Reinheit), das *ca.* 30% kaltverformt wurde. Eine Probe (die Vergleichssubstanz) wurde anschliessend 1 h bei 680 °C im Vakuum geglüht. Die differentielle, diffraktometrische Untersuchung bei Raumtemperatur ergab eine maximale Gitterkonstantenänderung der verformten gegenüber der ausgeheilten Probe von $\Delta a/a \approx -9 \cdot 10^{-5}$. Beide Proben wurden in Schritten von 50 °C gemeinsam jeweils 5 Minuten getempert und anschliessend wieder untersucht. Eine zweite Versuchsreihe erfolgte auf gleiche Weise mit entsprechend behandelten Proben, wobei die Temperaturen jeweils 25 °C höher lagen als in der ersten Serie. Die kombinierten Ergebnisse sind in Fig. 5 aufgetragen.

Man erkennt deutlich die allmähliche Annäherung der Gitterkonstanten des verformten Materials an die der Vergleichsproben. Bei *ca.* 650 °C ist im Rahmen der Messgenauigkeit schliesslich kein Gitterkonstantenunterschied $\Delta a/a$ mehr messbar.

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Determination of the Symmetry Elements of a Space Group from the 'General Positions' listed in *International Tables for X-ray Crystallography*, Vol. I.

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A simple prescription is given for determining the symmetry elements of a space group from the 'general positions' listed in *International Tables for X-ray Crystallography*, Vol. I. The method used is well known in analytical geometry. Its application to the data of I.T. allows more information to be extracted from them, in particular for the cubic space groups, where no drawings are given.

The description of a space group is possible in various ways. Two of these have gained wide acceptance and are given in *International Tables for X-Ray Crystallography* (1952) (here called I.T.):

(*a*) The entry 'general positions' gives for each point with the coordinates x,y,z (in an appropriate coordinate system) the coordinates of its images under the symmetry operations of the space group. Obviously a suitable choice from the infinite number of the symmetry operations has to be made.

(*b*) The geometric representation of the symmetry elements. On account of the periodicity of the lattice it is sufficient to list only the symmetry elements contained in a single unit cell. In I.T. this is done for all space groups except the cubic ones.

It is the purpose of this paper to describe a simple method for practical use to find (*b*) from a given (*a*). The user is assumed to have an elementary knowledge of crystallography. The only mathematical operation is the evaluation of a simple 3 × 3 determinant.

Procedure

In I.T. the general positions are given in the following form

$$r_1+a_{11}x+a_{12}y+a_{13}z;\quad r_2+a_{21}x+a_{22}y+a_{23}z;\quad r_3+a_{31}x+a_{32}y+a_{33}z\,. \qquad (1)$$

The r_i are rational numbers, the a_{ik} are ± 1 or 0.

Example: In space group $P6_122$ one finds, among others: $y-x,\ y,\ \frac{1}{2}-z$. This means $a_{11}=a_{33}=-1$, $a_{12}=a_{22}=+1$, $r_3=\frac{1}{2}$; all other a_{ik} and r_i are 0.

How does one find the symmetry element S of the operation σ which maps point xyz into the point with the coordinates given in (1)?

First one writes down the 'matrix' of the symmetry operation in the following way:

$$\mathbf{M}(\sigma)=\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & r_1 \\ a_{21} & a_{22} & a_{23} & r_2 \\ a_{31} & a_{32} & a_{33} & r_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right]=(\mathbf{A},\mathbf{r})\,. \qquad (2)$$

$\mathbf{A}=(a_{ik})$ describes uniquely a point symmetry operation ψ, where ψ is obtained from σ by removing all translation components. Such ψ have the origin as fixed point. $\mathbf{r}=(r_i)$ determines the 'position of the symmetry element in space' as well as the magnitude and direction of possible translation components.

The next step is the determination of the symmetry element F of ψ. In order to accomplish this, one first calculates the trace

Table 1. *Determination of the symmetry elements*

(i)	$F=1$	Translation with components (r_1, r_2, r_3)
(i)	$F=\bar{1}$	Inversion centre in $\langle \frac{1}{2}r_1, \frac{1}{2}r_2, \frac{1}{2}r_3\rangle$
(i)	$F=2$	One $a_{ii}=+1$, the other two $a_{kk}=-1$, $k\neq i$
	Direction of axis given by	$\mathbf{q}=\mathbf{a}$ for $i=1$; $\mathbf{q}=\mathbf{b}$ for $i=2$; $\mathbf{q}=\mathbf{c}$ for $i=3$.
	Screw vector	$r_i\mathbf{q}$
	Coordinates of a point on the axis	$\langle \frac{1}{2}r_1, \frac{1}{2}r_2, \frac{1}{2}r_3\rangle$
(i)	$F=m$	Two $a_{ii}=+1$, the third $a_{kk}=-1$, $k\neq i$.
	Normal to symmetry plane	$\mathbf{a}$ for $k=1$, $\mathbf{b}$ for $k=2$, $\mathbf{c}$ for $k=3$.
	Glide vector	$\frac{1}{2}\{(1+a_{11})r_1\mathbf{a}+(1+a_{22})r_2\mathbf{b}+(1+a_{33})r_3\mathbf{c}\}$.
	Coordinates of a point on symmetry plane	$\langle \frac{1}{2}r_1, \frac{1}{2}r_2, \frac{1}{2}r_3\rangle$

		(a)	(b)	(c)
(ii)	$F=2$			
	Direction of axis given by	$\mathbf{q}=[\mathbf{b}+a_{23}\mathbf{c}]$	$\mathbf{q}=[a_{31}\mathbf{a}+\mathbf{c}]$	$\mathbf{q}=[\mathbf{a}+a_{12}\mathbf{b}]$
	Screw vector	$\frac{1}{2}(r_2+a_{23}r_3)\mathbf{q}$	$\frac{1}{2}(r_3+a_{31}r_1)\mathbf{q}$	$\frac{1}{2}(r_1+a_{12}r_2)\mathbf{q}$
	Coordinates of a point on the axis	$\langle\frac{1}{2}(r_1, 0, -a_{23}r_2+r_3)\rangle$	$\langle\frac{1}{2}(-a_{31}r_3+r_1, r_2, 0)\rangle$	$\langle\frac{1}{2}(0, -a_{12}r_1+r_2, r_3)\rangle$
(ii)	$F=m$			
	Normal to symmetry plane	$[0\ 1\ -a_{23}]$	$[-a_{31}\ 0\ 1]$	$[1\ -a_{12}\ 0]$
	Glide vector	$\frac{1}{2}(r_2+a_{23}r_3)(\mathbf{b}+a_{23}\mathbf{c})+r_1\mathbf{a}$	$\frac{1}{2}(r_3+a_{31}r_1)(\mathbf{c}+a_{31}\mathbf{a})+r_2\mathbf{b}$	$\frac{1}{2}(r_1+a_{12}r_2)(\mathbf{a}+a_{12}\mathbf{b})+r_3\mathbf{c}$
	Coordinates of a point on symmetry plane	$\langle\frac{1}{2}(0, 0, -a_{23}r_2+r_3)\rangle$	$\langle\frac{1}{2}(-a_{31}r_3+r_1, 0, 0)\rangle$	$\langle\frac{1}{2}(0, -a_{12}r_1+r_2, 0)\rangle$
(ii)	$F=4$			
	Direction of axis	[100]	[010]	[001]
	Screw vector	$r_1\mathbf{a}$	$r_2\mathbf{b}$	$r_3\mathbf{c}$
	Coordinates of a point on the axis	$\langle\frac{1}{2}(0, r_2+a_{23}r_3, a_{32}r_2+r_3)\rangle$	$\langle\frac{1}{2}(a_{13}r_3+r_1, 0, r_3+a_{31}r_1)\rangle$	$\langle\frac{1}{2}(r_1+a_{12}r_2, a_{21}r_1+r_2, 0)\rangle$

(Remark: If the product (*a*) $a_{32}r_1$ or (*b*) $a_{13}r_2$ or (*c*) $a_{21}r_3$ has the value $(4n+1)/4$, n integer, a 4_1-axis is obtained; for $(4n+3)/4$ one obtains a 4_3-axis, for $(4n+2)/4$ a 4_2-axis.)

		(a)	(b)	(c)
(ii)	$F=\bar{4}$			
	Direction of inversion axis	[100]	[010]	[001]
	Coordinates of inversion point	$\langle\frac{1}{2}(r_1, r_2+a_{23}r_3, a_{32}r_2+r_3)\rangle$	$\langle\frac{1}{2}(a_{13}r_3+r_1, r_2, r_3+a_{31}r_1)\rangle$	$\langle\frac{1}{2}(r_1+a_{12}r_2, a_{21}r_1+r_2, r_3)\rangle$

(Remark: no translation components occur.)

		(a)	(b)
(iii)	$F=3$.		
	Direction of axis given by	$\mathbf{q}=a_{32}\mathbf{a}+a_{13}\mathbf{b}+a_{21}\mathbf{c}$	$\mathbf{q}=a_{23}\mathbf{a}+a_{31}\mathbf{b}+a_{12}\mathbf{c}$
	Screw vector	$\frac{1}{3}(a_{32}r_1+a_{13}r_2+a_{21}r_3)\mathbf{q}$	$\frac{1}{3}(a_{23}r_1+a_{31}r_2+a_{12}r_3)\mathbf{q}$
	Coordinates of point on the axis	$\langle\frac{1}{3}(r_1-a_{21}r_2, r_2-a_{32}r_3, r_3-a_{13}r_1)\rangle$	$\langle\frac{1}{3}(r_1-a_{31}r_3, r_2-a_{12}r_1, r_3-a_{23}r_2)\rangle$

[Remark: The symmetry operation belongs to a 3_1-axis if in (*a*) the screw vector is $[(3n+1)/3]\mathbf{q}$, in (*b*) $[(3n+2)/3]\mathbf{q}$, n integer. Similarly a screw vector $[(3n+2)/3]\mathbf{q}$ in (*a*) and $[(3n+1)/3]\mathbf{q}$ in (*b*) belongs to a 3_2-axis.)

		(a)	(b)
(iii)	$F=\bar{3}$		
	Direction of inversion axis	$-[a_{32}, a_{13}, a_{21}]$	$-[a_{23}, a_{31}, a_{12}]$
	Coordinates of inversion centre	$\langle\frac{1}{2}(r_1-a_{21}r_2+a_{13}r_3, a_{21}r_1+r_2-a_{32}r_3, -a_{13}r_1+a_{32}r_2+r_3)\rangle$	$\langle\frac{1}{2}(r_1+a_{12}r_2-a_{31}r_3, -a_{12}r_1+r_2+a_{23}r_3, a_{31}r_1-a_{23}r_2+r_3)\rangle$

(Remark: no translation components occur.)

(iv)	$F=2$	
	Direction of axis given by	$\mathbf{q}=(1+a_{11}+a_{12})\mathbf{a}+(1+a_{22}+a_{21})\mathbf{b}$
	Screw vector	$\frac{1}{2}[(1+a_{11}-a_{21}^2)r_1+(1+a_{22}-a_{12}^2)r_2]\mathbf{q}$
	Coordinates of a point on the axis	$\langle \frac{1}{2}r_1, \frac{1}{2}r_2, \frac{1}{2}r_3\rangle$
(iv)	$F=m$	
	Direction of normal to symmetry plane	$[1+a_{22}-a_{12}, 1+a_{11}-a_{21}, 0]$
	Glide vector	$\frac{1}{2}\{[(1+a_{11})r_1+a_{12}r_2]\mathbf{a}+[a_{21}r_1+(1+a_{22})r_2]\mathbf{b}+2r_3\mathbf{c}\}$
	Coordinates of a point on the symmetry plane	$\langle \frac{1}{2}r_1, \frac{1}{2}r_2, 0\rangle$

Table 1 (*cont.*)

(iv) $F=3$
Direction of axis [001]
Screw vector $r_3\mathbf{c}$
Coordinates of a point on the axis $\langle\frac{1}{3}[(1-a_{22})r_1+a_{12}r_2,\ a_{21}r_1+(1-a_{11})r_2,\ 0]\rangle$

(Remark: If $a_{21}r_3=(3n+1)/3$, n integer, a 3_1-axis is obtained; for $a_{21}r_3=(3n+2)/3$ one obtains a 3_2-axis.)

(iv) $F=6$
Direction of axis [001]
Screw vector $r_3\mathbf{c}$
Coordinates of a point on the axis $\langle a_{11}r_1+a_{12}r_2,\ a_{21}r_1+a_{22}r_2,\ 0\rangle$

(Remark: The symmetry operation belongs to a 6_1-, 6_2-, 6_3-, 6_4-, 6_5-axis, if $a_{21}r_3=(6n+1)/6$; $=(6n+2)/6$; $(6n+3)/6$; $(6n+4)/6$; $(6n+5)/6$ respectively.)

(iv) $F=\bar{3}$
Direction of inversion axis [001]
Coordinates of inversion centre $\langle a_{11}r_1+a_{12}r_2,\ a_{21}r_1+a_{22}r_2,\ r_3/2\rangle$

(Remark: no translation components occur.)

(iv) $F=\bar{6}$
Direction of inversion axis [001]
Coordinates of inversion point $\langle\frac{1}{3}\{(1-a_{22})r_1+a_{12}r_2,\ a_{21}r_1+(1-a_{11})r_2,\ \frac{3}{2}r_3\}\rangle$

(Remark: no translation components occur.)

$$\mathrm{tr}(\mathbf{A})=a_{11}+a_{22}+a_{33} \qquad (3)$$

and the determinant det(**A**). These two numbers determine F uniquely [see (4), where F is given in Hermann–Mauguin symbols].

F	1	2	3	4	6	$\bar{1}$	m	$\bar{3}$	$\bar{4}$	$\bar{6}$	
tr(**A**)	3	−1	0	1	2	−3	1	0	−1	−2	
det(**A**)	1	1	1	1	1	−1	−1	−1	−1	−1	(4)

In I.T., every matrix **A** belongs to one of four different types, which are defined as follows

$$\text{(i)}\quad \mathbf{A}=\begin{bmatrix}\pm1&0&0\\0&\pm1&0\\0&0&\pm1\end{bmatrix};$$

$$\text{(ii) }(a)\ \mathbf{A}=\begin{bmatrix}\pm1&0&0\\0&0&\pm1\\0&\pm1&0\end{bmatrix},$$

$$(b)\ \mathbf{A}=\begin{bmatrix}0&0&\pm1\\0&\pm1&0\\\pm1&0&0\end{bmatrix},$$

$$(c)\ \mathbf{A}=\begin{bmatrix}0&\pm1&0\\\pm1&0&0\\0&0&\pm1\end{bmatrix};$$

$$\text{(iii) }(a)\ \mathbf{A}=\begin{bmatrix}0&0&\pm1\\\pm1&0&0\\0&\pm1&0\end{bmatrix},$$

$$(b)\ \mathbf{A}=\begin{bmatrix}0&\pm1&0\\0&0&\pm1\\\pm1&0&0\end{bmatrix};$$

$$\text{(iv)}\quad \mathbf{A}=\begin{bmatrix}a_{11}&a_{12}&0\\a_{21}&a_{22}&0\\0&0&\pm1\end{bmatrix}$$ with one of the $a_{ik}=0$, the other three $a_{ik}=\pm1$; $i,k=1,2$.

Having determined F and the type of **A** one can go on to Table 1. This Table gives the full geometric characterization of the symmetry element S of the operation σ to which F and the type of **A** belong.

In order to make the procedure more comprehensible to the reader an example will now be given. We start with the values already listed in the text.

What kind of symmetry operation maps point x,y,z to $y-x,y,\frac{1}{2}-z$?

We find at once

$$\mathrm{tr}(\mathbf{A})=-1;\ \det(\mathbf{A})=\begin{vmatrix}-1&1&0\\0&1&0\\0&0&-1\end{vmatrix}=+1;$$

therefore $F=2$ from (4). (**A**) obviously is of type (iv). In the corresponding section of Table 1 we find the direction of the axis to be [120]. The screw vector equals **0** (2-axis) and the axis passes through the point $\langle 0,0,\frac{1}{4}\rangle$.

The (r_i) are not restricted to values less than unity; *e.g.*. we may have

$$x,y,z\rightarrow 5+y,3-x,{}^9/_4+z\ .$$

Application of the procedure gives: $F=4$; direction of axis [001]; screw vector $(\frac{9}{4})\mathbf{c}$; coordinates of a point on the axis $\langle 4,\bar{1},0\rangle$. The remark in Table 1 shows that the symmetry operation belongs to a 4_3-axis through $\langle 4,\bar{1},0\rangle$.

Appendix*

For settings other than those listed in I.T., matrices $\mathbf{M}=(\mathbf{A},\mathbf{r})$ can occur with (**A**)'s not belonging to one of the types (i) to (iv). In this case one can proceed as follows. (The formulae are valid for arbitrary unit cells; the *Procedure* given above is obtained as a special case for certain unit cells and settings.)

First F is determined from tr(**A**) and det(**A**) as described above under *Procedure*. Two cases are then distinguished.

(1) $\det(\mathbf{A})=+1$: n-fold rotation or screw axis. For $n>1$ the direction of the axis is given by the solutions **q** of the system of equations

$$(\mathbf{A}-\mathbf{E})\mathbf{q}=\mathbf{0} \text{ where } \mathbf{E} \text{ is the unit matrix.} \quad (5)$$

The translation component **t** (always parallel to **q**) is

$$\mathbf{t}=\frac{1}{n}\mathbf{B}\,\mathbf{r} \text{ with} \quad (6)$$

$$\mathbf{B}=\mathbf{A}^{n-1}+\mathbf{A}^{n-2}+\ldots+\mathbf{E}. \quad (7)$$

The points **x** on the axis are the solutions of the system of equations

$$\mathbf{A}\mathbf{x}+\mathbf{r}=\mathbf{x}+\mathbf{t}, \textit{ i.e.} \quad (8a)$$

$$(\mathbf{A}-\mathbf{E})\mathbf{x}=\left(\frac{1}{n}\mathbf{B}-\mathbf{E}\right)\mathbf{r}. \quad (8b)$$

For $n=2$, $\mathbf{x}=\frac{1}{2}\mathbf{r}$ is a special solution of (8*b*) and hence is a point on the axis.

The intersections of the axis with the planes (100), (010), and (001), if they exist (at least one does) are obtained by putting $x_1=0$, $x_2=0$, and $x_3=0$ respectively in (8*a*) or (8*b*).

(2) $\det(\mathbf{A})=-1$; inversion axis $\bar{n}$. There are three different cases.

$n=1$; see (i), $F=\bar{1}$.

$n=2$: $F=\bar{2}=\mathrm{m}$.

The vectors **q** normal to the mirror or glide plane are obtained by solving

$$(\mathbf{A}+\mathbf{E})\mathbf{q}=\mathbf{0}. \quad (9)$$

The translation component **t** is given by

$$\mathbf{t}=\tfrac{1}{2}(\mathbf{A}+\mathbf{E})\mathbf{r}. \quad (10)$$

The points **x** of the plane are the solutions of

$$\mathbf{A}\mathbf{x}+\mathbf{r}=\mathbf{x}+\mathbf{t}, \textit{ i.e.} \quad (11a)$$

$$(\mathbf{A}-\mathbf{E})\mathbf{x}=\tfrac{1}{2}(\mathbf{A}-\mathbf{E})\mathbf{r}. \quad (11b)$$

Special solution: $\mathbf{x}=\frac{1}{2}\mathbf{r}$.

Intersections with coordinate axes [100], [010], and [001], if existing (at least one does) are obtained by putting $\mathbf{x}=(x_1,0,0)$, $(0,x_2,0)$, and $(0,0,x_3)$ respectively in (11*a*) or (11*b*).

$n>2$: The inversion axes are at the same time rotation axes (4:2, $\bar{3}$ and $\bar{6}$:3). The direction of such a rotation axis is given by the solutions **q** of (9).

There are no translation components: $\mathbf{t}=\mathbf{0}$.

The inversion point **x** (centre of symmetry for $\bar{3}$; intersection of 3 and m for $\bar{6}$) is the (unique) solution of

$$\mathbf{A}\mathbf{x}+\mathbf{r}=\mathbf{x}, \textit{ i.e.} \quad (12a)$$

$$(\mathbf{A}-\mathbf{E})\mathbf{x}=-\mathbf{r}. \quad (12b)$$

We should like to thank Mr V. Gramlich and Dr W. E. Klee, Karlsruhe for their valuable help in finding a simple and understandable presentation.

* This section requires a basic knowledge of linear algebra.

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Étude Radiocristallographique Point par Point d'une Lame Monocristalline de $BaTiO_3$ par la Méthode de Lambot-Vassamillet et Influence du Champ Électrique

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The method allows observations of disorientations and parametral variations in barium titanate plates in connexion with the texture of domains. The effect of an applied electric field changed according to the texture of the region observed in the crystal, and it was possible to determine the piezoelectric behaviour on the microscopic scale.

Introduction

Diverses méthodes permettent l'étude de perturbations locales dans les cristaux par diffraction des rayons X. Le degré de perfection du cristal et la nature de l'imperfection étudiée conditionnent le choix de la méthode. Pour les cristaux de $BaTiO_3$, suffisamment imparfaits, on peut appliquer la théorie cinématique et le pouvoir