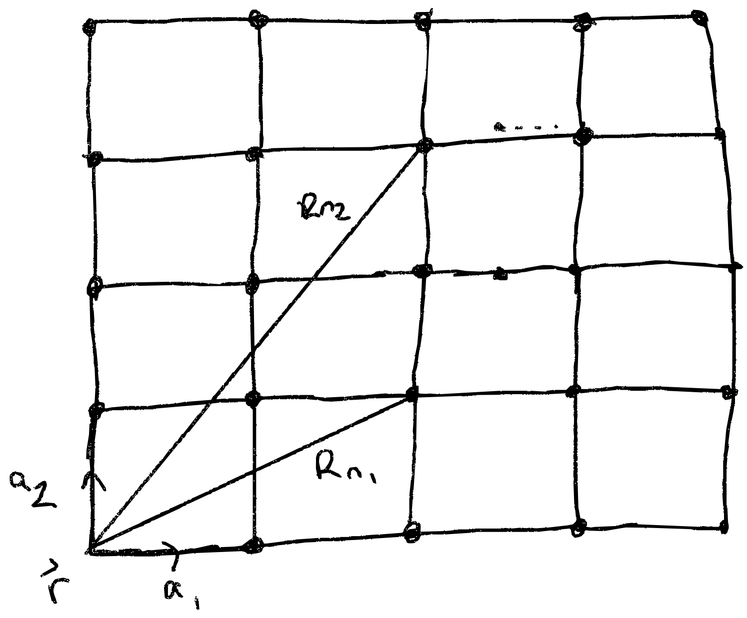
3.1

a) $\frac{\vec{R}_m + \vec{R}_n}{2}$ $\quad \frac{m_1+n_1}{2}\hat{a}_1 + \frac{m_2+n_2}{2}\hat{a}_2 + \frac{m_3+n_3}{2}\hat{a}_3$



$\vec{R}_{\vec{n}_1} = 2\vec{a}_1 + \vec{a}_2$

$\vec{R}_{n_2} = 2\vec{a}_1 + \vec{3a}_2$

$$\vec{R}_{l'} = \frac{\vec{R}_{\vec{l}} - (\vec{R}_{\vec{n}} + \vec{R}_{\vec{m}})}{2} = \sum_i \left[l_i - \tfrac{1}{2}(n_i+m_i)\right]\vec{a}_i$$

$-\vec{R}$

$\{\vec{R}_{\vec{n}}\}$

$\vec{R}_{\vec{n}} = n_1\vec{a}_1 + n_2\vec{a}_2 \; - - -$

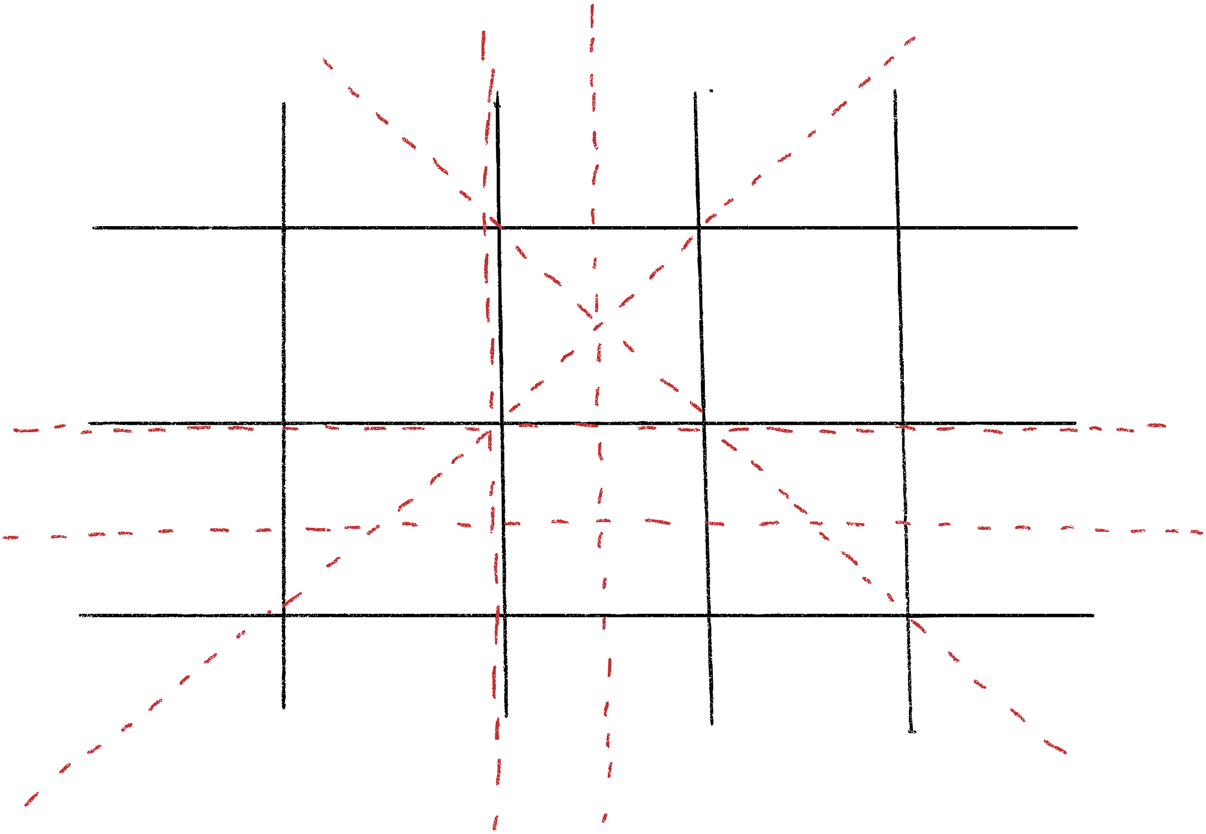
$$\vec{R}_{\vec{a}'} = \sum_i \left[a_i - \tfrac{1}{2}(n_i+m_i)\right]\vec{a}_i$$
$$\vec{R}_{\vec{b}'} = \sum_i \left[b_i - \tfrac{1}{2}(n_i+m_i)\right]\vec{a}_i$$

$-\vec{R}_{\vec{a}'} = \vec{R}_{\vec{b}'}$

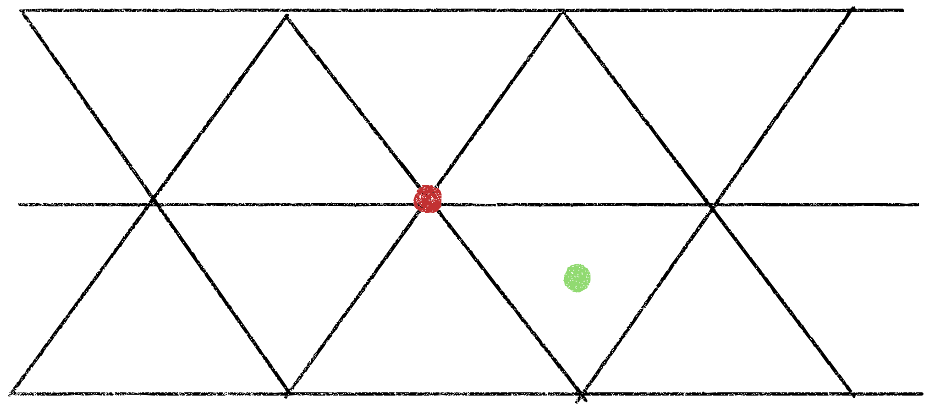
$$\sum_i \left[-a_i + \tfrac{1}{2}(n_i+m_i)\right]\vec{a}_i = \sum_i \left[b_i - \tfrac{1}{2}(n_i+m_i)\right]\vec{a}_i$$

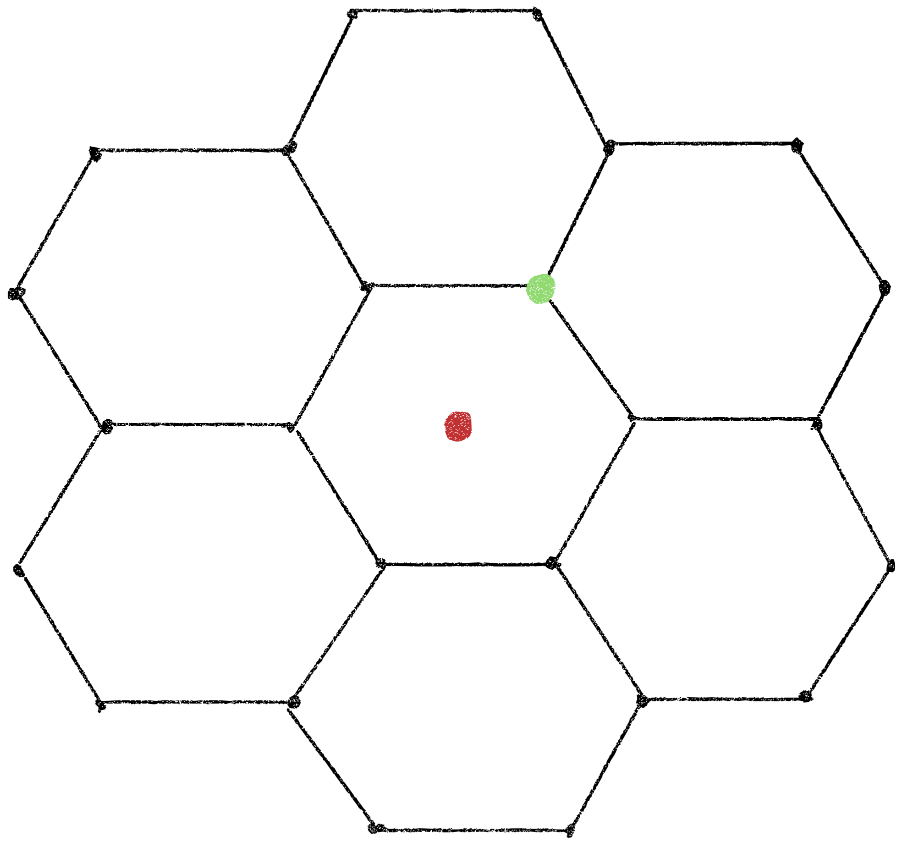
$$-a_i + \tfrac{1}{2}(n_i+m_i) = b_i - \tfrac{1}{2}(n_i+m_i)$$

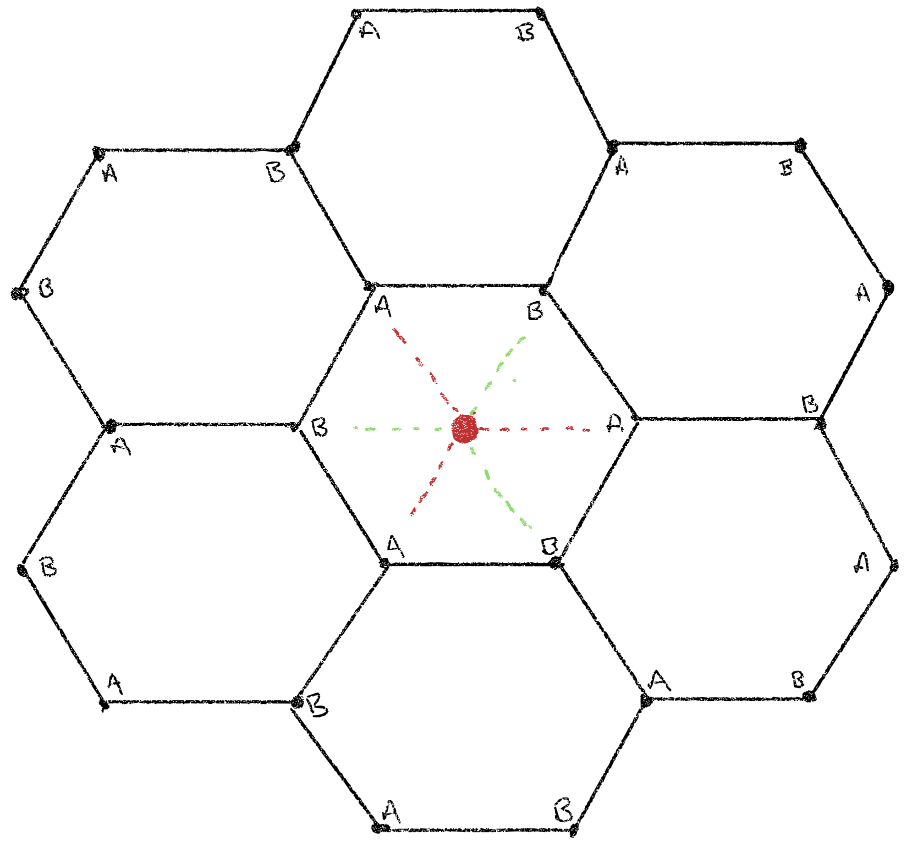
$b_i =$



and so on...






A
B
A
B
A
B
B
A
B
A
B
B
A
A
A
B
A
B
A
B
A
B
A
B
A
B

$$\frac{2\pi}{5}$$

$$\vec{R}_{\vec{n}} = n_1\vec{a}_1 + n_2\vec{a}_2$$

$$\hat{R}\left(\frac{2\pi}{5}\right)\vec{R}_{\vec{n}} = n_1\hat{R}\left(\frac{2\pi}{5}\right)\vec{a}_1 + n_2\hat{R}\left(\frac{2\pi}{5}\right)\vec{a}_2$$

$$\begin{pmatrix} \cos\frac{2\pi}{5} & -\sin\frac{2\pi}{5} \\ \sin\frac{2\pi}{5} & \cos\frac{2\pi}{5} \end{pmatrix}\begin{pmatrix} a_{1x} \\ a_{2x} \end{pmatrix}$$

$$\exists\ \vec{R}_{\vec{n}}, \vec{R}_{\vec{m}} \in \{\vec{R}_{\vec{n}}\} \text{ s.t.}$$

$$\hat{R}\left(\frac{2\pi}{5}\right)\vec{R}_{\vec{n}} = \vec{R}_{\vec{n}} + \vec{R}_{\vec{m}}$$

can't be integer

$$n_1\vec{a}_1' + n_2\vec{a}_2' = (n_1+m_1)\vec{a}_1 + (n_2+m_2)\vec{a}_2$$

$$n_1\begin{pmatrix} \cos & \sin \\ -\sin & \cos \end{pmatrix}\begin{pmatrix} a_{1x} \\ a_{1y} \end{pmatrix} + n_2\begin{pmatrix} \cos & \sin \\ -\sin & \cos \end{pmatrix}\begin{pmatrix} a_{2x} \\ a_{2y} \end{pmatrix}$$

$$n_1\hat{R}^{-1}\vec{a}_1 + n_2\hat{R}^{-1}\vec{a}_2 = (n_1+m_1)\vec{a}_1 + (n_2+m_2)\vec{a}_2$$

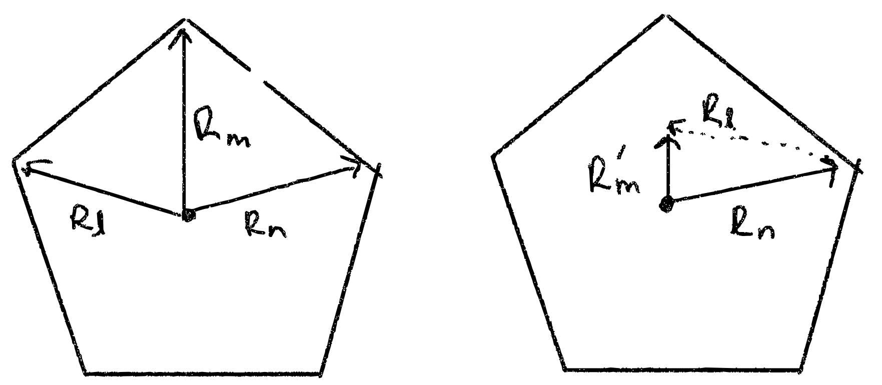
$$(n_1+m_1)\mathbb{1} = n_1\hat{R}^{-1}$$

$$\begin{pmatrix} n_1\cos - n_1 - m_1 & n_1\sin \\ -n_1\sin & n_1\cos - n_1 - m_1 \end{pmatrix} = 0$$

$$\left(\cos\frac{2\pi}{5} - 1 - \frac{m_1}{n_1}\right)^2 + \sin^2\frac{2\pi}{5} = 0$$

$$\cos^2 + \sin^2 + 1 + \frac{m_1^2}{n_1^2} - 2\cos - \frac{2n_1}{m_1}\cos + \frac{2n_1}{m_1} = 0$$

$$2\left(\cos - \frac{n_1}{m_1}\cos + \frac{n_1}{m_1}\right.$$



$$\sum_{\vec{q}} e^{i\vec{q}\cdot\vec{R}_n} = N, \quad N = \text{\# of reciprocal lattice vectors in } 1^{st} \text{ BZ}$$

$$\vec{q} = m_1\vec{g}_1 + m_2\vec{g}_2 + m_3\vec{g}_3$$

$$\vec{q}\cdot\vec{R}_n = 2\pi v, \quad v = n_1m_1 + n_2m_2$$

$$\sum_Q e^{iQR_n} \qquad R_n = na \quad 0 \le n \le N$$

$$Q = \frac{m}{N}\left(\frac{2\pi}{a}\right), \; m = 0, 1, 2, \ldots$$

$$-\frac{\pi}{a} \le q \le \frac{\pi}{a}$$

$$\sum_i \exp\left[\frac{m_i}{N}\left(\frac{2\pi}{a}\right)na\right] \quad \sum_i \exp\left[\frac{m_i}{N}(2\pi n)\right)$$

$$\vec{R}_n = n_1\vec{a}_1 \qquad n_1 a\hat{x}$$

$$\vec{G} = m_1\vec{b}_1, \quad b_i = \frac{2\pi}{a}\hat{x}$$

$$R_n = na\hat{x}$$

$$G = m\left(\frac{2\pi}{a}\right)$$

$$\sum_m \exp\left[m\left(\frac{2\pi}{a}\right)na\right] = \sum_m \exp\left[2\pi(mn)\right]$$

$$=$$

$$-\frac{\pi}{a} \le G \le \frac{\pi}{a}$$

$$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

$$G = m_1\vec{g}_1 + m_2\vec{g}_2 + m_3\vec{g}_3$$

$$\vec{g}_j = \frac{\vec{a}_j \times \vec{a}_k}{(\vec{a}_1\times\vec{a}_2)\cdot\vec{a}_3}$$

$$\vec{a}_n \cdot \vec{g}_m = 2\pi\delta_{nm}$$

$$\exp\left[\vec{G}\cdot\vec{R}_n\right] = \exp\left[2\pi\right]$$

$$\psi(\vec{r}+\vec{R}_n) = \psi(\vec{r})$$

$$e^{i\vec{k}\cdot\vec{R}_n}\psi(\vec{r}) = \psi(\vec{r})$$

$$e^{i\vec{k}\cdot\vec{R}_n} = 1$$

$$\sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}_n} =$$

$$k = \frac{m}{N}\left(\frac{2\pi}{a}\right), \quad R_n = na, 0 \le n \le N$$

$$e^{i\vec{q}\cdot\vec{R}_N} = 1$$

$$q_i N_i a_i = 2\pi m_i$$

$$\to q_i = \frac{m_i}{N_i}\left(\frac{2\pi}{a_i}\right)$$

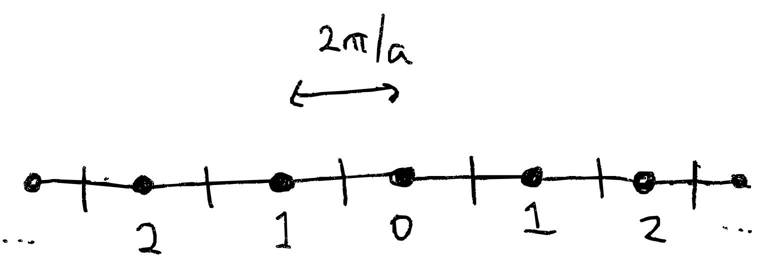
$$\sum_{n=-\infty}^{\infty} f(na) = \frac{1}{a}\sum_{l=-\infty}^{\infty}\tilde{f}(lG)$$

$$\sum_n f(x+na) = \sum_l g_l e^{ilGx}$$

$$= \sum_n f(y) = \sum_l g_l e^{ilGy}$$

$$\sum_n \int_{-\infty}^{\infty} dy\, f(y)e^{-ilGy} = \sum_l \int_{-\infty}^{\infty} dy\, g_l e^{ilGy}$$

$$\sum_n \tilde{f}(lG) =$$



$$G_m = m\left(\frac{2\pi}{a}\right)$$

$$\to e^{iG_m R_n} = e^{i2\pi nm}$$

$$\vec{g}_i = 2\pi \frac{\vec{a}_j \times \vec{a}_k}{\Omega_p}$$

$\leftarrow = 0$ unless $l = i$

$$\vec{a}_l \cdot \vec{g}_i = 2\pi \frac{\vec{a}_l \cdot (\vec{a}_j \times \vec{a}_k)}{|\vec{a}_i \cdot (\vec{a}_j \times \vec{a}_k)|}$$

$l = i, j, k$

$$= 2\pi \frac{\Omega_p}{\Omega_p} \delta_{l,i} = 2\pi \delta_{l,i}$$

$$\to \vec{G}_m \cdot \vec{R}_n = \sum_{i=1}^{3} m_i n_i \, \vec{g}_i \cdot \vec{a}_i = 2\pi \sum_{i=1}^{3} m_i n_i \quad \square$$

- reciprocal of FCC $\to$ BCC

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

$$\Omega_p = |(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3| = a^3/4$$

$$\frac{a^2}{4}\begin{vmatrix} i & j & k \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \frac{a^2}{4}\left[\hat{x} + \hat{y} - \hat{z}\right] \cdot \vec{a}_3$$

$$= \frac{a^3}{8}(2) = \frac{a^3}{4}$$

$$\vec{g}_1 = 2\pi \cdot \frac{4}{a^3}(\vec{a}_2 \times \vec{a}_3)$$

$$\frac{a^2}{4}\begin{vmatrix} i & j & k \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = \frac{a^2}{4}\left[-\hat{x} + \hat{y} + \hat{z}\right]$$

$$\vec{g}_1 = 2\pi \frac{4}{a^3} \cdot \frac{a^2}{4}$$

$$= \frac{2\pi}{a}(-\hat{x} + \hat{y} + \hat{z})$$

$$\vec{g}_2 = 2\pi \cdot \frac{4}{a^3}(\vec{a}_3 \times \vec{a}_1) \quad \frac{a}{4}\begin{vmatrix} i & j & k \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{vmatrix} = \frac{a^2}{4}\left[\hat{x} - \hat{y} + \hat{z}\right]$$

$$\vec{g}_2 = \frac{2\pi}{a}(\hat{x} - \hat{y} + \hat{z})$$

$$\vec{g}_3 = \frac{2\pi}{a}(\hat{x} + \hat{y} - \hat{z})$$

$\to$ the vector portions are the same as BCC

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

$$\Omega_p = |(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3| \quad \frac{a^2}{4}\begin{vmatrix} i & j & k \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{a^2}{4}(2\hat{x} + 2\hat{y})$$

$$= \frac{a^2}{2}(\hat{x} + \hat{y})$$

$$\frac{a^2}{2}(\hat{x} + \hat{y}) \cdot \frac{a}{2}(\hat{x} + y - \hat{z}) = \frac{a^3}{4}(2) = \frac{a^3}{2}$$

$$\vec{g}_1 = 2\pi \cdot \frac{2}{a^3}(a_2 \times a_3) = \frac{2\pi}{a} \cdot \frac{2}{a^2} \cdot \frac{a^2}{4}\begin{vmatrix} i & j & k \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix}$$

$$= \frac{2\pi}{a} \frac{1}{2}(2\hat{y} + 2\hat{z})$$

$$\vec{g}_1 = \frac{2\pi}{a}(\hat{y} + \hat{z})$$

$$\vec{g}_2 = \frac{2\pi}{a}(\hat{z} + \hat{x}) \quad \to \quad \underline{\underline{\text{FCC}}}$$

$$\vec{g}_3 = \frac{2\pi}{a}(x + \hat{y})$$

$$\vec{g}_i = 2\pi \frac{(\vec{a}_j \times \vec{a}_k)}{\Omega_p} \to \vec{G}_i = 2\pi m_i \frac{(\vec{a}_j \times \vec{a}_k)}{\Omega_p}$$

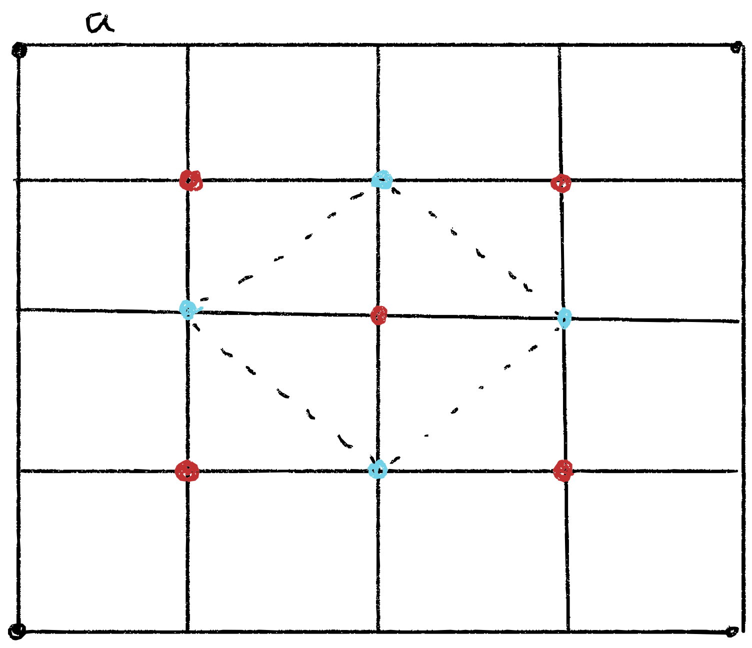
$$\to (\vec{R}_n)'_i = 2\pi \frac{(\vec{G}_j \times \vec{G}_k)}{\Omega_{BZ}} \varepsilon^{ijk}$$

$$(\vec{R}_n')_i = \frac{1}{(2\pi)^2}(2\pi)^2 m_i m_j \frac{\left[(a_k \times a_i) \times (a_i \times a_j)\right]}{\Omega_p}$$

$$= -m_i m_j \varepsilon^{ijk}\left[(a_i \times a_k) \times (a_i \times a_j)\right] / \Omega_p$$

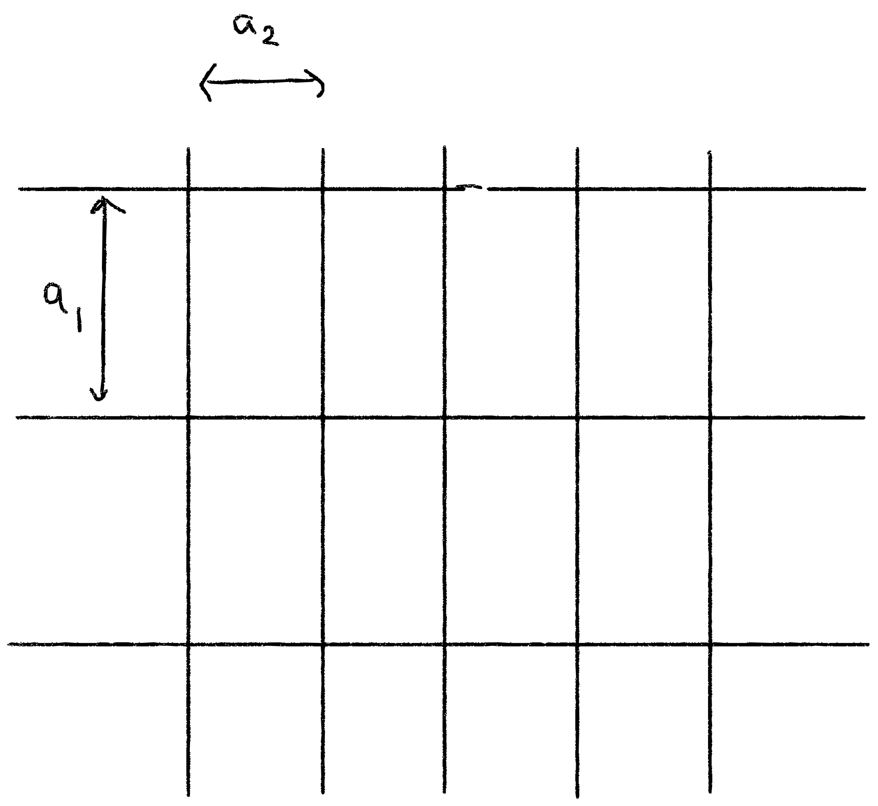
$$= m_i m_j \varepsilon^{ijk}\left[(a_i \cdot (a_j \times a_k))\vec{a}_i\right]$$

$$= m_i \vec{a}_i$$



ferro $\quad A_0 = a^2 \quad A_{BZ} = \frac{(2\pi)^2}{A_0} = \left(\frac{2\pi}{a}\right)^2$

anti-ferro $\quad A_0 = (a\sqrt{2})^2$
$= 2a^2 \quad A_{BZ} = \frac{(2\pi)^2}{A_0} = \frac{4\pi^2}{2a^2} = \frac{1}{2}\left(\frac{2\pi}{a}\right)^2$



Real Space