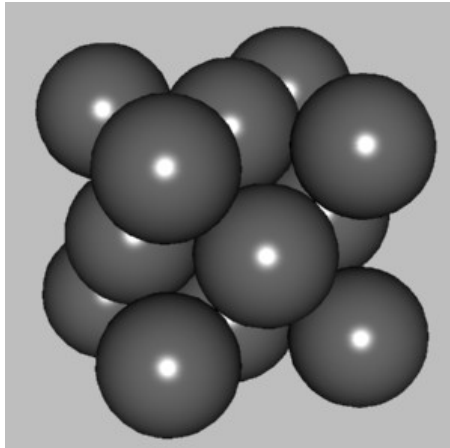


1) Calculate the packing efficiency of a face-centered cubic structure of atoms with a diameter of 1.00 Å (100 pm).



The atoms along the diagonal of a face touch each other !

Triangle:

$$a^2 + a^2 = (2d)^2$$

$$2a^2 = 4.00 \text{ Å}^2 \rightarrow a = 1.41 \text{ Å}$$

$$\text{Volume of the cell: } V = a^3 = (1.41 \text{ Å})^3 = 2.80 \text{ Å}^3$$

4 Atoms in the unit cell: 1/8 of the 8 corners and 6 face shared (= x 0.5) atoms.

The volume of a sphere is given as $V = \frac{4}{3} \pi r^3$

$$V_{\text{atom}} = \frac{4}{3} \pi (0.5 \text{ Å})^3 = 0.52 \text{ Å}^3$$

$$\text{Packing efficiency} = 2.08 \text{ Å}^3 / 2.80 \text{ Å}^3 = 74 \%$$

2) Copper has an atomic radius of 1.28 Å, an fcc crystal structure and an atomic weight of 63.5 g/mol. Calculate the theoretical density of Cu (measured value: 8.94 g/cm³).

$$\rho = n A / V N$$

n = number of atoms in unit cell; A = atomic weight

V = volume of the unit cell; N = Avogadro's number (6.023 x 10²³ atoms/mol)

cell length:

$$a^2 + a^2 = (2d)^2 = (4r)^2 \rightarrow a^2 = 8r^2 = 4r^2 \cdot 2$$

$$a = 2r \cdot 2^{0.5}$$

$$\text{cell volume: } a^3 = 8r^3 \cdot 2^{1.5} = 16r^3 \cdot 2^{0.5}$$

$$\text{radius: } r = 1.28 \text{ Å} = 128 \text{ pm} = 128 \cdot 10^{-12} \text{ m} = 128 \cdot 10^{-10} \text{ cm} = 1.28 \cdot 10^{-8} \text{ cm}$$

$$\text{density: } \rho = 4 \text{ atoms} \times 63.5 \text{ g/mol} / 16 \cdot 2^{0.5} (1.28 \cdot 10^{-8} \text{ cm})^3 \cdot 6.023 \cdot 10^{23} \text{ atoms/mol} = 8.89 \text{ g/cm}^3$$

3) What is the formula of a compound that crystallizes with lithium ions occupying all of the tetrahedral holes in a cubic-closed packed array of sulfide ions ?

There are 2N tetrahedral holes in ccp arrays $\rightarrow$ Li₂S

4) How many Cl^- ions surround a Na^+ ion and what is the geometric description of the coordination around the Na^+ ion? The ionic radii for Na^+ and Cl^- are 99 and 181 pm ($1 \text{ pm} = 10^{-12} \text{ m}$) respectively. What is the cation to anion radius ratio in this structure? In view of this ratio, do the neighboring chloride ions touch each other?

There are six Cl^- ions surrounding each Na^+ ion. Such a coordination forms an octahedron.

The cation to anion radius ratio = $99/181 = 0.547$. If the cations fit the *octahedral holes* precisely, the radius ratio would be 0.414. Thus the chloride ions do not touch each other.

5) How many ions of each are contained in the face-centered unit cell of NaCl? The specific gravity of NaCl is 2.165 g/cm^3 , what is the cell edge length of the unit cell.

Recall that the unit cells of ccp contains 4 atoms, it is easy to figure out that the unit cell contains 4 each of sodium and chloride ions.

The atomic masses for Na and Cl are 23.0 and 35.5 respectively. Assume the cell edge length to be a , then we have

$$\frac{4 * (23.0 + 35.5) \text{ g/mol}}{6.023 \times 10^{23} \text{ 1/mol} * a^3} = 2.165 \text{ g/cm}^3$$

Solving for a gives

$$a = 5.64 \times 10^{-8} \text{ cm} = 564 \text{ pm}$$