Condensed Matter Physics (Phy 771)

HW # 2 - solution

Dr. Gassem Alzoubi

① problem 2.1 Marder:

FCC: 4 LP/unit cell (primitive) located at

$(0,0,0)$, $\frac{a}{2}(1,1,0)$, $\frac{a}{2}(1,0,1)$, $\frac{a}{2}(0,1,1)$

$\downarrow \vec{a_1}$, $\downarrow \vec{a_2}$, $\downarrow \vec{a_3}$

$V_c = a^3$, $V_p = |\vec{a_1}\cdot(\vec{a_2}\times\vec{a_3})|$; $\vec{a_2}\times\vec{a_3} = \frac{a^2}{4}\begin{vmatrix} i & j & k \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{vmatrix}$

$= \frac{a^2}{4}\left[\hat{i}(0-1) - \hat{j}(1-0) + \hat{k}(1-0)\right]$

$= \frac{a^2}{4}\left[-\hat{i} - \hat{j} + \hat{k}\right]$

$= \frac{a^2}{4}(-1,-1,1)$

$\Rightarrow V_p = \left|\frac{a}{2}(1,1,0)\cdot\frac{a^2}{4}(-1,-1,1)\right|$

$= \frac{a^3}{8}|-1-1| = \frac{a^3}{4}$

$\Rightarrow \frac{V_c}{V_p} = \frac{a^3}{a^3/4} = 4$

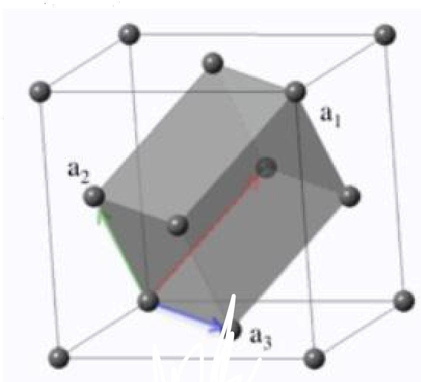
BCC: 2 LP / primitive cell located at $(0,0,0)$ and $\frac{a}{2}(1,1,1)$

primitive lattice vectors are

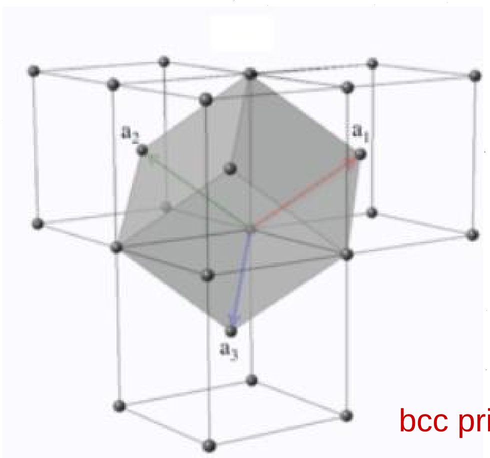
$\vec{a_1} = \frac{a}{2}(1,1,-1)$, $\vec{a_2} = \frac{a}{2}(-1,1,1)$, $\vec{a_3} = \frac{a}{2}(1,-1,1)$

$V_c = a^3$, $V_p = |\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}| = \frac{a^3}{2}$

$\Rightarrow \frac{V_c}{V_p} = \frac{a^3}{\frac{a^3}{2}} = 2$



fcc primitive unit cell

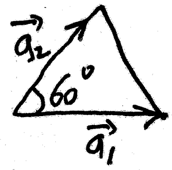


bcc primitive unit cell

② Problem 2.2 Marder

a)

$\vec{a}_1 = a(1,0,0)$ and



$\vec{a}_2 = a\cos 60\,\hat{i} + a\sin 60\,\hat{j}$

$= \frac{a}{2}\hat{i} + a\frac{\sqrt{3}}{2}\hat{j}$

$= a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right)$

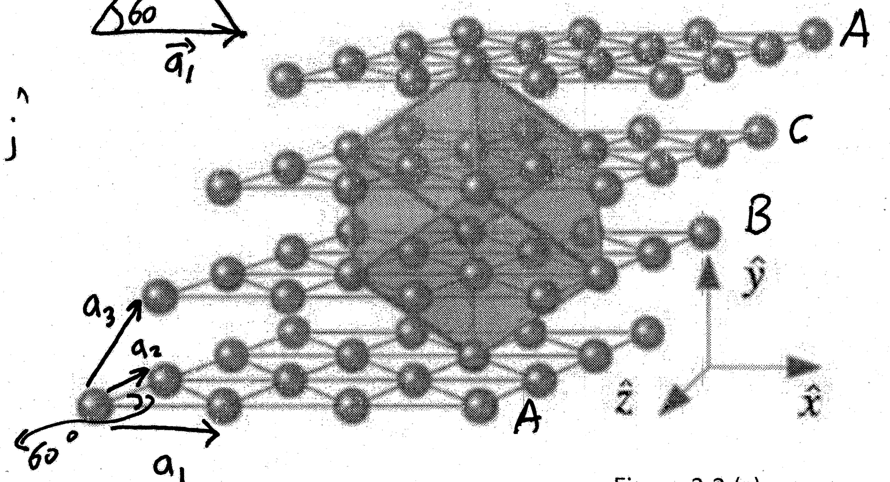
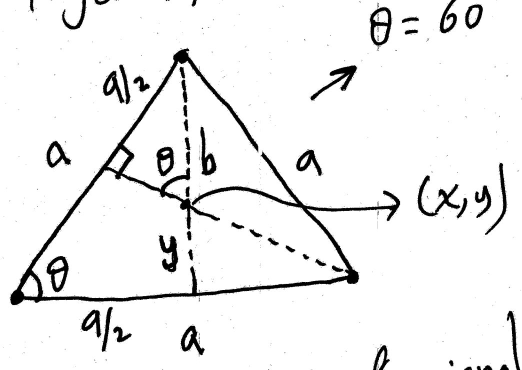
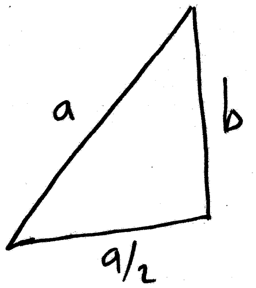


Figure 2.2 (c)

$\vec{a}_1$ and $\vec{a}_2$ generate 2D Hexagonal lattice (triangular lattice) which define layer A in the xy plane. Now we need to construct layer B such that the lattice points of layer B are located above the centers of triangles of layer A. So we need to find the third primitive vector $\vec{a}_3$. The projection of $\vec{a}_3$ on xy plane is represented by the center point of triangles of layer A.

from the figure, we see that $x = \frac{a}{2}$ and from left right triangle





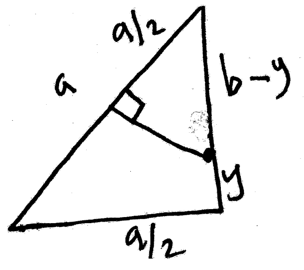
$\left(\frac{a}{2}\right)^2 + b^2 = a^2$

$\Rightarrow b^2 = \frac{3}{4}a^2$

$\Rightarrow b = \frac{\sqrt{3}}{2}a$

equilateral of triangle with sidelength a

we note that the two right triangles on left side are similar $\Rightarrow \frac{b-y}{a} = \frac{\frac{a}{2}}{b} \Rightarrow b - y = \frac{a^2}{2b} \Rightarrow y = b - \frac{a^2}{2b}$

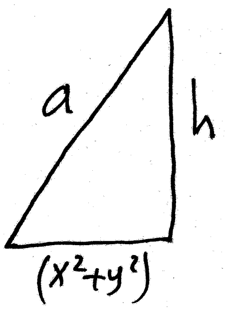


$\Rightarrow y = \frac{\sqrt{3}}{2}a - \frac{a^2}{2\frac{\sqrt{3}}{2}a} = a\left[\frac{\sqrt{3}}{2} - \frac{1}{\sqrt{3}}\right] = \frac{a}{2\sqrt{3}}$

$\Rightarrow (x,y) = \left(\frac{a}{2}, \frac{a}{2\sqrt{3}}\right)$

Now we need to find the z-component of $\vec{a_3}$

let the z-component be $h = \frac{c}{2}$, so from the tetrahedron shown in figure below, we see that



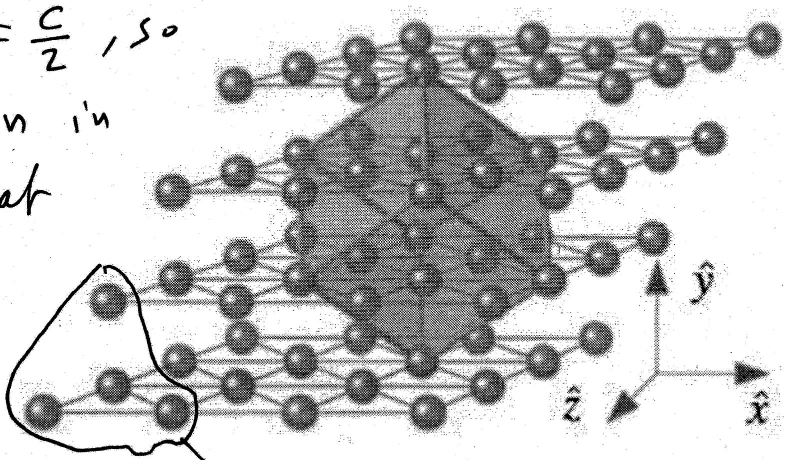
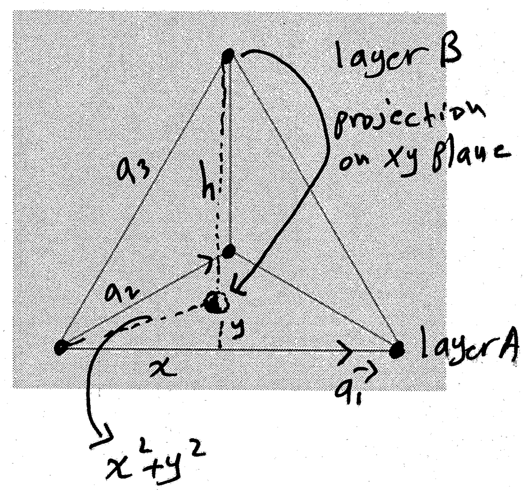


Figure 2.2 (c)

$$\Rightarrow h^2 = a^2 - (x^2+y^2) = a^2 - \left(\frac{a^2}{4} + \frac{a^2}{12}\right)$$

$$= a^2 - a^2\left\{\frac{4}{12}\right\} = a^2 - \frac{a^2}{3} = \frac{2}{3}a^2$$

$\Rightarrow h = \sqrt{\frac{2}{3}}\, a$, so the third primitive vector $\vec{a_3}$ reads



tetrahedron

$|\vec{a_1}| = |\vec{a_2}| = |\vec{a_3}| = a$

$$\vec{a_3} = \left(\frac{a}{2}, \frac{a}{2\sqrt{3}}, \sqrt{\frac{2}{3}}\, a\right)$$

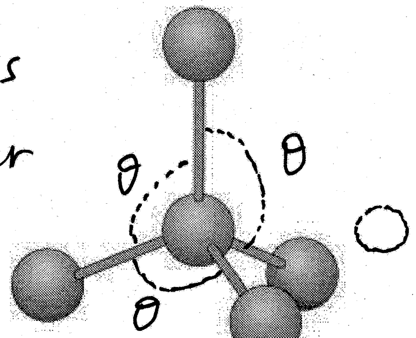
$$= a\left(\frac{1}{2}, \frac{1}{2\sqrt{3}}, \sqrt{\frac{2}{3}}\right)$$

the fcc lattice is a Bravias lattice, so all lattice points can be generated by $\vec{T} = n_1\vec{a_1} + n_2\vec{a_2} + n_3\vec{a_3}$.

Note that $c = 2h = 2\sqrt{\frac{2}{3}}\, a = \sqrt{\frac{8}{3}}\, a$

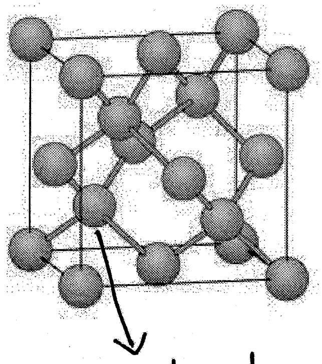
③ problem 2.3 Marder:

in diamond lattice, each Carbon atom is bonded to four other Carbon atoms in a tetrahedral shape as shown in figure.



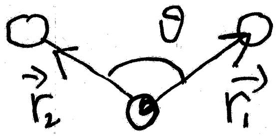
tetrahedron

Diamond lattice



$\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$

to find the angle between any two bonds, let us consider the two nearest neighbors of the origin which are $(1/4, 1/4, 1/4)$ and $(-1/4, -1/4, 1/4)$



i.e $\vec{r_1} = \frac{1}{4} a \hat{i} + \frac{1}{4} a \hat{j} + \frac{1}{4} a \hat{k}$

$= a(1/4, 1/4, 1/4)$, and

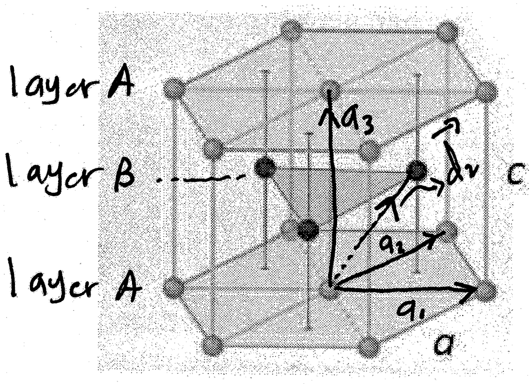
$\vec{r_2} = a(-1/4, -1/4, 1/4) \Rightarrow$

$$\cos\theta = \frac{\vec{r_1} \cdot \vec{r_2}}{|\vec{r_1}|\,|\vec{r_2}|} = \frac{a^2\left[-\frac{1}{16} - \frac{1}{16} + \frac{1}{16}\right]}{a\sqrt{\frac{3}{16}}\; a\sqrt{\frac{3}{16}}} = \frac{-\frac{a^2}{16}}{a^2\frac{3}{16}} = -\frac{1}{3}$$

$$\Rightarrow \theta = \cos^{-1}(-1/3) = 109.46^\circ$$

(4) problem 2.4 Marder

for simple hexagonal lattice, the primitive vectors are $\vec{a}_1 = a(1,0,0)$; $\vec{a}_2 = a(\frac{1}{2}, \frac{\sqrt{3}}{2}, 0)$ and $\vec{a}_3 = (0,0,c)$. but these 3 vectors gives the positions of lattice points only in layers of type A in the hcp ABAB structure, meaning that the 3 primitive vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$ don't encode all lattice points in the hcp ABAB structure. This is expected as the hcp lattice is Not a Bravias lattice.



hcp structure
ABABAB

To represent all lattice points in hcp, including lattice points in layers of type B, we need two additional primitive vectors $\vec{d}_1$ and $\vec{d}_2$; where

$\vec{d}_1 = (0,0,0)$ represents lattice points in layers of type A

$\vec{d}_2 = (\frac{a}{2}, \frac{a}{2\sqrt{3}}, \frac{c}{2})$ represents lattice points in layers of type B

Now the position of every point in the hcp ABAB lattice is given by

$$\vec{R} = \underbrace{\underbrace{n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3}_{\text{simple Hexagonal}} + \vec{d}_1 + \vec{d}_2}_{\text{for hcp}}$$

; n_1, n_2, n_3 are integers

Now for Hexagonal-Packed structures (hcp or fcc), we must have $|\vec{d_2}| = a$

$$\Rightarrow \frac{a^2}{4} + \frac{a^2}{12} + \frac{c^2}{4} = a^2$$

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

$$\Rightarrow \frac{c^2}{4} = \frac{2}{3}a^2 \Rightarrow \frac{c^2}{a^2} = \frac{8}{3} \Rightarrow \boxed{\frac{c}{a} = \sqrt{\frac{8}{3}}}$$

(5)

Problem 2.6 Marder: Packing fraction (F)

the packing fraction (F) is the volume of atoms in a unit cell divided by the volume of the unit cell

$$F = \frac{[\#\text{ of atoms/unit cell}][\text{volume of one atom}]}{\text{Volume of conventional unit cell}}$$

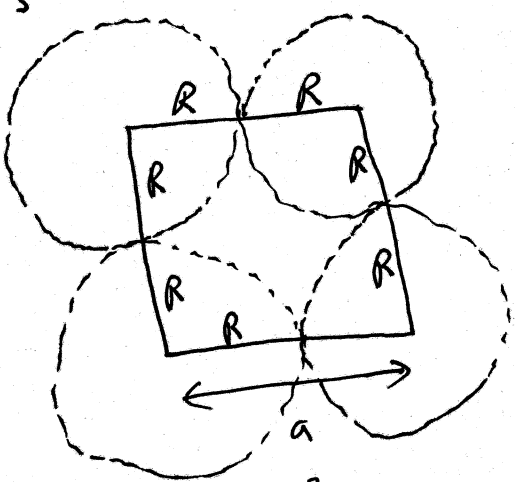
$$= \frac{Z \times \frac{4}{3}\pi R^3}{V_c}$$; R : radius of the atom
V_c : volume of conventional unit cell
Z : # of LP/unit cell

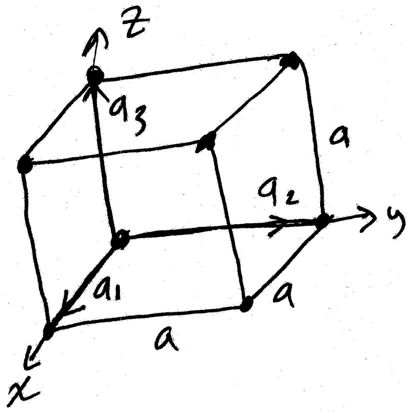
a) simple cube (SC):

$Z = 1$, $V_c = a^3$

$2R = a$

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



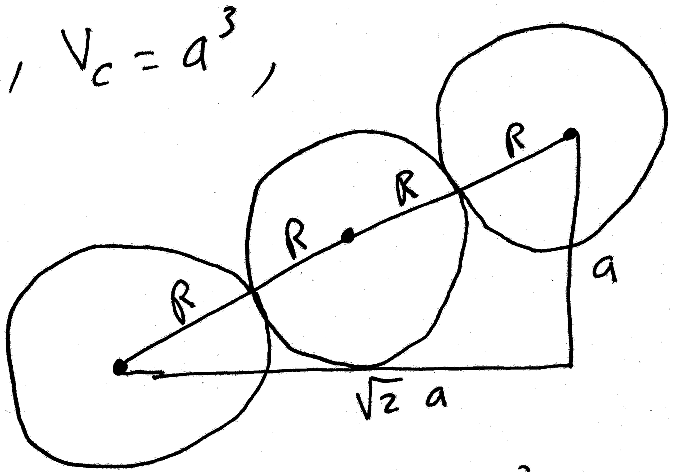


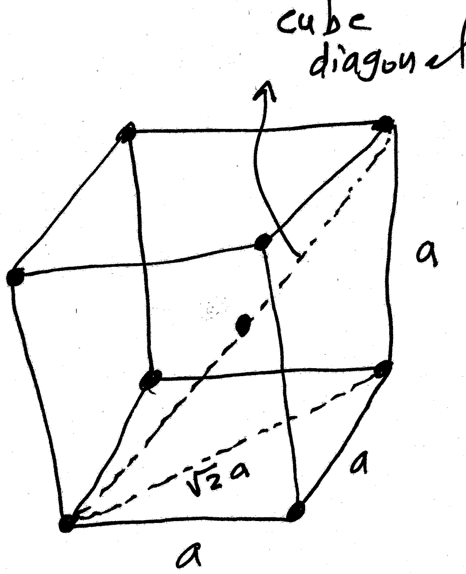
$$\Rightarrow F = \frac{1 \times \frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{a^3} = \frac{\pi}{6} = 0.52$$

spheres occupy 52 % of the volume of the cube and 48% are voids

b) Body-centered cubic (BCC):

$Z = 2$, $V_c = a^3$,





$$\Rightarrow (\sqrt{2}a)^2 + a^2 = (4R)^2$$

$$\Rightarrow a = \frac{4}{\sqrt{3}} R \Rightarrow F = \frac{2 \times \frac{4}{3}\pi R^3}{\left(\frac{4}{\sqrt{3}} R\right)^3} = 0.68$$

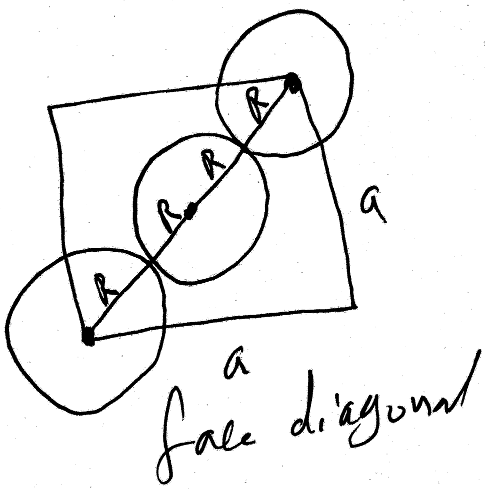
c) Face-centered cubic (FCC)

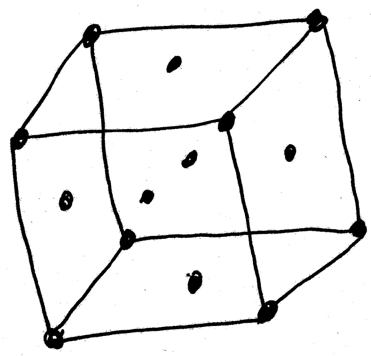
$Z = 4$, $V_c = a^3$

$(4R)^2 = a^2 + a^2$

$16R^2 = 2a^2$

$\Rightarrow a = \frac{4}{\sqrt{2}} R$





$$\Rightarrow F = \frac{4 \times \frac{4}{3}\pi R^3}{\left(\frac{4}{\sqrt{2}} R\right)^3} = 0.74$$

d) Hexagonal-closed packed (hcp)

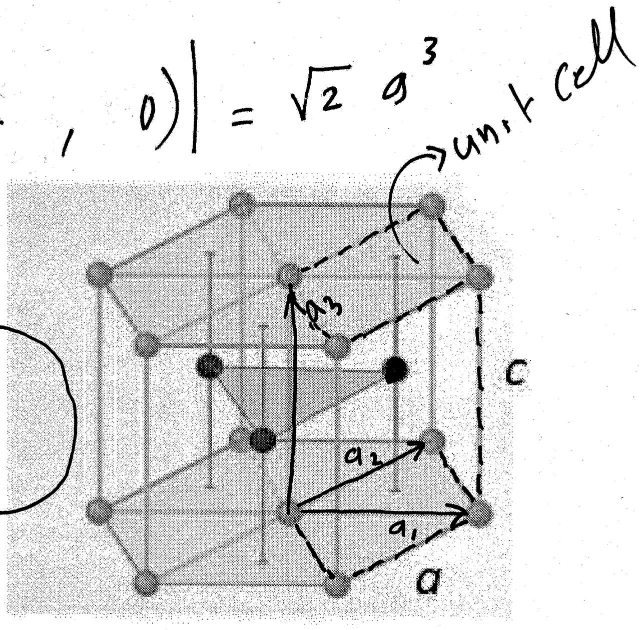
it is simple hexagonal with 2 LP/unit cell

$\vec{a_1} = a(1,0,0)$, $\vec{a_2} = a(1/2, \frac{\sqrt{3}}{2}, 0)$; $\vec{a_3} = (0,0,c)$
$= a(0,0,\sqrt{\frac{8}{3}})$

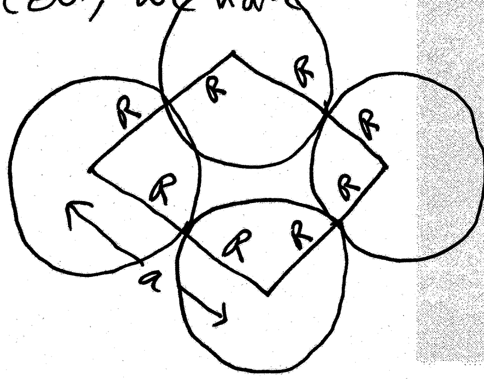
$Z = 2$

$V_c = |\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}|$; $\vec{a_2} \times \vec{a_3} = a^2(\sqrt{2}, -\sqrt{\frac{2}{3}})$

$= |a(1,0,0) \cdot a^2(\sqrt{2}, -\sqrt{\frac{2}{3}}, 0)| = \sqrt{2}\, a^3$



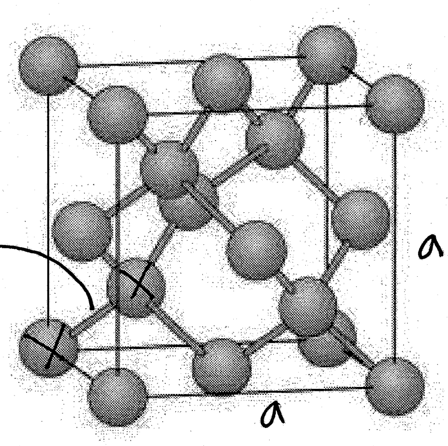
from base of unit cell, we have



$2R = a$

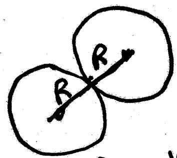
$\Rightarrow F = \dfrac{2 \times \frac{4}{3}\pi R^3}{\sqrt{2}\,(2R)^3} = \dfrac{\pi}{3\sqrt{2}} = 0.74$

e) Diamond: $Z = 8$, $V_c = a^3$



NN spacing $= |(\frac{a}{4}, \frac{a}{4}, \frac{a}{4}) - (0,0,0)| = \frac{\sqrt{3}}{4}a$

$R = \dfrac{\text{NN spacing}}{2} = \dfrac{\sqrt{3}}{8}a$



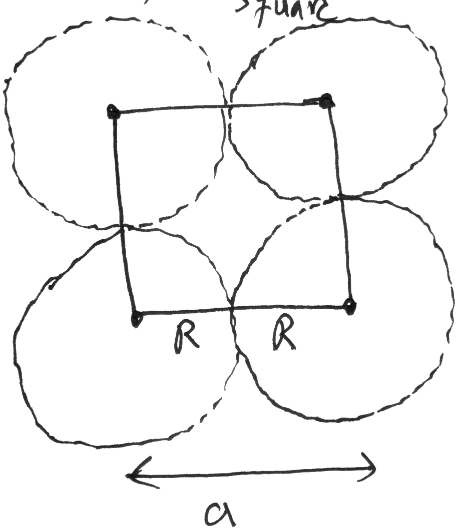
$2R = \frac{\sqrt{3}}{4}a \Rightarrow a = \frac{8R}{\sqrt{3}}$

$\Rightarrow F = \dfrac{8 \times \frac{4}{3}\pi R^3}{\left(\frac{8R}{\sqrt{3}}\right)^3} = \dfrac{\pi\sqrt{3}}{16} = 0.34$

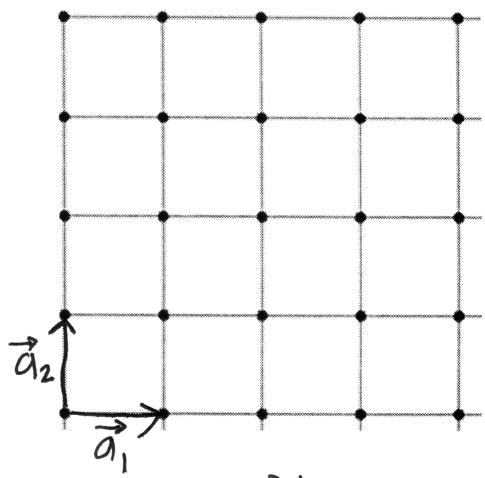
⑥ Packing fraction in 2D

a) Square lattice ; $\vec{a}_1 = a\hat{i}$, $\vec{a}_2 = a\hat{j}$

$Z=1$, $A_{square} = |\vec{a}_1 \times \vec{a}_2| = a^2$



$2R = a \Rightarrow R = \frac{a}{2}$



$|\vec{a}_1| = |\vec{a}_2| = a$

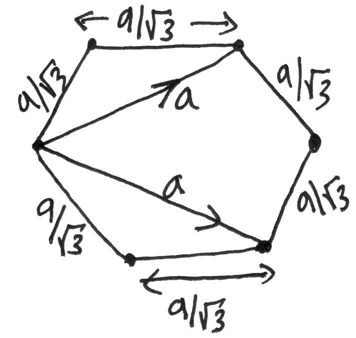
$$F = \frac{Z \times A_{sphere}}{A_{square}} = \frac{1 \times \pi R^2}{a^2} = \frac{1 \times \pi R^2}{(2R)^2} = \frac{\pi}{4} = 0.79$$

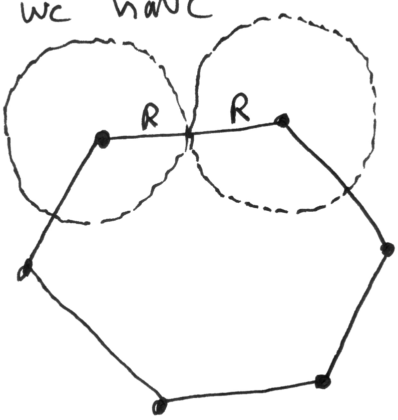
---

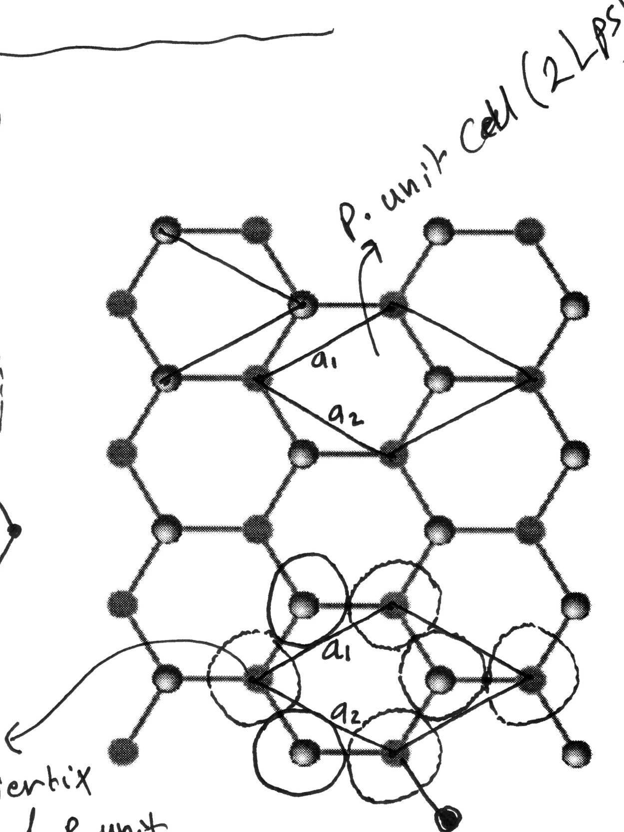
b) Graphene lattice (honeycomb lattice)

p. unit cell contains 2 LPs $\Rightarrow Z=2$

for Graphene lattice, we have







$\Rightarrow 2R = a/\sqrt{3} \Rightarrow R = \frac{a}{2\sqrt{3}}$

each vertix (atom) of p. unit cell is shared with 4 other p. unit. cells

$\vec{a}_1 = a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)$

$\vec{a}_2 = a\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$

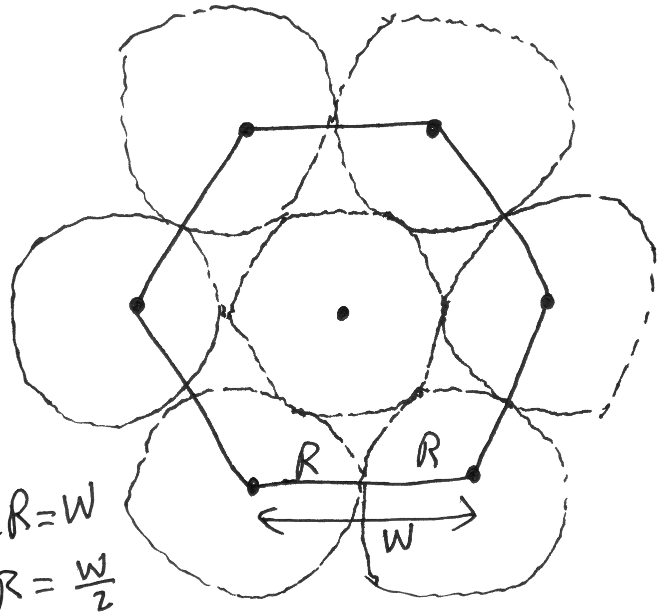
$|\vec{a}_1 \times \vec{a}_2| = \frac{\sqrt{3}}{2} a^2$

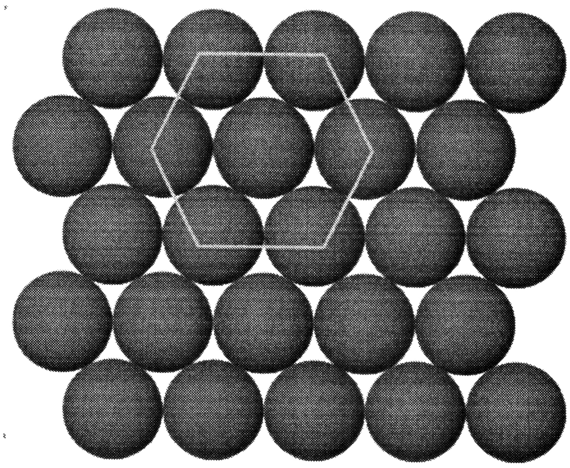
$|\vec{a}_1| = |\vec{a}_2| = a$

$$F = \frac{Z \times A_{sphere}}{A_{\substack{primitive\\cell}}} = \frac{Z \times \pi R^2}{|\vec{a}_1 \times \vec{a}_2|}$$

$$= \frac{2 \times \left(\frac{a}{2\sqrt{3}}\right)^2}{\frac{\sqrt{3}}{2} a^2} = \frac{\pi}{3\sqrt{3}} = 0.6$$

c) 2D hcp lattice





$2R = W$

$R = \frac{W}{2}$

for hcp lattice, there is an extra lattice point at the center of hexagon, so the coordination number is 6. Recall that for graphene lattice, there is no lattice point at the center and the coordination number is 3.

now each sphere on the vertix of hexagon is shared with 3 hexagons and the sphere at center is not shared with others, so $Z = 6 \times \frac{1}{3} + 1 = 2 + 1 = 3$

$$\Rightarrow F = \frac{Z \times A_{sphere}}{A_{hexagon}} = \frac{3 \times \pi R^2}{A_{hexagon}}$$; where $A_{hexagon}$ is

the area of one hexagon $\Rightarrow A_{hexagon} = \frac{3}{2}\sqrt{3}\, W^2$

$$F = \frac{3 \times \pi \frac{W^2}{4}}{\frac{3}{2}\sqrt{3}\, W^2} = \frac{\pi}{2\sqrt{3}} = 0.91$$, which is larger

that F for graphene lattice (0.6), due to the extra lattice point at center of hexagon.