HEXAGONAL FOUR-INDEX SYMBOLS

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Introduction

The purpose of this paper is to present a mathematical derivation of some properties of the four-index notation, for faces and zones, in the hexagonal system. No such treatment seems to be available in English, although adequate presentations can be found in other languages.

I. Face Symbol

In the hexagonal crystal system, a face is referred to the Bravais axes (Fig. 1) by means of the four-index symbol $(hk\bar{i}l)$, in which $i=h+k$.

Proof.—Let a straight line AB intersect the negative a_3-axis in a point C. Let its intercepts be $OA=a/h$, $OB=a/k$, $OC=a/i$. The equation of the line AB is

$$x/(a/h) + y/(a/k) = 1;$$

that of the line OC, the bisector of the angle AOB, is

$$x = y.$$

The co-ordinates, OM and ON, of the point C are thus $x=y=a/(h+k)$. Since the triangles OMC and ONC are equiangular, hence equilateral, the intercept OC is equal to either co-ordinate of the point C,

$$OC = a/i = a/(h+k),$$

so that $i=h+k$.

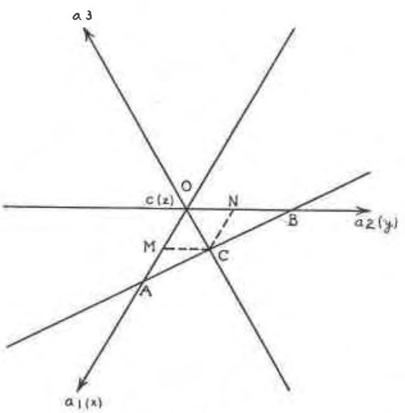

Fig. 1

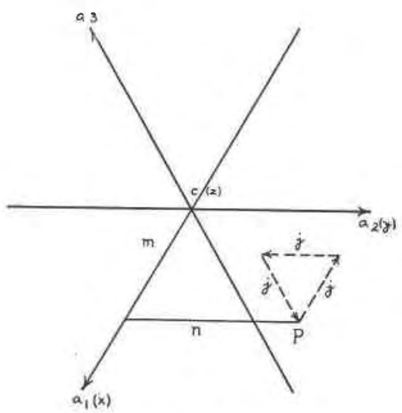

Fig. 2

II. Zone Symbol

A zone may likewise be expressed, in the four-index notation, by a symbol $[uv\bar{j}w]$, in which $j=u+v$.

Proof.—Let a point P in the $(a_1a_2a_3)$-plane (Fig. 2) be designated by the co-ordinates m, n, 0 (expressed in terms of the unit length a), which refer to the axes a_1, a_2, a_3, respectively. It is permissible to decrease (or increase) each of these co-ordinates by one and the same number, since the sum of the three vectors thus introduced is equal to zero. The point P can, therefore, be represented by the co-ordinates $m-j$, $n-j$, j, in which j is equal to any number, positive or negative. In particular, j may be chosen equal to $(m+n)/3$, so that the sum of the three co-ordinates

$$u = m - [(m + n)/3], \quad v = n - [(m + n)/3], \quad j = - (m + n)/3,$$

becomes equal to zero. The zone symbol $[mn0w]$ may, therefore, be written $[uv\bar{j}w]$, with $j=u+v$.

Remarks.—To pass from the four-index notation (axes a_1, a_2, a_3, c) to the three-index notation (axes a_1, a_2, c):

(1) In the case of a face symbol $(hk\bar{i}l)$, drop the third index and obtain (hkl);

(2) In the case of a zone symbol $[uv\bar{j}w]$, add j to the first three indices, so as to make the third index zero, and obtain $[u+j \cdot v+j \cdot w]$.

III. Equation of Zone Control

The equation of zone control is the relation between the indices of a zone $[uv\bar{j}w]$ and those of a face $(hk\bar{i}l)$ contained in the zone. Using the three-index notation, the face symbol is written (hkl) and the zone symbol $[u+j \cdot v+j \cdot w]$. It is known that the equation of zone control can then be expressed

$$h(u + j) + k(v + j) + lw = 0. \tag{1}$$

This can be written

$$hu + kv + (h + k)j + lw = 0$$

or, since $i=h+k$,

$$hu + kv + ij + lw = 0. \tag{2}$$

Because $j=u+v$, the latter equation may also be written

$$(h + i)u + (k + i)v + lw = 0. \tag{3}$$

The indices of a face $(hk\bar{i}l)$ situated at the intersection of two given zones $[u_1v_1\bar{j}_1w_1]$ and $[u_2v_2\bar{j}_2w_2]$ are found by means of equation (1). They must satisfy the equations:

$$(u_1 + j_1)h + (v_1 + j_1)k + w_1l = 0,$$
$$(u_2 + j_2)h + (v_2 + j_2)k + w_2l = 0.$$

The three indices h, k, l are therefore obtained by cross-multiplication:

$$\begin{array}{c|ccccccc|c}
(u_1+j_1) & (v_1+j_1) & & w_1 & & (u_1+j_1) & & (v_1+j_1) & w_1 \\
 & & \times & & \times & & \times & & \\
(u_2+j_2) & (v_2+j_2) & & w_2 & & (u_2+j_2) & & (v_2+j_2) & w_2 \\
\hline
 & & h & & k & & l & &
\end{array} \qquad (4)$$

and the superabundant index is $\bar{\imath} = -(h+k)$.

The indices of a zone $[uv\bar{\jmath}w]$ containing two given faces $(h_1k_1\bar{\imath}_1l_1)$ and $(h_2k_2\bar{\imath}_2l_2)$ are found by means of equation (3). They must satisfy the equations:

$$\begin{aligned}(h_1+i_1)u + (k_1+i_1)v + l_1w &= 0,\\ (h_2+i_2)u + (k_2+i_2)v + l_2w &= 0.\end{aligned}$$

The three indices u, v, w are therefore obtained by cross-multiplication:

$$\begin{array}{c|ccccccc|c}
(h_1+i_1) & (k_1+i_1) & & l_1 & & (h_1+i_1) & & (k_1+i_1) & l_1 \\
 & & \times & & \times & & \times & & \\
(h_2+i_2) & (k_2+i_2) & & l_2 & & (h_2+i_2) & & (k_2+i_2) & l_2 \\
\hline
 & & u & & v & & w & &
\end{array} \qquad (5)$$

and the *necessary* additional index is $\bar{\jmath} = -(u+v)$.

To check whether a given face $(hk\bar{\imath}l)$ is contained in a given zone $[uv\bar{\jmath}w]$, use equation (2).

Remarks.—Note that $(h+i \cdot k+i \cdot l)$ is *not* the three-index symbol of $(hk\bar{\imath}l)$ and that $[uvw]$ is *not* the three-index symbol of $[uv\bar{\jmath}w]$. In equation (2) the quantities h, k, i, l, on the one hand, u, v, j, w, on the other, play similar roles. This mathematical symmetry of equation (2) explains why it can be written in both forms (1) and (3). It also accounts for the fact that the same type of calculations permits finding the indices of a zone between two faces and those of a face at the intersection of two zones.

IV. Examples of Calculations

In beryl a face n is located at the intersection of two zones, between the faces $m(10\bar{1}0)$ and $v(21\bar{3}1)$ on the one hand, between the faces $a(11\bar{2}0)$ and $u(20\bar{2}1)$ on the other hand. What are its indices?

According to (5) we have

Indices of the first zone:

$$\begin{array}{c|cccc|c}
2 & 1 & 0 & 2 & 1 & 0 \\
 & & \times & \times & \times & \\
5 & 4 & 1 & 5 & 4 & 1 \\
\hline
 & & 1 & \bar{2} & 3 &
\end{array}$$

Indices of the second zone:

$$\begin{array}{c|cccc|c}
3 & 3 & 0 & 3 & 3 & 0 \\
 & & \times & \times & \times & \\
4 & 2 & 1 & 4 & 2 & 1 \\
\hline
 & & 3 & \bar{3} & \bar{6} &
\end{array}$$

The symbols of the two intersecting zones are $[1\bar{2}13]$ and $[1\bar{1}0\bar{2}]$.

According to (4) we have

Indices of the face n:

$$\begin{array}{cccccc} 0 & \bar{3} & 3 & 0 & \bar{3} & 3 \\ & \times & \times & \times & & \\ 1 & \bar{1} & \bar{2} & 1 & \bar{1} & \bar{2} \\ \hline & 9 & 3 & 3 & & \end{array}$$

The symbol of the face n is $(31\bar{4}1)$.

According to (2) the face $(31\bar{4}1)$ belongs to the zones $[1\bar{2}13]$ and $[1\bar{1}0\bar{2}]$ since

$$\begin{array}{cccc} 3 & 1 & \bar{4} & 1 \\ \times & \times & \times & \times \\ 1 & \bar{2} & 1 & 3 \\ \hline 3 & -2 & -4 & +3=0 \end{array} \qquad \begin{array}{cccc} 3 & 1 & \bar{4} & 1 \\ \times & \times & \times & \times \\ 1 & \bar{1} & 0 & \bar{2} \\ \hline 3 & -1 & +0 & -2=0 \end{array}$$

V. Addition and Subtraction Rule

In the three-index notation it is known that any face $(ph_1 \pm qh_2 \cdot pk_1 \pm qk_2 \cdot pl_1 \pm ql_2)$, where p and q are any integers, lies in a zone with the faces $(h_1k_1l_1)$ and $(h_2k_2l_2)$. The validity of this "addition and subtraction rule" is obviously unaffected by the use of the fourth, superabundant, index.

In the preceding example the indices of the face n could have been obtained simply as follows (taking $p=q=1$):

$$\begin{array}{cccc} 1 & 0 & \bar{1} & 0 \\ 2 & 1 & \bar{3} & 1 \\ \hline (3 & 1 & \bar{4} & 1) \end{array} \qquad \begin{array}{cccc} 1 & 1 & \bar{2} & 0 \\ 2 & 0 & \bar{2} & 1 \\ \hline (3 & 1 & \bar{4} & 1) \end{array}$$

By virtue of the duality principle between faces and zones, the addition and subtraction rule also holds good for four-index zone symbols. For instance the zone $[0\bar{1}15]$ passes through the intersection of the zones $[1\bar{2}13]$ and $[1\bar{1}0\bar{2}]$, since its indices are obtained by subtraction as follows:

$$\begin{array}{cccc} 1 & \bar{2} & 1 & 3 \\ 1 & \bar{1} & 0 & \bar{2} \\ \hline [0 & \bar{1} & 1 & 5] \end{array}$$

VI. Graphical Determination of a Zone Symbol from the Gnomonic Projection

In the three-index notation, the indices of a zone axis in the direct lattice (a_1, a_2, c) are the same as the indices of the plane perpendicular to the given zone axis in the reciprocal lattice (a_1^*, a_2^*, c^*). This follows from the very definition of the reciprocal lattice. The plane in question—the *zone plane*—contains all the normals to the faces in the zone. Its trace on the plane of the gnomonic projection is therefore the *zone line*.

The gnomonic projection is a representation of the reciprocal lattice (Mallard's Theorem). Indeed, since the scale of the projection is arbitrary, it is permissible to choose the plane of the gnomonic projection at a distance c^* above the origin; the gnomonic poles $(hk1)$ then constitute a net of the reciprocal lattice, namely its first layer. The natural axes of co-ordinates (P_1, P_2) of the gnomonic projection (Fig. 3) are parallel to the axes (a_1^*, a_2^*) of the reciprocal lattice. The zone plane passes through the origin; therefore, in order to find its indices in the reciprocal lattice, it is convenient to translate it parallel with itself until its intercept on the c^* axis is $-c^*$ or $c^*/\bar{1}$. After translation, the inter-

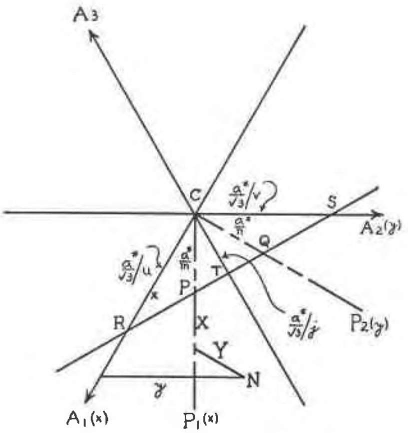

FIG. 3

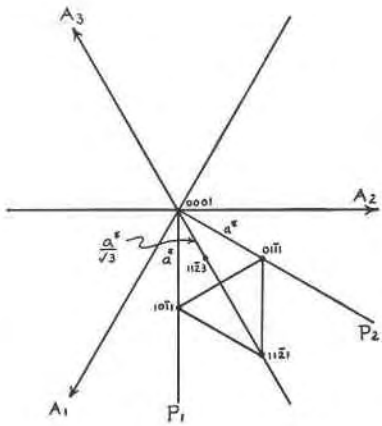

FIG. 4

cepts of the zone plane on the a_1^* and a_2^* axes of the reciprocal lattice are equal to the intercepts of the zone line on the P_1 and P_2 axes of the gnomonic projection. Let a^*/m and a^*/n be these intercepts, which can be determined graphically. The symbol of the zone plane in the reciprocal lattice is $(mn\bar{1})^*$. The symbol of the zone axis in the direct lattice (referred to the three axes a_1, a_2, c) is therefore $[mn\bar{1}]$. If the four axes, a_1, a_2, a_3, c, are used, the symbol may be written $[mn0\bar{1}]$ or preferably $[uv\bar{j}1]$, where u, v, j are the functions of m and n defined above (Section II). The necessity for carrying out the transformation $[mn0\bar{1}]$ to $[uv\bar{j}1]$ can be avoided and the latter symbol determined directly by graphical means, thanks to the following mathematical artifice.

Theorem.—In the plane of the gnomonic projection (Fig. 3) a zone line that intercepts a^*/m, a^*/n on the axes P_1, P_2 will intercept A/u, A/v, A/j (where $A = a^*/\sqrt{3}$) on the axes A_1, A_2, A_3.

Proof.—This theorem is easily proved by effecting a change of co-ordinates in the gnomonic plane. Let the old axes be P_1, P_2, with co-ordinates X, Y. Let the new axes be A_1, A_2, with co-ordinates x, y. The relation between the old and the new co-ordinates of any point N (Fig. 3) are

$$X + Y \sin 30° = x \cos 30°,$$
$$y - Y \cos 30° = x \sin 30°,$$

which can be written in the symmetrical forms

$$X = (2x - y)\sqrt{3}/3, \qquad Y = (2y - x)\sqrt{3}/3. \tag{6}$$

The equation of the zone line PQ in the old co-ordinate system is

$$X/(a^*/m) + Y/(a^*/n) = 1.$$

In the new co-ordinate system, it becomes, by virtue of relation (6) and after simple rearrangements,

$$x/\{(a^*/\sqrt{3})/[m - \tfrac{1}{3}(m+n)]\} + y/\{(a^*/\sqrt{3})/[n - \tfrac{1}{3}(m+n)]\} = 1$$

or

$$x/(A/u) + y/(A/v) = 1.$$

The intercepts on the axes A_1, A_2 are thus seen to be A/u and A/v. The intercept on the A_3 axis must be A/j, with $j = u + v$ (the proof of this is the same as that given in Section I).

Graphical method.—The indices $[uvj\bar{1}]$ of a zone line RS (Fig. 3) are obtained by measuring the intercepts A/u, A/v, A/j on the axes A_1, A_2, A_3. The unit length to be used, $A = a^*/\sqrt{3}$, is equal to one third the long diagonal of the reciprocal lattice mesh (a^*, a^*) built on the axes P_1, P_2 (see Fig. 4). It is equal to the distance of the pole $(11\bar{2}3)$ from the center of the gnomonic projection.

VII. Example

Given (Fig. 5) the poles $(10\bar{1}2)$ and $(01\bar{1}3)$ in gnomonic projection, find the symbol of the zone defined by these two faces.

Through the pole $(10\bar{1}1)$ pass a line parallel to the A_3 axis to obtain the unit length $A = a^*/\sqrt{3}$ on the A_1 axis. Measure the intercepts of the zone line RS on the axes A_1, A_2, A_3. They are: $CR = 3A$, $CS = 3A/4$, $-CT = -3A/5$. They can be written: $CR = A/(1/3)$, $CS = A/(4/3)$, $-CT = -A/(5/3)$. The intercept on the vertical axis is $-c^*$ by construction (see Section VI). The indices of the zone plane in the reciprocal lattice are therefore $(14\bar{5}\bar{3})^*$. The zone indices in the direct lattice are the same, $[14\bar{5}\bar{3}]$.

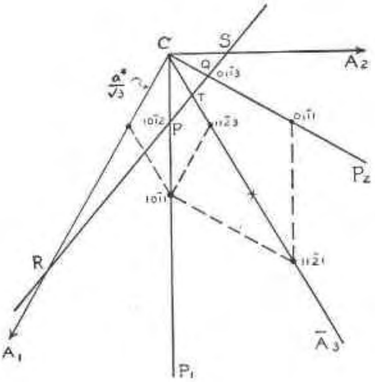

FIG. 5

VIII. REMARKS

The axes A_1, A_2, A_3 are *not* co-ordinate axes of the direct lattice. They are indeed parallel to the axes a_1, a_2, a_3 that pass through the origin. Their unit length, however, is $A = a^*/\sqrt{3}$, whereas the unit length a of the direct cell, expressed in terms of reciprocal lattice unit lengths, is $a = c^*a^*/V^* = c^*a^*/c^*a^{*2} \sin 60° = 2/a^*\sqrt{3}$ and not $a^*/\sqrt{3}$ as Wolfe implies (1944, pp. 52–53 and Fig. 4).

The four-index notation of hexagonal zones explained in Section II is due to Weber (1922). An excellent presentation is found in Terpstra's textbook (1927, pp. 201–204),[1] including the derivation of the equation of zone control in the four-index notation.

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TERPSTRA, P. (1927), *Leerboek der geometrische kristallografie*, 302 pp. P. Noordhoff, Groningen.

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WOLFE, C. W. (1944), Hexagonal zone symbols and transformation formulae: *Am. Mineral.*, **29**, 49–54.

[1] One misprint in Terpstra: on page 202, last line of the text, a minus sign is omitted. Read $\bar{\omega} = -(m+n)/3$.