Appendix E
3D Perspective View

Abstract This appendix describes a simple method to calculate a three dimensional perspective view on a two-dimensional screen of a collection of atom coordinates.

The specimen is clearly three dimensional (3D) but the electron microscope image is two dimensional (2D). The three dimensional structure of the specimen is projected into the final two-dimensional image making it difficult to determine if the original three dimensional structure of the specimen was properly described. The electron microscope image is in an x, y plane but the crystal structure is a set of (x_i, y_i, z_i) coordinates. The third dimension z can have a significant influence on the scattering within the specimen and influence the final image in rather nonintuitive ways. It is important to check that the full three dimensional structure of the specimen has been entered correctly.

A crystalline or amorphous specimen must be described as a detailed numerical list of atomic coordinates before an electron microscope image of the specimen can be simulated in the computer. Generating this set of numbers can be a rather tedious and difficult task. It is difficult to generate this list and even more difficult to determine if it is correct in the first place.

One particular type of diagnostic tool to determine if the specimen description is correct is to render a 3D perspective view of the entire specimen structure. Each atom can be drawn as a simple hard sphere and the entire structure can be rotated and viewed to inspect its three dimensional structure. A full rendering with shading and hidden surfaces can be difficult to calculate. There are a variety of sophisticated programs available for this procedure (for example RasMol [310] or jmol [189]). However, if some approximations are made there is a simple way to draw a reasonable approximation of the full 3D structure.

The specimen is assumed to be a collection of atoms in 3D. Each atom is drawn as a hard sphere at a particular set of coordinates (x_i, y_i, z_i) in 3D. This structure is viewed from a particular point in space as shown in Fig. E.1. The image seen by the viewer must be projected into a 2D image (the computer screen or a piece of paper).

E.J. Kirkland, *Advanced Computing in Electron Microscopy*,
DOI 10.1007/978-1-4419-6533-2_13,

If the viewer is close, then the structure will appear more distorted than if the viewer is far away. By varying the relative viewing position the three-dimensional nature of the structure can be investigated.

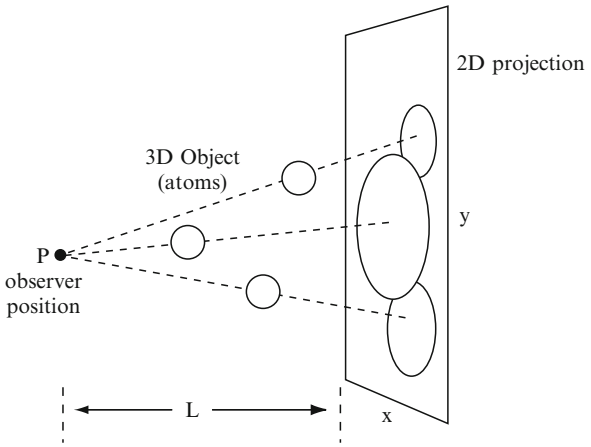

Fig. E.1 3D geometry of viewing a three dimensional collection of atoms (a specimen) as a two-dimensional projection

There are several approximations that make the 2D image simple to generate. First approximate a 3D sphere as a shaded circle. In 3D some atoms will be in front of other atoms and fully or partially hide those atoms in the back from the viewer. This is the so-called hidden surface problem. A simple approach to drawing hidden surfaces is to sort by depth and draw from the back forward. This is not particularly efficient but is simple to program and does a reasonable job of hiding the appropriate atoms. One particular situation that is not handled properly is the case where two adjacent atoms are at the same depth. One atom will be arbitrarily drawn on top of the other. This approach is simply enough to program on relatively simple and inexpensive personal computers (Kirkland [200]).

A 3D perspective view of the specimen is more useful if it can be rotated to see it from different angles. This should be done before drawing the 2D image for obvious reasons. Given a rotation angle ϕ and the tilt angle θ the initial set of atom coordinates (x_i, y_i, z_i) can be rotated about the point (x_0, y_0, z_0) (usually the center of the crystal) in two steps. First rotate by ϕ as:

$$\begin{aligned} x'_i &= (x_i - x_0)\cos\phi - (y_i - y_0)\sin\phi \\ y'_i &= (x_i - x_0)\sin\phi + (y_i - y_0)\cos\phi \end{aligned} \tag{E.1}$$

then tilt by θ as:

$$\begin{aligned} y''_i &= y'_i\cos\theta + (z_i - z_0)\sin\theta \\ z'_i &= -y'_i\sin\theta + (z_i - z_0)\cos\theta. \end{aligned} \tag{E.2}$$

Rotation and tilt produce a new set of coordinates (x_i', y_i'', z_i'). An angle of $(\phi, \theta) = (0,0)$ generates a view down the beam direction (the optic axis of the electron microscope). After rotation and tilt the z_i' coordinates are offset to yield $z > 0$ at the top or entrance surface and $z = 0$ at the bottom or exit surface. In Fig. E.1 the electrons are traveling from left to right with $z = 0$ on the right.

The position of each atom on the 2D viewing screen is not simply (x_i', y_i''). The three dimensional geometry between the viewer, the specimen and 2D viewing screen must be taken into account (for example Newman and Sproull [263]). If L is the distance from the viewer to the viewing screen and the specimen is in between the viewer and the viewing screen (as in Fig. E.1) then the actual coordinates on the viewing screen $(x_i, y_i)_s$ are:

$$x_{si} = \frac{Lx_i'}{L - z_i'}$$
$$y_{si} = \frac{Ly_i''}{L - z_i'} \tag{E.3}$$

by comparison of similar triangles as in Fig. E.2. The apparent size of each atom must also be scaled in a similar manner. If the actual 3D diameter of the atom is d_i then the diameter of the 2D circle is:

$$d_{si} = \frac{Ld_i}{L - z_i'} \tag{E.4}$$

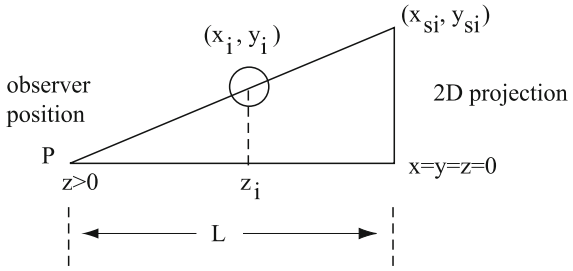

Fig. E.2 Similar triangles used to calculate the relative coordinates in a 3D perspective view

The final set of coordinates is sorted by depth z_i' and drawn from negative z_i' to positive z_i'. The sorting method of Shell is relatively easy to program and efficient enough for this purpose (Shell [318], Press et al. [288]). After sorting, each atom is drawn as a shaded circle. Each successive layer of atoms will overwrite the previous layer taking care of the hidden surface problem. Drawing a simple shaded circle is relatively easy and can mimic an actual 3D shaded sphere in a convincing manner. There are several possible ways to do this and two empirical schemes are listed later. If the output 2D perspective image is encoded as eight bits per pixel (integer valued)

with 255 being white and 0 being black then the grey scale intensity g inside each circle can follow:

$$g = 255 - 150\frac{r^2}{r_{\max}^2} \tag{E.5}$$

where r is the radius of the circle, and $r_{\max}$ is its maximum radius. This generates a white shaded circle on a black background. The entire background should be set to black before drawing any of the atoms. Alternately if an image is generated for printing on a postscript printer then the following postscript macros (Adobe Reference manual [170]) generates a black shaded circle on a white background:

```
%
% macro to make a unit circle at (0,0)
%
 /circle {newpath 0 0 1 0 360 arc
 closepath fill} def

%
%  macro to make a shaded sphere
%  call as-->  xscale yscale xpos ypos sp
%
/sp { gsave translate scale
   0.0 0.04 1 { sqrt 1 exch sub setgray circle
   0.98 0.98 scale  } for grestore } def
```

The first macro called "circle" draw a circle and fills it in with the current color or grey level. The second macros called "sp" draws a series of solid circle one on top of the other. Each successive circle is slightly smaller and slightly blacker to generate the shading. The "sp" macro is given a short name because it must be called many times and a shorter name will use less disk space and transfer quicker to the printer. Figure E.3 shows an example of a 3D view looking down the 110 direction of the silicon lattice.

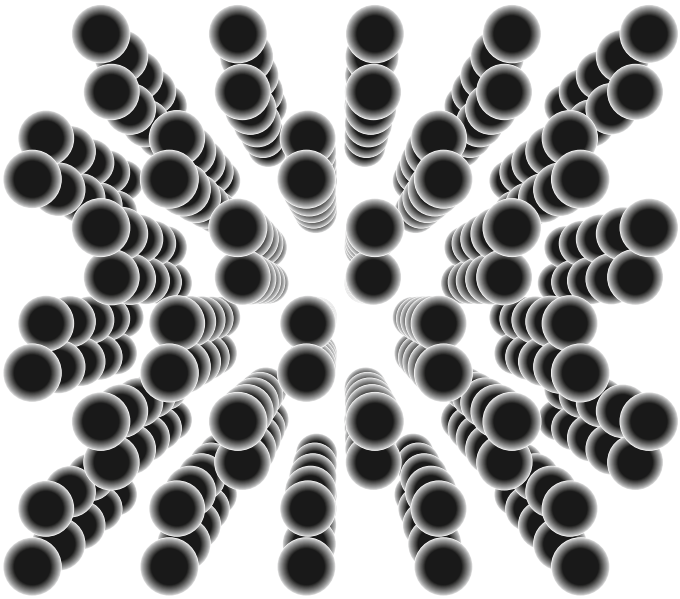

Fig. E.3 A 3D perspective view looking down the (110) direction of silicon (drawn in postscript format). Each silicon atom is drawn as a *shaded hard sphere (black)*