APPENDIX A

UNIT CELLS

Crystallography is the study of the structure of crystals; it includes the ways of describing the structure of a crystal, the principles that govern the different types of structures possible, the structures of crystals of specific substances, and the methods by which structures are determined.

A knowledge of crystallography is important in numerous scientific fields, including metallurgy, materials science, ceramics, physics and chemistry. Although each of these fields has its own special requirements, there is a basic core of knowledge common to them all. This consists of the description of the structure in terms of the smallest unit that can be used to represent it and the three-dimensional lattice with which the atom sites may be associated, and (2) the accepted method for determining planes and directions in crystal structures. It is (1) that will be further addressed here.

All crystal structures are periodic arrays of atoms, ions, or molecules, for which an imaginary box, the unit cell, may be constructed. The unit cell is the basic unit of the crystal structure. Consider the array shown in Figure 1 in which circles have been used to represent atoms, ions, or molecules. Three valid unit cells have been outlined that can be used to represent the array. The criterion for a valid unit cell is that if any of the three unit cells is moved along any of its edges by the length of the edge, the entire pattern is reproduced. Note that each unit cell contains one complete circle and that only the shaded portion of the circle lies within the unit cell.

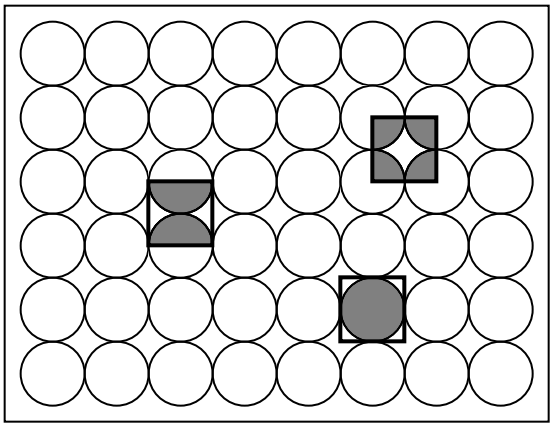

Figure 1: *A Cartesian array of circles with three valid unit cells, each containing a total of one circle.*

There are four properties of unit cells that may be generalized from the figure above.

1. The opposite sides of a unit cell are parallel.

2. Each unit cell contains an integer number of structural units (circles, atoms, ions, etc.)- in this case, one.

3. The unit cells fit together so as to fill space completely and they are identical to one another.

4. The corners of the unit cell can be anywhere.

Figure 2 below contains an oblique array of circles with a valid unit cell. Note that the unit cell selected possesses all four properties of a valid unit cell listed above.

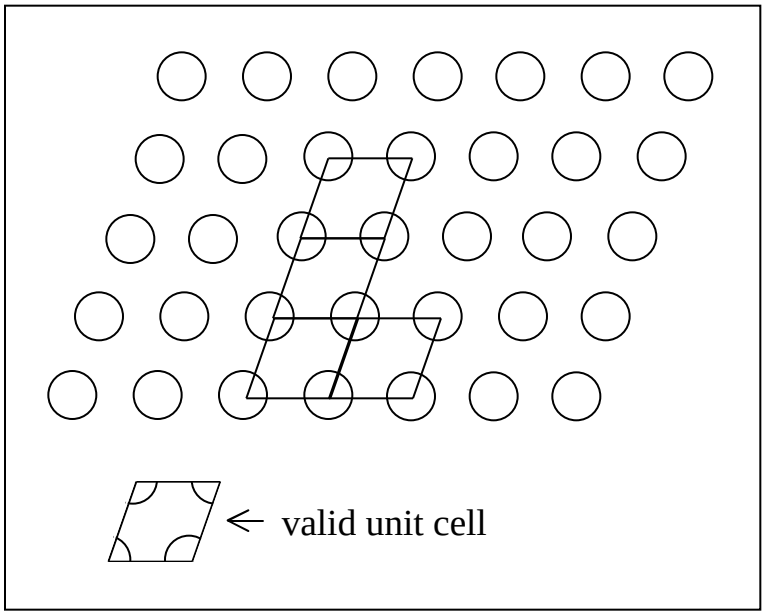

Figure 2: *An oblique array of circles with a valid unit cell.*

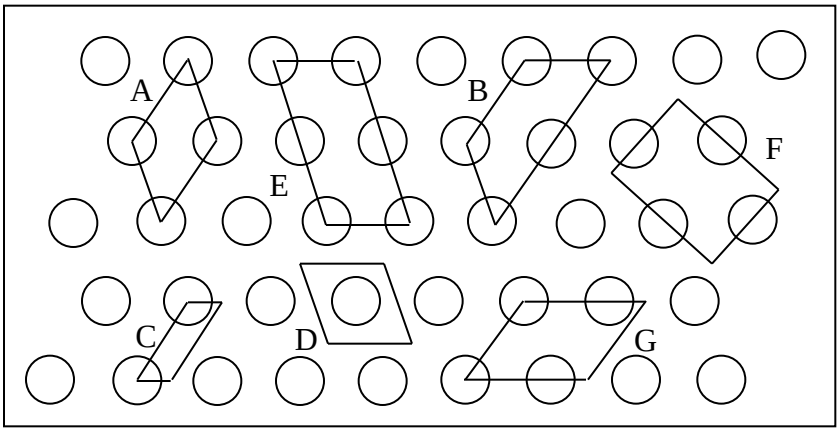

Figure 3. *An oblique array of circles with some valid and invalid unit cells.*

Note that in Figure 3 above, B, C, and G are not valid unit cells. B does not have parallel sides. C does not contain at least one complete structural unit (circle). Neither B, C, nor G fill space completely when shifted while still retaining the same arrangement of circles in each unit cell.

SUGGESTIONS

In order for students to identify a unit cell in the three-dimensional models that they are to construct, a presentation of the material above during the class session prior to Investigation 2

is probably necessary. Making overheads of the enlarged images contained here is also a good idea.