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Computing and drawing crystal shapes

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Abstract

A computerized (Fortran) method for plotting crystal shapes is based on the following procedures. Each face is represented by an equation, the coefficients of which are derived from the (*hkl*) indices and the central distance. The central distances may be measured (actual shape) or represent relative growth velocities (ideal growth shape) or surface energies (equilibrium shape). All triplets of face equations are solved to give the possible corners, then the smallest polyhedron is found by eliminating corners which are further from the center than any face. A drawing is made by connecting corners which have two faces in common. Matrix methods are used to convert face indices from the crystal axial system to a working cartesian coordinate system, and to rotate the image of the crystal to any desired orientation. Projection may be orthographic or perspective. Twins may be drawn with a composition plane, or as interpenetrating individuals. Shaded, rather than line, drawings may also be made.

Introduction

The growth shape of a crystal depends on the relative growth velocities of the various faces, which determine the relative center-to-face distances. The equilibrium shape depends on the surface energies, whose relative values may also be taken by the Wulff (1901) theorem to give the relative center-to-face distances. Various special and general methods exist for predicting relative growth velocities or surface energies (Donnay and Harker, 1936; Hartman and Perdok, 1955; McLachlan, 1974; Dowty, 1976), but even given these values, one is still faced with the rather tedious geometric or mathematical problem of determining the configuration of edges and corners which define the crystal polyhedron. Computer methods are ideally suited for this task. Several investigators have independently developed at least parts of a general analytical procedure for determining and plotting crystal shape (Keester and Giddings, 1971; Felius, 1976; Schneer, 1978), but no comprehensive account of such a procedure seems to have been offered.

Many ingenious graphical methods have been developed for making drawings of idealized crystals (see Terpstra and Codd, 1961), but all can be very time-consuming. The computerized matrix methods outlined in this paper allow rapid and routine orthographic or perspective drawing of any desired crystal shape, viewed from any angle. The computer programs are written in Fortran.

Basic mathematical methods

Coordinate systems

Crystallographic calculations are easily done with matrix algebra (Bond, 1946). For some operations, such as symmetry transforms, it is most convenient to use the system of base vectors (coordinate system) of the crystal axes, but for most it is better to use a cartesian system. A vector, or a point whose location with respect to the center of coordinates is represented by a vector, can be converted from one system to another with a transformation matrix **M**:

$$\mathbf{V}_x = \mathbf{M}\mathbf{V}_a\,;\ \mathbf{V}_a = \mathbf{M}^{-1}\,\mathbf{V}_x \qquad (1)$$

where $\mathbf{V}_a$ is the vector in the crystal system and $\mathbf{V}_x$ is the vector in the cartesian system; $\mathbf{M}^{-1}$ is the inverse of the matrix **M**. The matrix depends on the mutual orientation of the coordinate systems. The orientation used for this work is c (crystal) parallel to z (cartesian) and b (crystal) in the y–z (cartesian) plane (Fig. 1); then x (cartesian) is parallel to a^* (crystal), and if the projection is made along x, the (100) face

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is perpendicular to the view direction in a drawing. The transformation matrix is

$$\mathbf{M} = \begin{vmatrix} a\cos\nu_1 & 0 & 0 \\ a\cos\nu_2 & b\sin\alpha & 0 \\ a\cos\beta & b\cos\alpha & c \end{vmatrix} \qquad (2)$$

$$\nu_1 = \frac{\sqrt{1-\cos^2\alpha-\cos^2\beta-\cos^2\gamma+2\cos\alpha\cos\beta\cos\gamma}}{\sin\alpha}$$

$$\nu_2 = \frac{\cos\gamma-\cos\alpha\cos\beta}{\sin\alpha}$$

This orientation is somewhat different from that used by Bond (1946) and Terpstra and Codd (1961), but the matrix was derived in the same way.

The orientation of a face is specified in the crystal system with the Miller indices (*hkl*), but the vector [*hkl*] is not in general perpendicular to the face except in the cubic system. However, the vector $\mathbf{V}_{hx}$ in the cartesian system which is perpendicular to the face can be obtained by multiplying the vector $\mathbf{V}_h$ = [*hkl*] by the transpose of the inverse of the matrix **M** above (Bond, 1946), or by premultiplication instead of postmultiplication:

$$\mathbf{V}_{hx} = \mathbf{V}_h\mathbf{M}^{-1} \qquad (3)$$

In the cartesian system, the equation of the plane (*hkl*) is then

$$Ax + By + Cz = D\sqrt{A^2+B^2+C^2} \qquad (4)$$

where A, B, and C are the components in the *x*, *y*, and *z* directions respectively of the vector $\mathbf{V}_{hx}$, and D is the perpendicular distance from the plane to the origin (the central distance).

Rotation matrices

In obtaining different view angles of crystals or in generating twins it is necessary to be able to rotate vectors, points, or planes about various directions. This is also done with matrix multiplication in the cartesian system:

$$\mathbf{V}'_x = \mathbf{R}\mathbf{V}_x \qquad (5)$$

where the vector may represent an axis, a point, or the normal to a face. Matrices for rotation about the cartesian axes are easily derived intuitively, but for twin operations it is desirable to have a more general means of obtaining the rotation matrix. A general expression for the rotation matrix found by Morgan (1976) is:

$$\mathbf{R} = \begin{vmatrix} \rho_{11} & \rho_{12} & \rho_{13} \\ \rho_{21} & \rho_{22} & \rho_{23} \\ \rho_{31} & \rho_{32} & \rho_{33} \end{vmatrix} \qquad (6)$$

$$\begin{aligned}
\rho_{11} &= 1 - 2r_y^2\sin^2\theta/2 - 2r_z^2\sin^2\theta/2 \\
\rho_{12} &= 2r_xr_y\sin^2\theta/2 - 2r_z\sin\theta/2\cos\theta/2 \\
\rho_{13} &= 2r_xr_z\sin^2\theta/2 + 2r_y\sin\theta/2\cos\theta/2 \\
\rho_{21} &= 2r_xr_y\sin^2\theta/2 + 2r_z\sin\theta/2\cos\theta/2 \\
\rho_{22} &= 1 - 2r_x^2\sin^2\theta/2 - 2r_z^2\sin^2\theta/2 \\
\rho_{23} &= 2r_yr_z\sin^2\theta/2 - 2r_x\sin\theta/2\cos\theta/2 \\
\rho_{31} &= 2r_xr_z\sin^2\theta/2 - 2r_y\sin\theta/2\cos\theta/2 \\
\rho_{32} &= 2r_yr_z\sin^2\theta/2 + 2r_x\sin\theta/2\cos\theta/2 \\
\rho_{33} &= 1 - 2r_x^2\sin^2\theta/2 - 2r_y^2\sin^2\theta/2
\end{aligned}$$

where r_x, r_y, and r_z are the components of the vector of unit length in the cartesian system representing the axis of rotation, and θ is the angle of rotation. The sense of the rotation, which will be assumed throughout this paper, is clockwise looking outward from the origin along the axis.

Symmetry

It is desirable to take advantage of crystal symmetry so that only one face per form need be entered into the computer program. The generation of equivalent faces is also carried out by matrix multiplication:

$$\mathbf{V}'_h = \mathbf{S}_f\mathbf{V}_h \qquad (7)$$

where $\mathbf{V}_h$ represents the indices (*hkl*). In a system devised by L. W. Finger for the crystal-structure refinement program RFINE (Finger and Prince, 1975), the information for symmetry transforms is obtained from the *International Tables for X-Ray Crystallography*, Volume I. The atomic positions in the general equipoint of each space group give the symmetry matrices of the crystal and all their possible products. Thus the position *y*, *y*–*x*, $\bar{z}$ gives the matrix

$$\mathbf{S}_p = \begin{vmatrix} 0 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & \bar{1} \end{vmatrix} \qquad (8)$$

The elements of such matrices will be integers if the operation is carried out in the crystal coordinate system. In the computer program, the information is

read in just as given in the *Tables*. The matrices ($\mathbf{S}_p$) thus derived apply to points or vectors, rather than faces. They also may contain translational operations which are ignored for the purposes of determining equivalent faces, although it is useful to have a file of space-group symmetry cards for use in RFINE and other programs which use this system (Dowty, 1976). Because the face indices are the reciprocals of the axial intercepts, the desired matrix $\mathbf{S}_f$ is the inverse of the space-group symmetry matrix $\mathbf{S}_p$. However, the inverse of a symmetry matrix is the transpose, so that $\mathbf{S}_f = \mathbf{S}_p^T$.

General procedure

The requisite information, or input to the computer program, is the symmetry information, unit-cell parameters, and the indices of one face of each form with its central distance. If the object is to determine the growth or equilibrium shape, more faces may be entered than are likely to be present on the crystal.

The indices of symmetry-equivalents to each face are first generated; then the equations of all faces in the cartesian system are derived from equations (3) and (4). To determine the crystal shape, every possible corner, or junction of three faces, is considered, which involves a triple loop in the computer program. The coordinates of the corners are found by solution of the three simultaneous face equations. This is most conveniently done by inverting the matrix of the coefficients. In order for a corner actually to be present on the crystal, it must lie on or inside any and all faces. Thus the perpendicular distance δ of each corner from each face is computed by the formula

$$\delta = \frac{A\epsilon_x + B\epsilon_y + C\epsilon_z}{\sqrt{A^2 + B^2 + C^2}} - D \qquad (9)$$

where ϵ_x, ϵ_y, and ϵ_z are the x, y, and z coordinates of the corner. If this distance is greater than zero (within the precision of the calculation) for any face, that corner does not exist on the crystal.

It is necessary to check each new corner against the list which is being built up, since if more than three faces meet at a corner, many triplets of faces give the same solution (*e.g.* a corner with four faces appears in four triplets). The overall procedure can be time-consuming if the number of faces is very large—the number of permutations of n faces taken three at a time is $n(n-1)(n-2)/3$, and each such permutation must be checked against the list of valid corners and the distance from each face computed. The labor is somewhat reduced if triplets involving parallel and opposite faces [for which $(\epsilon_x)_1 + (\epsilon_x)_2 = (\epsilon_y)_1 + (\epsilon_y)_2 = (\epsilon_z)_1 + (\epsilon_z)_2 = 0$] are identified and rejected.

The result of the procedure is a list of valid corners, each with xyz coordinates and at least three appertaining faces. The forms present on the growth or equilibrium shape are determined from the list of faces. If the object is to make a drawing, the edges between corners must be identified. This is done by considering all possible pairs of corners, a double loop in the program. An edge exists between any two corners which have two faces in common. A list of edges is compiled, in terms of the coordinates of the two corners, and a drawing is made by connecting each pair of corners with a straight line, either by hand or by machine.

Of course, the actual drawing is a projection. This operation is done most simply, for orthographic projection, by neglecting one of the cartesian coordinates, conventionally x. Before making the projection, it is customary to rotate the crystal to a suitable view orientation. For a standard view, the crystal is rotated $-\arctan(1/3)$ about z, then $\arctan(1/6)$ about y (Terpstra and Codd, 1961). This gives a view of the crystal in effect from the front (a^* axis), but from a direction slightly upwards and to the right (Fig. 1). Any other view may be obtained by adding appropriate values to the rotations about the cartesian axes. In practice, all the separate rotation matrices are multiplied together into a single orientation

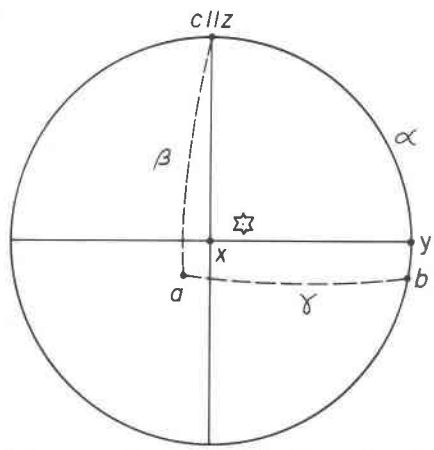

Fig. 1. Stereogram (upper hemisphere) showing orientation of crystallographic axes (a,b,c) and cartesian axes (x,y,z) for crystallographic calculations and plotting. The star shows the standard projection direction for orthographic drawings.

matrix, and this is applied to the coordinates of each corner.

If an edge is on the front side of the crystal, within its outline in projection, the normals of both its faces will make angles of less than 90° with the projection direction, *i.e.* they will have positive x components. If the edge is on the drawing outline, one face normal will have a positive x component and the other a negative one. If the edge is on the back, both face normals will have negative x components. Thus back edges can be identified and either omitted entirely or drawn with dashed lines. Before making this test, the face normals are multiplied by the orientation matrix.

Stereo pairs are easily drawn by rotating an appropriate amount on the z axis (Fig. 2). Once a set of corners and faces has been determined, which is the principal labor of the procedure, its orientation can be changed simply by multiplying each corner and face by the new orientation matrix.

For stereo pairs, it appears to be more satisfactory to use perspective rather than orthographic projection. In this case, the y (horizontal) and z (vertical) coordinates of each corner are transformed before drawing, but after rotation, by the equations

$$y' = \epsilon_y\left(\frac{\zeta}{\zeta - \epsilon_x}\right); \; z' = \epsilon_z\left(\frac{\zeta}{\zeta - \epsilon_x}\right) \tag{10}$$

where ζ is the distance from the projection point (the eye) to the center of the crystal and the projection is onto the plane $x = 0$ (Fig. 3). This method does not give perfectly true perspective, since straight lines are still drawn instead of curved ones, but the curvature is negligible except for very close views. The distance from the crystal center to the projection point should also be used to determine μ, the stereo rotation angle:

$$\sin(\mu/2) = \lambda/(2\zeta) \tag{11}$$

where λ is the interocular distance, usually about 2¼ inches. With perspective projection, determining back edges must be done by computing the dot product of the face normals and the vector $\mathbf{V}_{pc}$ from the

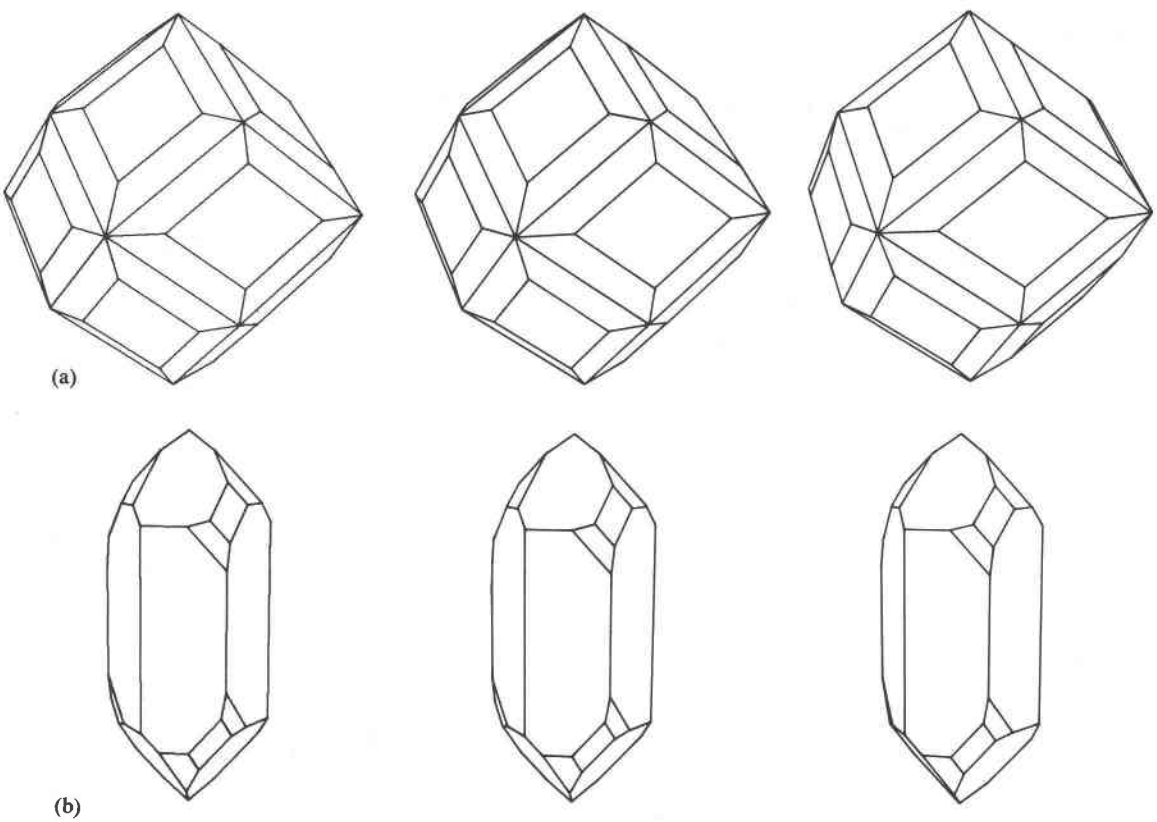

Fig. 2. Computer drawings of crystals. In Figs. 2 and 4, the two images on the right are a stereo pair, traced from the machine plot, and the image on the left is the original machine plot of the left-eye image. (a) Above: cubic crystal, class m3m showing the rhombic dodecahedron {110} and hexoctahedron {321}. (b) Below: quartz, class 32, showing the hexagonal prism $\{10\bar{1}0\}$, rhombohedra $\{10\bar{1}1\}$ and $\{01\bar{1}1\}$, the trigonal dipyramid $\{11\bar{2}1\}$ and the trigonal trapezohedron $\{51\bar{6}1\}$.

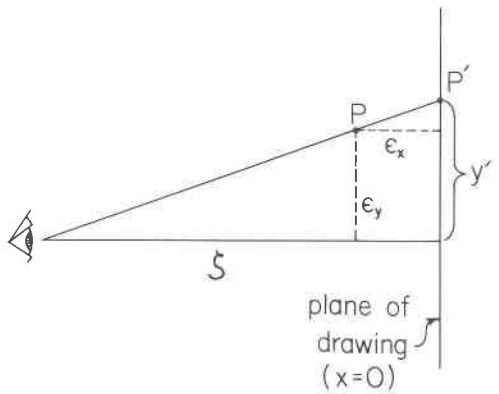

Fig. 3. Perspective projection of a point P (normally a crystal corner) with coordinates ϵ_x, ϵ_y, ϵ_z, into the point P′ with coordinates y', z' in the plane of the drawing (x = 0); see equations (10). The x axis is horizontal and the y axis is vertical on the page; view is down the z axis.

projection point to either corner. If

$$\cos\phi = \frac{\mathbf{V}_{pc} \cdot \mathbf{V}_{hx}}{|\mathbf{V}_{pc}|\,|\mathbf{V}_{hx}|} \qquad (12)$$

is positive, the face represented by $\mathbf{V}_{hx}$ is in back.

Twins

Twins are most easily and consistently described by the system of Friedel (1926; see also Cahn, 1954), in which only rational lines or planes may be twin operators. To produce a second crystal related to the original one by rotation, a twin rotation matrix is derived from (6) above, after transforming the indices of the twin axis to the cartesian system, and the coordinates of each corner are multiplied by this twin matrix. A reflection twin is generated by utilizing the identity of a mirror plane and a two-fold rotary-inversion axis. The crystal is rotated by 180° about the normal to the twin plane, then inverted. In practice, the rotation and inversion matrices are combined by multiplication into one twin matrix.

An idealized contact twin with a composition plane is obtained by inserting a plane with the desired orientation and a distance of zero, *i.e.* passing through the center, into the list of faces before solving for corners. The twin matrix is then applied to the corners and faces of this completed half-crystal, and if the twin is by reflection, the two halves will match. To determine front and back edges, each half-crystal is treated independently. In order to prevent the trace of the composition plane on the back of the crystal from showing through in the drawing, edges which are defined by the composition plane and any regular face whose normal is greater than 90° from the projection direction are rejected. In some cases, edges or parts of edges involved in re-entrant faces will still need to be removed from the drawing.

If the twin is by rotation of 180°, a composition plane parallel to the twin axis will have a parallel orientation in the two individuals, but the remainder of the faces will not necessarily match at the boundary. In many cases the structures of the two individuals in a rotation twin will match without dislocation only if the composition plane is the rhombic section, which, though parallel to the twin axis, may be irrational. The rhombic section is the plane passing through the twin axis [*hkl*] and the line or vector $\mathbf{V}_{tp}$ perpendicular to the twin axis in the plane (*hkl*). The orientation of this plane may be found with a sequence of vector multiplications. If the twin axis [*hkl*] is the vector $\mathbf{V}_{ta}$ and the normal to the plane (*hkl*) is the vector $\mathbf{V}_h$,

$$\mathbf{V}_{tp} = \mathbf{V}_{ta} \times \mathbf{V}_h \quad \text{and} \quad \mathbf{V}_{rs} = \mathbf{V}_{tp} \times \mathbf{V}_{ta} \qquad (13)$$

where $\mathbf{V}_{rs}$ is the normal to the rhombic section.

Interpenetration twins can be drawn by not specifying a composition plane, and carrying out the twin operation on the entire crystal (Fig. 4). Here it is almost always necessary to draw in lines of junction between the individuals, and to remove some edges of each crystal which are masked by the other(s). With some ingenuity twin configurations involving composition planes not passing through the center of the crystal, such as multiple lamellar twins, may be drawn by making independent drawings of the individuals and superimposing them.

Shaded drawings

Line drawings of crystals, even when they are stereo-pair perspective, do not closely resemble real crystals; they give the impression of cardboard or paper models with inked edges. Shaded drawings that may be more pleasing to some tastes can be made if a suitable plotter is available (Fig. 5).

In the main program, before performing any orientation or stereo rotations, the cosine of the angle between each face normal and an illumination direction is calculated. The illumination direction is specified in standard crystal vector notation [*uvw*]. These illumination cosines are punched on cards, as well as the x and y coordinates of the two corners defining each edge. A second program reads these data, and converts the corner coordinates into equations of lines in the plane of the plot. Shading densities for each face are derived from the illumination cosines. The plotting area is scanned point-by-point on a fine

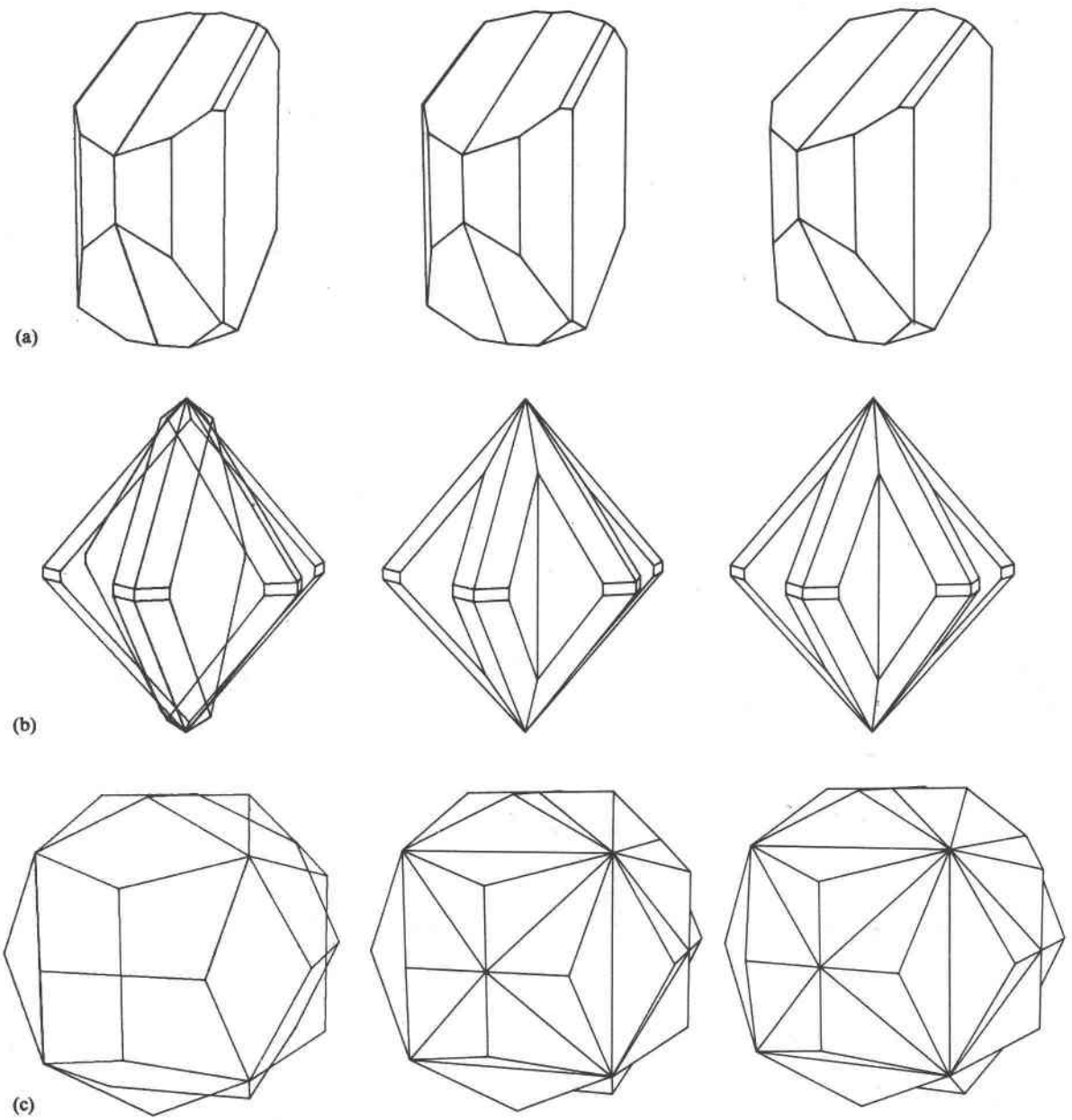

Fig. 4. (a) Andesine, class $\bar{1}$, albite twin by reflection on (010), showing the pinacoids {010}, {001}, {$\bar{2}$01}, {110}, {$\bar{1}$10}, {11$\bar{1}$}, {$\bar{1}$11}, {130}, {$\bar{1}$30}, {021} and {02$\bar{1}$}. (b) Aragonite or cerussite (class mmm) "sixling" twin; actually two twins by reflection on (110) and ($\bar{1}$10). Forms shown are the pinacoid {010}, prism {110} and dipyramid {111}. (c) Cubic crystal, class m3, "iron cross" twin; pentagonal dodecahedron {210} twinned by rotation on [011].

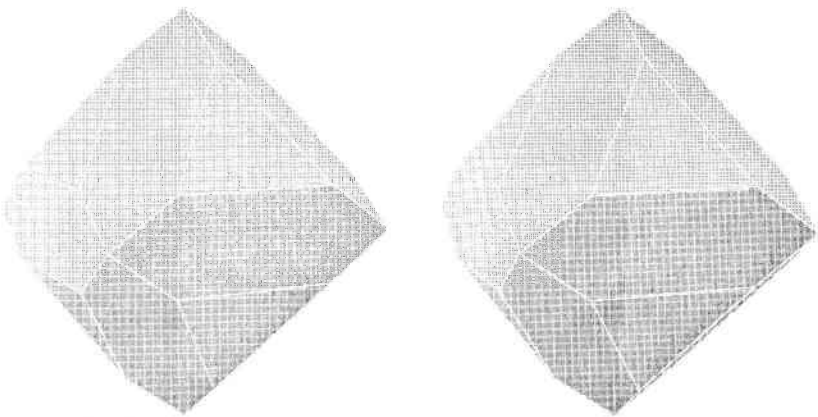

Fig. 5. Shaded drawing of a cubic crystal showing the dodecahedron {110} and the octahedron {111}.

grid, and a rather complicated algorithm uses the edge equations to determine in which face each point lies. The shading density for the face then determines whether a dot should be placed at that point.

Copies of the computer program are available from the author.

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