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Determination of the Crystal Elements from Angle Measurements

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Websky gave a crystallographic method to find the crystal elements from the angle measurements between four arbitrary crystal faces, using the Gauss-Miller relation on anharmonic ratios of four tautozonal faces. We extend this relation to five arbitrary faces and apply it to the same problem.

Introduction

The values of five independent angles between four, appropriately indexed faces (Brezina, 1884, p. 205) are necessary for the deduction of the crystal elements a/b, c/b, α, β, γ of a triclinic crystal. This number is reduced for symmetrical axial crosses but, these cases being simpler, we consider the triclinic system.

The calculation methods are divided into two groups, the mathematical and the crystallographic. In the first methods the cosines of the five angles are expressed in terms of the crystal elements or as functions of these; one may choose as the functions z_{ik} (Hecht, 1887, 1891) or g^* (de Jong & Bouman, 1939, who denote our g^* by g'). The calculations are laborious and usually these methods are avoided.

A crystallographic method is due to Websky and makes use of the Gauss-Miller anharmonic-ratios relation between the sines of the included angles of four tautozonal faces and their indices (Gauss, 1831, p. 308; Miller, 1839, p. 12). The method is described by Liebisch (1881, p. 159).

Instead of using the above-mentioned anharmonic ratios, which are concerned essentially with two-dimensional cases, we can apply with advantage three-dimensional anharmonic ratios between arbitrary faces. We shall in the first place derive these relations.

Spatial anharmonic ratios

Five arbitrary faces, of which no three are tautozonal, may be symbolized $h_0(h_0k_0l_0)$, $h_1(h_1k_1l_1)$, $h_2(h_2k_2l_2)$, $h_3(h_3k_3l_3)$ and $h_4(h_4k_4l_4)$. In the reciprocal lattice these faces are represented by five lattice points; a radius vector from the origin O^* to $h_0k_0l_0$ is perpendicular to the face h_0, and each point $nh_0nk_0nl_0$, where n is an integer, lies on the radius vector and also represents the crystal face in question.

We now consider on each of the five radius vectors the point of which the first index possesses the value $h_0h_1h_2h_3h_4$; these five points, called H_0, H_1, H_2, H_3 and H_4, all lie in a plane parallel to the axial plane B^*C^* (Fig. 1). Then we may distinguish five quadruples of tetrahedra: each tetrahedron has its summit in O^*, while the base is in the plane parallel to B^*C^*; each quadruple possesses a common edge, namely one of the radius vectors O^*H_0, O^*H_1, etc.

We consider the quadruple with the common edge O^*H_0 and write down the following anharmonic ratio of the volumes of the four tetrahedra:

$$\frac{V_{102}}{V_{203}}:\frac{V_{104}}{V_{304}}=\frac{V_{102}\,V_{304}}{V_{203}\,V_{104}},$$

where V_{102} is the volume of the tetrahedron $O^*H_1H_0H_2$.

Now the volume of a tetrahedron is on the one hand

$$V=\tfrac{1}{6}r_1r_2r_3 \operatorname{Sin}(123),$$

and on the other

$$V=\tfrac{1}{3}\ \text{base}\times\text{height}.$$

In these formulae r_1, r_2 and r_3 are the lengths of the radius vectors and Sin (123) is the spatial sine of the solid angle between r_1, r_2 and r_3. We have for Sin (123)

$$\begin{aligned}\operatorname{Sin}(123) &= \sqrt{\begin{vmatrix}1 & \cos(12) & \cos(13)\\ \cos(21) & 1 & \cos(23)\\ \cos(31) & \cos(32) & 1\end{vmatrix}}\\ &= \sqrt{\{1-\cos^2(12)-\cos^2(23)-\cos^2(31)} \\ &\qquad \overline{+2\cos(12)\cos(23)\cos(31)\}}\\ &= \sin(12)\sin(23)\sin(123), \qquad (1)\end{aligned}$$

where cos (12) is the cosine of the angle between r_1 and r_2 and sin (123) is the sine of the angle on the edge r_2 between the planes (12) and (23).

The heights of the tetrahedra are equal and the volumes proportional to the areas of their bases. Hence

$$\frac{\frac{1}{6}r_1r_0r_2\operatorname{Sin}(102).\frac{1}{6}r_3r_0r_4\operatorname{Sin}(304)}{\frac{1}{6}r_2r_0r_3\operatorname{Sin}(203).\frac{1}{6}r_1r_0r_4\operatorname{Sin}(104)}=\frac{\operatorname{Sin}(102)\operatorname{Sin}(304)}{\operatorname{Sin}(203)\operatorname{Sin}(104)}$$

$$=\frac{\text{area}\,\triangle H_1H_0H_2.\text{area}\,\triangle H_3H_0H_4}{\text{area}\,\triangle H_2H_0H_3.\text{area}\,\triangle H_1H_0H_4}. \qquad (2)$$

Now the area of a triangle, of which the vertices are three points m_1n_1, m_2n_2, and m_3n_3 of a net-plane whose primitive parallelogram has the area A_p, is

$$\text{area}\,(123)=\tfrac{1}{2}\begin{vmatrix}m_1 & n_1 & 1\\ m_2 & n_2 & 1\\ m_3 & n_3 & 1\end{vmatrix}A_p.$$

On substituting this in (2) we find:

$$\frac{\text{Sin }(102)\text{ Sin }(304)}{\text{Sin }(203)\text{ Sin }(104)}$$

$$=\frac{\begin{vmatrix} k_1h_0h_2h_3h_4 & l_1h_0h_2h_3h_4 & 1 \\ k_0h_1h_2h_3h_4 & l_0h_1h_2h_3h_4 & 1 \\ k_2h_0h_1h_3h_4 & l_2h_0h_1h_3h_4 & 1 \end{vmatrix} \begin{vmatrix} k_3h_0h_1h_2h_4 & l_3h_0h_1h_2h_4 & 1 \\ k_0h_1h_2h_3h_4 & l_0h_1h_2h_3h_4 & 1 \\ k_4h_0h_1h_2h_3 & l_4h_0h_1h_2h_3 & 1 \end{vmatrix}}{\begin{vmatrix} k_2h_0h_1h_3h_4 & l_2h_0h_1h_3h_4 & 1 \\ k_0h_1h_2h_3h_4 & l_0h_1h_2h_3h_4 & 1 \\ k_3h_0h_1h_2h_4 & l_3h_0h_1h_2h_4 & 1 \end{vmatrix} \begin{vmatrix} k_1h_0h_2h_3h_4 & l_1h_0h_2h_3h_4 & 1 \\ k_0h_1h_2h_3h_4 & l_0h_1h_2h_3h_4 & 1 \\ k_4h_0h_1h_2h_3 & l_4h_0h_1h_2h_3 & 1 \end{vmatrix}}$$

$$=\frac{\begin{vmatrix} h_1k_1l_1 \\ h_0k_0l_0 \\ h_2k_2l_2 \end{vmatrix} \begin{vmatrix} h_3k_3l_3 \\ h_0k_0l_0 \\ h_4k_4l_4 \end{vmatrix}}{\begin{vmatrix} h_2k_2l_2 \\ h_0k_0l_0 \\ h_3k_3l_3 \end{vmatrix} \begin{vmatrix} h_1k_1l_1 \\ h_0k_0l_0 \\ h_4k_4l_4 \end{vmatrix}} \qquad (3)$$

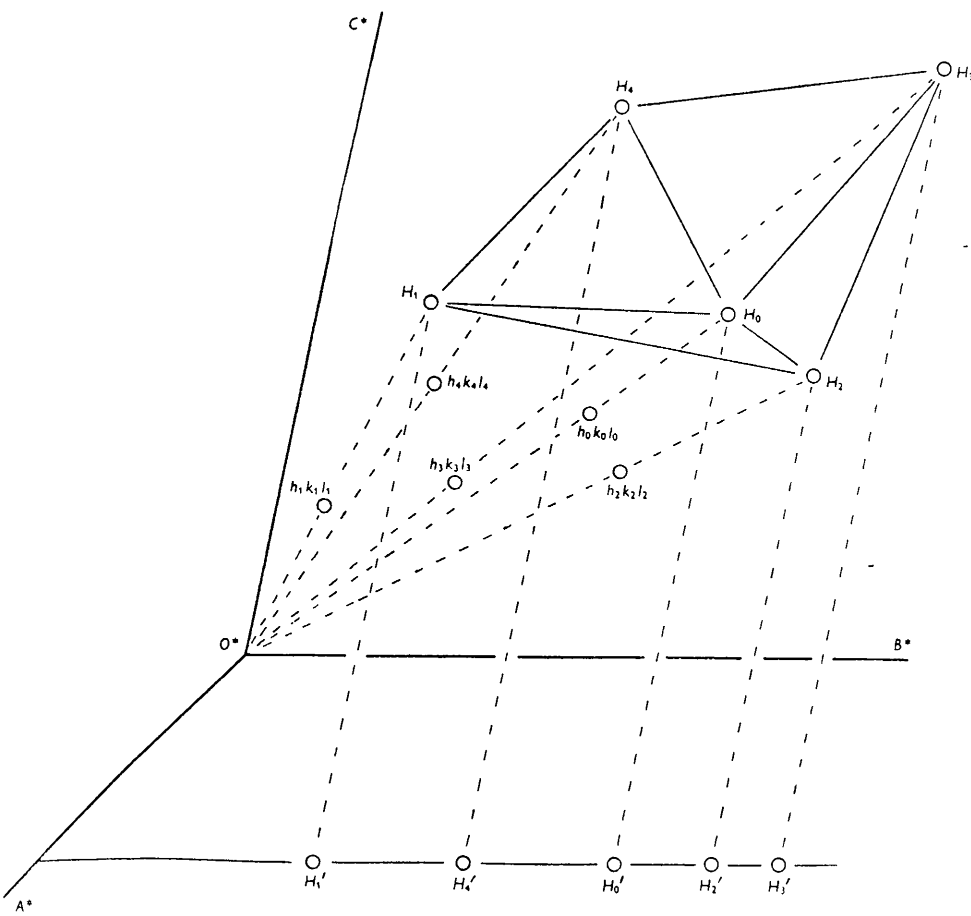
This and the similar anharmonic ratios may be considered as the spatial analogues of the Gauss-Miller relations. Their rationality was pointed out by Gauss (cf. Liebisch, 1881, p. 69), but he did not derive their values.

Replacing the Sines by their values (1), we find finally the useful formula

$$\frac{\sin (102) \sin (304)}{\sin (203) \sin (104)} = \frac{\begin{vmatrix} h_1k_1l_1 \\ h_0k_0l_0 \\ h_2k_2l_2 \end{vmatrix} \begin{vmatrix} h_3k_3l_3 \\ h_0k_0l_0 \\ k_4h_4l_4 \end{vmatrix}}{\begin{vmatrix} h_2k_2l_2 \\ h_0k_0l_0 \\ h_3k_3l_3 \end{vmatrix} \begin{vmatrix} h_1k_1l_1 \\ h_0k_0l_0 \\ h_4k_4l_4 \end{vmatrix}} \qquad (4)$$

We observe that sin (102) is the sine of the angle between two planes, the first being the plane through the perpendiculars to h_1 and h_0 and the second the plane through the perpendiculars to h_0 and h_2: in other words, the sine of the angle between the zone planes $[h_1h_0]$ and $[h_0h_2]$ and in the stereographic projection the angle between the zone circles $[h_1h_0]$ and $[h_0h_2]$.

Formula (4) enables us, without calculating crystal elements or other constants, to derive the symbol of a fifth face, when we are given five (and hence also six)



$H_1 \equiv (h_1h_0h_2h_3h_4,\ k_1h_0h_2h_3h_4,\ l_1h_0h_2h_3h_4)$

$H_1' \equiv (h_1h_0h_2h_3h_4,\ k_1h_0h_2h_3h_4,\ 0)$

Fig. 1.

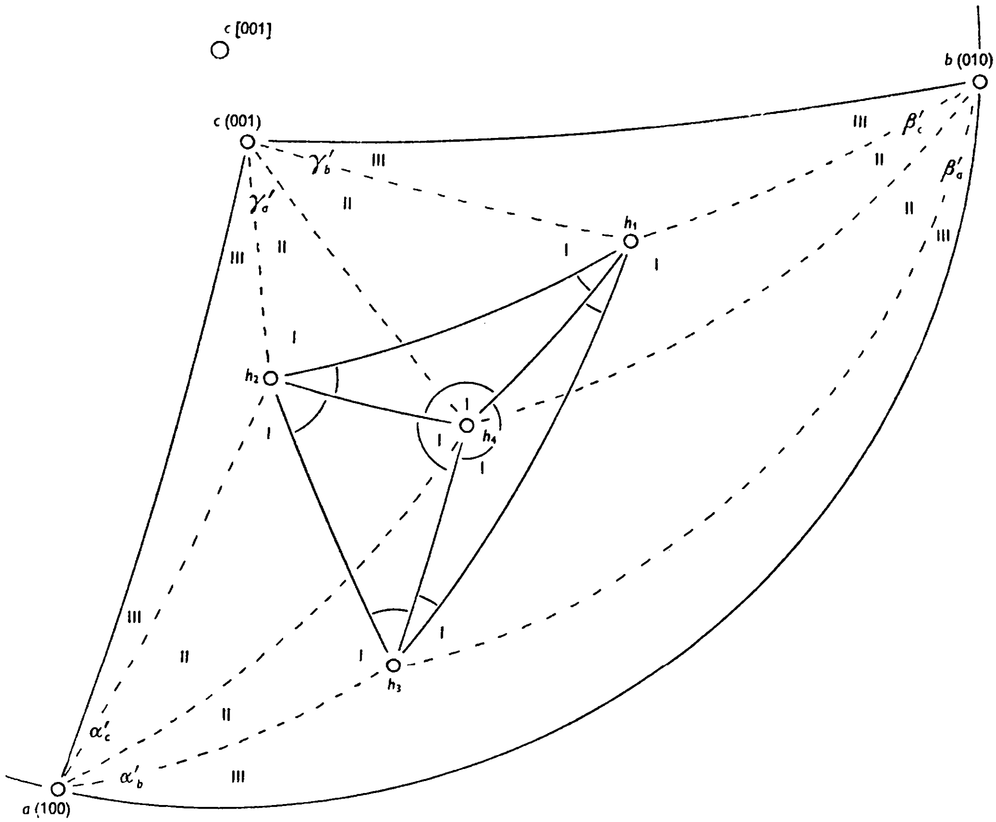

c [001]
c (001)
b (010)
a (100)
h_1
h_2
h_3
h_4
γ'_b
γ'_a
β'_c
β'_a
α'_c
α'_b

Fig. 2.

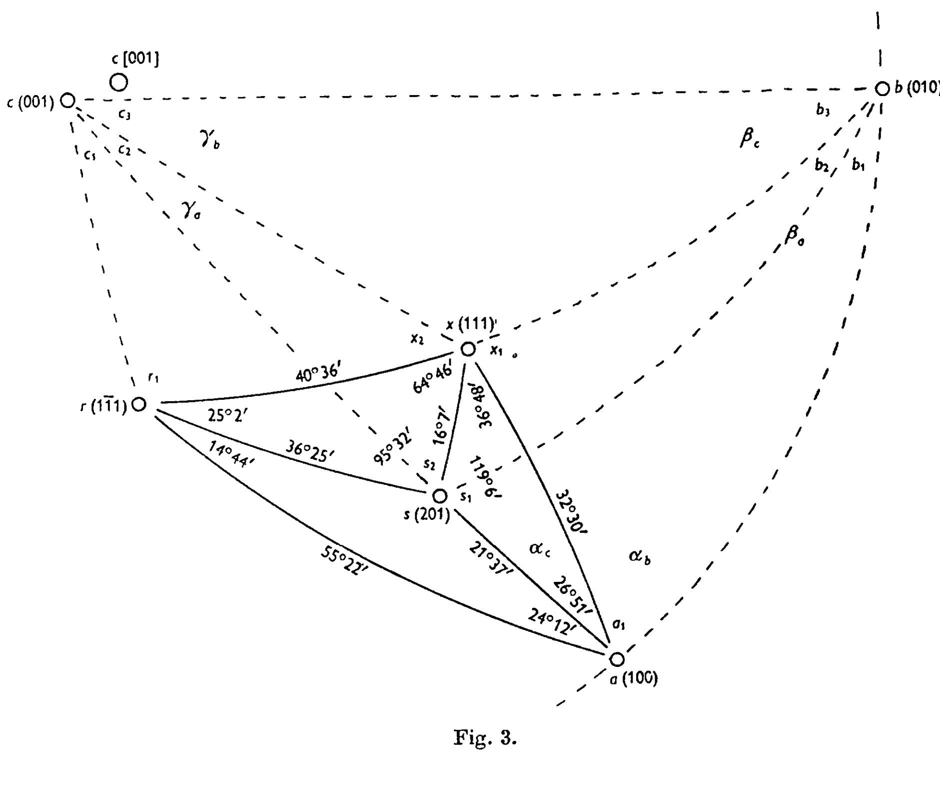

c [001]
c (001)
b (010)
x (111)
r (1$\bar{1}$1)
s (201)
a (100)
c_1 c_2 c_3
b_1 b_2 b_3
x_1 x_2
r_1
s_1 s_2
a_1
γ_b
γ_a
β_c
β_a
α_c
α_b
40°36′
64°46′
25°2′
36°48′
16°7′
95°32′
36°25′
14°44′
119°6′
32°30′
55°22′
21°37′
26°51′
24°12′

Fig. 3.

angles between four symbolized faces together with the angles between the fifth face and two of the four known faces (de Jong, 1946).

Application

An application of (4) may be encountered in the *Second crystallographic method* of determining the crystal elements.

Assume that five (six) angles between h_1, h_2, h_3 and h_4 have been measured (Fig. 2).

Our aim is to calculate the angles α_b', α_c', β_a', β_c', γ_a' and γ_b' and to derive from these quantities the crystal elements in the usual way.

To that end we calculate the nine angles between the known arcs, denoted by the full lines, using the spherical rule of cosines or a derivative. Then applying (4) twice in h_1, h_2, h_3 and three times in h_4, we find the nine angles denoted I. Now the triangles h_2ah_4, h_3ah_4, h_1bh_4, h_3bh_4, h_1ch_4 and h_2ch_4 are known, and we calculate by means of spherical trigonometry the six angles II. Applying (4) twice in each of the points a, b and c, we get the six angles III and hence α_b', etc.

In particular cases the manipulations are often reduced, as in the following example.

Example. Suppose the six angles between the four faces a, x, r and s of axinite (Dana, 1914, p. 527) have been measured (Fig. 3).

By means of spherical trigonometry the inscribed zone angles are computed. Then applying (4) once in a and r and twice in x and s, we find the six angles a_1, r_1, x_1, x_2, s_1, and s_2.

For example, in a we have:

$$\frac{\sin 24^\circ 12' \sin a_1}{\sin 26^\circ 51' \sin (51^\circ 3' + a_1)} = \frac{\begin{vmatrix} 1 & \bar{1} & 1 \\ 1 & 0 & 0 \\ 2 & 0 & 1 \end{vmatrix} \begin{vmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{vmatrix}}{\begin{vmatrix} 2 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \end{vmatrix} \begin{vmatrix} 1 & \bar{1} & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{vmatrix}} = 1,$$

whence $a_1 = 70^\circ 16'$.

Similarly,

$$r_1 = 104^\circ 43', \quad x_1 = 78^\circ 25', \quad x_2 = 48^\circ 37',$$
$$s_1 = 65^\circ 58', \quad s_2 = 60^\circ 54'.$$

Now in the triangle abs one side and two angles are known and we derive trigonometrically $b_1 = 26^\circ 42'$.

In the same way $b_2 = 18^\circ 1'$; $c_1 = 28^\circ 37'$; $c_2 = 15^\circ 31'$.

Formula (4) in b gives $b_3 = 43^\circ 28'$ and in c similarly $c_3 = 32^\circ 59'$.

So we have the angles

$$\alpha_b = a_1 = 70^\circ 16', \qquad \beta_c = b_3 = 43^\circ 28',$$
$$\alpha_c = 26^\circ 51', \qquad \gamma_a = c_2 = 15^\circ 31',$$
$$\beta_a = b_1 + b_2 = 44^\circ 43', \qquad \gamma_b = c_3 = 32^\circ 59',$$

and the crystal elements are

$$\alpha = 180^\circ - (\alpha_b + \alpha_c) = 82^\circ 53',$$
$$\beta = 180^\circ - (\beta_a + \beta_c) = 91^\circ 49',$$
$$\gamma = 180^\circ - (\gamma_a + \gamma_b) = 131^\circ 30',$$
$$a/b = \sin \gamma_a / \sin \gamma_b = 0{\cdot}4914,$$
$$c/b = \sin \alpha_c / \sin \alpha_b = 0{\cdot}4797.$$

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