731 Homework #5

Due October 9th , 2006

1. A&M, problem 5.1 a + b + c = 15 pts
2. A&M, problem 5.2 a + b + c = 15 pts
3. A&M, problem 5.3 a + b = 10 pts
4. A&M, problem 5.4 10 pts

50 pts

HW # 5 solutions :

$\boxed{5.1}$.

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

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

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

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

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

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

$$= \frac{(4\pi)^2}{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)} \frac{[((\vec{b}_2 \cdot \vec{a}_2)\vec{a}_1 - \cancel{(\vec{b}_2 \vec{a}_1)} \vec{a}_2)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$; From (a) →

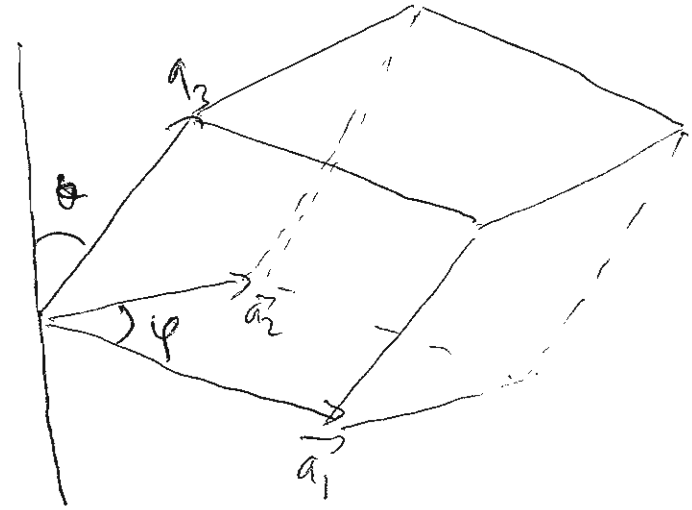
$$\vec{b}_1 (\vec{b}_2 \times \vec{b}_3)(\vec{a}_1 (\vec{a}_2 \times \vec{a}_3) = (2\pi)^3$$

$$2\pi \frac{\vec{b}_2 \times \vec{b}_3}{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)} = \frac{1}{2\pi} \vec{b}_2 \times \vec{a}_1 \times \vec{a}_2$$

$$\Rightarrow 2\pi \frac{\vec{b}_2 \times \vec{b}_3}{\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)} = \frac{1}{2\pi} \left(\vec{a}_1 (\vec{b}_2 \vec{a}_2 - \vec{a}_2 (\vec{b}_2 \cdot \vec{a}_1) \right)$$

$$= \frac{8\pi^3 \quad \vec{a}_1}{b_1(\vec{b}_2 \times \vec{b}_3)(\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3))} = \vec{a}_1.$$

c)



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

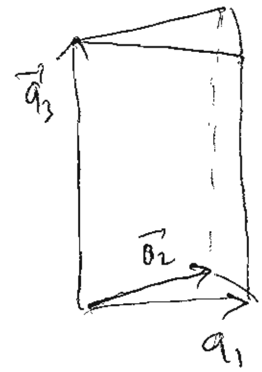
$$h = |\vec{a}_3| \cos\theta.$$

$$\text{Volume} = A.h = |\vec{a}_1 \times \vec{a}_2|\,|\vec{a}_3| \cos\theta$$

$$= |(\vec{a}_1 \times \vec{a}_2).\vec{a}_3| = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3|$$

$\boxed{5.2}$ (5)

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



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

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_2}{\vec{a}_1 (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{\frac{\sqrt{3}}{2}a}\hat{y}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{c}\hat{z}$$

$$\Rightarrow a' = \frac{4\pi}{\sqrt{3}a} \; ; \quad c' = \frac{2\pi}{c} \Rightarrow \text{rotate } 30^\circ.$$

b) $+ \; \frac{c'}{a'} = \frac{c}{a} \Rightarrow \frac{2\pi/c}{4\pi/\sqrt{3}a} = \frac{\sqrt{3}}{2}\frac{a}{c} = \frac{c}{a}$.

$$\frac{c}{a} = \sqrt{\frac{\sqrt{3}}{2}}$$

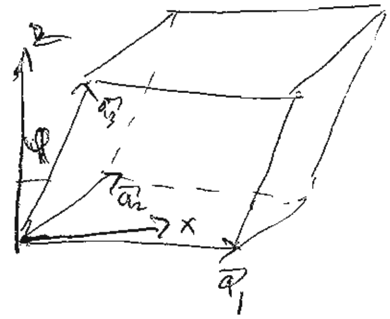
$$+ \; \frac{c}{a} = \sqrt{\frac{8}{3}} \Rightarrow \frac{c'}{a'} = \frac{\sqrt{3}}{2}\sqrt{3/8} = \frac{\sqrt{9}}{2\sqrt{8}}$$

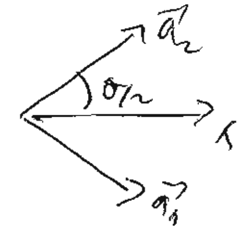
c)

$$\vec{a}_1' = a\cos\tfrac{\theta}{2}\,\hat{x} - a\sin\tfrac{\theta}{2}\,\hat{y}$$

$$\vec{a}_2' = a\cos\tfrac{\theta}{2}\,\hat{x} + a\sin\tfrac{\theta}{2}\,\hat{y}$$

$$\vec{a}_3' = a\cos\varphi\,\hat{x} + a\sin\varphi\,\hat{z}.$$





$$\vec{a}_2'\cdot\vec{a}_3' = a^2\cos\tfrac{\theta}{2}\cos\varphi = a^2\cos\theta \Rightarrow \cos\varphi = \frac{\cos\theta}{\cos\theta/2}$$

$$\sin\varphi = \sqrt{1 - \frac{\cos^2\theta}{\cos^2\theta/2}}$$

$$\Rightarrow \vec{a}_1'\cdot(\vec{a}_2'\times\vec{a}_3') = a^3\sin\theta\sin\varphi$$

$$\Rightarrow \vec{b}_1' = 2\pi\frac{\vec{a}_2'\times\vec{a}_3'}{\vec{a}_1'\cdot(\vec{a}_2'\times\vec{a}_3')} = \left(\frac{2\pi}{a}\right)\left(\frac{\hat{x}}{2\cos\theta/2} - \frac{\hat{y}}{2\sin\theta/2} - \frac{\hat{z}}{2\cos\frac{\theta}{2}}\cot\varphi\right)$$

$$\vec{b}_2 = 2\pi\frac{\vec{a}_3'\times\vec{a}_1'}{\vec{a}_1'\cdot(\vec{a}_2'\times\vec{a}_3')} = \left(\frac{2\pi}{a}\right)\left(\frac{\hat{x}}{2\cos\theta/2} + \frac{\hat{y}}{2\sin\theta/2} - \frac{\hat{z}}{2\cos\theta/2}\cot\varphi\right)$$

$$\vec{b}_3' = 2\pi\frac{\vec{a}_1'\times\vec{a}_2'}{\vec{a}_1'\cdot(\vec{a}_2'\times\vec{a}_3')} = \left(\frac{2\pi}{a}\right)\left(\frac{\hat{z}}{\sin\varphi}\right)$$

$$\left\{\begin{array}{l}|a_1| = |a_2| = |a_3| \\ \text{Same angle}\end{array}\right. \Rightarrow |\vec{a}_1'\times\vec{a}_2'| = |\vec{a}_2'\times\vec{a}_3'| = |\vec{a}_3'\times\vec{a}_1'|$$

$$\Rightarrow |\vec{b}_1'| = |\vec{b}_2'| = |\vec{b}_3'| = \frac{2\pi}{a}\cdot\frac{1}{\sin\varphi} = \frac{2\pi}{a}\frac{1}{\sqrt{1-\frac{\cos^2\theta}{\cos^2\theta/2}}}$$

⑤

$$(\vec{b_1}\cdot\vec{b_2}) = \frac{(2\pi)^2}{|\vec{a_1}\cdot(\vec{a_2}\times\vec{a_3})|^2}(\vec{a_2}\times\vec{a_3})(\vec{a_3}\times\vec{a_1})$$

$$= \frac{(2\pi)^2}{|\vec{a_1}\cdot(\vec{a_2}\times\vec{a_3})|^2}\left(\vec{a_3}\cdot(\vec{a_1}\times(\vec{a_2}\times\vec{a_3}))\right)$$

$$= \frac{(2\pi)^2}{|\vec{a_1}\cdot(\vec{a_2}\times\vec{a_3})|^2}\left[(\vec{a_3}\vec{a_2})(a_1\cdot\vec{a_3}) - |\vec{a_3}|^2(\vec{a_1}\cdot\vec{a_2})\right]$$

From

$$\vec{a_1}\vec{a_2} = \vec{a_2}\cdot\vec{a_3} = \vec{a_3}\,\vec{a_1} \Rightarrow \vec{b_2}\cdot\vec{b_3} = \vec{b_3}\cdot\vec{b_1}$$

$\Rightarrow$ $\vec{b_1}, \vec{b_2}, \vec{b_3}$ have same angle between.

$\Rightarrow$ reciprocal lattice is also trigonal.

$$\cos\theta^* = \frac{\vec{b_2}\cdot\vec{b_3}}{|\vec{b_2}||\vec{b_3}|} = \frac{\left(\frac{2\pi}{a}\right)^2\left(-\frac{1}{\cos\theta/2}\frac{\cot\varphi}{\sin\varphi}\right)}{\left(\frac{2\pi}{a}\right)^2\frac{1}{\sin^2\varphi}} = -\frac{\cos\theta}{2\cos\frac{\theta}{2}}$$

$$= -\frac{\cos\theta}{2\cos^2\theta/2} = -\frac{\cos\theta}{1+\cos\theta}.$$

$$a^* = |\vec{b_3}| = \frac{2\pi}{a}\frac{1}{\sqrt{1-\frac{\cos^2\theta}{\cos^2\theta/2}}} = \frac{2\pi}{a}\frac{1}{\sqrt{1+2\cos\theta\cos\theta^*}}$$

5.3

a) V is volume of a primitive cell containing only 1 lattice point. $\rightarrow$ $\frac{V}{d}$ is area of a primitive cell, containing only 1 lattice point in a plane

$\frac{d}{V}$ is density of lattice points

b) V is given. greatest density depend on d

in FCC $\Rightarrow$ $d = |\vec{K}_\perp|$.

greatest d : $\vec{K}_\perp = \vec{b}_1 + \vec{b}_2 + \vec{b}_3$

$\{1,1,1\}$ plane

BCC : $\{1\,1\,0\}$

5.4 assume $\vec{k} = p/q\ \vec{k_0}$, $\frac{p}{q}$ is not integer

$$\vec{K} = \Big(\overset{\text{integer}}{n} + \frac{r}{q}\Big)\vec{k_0} \qquad 0<r<q$$

$(\vec{k} - n\vec{k_0}) = \frac{r}{q}\vec{k_0} \Rightarrow \frac{r}{q}\vec{k_0}$ is also a lattice vector

$\left|\frac{r}{q}\vec{k_0}\right| < |\vec{k_0}|$

$\Leftrightarrow$ Contradicts. $\vec{k_0}$ is shortest lattice vector

$\Rightarrow$ p/q must be integer