Skills to Develop

- Use the packing of spheres to model the fcc crystal structure.
- Practice solving problems related to crystal structures.

Closest Packing and Crystal Structures

We use models for sciences. Some models are mathematical formulas, some are theories, and some are physical representations.

The arrangements of molecules, atoms or ions are called **crystal structures**. The packing of spheres is often used to model metal crystal structures. Atoms, molecules, and ions are too small, so we use balls and sticks to represent them. These models enable us to see the invisible world of atoms and molecules.

There are two types of closest packing, the hexagonal and the face-centered closest packing, and they are called hcp and fcc (or ccp) respectively. The hcp packing has an ABABAB... two-layer sequence, where A and B represent the location of the layers. In other words, the third layer is exactly above the first layer in hcp. The fcc packing has a three-layer sequence, ABCABC... rather than the two-layer sequence of the hcp. The two types of packing are shown below:
Since these structures have been discussed in Solids, work on the questions below.

**Confidence Building Questions**

1. There are two types of closest packing of spheres: face-centered-cubic (fcc with the ABCABC... sequence) and the hexagonal closest packing (hcp with the ABAB... sequence) How many neighbors are there for a sphere in these packings?

   Hint: 12

   **Skill -**
   Draw diagrams of closest packing and draw the polyhedra of neighbouring atoms. One each for the fcc and hcp type.

2. If the radii of the spheres are 1.5 Å, what will be the distance between centers of neighboring spheres?

   Hint: The bond distance is 3.0 Å

   **Discussion -**
   The covalent radius is half the covalent bond length between two atoms of the same element.
3. If the radius of an atom is 123 pm, calculate the volume of the atom. Assume the atom to be a sphere.

Hint: \( V = 7.79 \times 10^6 \text{ cubic pm} \)

**Discussion -**

The volume of a sphere with radius \( r \) is \( \frac{4}{3} \pi r^3 \). The chemical literature uses the unit Angstrom or Å (\( = 10^{-10} \text{ m} \)). 1 Å = 100 pm.

4. Nickel atoms pack in a fcc lattice in its crystal structure. Its density is 8.90 g/mL. The unit cell edge is 352 pm. Its molar mass is 58.7 g/mol. Calculate Avogadro’s number from these data.

Hint: The calculated Avogadro’s number is 6.023e23

**Discussion -**

You can almost guess Avogadro’s number, but make sure you know how to calculate it from the given data.

5. The crystal structure of calcium is face centered cubic. Its cell edge is 557 pm. Calculate the radius (in pm) of the calcium atoms, assuming they are spheres.

Hint: 197 pm

**Discussion -**

Find the relationship: \( 2 \times \sqrt{2} \times \text{radius of Ca} = \text{edge} \).

6. The crystal structure of calcium is face centered cubic. Its cell edge is 557 pm. Calculate the density of \( \text{Ca} \) in g/cm\(^3\). Atomic mass, \( \text{Ca} \), 40.08; Avogadro’s number 6.022e23

Hint: 1.54 g/mL

**Discussion -**

mass = 4 * 40.08 / 6.023e23 g
volume = (557e-10 cm)\(^3\)
density = mass / volume.

7. The density of silver (atomic mass: \( \text{Ag} \), 107.9) is 10.6 g/cm\(^3\), and it has a face centered cubic structure. Calculate the edge of the cubic unit cell in pm. (Avogadro’s number 6.022e23)

Hint: a = 400 pm

**Discussion -**

Volume of cell = mass / density, and there are 4 atoms per unit cell.

Calculate the number of atoms per unit cell from the density and a cell edge of 408 pm.

8. Iron has a body-centered-cubic structure, with unit cell edge of 287 pm. Calculate its density in g / cm\(^3\). Atomic mass, \( \text{Fe} \), 55.85; Avogadro’s number 6.022e23

Hint: density = 7.85 g/mL

**Discussion -**
Mass = 2 * 55.85/6.022e23 = 1.855e-22 gm
Volume = 2.36e-23 cm³
Density = ?
Iron transforms from a bcc structure to fcc structure at 910 C. The volume shrinks as the structure transforms from bcc to fcc; explain!

Contributors

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