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A GRAPHICAL DERIVATION OF THE CRYSTALLOGRAPHIC ROTATION AXES

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Abstract

The reason why axes of order $n=5$ and $n>6$ cannot occur in lattices is that, in a semi-circle, only one chord can be equal in length to the radius and parallel to the diameter.

Sommaire

L'inexistence d'axes d'ordre $n=5$ et $n>6$ dans les réseaux découle du fait que, dans un demi-cercle, une seule corde de longueur égale au rayon est parallèle au diamètre.

Introduction

The proof that the only rotation axes of symmetry that are possible in crystals are of order 1, 2, 3, 4, 6 need not postulate the existence of a lattice: this so-called *crystallographic restriction* is a consequence of Haüy's law of Rationality[1], which is less restrictive than the lattice. For this reason, as was pointed out by G. Friedel (1926), it is erroneous to conclude that the fact of the non-existence of rotation axes of order 5 or greater than 6 *proves* the existence of a lattice[2].

Nowadays, since the existence of a lattice in every crystal is a datum of observation, we are justified in using it as the basis of the mathematical proof, which is thereby considerably simplified. The following derivation postulates the lattice and recognizes the fact that any lattice has a symmetry center at every node (by lattice construction every row through a given node is centrosymmetric in it). The proof also accepts the lemma that the order n of a rotation axis must be an integer (an n-fold axis acting on a node outside the axis generates n nodes in all, which lie at the vertices of a regular polygon, an n-gon, in a net plane normal to the axis).

The Proof

Let an n-fold rotation axis of the crystal be perpendicular to the plane of the paper (Fig. 1) and intersect it at B. Consider the crystal lattice constructed on B, which is taken as the initial node. (The lattice, being the geometrical representation of the translation group, can indeed begin anywhere.) Let C be one of the nodes closest to B in the net. Set $BC=a$. No row in the net can have an internodal spacing shorter than a. Since C is translation equivalent to B, there must pass an n-fold axis through C. It follows that no node other than B and C can exist *inside* the semi-circles of radius a drawn around B and C, on the same side of BC. For convenience let ω designate the smallest rotation $360°/n$ that can be performed around an n-fold axis.

I. The permissible cases

Consider $n=6$. Rotate node C around B through $\omega=60°$, both counterclockwise to node F and clockwise to node E′ (not shown, but centrosymmetrical of E with respect to node B, so that as E′ is a node so is E). Likewise rotate B around C through 60° in both senses, thus determining two rows CF and CG. The triangles BCF, EFB and FGC are equilateral, the nodes E, F, G form a row parallel to BC, and the construction has yielded an hexagonal net, thus showing that the 6-fold axis is compatible with

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[1]The proof that is based on Haüy's law of Rationality, available in Friedel (1926), Hilton (1903) and de Jong (1959), leads to the condition that cos ω, $\omega=360°/n$ with n an integer, must be rational. The proof that 0, ±½, ±1 are the only rational values of cos ω was first "given by N. Budaiev to Gadolin, read March 19, 1867, and published in 1871." It can be found in *Ostwald's Klassiker* No 75 (Anhang B). Richmond's later proof is given by Coxeter (1969, p. 443).

[2]This fallacy is found, for instance, in P. Niggli (1920): "Dieser Satz ermöglicht uns die erste Nachprüfung der Annahme die Kristalle . . . seien aus Raumgittern aufgebaut."

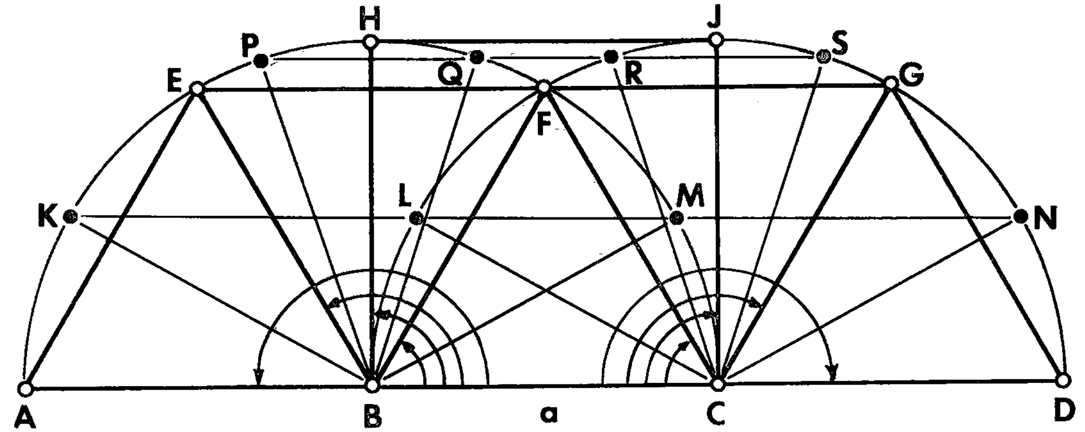

FIG. 1. Net plane perpendicular to which n-fold axes are considered at B and C. BC=a is the shortest internodal distance. Rotations of $\pm\omega$, $\omega=360°/n$, yield new nodes (white circlets) on rows parallel to BC: row EFG for $n=6$ and $n=3$, row HJ for $n=4$, row ABCD for $n=2$ and $n=1$. Black circlets are points generated for $n=5$ and $n>6$; they lie on lines, PQRS and KLMN, that are *not* rows.

the lattice. Note that the same hexagonal net would also be generated for $n=3$, so that the 3-fold axis is also possible.

For $n=4$, a similar construction with $\omega=90°$ leads to row HJ parallel to BC and the square BCHJ is the mesh of a tetragonal net: the 4-fold axis is thus permissible.

For $n=2$ the rotations through $\omega=180°$ around B and C bring C onto A and B onto D. The two new nodes being part of row BC, the 2-fold axis is permissible.

For $n=1$ and $\omega=360°$, the construction brings B onto itself and C onto itself, thus yielding the same row as for $n=2$. Both the 2-fold axis and the (trivial) 1-fold axis are thus shown to be possible.

II. The forbidden cases

For $n=5$, $\omega=72°$, the above construction yields points P and Q, by rotations of C around B, and points R and S, by rotations of B around C. The points PQRS are seen to be collinear on a line parallel with BC, but they do not form a row because they are not equidistant and their spacings are less than a. (PR=QS=a, whence PQ=RS<a and QR<a).

For $n>6$, $\omega<60°$, the construction generates, on a line parallel with BC, points such as KLMN, which are collinear but not equidistant. (KL=MN=a, but LM<a).

Cases $n=5$ and $n>6$ are thus ruled out.

Geometrically the ultimate reason why these cases are eliminated is thus that, *in a semi-circle, there exists only one chord that is equal to the radius and parallel to the diameter.*

Remark

The treatment of the forbidden cases acquires more unity (as suggested to us by Dr. Yvon Le Page) if one takes advantage of the centrosymmetry of a net in any node. A pentagon of points related by a 5-fold axis passing through a node B, for instance, thus generates a decagon by inversion through B, and the 5-axis turns into a 10-axis. The case $n=5$ is simply ruled out because it implies $n=10$, which is impossible as $n>6$.

ADVANTAGES OF THE PROPOSED PROOF

The proof given here does more than eliminate the forbidden cases: it shows the geometrical outcome in the permitted cases, and enables the different nets that are possible in the plane to be enumerated and visualized. In addition to the *hexagonal net* and the *tetragonal net* shown on the drawing, three more nets can be derived from the only condition that each one must contain row BC. This row provides the shortest vector BC=a; vector b, defined as the next shortest in the net, can be taken: either (i) perpendicular to a (along BH) or (ii) oblique to a, in which case its projection onto a is either (1) of length $a/2$ or (2) of any other length. The additional nets thus found are, respectively, the *rectangular net*, the *primitive rhombic* (or centered–rectangular) *net* and the *parallelogrammic net*.

HISTORICAL SURVEY

This historical survey does not claim to be exhaustive. Its purpose is simply to trace the origin of a number of proofs, some of which are encountered in present-day literature without any reference to their source. We shall consider two kinds of proofs: geometrical and analytical.

Geometrical proofs

Among the geometrical proofs, that of Barlow (1901) is particularly attractive. It can be explained by means of our Figure 1. Two n-fold axes, perpendicular to the plane of the paper at Q and B, are situated at minimum distance a apart. Axis Q, rotated through $\omega=2\pi/n$ clockwise around B, gives C; B, rotated through ω around C, gives R. If R coincides with Q (in F), we have $n=6$. If R does not coincide with Q, line QR is parallel to BC and the distance QR must be equal to ka, k an integer. Case $k=1$ corresponds to HJ$=a$, which requires $\omega=\pi/2$, whence $n=4$. Case $k\geqslant 2$ demands $\omega>\pi/2$, whence $n<4$ (EG$=2a$ yields $n=3$; AD$=3a$, $n=2$ and $n=1$.) This proof has been used in English text-books, such as Wells (1956). Coxeter (1961) gives "Barlow's elegant proof" with its reference. Fejes Tóth (1964) credits William Barlow for a "simple direct proof of the crystallographic restriction", gives the proof but omits the bibliographic reference.

Popov & Shafranovskii (1964) prove the incompatibility of a 5-axis with a lattice by forming the pentagon of "equivalent atoms" nearest to a given 5-axis and constructing, on two consecutive sides of the pentagon, a parallelogram which generates a sixth atom; this atom is closer to the given 5-axis than the postulated minimum distance. The cases $n\geqslant 7$ are ruled out in like manner. This proof is found in Shafranovskii (1968) and Flint (1968).

Coxeter (1969, p. 207) points out that the crystallographic restriction is, in a sense, a theorem of affine geometry: the only affinely regular n-gons that are affinely constructible (i.e., with the "parallel ruler") are those with $n=2$, 3, 4, 6. It thus appears that the two distinct crystallographic constraints, the existence of a lattice versus the law of Rationality, correspond to two different geometries, the Euclidean geometry, with its five postulates, versus the affine geometry, which has no circles and no right angles.

Analytical proofs

As mentioned above, the proof based on the law of Rationality (Gadolin 1871) rests on the condition that cos ω, $\omega=2\pi/n$, must be rational, thereby requiring finding which rational values of cos ω correspond to integral values of n (a non-trivial task). Most proofs based on the existence of a lattice, on the other hand, establish (after Bravais 1850) the condition that cos ω must be equal to half an integer or, equivalently, that sin $(\omega/2)$ must be equal to half the square root of an integer. Finally two proofs were found (Fedorov 1891; Cesàro 1902) that apparently were not followed by later text-book authors.

Bravais (1850) considers two n-axes B and C, perpendicular to the plane of the paper (Fig. 1) and separated by the minimum distance a. He rotates B around C through BCS $= -\omega$ to S and through $+\omega$ to S′ (S′, not shown on the Figure, is the mirror-image of S in the row BC). It follows that BS and BS′ are lattice vectors, whose vector sum BT determines a node T (not shown) on row BC. Distance BT must be equal to ka, k an integer, but BT is equal to $2a(1-\cos\omega)$ or $4a\sin^2(\omega/2)$. The condition thus expressed immediately yields the desired values of n. The method has been widely used in French text-books; e.g., Mallard (1879), Buttgenbach (1953), Mélon (1949) and Brasseur (1967).

Whereas Bravais and his followers make use of two rotations of opposite senses, through an angle ω, around a single n-axis C to get two lattice vectors whose sum will yield the additional node on the original row BC, later authors (Niggli 1920; Buerger 1956; Azároff 1960) use the rotations $+\omega=$CBQ and $-\omega=$BCR around two distinct axes, B and C respectively, to generate a new row QR, parallel to the original row. The condition that QR$=a(1-2\cos\omega)$ must be euqal to $k'a$ yields $\cos\omega=k''/2$, with $k''=1-k'$ and both k' and k'' integers.

Sands (1969) modifies the figure by considering a string of equivalent n-axes in a row AB . . . CD and letting the rotations through $+\omega$ and $-\omega$ be performed around A and D respectively to generate E and G (Fig. 1). The condition that EG$=$AD$-2a\cos\omega$ must be a multiple of a becomes, by letting EG$=la$ and AD$=ma$, $\cos\omega=(m-l/2$, m and l integers.

Buerger (1970) offers the simplest variant: three axes A, B, C are considered (Fig. 1); rotations through $-\omega$ and $+\omega$ around a single axis B carry A to P and C to Q. PQ is parallel to AB; it must be a row, so that PQ$=2a\cos\omega$ must be equal to ka, whence $\cos\omega=k/2$, k an integer.

Fedorov (1891) considers a series of n-axes A, E, F, C, . . . as occupying the i vertices of a regular polygon around an i-axis at B, so that ABE$=2\pi/i$ (Fig. 1). Axis A, rotated through $\omega=2\pi/n$ around axis E, generates axis F; likewise, E rotated around F, creates C, etc.

Triangle ABE yield $(\pi/i)+(\pi/n)=\pi/2$, whence

$$n=2i/(i-2),$$

where i and n must be integers. For i = 2, 3, 4, (5), 6, ∞, one finds n = 2, 6, 4, (10/3), 3, 2, so than $n=5$ is ruled out. For $6<i<\infty$, set $i=6+k$, k a positive integer; this gives[4]

$$n = (12+2k)/(4+k) = 3-[k/(4+k)],$$

which requires $2<n<3$, so that n cannot be an integer.

An original proof, somewhat analogous to that of Fedorov, was proposed by Cesàro (1902). Two n-axes, B and C, are separated by minimum distance a (Fig. 1). Rotate C around B, through ω=CBQ=$2\pi/n$; further rotations through ω would generate additional n-axes whose traces would lie on the circle of radius a drawn around B. Now rotate Q through ω around C; this rotation will bring Q onto a new axis Q′. Point Q′ cannot lie inside the circle, except at its center B, when ϕ=QCB must equal ω, Q is at F, and n equals 6. If Q′ lies *on* the circle, it will be symmetrical of Q in the row BC, thus requiring ω=QCQ′ to be equal to 2ϕ; bisecting QBC, we get $(\omega/2)+\phi=\pi/2$ or $\omega+2\phi=\pi$, in which we replace 2ϕ by ω and obtain $2\omega=\pi$ or $n=4$, in which case Q is at H. Finally if Q′ lies outside the circle, ω=QCQ′ must exceed 2ϕ, which gives $n<4$.

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[4]Erratum: in both the Russian text (1949) and the English translation (1971), the formula reads $n=(2+2k)/(4+k)$.