Crystallography (Prof. Aron Walsh)

Exercise: Packing

1. What is the coordination number in:
   a. the face-centred cubic (fcc) structure 12
   b. the hexagonal closed-packed (hcp) structure 12
   c. the body-centred cubic (bcc) structure 8

2. How many atoms per unit cell are there in:
   a. the face-centred cubic (fcc) structure $\overbrace{8\times\frac{1}{8}}^{\text{corners}} + \overbrace{6\times\frac{1}{2}}^{\text{faces}} = 1+3 = 4$
   b. the hexagonal closed-packed (hcp) structure 2
   c. the body-centred cubic (bcc) structure $8\times\frac{1}{8} + 1_{\text{body centre}} = 2$

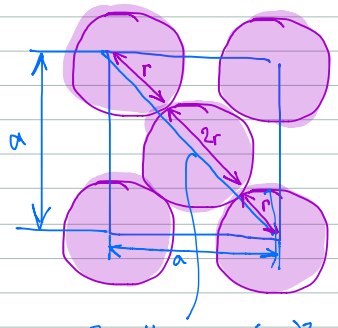
3. Calculate the packing fraction for the body-centred cubic (bcc) structure.

see below

3. Packing fraction:

FCC: Volume of cell = a^3 (where a is unit cell side length)

As a reminder



By pythagoras: $(4r)^2 = a^2 + a^2$

Atoms touch along face diagonal.

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

$r = \frac{\sqrt{2}}{4}a$ ← (1)

Volume of sphere = $4/3\,\pi r^3$

↓ Substitute (1)

Volume of atom = $4/3\,\pi\left(\frac{\sqrt{2}}{4}a\right)^3 = \frac{\pi a^3}{12\sqrt{2}}$

FCC contains 4 atoms so volume of atoms:

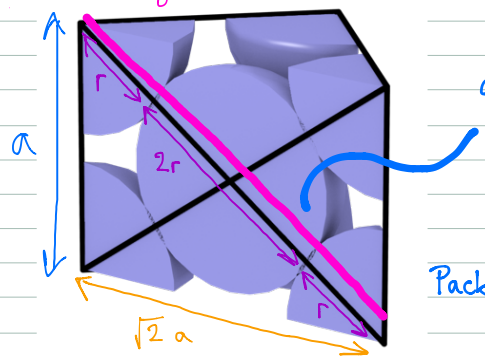
$$V_{atom} = 4 \times \frac{\pi a^3}{12\sqrt{2}} = \frac{\pi a^3}{3\sqrt{2}}$$

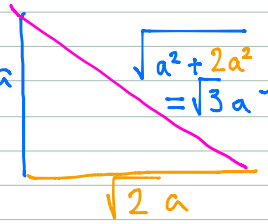
Divide volume of atoms by volume of cell to obtain packing fraction:

$$\text{Packing fraction} = \frac{1}{a^3}\frac{\pi a^3}{3\sqrt{2}} = \frac{\pi}{3\sqrt{2}} = \underline{0.740}$$

Main answer:

Packing fraction Bcc:





$4r = \sqrt{3}a$

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

Volume of atoms = $2 \times \frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}a\right)^3 = \frac{1}{8}\sqrt{3}\pi a^3$

Packing fraction = $\frac{1}{a^3}\frac{1}{8}\sqrt{3}\pi a^3 = \frac{\sqrt{3}}{8}\pi = \underline{0.680}$