denoted by the triple $\begin{bmatrix} x \\ y \\ z \end{bmatrix}$

(or by $\begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix}$ when dealing with a 4×4

matrix representation). For convenience, r will

be identified with the symbol $\begin{bmatrix} x \\ y \\ z \end{bmatrix}$ and

simply be written $r = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ with the basis

being understood. Consequently, we will not be distinguishing between a vector r and its end-

point $\begin{bmatrix} x \\ y \\ z \end{bmatrix}$.

A space-group operation α is composed of a point-group operation, β , (i.e., a distance-preserving mapping that leaves at least one point fixed) and a translational operation δ such that $\delta(r) = r + d$ for all r . That is, $\alpha = \delta\beta$. The *symmetry element* of the point operation β is defined to be the set of all points left fixed by β (i.e., a point e is on the symmetry element of β if and only if $\beta(e) = e$). The *symmetry element* of α is defined to be that of β . A point operation is either the identity (having all space as its symmetry element) or a rotation (having its axis, a straight line, as its symmetry element) or a rotoinversion (having a point as its symmetry element unless it is a reflection, in which case a plane is its symmetry element).

The vector d generated by the translational operation δ parallels the symmetry element of β . Note that the symmetry element of β need not contain the origin, 0 . However, by translating the symmetry element of β so that it contains the origin we can define a point-group operation σ such that (1) the symmetry ele-

*It is a pleasure to dedicate this paper to Professor J. D. H. Donnay on the occasion of his 75th birthday as a tribute to his pioneering contributions in the fields of crystallography and mineralogy.

TABLE 1. SYMBOLS USED

α, β, δ	$\alpha = \delta\beta$, where α is a space-group operation, β is the point-group operation part of α and δ is the translational part of α .
σ	a point-group operation identical with that of β except $\sigma(\mathbf{0}) = \mathbf{0}$.
η	translational operation that moves the symmetry element of σ to that of β .
ξ	used to denote a point on the symmetry element of β .
ξ	used to denote the vector generated by δ .
$M(\alpha)$	matrix representation of α .
R	matrix representation of σ .
ξ	ξ is the vector such that $M(\alpha) = \{R, \xi\}$.

Note that in the text, vectors have been set in bold-face type.

ment of σ contains $\mathbf{0}$, (2) the symmetry element of σ parallels that of β , and (3) the motion of σ about its symmetry element is the same as that of β about its symmetry element. A translational operation η moves the symmetry element of σ to that of β if and only if $\eta(\mathbf{r}) = \mathbf{r} + \mathbf{e}$ for some point $\mathbf{e}$ on the symmetry element of β . Furthermore, in this case $\beta = \eta\sigma\eta^{-1}$ (Buerger 1963, p. 196). The notational conventions made above are summarized in Table 1.

Example 1

In space group $I4_1$ (No. 80), there exists a quarter-turn screw operation 4_1 , which we will call α , whose symmetry element passes through the point $-\frac{1}{4}\mathbf{a} + \frac{1}{4}\mathbf{b}$ and parallels $\mathbf{c}$. Hence $\alpha = \delta\beta$ where β is the quarter turn whose symmetry element parallels the $\mathbf{c}$ axis and passes through the point $-\frac{1}{4}\mathbf{a} + \frac{1}{4}\mathbf{b}$ and δ is the translational operation such that $\delta(\mathbf{r}) = \mathbf{r} + \frac{1}{4}\mathbf{c}$ for all $\mathbf{r}$ in space. Accordingly, σ is a quarter-turn rotation about the $\mathbf{c}$ axis containing $\mathbf{0}$. Moreover, an arbitrary vector on the symmetry element of β is of the form $\mathbf{e} = -\frac{1}{4}\mathbf{a} + \frac{1}{4}\mathbf{b} + z\mathbf{c}$ where z is any real number. Hence choosing $z = 0$, η can be taken to be the translation that moves each point $\mathbf{r}$ in space to $\mathbf{r} - \frac{1}{4}\mathbf{a} + \frac{1}{4}\mathbf{b}$. Inasmuch as $\delta(\mathbf{r}) = \mathbf{r} + \frac{1}{4}\mathbf{c}$, we have $\mathbf{d} = \frac{1}{4}\mathbf{c}$.

In general, each space-group operation $\alpha = \delta\beta$ can be described by a 4×4 matrix, $M(\alpha)$, of the form

$$M(\alpha) = \begin{bmatrix} l_{11} & l_{12} & l_{13} & t_1 \\ l_{21} & l_{22} & l_{23} & t_2 \\ l_{31} & l_{32} & l_{33} & t_3 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \{R, \mathbf{t}\}$$

where the matrix

$$R = \begin{bmatrix} l_{11} & l_{12} & l_{13} \\ l_{21} & l_{22} & l_{23} \\ l_{31} & l_{32} & l_{33} \end{bmatrix}$$

represents the point-group operation σ . Because of the choice of basis made in the *International Tables*, Vol. I for each space group,

the elements of R will always be 1, 0 or -1. Whereas the interpretation of the vector

$$\mathbf{t} = \begin{bmatrix} t_1 \\ t_2 \\ t_3 \end{bmatrix}$$

is not as obvious as that of R , it is important in the analysis of $M(\alpha)$. First note that $\mathbf{t}$ is the image of the origin, $\mathbf{0}$, under the space-group operation α , i.e., $\mathbf{t} = \alpha(\mathbf{0})$ because

$$M(\alpha) \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} t_1 \\ t_2 \\ t_3 \\ 1 \end{bmatrix}$$

To find the connection between δ and $\mathbf{t}$, recall that $\mathbf{d}$ is the vector such that $\delta(\mathbf{r}) = \mathbf{r} + \mathbf{d}$ for all $\mathbf{r}$. Let $\mathbf{e}$ be a vector on the symmetry element of β and define η such that $\eta(\mathbf{r}) = \mathbf{r} + \mathbf{e}$. Then $\alpha(\mathbf{r}) = \delta\beta(\mathbf{r}) = \beta(\mathbf{r}) + \mathbf{d}$. If we replace β by $\eta\sigma\eta^{-1}$, we obtain

$$\begin{aligned} \alpha(\mathbf{r}) &= \eta\sigma\eta^{-1}(\mathbf{r}) + \mathbf{d} \\ &= \eta[\sigma(\mathbf{r} - \mathbf{e})] + \mathbf{d} \\ &= \sigma(\mathbf{r} - \mathbf{e}) + \mathbf{e} + \mathbf{d}. \end{aligned}$$

when $\mathbf{r} = \mathbf{0}$

$$\begin{aligned} \alpha(\mathbf{0}) &= \sigma(\mathbf{0}) - \sigma(\mathbf{e}) + \mathbf{e} + \mathbf{d} \\ &= \mathbf{e} - \sigma(\mathbf{e}) + \mathbf{d}. \end{aligned}$$

Inasmuch as $\alpha(\mathbf{0}) = \mathbf{t}$, we have the equality $\mathbf{t} = \mathbf{e} - \sigma(\mathbf{e}) + \mathbf{d}$. Because R is the matrix representation of σ , this equality becomes

$$\mathbf{t} = (I_3 - R)\mathbf{e} + \mathbf{d} \quad (1)$$

$$\text{where } I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

THE METHOD FOR CONSTRUCTING THE MATRIX $M(\alpha)$ GIVEN α

Given some space-group operation α (and hence given δ and β) we wish to construct $M(\alpha)$. Considering β first, we translate β in such a way that its symmetry element contains the origin (this translated operation is σ). The R part of $M(\alpha)$ is found by observing that

$$R\mathbf{a} = \begin{bmatrix} l_{11} & l_{12} & l_{13} \\ l_{21} & l_{22} & l_{23} \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} l_{11} \\ l_{21} \\ l_{31} \end{bmatrix}$$

$$\text{and similarly that } R\mathbf{b} = \begin{bmatrix} l_{12} \\ l_{22} \\ l_{32} \end{bmatrix} \text{ and } R\mathbf{c} =$$

$$\begin{bmatrix} l_{13} \\ l_{23} \\ l_{33} \end{bmatrix}. \text{ Therefore, the columns of } R \text{ are}$$

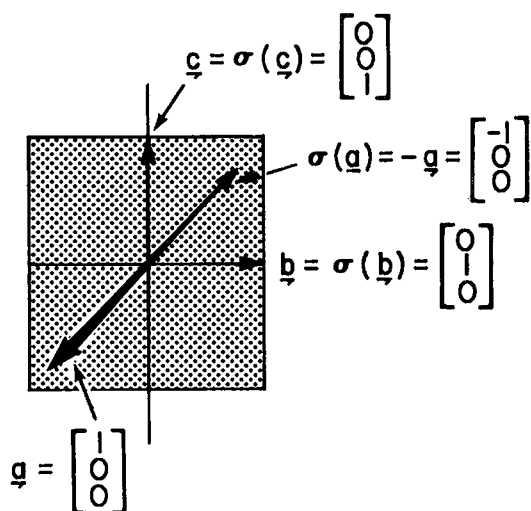


FIG. 2. The effect of a reflection σ over a plane containing $\mathbf{b}$ and $\mathbf{c}$. Inasmuch as σ sends $\mathbf{a}$ into $-\mathbf{a}$, $\mathbf{b}$ into $\mathbf{b}$ and $\mathbf{c}$ into $\mathbf{c}$,

$$R = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1/4 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1/2 \\ 1/2 \end{bmatrix} = \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \end{bmatrix}$$

$$M(\alpha) = \begin{bmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Having found $M(\alpha)$ it is easy to locate the image of an arbitrary point $\mathbf{r} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ under α by performing the multiplication

$$\begin{bmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix} = \begin{bmatrix} 1/2 - x \\ 1/2 + y \\ 1/2 + z \\ 1 \end{bmatrix}$$

Hence, the n glide sends each point in space

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} \text{ to } \begin{bmatrix} 1/2 - x \\ 1/2 + y \\ 1/2 + z \end{bmatrix}$$

CONSTRUCTING α GIVEN ITS MATRIX REPRESENTATION $M(\alpha)$

Given $M(\alpha)$ (and hence also the basis vectors) we wish to find δ and β . As $M(\alpha)$ is given, we know R and $\mathbf{t}$. From the matrix R , σ can be easily found by inspection (recall that the columns of R are the images of the basis

vectors). If $\mathbf{e}$ is determined, because η can be chosen such that $\eta(\mathbf{r}) = \mathbf{r} + \mathbf{e}$, then $\beta = \eta\sigma\eta^{-1}$ would be determined. We begin by finding $\mathbf{d}$ (and hence δ) and then find $\mathbf{e}$. Let n be the order of R , i.e., n is the smallest positive integer for which $R^n = I_3$ is true. Consider the effect of operating on equation (1) with successive powers of R going from 1 to n (recall that $R(\mathbf{d}) = \mathbf{d}$):

$$\begin{aligned} R\mathbf{t} &= (R - R^2)\mathbf{e} + \mathbf{d} \\ R^2\mathbf{t} &= (R^2 - R^3)\mathbf{e} + \mathbf{d} \\ &\vdots \\ R^{n-1}\mathbf{t} &= (R^{n-1} - I_3)\mathbf{e} + \mathbf{d} \\ R^n\mathbf{t} &= (I_3 - R)\mathbf{e} + \mathbf{d} \end{aligned}$$

Upon summation, the left member becomes $\sum_{i=1}^n R^i\mathbf{t}$ whereas the coefficient of $\mathbf{e}$ becomes

$$(R - R^2) + (R^2 - R^3) + \dots + (R^{n-1} - I_3) + (I_3 - R) = 0. \text{ Therefore,}$$

$$\sum_{i=1}^n R^i\mathbf{t} = n\mathbf{d}$$

and so

$$\mathbf{d} = \frac{1}{n} \sum_{i=1}^n R^i\mathbf{t} \quad (2)$$

Now that R and $\mathbf{d}$ have been found, $\mathbf{e}$ can be found using equation (1) rewritten as:

$$(I_3 - R)\mathbf{e} = \mathbf{t} - \mathbf{d}.$$

In general, there is more than one solution for $\mathbf{e}$. In fact the solution set is exactly the set of points in the symmetry element of β . If the symmetry element of β is a point, then the solution will be unique. On the other hand, if the symmetry element of β is a line or a plane, then the solution set will be infinite. Now that R and $\mathbf{d}$ have been found, $\mathbf{e}$ can be identified from $M(\alpha)$. Given the general equivalent position for any space-group operation α listed in the *International Tables*, Vol. I, $M(\alpha)$ can be easily found, from which the method yields the corresponding δ and β .

Example 4

To discover the nature (i.e., δ and β) of the space-group operation α in space group

$I4_1/amd$ (No. 141) that maps each point $\begin{bmatrix} x \\ y \\ z \end{bmatrix}$

in space into $\begin{bmatrix} y \\ 1/2 + x \\ 1/4 + z \end{bmatrix}$, $M(\alpha)$ must be

found. From the definition of α .

$$\begin{bmatrix} l_{11} & l_{12} & l_{13} & t_1 \\ l_{21} & l_{22} & l_{23} & t_2 \\ l_{31} & l_{32} & l_{33} & t_3 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ 1 \end{bmatrix} = \begin{bmatrix} y \\ \frac{1}{2} + x \\ \frac{1}{4} + z \\ 1 \end{bmatrix}$$

which upon multiplication leads to the system of polynomial identities (in indeterminates x , y and z):

$$\begin{aligned} l_{11}x + l_{12}y + l_{13}z + t_1 &= y \\ l_{21}x + l_{22}y + l_{23}z + t_2 &= \frac{1}{2} + x \\ l_{31}x + l_{32}y + l_{33}z + t_3 &= \frac{1}{4} + z. \end{aligned}$$

Equating corresponding coefficients, we have $l_{12} = 1$, $l_{21} = 1$ and $l_{33} = 1$, $t_2 = \frac{1}{2}$, $t_3 = \frac{1}{4}$ (the t_i s are the constant terms of the polynomials) and all the rest are zero. Hence,

$$M(\alpha) = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

From R we see that σ is a mirror operation that interchanges **a** and **b** and leaves **c** fixed and, hence, is a mirror operation whose symmetry element is a plane containing **c** and bisecting **a** and **b**. Therefore, the symmetry element of σ parallels $(1\bar{1}0)$. The order of R is 2 since $R \neq I_3$ and $R^2 = I_3$. To solve for **d**, equation (2) is employed:

$$\begin{aligned} d &= \frac{1}{2} \sum_{i=1}^2 R^i t = \frac{1}{2} (Rt + R^2 t) \\ &= \frac{1}{2} \left(\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{bmatrix} \right) \\ &= \begin{bmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{bmatrix} \end{aligned}$$

This result tells us that α is a diamond-glide operation. The symmetry element of β (in this case a plane) will now be found by adapting equation (1):

$$\begin{aligned} (I_3 - R)e &= t - d \\ \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix} &= \begin{bmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{4} \end{bmatrix} - \begin{bmatrix} \frac{1}{4} \\ \frac{1}{4} \\ \frac{1}{4} \end{bmatrix} \\ &= \begin{bmatrix} -\frac{1}{4} \\ \frac{1}{4} \\ 0 \end{bmatrix} \end{aligned}$$

Solving this system of equations, we find that

any vector of the form $\begin{bmatrix} e_1 \\ e_1 + \frac{1}{4} \\ e_3 \end{bmatrix}$ for

real numbers e_1 and e_3 is a solution. As expected, this solution describes a plane. Choosing a convenient vector in this set for our solution, we let

$$e = \begin{bmatrix} 0 \\ \frac{1}{4} \\ 0 \end{bmatrix} \quad (\text{where } e_1 \text{ and } e_3 \text{ were both chosen as } 0).$$

Hence, the mirror plane of β associated with the diamond-glide operation α parallels

$(1\bar{1}0)$ and passes through the point $\begin{bmatrix} 0 \\ \frac{1}{4} \\ 0 \end{bmatrix}$ and

δ is the translational operator that maps each vector **r** to $\mathbf{r} + \frac{1}{4}\mathbf{a} + \frac{1}{4}\mathbf{b} + \frac{1}{4}\mathbf{c}$.

APPLICATION OF THE METHOD

In the final two examples of the application of the method, the problem of determining the nature of the composition of two space-group operations is considered.

Example 5

For space group $R\bar{3}c$ (No. 167, hexagonal basis), we will form the composition of space-group operations α_1 and α_2 where α_1 is the half-turn with its axis parallel to **b** passing through the point $e = \frac{1}{4}\mathbf{c}$ and α_2 is the translational operation that maps **r** to $\mathbf{r} + \frac{1}{3}\mathbf{a} + \frac{2}{3}\mathbf{b} - \frac{1}{3}\mathbf{c}$ for all **r**. We begin by constructing $M(\alpha_1)$ and $M(\alpha_2)$. If $\alpha_1 = \delta_1\beta_1$, then as α_1 lacks a translation component (being a pure rotation), δ_1 is the identity mapping and so $\mathbf{d} = \mathbf{0}$. Inasmuch as β_1 is a half turn (Fig. 3), the matrix representation for σ_1 (a half turn about **b**) is

$$R_1 = \begin{bmatrix} -1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

$$\text{As } e = \frac{1}{4}\mathbf{c} = \begin{bmatrix} 0 \\ 0 \\ \frac{1}{4} \end{bmatrix}, \text{ by equation (1)}$$

$$t = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ \frac{1}{4} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \end{bmatrix}$$

$$M(\alpha_1) = \begin{bmatrix} -1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

As α_2 is a pure translational operation, application of the method yields

$$M(\alpha_2) = \begin{bmatrix} 1 & 0 & 0 & \frac{1}{3} \\ 0 & 1 & 0 & \frac{2}{3} \\ 0 & 0 & 1 & -\frac{1}{3} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

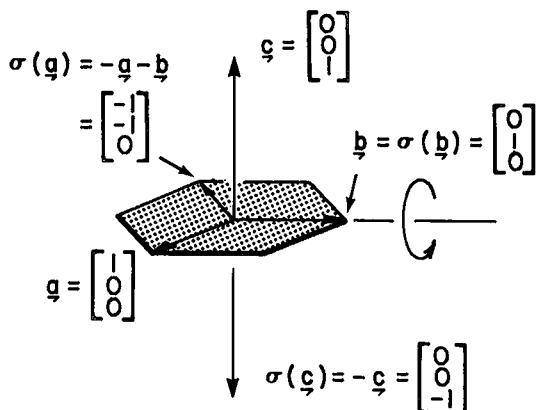


FIG. 3. The effect of a half-turn σ about $\mathbf{b}$ on the basis vectors of a hexagonal crystal. The half turn σ rotates $\mathbf{a}$ into self-coincidence with $-\mathbf{a}$, $\mathbf{b}$ into itself and $\mathbf{c}$ into $-\mathbf{c}$, i.e.,

$$\sigma \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 0 \end{bmatrix}, \quad \sigma \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

and $\sigma \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix}.$

Therefore,

$$M(\alpha_2\alpha_1) = M(\alpha_2)M(\alpha_1) = \begin{bmatrix} -1 & 0 & 0 & \frac{1}{3} \\ -1 & 1 & 0 & \frac{2}{3} \\ 0 & 0 & -1 & \frac{1}{6} \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

To discover the nature of $\alpha = \alpha_2\alpha_1$ where $\alpha = \delta\beta$, we apply the second half of the method. As the R for α is the same as that for α_1 , then β is a half turn parallel to $\mathbf{b}$. To find $\mathbf{d}$, equation (2) is applied. As the order of R is 2,

$$\mathbf{d} = \frac{1}{2} \sum_{i=1}^2 R^i \mathbf{t} = \frac{1}{2} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{1}{2} \\ 0 \end{bmatrix}$$

Therefore, δ is the translational operation that maps each point $\mathbf{r}$ to $\mathbf{r} + \frac{1}{2}\mathbf{b}$. Hence, α is a half-turn screw operation. To find the symmetry element (rotation axis) of β , equation (1) is used:

$$(I_3 - R)\mathbf{e} = \mathbf{t} - \mathbf{d}$$

$$\begin{bmatrix} 2 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{3} \\ \frac{2}{3} \\ \frac{1}{6} \end{bmatrix} - \begin{bmatrix} 0 \\ \frac{1}{2} \\ 0 \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{3} \\ \frac{1}{6} \\ \frac{1}{6} \end{bmatrix}.$$

The solution of this system is the set of all vectors of the form $\begin{bmatrix} \frac{1}{6} \\ e_2 \\ \frac{1}{6} \end{bmatrix}$ where e_2 is any

real number. Taking $e_2 = 0$, note that the axis of the half-turn β passes through the point $\frac{1}{6}\mathbf{a} + \frac{1}{2}\mathbf{c}$. Hence, a half-turn with its rotation axis parallel to $\mathbf{b}$ and passing through the point $\frac{1}{6}\mathbf{a}$ combined with a translational operation that generates the vector $\frac{1}{6}\mathbf{a} + \frac{1}{2}\mathbf{b} - \frac{1}{6}\mathbf{c}$ is equivalent to a half-turn screw operation with its rotation parallel to $\mathbf{b}$ and passing through the point $\frac{1}{6}\mathbf{a} + \frac{1}{2}\mathbf{c}$.

Example 6

As a last example, the composition, α , of two space-group operations α_1 and α_2 contained in the cubic space group $F4_32$ (No. 210) is examined. Let α_1 be a half-turn screw operation ($\mathbf{d} = \frac{1}{4}\mathbf{b} + \frac{1}{4}\mathbf{c}$) such that the symmetry axis of β_1 parallels $[011]$ and passes through the point $\mathbf{e} = \frac{1}{8}\mathbf{a}$ and let α_2 be a quarter-turn screw operation ($\mathbf{d} = \frac{1}{4}\mathbf{b}$) such that the symmetry axis of β_2 parallels $[010]$ and passes through the point $\mathbf{e} = \frac{1}{4}\mathbf{a}$. This information and an understanding of how the basis vectors transform leads to

$$M(\alpha_1\alpha_2) = \begin{bmatrix} -1 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 1 & \frac{1}{4} \\ 0 & 1 & 0 & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 & \frac{1}{4} \\ 0 & 1 & 0 & \frac{1}{4} \\ -1 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$M(\alpha) = \begin{bmatrix} 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

The nature of the σ associated with α may be deduced by examining the columns of R . In this case, as $\sigma(\mathbf{a}) = -\mathbf{b}$, $\sigma(\mathbf{b}) = \mathbf{c}$ and $\sigma(\mathbf{c}) = -\mathbf{a}$ (Fig. 4), it can be shown that σ may be viewed either as a third-turn about $[1\bar{1}\bar{1}]$ or a negative third-turn about $[\bar{1}11]$. In some instances, this may not, however, be an obvious result. Nevertheless, by examining the determinant and the diagonal elements of R , the proper or improper character and the turn angle ρ of the point-group operation are found as follows. For any space-group operation, the proper or improper character of σ is ascertained by evaluating the determinant of R , $\det R$. If $\det R = +1$, then σ is a rotation whereas if $\det R = -1$, then σ is a rotoinversion (Bradley & Cracknell 1972). In this example, as

$$\det R = \begin{vmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{vmatrix} = +1,$$

it can be concluded that σ is a rotation.

By definition, if P is some rotation about an

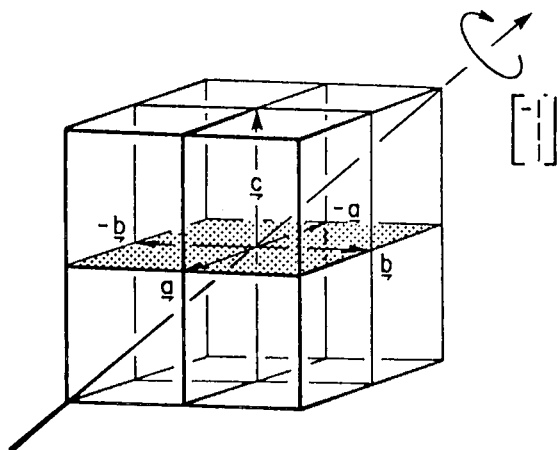


FIG. 4. The effect of a negative-third turn σ along the vector $\begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix}$ on the basis of a cubic crystal. The negative third turn σ rotates $\mathbf{a}$ into $-\mathbf{b}$, $\mathbf{b}$ into $\mathbf{c}$ and $\mathbf{c}$ into $-\mathbf{a}$.

axis containing $\mathbf{0}$ and if i is an inversion over $\mathbf{0}$ such that $i(\mathbf{r}) = -\mathbf{r}$ for all $\mathbf{r}$, then $\Phi = Pi = iP$ is a roto-inversion (cf., Boisen & Gibbs 1976 for a discussion of these ideas). In this case we assign as the turn angle of Φ the turn angle of P and as the rotation axis of Φ the rotation axis of P . When $\det R = -1$, indicating that σ is a rotoinversion, it will be convenient to convert R to a matrix representing a rotation by multiplying each of its entries by -1 . When this is done, the turn angle ρ and the orientation of the rotation axis of the roto-inversion are found in exactly the same way as done for a rotation. The turn angle, ρ , of σ for any space-group operation is obtained from the trace of R , $\text{tr } R = l_{11} + l_{22} + l_{33}$, such that (cf., Benson & Grove 1971, p. 21)

$$\rho = \pm \cos^{-1} [\frac{1}{2} (\text{tr } R - 1)].$$

In our example, since $\text{tr } R = 0$, we may conclude that $\rho = \pm 120^\circ$. Hence, as asserted earlier, σ is either a third-turn rotation or a negative third-turn rotation depending on the chosen orientation of the axis. The points $\mathbf{e}$ on the rotation axis of a nonidentity rotation σ satisfy the equation

$$(I_3 - R)\mathbf{e} = \mathbf{0} \quad (3)$$

as for σ the $\mathbf{d}$ and $\mathbf{t}$ of equation (1) are both equal to $\mathbf{0}$. Hence,

$$\begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

The solution to this system is the set of all

vectors of the form $\begin{bmatrix} -e_3 \\ e_3 \\ e_3 \end{bmatrix}$. If we set $e_3 = 1$, the vector $\mathbf{e} = \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix}$ defines the

orientation of the rotation axis. However, there are two choices that can be made for the positive end of the rotation axis of σ , i.e., $-\mathbf{a} + \mathbf{b} + \mathbf{c}$ or $\mathbf{a} - \mathbf{b} - \mathbf{c}$. If the vector $\mathbf{a} - \mathbf{b} - \mathbf{c}$ is chosen to point along the positive end of the rotation axis, then we see that σ is a third turn by observing that a positive rotation of 120° about the axis maps $\mathbf{a}$ into $-\mathbf{b}$. On the other hand, if $-\mathbf{a} + \mathbf{b} + \mathbf{c}$ is chosen to point along the positive end of the rotation axis, then σ is seen to be a negative-third turn by observing that a rotation of -120° about the axis also maps $\mathbf{a}$ into $-\mathbf{b}$. To find the $\mathbf{d}$ associated with α , we use equation (2). Since the order of R is 3,

$$\mathbf{d} = \frac{1}{3} \sum_{i=1}^3 R^i \mathbf{t} = \frac{1}{3} \begin{bmatrix} -1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -\frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{bmatrix}$$

and we see that δ defines a translation of space along the vector $-\mathbf{a} + \mathbf{b} + \mathbf{c}$. The convention is that the translational component of a screw operation translates space along the positive end of its symmetry axis. The choice of a positive direction on σ should be consistent with this convention on α and, hence, we may conclude the σ is a negative-third-turn operation about the vector $-\mathbf{a} + \mathbf{b} + \mathbf{c}$ because $\delta(\mathbf{r}) = \mathbf{r} - \frac{1}{3}\mathbf{a} + \frac{1}{3}\mathbf{b} + \frac{1}{3}\mathbf{c}$ for all $\mathbf{r}$ in space. However, in the absence of a nonzero translation component (i.e., $\mathbf{d} = \mathbf{0}$), the choice of the positive direction of the rotation axis for σ is arbitrary; hence, either one is "correct."

To find the set of points defining the rotation axis of β , equation (1) is used:

$$(I_3 - R)\mathbf{e} = \mathbf{t} - \mathbf{d}$$

$$\begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{3} \\ \frac{1}{6} \\ \frac{1}{6} \end{bmatrix}.$$

The solution set to this system is the set of all vectors of the form

$$\mathbf{e} = \begin{bmatrix} \frac{1}{3} - e_3 \\ e_3 \\ \frac{1}{6} \end{bmatrix}$$

where e_3 is any real number. Setting $e_3 = 0$, it is seen that the symmetry axis of the third turn passes through the point $\mathbf{e} = \frac{1}{3}\mathbf{a} - \frac{1}{6}\mathbf{b}$. Hence, the composition of α_2 followed by α_1 is

equivalent to a negative-third-turn screw operation taking place about a line paralleling $[\bar{1}11]$ and passing through the point $\frac{1}{3}\mathbf{a} - \frac{1}{6}\mathbf{b}$.

SUMMARY OF METHOD

Given the motion of a space-group operation $\alpha = \delta\beta$, the method yields its matrix representation $M(\alpha) = \{R, \mathbf{t}\}$. The elements of R are found by examining the images of the basis vectors under σ (the parallel operation to β through $\mathbf{0}$), and $\mathbf{t} = (I_3 - R)\mathbf{e} + \mathbf{d}$ where $\mathbf{e}$ is a point on the symmetry element of β and $\mathbf{d}$ is the vector generated by δ .

On the other hand, given a matrix $M(\alpha) = \{R, \mathbf{t}\}$, the method reveals the motion (*i.e.* δ and β) of α . From the matrix R , σ is found by inspection (as R is the matrix representation for σ). As R and $\mathbf{t}$ are given, $\mathbf{d}$ can be found by the formula

$$\mathbf{d} = \frac{1}{n} \sum_{i=1}^n R^i \mathbf{t}$$

where n is the smallest positive integer for which $R^n = I_3$ is true. Substituting R , $\mathbf{d}$ and $\mathbf{t}$ into the equation $(I_3 - R)\mathbf{e} = \mathbf{t} - \mathbf{d}$ and solving we obtain as the solution for $\mathbf{e}$, the set of all points on the symmetry element of β . Hence, both δ and β are determined.

ACKNOWLEDGMENTS

We thank Professor P. H. Ribbe and Dr. R. J. Hill of V.P.I. & S.U., Dr. G. E. Brown, M. Hochella and M. Taylor of Stanford University and Dr. P. Bayliss of the University of Calgary for reviewing the manuscript and making a

number of helpful suggestions for improvement. The Earth Sciences Section of N.S.F. is thanked for supporting this study with grant DES75-14912. We are also grateful to Mrs. Ramonda Haycocks for typing the manuscript and Mrs. Sharon Chiang for drafting the figures.

REFERENCES

- BENSON, C. T. & GROVE, L. C. (1971): *Finite Reflection Groups*. Bogden & Quigley, Tarrytown-on-Hudson, New York.
- BLOSS, F. D. (1971): *Crystallography and Crystal Chemistry. An Introduction*. Holt, Rinehart & Winston, New York.
- BOISEN, M. B., JR. & GIBBS, G. V. (1976): A derivation of the 32 crystallographic point groups using elementary group theory. *Amer. Mineral.* **61**, 145-165.
- BRADLEY, C. J. & CRACKNELL, A. P. (1972): *The Mathematical Theory of Symmetry in Solids. Representation Theory for Point Groups and Space Groups*. Clarendon Press, Oxford.
- BUERGER, M. J. (1963): *Elementary Crystallography. An Introduction to the Fundamental Geometrical Features of Crystals*. John Wiley & Sons, New York.
- HENRY, N. F. M. & LONSDALE, K., eds. (1969): *International Tables for X-ray Crystallography*. 1. *Symmetry Groups* (3rd ed.). Int. Union Cryst., The Kynoch Press, Birmingham, England.
- WONDRATSCHEK, H. & NEUBÜSER, J. (1967): Determination of the symmetry elements of a space group from the 'general positions' listed in *International Tables for X-ray Crystallography*, Vol. I. *Acta Cryst.* **23**, 349-352.

Received August, 1977; revised manuscript accepted December 1977.