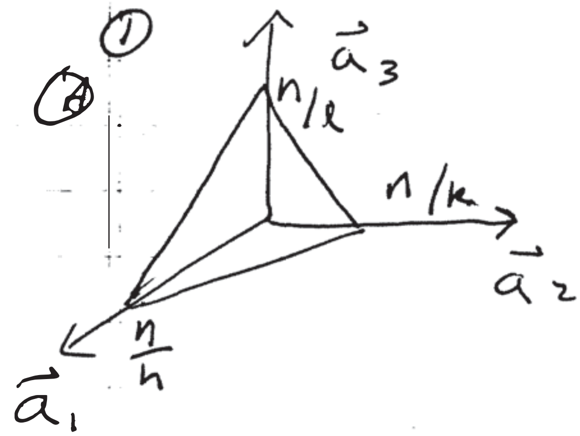
HW 3 Solutions: Chapter 2:

1

(a)



IN GENERAL, THE PLANE HAS INTERCEPTS

$$\frac{n}{h}, \quad \frac{n}{k}, \quad \frac{n}{\ell}.$$

WITH THE $\vec{a}_1$, $\vec{a}_2$ & $\vec{a}_3$. AXES, WHERE n IS AN INTEGER

TWO VECTORS WHICH LIE IN THE PLANE ARE

$$\vec{V}_1 = \frac{n}{h}\vec{a}_1 - \frac{n}{k}\vec{a}_2$$

AND

$$\vec{V}_2 = \frac{n}{h}\vec{a}_1 - \frac{n}{\ell}\vec{a}_3$$

SINCE $\vec{V}_1 \cdot \vec{G} = 0$ AND

$$\vec{V}_2 \cdot \vec{G} = 0$$

WHERE

$$\vec{G} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3$$

(RECALL $\vec{a}_i \cdot \vec{b}_j = 2\pi\,\delta_{ij}$)

IT FOLLOWS $\boxed{\vec{G} \text{ IS } \perp \text{ TO THE PLANE}}$

(B) IF $\hat{n}$ IS THE UNIT NORMAL TO THE PLANE, THEN THE DISTANCE BETWEEN THE PLANES IS:

$$\hat{n} \cdot \frac{\vec{a}_1}{h} = \hat{n} \cdot \frac{\vec{a}_2}{k} = \hat{n} \cdot \frac{\vec{a}_3}{\ell}$$

(PROVIDED h, k OR $\ell \neq 0$. IF $h = 0$, TAKE THE $\vec{a}_2$ COMPONENT ETC.)

NOW $\hat{n} = \dfrac{\vec{G}}{|\vec{G}|}$ SO

$$\boxed{d(hk\ell) = \frac{2\pi}{|\vec{G}|}}$$

USING $\vec{a}_i \cdot \vec{b}_j = 2\pi\,\delta_{ij}$

(NOTE: $|\vec{G}|$ MAY NOT EQUAL $\sqrt{h^2 + k^2 + \ell^2}$ SINCE $\vec{b}_1, \vec{b}_2, \vec{b}_3$ MAY NOT FORM AN ORTHONORMAL SYSTEM).

(C) FOR A CUBIC SYSTEM

$\vec{a}_1 = a\hat{x}$ $\qquad \vec{b}_1 = \frac{2\pi}{a}\hat{x}$

$\vec{a}_2 = a\hat{y}$ $\qquad \vec{b}_2 = \frac{2\pi}{a}\hat{y}$

$\vec{a}_3 = a\hat{z}$ $\qquad \vec{b}_3 = \frac{2\pi}{a}\hat{z}$

SO THAT

$$\boxed{d(hk\ell) = \frac{a}{\sqrt{h^2+k^2+\ell^2}}}$$

(2)

(A) $\vec{a}_1 = \sqrt{3}\,\frac{a}{2}\,\hat{x} + \frac{a}{2}\,\hat{y}$

$\vec{a}_2 = -\frac{\sqrt{3}}{2}\,a\,\hat{x} + \frac{a}{2}\,\hat{y}$

$\vec{a}_3 = c\,\hat{z}$

$$V = \vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3 = \begin{vmatrix} \frac{\sqrt{3}}{2}a & \frac{a}{2} & 0 \\ -\frac{\sqrt{3}}{2}a & \frac{a}{2} & 0 \\ 0 & 0 & c \end{vmatrix}$$

$$= a^2 c \left\{ \frac{\sqrt{3}}{4} - \left(-\frac{\sqrt{3}}{4}\right) \right\}$$

$$\boxed{V = \frac{\sqrt{3}}{2}\,a^2 c}$$

(B)

$$\vec{b}_1 = \frac{2\pi}{V} \vec{a}_2 \times \vec{a}_3$$

$$= \frac{2\pi}{\left(\frac{\sqrt{3}}{2}a^2 c\right)} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ -\frac{\sqrt{3}}{2}a & \frac{a}{2} & 0 \\ 0 & 0 & c \end{vmatrix} = \boxed{\frac{2\pi}{\sqrt{3}\,a}\hat{x} + \frac{2\pi}{a}\hat{y}}$$

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

$$= \frac{2\pi}{\frac{\sqrt{3}}{2}a^2 c} \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 0 & 0 & c \\ \frac{\sqrt{3}}{2} & \frac{a}{2} & 0 \end{vmatrix} = \boxed{-\frac{2\pi}{\sqrt{3}\,a}\hat{x} + \frac{2\pi}{a}\hat{y}}$$

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

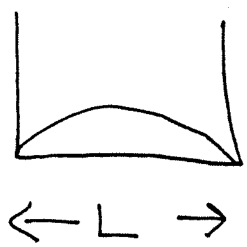
$$= \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\sqrt{3}}{2}a & \frac{a}{2} & 0 \\ -\frac{\sqrt{3}}{2}a & \frac{a}{2} & 0 \end{vmatrix} \frac{2\pi}{\frac{\sqrt{3}}{2}a^2 c}$$

$$= \frac{2\pi}{\frac{\sqrt{3}}{2}a^2 c} \frac{\sqrt{3}}{2} a^2 \hat{z} = \boxed{\frac{2\pi}{c}\hat{z}}$$

CHAPTER 3

(1) THE GROUND STATE ENERGY IS

$$\frac{\hbar^2 k^2}{2M} = \frac{\hbar^2 \left(\frac{2\pi}{\lambda}\right)^2}{2M}$$



IN THE GROUND STATE $L = \frac{\lambda}{2} \Rightarrow$

$$\boxed{E_{GROUND} = \frac{\hbar^2}{2M}\left(\frac{\pi}{L}\right)^2}$$

(2) THE FCC COHESIVE ENERGY IS CALCULATED IN THE TEXT.

FOR THE BCC,

$$\left.\frac{dU}{dR}\right|_{R_0} = 0 \Rightarrow$$

$$(12)(9.11418)\frac{\sigma^{12}}{R^{13}} - (6)(12.2533)\frac{\sigma^6}{R^7} = 0$$

$$\Rightarrow \frac{R_0^6}{\sigma^6} = 1.488$$

THUS, THE COHESIVE ENERGY FOR THE B.C.C. IS:

$$U = -2N\xi\left(4.116 \qquad\right)$$

COMPARING THIS WITH THE FCC

$$\boxed{\frac{U_{Bcc}}{U_{Fcc}} = 0.956}$$

(THUS FCC IS MORE STABLE CRYSTAL i.e. MORE COHESIVE ENERGY)