Oct 7, 2015

39/40

5.1 $\vec{b}_1 = 2\pi \dfrac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$ $\quad \vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$

(a)

show $\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \dfrac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$

$$\vec{A} \cdot (\vec{B} \times \vec{C}) = \vec{B} \cdot (\vec{C} \times \vec{A}) = \vec{C} \cdot (\vec{A} \times \vec{B}) \ \& \ \vec{A} \times (\vec{B} \times \vec{C}) = (\vec{A} \cdot \vec{C})\vec{B} - (\vec{A} \cdot \vec{B})\vec{C}$$

$$\vec{b}_2 \times \vec{b}_3 \propto \underbrace{(\vec{a}_3 \times \vec{a}_1)}_{A} \times (\underset{B}{\vec{a}_1} \times \underset{C}{\vec{a}_2}) = [(\vec{a}_3 \times \vec{a}_1) \cdot \vec{a}_2]\vec{a}_1 - [(\vec{a}_3 \times \vec{a}_1) \cdot \vec{a}_1]\vec{a}_2$$

$$\hookrightarrow \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) \overset{\text{ortho}}{=} \left(\frac{2\pi}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \right)^2 [(\vec{a}_3 \times \vec{a}_1) \cdot \vec{a}_2] \cdot 2\pi \overset{\text{cyclic}}{=} (2\pi)^3 \frac{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}{[\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)]^2}$$

$$\Rightarrow \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \frac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \quad \checkmark$$

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

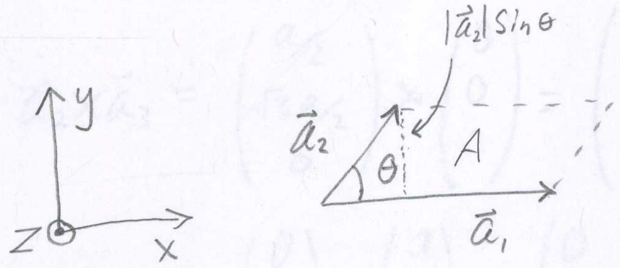
$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \Rightarrow \vec{b}_2 \times \vec{b}_3 \propto \vec{b}_2 \times (\vec{a}_1 \times \vec{a}_2) = \underbrace{(\vec{b}_2 \cdot \vec{a}_2)}_{=2\pi}\vec{a}_1 - \underbrace{(\vec{b}_2 \cdot \vec{a}_1)}_{=0}a_2$$

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

$\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \dfrac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$ from above

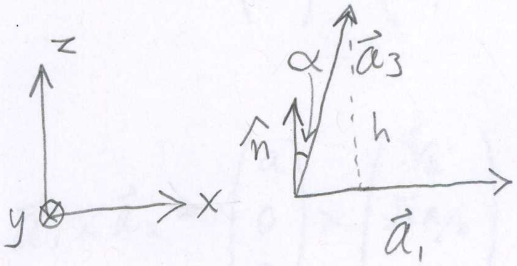
$$\hookrightarrow 2\pi \frac{\vec{b}_2 \times \vec{b}_3}{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)} = 2\pi \vec{a}_1 \frac{(2\pi)^2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \cdot \frac{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}{(2\pi)^3} = \vec{a}_1 \quad \checkmark$$

5.1 c) a general bravias cell is a 3-D parallelepiped.



A = area of base

$A = |\vec{a}_1|\cdot|\vec{a}_2|\sin\theta = |\vec{a}_1 \times \vec{a}_2|$



$\bar{V}$ = volume = $A\cdot h$

$h = |\vec{a}_3|\cos\alpha$

$\hat{n}$ normal to plane containing $\vec{a}_1, \vec{a}_2$

$\Rightarrow \hat{n} = \dfrac{\vec{a}_1\times\vec{a}_2}{|\vec{a}_1\times\vec{a}_2|}$

$\vec{a}_3\cdot\hat{n} = |\vec{a}_3||\hat{n}|\cos\alpha = |\vec{a}_3|\cos\alpha = h$

$\hookrightarrow \bar{V} = \left(|\vec{a}_1\times\vec{a}_2|\right)\cdot\left(\vec{a}_3\cdot\left[\dfrac{\vec{a}_1\times\vec{a}_2}{|\vec{a}_1\times\vec{a}_2|}\right]\right) = \vec{a}_3\cdot(\vec{a}_1\times\vec{a}_2) = \vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)$

$\square$

/2

5.2 a)

$\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = \frac{a}{2}\hat{x} + \frac{\sqrt{3}}{2}\hat{y}$, $\vec{a}_3 = c\hat{z}$

$\Rightarrow \vec{a}_1 \times \vec{a}_2 = (0, 0, \sqrt{3}a^2/2)$, $\vec{a}_2 \times \vec{a}_3 = (\frac{\sqrt{3}ac}{2}, \frac{-ac}{2}, 0)$

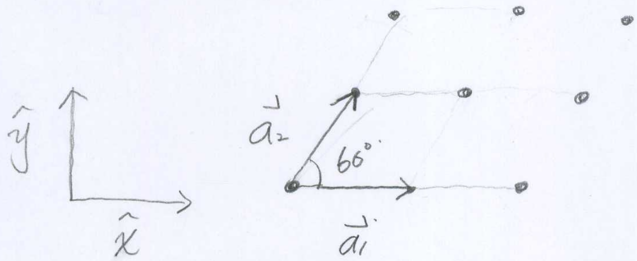
$\vec{a}_3 \times \vec{a}_1 = (0, ac, 0)$ & $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = \frac{\sqrt{3}}{2}a^2c$

$$\Rightarrow \vec{b}_1 = 2\pi \frac{(\frac{\sqrt{3}ac}{2}, \frac{-ac}{2}, 0)}{\sqrt{3}/2\, a^2c} = \frac{2\pi}{a}(\hat{x} - \frac{1}{\sqrt{3}}\hat{y}) \Rightarrow |\vec{b}_1| = \frac{4\pi}{a\sqrt{3}}$$

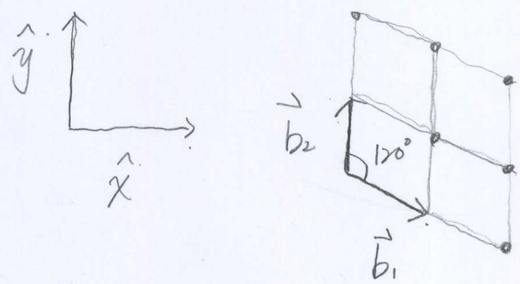
$$\vec{b}_2 = 2\pi \frac{(0, ac, 0)}{\sqrt{3}/2\, a^2c} = \frac{2\pi}{a}(\frac{2}{\sqrt{3}}\hat{y}), \quad |\vec{b}_2| = \frac{4\pi}{a\sqrt{3}}$$

$$\vec{b}_3 = 2\pi \frac{(0, 0, \frac{\sqrt{3}}{2}a^2)}{\sqrt{3}/2\, a^2c} = \frac{2\pi}{c}\hat{z}, \quad |\vec{b}_3| = \frac{2\pi}{c}$$

For Bravais lattice (2D)



For reciprocal lattice (2D)

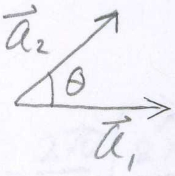


By comparing these two lattice: we find the reciprocal lattice has the same with Bravais lattice with a 30° rotation ※

5.2 b)

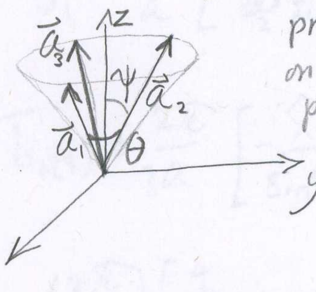
$$\frac{c}{a} = \frac{c'}{a'} = \frac{\left(\frac{2\pi}{c}\right)}{\left(\frac{4\pi}{\sqrt{3}a}\right)} = \frac{\sqrt{3}a}{2c} \quad \text{ie } c^2 = \frac{\sqrt{3}}{2}a^2, \text{ or } \frac{c}{a} = \frac{\sqrt[4]{3}}{\sqrt{2}}$$

$$\frac{c}{a} = \sqrt{\frac{8}{3}} \Rightarrow \frac{c'}{a'} = \frac{2\pi}{\sqrt{8}} \cdot \frac{\sqrt{3}\sqrt{3}}{4\pi} = \frac{1}{2} \cdot \frac{3}{2\sqrt{2}} = \frac{3\sqrt{2}}{8}$$

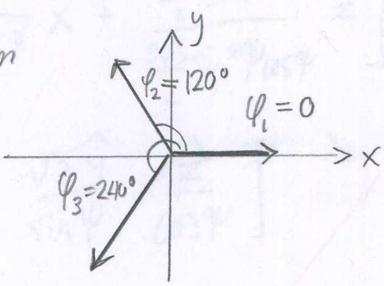


c) $\vec{a}_i \cdot \vec{a}_j = a^2 \cos\theta \;(i \neq j)$

$|\vec{a}_i \times \vec{a}_j| = a^2 \sin\theta \;(i \neq j)$



projection on x-y plane:



In spherical coordinates, the $\vec{a}_i$s have common length a, common polar angle ψ, & azumuthal angles above.

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r\sin\psi\cos\varphi \\ r\sin\psi\sin\varphi \\ r\cos\psi \end{pmatrix} \Rightarrow \vec{a}_1 = \begin{pmatrix} a\sin\psi \\ 0 \\ a\cos\psi \end{pmatrix}, \quad \vec{a}_{2(3)} = \begin{pmatrix} -\frac{1}{2}a\sin\psi \\ (-)\frac{\sqrt{3}}{2}a\sin\psi \\ a\cos\psi \end{pmatrix}$$

$$\vec{a}_1 \cdot \vec{a}_2 = a^2\left(-\frac{1}{2}\sin^2\psi + \cos^2\psi\right) = a^2\cos\theta$$

$$\Rightarrow \cos\theta = \cos^2\psi - \frac{1}{2}\sin^2\psi$$ $\longrightarrow$ this defines the polar angle

/4

5.2 b) continued

$$\vec{a}_2 \times \vec{a}_3 = \begin{pmatrix} a^2\sqrt{3}\sin\psi\cos\psi \\ 0 \\ a^2\frac{\sqrt{3}}{2}\sin^2\psi \end{pmatrix}, \quad \vec{a}_3\times\vec{a}_1 \; (\vec{a}_1\times\vec{a}_2) = \begin{pmatrix} -a^2\frac{\sqrt{3}}{2}\sin\psi\cos\psi \\ (-)a^2\frac{3}{2}\sin\psi\cos\psi \\ a^2\frac{\sqrt{3}}{2}\sin^2\psi \end{pmatrix}$$

$$\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3) = a\sin\psi(\sqrt{3}a^2\sin\psi\cos\psi) + a\cos\psi\left(\frac{\sqrt{3}}{2}a^2\sin^2\psi\right)$$
$$= \frac{3\sqrt{3}}{2}a^3\sin^2\psi\cos\psi$$

$$\Rightarrow \vec{b}_1 = \frac{2\pi}{a}\left[\frac{\sqrt{3}\sin\psi\cos\psi}{\frac{3\sqrt{3}}{2}\sin^2\psi\cos\psi}\hat{x} + \frac{\frac{\sqrt{3}}{2}\sin^2\psi}{\frac{3\sqrt{3}}{2}\sin^2\psi\cos\psi}\hat{z}\right] = \frac{2\pi}{3a}\left[\frac{2\hat{x}}{\sin\psi} + \frac{\hat{z}}{\cos\psi}\right]$$

$$\& \; \vec{b}_{2(3)} = \frac{2\pi}{3a}\left[-\frac{\hat{x}}{\sin\psi} \overset{+}{(-)} \frac{\sqrt{3}\hat{y}}{\sin\psi} + \frac{\hat{z}}{\cos\psi}\right]$$

$$|\vec{b}_i| = \left(\frac{2\pi}{3a}\right)\left[\frac{4}{\sin^2\psi} + \frac{1}{\cos^2\psi}\right]^{\frac{1}{2}}$$

$$\vec{b}_1\cdot\vec{b}_2 = \left(\frac{2\pi}{3a}\right)^2\left[\frac{4}{\sin^2\psi} + \frac{1}{\cos^2\psi}\right]\cos\theta^* = \left(\frac{2\pi}{3a}\right)^2\left[-\frac{2}{\sin^2\psi} + \frac{1}{\cos^2\psi}\right]$$

$$\hookrightarrow \cos\theta^* = \left[-\frac{2}{\sin^2\psi} + \frac{1}{\cos^2\psi}\right]\cdot\left[\frac{4}{\sin^2\psi} + \frac{1}{\cos^2\psi}\right]^{-1} = \left[\frac{-2\cos^2\psi + \sin^2\psi}{\sin^2\psi\cos^2\psi} \cdot \frac{\sin^2\psi\cos^2\psi}{4\cos^2\psi + \sin^2\psi}\right]$$

$$= -\frac{2(\cos^2\psi - \frac{1}{2}\sin^2\psi)}{2(2\cos^2\psi + \frac{1}{2}\sin^2\psi)} = -\frac{\cos\theta}{\left[\underbrace{(\cos^2\psi - \frac{1}{2}\sin^2\psi)}_{\cos\theta} + \underbrace{(\cos^2\psi + \sin^2\psi)}_{1}\right]}$$

$$\Rightarrow \boxed{\cos\theta^* = -\frac{\cos\theta}{1+\cos\theta}} \checkmark$$

5

$$|\vec{b}_i| = \frac{2\pi}{a}\left[\frac{4}{9\sin^2\psi} + \frac{1}{9\cos^2\psi}\right]^{\frac{1}{2}} = \frac{2\pi}{a}\left[\frac{9\sin^2\psi\cos^2\psi}{4\cos^2\psi+\sin^2\psi}\right]^{-\frac{1}{2}}$$

$$a^{*} = \frac{2\pi}{a}\left[1+2\cos\theta\cos\theta^{*}\right]^{-\frac{1}{2}} = \frac{2\pi}{a}\left[1+2\left(\cos^2\psi-\tfrac{1}{2}\sin^2\psi\right)\left(\frac{\sin^2\psi-2\cos^2\psi}{4\cos^2\psi+\sin^2\psi}\right)\right]^{-\frac{1}{2}}$$

$$= \frac{2\pi}{a}\left(\frac{1}{4\cos^2\psi+\sin^2\psi}\right)^{-\frac{1}{2}}\left[4\cos^2\psi+\sin^2\psi+2\left(\sin^2\psi\cos^2\psi-2\cos^4\psi - \tfrac{1}{2}\sin^4\psi+\sin^2\psi\cos^2\psi\right)\right]^{-\frac{1}{2}}$$

$$= \frac{2\pi}{a}\left(\frac{1}{4\cos^2\psi+\sin^2\psi}\right)^{-\frac{1}{2}}\left[4\cos^2\psi\left(1-\cos^2\psi\right)+\sin^2\psi\left(1-\sin^2\psi\right)+4\sin^2\psi\cos^2\psi\right]^{-\frac{1}{2}}$$

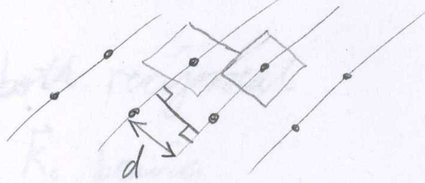
$$= \;'' \;\left[4\cos^2\psi\sin^2\psi+\sin^2\psi\cos^2\psi+4\sin^2\psi\cos^2\psi\right]^{-\frac{1}{2}}$$

$$= \frac{2\pi}{a}\left(\frac{9\cos^2\psi\sin^2\psi}{4\cos^2\psi+\sin^2\psi}\right)^{-\frac{1}{2}} = |\vec{b}_i|$$

$$\Rightarrow |\vec{b}_i| = a^{*} = \frac{2\pi}{a}\left[1+2\cos\theta\cos\theta^{*}\right]^{-\frac{1}{2}}$$

/6

3 a) Density of lattice points: $\rho_A = \frac{N/s}{A}$



N = total # of points in volume

s = # of planes in volume

A = Area of plane

$N = \frac{V}{v}$, V = total volume, v = primitive cell volume

$V = A \cdot d \cdot s \Rightarrow \rho_A = \frac{A \cdot d \cdot s}{v \cdot s} \cdot \frac{1}{A} = \frac{d}{v}$ ✓

b) $d = \frac{2\pi}{K} \Rightarrow$ smallest $|\vec{K}|$ gives largest d, giving largest density for a given v.

FCC: $\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z}-\hat{x})$, $\vec{b}_2 = \frac{2\pi}{a}(\hat{z}+\hat{x}-\hat{y})$, $\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$ (5.12)

$|\vec{K}| = |h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3| \geq \left(\frac{2\pi}{a}\right)\sqrt{3} = |\vec{b}_i|$

$h=k=l=1$: $\vec{K} = \frac{2\pi}{a}(\hat{x}+\hat{y}+\hat{z})$, $|\vec{K}| = \left(\frac{2\pi}{a}\right)\sqrt{3}$ = min length

$(1,1,1) \in \{111\}$ ✓

BCC: $\vec{b}_1 = \frac{2\pi}{a}(\hat{y}+\hat{z})$, $\vec{b}_2 = \frac{2\pi}{a}(\hat{z}+\hat{x})$, $\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y})$ (4.5)

$|K| \geq \left(\frac{2\pi}{a}\right)\sqrt{2}$

$h=1, k=-1, l=0$: $\vec{K} = \frac{2\pi}{a}(\hat{y}-\hat{x})$, $|\vec{K}| = \frac{2\pi}{a}\sqrt{2}$ = min length

$(1\bar{1}0) \in \{110\}$ ✓

7

5.4

Let $\vec{K_0} = h\vec{b_1} + k\vec{b_2} + l\vec{b_3}$ & $\vec{K} = H\vec{b_1} + K\vec{b_2} + L\vec{b_3}$ & $\vec{K_0} \neq \vec{K}$

$\boxed{\text{Assume: } \vec{K_0} \text{ is the only shortest vector on a specified direction}}$

1. then, h, k, l has no common factor.

2. Also if $\vec{K} \parallel \vec{K_0}$, then $\vec{K} = H\vec{b_1} + K\vec{b_2} + L\vec{b_3} = A(h\vec{b_1} + k\vec{b_2} + l\vec{b_3})$.

3. In this case, if $\vec{A}$ is not a integer, it means. H, K, L have no common factor, which indicates $\vec{K}$ is also the shortest vector in direction of $\frac{\vec{K}}{|\vec{k}|}$. This is contradict to assumption.

$\boxed{\text{Hence A must be a integer ※}}$