# Solid State Modeling

## PURPOSE

**A** To explore some simple solid state structures.

**B** To explore unit cell stoichiometry.

## GOALS

**1** To visualize the three dimensional arrangement of atoms and ions in common solid state structures.

**2** To determine the stoichiometry of unit cells.

**3** To gain a working knowledge of unit cells, packing efficiency, coordination numbers and their relationship to each other.

## INTRODUCTION

The solid state is the least energetic of the three common states of matter. Atoms and ions are packed together in a regular arrangement. The arrangement is normally one that minimizes the energy of the particles by maximizing the interaction of positive and negative charges. Maximizing the contact between atoms, which maximizes the dispersion forces holding atoms and molecules together, also minimizes energy. Thus, atoms and ions are often packed in a spatially efficient manner with alternating charges. When this ordered arrangement extends throughout the entire crystal in very well defined and repeating patterns (**a crystal lattice**), the solid is considered **crystalline.** If the arrangement is not as repetitive (local order), the solid is **amorphous**. This experiment deals only with crystalline solids.

Although this description might lead you to believe that there is only one best way to arrange atoms to minimize their energies, there are actually many different ways atoms and ions can pack to achieve this. The arrangement a particular compound or material chooses depends to a large extent on the size and charge of the particles.

The three simplest and common lattices are:

- **Simple cubic or primitive** in which identical particles are found on the eight corners of a cube.
- **Body centered cubic** in which identical particles are found on the eight corners plus one in the center of the cube.
- **Face centered cubic** in which identical particles are found on the eight corners plus the six faces of the cube.

In this modeling experiment, you will build models of a few of the packing arrangements that simple materials can take. The models will focus on the **unit cell** of these structures. The unit cell is the smallest repeating unit in the three dimensional array. You will also explore **unit cell**

**stoichiometry.** We normally think of the stoichiometry of a substance as the ratio of moles of each element. This is reflected in the chemical formula of that substance. This same ratio must also hold in the smallest repeating unit of the solid state, the unit cell. The models will help you visualize the number of each atom or ion inside a unit cell and help you determine the stoichiometry.

Packing efficiency and coordination number will also be investigated. The **packing efficiency** of a unit cell is the fraction of the volume of the unit cell that is occupied by atoms, ions or molecules (commonly expressed as the percent). Thus, as more atoms are packed into a volume, the packing efficiency increases. The **coordination number** is the number of atoms surrounding another atom in a crystal lattice. The coordination number can also predict trends in packing efficiency. As the coordination number increases, the packing efficiency increases as well. The space in a unit cell that is not occupied by an atom is referred to as the **void volume.** As void volume increases, packing efficiency decreases.

In Part A of the experiment, you will build some simple structures that metallic elements pack in. You may have encountered these in the lecture class. Part B is an exercise in exploring unit cell stoichiometry: finding the ratio of two different ions inside a few unit cells.

# EQUIPMENT

**1** Solid-State Model Kit

**1** ruler

### About the model kit.

This model kit was developed by the Institute for Chemical Education at the University of Wisconsin - Madison. The instruction pages that follow are reprinted with permission from the Institute for Chemical Education (ICE), John W. Moore, director. The Chemistry Department of North Carolina State University wishes to express thanks to ICE for permission to reproduce these pages.

**Contents of the model kit.** When you open the model kit, you will notice a series of boxes and/or bags containing different colored spheres. These will be our atoms and ions. There are also two square plastic blocks with holes drilled in them. These will be the bases. Notice that one has a circular sticker and the other a semicircular sticker. There are also a number of square paper templates with holes punched in them. Each has either a circle or semicircle in the corner and a letter to identify it. There is also a long plastic tube with metal rods in it.

**Assembling the structure base.** Instructions for assembling each solid state base appear on the ensuing pages. In each case, a paper template is placed on top of one of the bases, with the circle or semicircle aligned. The metal rods are then inserted into specific holes in the template, as instructed. The structure is then built up, layer by layer.

**Taking a model apart.** To take a model apart, invert the structure and allow the spheres to slowly slide off the rods. Try to make sure the spheres do not roll away. Remove the rods by grasping near the base and pulling without bending or wiggling.

**Instructions for assembling the solid state structures.** Instructions for each of the structures in this lab are given on the ensuing pages. For each structure, pictures are reproduced from the instruction manual that accompanies the model kits. They include a picture of the template in the upper right hand corner and the pattern of holes that are used on that template in the upper left hand corner.

Next to each hole in the pattern is a number, which corresponds to a layer of atoms. Building the layers in numerical order forms structures. Usually the top layer of the structure is a repeat of layer number 1, and is referred to as layer 1'. You will notice that some of the numbers are black and others are white. The black and white numbers correspond to different color spheres, as given by the key at the bottom left corner. This experiment will be using the colorless, green and blue spheres.

There is also a picture of the "unit cell layers". This shows a picture of the arrangement of each layer of the unit cell. **Use the instructions provided to assemble each structure using the entire shaded area of the template.** Do not build your structures based on the "unit cell layers", because it will not give a large enough portion of the structure to allow you to answer the questions for the non-cubic cells.

Follow the typed instructions for each structure. These will give you step by step instructions on building the models. Also, you will be asked to view the structures as you assemble them and answer questions about them.

## REAGENTS

No chemicals will be used in this experiment.

## SAFETY

None of the materials being used in this experiment present a safety hazard. However, the work is being done in a laboratory and the usual rules about eye protection and proper clothing apply.

Gloves will not be provided for this experiment as no chemicals are involved.

## WASTE DISPOSAL

Since no chemicals are being used in this experiment, there will not be any waste for disposal.

## PRIOR TO CLASS

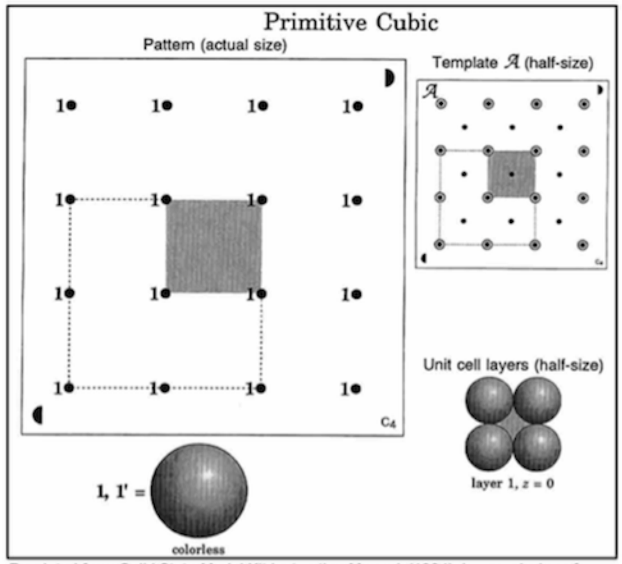
Please complete WebAssign prelab assignment. Check your WebAssign Account for due dates. Students who do not complete the WebAssign prelab are required to bring and hand in the prelab worksheet.

## LAB PROCEDURE

You will notice the format of this lab experiment is different than other experiments. You will build a series of solid state structures. Directions for building each structure are intermingled with questions to help you with your observations. Please answer the questions in your lab manual along with any other observations you make while you are building the structures.

Please print the worksheet for this lab. You will need this sheet to refer to.

## Part A: Some Simple Structures



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*Structure 1: Simple (primitive) cubic (use template A)*

- Position the semicircle on template A in the same corner as the matching semicircle on the base, and align the holes.
- Insert rods in the 4 *circled* holes in the shaded region.
- Place a single atom on one of the 4 rods.

**Question A1:** Looking from above, how much of the atom is inside the shaded region?

**Question A2:** The corner of a cubic unit cell such as this one is *defined by the center (nucleus) of the atom at the corner.* How much of this atom is above the nucleus **and** inside the shaded region (inside the unit cell)?

- Build the rest of layer **1.**
- Complete the unit cell by repeating the first layer (**1'**).

**Question A3:** How many total atoms are inside the unit cell (where the corners of the cubic unit cell are defined by the centers of the eight spheres)?

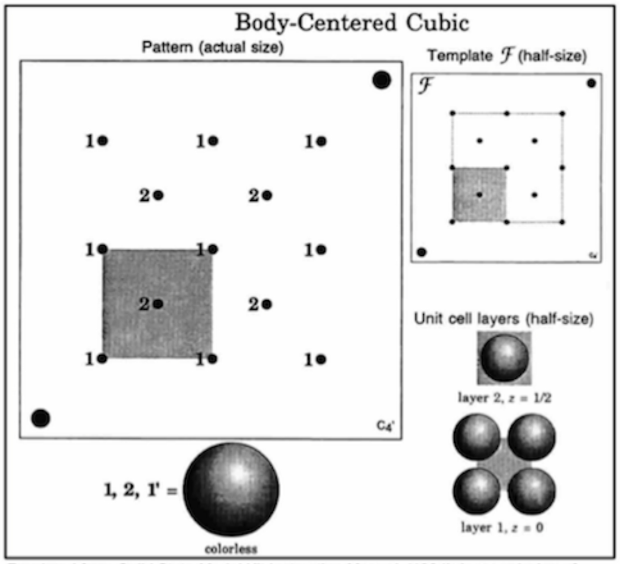
**Question A4:** Using a ruler, measure the length of a side of your unit cell in cm. (Remember, the unit cell is defined by the nuclei of the atoms!) What is the volume of your unit cell?

**Question A5:** We will define "atom density" for our unit cells as the number of spheres that can pack into a cubic centimeter. What is the "atom density" (spheres/$cm^3$) for your simple cubic cell?

**NOTE:** Keep this structure assembled to compare with the next structure.

*Structure 2: Body centered cubic (**use template F**)*

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- Position the circle on template **F** in the same corner as the matching circle on the base, and align the holes.
- Insert rods in **all 5 holes in the shaded region.**
- Place a single atom at **one** of the layer **1** positions.

**Question A6:** Noting as before that the corner of the unit cell is defined by the nucleus of this atom, how much of this atom is inside the unit cell?

- Complete layer **1** and then layer **2**.
- Complete the unit cell by repeating the first layer (**1'**).

**Question A7:** Focus on the layer 2 atom. How much of this atom is inside the unit cell?

**Question A8:** How many total atoms are inside the unit cell?

**Question A9:** Using a ruler, measure the length of a side for this unit cell. What is the volume (in $cm^3$) of this unit cell?

**Question A10:** What is the "atom density" (spheres/$cm^3$) for your body centered cubic cell?

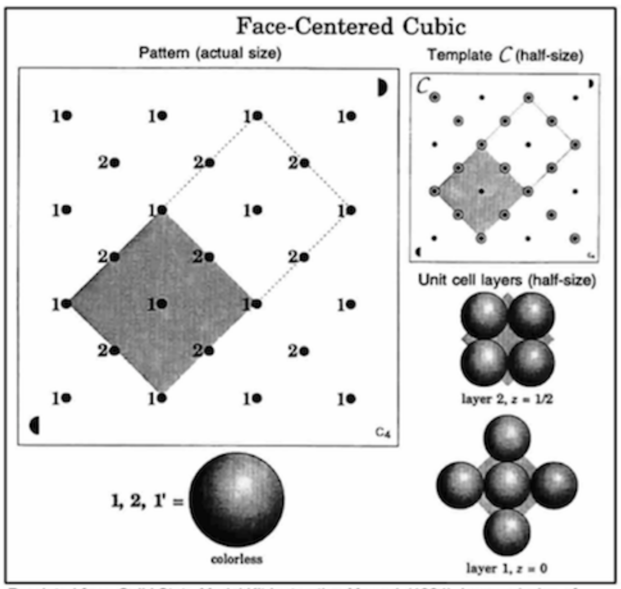
**Question A11:**

**a** Comparing this structure (body centered cubic) to the last structure (simple cubic), which one *appears* to have less void volume?

**b** Compare your observation to your calculated “atom densities” for these two structures. Do your calculations confirm your observation?

**NOTE:** Keep this structure assembled to compare with the next structure.

*Structure 3: Face centered cubic (**use template C**)*

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- Carefully disassemble your simple cubic structure.
- Position the semicircle on template **C** in the same corner as the matching semicircle on the base, and align the holes.
- Insert rods in **all 9 holes in the shaded region.**
- Place a single atom at one of the layer 1 positions. Noting as before that the corner of the unit cell is defined by the nucleus of this atom, how much of this atom is inside the unit cell?
- Build each layer in numerical order. Finish each layer before starting the next layer.
- Complete the unit cell by repeating the first layer (**1’**).

**Question A12:** Focus on a layer 2 atom. How much of this atom is inside the unit cell?

**Question A13:** How many total atoms are inside the unit cell?

**Question A14:** Using a ruler, measure the length of a side of this unit cell. What is the volume (in $cm^3$) of this unit cell?

**Question A15:** What is the "atom density" (in spheres/cm$^3$) for your face centered cell?

**Question A16:**

**a** Comparing this structure (face centered cubic) to the last structure (body centered cubic), which one *appears* to have less void volume?

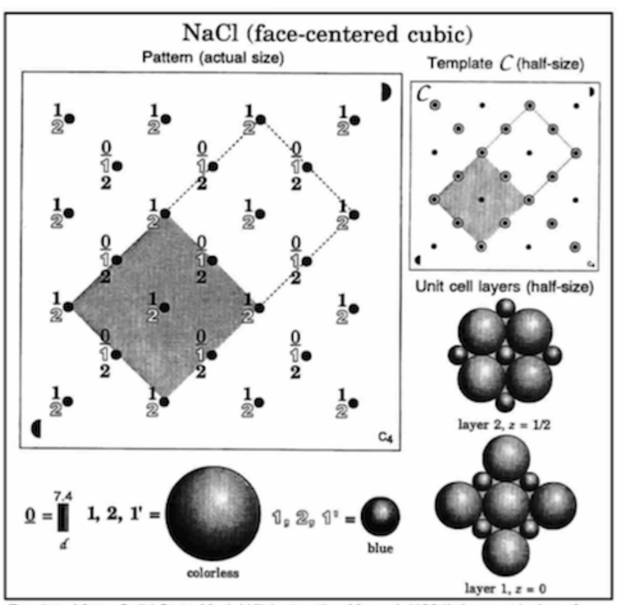
**b** Compare your observation to your calculated "atom densities" for these two structures. Do your calculations confirm your observation?

**Question A17:** Comparing the "atom densities" of all three cubic unit cells, rank them in packing efficiency, with the most efficiently packed cell listed first.

- Carefully disassemble the two remaining structures.

## Part B: Unit Cell Stoichiometry

*Structure 4: Sodium Chloride (**use template C**)*



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- Position the semicircle on template **C** in the same corner as the matching semicircle on the base, and align the holes.
- Insert rods in **all 9 holes in the shaded region.**
- Build each layer in numerical order: **0**, **1**, 1, **2** and 2. (Layer **0**, grey straw spacers, must be assembled first!) Finish each layer before starting the next layer.
- Complete the unit cell by repeating the first layer (**1'**, 1').

**Question B1:** Focus on *only* the colorless spheres. What type of cubic structure do they appear to be arranged in?

**Question B2:** Focus on *only* the blue spheres. What type of cubic structure do they appear to be arranged in? (You may need to build another set of layers 2 and 2 to see this.)

**Question B3:**

**a** How many colorless spheres are inside the unit cell?

**b** How many blue spheres are inside the unit cell?

**c** What is the ratio of colorless to blue spheres in the unit cell?

**d** What is the chemical formula for sodium chloride?

**e** Do your results in part c reflect the correct stoichiometry in sodium chloride?

**f** Based on your knowledge of trends in ionic radii, which spheres represent sodium ions and which represent chloride ions?

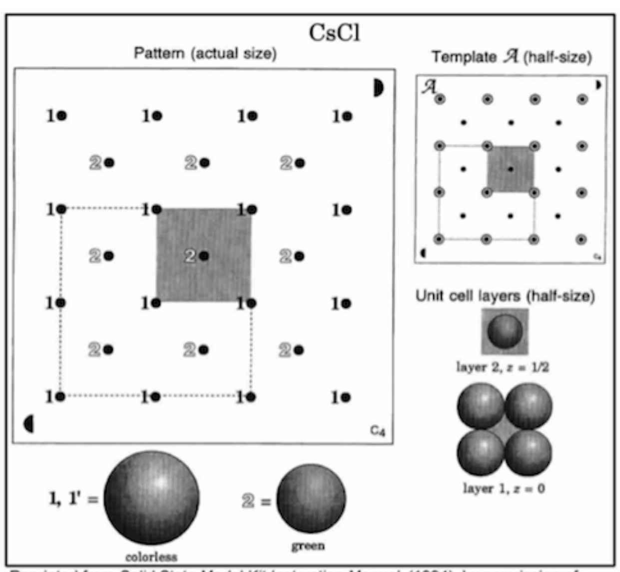
**Question B4:**

**a** Focus on the central, colorless sphere of layer 1'. How many blue spheres are in contact with it? (You may need to build another set of layers 2 and 2 to see this.) This is its coordination number.

**b** Focus on the central, blue sphere of layer 2. How many colorless spheres are in contact with it?

- Carefully disassemble this structure.

*Structure 5: Cesium Chloride (**use template A**)*

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- Position the semicircle on template **A** in the same corner as the matching semicircle on the base, and align the holes.
- Insert rods in **all 5 holes in the shaded region.**
- Build each layer in numerical order: **1** and **2**. Finish each layer before starting the next layer.
- Complete the unit cell by repeating the first layer (**1'**).

**Question B5:** Focus on *only* the colorless spheres. What type of cubic structure do they appear to be arranged in?

**Question B6:**

**a** How many colorless spheres are inside the unit cell?

**b** How many green spheres are inside the unit cell?

**c** What is the ratio of colorless to green spheres in the unit cell?

**d** What is the chemical formula for cesium chloride?

**e** Do your results in part c reflect the correct stoichiometry in cesium chloride?

**f** Based on your knowledge of trends in ionic radii, which spheres represent cesium ions and which represent chloride ions?

- Carefully remove the four colorless atoms of layer **1'**.
- Insert rods in to the **remaining 8 holes in the region indicated by the dashed square.**
- Complete layer **1** with colorless spheres. Note: There should be nine total.
- Complete layer **2** with four green spheres.
- Repeat layers **1** and **2**.

**Question B7:** Focus only on the cube made by the 8 green spheres.

**a** What type of cubic structure do the green spheres appear to be arranged in?

**b** What is the ratio of colorless to green spheres?

**Question B8:** Using a ruler, compare the length of the side of a cube with colorless spheres on the corners to one with green spheres.

**a** Do they have the same volume?

**b** Are these both acceptable unit cells for cesium chloride? Why or why not?

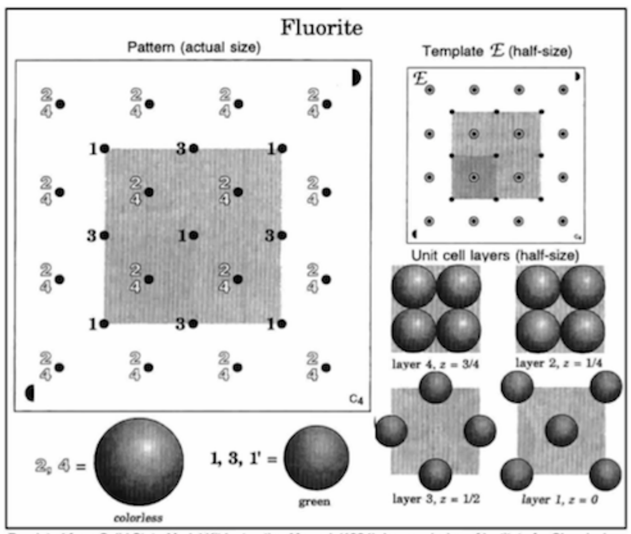
**Question B9:**

**a** Focus on one of the green spheres in layer 2. How many colorless spheres are in contact with it?

**b** Focus on the colorless sphere at the center of the green cornered cube. How many green spheres are in contact with it?

- Carefully disassemble this structure.

*Structure 6: Fluorite (calcium fluoride)* (***use template E***)

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- Position the semicircle on template **E** in the same corner as the matching semicircle on the base, and align the holes.
- Insert rods in **all 13 holes in the shaded region.**
- Build each layer in numerical order, **1** through **4**. Finish each layer before starting the next layer.
- Complete the unit cell by repeating the first layer (**1'**).

**Question B10:**

**a** Focus on *only* the colorless spheres. What type of cubic structure do they appear to be arranged in?

**b** Focus on *only* the green spheres. What type of cubic structure do they appear to be arranged in?

**Question B11:** Putting the two ions together in this arrangement gives the "fluorite" structure. The name is derived from the mineral fluorite, which contains calcium fluoride.

 

**a** How many colorless spheres are inside the unit cell?

**b** How many green spheres are inside the unit cell?

**c** What is the ratio of colorless to green spheres in a unit cell?

**d** What is the chemical formula of calcium fluoride?

**e** Do your results in part c reflect the correct stoichiometry in calcium fluoride?

**f** Which spheres represent calcium ions and which represent fluoride ions?

- Carefully disassemble this structure.
- Reassemble the contents of the model kit and return it to where you found it at the beginning of the lab period.
- Before leaving, go to a computer in the laboratory and enter your results in the InLab assignment. If all results are scored as correct, log out. If not all results are correct, try to find the error or consult with your teaching assistant. When all results are correct, note them and log out of WebAssign. The InLab assignment must be completed by the end of the lab period. If additional time is required, please consult with your teaching assistant.