Crystal Structures

Experiment
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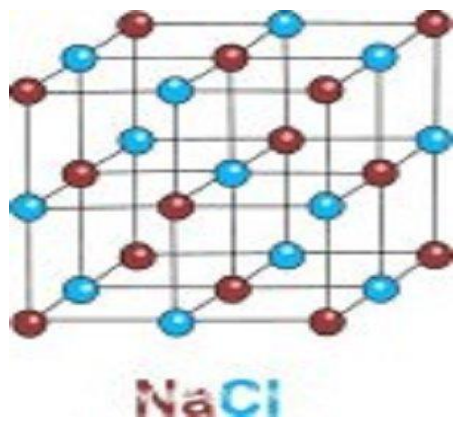
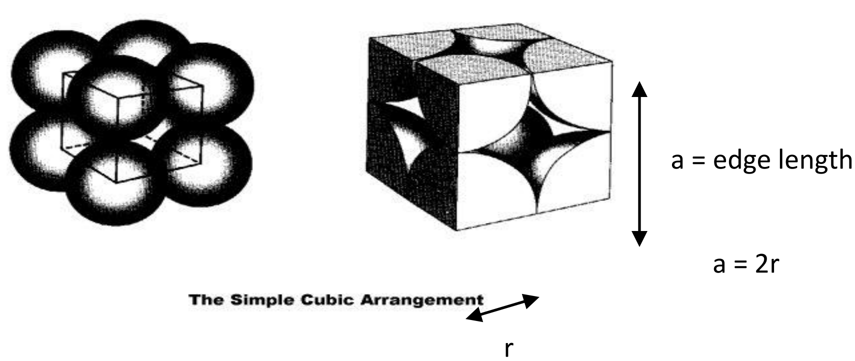
Solid materials exist as a *crystalline lattice*. A crystalline lattice is an orderly arrangement of particles in a three dimensional arrangement. The particles making up the crystal lattice may be atoms, molecules, or ions. The *unit cell* is the smallest part of the lattice that represents the entire array. Repeating the unit cell in three directions in space produces the crystal lattice. Shown below is a crystal lattice for sodium chloride formed from simple cubic unit cells.



The unit cell contains pockets of empty space which varies depending upon the type of unit cell. The arrangement of the atoms within a unit cell is called *packing*. Assuming the shape of an atom to be a sphere, any type of packing of the atoms within a unit cell would leave space in between the atoms. In order to find out how much space in a cube is occupied by the atoms, both the volume of the unit cell and the volume of the atomic sphere must be determined. The total volume of the sphere must account for all of the atoms (spheres) are contained within the unit cell. In this experiment, the percentage of space occupied by the atoms will be determined for the following three unit cells: simple cubic, face-centered cubic, and body-centered cubic.

<u>Simple Cubic Unit Cell</u>

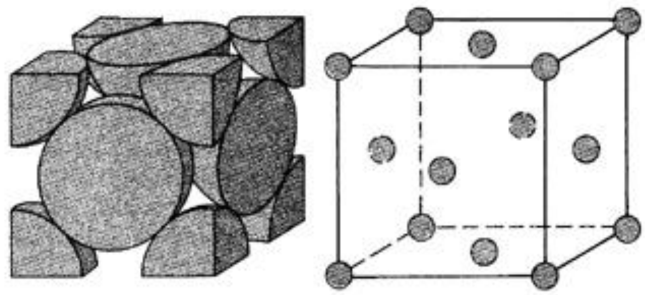


The Simple Cubic Arrangement

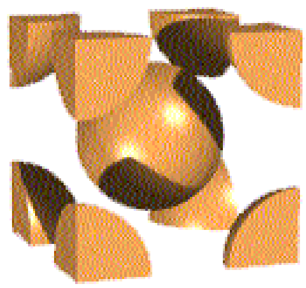
$V = 8r^3$

Face-Centered Unit Cell

$V = 16\sqrt{2}r^3$



Body-Centered Unit Cell



$V = \frac{64\sqrt{3}}{9}r^3$

Materials

Simple unit cell model | Face-centered unit cell model | Body-centered unit cell model

Procedure

The volume of a sphere is $4/3\ \pi r^3$. Assume that the radius of each sphere is 1.00 cm. ($1\ cm^3 = 1\ mL$)

Simple Cubic

1. Find the volume of the space occupied in the unit cell:

   a) Count the number of atoms(spheres) inside the unit cell.

   b) Calculate the total volume of the spheres inside the unit cell.

2. Find the volume of the unit cell using the above volume formula.

3. Calculate the percentage of space occupied in the unit cell.

$$\%\ space\ occupied\ by\ the\ spheres = \frac{V_{spheres}}{V_{Cell}} \times 100$$

Face-Centered Cubic

1. Find the volume of the space occupied in the unit cell:

    a) Count the number of atoms(spheres) inside the unit cell.

    b) Calculate the total volume of the spheres inside the unit cell.

2. Find the volume of the unit cell using the above volume formula.

3. Calculate the percentage of space occupied in the unit cell.

$$\%\ space\ occupied\ by\ the\ spheres = \frac{V_{spheres}}{V_{Cell}} \times 100$$

Body-Centered Cubic

1. Find the volume of the space occupied in the unit cell:

    a) Count the number of atoms(spheres) inside the unit cell.

    b) Calculate the total volume of the spheres inside the unit cell.

2. Find the volume of the unit cell using the above volume formula.

3. Calculate the percentage of space occupied in the unit cell.

$$\%\ space\ occupied\ by\ the\ spheres = \frac{V_{spheres}}{V_{Cell}} \times 100$$

Results

Assuming that the above solids are all aluminum, calculate the density for each unit cell.

$$d = \frac{mass}{volume} = \frac{g}{mL}$$

$$mass = \#\ of\ atoms\ \times \frac{mol}{6.02x10^{23}} \times \frac{26.98g}{mol}$$

Tabulate the Data.

Cube	# of Atoms	Vol of spheres	Vol of cell	% occupied	Density (g/mL)
Simple					
Face-centered					
Body-centered					

No written report required for this experiment.