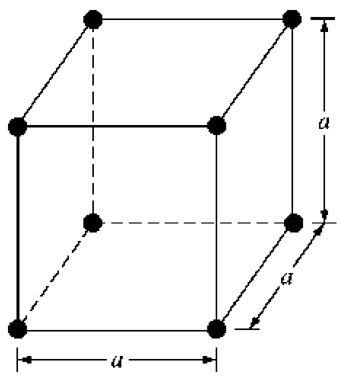
1.9 (*a*) A crystal with a simple cubic lattice structure is composed of atoms with an effective radius of r = 2.25 Å and has an atomic weight of 12.5. Determine the mass density assuming the atoms are hard spheres and nearest neighbors are touching each other. (*b*) Repeat part (*a*) for a body-centered cubic structure.

Hint: You will need to know Avogadro's number (see Appendix B.3 or 6.022×10^{23} atoms per gram molecular weight).

a)



Nearest neighbors are at corners, Therefore,

$r + r = a \Rightarrow a = 2r = 2(2.25\,Å) = 4.5\,Å$

$\#$ atoms per unit cell $= 8 \text{ corners}\left(\frac{1/8 \text{ atom}}{\text{corner}}\right) = 1 \text{ atom}$

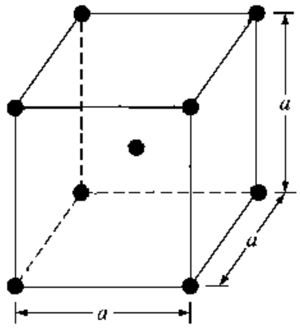
atom vol. density $= \frac{1 \text{ atom}}{a^3} = \frac{1}{(4.5 \times 10^{-10} m)^3} = 1.097 \times 10^{28} \frac{\text{atoms}}{m^3}$

Mass density $= \frac{\text{Atomic weight} \cdot \text{atom vol. density}}{\text{Avogadro's number}}$

$= \frac{1.0974 \times 10^{28}\,(12.5)}{6.022 \times 10^{23} \text{ atom/g}}$

Mass density $= 227{,}788.46 \text{ g/m}^3 = 0.2278 \text{ g/cm}^3$

b)



Here, the nearest neighbors are along the diagonal of the cube. Therefore,

$$d = \sqrt{a^2+a^2+a^2} = \sqrt{3}\, a = r + 2r + r = 4r$$

$$\hookrightarrow a = \frac{4}{\sqrt{3}} r = \frac{4}{\sqrt{3}} 2.25\,\text{Å} = 5.19615\,\text{Å}$$

$$\#\text{ atoms per unit cell} = 8 \text{ corners}\left(\frac{\frac{1}{8}\text{ atom}}{\text{corner}}\right) + 1 \text{ atom in center}$$

$$= 2 \text{ atoms}$$

$$\text{atom vol. density} = \frac{2 \text{ atoms}}{a^3} = \frac{2}{(5.2\times10^{-10}\,m)^3} = 1.425556\times10^{28}\,\frac{\text{atoms}}{m^3}$$

$$\text{Mass density} = \frac{\text{At. wt (atom vol. dens)}}{\text{Avogadro's }\#}$$

$$= \frac{12.5\,(1.426\times10^{28})}{6.022\times10^{23}}$$

$$\underline{\underline{\text{Mass density} = 295{,}905.9\,\frac{g}{m^3} = 0.2959\,g/cm^3}}$$