5. TECHNICAL DETAILS

Publications by Heading,[8] Springer,[9] Todd,[10] and Korn and Korn[11] provide background on many of the projective and analytical geometry concepts discussed in this section.

5.1 HOW ORTEP DRAWS ELLIPSOIDS

Fig. 3.1 illustrates various ellipsoid graphical representations that can be drawn with ORTEP. The major components in the representations are the three principal ellipses and the boundary (outline) ellipse. The principal ellipses have a front half and a back (hidden) half. The entire boundary ellipse is visible.

An ellipse is approximated by connecting a series of points on the ellipse with straight line segments. Points on an ellipse having a general orientation in three dimensions are computed; then each of these points is projected onto the drawing board for plotting.

The basic algorithm for finding the points along a given general ellipse utilizes the properties of conjugate diameters. Assume that we have the three principal axis vectors $\mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3$ of the general ellipsoid and a vector $\mathbf{V}_4$ from the center of the ellipsoid to the viewpoint. The vector $\mathbf{V}_5$ normal to the polar plane (see Fig. 5.1), whose pole is the viewpoint, can be obtained from

$$\mathbf{V}_5 = \mathbf{A}\,\mathbf{V}_4\,, \tag{5.1.1}$$

where $\mathbf{A}$ is the matrix for the ellipsoid that is defined by

$$\mathbf{X}^{\mathrm{T}}\,\mathbf{A}\,\mathbf{X} = d\,, \tag{5.1.2}$$

where d is a constant.

The boundary ellipse is defined by two conjugate vectors, one of which is any vector $\mathbf{V}_6$ perpendicular to $\mathbf{V}_5$ and the second is $\mathbf{V}_7$, where

$$\mathbf{V}_7 = \mathbf{V}_5 \times \mathbf{A}\,\mathbf{V}_6\,. \tag{5.1.3}$$

The assumption made for this boundary ellipse derivation is that the view distance is large compared to the ellipsoid size. Therefore, the boundary ellipse defined above always lies on the diametral polar plane (see Fig. 5.1).

A principal ellipse that lies in the plane of the principal axis vectors $\mathbf{V}_1$ and $\mathbf{V}_2$ will have the third principal axis vector $\mathbf{V}_3$ normal to the plane of the ellipse. The intersection of this principal ellipse with the boundary ellipse is along the vector $\mathbf{V}_8$ where

$$\mathbf{V}_8 = \mathbf{V}_5 \times \mathbf{V}_3\,. \tag{5.1.4}$$

This vector divides the front and back (hidden) sides of the principal ellipse. A vector conjugate to $\mathbf{V}_8$ and in the principal plane containing $\mathbf{V}_1$ and $\mathbf{V}_2$ is $\mathbf{V}_9$, where

$$\mathbf{V}_9 = \mathbf{V}_3 \times \mathbf{A}\,\mathbf{V}_8\,. \tag{5.1.5}$$

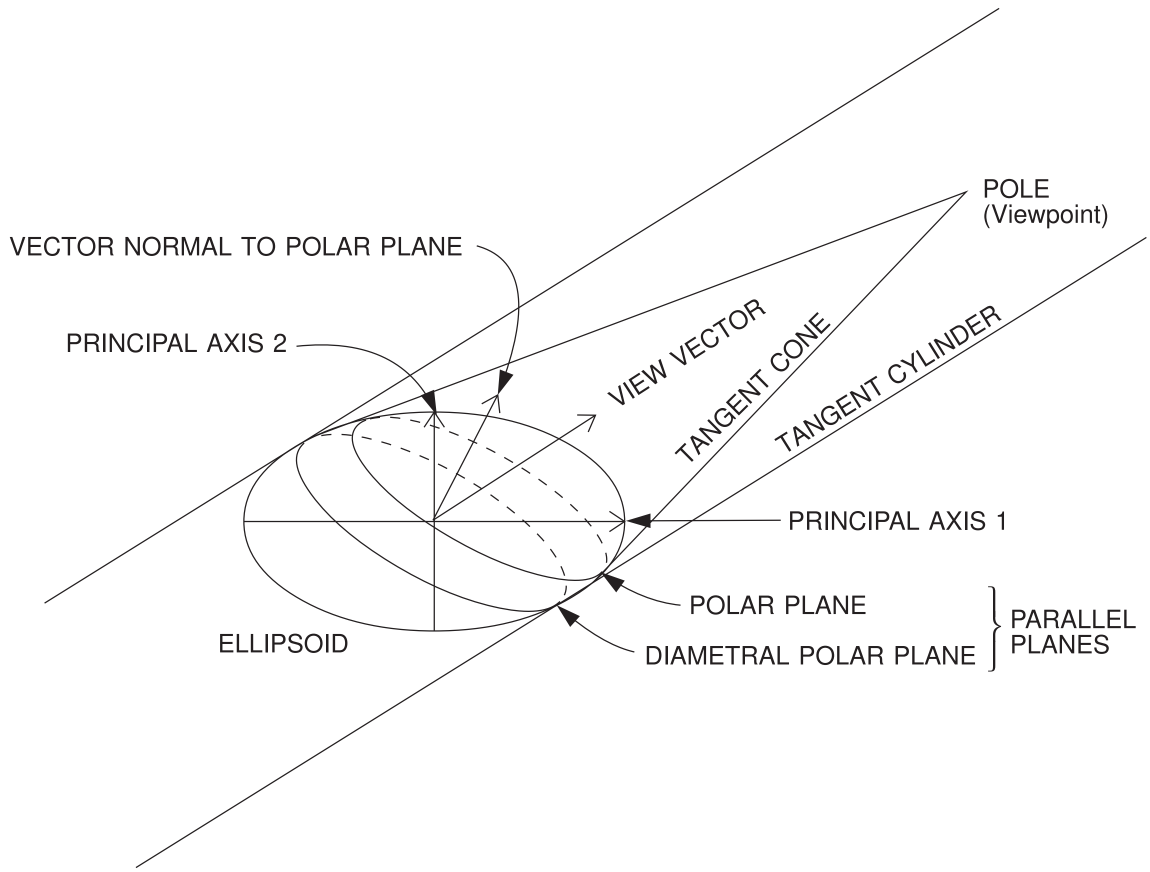

Fig. 5.1. Polar planes formed by tangent cylinder and tangent cone.

After the conjugate vectors have been found, their lengths are adjusted to make them satisfy Eq. 5.1.2 by letting $\mathbf{X} = s\,\mathbf{I}$, where $\mathbf{I}$ is a unit vector. Solving for s, we obtain

$$s = [\,d\,/\,(\mathbf{I}^{\mathrm{T}}\,\mathbf{A}\,\mathbf{I})]^{1/2}\,. \tag{5.1.6}$$

A conjugate vector pair is expanded into an ellipse by subroutine RADIAL. Since an ellipse is centrosymmetric, the two conjugate vectors and their negatives give four vectors whose endpoints lie on the ellipse. By performing a vector sum of two adjacent vectors and dividing the resultant vector components by $\sqrt{2}$, we can obtain an additional vector. After doing this for all adjacent pairs, we then have a total of eight vectors. This process can be repeated as many times as desired except that the scaling constant will be different for each cycle. The constant is described by

$$\mathrm{CONST}_i = \sqrt{2[\,1 + \cos(\pi/2^i)]} \;= 2\cos(\pi/2^{i+1})\,, \tag{5.1.7}$$

where i is the cycle number.

This total process may be thought of as taking a planar radial set of equally spaced unit vectors and performing a deformation and scaling on the space in which it is described. In geometry, this deformation is called an affine transformation.

Complete details on drawing ellipsoids can be obtained from the FORTRAN coding of subroutines F700 and RADIAL.

5.2 ELLIPSE RESOLUTION

With printer/plotter resolution improvements, highly complex stereo drawings with each image of the pair about 2.25 inches wide can now be produced directly without photographic reduction. As a result, it has become necessary to adjust the resolution (smoothness) of the plotted elliptical curves in ORTEP to take full advantage of the output devices' capabilities.

ORTEP produces its ellipses by "stretching" an equal-area circle to the shape of the ellipse. (Since ORTEP draws all its shapes with straight lines, the circle is, in fact, a polygon, and the smoothness of the ellipse depends on the number of vertices, or spokes, in the polygon.) ORTEP can produce circles having 16, 32, 64, and 128 spokes. The selection is a function of the radius of the circle. The default radii for changing to circles with fewer spokes are 0.09375 in. (128 $\rightarrow$ 64), 0.375 in. (64 $\rightarrow$ 32), and 0.75 in. (32 $\rightarrow$ 16). These default values are smaller than those in OR TEP-II.[2]

The smoothness of ellipses can be altered with the new 304 instruction in ORTEP-III, which allows the user to enter a smoothness factor. A factor of 1 sets the circle radii for changing to other spoke angles to the default values given above. A factor less than 1 produces smoother ellipses, and values greater than 1 produce ellipses with more "jaggies". If the factor is 0, all ellipses, regardless of their size, will be drawn from circles having 128 spokes.

Fig. 5.2 shows three groups of ellipses produced with smoothness factor settings of 3, 2, and 0. Although perfectly smooth ellipses are the ideal, it may be necessary to balance their appearance against the computational time to produce them and the sizes of the resultant files containing the ORTEP illustration. Table 5.1 shows the sizes of the EPS and HPGL files of the concentric ellipses in Fig. 5.2 as a function of the smoothness factor. Computational time was not determined for these examples, but it may become a significant factor on slower computers.

Table 5.1. Size of ORTEP illustration files as a function of ellipse smoothness factor settings.

Smoothness Factor	Size of EPS File	Size of HPGL File
0.	35544	28558
0.5	29400	23566
1.	21464	17118
2.	11992	9422
3.	8408	6510
5.	7640	5886
10.	5848	4430

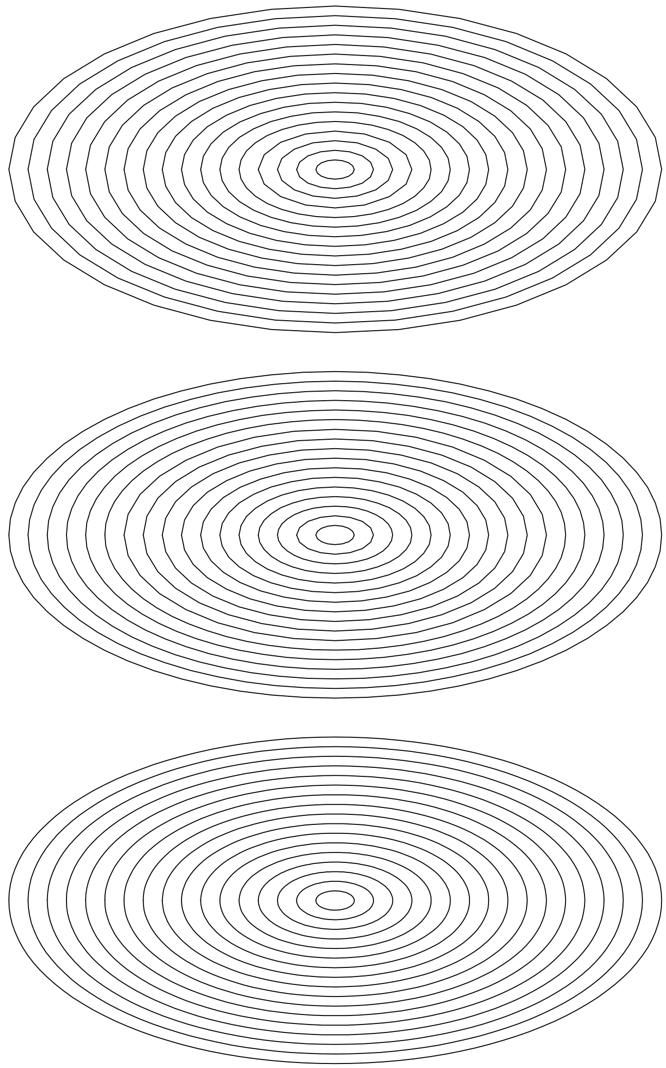

Fig. 5.2. Three sets of concentric ellipses produced by ORTEP with smoothness factor settings of 3, 2, and 0, respectively, starting from the top.

5.3 HOW ORTEP DRAWS BONDS

The major difficulty when drawing bonds is obtaining the intersection where the bond penetrates the ellipsoid. Three quadrics are used in subroutine BOND to calculate bond intersection. These three are the ellipsoid, the tangent cylinder, and the tangent cone.

The ellipsoid is described in matrix notation as

$$\mathbf{X}^{\mathrm{T}}\mathbf{A}\,\mathbf{X} = d\,, \tag{5.3.1}$$

where d is a constant and $\mathbf{X}$ is any vector from the center to the surface of the ellipsoid. The matrix $\mathbf{A}$ is 3×3 symmetrical with components a_{ij} $(i,j = 1, 2, 3)$.

The elliptic cylinder tangent to the ellipsoid and with its axis along z is described by

$$\mathbf{X}^{\mathrm{T}}\mathbf{B}\,\mathbf{X} = d\,, \tag{5.3.2}$$

where

$$\mathbf{B} = \begin{pmatrix} a_{11} - \dfrac{a_{13}a_{31}}{a_{33}} & a_{12} - \dfrac{a_{23}a_{31}}{a_{33}} & 0 \\ a_{12} - \dfrac{a_{13}a_{32}}{a_{33}} & a_{22} - \dfrac{a_{23}a_{32}}{a_{33}} & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{5.3.3}$$

and d is the constant used in Eq. 5.3.1. The tangent cylinder is used when it is necessary to terminate the bond at the boundary of the ellipsoid *when a parallel projection is used.*

To find the intersection of a cylindrical bond along $\mathbf{Vb}$ with radius r with either the ellipsoid or the tangent cylinder, we proceed as follows:

1. Form a radial set of vectors $\mathbf{Vr}_j$ of length r normal to $\mathbf{Vb}$.

2. Take a unit vector $\mathbf{I}$ parallel to $\mathbf{Vb}$ and let

$$\mathbf{X}_j = \mathbf{Vr}_j + s\,\mathbf{I}\,, \tag{5.3.4}$$

where s is a constant to be determined. Substituting in Eq. 5.3.1, we obtain

$$s^2\,\mathbf{I}^{\mathrm{T}}\mathbf{A}\,\mathbf{I} + 2s\mathbf{Vr}^{\mathrm{T}}\mathbf{A}\,\mathbf{I} + \mathbf{Vr}^{\mathrm{T}}\mathbf{A}\,\mathbf{Vr} - d = 0\,; \tag{5.3.5}$$

and solving for s, we get

$$s = \frac{-\mathbf{Vr}^{\mathrm{T}}\,\mathbf{A}\,\mathbf{I} + \sqrt{(\mathbf{Vr}^{\mathrm{T}}\,\mathbf{A}\,\mathbf{I})^2 - (\mathbf{I}^{\mathrm{T}}\,\mathbf{A}\,\mathbf{I})(\mathbf{Vr}^{\mathrm{T}}\,\mathbf{A}\,\mathbf{Vr} - d)}}{\mathbf{I}^{\mathrm{T}}\,\mathbf{A}\,\mathbf{I}}\,. \tag{5.3.6}$$

The elliptic cone that is tangent to the ellipsoid and has its apex on the viewpoint can be obtained from the matrix $\mathbf{A}$ and the vector $\mathbf{Vu}$, which extends from the center of the ellipsoid to the viewpoint. This is performed in the following steps:

1. The ellipsoid is transformed with a rotation matrix to a new Cartesian frame of reference that has the z axis along the view vector $\mathbf{Vu}$.

2. The tangent cone can now be described as

$$\mathbf{Y}^{\mathrm{T}}\mathbf{C}\,\mathbf{Y} = 0\,, \tag{5.3.7}$$

where $\mathbf{Y}$ is a vector originating from the vertex (viewpoint) of the cone and

$$\mathbf{C} = \begin{pmatrix} a_{11} + \dfrac{a_{13}a_{31}}{K-a_{33}} & a_{12} + \dfrac{a_{13}a_{32}}{K-a_{33}} & \dfrac{Ka_{13}}{K-a_{33}} \\ a_{21} + \dfrac{a_{23}a_{31}}{K-a_{33}} & a_{22} + \dfrac{a_{23}a_{32}}{K-a_{33}} & \dfrac{Ka_{23}}{K-a_{33}} \\ \dfrac{Ka_{31}}{K-a_{33}} & \dfrac{Ka_{32}}{K-a_{33}} & \dfrac{Ka_{33}}{K-a_{33}} \end{pmatrix}, K = d/(\mathbf{Vu}^{\mathrm{T}}\,\mathbf{Vu})\,. \tag{5.3.8}$$

3. The frame of reference is rotated back to its original orientation with a rotation matrix that is the inverse of the one used in step 1. Note that the origin is now on the viewpoint rather than on the ellipsoid center.

To find the length, s, of a vector $s\mathbf{I}$ extending from any point p inside the cone to the surface of the cone, we let

$$\mathbf{Y} = \mathbf{Vp} + s\mathbf{I} \tag{5.3.9}$$

and obtain from Eq. 5.3.7

$$(\mathbf{Vp} + s\mathbf{I})^{\mathrm{T}}\ \mathbf{C}\,(\mathbf{Vp} + s\mathbf{I}) = 0\ ; \tag{5.3.10}$$

then solving for s, we obtain

$$s = \frac{-\mathbf{Vp}^{\mathrm{T}}\mathbf{C}\mathbf{I} + \sqrt{(\mathbf{Vp}^{\mathrm{T}}\mathbf{C}\mathbf{I})^2 - (\mathbf{I}^{\mathrm{T}}\mathbf{C}\mathbf{I})(\mathbf{Vp}^{\mathrm{T}}\,\mathbf{C}\mathbf{Vp})}}{\mathbf{I}^{\mathrm{T}}\mathbf{C}\mathbf{I}} \tag{5.3.11}$$

The vector $\mathbf{Vp}$ from the vertex to p is formed by

$$\mathbf{Vp} = -\mathbf{Vu} + \mathbf{Vr}\,, \tag{5.3.12}$$

where $\mathbf{Vr}$ is any member of a radial set such as that described for the regular ellipsoid intersection.

5.4 OPTIMAL PARAMETERS FOR STEREOSCOPIC DRAWINGS

For optimal viewing of stereoscopic drawings, the origins of the two views should be separated by 2.2-2.4 in. and the stereo rotation between the two should be 5°-6°.

Fig. 5.3 was created when it was common practice to produce "large" ORTEP drawings that would be photographically reduced to give the optimal origin separation.[1,2] The reduced drawings would then typically be viewed with a stereoscope. Under these circumstances, Fig. 5.3 provides a picture of the relationship among the various parameters that must be taken into consideration when producing the drawing.[12,13]

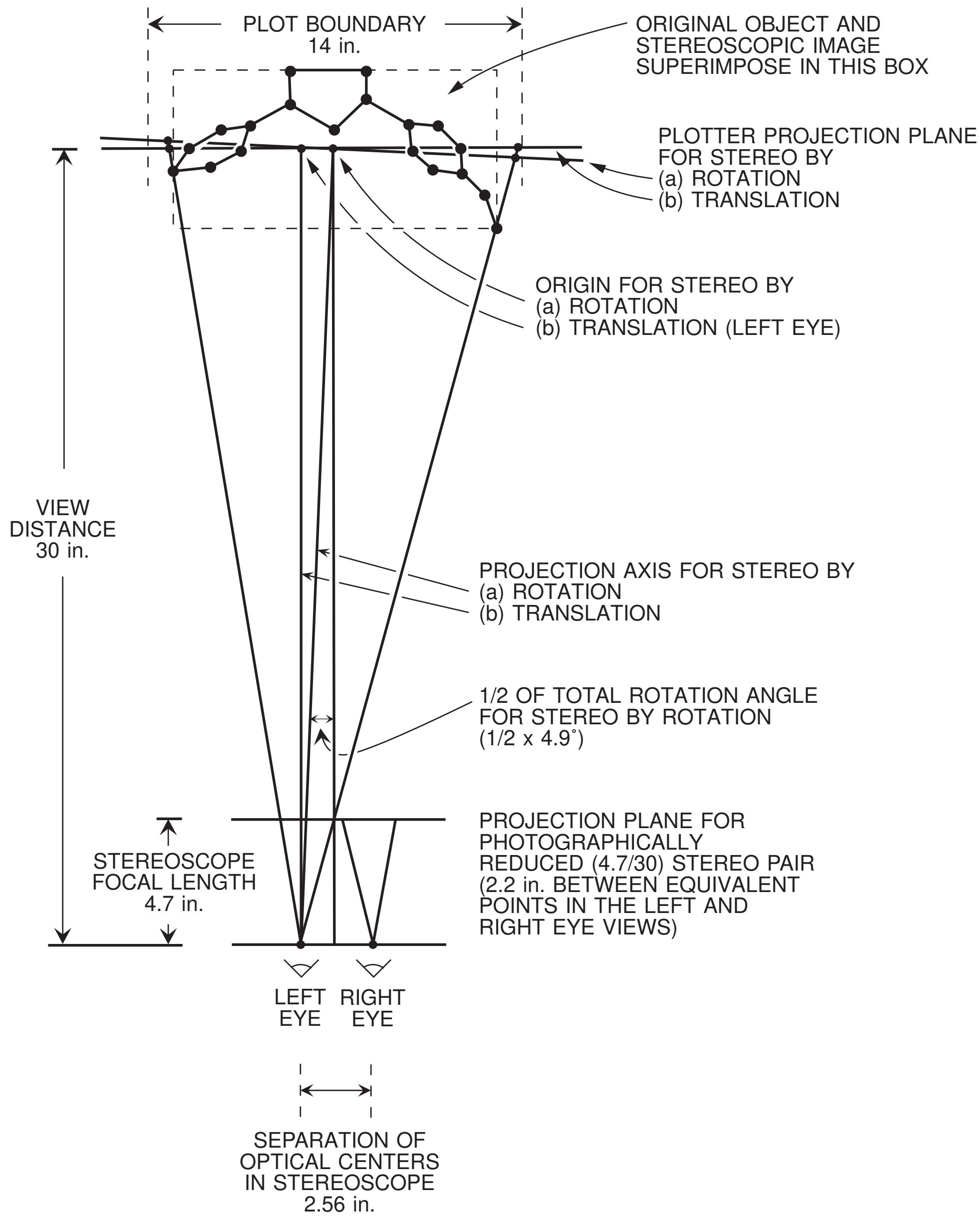

Fig. 5.3. Geometrical relations among the stereoscopic perspective projection parameters for a typical ORTEP drawing.

In Fig. 5.3, the available plotting area for each projection is assumed to be 14 in. horizontally and at least 11 in. vertically. The scaled mathematical object is within a box 12 in. wide, 9 in. (or more) high, and 6 in. deep with the plane of the plotter halfway back into the box. The stereoscopic image seen through a stereoscope with a 4.7-in. focal length and a 2.56-in. separation between optical centers should appear superimposed on the original object. The parameters for both “translation stereo” and “rotation stereo” are shown. The appropriate linear dimensions can be scaled to accommodate other plotting areas and still produce the same final stereoscopic image.

With the advent of high resolution printers/plotters, the need to reduce large drawings has diminished, and high quality drawings with the optimal origin separation can be produced directly. For those who view such drawings without the aid of a stereoscope, the viewing distance set in ORTEP should be the actual physical distance that will be used to view the pair. If a stereoscope is used for viewing, the viewing distance set in ORTEP is a function of the device's focal length and the location of the drawing's origin.

The cubane example in Section 2.4 can be used as a tool for determining the optimal view distance parameter. When the stereo cubane drawing is observed under usual viewing conditions, users should compare the front and back faces to decide if the molecule actually looks like a cube. If the faces appear out of proportion with each other, adjust the view distance parameter until the cube looks correct.

Theoretically, the best stereoscopic fidelity is obtained by translation of the origin rather than by stereo rotation of the object; however, the comparison of results given in Fig. 5.4 shows that the differences are indeed minor and nearly impossible to detect.

A

B

C

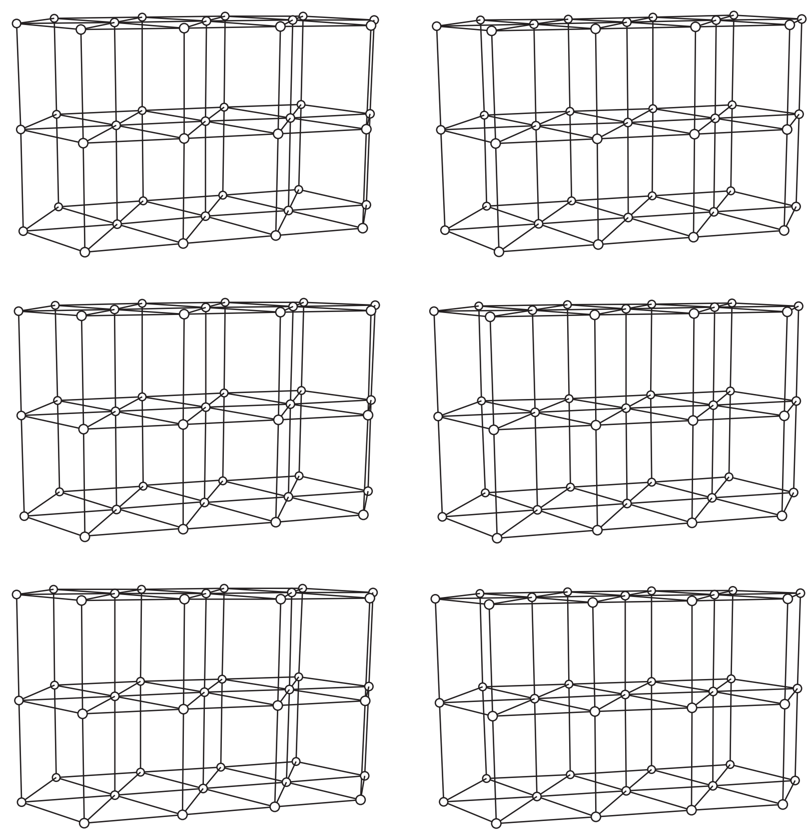

Fig. 5.4. Stereoscopic drawings of a hexagonal lattice with different stereoscopic parameters. (A) Stereo rotation of 4.9°, (B) stereo translation of 2.56 in., and (C) stereo rotation of 6.0°.

The top and middle drawings of Fig. 5.4 utilize the parameters derived in Fig. 5.3 and demonstrate that the differences predicted[13] for translation and rotation stereo are not discernible in practice. The bottom stereo drawing illustrates the slight exaggeration in depth that occurs when a larger stereo rotation angle is used.

Fig. 5.4A was produced with the following stereo-rotation instructions for the left and right eye views,

```
503         2     2.45

503         2    -2.45
```

and stereo translation instructions were used for Fig. 5.4B.

```
504    -1.28         0         0

504     2.56         0         0
```

Remember that the 504 instruction (see 3.3.6.4) changes the origin of the *reference* Cartesian system while the 503 instruction (see 3.3.6.3) rotates the *working* Cartesian system. If additional drawings are to be made following a stereo translation, the reference system origin should be returned to its original position in order to prevent confusion.

```
504    -1.28         0         0
```

Also keep in mind that the 504 instruction (see 3.3.6.4) should not be used when the ellipsoids have internal structure because the octants selected for shading may not be the same in both views.