Solid State Structures

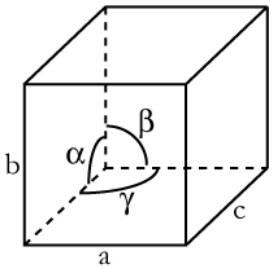
An inorganic compound's three-dimensional structure can play an important role in determining its properties. In this week's experiment you will study the structures of these compounds using physical models that you can manipulate by hand and computer-rendered representations that you can manipulate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

Pre-lab Assignment. Answer the following questions in your lab notebook. For the figure on the right, if 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—then to two decimal places, what is the area of the shaded portion of the square? For the figure on 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? Be prepared to share your work at the beginning of the lab.

Procedure. Following a demonstration of the software, you and a partner will complete exercises at 12 stations, filling out a report form as you go. You must complete Stations 1–4 before your begin work on other stations, which you then 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 model and the computer model as you work.

Station 1. Three Basic Cubic Systems: Simple Cubic. A crystalline solid is built from a simple array of atoms that repeats itself in three directions. The simplest array is a unit cell and the entire structure is a lattice. To understand a lattice's structure, 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 in length(a = b= c) and all angles are right angles (α = β = γ = 90°). Within the cubic system there are three different ways to arrange atoms: 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 that forms when this unit cell is the building block. There is also a physical model in the room to inspect.

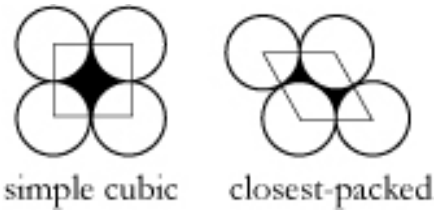
For questions 5–7 on the report form, open the unit cell's space-filling model (filenames that end with SF are space-filling models). The spaces between the atoms in a unit cell are holes. For many ionic solids the anions, which are larger, define the lattice and the cations occupy the holes. If a hole 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 that forms 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 that forms 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 on the right that show 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 the circles have a radius of 0.5 cm, that the unit cells' dimensions are defined by the square and the rhombus that overlay 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 model and the physical model, and answer the questions on the report form. The green balls are chloride ions and the yellow balls are sodium ions. For questions 2 and 3, the coordination number for sodium ions is the number of chloride ions that surround it, and the coordination number for chloride ions is the number of sodium ions that surround it.

Station 6. CsCl Lattice. Examine the structure of the CsCl lattice using the computer model and the physical model, and answer the questions on the report form. The green balls are chloride ions and the grey balls are cesium ions.

Station 7. Zinc Blende Structure. Examine the structure of the zinc blende (ZnS) lattice using the computer model and the physical model, and answer the questions on the report form. The yellow balls are sulfide ions and the grey balls are zinc ions. The corners of the unit cell are marked by red dots.

Station 8. Fluorite Structure. Examine the structure of the fluorite lattice (CaF_2) using the computer model and the physical model, and answer the questions on the report form. The green balls are fluoride ions and the grey balls are calcium ions.

Station 9. Wurtzite Structure. Examine the lattice structure of Wurtzite—another ionic lattice of zinc and sulfide ions—using the computer model and the physical models, and answer the questions on the report form. The yellow balls are sulfide ions and the grey balls are zinc ions.

Station 10. Rutile Structure. Examine the lattice structure of rutile using the computer model and the physical model, and answer the questions on the report form. The silver balls are titaniums 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 that is 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 model and the physical model, and answer the questions on the report form.