NOMOGRAPHS FOR TRICLINIC CELL COMPUTATIONS

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Some of the equations used in computing the constants of triclinic cells, although rather involved, can be readily handled by nomographs. Given these nomographs one has a method of solving many triclinic cell problems very quickly with an accuracy of a fraction of a degree. Two types of problem are common. In the first type we are given the cell edge ratios and angles and wish to make a gnomonic projection to help in identifying a crystal that has been measured on an optical goniometer. In the second type of problem we are given certain atomic plane spacings and wish to compute the cell edges and angles and perhaps also to compute other atomic plane spacings.

We will consider the first type of problem first. As an example let us assume a crystal for which $a:b:c=0.900:1:0.800$, $\alpha=100°$, $\beta=95°$, $\gamma=105°$. The reciprocal angle chart, Fig. 1 gives us the reciprocal cell angles: α^*, β^*, γ^*. To find α^* we join the point β, γ of the grid to the point α of the linear α scale. This line crosses the linear scale α^* at a point that indicates the value of α^*. In our example the point 95°, 105° is found (on the right side of the grid because 95 and 105 are "like" in being greater than a right angle) and when joined to the point $\alpha=100°$ we find the line crosses the α^* scale at $\alpha^*=78.2°$. The point 105°, 100° of the grid joined to 95° on the center scale gives $\beta^*=82.0$ on the lower scale. Similarly we find $\gamma^*=73.8°$.

With a slide rule, we now evaluate the four quantities

$$V_1 = -\sin\alpha^* \cos\beta = 0.0853$$
$$V_2 = \sin\alpha^* \sin\beta = 0.975$$
$$A = \frac{\sin\alpha}{a\sin\beta} = 1.098$$
$$C = \frac{\sin\gamma}{c\sin\beta} = 1.212$$

We can now easily write the matrix $\overline{m}^{-1}$:

$$\overline{m}^{-1} = \begin{Bmatrix} A\sin\gamma^* & 0 & CV_1 \\ A\cos\gamma^* & 1 & C\cos\alpha^* \\ 0 & 0 & CV_2 \end{Bmatrix} = \begin{Bmatrix} 1.055 & 0 & .103 \\ .307 & 1 & .247 \\ 0 & 0 & 1.182 \end{Bmatrix}.$$

To make a gnomonic projection, on, say the plane perpendicular to the c axis, we evaluate the product $\overline{m}^{-1}\begin{Bmatrix} h \\ k \\ l \end{Bmatrix}$ for a number of planes (hkl). On coordinate paper we plot x/z, y/z for each point. This is the gnomonic projection.

For example, for the plane (112) of the crystal we have been considering:

$$\begin{Bmatrix} 1.055 & 0 & .103 \\ .307 & 1 & .247 \\ 0 & 0 & 1.182 \end{Bmatrix} \begin{matrix} (1) \\ (1) \\ (2) \end{matrix} = \begin{Bmatrix} 1.055 \times 1 + 0 \times 1 + .103 \times 2 \\ .307 \times 1 + 1 \times 1 + .247 \times 2 \\ 0 \times 1 + 0 \times 1 + 1.182 \times 2 \end{Bmatrix} = \begin{Bmatrix} 1.261 \\ 1.801 \\ 2.364 \end{Bmatrix}.$$

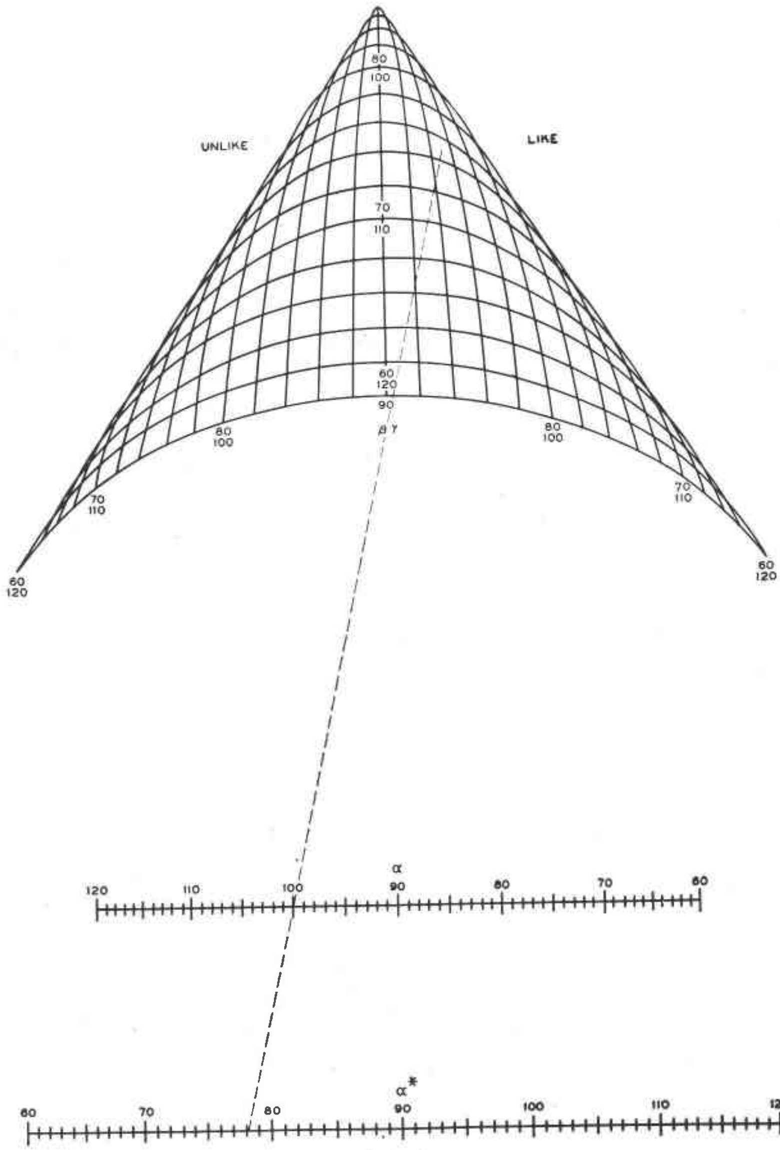

Fig. 1

The point $x=1.261/1.182=1.067$. $y=1.801/2.364=.762$ is the gnomonic projection of the plane (112).

If now, by x-rays we determine the value of d_{010} we can divide all terms of $\overline{m}^{-1}$ by d_{010} to obtain the matrix $\overline{M}^{-1}$. This matrix then gives all atomic spacings readily. We will illustrate the use of charts with this $\overline{M}^{-1}$ matrix by means of the next example, the second type of problem.

Let us assume that the measured reciprocal cell constants of a crystal are: $A_0=1/d_{100}=0.170$, $B_0=1/d_{010}=0.150$, $C_0=1/d_{001}=0.200$, $D_{01\bar{1}}==1/d_{01\bar{1}}=0.220$, $D_{10\bar{1}}=1/d_{10\bar{1}}=.260$ and $D_{110}=1/d_{110}=.204$. We know that the reciprocal cell angle α^* is determined by the ratios of B_0, C_0 and D_{011} (or $D_{01\bar{1}}$). We write these as a ratio in this order, then divide all three terms by the larger of the first two as B_0:C_0:$D_{01\bar{1}}=0.150:0.200:0.220$ $=0.75:1:1.10=e:l:g$ (or $l:e:g$ if the first number had been the larger of the first two). We then turn to the parallelogram chart, Fig. 2, and run

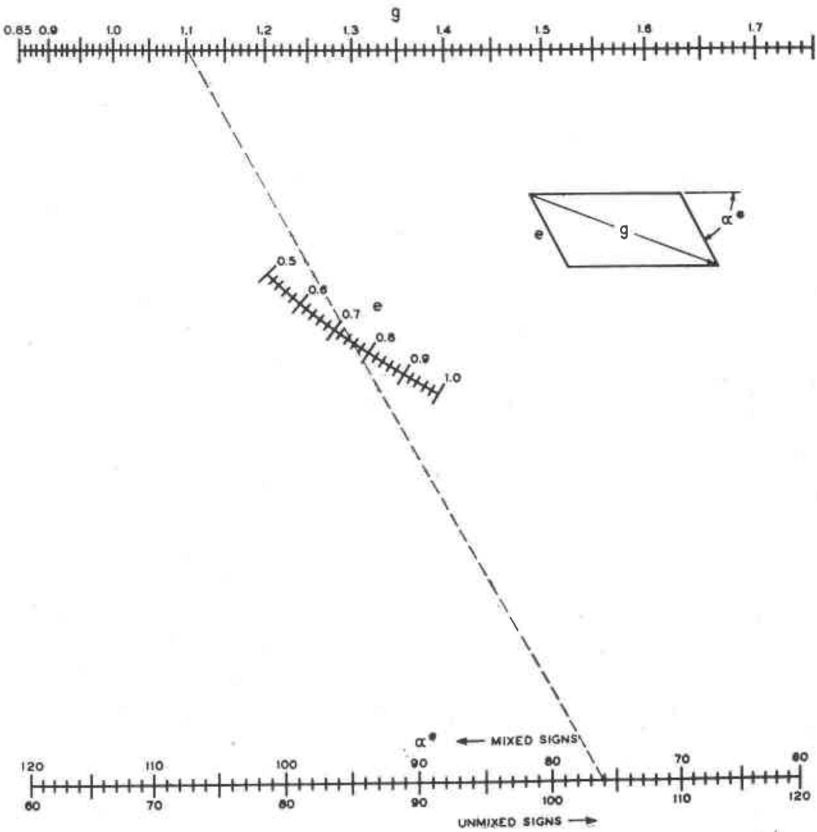

FIG. 2

a line through $g=1.10$ and $e=0.75$, then observe that this line cuts the α^* scale at 76.4°. (We read the upper numbers because $d_{01\bar{1}}$ has mixed signs.) Similarly $C_0:A_0:D_{10\bar{1}}=0.200:0.170:0.260=1:0.85:1.30$ gives $\beta^*=88.9°$ and $A_0:B_0:D_{110}=0.170:0.150:0.204=1:0.882:1.20$ gives $\gamma^*=101.1°$, (the lower numbers are read because D_{110} has unmixed signs).

To find α, β, γ from the angles α^*, β^*, γ^*, that we have just determined we use the reciprocal angle chart, Fig. 1 as before, merely considering starred angles to be unstarred and vice versa. The chart gives $\alpha=104.1°$, $\beta=93.8°$, $\gamma=78.4°$. A slide rule now gives us

$$a_0 = \frac{1}{A \sin\beta \sin\gamma^*} = \frac{1}{A \sin\beta^* \sin\gamma}, \quad \text{also}$$

b_0 and c_0 from the similar equations derived by permuting the letters. These equations give for our example, $a_0=6.01$, $b_0=7.00$, $c_0=5.16$. We now compute

$$V_1 = -\sin\alpha^* \cos\beta$$
$$V_2 = \sin\alpha^* \sin\beta$$

for our example, getting $V_1=.0642$, $V_2=.970$.

We may now form the matrix $\overline{M}^{-1}$:

$$\overline{M}^{-1} = \begin{Bmatrix} A_0 \sin\gamma^* & 0 & C_0V_1 \\ A_0\cos\gamma^* & B_0 & C_0\cos\alpha^* \\ 0 & 0 & C_0V_2 \end{Bmatrix} = \begin{Bmatrix} .1668 & 0 & .0128 \\ -.0326 & .150 & .0470 \\ 0 & 0 & .1940 \end{Bmatrix}.$$

We will illustrate the computation of a plane spacing for the plane (312).

$$\begin{Bmatrix} .1668 & 0 & .0128 \\ -.0326 & .150 & .0470 \\ 0 & 0 & .1940 \end{Bmatrix} \begin{matrix} (3) \\ (1) \\ (2) \end{matrix} = \begin{Bmatrix} .1668\times 3 + 0\times 1 + .0128\times 2 \\ -.0326\times 3 + .150\times 1 + .0470\times 1 \\ 0\times 3 + 0\times 1 + .1940\times 2 \end{Bmatrix}$$

$$= \begin{Bmatrix} .5260 \\ .1462 \\ .3880 \end{Bmatrix} = \begin{Bmatrix} D_1 \\ D_2 \\ D_3 \end{Bmatrix}.$$

The square root of the sum of the squares of these numbers is $1/d_{312}$ but the nomograph, Fig. 3 gives this value, $D_{312}=1/D_{312}$ much more easily and gives the Bragg angle for copper Kα besides.

We locate two of the three numbers on scales D_1 and D_2 and make a mark where a line joining these points crosses the ungraduated line. This crossing point is then joined to the third D value located on scale D_3 by a line that crosses scale D_{hkl}. This last crossing point gives $1/d_{hkl}$ below the line and the Bragg angle for copper Kα above the line. In our example this last crossing point is at $D_{hkl}=0.668$, hence, $d_{312}=1.497$ and above the line we read $\theta=31.0$.

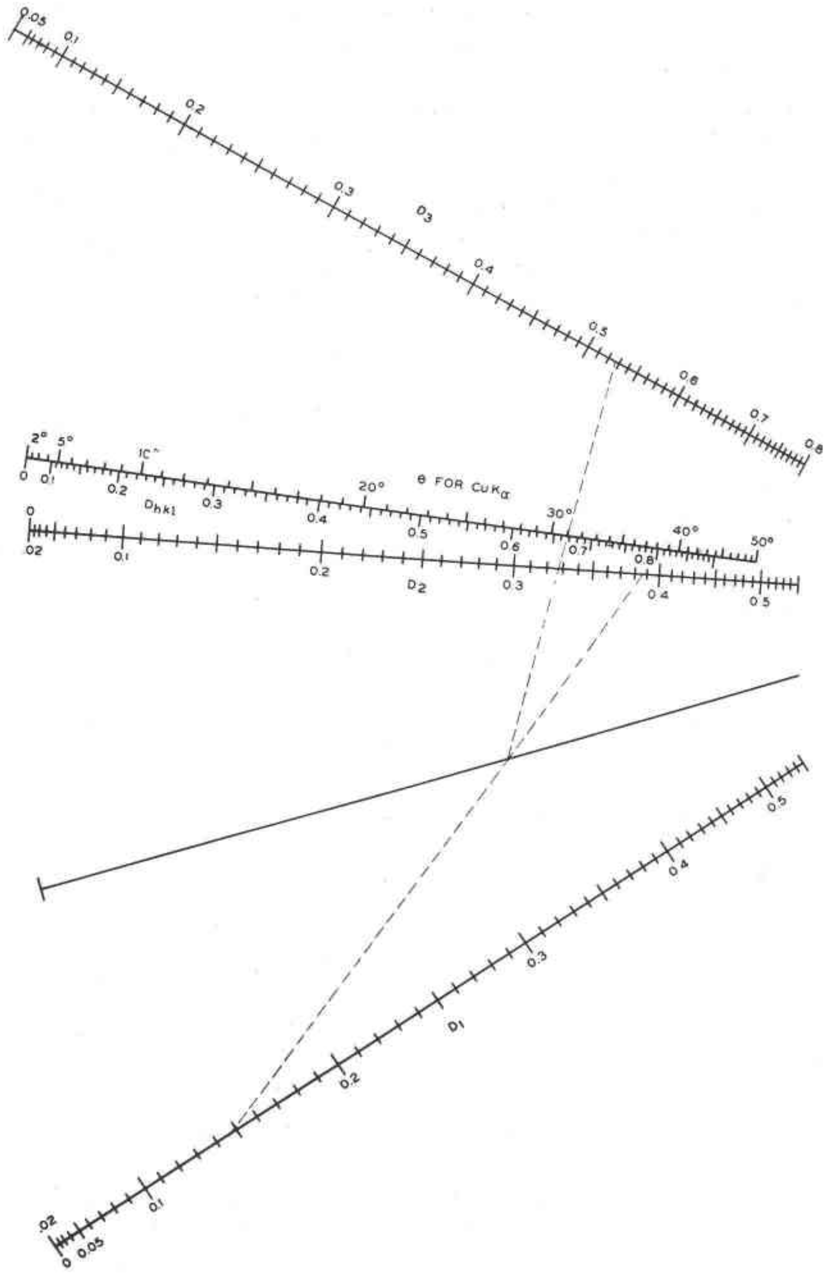
D3
θ FOR CuKα
D_{hkl}
D2
D1
0.05
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
2°
5°
10°
20°
30°
40°
50°
.02
0.05

FIG. 3

While the charts published with this paper will be adequate for most purposes some workers may wish to prepare their own charts. The charts here presented may be photostated and hence enlarged to any convenient scale. Photographic distortion is immaterial as long as all straight lines are reproduced as straight. For those who wish to replot the charts we give the formulae

The Reciprocal Angle Chart.

The Grid: $x = \dfrac{\cos\beta\cos\gamma}{5/4 - \sin\beta\sin\gamma}$, $y = \dfrac{1}{5/4 - \sin\beta\sin\gamma}$

The α Scale: $x = 0.8\cos\alpha$, $y = .3$

The α^* Scale: $x = \cos\alpha^*$, $y = 0$

The Parallelogram Chart.

g scale: $x = 4/9g^2 - 5/6$, $y = 1$

e scale: $x = \dfrac{e^2 - 7/8}{2e + 9/4}$, $y = \dfrac{9/4}{2e + 9/4}$

α^* scale: $x = -\cos\gamma^*$, $y = 0$

The D Chart.

D_1 scale: $x = \dfrac{D_1^2}{1 + 10D_1^2}$, $y = \dfrac{-8.5}{1 + 10D_1^2}$

D_2 scale: $x = \dfrac{D_2^2}{1 + 10D_2^2}$, $y = \dfrac{1.5}{1 + 10D_2^2}$

D_3 scale: $x = \dfrac{D_3^2}{2 + 10D_3^2}$, $y = \dfrac{17}{2 + 10D_3^2}$

D_{hkl} scale: $x = \dfrac{D^2}{4 + 10D^2}$, $y = \dfrac{10}{4 + 10D^2}$

θ scale: $x = \dfrac{(2/\lambda)^2\sin^2\theta}{4 + 10(2/\lambda)^2\sin^2\theta}$.

In plotting these we do not need to plot x and y to the same scale. The derivation of these formulae will not be given here; it is a straightforward application of the methods given by the author in a recent paper—"A simple procedure for the making of alinement charts," *Journal of Applied Physics*, 83–86 (January 1948).