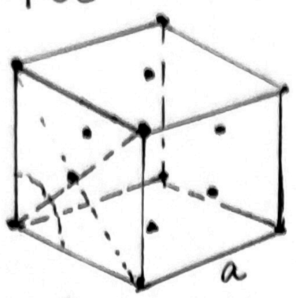
Problem set 2.

Problem 1.

(1.a) FCC

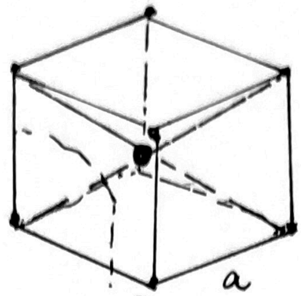


$R = \frac{a}{2\sqrt{2}}$, $V_{sph} = \frac{4}{3}\pi R^3$

$N = \frac{1}{8}\times 8 + 6\times\frac{1}{2} = 4$

$\frac{V_{occ}}{V_{cub}} = \frac{4\times V_{sph}}{V_{cub}} = \frac{\pi}{3\sqrt{2}} = 0.74$

BCC



$R = \frac{\sqrt{3}}{4}a$, $V_{sph} = \frac{4}{3}\pi R^3$

$N = \frac{1}{8}\times 8 + 1 = 2$

$\frac{V_{occ}}{V_{cub}} = \frac{2\times V_{sph}}{V_{cub}} = \frac{\sqrt{3}}{8}\pi = 0.68$

(2.b) coordination number

FCC: $3\times 4 = 12$

BCC: 8

atomer per cell

FCC: 4 BCC: 2

(1.k) primitive vectors of FCC

$\vec{a_1} = \frac{a}{2}(\vec{y} + \vec{z})$

$\vec{a_2} = \frac{a}{2}(\vec{z} + \vec{x})$

$\vec{a_3} = \frac{a}{2}(\vec{x} + \vec{y})$

Obviously, $|\vec{a_1}| = |\vec{a_2}| = |\vec{a_3}| = \frac{1}{\sqrt{2}}a$

$\cos\theta = \frac{\vec{a_i}\cdot\vec{a_j}}{|\vec{a_i}||\vec{a_j}|} = \frac{a^2/4}{a^2/2} = \frac{1}{2}$

$\theta = \pi/3 \longrightarrow \vec{a_1}, \vec{a_2}, \vec{a_3}$ form a regular tetrahedron

(1.d) primitive vectors of BCC

$\vec{a_1'} = \frac{a}{2}(\vec{z} + \vec{y} - \vec{x})$

$\vec{a_2'} = \frac{a}{2}(\vec{z} + \vec{x} - \vec{y})$

$\vec{a_3'} = \frac{a}{2}(\vec{x} + \vec{y} - \vec{z})$

Reciprocal space

$\vec{b_1} = \frac{2\pi}{\Omega}\vec{a_2}\times\vec{a_3}$

$\vec{b_2} = \frac{2\pi}{\Omega}\vec{a_3}\times\vec{a_1}$

$\vec{b_3} = \frac{2\pi}{\Omega}\vec{a_1}\times\vec{a_2}$ where $\Omega = \vec{a_1}\cdot(\vec{a_2}\times\vec{a_3})$

Note that

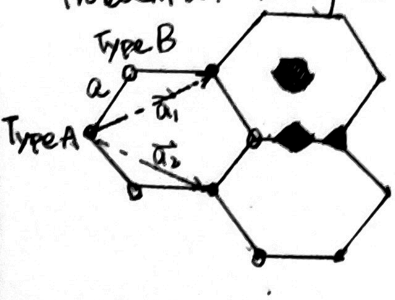
$\vec{a_i}\cdot\vec{b_j} = \begin{cases} 2\pi, & i=j \\ 0, & i\neq j \end{cases}$, $\vec{a_i}\cdot\vec{b_j} = 2\pi\delta_{ij}$

And

$\vec{a_i}\cdot\vec{a_i'} = \frac{a^2}{4}$, $\vec{a_i}\cdot\vec{a_j'} = 0$ if $i\neq j$

Therefore, reciprocal lattice of FCC is BCC and vice versa.

Problem 2. honey comb lattice



(1.a) Type A and Type B are not equivalent in the sense of Bravais lattice

$$\vec{a_1} = \frac{3}{2}a\vec{x} + \frac{\sqrt{3}}{2}a\vec{y}$$

$$\vec{a_2} = \frac{3}{2}a\vec{x} - \frac{\sqrt{3}}{2}a\vec{y}$$

(2.b)

	Bravais lattice	Point group
6-fold	1 (hexagon center)	1 (center)
3-fold	2 (Vertexes A, B)	1 (A and B equivalent under C_2).
2-fold	3 (edges)	1 (edges equivalent under C_3)

When A, B become unequivalent,

2-fold → violated

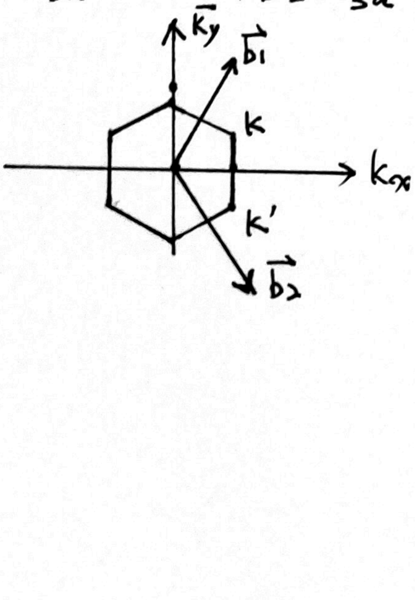
3-fold → two unequivalent ones

6-fold → 3-fold

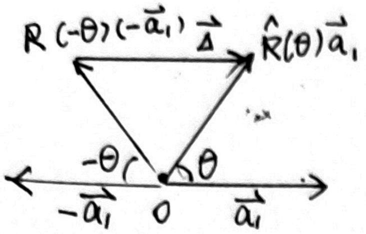
Symmetry reduces to 3 3-folds.

(2.c) Reciprocal space

$$\vec{b_1} = \frac{2\pi}{3a}(1, \sqrt{3}), \quad \vec{b_2} = \frac{2\pi}{3a}(1, -\sqrt{3})$$



Problem 3.



Take $\vec{a}_1 = \vec{x}$ as primitive vector

Assume this lattice is invariant under rotation of θ s.t.

$\hat{R}(\theta)\vec{a}_1 = \cos\theta\,\vec{x} - \sin\theta\,\vec{y}$

$\hat{R}(-\theta)(-\vec{a}_1) = -\cos\theta\,\vec{x} - \sin\theta\,\vec{y}$

The above vectors are belong to Bravais lattice.

$\vec{\Delta} = \hat{R}(\theta)\vec{a}_1 - \hat{R}(-\theta)(-\vec{a}_1) = 2\cos\theta\,\vec{x}$

Displacement $\vec{\Delta}$ ~~is~~ parallel to $\vec{a}_1$ so it has to be multiples of $\vec{x}$

$\vec{\Delta} = 2\cos\theta\,\vec{x} = N\cdot\vec{x}$

$\cos\theta \in [-1,1]$, the only allowed values are $N = -2, -1, 0, +1, +2$

N	$\cos\theta$	θ	
-2	-1	π	2-fold
-1	$-\frac{1}{2}$	$\frac{2}{3}\pi$	3-fold
0	0	$\pi/2$	4-fold
$+1$	$+\frac{1}{2}$	$\pi/3$	6-fold
$+2$	$+1$	$0, 2\pi$	1-fold

Thus 5-fold is not allowed in Bravais lattice

Problem 4

$\vec{R}_{\vec{n}} \pm \vec{R}_{\vec{m}} = (n_1 \pm m_1)\vec{a}_1 + (n_2 \pm m_2)\vec{a}_2 + (n_3 \pm m_3)\vec{a}_3 = \vec{R}_{\vec{n}\pm\vec{m}}$