Physics 211A HW2 Solutions Fall 2014

1) Ch. 2, Prob 1

fcc: $\vec{v}_1 = 0$, $\vec{v}_2 = \frac{a}{2}(\hat{x}+\hat{y})$, $\vec{v}_3 = \frac{a}{2}(\hat{x}+\hat{z})$, $\vec{v}_4 = \frac{a}{2}(\hat{y}+\hat{z})$

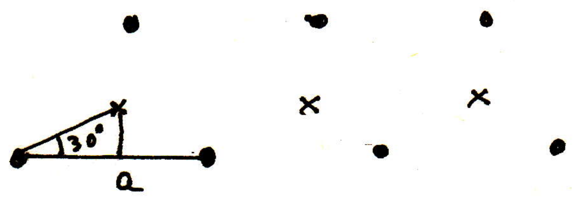
bcc: $\vec{v}_1 = 0$, $\vec{v}_2 = \frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

(b) Volume of conventional unit cell $= a^3$

fcc has 4 atoms in conv unit cell $\Rightarrow$ volume of primitive unit cell $= a^3/4$

bcc " 2 - - - - - - - - - $= a^3/2$

2) Ch. 2, Prob. 4 : hcp



Next layer has atoms at x's, with height $\frac{c}{2}$ $\Rightarrow$ at points $\left(\frac{a}{2}, \frac{a}{2\sqrt{3}}, \frac{c}{2}\right)$. We want the distance to $(0,0,0)$ to be $= a$, so that spheres of radius $\frac{a}{2}$ will touch. $\Rightarrow$

$$d^2 = \left(\frac{a}{2}\right)^2 + \left(\frac{a}{2\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = a^2 \Rightarrow \frac{1}{4} + \frac{1}{12} + \frac{1}{4}\left(\frac{c}{a}\right)^2 = 1$$

$$\Rightarrow \frac{c}{a} = \sqrt{\frac{8}{3}}$$

Ch 2, prob 6

simple cubic: $r = \frac{a}{2}$ is radius of atoms.

packing fraction: $\frac{\text{volume of atom}}{\text{volume of space per atom}} = \frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6} = 0.52$

bcc: nn distance $= \sqrt{3\left(\frac{a}{2}\right)^3} = \frac{a\sqrt{3}}{2} \Rightarrow r = \frac{\sqrt{3}}{4}a \Rightarrow$

$\Rightarrow$ p.f. $= \frac{2 \times \frac{4}{3}\pi r^3}{a^3} = \frac{\sqrt{3}}{8}\pi = 0.68$

2 atoms in a^3 volume

fcc: nn distance $= \sqrt{2\left(\frac{a}{2}\right)^2} = \frac{a}{\sqrt{2}} \Rightarrow r = \frac{a}{2\sqrt{2}}$

and 4 atoms in unit cell $\Rightarrow$

p.f. $= 4 \times \frac{4}{3}\pi \times \left(\frac{1}{2\sqrt{2}}\right)^3 = \frac{\pi}{3\sqrt{2}} = 0.74$

hcp: in ABCABC stacking it's an fcc lattice, packing fraction is the same as in ABABAB stacking $\Rightarrow$ 0.74

diamond: body diagonal length is $\sqrt{3}a$, two fcc lattices shifted by 1/4 of body diagonal $\Rightarrow$ nn distance is $r = \frac{\sqrt{3}}{8}a \Rightarrow$

we have $2 \times 4 = 8$ atoms per volume $a^3 \Rightarrow$

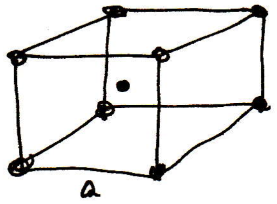
p.f. $= 8 \times \frac{4}{3}\pi\left(\frac{\sqrt{3}}{8}\right)^3 = \frac{\sqrt{3}\pi}{16} = 0.34$

Ch. 2, prob 7

$\phi(r) = e^{-r}\left(\frac{1}{r^3} - 1\right) \qquad r \le 1.5$

r	$\phi(r)$	
1.45	−0.1576	← minimum of $\phi(r)$
1.5	−0.1570	
1.3	−0.1484	
1.06	−0.056	

bcc



nn distance $= r_{nn} = \frac{\sqrt{3}}{2} a$, 8 nn

nnn distance $= r_{nnn} = a$, 6 nn

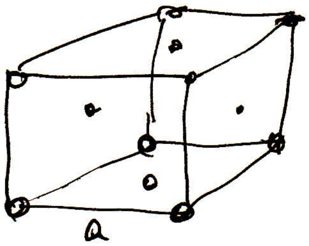
$\Rightarrow r_{nnn} = \frac{2}{\sqrt{3}} r_{nn} = 1.155\, r_{nn}$

If we take $r_{nn} = 1.45$, $r_{nnn} = 1.67 > 1.5 \Rightarrow \sum_j \phi(r_{ij}) = 8\,\phi(1.45) = -1.261$

If we take $r_{nnn} = 1.5 \Rightarrow r_{nn} = 1.30 \Rightarrow \sum_j \phi_{ij} = 8\,\phi(1.3) + 6\,\phi(1.5) =$

$= 8 \times (-0.148) + 6 \times (-0.157) = \boxed{-2.126}$

fcc



$r_{nn} = \frac{a}{\sqrt{2}}$, $r_{nnn} = a \Rightarrow r_{nnn} = 1.414\, r_{nn}$

12 nn, 6 nnn

If we take $r_{nn} = 1.45$, $r_{nnn} > 1.5 \Rightarrow \sum_j \phi_{ij} = 12\,\phi(1.45) = \boxed{-1.891}$

If we take $r_{nnn} = 1.5 \Rightarrow r_{nn} = 1.061 \Rightarrow$

$\sum_j \phi_{ij} = 12\,\phi(1.06) + 6\,\phi(1.5) = 12 \times (-0.056) + 6 \times (-0.157) = \boxed{-1.615}$

hcp is same as fcc

So lowest energy is for bcc, $a = 1.5$. $\sum_j \phi_{ij} = -2.126$

Ch. 3, probl

fcc : $\vec{a}_1 = \frac{a}{2}(1,1,0)$, $\vec{a}_2 = \frac{a}{2}(1,0,1)$; $\vec{a}_3 = \frac{a}{2}(0,1,1)$

$\vec{a}_1 = \frac{a}{2}(\hat{x}+\hat{y})$, $\vec{a}_2 = \frac{a}{2}(\hat{x}+\hat{z})$, $\vec{a}_3 = \frac{a}{2}(\hat{y}+\hat{z})$

$\hat{x} \times \hat{y} = \hat{z}$, $\hat{y} \times \hat{z} = \hat{x}$, $\hat{z} \times \hat{x} = \hat{y}$

$\vec{a}_1 \times \vec{a}_2 = \frac{a^2}{4}(\hat{x}+\hat{y}) \times (\cancel{\hat{y}}+\hat{z}) = \frac{a^2}{4}(-\hat{y} - \hat{z} + \hat{x})$

$\vec{a}_2 \times \vec{a}_3) = \frac{a^2}{4}(\hat{x}+\hat{z}) \times (\hat{y}+\hat{z}) = \frac{a^2}{4}(\hat{z} - \hat{y} - \hat{x})$

$\vec{a}_3 \times \vec{a}_1 = \frac{a^2}{4}(\hat{y}+\hat{z}) \times (\hat{x}+\hat{y}) = \frac{a^2}{4}(-\hat{z}+\hat{y}-\hat{x})$

$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{a^3}{8}(\hat{x}+\hat{y}) \cdot (\hat{z} - \hat{y} - \hat{x}) = -\frac{a^3}{4} = \vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1) = \vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)$

$$\vec{b}_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)} = \frac{2\pi \frac{a^2}{4}}{\frac{a^3}{4}}(\hat{x}+\hat{y}-\hat{z}) = \frac{4\pi}{a} \cdot \frac{1}{2}(\hat{x}+\hat{y}-\hat{z})$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{a_2 \cdot (a_3 \times \vec{a}_1)} = \frac{4\pi}{a} \cdot \frac{1}{2} \cdot (\hat{z}+\hat{x}-\hat{y})$$

$$\vec{b}_3 = 2\pi \frac{(\vec{a}_1 \times \vec{a}_2)}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)} = \frac{4\pi}{a} \cdot \frac{1}{2} \cdot (\hat{y}+\hat{z}-\hat{x})$$

= basis vectors of bcc with lattice spacing $\frac{4\pi}{a}$

and vice-versa, since $\frac{4\pi}{4\pi/a} = a$

(b) Al is fcc, $a = 4.05\,\text{Å}$ $\Rightarrow$ reciprocal lattice is bcc,

$\frac{4\pi}{a} = 3.10\,\text{Å}^{-1}$. Magnitude of primitive vectors of reciprocal lattice is $\frac{4\pi}{a}\frac{\sqrt{3}}{2} = 2.68\,\text{Å}^{-1}$. Vectors are $\frac{4\pi}{a}\left(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right)$,

$\frac{4\pi}{a}\left(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$, $\frac{4\pi}{a}\left(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right)$

Be is hexagonal, reciprocal lattice vectors are

$\frac{2\pi}{a}\left(1, -\frac{1}{\sqrt{3}}, 0\right)$; $\frac{2\pi}{a}\left(0, \frac{2}{\sqrt{3}}, 0\right)$; $\frac{2\pi}{c}(0, 0, 1)$

$a = 2.29\,\text{Å}$, $c = 3.59\,\text{Å}$ $\Rightarrow$ $\frac{2\pi}{c} = 1.75\,\text{Å}^{-1}$, $\frac{4\pi}{\sqrt{3}a} = 3.16\,\text{Å}^{-1}$

bcc iron, $a = 2.87\,\text{Å}$, $\Rightarrow$ reciprocal lattice is fcc,

$\frac{4\pi}{a} = 4.38\,\text{Å}^{-1}$, magnitude of primitive vectors of reciprocal lattice is $\frac{4\pi}{a}\frac{1}{\sqrt{2}} = 3.10\,\text{Å}^{-1}$. Vectors are $\frac{4\pi}{a}\left(\frac{1}{2}, \frac{1}{2}, 0\right)$,

$\frac{4\pi}{a}\left(\frac{1}{2}, 0, \frac{1}{2}\right)$, $\frac{4\pi}{a}\left(0, \frac{1}{2}, \frac{1}{2}\right)$

Ch. 3, prob 2 : for hexagonal lattice primitive vectors Eq. (2.5)

$$\vec{a}_1 = a\left(\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}\right), \quad \vec{a}_2 = a\left(\frac{\sqrt{3}}{2}\hat{x} - \frac{1}{2}\hat{y}\right), \quad \vec{a}_3 = c\hat{z}$$

$$\vec{a}_2 \times \vec{a}_3 = ac\left(-\frac{\sqrt{3}}{2}\hat{y} - \frac{1}{2}\hat{x}\right), \quad \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = -a^2 c\frac{\sqrt{3}}{2}$$

$$\vec{a}_3 \times \vec{a}_1 = ac\left(\frac{\sqrt{3}}{2}\hat{y} - \frac{1}{2}\hat{x}\right), \quad \vec{a}_1 \times \vec{a}_2 = -a^2\frac{\sqrt{3}}{2}\hat{z}$$

$$\vec{b}_1 = 2\pi\frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{x} + \hat{y}\right)$$

$$\vec{b}_2 = 2\pi\frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} = \frac{2\pi}{a}\left(\frac{1}{\sqrt{3}}\hat{x} - \hat{y}\right)$$

$$\vec{b}_3 = 2\pi\frac{\vec{a}_1 \times \vec{a}_2}{a_1 \cdot a_2 \times a_3} = \frac{2\pi}{c}\hat{z}$$

$$\vec{q} = n_1\vec{b}_1 + n_2\vec{b}_2 + n_3\vec{b}_3$$

For hcp, $c = \sqrt{\frac{8}{3}}\,a = 2\sqrt{\frac{2}{3}}\,a$

For basis vectors eq. (2.6)

$$\vec{v}_1 = \vec{0}, \quad \vec{v}_2 = \frac{a}{\sqrt{3}}\hat{x} + \frac{c}{2}\hat{z}$$

the modulation introduced by the basis is

$$F_{\vec{q}} = \left|1 + e^{i\vec{q}\cdot\vec{v}_2}\right|^2$$

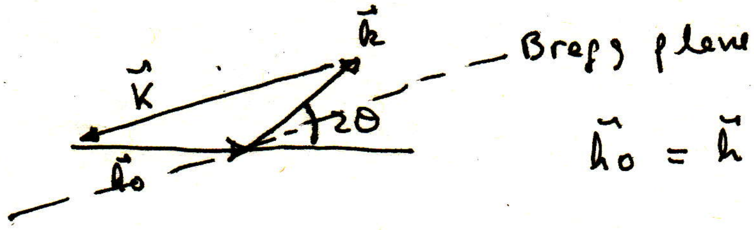
$$\vec{b}_1 \cdot \vec{v}_2 = \frac{2\pi}{3}; \quad \vec{b}_2 \cdot \vec{v}_2 = \frac{2\pi}{3}; \quad \vec{b}_3 \cdot \vec{v}_2 = \pi$$

$$\vec{q} \cdot \vec{v}_2 = n_1\vec{b}_1 \cdot \vec{v}_2 + n_2\vec{b}_2 \cdot \vec{v}_2 + n_3\vec{b}_3 \cdot \vec{v}_2 = \frac{2\pi}{3}n_1 + \frac{2\pi}{3}n_2 + \pi n_3$$

$$\Rightarrow F_{\vec{q}} = \left|1 + e^{i\left(\frac{2\pi}{3}n_1 + \frac{2\pi}{3}n_2 + \pi n_3\right)}\right|^2$$

Get extinction when $\dfrac{2(n_1+n_2)+3n_3}{3}$ = odd integer.

Ch. 3, prob 3



$\vec{k}_0 = \vec{k} + \vec{K}$

Bragg condition: $2d\sin\theta = n\lambda$

$\vec{K} = \vec{k}_0 - \vec{k}$

$K^2 = 2k_0^2 - 2\vec{k}_0 \cdot \vec{k} = 2k_0^2(1-\cos 2\theta) = 4k_0^2\sin^2\theta$

$\Rightarrow \quad K = 2k_0\sin\theta$

$K = \frac{2\pi}{d}n \quad , \quad k_0 = \frac{2\pi}{\lambda} \quad \Rightarrow$ Bragg condition

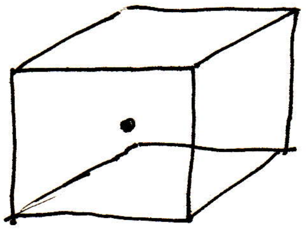
Problem on powder method

the scattering condition is $K = 2k_0 \sin\frac{\phi}{2}$

From the table of angles we construct a table for ratios of reciprocal lattice vector magnitudes, i.e. $K_2/K_1 = \sin\frac{\phi_2}{2} / \sin\frac{\phi_1}{2}$

	A	B	C
K_2/K_1	1.156	1.408	1.634
K_3/K_1	1.633	1.725	1.921
K_4/K_1	1.917	2	2.311

fcc: reciprocal is bcc. For cube length a in bcc, the shortest lattice vectors have length: $\frac{\sqrt{3}}{2}a,\ a,\ \sqrt{2}a,\ \frac{\sqrt{11}}{2}a \equiv K_1, K_2, K_3, K_4$



$\Rightarrow \frac{K_2}{K_1} = \frac{2}{\sqrt{3}} = 1.15$

$\frac{K_3}{K_1} = \frac{2\sqrt{2}}{\sqrt{3}} = 1.63$; $\frac{K_4}{K_1} = \frac{\sqrt{11}}{\sqrt{3}} = 1.915$

$\Rightarrow$ A is fcc

bcc: reciprocal is fcc. For cube length a in fcc, the shortest lattice vectors have length $\frac{a}{\sqrt{2}},\ a,\ \sqrt{\frac{3}{2}}a,\ \sqrt{2}a = K_{1,2,3,4} \Rightarrow$

$\frac{K_2}{K_1} = \sqrt{2} = 1.41$, $\frac{K_3}{K_1} = \sqrt{3} = 1.73$, $\frac{K_4}{K_1} = 2 \Rightarrow$ B is bcc

Diamond structure is fcc with 2 atom basis, $n_1+n_2+n_3 = 2, 6, 10 \ldots$ are absent $\Rightarrow$ C is diamond

$\lambda = 1.5\,\mathring{A} \Rightarrow q = \frac{2\pi}{\lambda} = 4.189\,\mathring{A}^{-1} = k_0$

A is fcc, reciprocal is bcc with conventional unit cell $\frac{4\pi}{a}$

Shortest reciprocal lattice vector is $\frac{4\pi}{a}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$ with

magnitude $K_1 = \frac{\cancel{4}^{2}\pi}{a}\frac{\sqrt{3}}{2}$

From $K_1 = 2k_0 \sin\frac{\phi}{2}$, $\phi = 42.2° \Rightarrow K_1 = 3.02\,\mathring{A}^{-1}$

$\Rightarrow a = \frac{2\pi\sqrt{3}}{K_1} \Rightarrow \boxed{a = 3.60\,\mathring{A}}$

B is bcc, reciprocal is fcc with conv unit cell $\frac{4\pi}{a}$

Shortest reciprocal lattice vector is $\frac{4\pi}{a}\left(\frac{1}{2}, \frac{1}{2}, 0\right)$ with

magnitude $\frac{4\pi}{a}\frac{1}{\sqrt{2}} = K_1$. $\phi = 28.8° \Rightarrow K_1 = 2.084\,\mathring{A}^{-1}$

$\Rightarrow \cancel{a = \frac{\sqrt{2}K_1}{4\pi}}$ $a = \frac{4\pi}{\sqrt{2}K_1} = \boxed{4.26\,\mathring{A}}$

C is diamond, reciprocal is bcc. Smallest angle corresponds

to vector of length $K = \frac{4\pi}{a}\frac{\sqrt{3}}{2}$, and it is $42.8° \Rightarrow$

$K = 2k_0 \sin\frac{\phi}{2} = 3.06\,\mathring{A}^{-1} \Rightarrow a = \frac{4\pi\sqrt{3}}{K\cdot 2} = \boxed{3.56\,\mathring{A}}$

For zincblende structure there would be no extinctions,

so there would be a ring for $K = \frac{4\pi}{a} \Rightarrow \boxed{\phi = 49.8°}$