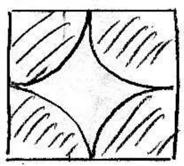
Physics 481: Condensed Matter Physics - Homework Solutions 2

Homework 2.1

a) square: 1 atom per cell



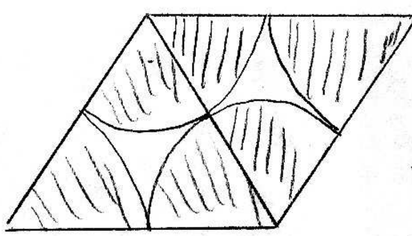
$r = \frac{a}{2}$

$A_{sphere} = \pi \left(\frac{a}{2}\right)^2 = \frac{\pi}{4} a^2$

$A_{square} = \quad = a^2$

packing fraction $\pi/4 = 78.5\%$

hexagonal: 1 atom per cell



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

$A_{sphere} = \frac{\pi}{4} a^2$

$A_{rhombus} = a^2 \sin(60°) = a^2 \frac{\sqrt{3}}{2}$

packing fraction $\frac{\pi}{4} \frac{2}{\sqrt{3}} = \frac{\pi}{2\sqrt{3}} = 90.7\%$

- Simple cubic $r = 1$, one sphere per cube

$$f = \frac{1}{8}\, 4\pi/3 = 0.5235$$

- bcc $r = \frac{1}{2}\sqrt{3}$, two spheres per cube

$$f = \frac{2}{8}\,\frac{4\pi}{3}\left(\frac{1}{2}\sqrt{3}\right)^3 = \frac{\sqrt{3}\,\pi}{8} = 0.6800$$

- fcc $r = \frac{1}{2}\sqrt{2}$, four spheres per cube

$$f = \frac{4}{8}\,\frac{4\pi}{3}\left(\frac{1}{2}\sqrt{2}\right)^3 = \frac{\sqrt{2}}{3\cdot 2}\,\pi = 0.7403$$

- hcp primitive unit cell :

$$V = a^2 \sin 60° \cdot c = a^2\,\frac{1}{2}\sqrt{3}\,\sqrt{\frac{8}{3}}\,a$$

$$V = \sqrt{2}\,a^3$$

$$r = \frac{1}{2}\sqrt{\frac{a^2}{4} + \frac{a^2}{12} + \frac{8}{12}a^2} = \frac{a}{2}$$, 2 spheres per cell

$$f = \frac{2}{\sqrt{2}}\,\frac{4\pi}{3}\,\frac{1}{8} = \frac{\sqrt{2}}{3\cdot 2}\,\pi = 0.7403$$

- diamond $r = \frac{1}{4}\sqrt{3}$, 8 spheres per cube

$$f = \frac{8}{8}\,\frac{4\pi}{3}\left(\frac{1}{4}\sqrt{3}\right)^3 = \frac{\sqrt{3}\,\pi}{16} = 0.3400$$

Problem 2.2

a) $\vec{b}_1 = 2\pi \dfrac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$, $\vec{b}_2 = 2\pi \dfrac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$\vec{a}_1 \cdot \vec{b}_1 = 2\pi$, $\vec{a}_1 \cdot \vec{b}_2 = 0$, $\vec{a}_1 \cdot \vec{b}_3 = 0$

analogously for the others

b) $V = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$

$$V_R = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \vec{b}_1 \cdot \left(\vec{b}_2 \times \frac{2\pi}{V}(\vec{a}_1 \times \vec{a}_2)\right)$$

$$= \frac{2\pi}{V} \vec{b}_1 \cdot \left(\vec{a}_1 \underbrace{(\vec{b}_2 \cdot \vec{a}_2)}_{2\pi} - \vec{a}_2 \underbrace{(\vec{a}_1 \cdot \vec{b}_2)}_{0}\right)$$

$$= \frac{(2\pi)^3}{V}$$

Homework 2.3.

a) fcc $\quad V = \frac{a^3}{8} \begin{vmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{vmatrix} = \frac{a^3}{4}$ $\quad$ 4 particles per cell

bcc $\quad V = \frac{a^3}{8} \begin{vmatrix} 1 & 1 & -1 \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{a^3}{8} \left| 1 - (-3) \right| = \frac{a^3}{2}$

2 particles per cell

b) fcc $\quad \vec{b}_1 = \frac{2\pi}{V}\frac{a^2}{4} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{vmatrix} = \frac{2\pi}{a}\left(\hat{z} - \hat{x} - \hat{y} \right)$

$$\vec{b}_2 = \frac{2\pi}{a} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \frac{2\pi}{a}\left(\hat{y} - \hat{x} - \hat{z} \right)$$

$$\vec{b}_3 = \frac{2\pi}{a} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{vmatrix} = \frac{2\pi}{a}\left(\hat{x} - \hat{y} - \hat{z} \right)$$

this is a bcc lattice with cubic lattice constant $\frac{4\pi}{a}$