THE THEORY OF DETERMINANTS APPLIED TO CRYSTALLOGRAPHY

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An example of the usefulness of determinants in crystallography is furnished by the derivation of the equation of zone control and of its applications. The application of the elementary properties of determinants leads, moreover, to several new zonal relations.

Three faces (hkl), $(h'k'l')$, $(h''k''l'')$ lie in a zone if the three parallel planes passed through the origin intersect along the same straight line. Analytically expressed, the condition is that the three linear homogeneous equations

$$h\frac{x}{a}+k\frac{y}{b}+l\frac{z}{c}=0$$

$$h'\frac{x}{a}+k'\frac{y}{b}+l'\frac{z}{c}=0$$

$$h''\frac{x}{a}+k''\frac{y}{b}+l''\frac{z}{c}=0$$

must yield one system of solutions. This will be the case if the *coefficient determinant*[1] be equal to zero or if

$$\begin{vmatrix} h & k & l \\ h' & k' & l' \\ h'' & k'' & l'' \end{vmatrix}=0$$

for when the elements of a row are multiplied by the same factor, the determinant is multiplied by that factor.

A determinant of the 3rd order is easily expanded according to the Rule of Sarrus. The above condition becomes

$$hk'l''+kl'h''+lh'k''-lk'h''-hl'k''-kh'l''=0.$$

If expansion be effected in terms of the co-factors of the elements of the first horizontal row, the condition for tautozonality is written:

$$\begin{vmatrix} k' & l' \\ k'' & l'' \end{vmatrix} h+\begin{vmatrix} l' & h' \\ l'' & h'' \end{vmatrix} k+\begin{vmatrix} h' & k' \\ h'' & k'' \end{vmatrix} l=0.$$

[1] A good and amply sufficient introduction to the theory of determinants and its application to the treatment of systems of linear equations is found in the first two chapters of Arnold Dresden: Solid Analytical Geometry and Determinants, 1930.

Developing and substituting

$$u = k'l'' - l'k'', \quad v = l'h'' - h'l'', \quad w = h'k'' - k'h'',$$

it assumes the usual form:

$$uh + vk + wl = 0$$

known as the *equation of zone control.*

The outlined method of derivation makes it immediately apparent why the symbol $[uvw]$ of a zone defined by two intersecting faces $(h'k'l')$ and $(h''k''l'')$ can be obtained by cross-multiplying the face indices. This so-called *process of cross-multiplication*, whose magic virtues seem so mysterious to most students, is hence reduced to its proper place of a mere mnemonic rule.

Laws of Addition and Subtraction[2]

(1) *The faces* $(h'+h''\cdot k'+k''\cdot l'+l'')$ *and* $(h'-h''\cdot k'-k''\cdot l'-l'')$ *are tautozonal with* $(h'k'l')$ *and* $(h''k''l'')$.

The proof. We have:

$$\begin{vmatrix} h'+h'' & k'+k'' & l'+l'' \\ h' & k' & l' \\ h'' & k'' & l'' \end{vmatrix} = 0,$$

for this determinant is equal to the sum of two determinants,

$$\begin{vmatrix} h' & k' & l' \\ h' & k' & l' \\ h'' & k'' & l'' \end{vmatrix} \text{ and } \begin{vmatrix} h'' & k'' & l'' \\ h' & k' & l' \\ h'' & k'' & l'' \end{vmatrix},$$

both equal to zero as they have two parallel rows identical.

The same proof holds true if the $-$ sign be substituted for the $+$ sign and the word "difference" for the word "sum" in the above.

Example: In axinite,[3] face $s(201)$ lies in a zone with $m(110)$ and $r(1\bar{1}1)$, and is also tautozonal with $M(1\bar{1}0)$ and $x(111)$. Its indices are determined by the Law of Addition.

Face $M(1\bar{1}0)$, whose indices are derived by the Law of Subtraction from those of $s(201)$ and $x(111)$, lies in a zone with s and x.

(2) *The faces* $(mh'+nh''\cdot mk'+nk''\cdot ml'+nl'')$ *and* $(mh'-nh''\cdot mk'-nk''\cdot ml'-nl'')$ *are tautozonal with* $(h'k'l')$ *and* $(h''k''l'')$, *where* m *and* n *will usually be simple integers owing to the restrictions of the Law of Haüy.*

[2] See Rogers, A. F., *Am. Mineral.*, vol. **11**, p. 303, 1926.

[3] The orientation and axial elements adopted here for axinite are those given by Dana.

The proof. Let

$$D=\begin{vmatrix} mh'\pm nh'' & mk'\pm nk'' & ml'\pm nl'' \\ h' & k' & l' \\ h'' & k'' & l'' \end{vmatrix},$$

where the elements of the first horizontal row are taken with + signs or − signs only. We may write

$$D=m\begin{vmatrix} h' & k' & l' \\ h' & k' & l' \\ h'' & k'' & l'' \end{vmatrix} \pm n\begin{vmatrix} h'' & k'' & l'' \\ h' & k' & l' \\ h'' & k'' & l'' \end{vmatrix}=0.$$

EXAMPLE: In axinite, twice the indices of $m(110)$, plus the indices of $z(1\bar{1}2)$, yield the symbol (312) of a face W in a zone with m and z.

Twice the indices of $y(021)$, minus the indices of $r(1\bar{1}1)$, give $(\bar{1}51)$ the symbol of face q which occurs in the zone ry.

The following fact has not yet been mentioned, as far as the writer is aware: it is sufficient to know that three faces lie in a zone to be in a position to state that other groups of three faces are also tautozonal.

The value of a determinant does not change if the columns are made into lines[4] and conversely. For instance, if

$$\begin{vmatrix} h & k & l \\ h' & k' & l' \\ h'' & k'' & l'' \end{vmatrix}=0.$$

we may also write

$$\begin{vmatrix} h & h' & h'' \\ k & k' & k'' \\ l & l' & l'' \end{vmatrix}=0$$

Hence,

THEOREM A: *If three faces (hkl), $(h'k'l')$, $(h''k''l'')$ be tautozonal, the faces $(hh'h'')$, $(kk'k'')$, $(ll'l'')$ also lie in a zone.*

EXAMPLE: In axinite, the faces $h(3\bar{1}0)$, (112), $s(201)$, $g(023)$, and $e(\bar{1}11)$ all lie in zone $[\bar{1}\bar{3}2]$. Making columns into lines in the determinant yielded by the first three faces leads to faces $W(312)$, $M(\bar{1}10)$, and $y(021)$ of zone $[\bar{1}\bar{1}2]$.

[4] Horizontal and vertical rows of a determinant are called *lines* and *columns*, respectively.

By using faces s, g, e instead, the symbols $(20\bar{1})$, $y(021)$, $\nu(131)$ are obtained: $(20\bar{1})$ is a possible face of zone $[1\bar{1}2]$ to which y and ν also belong.

The value of a determinant remains unchanged in absolute magnitude but its sign is changed when two parallel rows are interchanged.

Applying this property to two columns, we have:

THEOREM B: *If three faces (hkl), $(h'k'l')$, $(h''k''l'')$ lie in a zone, then other groups of three tautozonal faces may be obtained by interchanging any two (but the same two) indices in the symbols of the three given faces.*

The proof. The determinants

$$\begin{vmatrix} h & l & k \\ h' & l' & k' \\ h'' & l'' & k'' \end{vmatrix}, \quad \begin{vmatrix} l & k & h \\ l' & k' & h' \\ l'' & k'' & h'' \end{vmatrix}, \quad \begin{vmatrix} k & h & l \\ k' & h' & l' \\ k'' & h'' & l'' \end{vmatrix},$$

are all three equal to zero.

It immediately follows that the symbol of the new zone will in each case be obtained by interchanging the corresponding zone indices in the symbol of the original zone. If $[uvw]$ be the symbol of the given zone, then the three zones obtained by theorem B are respectively $[uwv]$, $[wvu]$, and $[vuw]$.

EXAMPLE: In axinite, faces $w(1\bar{3}0)$, $r(1\bar{1}1)$, and $y(021)$ lie in zone $[\bar{3}\bar{1}2]$. Faces $h(\bar{3}10)$, $e(\bar{1}11)$, and $s(201)$ lie in zone $[\bar{1}\bar{3}2]$.

REMARKS: If two indices are equal in a zone symbol, then by interchanging corresponding indices in the face-symbol of a face in the zone, another face in the same zone is obtained. This can also be derived by inspection of the equation of zone control.

EXAMPLE: In axinite, faces $s(201)$ and $i(3\bar{1}1)$ belong to zone $Ms[\bar{1}\bar{1}2]$. Faces $y(021)$ and $V(\bar{1}31)$ also lie in the same zone.

Now by applying the theorem B twice in succession it is found that if

$$\begin{vmatrix} h & k & l \\ h' & k' & l' \\ h'' & k'' & l'' \end{vmatrix} = 0,$$

the following is also true

$$\begin{vmatrix} k & l & h \\ k' & l' & h' \\ k'' & l'' & h'' \end{vmatrix} = 0, \text{ and } \begin{vmatrix} l & h & k \\ l' & h' & k' \\ l'' & h'' & k'' \end{vmatrix} = 0.$$

Hence,

THEOREM C: *If three faces (hkl), (h'k'l'), (h''k''l'') lie in a zone, two other groups of tautozonal faces are given by the cyclic permutations of the indices in the original three face symbols.*

It is easy to see that the zone indices follow the same permutation as the face indices. If [*uvw*] be the symbol of the original zone, then the two new zones yielded by theorem C are respectively [*vwu*] and [*wuv*].

EXAMPLE: In axinite, faces $a(100)$, $\alpha(210)$, and $m(110)$ lie in zone [001]. Faces $b(010)$, $y(021)$, and $f(011)$ lie in zone [100].

When the three zone indices are equal [111], the faces whose symbols are obtained by permuting the indices of the given faces lie in the original zone.

REMARKS: *If three faces (hkl), (h'k'l'), (h''k''l'') are known to lie in a zone, five additional groups of three tautozonal faces can be formed by applying theorems B and C to faces (hh'h''), (kk'k''), (ll'l'').*

Another proposition can be derived from the following: The value of a determinant remains unchanged when the elements of a row multiplied by a common factor are added to the elements of a parallel row.

This property applied to columns gives

THEOREM D: *If three faces (hkl), (h'k'l'), (h''k''l'') lie in a zone, then the three faces in any of the following groups are also tautozonal:*

$$\begin{array}{llll} (Hkl), & (H'k'l'), & \text{and} & (H''k''l''); \\ (hKl), & (h'K'l'), & \text{and} & (h''K''l''); \\ (hkL), & (h'k'L'), & \text{and} & (h''k''L''); \end{array}$$

where a capital letter (H, for instance) stands for the corresponding small letter (h) plus any multiple m of either one of the remaining indices (k or l). The same factor m must be used for the other capital letters (H', H'') of the group, and also the same remaining index (k', k'' or l', l'').

The proof. We have:

$$\begin{vmatrix} h+mk & k & l \\ h'+mk' & k' & l' \\ h''+mk'' & k'' & l'' \end{vmatrix} = \begin{vmatrix} h & k & l \\ h' & k' & l' \\ h'' & k'' & l'' \end{vmatrix} + m \begin{vmatrix} k & k & l \\ k' & k' & l' \\ k'' & k'' & l'' \end{vmatrix} = 0.$$

The same proof can be adapted to all cases.

It may be of interest to derive the symbol of the zone obtained in this manner and see under what condition the new zone will be the same as the original.

Let $[uvw]$ be the symbol of the zone containing the three faces (hkl), $(h'k'l')$, $(h''k''l'')$. Let $[UVW]$ be the symbol of the zone in which $(h+mk\cdot k\cdot l)$, $(h'+mk'\cdot k'\cdot l')$, $(h''+mk''\cdot k''\cdot l'')$ are found. Expanding the above determinant we get

$$U=\begin{vmatrix} k' & l' \\ k'' & l'' \end{vmatrix}=u,\quad V=\begin{vmatrix} l' & h'+mk' \\ l'' & h''+mk'' \end{vmatrix}=v-mu,\quad W=\begin{vmatrix} h'+mk' & k' \\ h''+mk'' & k'' \end{vmatrix}=w$$

This result can readily be generalized into the following rule.

RULE: *If m times the pth index be added to the qth index in each original face symbol* (pth and qth being any two different ordinal numbers out of 1st, 2nd, and 3rd), *then the symbol of the new zone is derived from the original zone symbol by subtracting m times the qth index from the pth.*

A sufficient condition for the new zone to coincide with the original zone is that the qth index of the original zone symbol be equal to zero.

For instance, if m times the 2nd index be added to the 1st index in each face symbol of three tautozonal faces, then m times the 1st index must be subtracted from the 2nd index in the original zone symbol $[uvw]$ in order to obtain the symbol $[u\cdot v-mu\cdot w]$ of the new zone. The two zones will coincide if the original zone symbol is of the form $[Cvw]$.

It goes without saying that, in all cases, the resultant indices must be cleared of common factors if necessary and, in case m should not be chosen an integer, the indices should be cleared of common denominators.

EXAMPLE: In axinite, faces $s(201)$, $e(\bar{1}11)$, and $h(3\bar{1}0)$ lie in zone $[\bar{1}\bar{3}2]$. Take $m=-1$, let $p=2$ and $q=3$. It will be found that faces $s(201)$, $M(\bar{1}10)$, and $i(3\bar{1}1)$ lie in zone $[\bar{1}\bar{1}2]$. In the face symbols, the 2nd index is subtracted from the 3rd; in the zone symbol, the 3rd index is added to the 2nd.

It may be well to recall that to all these properties of tautozonal faces, perfectly similar properties correspond for coplanar edges on account of the known duality principle.

The starting point is the condition for three edges to be coplanar (or, in other words, for three zones to include the same face; for three zone circles to intersect in one point; for three lattice rows to lie in the same reticular plane):

$$\begin{vmatrix} u & v & w \\ u' & v' & w' \\ u'' & v'' & w'' \end{vmatrix} = 0.$$

The developments are the exact duplication of the above. They are omitted here for the sake of brevity.

Finally, one should not lose sight of the fact that the word "face" is here used in its broadest sense covering all planes (evidence of discontinuous vectorial properties) which obey Haüy's Law of Rationality: cleavage planes, twinning planes, gliding planes, x-ray "reflection" planes, as well as actual bounding faces. The meaning of the term "edge" is similarly extended: the intersection of two possible crystal planes, from the standpoint of rationality of indices.

NOTES AND NEWS

OCTAHEDRITE AS AN ALTERATION PRODUCT OF TITANITE

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In 1930 Dr. Hugh S. Spence of the Department of Mines of Canada described[1] a pegmatite rich in thucholite derived from uraninite from Henvey Township, Ontario. An important constituent of this pegmatite was an altered titanite intimately associated with thucholite. Dr. Spence submitted samples of this titanite to the Harvard Mineralogical Museum for examination as to the nature of its alteration, and the microscopic study of these specimens was entrusted to the author since the unusual type of alteration-product seemed to merit detailed description.

According to Dr. Spence the titanite is intimately associated with uraninite and thucholite in the centres of core-like masses of oligoclase which are distributed through the main mass of microcline. The titanite is in massive form, in aggregates of coarse crystals, pieces up to three pounds in weight having been found.

The specimens submitted are rough crystals or fragments bounded more or less by parting surfaces, the largest piece measuring 8 by 4 by 1.5 cms. They are dark green to yellowish green in color and none of them shows any of the original titanite substance. A clay-like substance not definitely determined is the main con-

[1] A remarkable occurrence of thucholite and oil in a pegmatite dyke, Parry Sound District, Ontario. *Am. Mineral.*, vol. **15**, pp. 499–520, 1930.