Answer on Question #71693, Chemistry / General Chemistry

Question: What fraction of the total volume of a cubic closest packed structure is occupied by atoms? Hint: Vsphere = $4/3\pi r^3$

Answer: 74.05 %

Solution: The atoms in a cubic closest packed structure (or face-centered cubic structure) are located at the corners of a unit cell and in the center of each of the faces of a unit cell; a cube with side a. There are eight atoms occupying the corners of the cube. There are six atoms occupying the center of the six faces of the cube. But only $8 \cdot \frac{1}{8} + 6 \cdot \frac{1}{2} = 4$ atoms are within the unit cell so that the number of atoms equals four per unit cell.

The packing density (or fraction of the total volume is occupied by atoms) can be calculated using the formula $\frac{Volume \text{ of atoms}}{Volume \text{ of a unit cell}} = \frac{N \cdot \frac{4}{3} \pi r^3}{a^3}$, where N – a number of atoms per unit cell (in our case N = 4), r - radius of atom.

In accordance with the Pythagorean theorem, the length of the diagonal of the front face of the cube is equal to $a\sqrt{2}$ or 4r (see the figure below). So $r = \frac{a\sqrt{2}}{4}$.



$$\frac{\text{Volume of atoms}}{\text{Volume of a unit cell}} = \frac{4 \cdot \frac{4}{3} \pi (\frac{a\sqrt{2}}{4})^3}{a^3} = \frac{32\sqrt{2} \cdot \pi \cdot a^3}{192 \cdot a^3} = \frac{32\sqrt{2} \cdot 3,1416 \cdot a^3}{192 \cdot a^3} = 0.7405$$

It means that 74.05 % of the total volume of a cubic closest packed structure is occupied by atoms.

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