**Solid State Structures**

An inorganic compound’s three-dimensional structure can play an important role in determining its properties. In this week’s experiment you will study the structures of these compounds using physical 3-D models that you can manipulate by hand and computer-rendered 3-D representations that you can manipulate using the program Crystal Maker.

**Pre-lab Assignment**

Answer the following questions in your lab notebook. What is the Pythagorean theorem and why is it useful? For the figure shown to the right, each side of the square has a length of 1.00 cm and the circle fits exactly within the square (that is, it is tangent to each of the square’s four sides). To two decimal places, what is the area of the shaded portion of the square? For the figure to the left, which shows a rectangular solid with sides of 1.00 cm 🞨 1.00 cm 🞨 3.00 cm, what is the distance between the two dots?

**Procedure**

Following a demonstration of the software, you and a partner will complete exercises at 13 stations, filling out a report form as you go. You must complete Stations 1–4 before beginning working on other stations, which you may complete in any order. For most stations there is both a physical model and a computer model. There are many ways to represent atoms on a computer screen, two of which you will use in this lab: a ball and stick model (which makes it easier to see the unit cell) and a space-filling model (which makes it easier to evaluate the interactions between atoms). Feel free to move back and forth between the physical and computer models as you work.

**Station 1. Three Basic Cubic Systems: Simple Cubic**

A crystalline solid is built up from a simple array of atoms that repeats itself in three directions (up/down, left/right, and forward/backward). The simplest repeating array is called a unit cell and the entire structure is called a lattice. To understand the structure of a lattice, you need only examine the unit cell.

There are seven basic lattice systems, which are determined by the relative lengths of the unit cell’s three sides (a, b, and c in the figure to the right) and the relative size of the three angles (α, β, and γ) between the sides. In the basic cubic system, all sides of the unit cell are equal to each other (a = b= c), and all angles are right angles (α = β = γ = 90°). Within the cubic system there are three different ways atoms can be arranged: simple cubic, body-centered cubic, and face-centered cubic.

Open the file for the ball and stick model of the simple cubic unit cell and answer questions 1–4 on the report form. As you look at these models, try to imagine the three-dimensional lattice formed when using this unit cell as a building block. There is also a physical model in the room to inspect.

For questions 5–7 on the report form, open the unit cell’s space-filling model (file names ending with SF are space-filling models). The spaces between the atoms of a unit cell are called holes. For many ionic solids the larger anions define the lattice and the smaller cations occupy the holes. If a hole is surrounded by eight equidistant atoms, it is a **cubic hole**; if it surrounded by six equidistant atoms it is an **octahedral hole**; and if it surrounded by four equidistant atoms, it is a **tetrahedral hole**.

**Station 2. Three Basic Cubic Systems: Face-Centered Cubic (fcc)**

Open the files for the ball and stick model and the space-filling model of the fcc unit cell and answer the questions on the report form. As you look at these models, try to imagine the three-dimensional lattice formed when using this unit cell as a building block. There is also a physical model in the room to inspect.

**Station 3. Three Basic Cubic Systems: Body Centered Cubic (bcc)**

Open the ball and stick model and the space-filling model for the bcc unit cell and answer the questions on the report form. As you look at these models, try to imagine the three-dimensional lattice formed when using this unit cell as a building block. There is also a physical model in the room to inspect. Notice that in the space filling model, atoms on the face diagonal of the unit cell don’t touch, unlike the fcc example.

**Station 4. Closest Packing**

Consider the figures to the right, which shows a two-dimensional slice through a simple cubic unit cell and a closest-packed unit cell, and answer questions 1–4 on the report form. Assume that the circles have a radius of 0.5 cm, that the unit cells’ dimensions are shown by the square and the rhombus overlaying the circles, and that the black areas are holes.

There are two types of closest packing: hexagonal (hcc) and cubic (ccc). Open the files for each of these lattices and answer questions 5–7. Physical models are also available in the room. Carefully examine the layers in both models and look for patterns. For example, is the third layer the same as the first layer or the second layer? Is the fourth layer the same as the first layer, the second layer, or the third layer? Identify the pattern for each type of packing using a label such as ***abcd***, where each letter indicates a unique layer. A packing of ***abcd***, for example, means that there are four unique layers and that the fifth layer is identical to the first layer.

**Station 5. NaCl Lattice**

Examine the structure of the NaCl lattice using the computer and physical models and answer the questions on the report form. You may assume that the green balls are chlorine and the yellow balls are sodium. For questions 2 and 3, the coordination number for sodium ions is the number of chloride ions surrounding it, and the coordination number for chloride ions is the number of sodium ions surrounding it.

**Station 6. CsCl Lattice**

Examine the structure of the CsCl lattice using the computer and physical models and answer the questions on the report form. You may assume that the green balls are chlorine and the grey balls are cesium.

**Station 7. Zinc Blende Structure**

Examine the structure of the zinc blende (ZnS) lattice using the computer and physical models and answer the questions on the report form. You may assume that the yellow balls are sulfur and the grey balls are zinc. The corners of the unit cell are marked by red dots in the physical model.

**Station 8. Fluorite Structure**

Examine the structure of the fluorite lattice (CaF2) using the computer and physical models and answer the questions on the report form. You may assume that the green balls are fluorine and the grey balls are calcium.

**Station 9. Wurtzite Structure**

Examine the lattice structure of Wurtzite, another ionic lattice formed by zinc and sulfide ions, using the computer and physical models and answer the questions on the report form. You may assume that the yellow balls are sulfur and the grey balls are zinc.

**Station 10. Rutile Structure**

Examine the lattice structure of rutile using the computer and physical models and answer the questions on the report form. You may assume that the silver balls are titanium and the red balls are oxygen. Rutile differs from the other unit cells you have studied in that one of the unit cell’s sides has a length different from its other two sides. On the physical model, the atoms that form the corners of the unit cell are shown with red dots.

**Station 11. Diamond Structure**

Examine the lattice structure for diamond using the computer and physical models and answer the questions on the report form.

**Station 12. Calcite Structure**

Examine the lattice structure for calcite (CaCO3) using the computer and physical models and answer the questions on the report form. Note that only the computer model shows the full unit cell! To easily see the unit cell outline on the computer you can hide the atoms by unclicking their boxes in the visualizer.