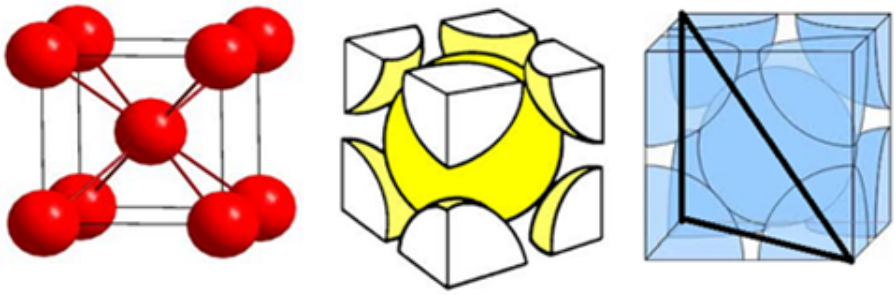
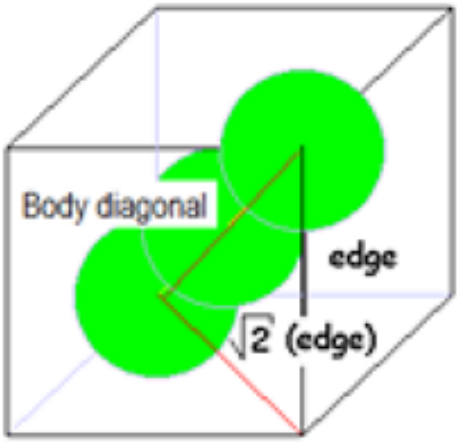
Figure 7. Body Centered Cubic Unit Cell



As can be seen from the drawings, the body centered cube has 1/8 of an atom at each corner and one atom in the center for a total of two atoms per unit cell. The cube diagonal is four times the radius of an atom (4r) and can be shown to be $3^{1/2}$ times the edge length of the cube.

Figure 8. Body Centered Cubic Unit cell Calculations



$$4r = body\ diagonal\ of\ the\ cube$$

$$4r = \sqrt{edge^2 + face\ diagonal^2}$$

$$face\ diagonal^2 = edge^2 + edge^2 = 2\ edge^2$$

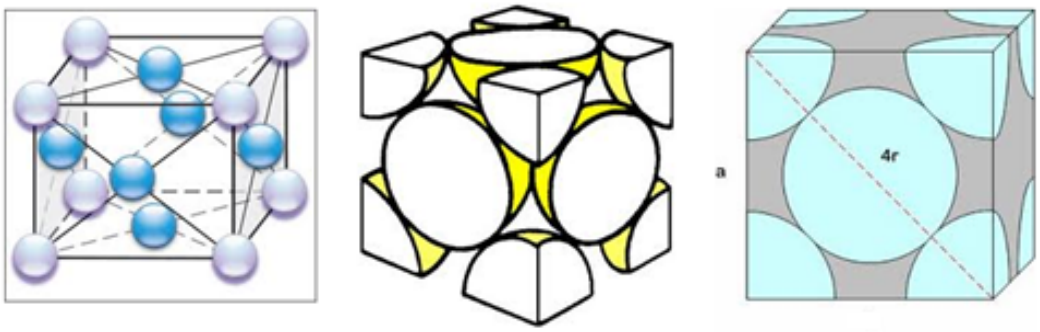
$$4r = \sqrt{edge^2 + 2\ edge^2} = \sqrt{3\ edge^2}$$

$$4r = \sqrt{3}\ edge$$

$$edge = r\frac{4}{\sqrt{3}}$$

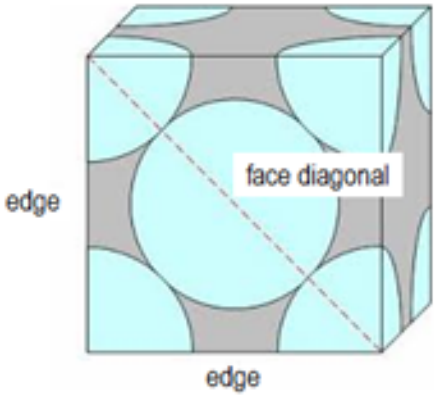
The face centered cube has 1/8 of an atom in each corner and ½ in each of the six faces for a total of 4 atoms per unit cell.

Figure 9. Face Centered Cubic unit cell



A face diagonal is four times the radius of an atom and is $2^{1/2}$ times the edge length of the cube.

Figure 10. Face Centered Cubic Unit cell Calculations



$$4r = face\ diagonal\ of\ the\ cube$$
$$4r = \sqrt{edge^2 + edge^2}$$
$$4r = \sqrt{2}\ edge$$
$$edge = r\frac{4}{\sqrt{2}}$$

After you determine the density of a metal cylinder by methods used in earlier laboratory assignments and the crystal structure of the metal is known, it is possible with proper mathematical manipulation to calculate the atomic radius of the element. The calculation involves the use of the atomic mass, Avogadro's number, the number of atoms per unit cell and the density.

For example, chromium with a density of 7.19 g/cm^3 crystallizes as a body centered cubic crystal. The volume V of its unit cell is:

$$V = \frac{1}{density\ of\ the\ metal} \times molar\ mass\ of\ metal \times \frac{1}{Avogadro's\ Number} \times atoms\ in\ unit\ cell$$

$$V = \frac{1\ cm^3}{7.19\ g} \times \frac{52.0\ g}{1\ mole} \times \frac{1\ mol}{6.022 \times 10^{23} atoms} \times \frac{2\ atoms}{unit\ cell} = 2.40 \times 10^{-23}\ cm^3$$

The edge of the unit cell (a) is the cube root of the volume [$V^{1/3}$]

$$edge\ (a) = \sqrt[3]{V} = \sqrt[3]{2.40 \times 10^{-23}\ cm^3} = 2.89 \times 10^{-8}\ cm$$

$$atomic\ radius = r = \frac{\sqrt{3}}{4} \text{ a (cell length)}$$

$$(2.89 \times 10^{-8}\ cm) = 1.25 \times 10^{-8}\ cm = 125\ pm$$

In this experiment you will investigate the three-dimensional shape of several unit cells, explore the packing efficiency, how the spaces or holes between atoms can be filled, and the coordination number which is the number of atoms a single atom in the structure is in direct contact with.

IV. Density and atomic radius.

Density is an intensive physical property that is unique to a substance and often can be used to identify the material. Density is the relationship between mass and volume.

$$density = \frac{mass\ of\ object}{volume\ of\ object}$$

The mass of the substance is always measured in grams and the volume of most liquids and solids are measured in either mL or cm^3. Therefore the units of density can be written as either g/mL or g/cm^3. The density is considered to be the mass of 1 mL or 1 cm^3 (Remember 1 mL = 1 cm^3).

The volume of a solid can be determined using two different methods, direct measurement followed by calculation of the regularly shaped object or by water displacement. The method used to determine the volume is dependent upon the nature of the substance. Solids of regular shape such as a cube can be measured with a precision tool and the volume of the cube calculated as the length × width × height of the cube. Solids that do not have a regular shape have to be placed into a container filled with a liquid that is then displaced by the solid. Several criteria are important to determining the volume by displacement. First the solid and liquid cannot undergo a chemical reaction, the solid cannot dissolve in the liquid and the solid should be of greater density than the liquid. If any of the criteria are not met, the volume cannot be determined without changing one of the substances.

Data and Results:

For regularly shaped objects such as a cylinder, it is possible to measure the dimensions and use a formula to calculate its volume. The volume of a cylinder is calculated by $V=\pi r^2 L$, where r is the radius of the cylinder and L is the length. The volume of the cube, $V = Length^3$.

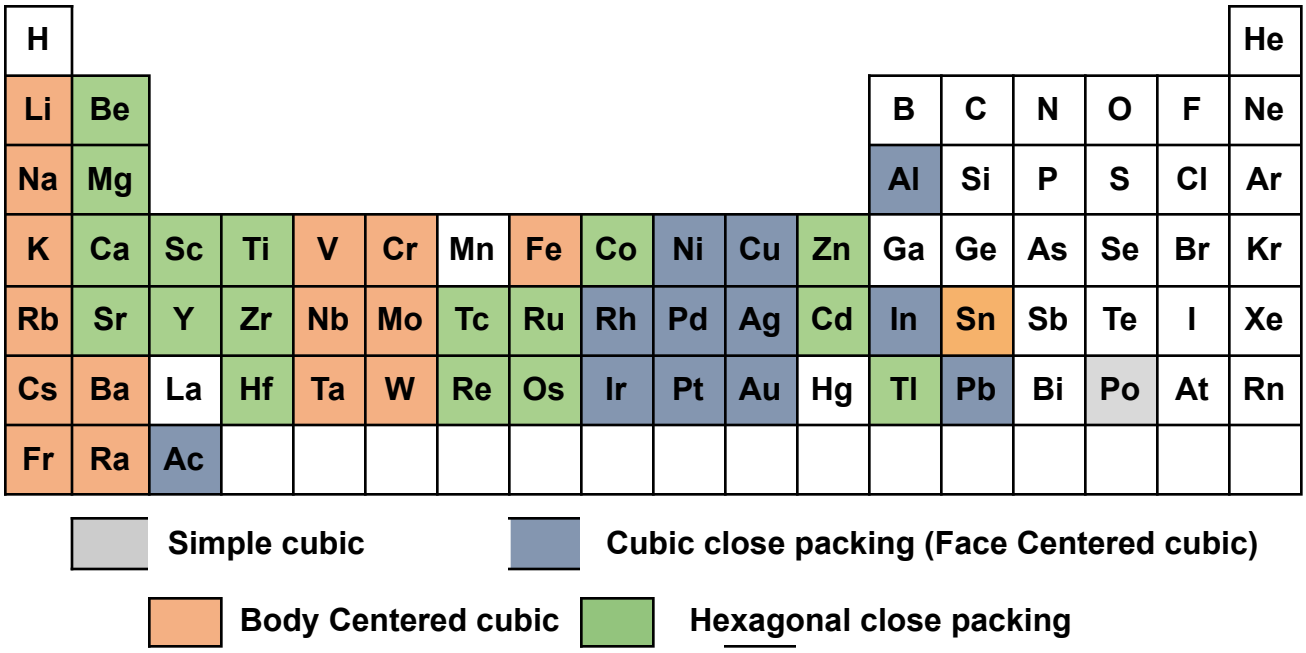
Use a micrometer or Vernier calipers to measure a cylinder or cube and calculate its volume and density. Remember that the units of volume can be mL or cm^3. Remember that a micrometer measures in mm not cm.

Determine the density of a metallic element provided by your instructor. Determine the volume and mass of the metal. Compare your experimental density to values to possible metals and identify your metal.

Using the information from the table below, your experimental density, the atomic mass and Avogadro's number, calculate the atomic radius of the metal. Compare your calculated atomic radius to the known value of the atomic radius for your unknowns. (give a properly cited reference for the book value of the atomic radius)

Calculate the percent error of the atomic radius using your calculated values.

Figure 11. Unit cell structure of elements



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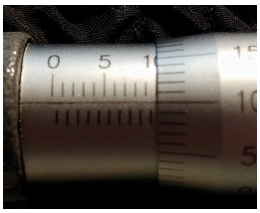
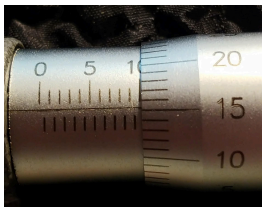
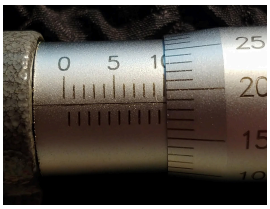
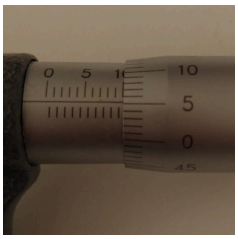
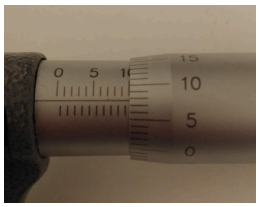
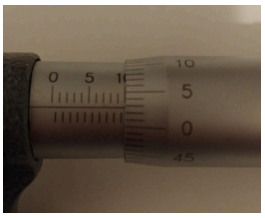
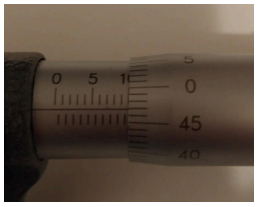
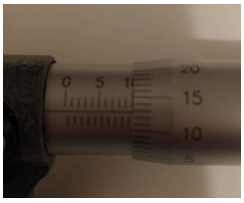
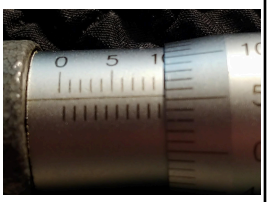
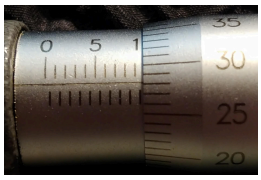
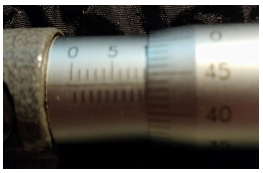
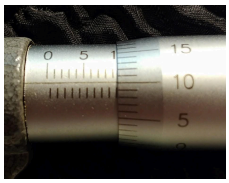
Given the following measurements for several metals, choose one unknown that is Body centered cubic (BCC) and one unknown metal that is cubic close packed (CCP) to complete this assignment.

Unknown and packing	Mass	Length of cube - side A	Length of cube - side B	Length of cube - side C
				

1 - CCP - FCC				
2 - BCC				
3 - CCP				
4 - CCP				

5 - BCC				
6 - BCC