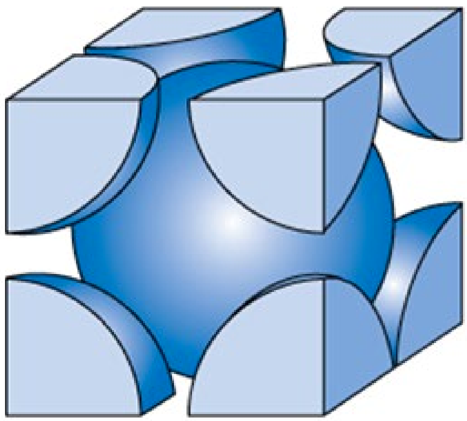
Tutorial 1

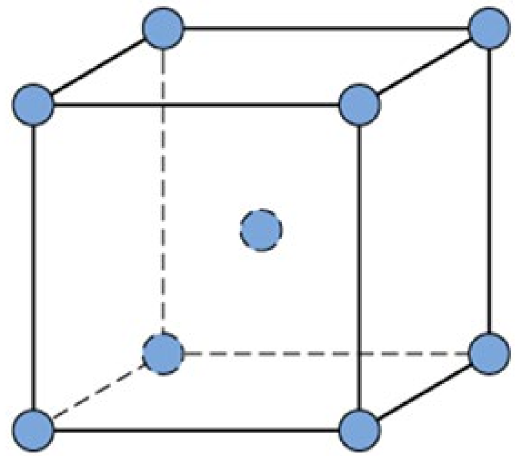
Solutions

ENGG103 AUT 2022

Crystal Structure

BCC



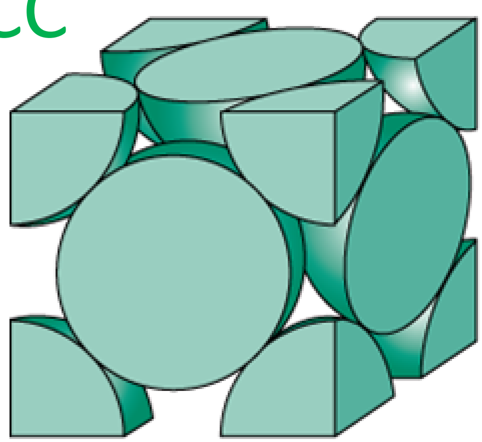


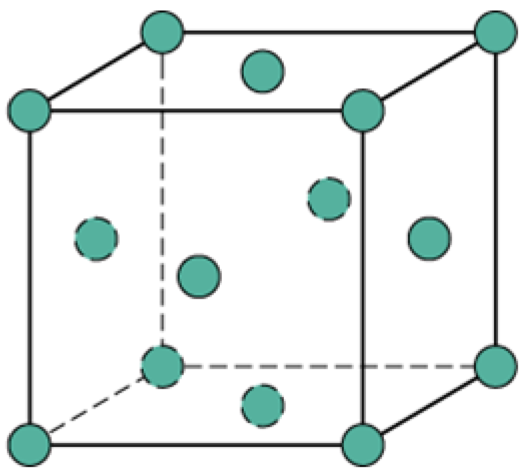
- One atom at the eight corners of a cube and one in the centre of the cube

Close packed directions are cube diagonals, but no close-packed planes.

BCC packing is less dense than FCC

FCC





- One atom at the eight corners of a cube and one in the centre of each of the six faces

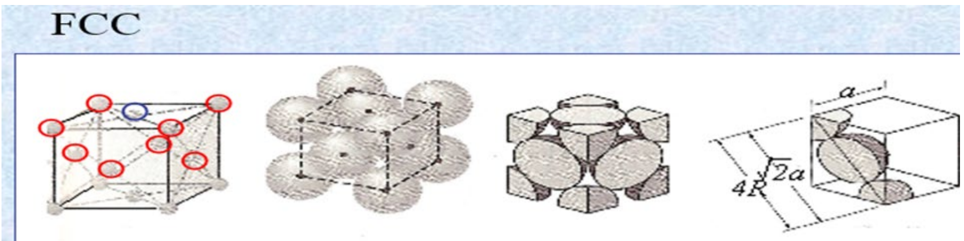
Close packed directions are face diagonals

Q 1.2

Calculate the atomic Packing Factor (APF) of FCC.

It can be defined as the ratio between the volume of the basic atoms of the unit cell (which represent the volume of all atoms in one unit cell) to the volume of the unit cell it self.

$$\frac{Volume\ of\ atoms}{Volume\ of\ the\ unit\ cell} = \frac{\frac{4}{3}\pi r^3}{a^3}$$



A face centered cubic (FCC) lattice contains six additional atoms in the center of all six faces of the cube. Since only half of the atoms is within the cube the total number of atoms per unit cell equals four.

number of atoms = 4

volume of four atoms = $4 * \frac{4}{3}\pi r^3$

The atoms touch along the diagonal of the faces of the cube, which equals $\sqrt{2}$a . The radius is one quarter of the diagonal.

r = $\frac{a\sqrt{2}}{4} = \frac{a}{2\sqrt{2}}$

$$= \frac{4 * \frac{4}{3}\pi\left(\frac{a}{2\sqrt{2}}\right)^3}{a^3} = \frac{\frac{16\pi r^3}{3}}{(2\sqrt{2}r)^3} = \frac{16\pi r^3}{3} \times \frac{1}{8\sqrt{2}r^3} = 0.74$$

Packing Density = 74% or APF = 0.74

Q 1.2

Calculate the atomic Packing Factor (APF) of BCC.

It can be defined as the ratio between the volume of the basic atoms of the unit cell (which represent the volume of all atoms in one unit cell) to the volume of the unit cell it self.

$$\frac{Volume\ of\ atoms}{Volume\ of\ the\ unit\ cell} = \frac{\frac{4}{3}\pi r^3}{a^3}$$

A body centered cubic (BCC) lattice contains an additional atom in the middle and therefore contains two atoms per unit cell.

number of atoms = 2

volume of four atoms = 2 * $\frac{4}{3}\pi r^3$

The atoms touch along the body diagonal, which equals $\sqrt{3}$a . The radius is one quarter of the body diagonal.

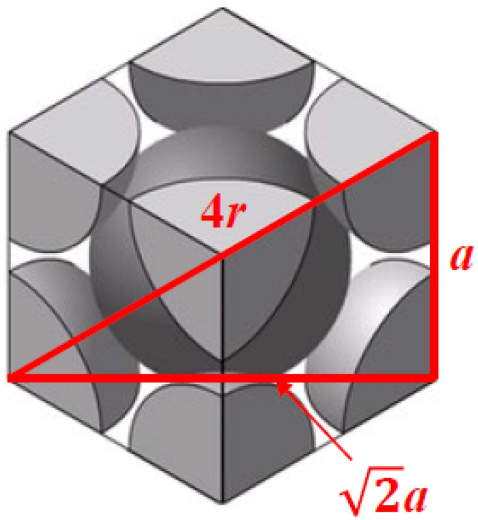
r = $\frac{a\sqrt{3}}{4}$

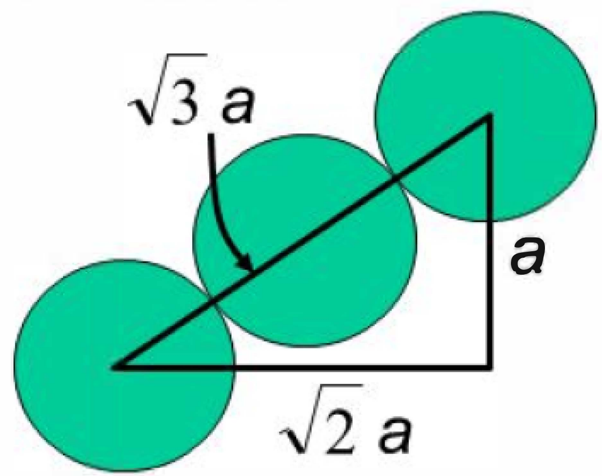
$$= \frac{2*\frac{4}{3}\pi(\frac{a\sqrt{3}}{4})^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{\frac{8\pi r^3}{3}}{(\frac{4r}{\sqrt{3}})^3} = \frac{\sqrt{3}\pi}{8} = 0.68$$

Packing Density = 68% or APF = 0.68

a) Given that the atomic radius of an iron atom is *r* (Fe) = 0.126 nm, calculate the lattice constant *a* for the iron unit cell.

The atoms in a BCC unit cell touch each other across the diagonal, as shown below. Pythagoras' theorem can now be used to determine the relationship between a and r.





$$\therefore\ \sqrt{3}a = 4r$$

$$\therefore\ a = \frac{4r}{\sqrt{3}} = \frac{4(0.126\ \text{nm})}{\sqrt{3}} = \mathbf{0.291\ nm}$$

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b) Given the atomic mass of iron is m_a (Fe) = 55.85 g/mol, calculate the theoretical density of iron. (Hint: Consider first the mass per atom and then the number of atoms in a unit cell).

The BCC unit cell contains an equivalent of: $8(\frac{1}{8}) + 1 =$ **2 atoms**

The atomic mass of iron is 55.85 g/mol. Therefore:

the mass of one mole of Fe atoms is 55.85 g/mol, or

the mass of 6.022×10^{23} Fe atoms is 55.85 g/mol.

The mass of the two equivalent atoms in the BCC unit cell is therefore:

$2(55.85/6.022 \times 10^{23}) = \mathbf{1.855 \times 10^{-22}\ g}$

The volume of the Fe unit cell:

volume $= a^3 = (0.291\text{ nm})^3 = \mathbf{0.0246\ nm^3}$

The theoretical density is therefore:

$\rho = \text{mass/volume} = (1.855 \times 10^{-22})/0.0246 = 7.541 \times 10^{-21}\text{ g/nm}^3 =$ **7541 kg/m^3**

c) Comment on why the calculated density may differ from the published value of 7850 kg/m^3 for plain-carbon steel.

Calculation of the theoretical density of steel does not take into account the fact that crystal structures always contain defects. The presence of interstitially dissolved carbon atoms in steel, vacancies and dislocations can affect the measured density values.

2.11 Magnesium

$A_{mg} = 24.305$ g/mol $\qquad N_A = 6.022 \times 10^{23}$ atoms/mol

$\rho = 1.74$ g/cm^3 $\qquad K_B = 8.62 \times 10^{-5}$ eV/K

$Q_v = 0.89$ eV/atom

$T = 450°C = 723$ K

$$N = \rho \left(\frac{N_A}{A_{mg}} \right)$$

$$= (1.74) \left(\frac{6.022 \times 10^{23}}{24.305} \right) \frac{g}{cm^3} \frac{atoms}{mol} \frac{mol}{g}$$

$$N_s = 4.31 \times 10^{22} \text{ atoms/cm}^3$$

$$N_v = N_s \exp\left(\frac{-Q_v}{k_B T} \right)$$

$$= (4.31 \times 10^{22}) \exp(-14.28)$$

$$= (4.31 \times 10^{22})(6.281 \times 10^{-7})$$

$$N_v = 2.707 \times 10^{16} \text{ vacancies/cm}^3$$

At temp =600°C

$$\frac{N_v}{N_s} = (e^{\left(-\frac{0.89}{(8.62\times10^{-5})(873)}\right)})$$

$$\frac{N_v}{N_s} = (e^{(-11.83)})$$

$$\frac{N_v}{N_s} = 7.283 \times 10^{-6}$$