Plotting stereoscopic phase diagrams

Frank S. Spear

Department of Earth and Planetary Sciences
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

Abstract

An algorithm for calculating the x–y plotting coordinates of a rock or mineral given the composition in four-component barycentric coordinates is presented. The algorithm permits the plotting of stereoscopic four-component (tetrahedral) phase diagrams from any perspective desired and with any amount of foreshortening and stereoshift desired.

Introduction

The phase relations of chemical systems containing four or more components can be difficult to visualize unless a suitable projection through a ubiquitous phase can be found (*e.g.,* Thompson, 1957; Greenwood, 1975). Even after projection some systems cannot be represented with fewer than four components (*e.g.,* Spear, 1977; Rumble, 1978). Plotting mineral assemblages in four-component systems by means of perspective drawings of tetrahedra can be imprecise and time-consuming. Moreover, the visualization of phase volumes is greatly facilitated by stereoscopic viewing of tetrahedral phase diagrams, and plotting these types of diagrams is impossible without the aid of a suitable algorithm to calculate the plotting coordinates. This note presents such an algorithm.

The algorithm is designed so that the tetrahedron can be viewed from any perspective desired. In this respect, the algorithm differs from that contained in the program PROTEUS (H. J. Greenwood, personal communication), which provides for only two different stereoscopic views of tetrahedra. Arem (1971) presented a method for plotting stereoscopic four-component phase diagrams using the FORTRAN program ORTEP (Johnson, 1965). The approach outlined here provides an analytical solution for the calculation of plotting coordinates, instead of a graphical solution as outlined by Arem, and does not require any special computer program.

The algorithm is relatively simple and the only inputs required are three of the four barycentric coordinates (that is, the composition of the rock or mineral in the tetrahedron normalized to 1.0), the desired viewing distance, two angles to specify the desired rotation of the tetrahedron, and one angle specifying the desired amount of stereoshift. The algorithm is ideally suited for computer systems with x–y plotters. I currently have two working programs, available on request, for performing the calculations. One program, written for an HP-97 programmable pocket calculator, calculates the plotting coordinates only; the user must plot the diagram by hand on x–y graph paper. The other program, written in PDP-11 BASIC, is interfaced to an x–y plotter.

Plotting tetrahedral diagrams

The plotting of tetrahedra in perspective requires three steps: (1) conversion from barycentric (A,B,C,D) to cartesian (X,Y,Z) coordinates; (2) rotation of the cartesian coordinate system to the desired viewing point; and (3) projection from the perspective point onto the perspective plane. The analytical techniques used here are formulated in many standard texts on analytical geometry (*e.g.,* Schwartz, 1967, p. 585–588). Nye (1957, p. 8–11) presents a good discussion of the use of direction cosines in the transformation of coordinate systems. The construction of stereoscopic pairs simply involves the construction of two perspective drawings, each made from a slightly different perspective point. When the two images are viewed, each by a separate eye, the image appears in 3-D.

Conversion from barycentric to cartesian coordinates

The transformation is made by noting that the desired point to be plotted (a,b,c,d), be it an apex of the

tetrahedron or a mineral or rock composition, lies on the intersection of three planes: $A = a$, $B = b$ and $D = d$ (it also lies on the fourth plane $C = c$, but this plane is not independent of the other three). The right-handed cartesian coordinate system is established with the origin in the center of the tetrahedron (0.25, 0.25, 0.25, 0.25 in barycentric coordinates) with the three axes (X, Y, Z) oriented as shown in Figure 1. Unit distance is taken as the distance from the base to the apex of the tetrahedron.

Each of the three planes that intersect at the point of interest can be obtained by finding the normal to any one and the position of a point on it; the most convenient point to choose is the point where the normal intersects the plane. The equation of the plane is given by:

$$X_0X + Y_0Y + Z_0Z = (X_0^2 + Y_0^2 + Z_0^2)$$

where (X_0, Y_0, Z_0) are the coordinates of the point at which the normal vector $\{X_0, Y_0, Z_0\}$ intersects the plane.

The plane $D = d$ has the normal vector $\{0, 0, d - 0.25\}$ (Fig. 2) and thus the equation of the plane is $Z = (d - 0.25)$. The plane $B = b$ has the normal (determined by projection onto the Y and Z axes) $\{0, (b - 0.25) \cos 19.47, - (b - 0.25) \cos 70.53\}$ (Fig. 2) and thus the equation of the plane is

$$0.9428Y - 0.3333Z = (b - 0.25)$$

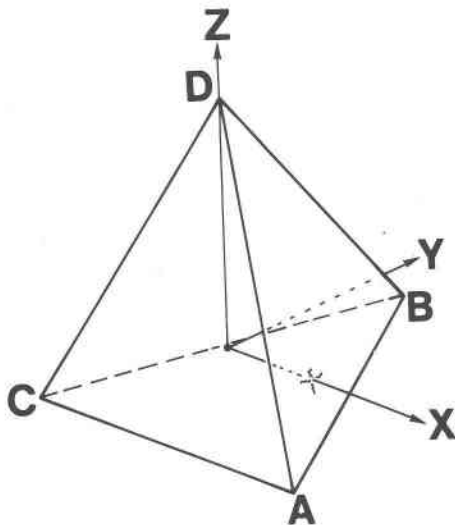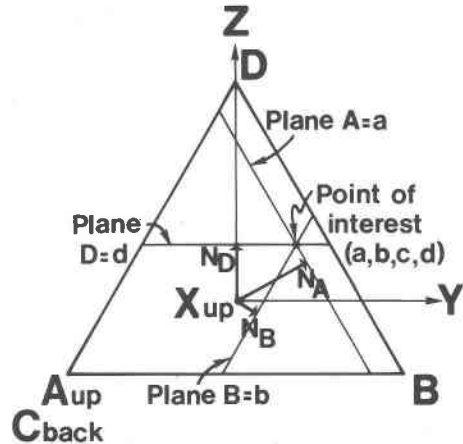The plane $A = a$ has the normal $\{(a - 0.25) \cos 19.47$

Fig. 2. Construction of tetrahedron taken through D, B and at the mid-point between A and C, showing the intersection of the three planes A=a, B=b, and D=d at the point of interest. N_D, N_A, and N_B represent the normal vectors to the three planes.

$\cos 30, -(a - 0.25) \cos 19.47 \cos 60, -(a - 0.25) \cos 70.53\}$ and the equation of the plane is

$$0.8165X - 0.4714Y - 0.3333Z = (a - 0.25)$$

Solving these three equations for X, Y and Z gives:

$$X = [(a - 0.25) + \tfrac{1}{2}(b - 0.25)$$
$$+ \tfrac{1}{2}(d - 0.25)]/0.8165 \quad (1a)$$

$$Y = [(b - 0.25) + \tfrac{1}{3}(d - 0.25)]/0.9428 \quad (1b)$$

$$Z = (d - 0.25) \quad (1c)$$

Rotation of cartesian coordinate system

Rotation of the tetrahedron into the desired viewing position is accomplished with direction cosine transformation matrices. The rotation can be broken into two parts: a rotation around Z and a rotation around X. These two rotations are sufficient to bring the tetrahedron into any orientation. The transformation equations for the first rotation are:

$$X' = X \cdot \cos\alpha - Y \cdot \sin\alpha$$
$$Y' = X \cdot \sin\alpha + Y \cdot \cos\alpha$$
$$Z' = Z$$

and for the second rotation are:

$$X'' = X'$$
$$Y'' = Y'\cos\theta + Z'\sin\theta$$
$$Z'' = -Y'\sin\theta + Z'\cos\theta$$

where α and θ are the angles for the first and second rotations, respectively.

Fig. 1. Perspective drawing of a tetrahedron showing relationship of cartesian to barycentric coordinate systems. The origin $(X,Y,Z) = (0,0,0)$ is set at $(a,b,c,d) = (0.25,0.25,0.25,0.25)$.

Projection onto the perspective plane

The perspective plane is taken as the X,Y plane ($Z = 0$) with the perspective point an arbitrary distance along the Z axis. The projection is made by adding some multiple of the vector $\bar{L}$, which is the vector from the perspective point, $\bar{E} = (0,0,e)$, to the point of interest, $\bar{P} = (X'',Y'',Z'')$, from the vector representing the point of interest and solving for the intersection with the X–Y plane. The vector $\bar{L}$ is given as $\bar{P}-\bar{E}$ or $\bar{L} = [X'', Y'',(Z'' - e)]$. The projected coordinates are thus:

$$X''' = X'' \frac{e}{(e - Z'')} \qquad Y''' = Y'' \frac{e}{(e - Z'')}$$

The X–Y plotting coordinates for any point (X,Y,Z) rotated through angles α and β and projected from an arbitrary perspective point $(0,0,e)$ are given as:

$$X''' \, e/(e - Z'') = (X\cos\alpha - Y\sin\alpha) \, e/(e - Z'') \quad (2a)$$

$$Y''' = Y'' \, e/(e - Z'')$$

$$= (X\sin\alpha\cos\theta + Y\cos\alpha\cos\theta + Z\sin\theta) \, e/(e - Z'') \quad (2b)$$

where

$$Z'' = -X\sin\alpha\sin\theta - Y\cos\alpha\sin\theta + Z\cos\theta \qquad (2c)$$

Stereoscopic phase diagrams

The plotting of stereoscopic phase diagrams involves plotting two diagrams, each drawn from a slightly different perspective point. This is most easily accomplished through a third rotation around the Y axis, the left "eye" requiring a clockwise rotation (looking down Y) and the right "eye" requiring a counterclockwise rotation. Incorporating this third rotation into equations 2 yields the following equations for the plotting coordinates of the left and right diagrams respectively:

$$X_{Left} = (X'' \cos\gamma/2 + Z'' \sin\gamma/2) \, e/(e - Z_{Left}) \qquad (3a)$$

$$Y_{Left} = Y'' \, e/(e - Z_{Left}) \qquad (3b)$$

where

$$Z_{Left} = -X'' \sin\gamma/2 + Z'' \cos\gamma/2 \qquad (3c)$$

and

$$X_{Right} = (X'' \cos\gamma/2 - Z'' \sin\gamma/2)e/(e - Z_{Right}) \qquad (4a)$$

$$Y_{Right} = Y'' \, e/(e - Z_{Right}) \qquad (4b)$$

where

$$Z_{Right} = (X'' \sin\gamma/2 + Z'' \cos\gamma/2) \qquad (4c)$$

In the above equations (2, 3, and 4) the angles α and θ determine the orientation of the tetrahedron; these angles can be any value from $-360°$ to $+360°$, as desired. The angle γ determines the amount of stereoshift and the quantity e determines the amount of foreshortening. For example, an individual with an interpupillary distance of 6 cm viewing an object from 20 cm (e) would have an interpupillary angle (γ) of $17.06°$. These values produce an acceptable stereo image, but may be altered to suit individual preferences.

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