

Name: _____

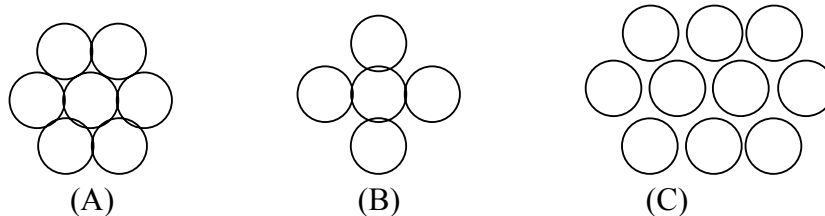
Introduction to Crystal Structures (Packing of Spheres)

Introduction

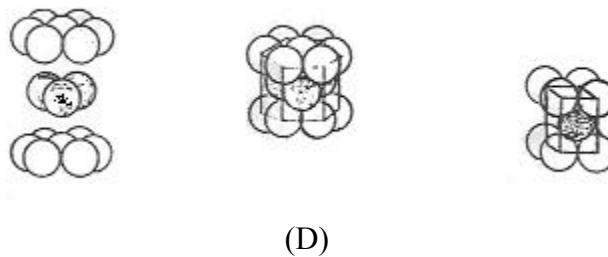
A crystalline solid is a substance which is composed of a basic unit which is repeated in three dimensions (3D) in an ordered fashion. The basic 3D repeating pattern is called the unit cell and can be composed of atoms, ions, or molecules. The collection of particles which make up the **unit cell** must meet three requirements:

1. they must indicate the coordination number
2. they must be consistent with the empirical formula
3. they must generate the crystal structure when repeated in three dimensions

These particles can also be considered as uniform, hard spheres which may form different structures depending on how they are packed. One of the controlling aspects of the packing of spheres is how they are arranged within each layer. In some layers all of the spheres are touching and each sphere is surrounded by six others. This is the most efficient way to pack spheres and is called **closest packing** (see figure A). Layers can also be fashioned from spheres which do not make such efficient use of the available space; in these layers one sphere will be in contact with only four other spheres (see figure B). The least efficient packing of sphere layers occurs when no contact at all exists between the spheres (see figure C). The arrangement of the spheres in two dimensional sheets represents only one aspect of the overall crystal structure; how the two dimensional sheets are stacked must also be considered.

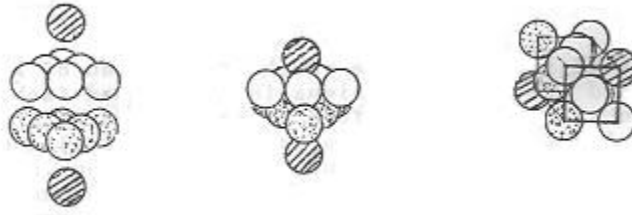


Two different types of closest packed structures can be generated depending on how close-packed layers of spheres are stacked. The **hexagonal close-packed** structure is built by placing one layer of spheres in the depressions formed by a first layer and then adding a third directly above the first. A hexagonal prism is generated by the repeating pattern defined by the **hexagonal** unit cell (see figure D).



Name: _____

The **cubic closed-packed** structure is similar to the hexagonal close-packed structure except that the third layer sits in different depressions than the first. This structure is represented by the face-centered cubic unit cell (see figure E).

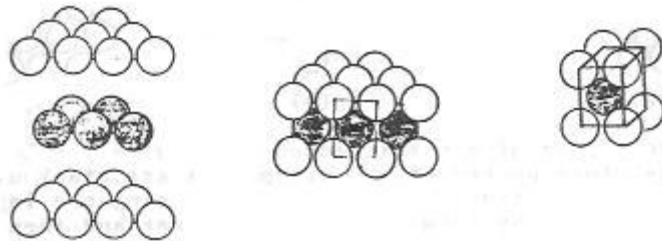


(E)

In the close-packed structures holes are formed as the result of the spheres being placed on top of each other; they are referred to as voids or interstices. There are two types of voids depending on the number of spheres surrounding the void:

- **Tetrahedral voids** are formed when one sphere in one layer is fit over three spheres in another generating a void which is surrounded by four spheres.
- **Octahedral voids** are formed when three spheres in one layer are fit over three spheres in another generating a void which is surrounded by six spheres.

The **body-centered cubic** cell (see figure F) is generated from packing of layers similar to that for the hexagonal close-packed structure except that the layers are composed of spheres that **do not** touch (see figure C). Here the body diagonal (that which connects the top left back corner of the cube to the bottom right front corner) is the only place in the unit cell where spheres are touching.



(F)

Placement of layers of spheres which have four nearest neighbors (see figure B) directly on top of each other generates the simplest of three structures and is composed of a **simple cubic** unit cell (see figure G).



(G)

Name: _____

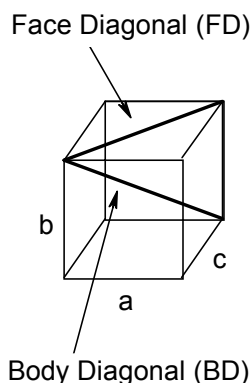
Purpose

The purpose of this laboratory experiment is to allow the student to gain an understanding of the concepts of the packing of spheres by building and examining models of some of these structures.

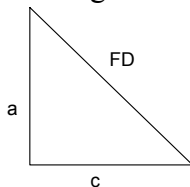
Procedure

Working in pairs, carefully insert wires into the centers of Styrofoam balls. Note which size balls you are instructed to use for each structure. Answer each question in the space provided.

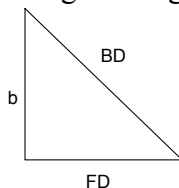
It may be helpful to remember the following geometric relationships. In reality there are seven different types of unit cells, but we will only be dealing with the cubic unit cell. So, remember that it has to be a cube. **SHOW ALL WORK!**



The face diagonal makes a right triangle with sides a and b.



The body diagonal makes a right triangle with the FD and side c.



You also have to remember some geometry.

For a right triangle $A^2 + B^2 = C^2$.

Volume of a cube = S^3 , where S is the length of a side of the cube.

Volume of a sphere = $\frac{4}{3}\pi r^3$

Name: _____

Simple Cubic

1. Using your largest spheres, construct a single simple cubic unit cell lattice. Using dots to represent the center of each atom, draw a diagram to represent your model.

2. How many atoms are contained in the simple cubic unit cell?

3. Express the length of the side of the cube in terms of sphere radii.

4. Express the body diagonal (BD) of your unit cell in terms of sphere radii.

5. Calculate the volume of the simple cube unit cell in terms of sphere radii.

6. Calculate the volume actually occupied by spheres in the simple cubic unit cell in terms of sphere radii.

7. The spheres occupy what % of the total available volume in the simple cubic cell.

Name: _____

Body Centered Cubic

1. Construct a body centered cubic cell. (start with the center sphere and work outwards).
Using dots to represent the center of each atom, draw a diagram to represent your model.

2. How many atoms are contained in the body centered cubic unit cell?

3. Are the spheres in contact along the edge, face diagonal, or body diagonal?

4. Express the body diagonal (BD) of your unit cell in terms of sphere radii.

5. Express the length of the side of the cube in terms of sphere radii.

6. Calculate the volume of the body centered cubic unit cell in terms of sphere radii.

7. Calculate the volume actually occupied by spheres in the body centered cubic unit cell in terms of sphere radii.

8. The spheres occupy what % of the total available volume in the body centered cubic cell.

Name: _____

Face Centered Cubic

1. Using your spheres, construct a face centered cubic unit cell lattice. Using dots to represent the center of each atom, draw a diagram to represent your model.

2. How many atoms are contained in the face cubic unit cell?

3. Express the face diagonal (FD) of your unit cell in terms of face radii.

4. Express the length of the side of the cube in terms of sphere radii.

5. Calculate the volume of the face cube unit cell in terms of sphere radii.

6. Calculate the volume actually occupied by spheres in the face cubic unit cell in terms of sphere radii.

7. The spheres occupy what % of the total available volume in the face cubic cell.

Name: _____

Unknown Unit Cell 1



Construct three close-packed layers using your largest spheres as show in Diagrams 1, 2, and 3.

1. What is the coordination number in a two dimensional closed-packed layer.

Position layer 2 on top of layer 1 so that the second is nestled in the depressions of the first, note the holes that are formed by the placement of one sphere on top of the three others.

2. Place layer 3 on top of your second layer so that it is directly above the first. What type of structure does this represent?

3. What is the coordination number of a 3D close packed structure?

4. Note the holes that are formed by three spheres arranged  above three others arranged . What kind of void is this hole?

5. Which of the two types of voids is larger?

6. How many spheres surround the larger void?

7. What is the coordination number of an ion in a tetrahedral void?

8. What is the coordination number of an ion in an octahedral void?

Name: _____

Unknown Unit Cell 2

1. Construct two layers as shown in figure 3 and arrange one layer so that it rests in some of the depressions of the other. Position one sphere on top of the layers so that it is not directly above layer 1 nor 2. Invert this structure and place another sphere, as a 4th layer directly above the first. What kind of structure does this represent?

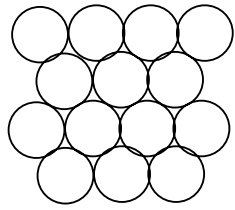
2. What is the coordination number of this 3D structure?

3. What is the unit cell described by this packed structure?

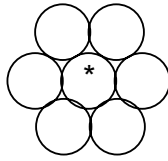
4. Is the stacking of the closed-packed planes along the edge or diagonal of the cube?

Name: _____

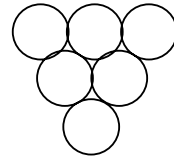
Diagrams



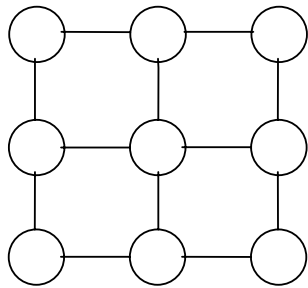
1



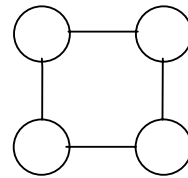
2



3



4



5