STEREOSCOPIC DRAWINGS OF CRYSTAL STRUCTURES

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Abstract

A method is presented for getting stereoscopic pairs of atomic structure views given the coordinates of the atoms and cell constants.

Stereoscopic pairs of pictures of crystal structures take much less space to store than do actual models. A box $4'' \times 7'' \times 8''$ can hold 200 such views in individual envelopes, while 200 three dimensional models might require fifty square feet of shelf space.

One could produce the stereoscopic views by photographing an actual model or one can draw them directly, avoiding the work of construction of the three dimensional models. We turn then to the analysis of the simplest case, that of representing a point p in three dimensional space as two points on a plane, one point as seen by the right eye, the other as seen by the left eye.

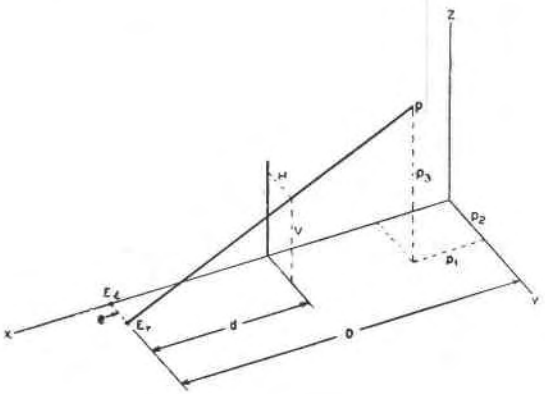

Fig. 1

Consider a rectangular coordinate system XYZ, Fig. 1. The two eyes are in the XYZ plane at a distance D from the Y axis, the left eye is on the axis at E_l, the right eye at a distance e from it at E_r. The plane of projection is parallel to the YZ plane and is at a distance d from the eyes. The right eye will see point p by looking along the line E_r–p, hence p can be represented by the point (x, y, z) where this line passes through the plane of projection. A similar line from E_l to p would give the point $(x'y'z')$ where this line passes through the projection plane, this point (x', y', z') represents p as seen by the left eye.

In solid analytical geometry it is shown that for any point (x, y, z) on the line joining points (x_1, y_1, z_1) and (x_2, y_2, z_2), the values of x, y, y

satisfy the equation:

$$\frac{x - x_1}{x_2 - x_1} = \frac{y - y_1}{y_2 - y_1} = \frac{z - z_1}{z_2 - z_1} = r,$$

For the right eye (see Fig. 1)

$$\begin{aligned} x &= D - d, & x_1 &= p_1, & x_2 &= D \\ y &= H, & y_1 &= p_2, & y_2 &= e \\ z &= V, & z_1 &= p_3, & z_2 &= 0. \end{aligned}$$

For the left eye y_2 becomes zero and H becomes H'. If we substitute $1-s$ in place of r (for later convenience) we now find:

$$s = \frac{d}{D - p_1} \tag{1}$$

$$H' = sp_2 \tag{2}$$

$$H = H' + e(1 - s) \tag{3}$$

or

$$H = H' + f$$

$$V = sp_3 \tag{4}$$

although $f = e(1-s)$ it will be read from a chart, Fig. 3, instead of being computed. In this chart f has been arbitrarily increased by 2 cms. to allow for the prism deviation of the stereoscopic viewer. We will assume that $D = 125$ cms., $d = 25$ cms. and $e = 6$ cms. Also we assume that the object viewed is in the upper near quadrant and that the values of p_1, p_2 and p_3 are between 0 and 10 cms. but the assumptions of this sentence can be violated a little.

FIG. 2

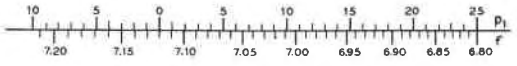

FIG. 3

If we consider the object being viewed as standing squarely in the corner at the origin the resulting projection will not be very pleasing. A very satisfactory result will follow, however, if the object is turned so that it is viewed at the clinographic angle. This "turning" can be accomplished if the coordinates p_1, p_2, p_3 are those computed for a clinographic projection.

Consider a rectangular coordinate system x, y, z associated with a crystal being drawn. Let z lie along the crystallographic c axis and x lie in the plane of a and c. If a vector R having components on the x, y, z axes of R_1, R_2, R_3, respectively, is written in matrix form as

$$(R)_x = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \end{bmatrix}$$

then the components on a set of clinographic axes is given* by means of the matrix multiplication

$$(R)_c = K \begin{bmatrix} R_1 \\ R_2 \\ R_3 \end{bmatrix} \tag{5}$$

where

$$K = \begin{bmatrix} 18/\sqrt{370} & 6/\sqrt{370} & -1/\sqrt{37} \\ -1/\sqrt{10} & 3/\sqrt{10} & 0 \\ -3/\sqrt{370} & -1/\sqrt{370} & 6/\sqrt{37} \end{bmatrix} \tag{6}$$

or

$$K = \begin{bmatrix} .9358 & .3120 & .1644 \\ -.3162 & -.9487 & 0 \\ -.1560 & -.0520 & .9864 \end{bmatrix}. \tag{6a}$$

The components of the vector R on the x, y, z system can be computed from its components on the a, b, c system by means of the matrix equation:

$$(R)_x = M(R)_a \tag{7}$$

where M is a matrix† peculiar to the crystal. Whence:

$$(R)_c = K(R)_x = KM(R)_a. \tag{8}$$

We now illustrate the foregoing by preparing a picture of cassiterite. For cassiterite $a:c = 1:0.6723$, hence the matrix M takes the value:

$$M' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & .6723 \end{bmatrix}$$

* See Computation of Interfacial Angles, Interzonal Angles and Clinographic Projection by Matrix Methods: *Am. Mineral.*, **31**, 31–42 (1946).

† Computations of Interfacial Angles, etc., *Am. Mineral.*, **31**, 31–42 (1946).

tin atoms are at the points.**

$$\begin{bmatrix}0\\0\\0\end{bmatrix}_a, \begin{bmatrix}1\\0\\0\end{bmatrix}_a, \begin{bmatrix}0\\1\\0\end{bmatrix}_a, \begin{bmatrix}1\\1\\0\end{bmatrix}_a, \begin{bmatrix}0\\0\\1\end{bmatrix}_a, \begin{bmatrix}1\\0\\1\end{bmatrix}_a, \begin{bmatrix}0\\1\\1\end{bmatrix}_a, \begin{bmatrix}1\\1\\1\end{bmatrix}_a \text{ and } \begin{bmatrix}1/2\\1/2\\1/2\end{bmatrix}_a$$

while oxygen atoms are at the points

$$\begin{bmatrix}u\\u\\0\end{bmatrix}_a, \begin{bmatrix}1-u\\1-u\\0\end{bmatrix}_a, \begin{bmatrix}1/2-u\\1/2+u\\1/2\end{bmatrix}_a, \text{ and } \begin{bmatrix}1/2+u\\1/2-u\\1/2\end{bmatrix}_a$$

where $u=0.30$.

To compute the components of $(R)_c$ by equation (8a) we will need the product KM:

$$KM = \begin{bmatrix}.9358 & .3120 & .1644\\ -.3162 & .9487 & 0\\ -.1560 & -.0520 & .9864\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\0 & 1 & 0\\0 & 0 & .6723\end{bmatrix}$$

or

$$KM = \begin{bmatrix}.9358 & .3120 & .1105\\ -.3162 & .9487 & 0\\ -.1560 & -.0520 & .6632\end{bmatrix}.$$

To avoid the further use of subscripts denoting the different axial systems we will henceforth refer to the vector from the origin to a point being represented as P if stated on the crystallographic axes a, b, c and p if stated on the clinographic axes. Hence the equation (8) becomes

$$p = KMP. \tag{8a}$$

If the cell is to be 10 cms. on a side we multiply all components on the a system by 10 so that, for the P corresponding to the point $\begin{pmatrix}1\\0\\0\end{pmatrix}_a$ we have

$$P = \begin{bmatrix}10\\0\\0\end{bmatrix}$$

whence

$$p = KMP = \begin{bmatrix}9.358\\-3.162\\-1.560\end{bmatrix}.$$

** Wyckoff, R. W. G., *The Structure of Crystals*, 2nd ed. p. 239, The Chemical Catalog Co.

Using $p_1 = 9.358$, reference to figures 2 and 3 give us:

$$s = .2163$$
$$f = 7.015$$

Finally

$$H' = sp_2 = -.684$$
$$H = H' + f = 6.331$$
$$V = sp_3 = -.337$$

The following tabular form is a considerable aid in keeping straight the mass of figures. It also helps in allowing all of one kind of computation to be finished before another kind is started. For instance all the p's were computed before any of the s's were determined, then all the s's were taken from Fig. 2, etc. Since hexagonal crystals are traditionally viewed differently than other crystals (i.e. 30° further around with respect to the a axis), we set up a special KM matrix for this case. We use

$$(KM)_h = K\begin{pmatrix} 1/2\sqrt{3} & 0 & 0 \\ -1/2 & 1 & 0 \\ 0 & 0 & c \end{pmatrix}$$
$$= \begin{pmatrix} .6544 & .3120 & .1644c \\ -.7482 & .9487 & 0 \\ -.10908 & -.0520 & .9864c \end{pmatrix}$$

where c is the axial ratio. The procedure is the same as before and one will get values of H, H' and V as in the previous case.

If the points (H, V) and (H', V) are plotted on metric graph paper, the unit being a centimeter the resulting pictures are right for viewing in the old fashioned parlor stereoscope. Better results are achieved however, by one of two other methods. The easiest method is to plot the data on tracing paper on an enlarged scale, then photograph the drawings down to proper size, thus reducing the errors of drawing. The second method is to employ special methods of precision drawing.

Precision Drawing Method

In the precision drawing method the data is plotted on a transparent plastic sheet laid over the graph paper. (Cellulose acetate 15 or 20 thousandths of an inch thick serves nicely.) The points (H, V) and (H', V) are plotted with a sharp pointed tool like a machinist's scriber, using a magnifying glass to reduce the errors. One should look at the scriber (which rests lightly on the plastic slide) studying its position from two different angles. When-satisfied that the position is right the scriber is pressed into the plastic. We wish now to make a circle about the point, the size of the circle indicating the kind of atom the point repre-

sents. Ordinary dividers are not well suited to this purpose. They are too difficult to reset to the same size as before in case one has changed to another size. Also they are clumsy, if one wishes a circle of say 1/16″ diameter they slip and scar the sheet. A *circler* shown in Fig. 4 works well. It is a pin fitting nicely into a tube. The pin has an accurately centered conical point; the tube has a cutting lip. The tube is pushed up away from the point, the point is introduced into the hole, the pin forced firmly into the hole in an erect position, then with the other hand the tube is pushed down and rotated thus leaving a small ring engraved in the plastic. One needs several sizes of this tool.

FIG. 4

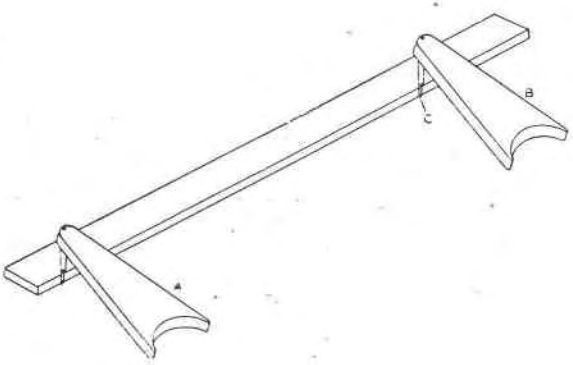

FIG. 5

Another difficulty is that of accurately joining points by lines. This difficulty is resolved by using two *joiners*, i.e. two special scribers with a support that holds them perpendicular to the table. These scribers, Fig. 5, have an accurately turned cylinder *C* near the point, the diameter of *C* is the same for both scribers of the pair, the conical point is true with the cylinder. A scriber is inserted in each of two holes that are to be joined, they are held down with a finger pressing at *p* on each, then a straight edge is pressed against both cylinders by pressure at the arrow, Fig. 5. When firm contact is made, the straight edge is held down, the near

FIG. 6

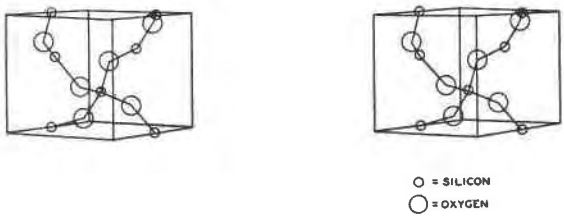

FIG. 7

S_n ATOMS

P =	0	10	0	10	0	10	0	10	5
	0	0	10	10	0	0	10	10	5
	0	0	0	0	10	10	10	10	5
p =	0	9.358	3.120	12.478	1.105	10.465	4.225	13.583	6.791
	0	−3.162	9.487	6.325	0	−3.162	9.457	6.325	3.162
	0	−1.560	−.520	−2.080	6.632	5.072	6.112	4.552	2.276
s =	.200	.2163	.2051	.2222	.2018	.2183	.2071	.2242	.2114
f =	7.120	7.015	7.087	6.977	7.106	7.003	7.075	6.965	7.046
$H' = sp_2$	0	−.684	1.945	1.405	0	−.690	1.965	1.418	.668
H = H′ + f	7.120	6.331	9.032	8.382	7.108	6.313	9.040	8.383	7.714
$V = sp_3$	0	−.337	−.107	−.462	1.337	1.107	1.265	1.022	.480

O ATOMS

3	7	2	8	3	7
3	7	8	2	3	7
0	0	5	5	10	10
3.743	8.735	4.920	8.663	4.848	9.840
1.898	4.428	6.959	− .632	1.900	4.428
−.624	−1.456	2.588	+1.964	6.008	5.176
.2062	.2150	.2081	.2150	.208	.217
7.080	7.024	7.067	7.024	7.068	7.011
.392	.952	1.448	− .136	.395	.961
7.472	7.976	8.515	6.888	7.463	7.972
−.129	− .313	.539	.422	1.250	1.123

scriber is removed and the far one moved towards the operator, scratching as it goes, until it falls in the second hole.

With two of these devices one can draw the views quite accurately, locating each point to within 2 or 3 thousandths of an inch. In making stereo views a mistake may occur, such as misplotting a point. The best procedure is to finish the drawings, view the pair in the stereo viewer and mark all the points that seem to float in space or fail to blend. The slide is then replaced over the graph paper and the points in error are checked for correspondence with the entries in the data table. If the positions correspond with the tables, the data are of course recomputed. The correct data is conspicuously written on the slide and a new piece of plastic is fastened over the old slide. Using the magnifier a new slide is copied from the old making the corrections. Before unclamping the new slide slip a piece of white paper between the two slides and view by reflected light to make sure that there are no omissions.

Figures (6) and (7) show cassiterite and quartz drawn by the precision method.