2.47: Calculating the Atomic Radius of Gold

Three experimental facts are required to determine the atomic radius of a metallic element such as gold: density, molar mass and crystal structure.

The crystal structure of gold is face-centered cubic. Its unit cell, or basic repeating unit, shows that it contains four gold atoms and that the gold atoms touch along the face diagonal. In terms of the gold atom radius, the unit cell dimension is $2\sqrt{2}R$.

As noted above, this calculation will require, in addition to the crystal structure, the density and molar mass of gold, which are given below along with Avogadro's number.

- Density: $19.32 \frac{\text{gm}}{\text{cm}^3}$
- Molar mass: 197.0gm
- Atoms per mole: $6.022(10)^{23}$

Assuming that atomic gold is a sphere, as shown above, we can calculated its atomic volume.

- Atomic volume: $V_{Atom} = \frac{4}{3}\pi R^3$

However, the effective volume of a gold atom is 25% of the unit cell volume, $(2\sqrt{2}R)^3$.

- Effective atomic volume: $V_{Aeffective} = \frac{(2\sqrt{2}R)^3}{4} \rightarrow V_{Aeffective} = 4(2)^{\frac{1}{2}}R^3$

The next step involves calculating the packing efficiency of the face-centered cubic structure - in other words, the ratio of the atomic and effective atomic volumes. We see that only 74% of the space is occupied by gold atoms.

- Ratio of atomic and effective atomic volumes according to the fcc model:

$$\frac{V_{Atom}}{V_{Aeffective}} = \frac{\frac{4}{3}\pi R^3}{4 \times 2^{\frac{1}{2}}R^3}\text{float}, 2 \rightarrow \frac{V_{Atom}}{V_{Aeffective}} = .74$$

Next the reciprocal of the density, along with the molar mass and Avogadro's number is used to calculate the experimental effective volume of an individual gold atom.

- Experimental effective atomic volume:

$$V_{ExEffective} = \frac{1cm^3}{19.32gm} \frac{197.0gm}{6.022\ 10^{23}} \quad V_{ExEffective} = 1.693 \times 10^{-23} cm^3$$

According to the fcc model the atomic volume is 74% of the experimental effective atomic volume. This allows the calculation of the atomic radius of gold.

$$\frac{4}{3}\pi R^3 = 0.74 V_{ExEffective} \quad R = \left(\frac{0.74 V_{ExEffective}}{\frac{4}{3}\pi}\right)^{\frac{1}{3}} \quad R = 144 \text{pm}$$

This is in agreement with the literature value (see Figure 5.19 page 176 in Chemistry, 5th edition, by McMurry and Fay).

- Define picometer: $\text{pm} = 10^{-12}\text{m}$