Phys 460 Problem Set # 4

Solutions

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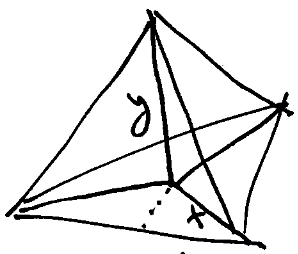
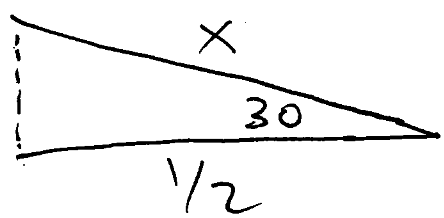
1) $\frac{c}{a}$ = twice the height of a regular tetrahedron of unit edge:





$$\frac{\frac{1}{2}}{x} = \cos 30 = \frac{\sqrt{3}}{2}$$

$$x = \frac{1}{\sqrt{3}} \qquad y = \sqrt{1-x^2} = \sqrt{\frac{2}{3}}$$

$$\frac{c}{a} = 2y = \sqrt{\frac{8}{3}}.$$

2a) <u>simple cubic</u>: The sphere inscribes the cube.

$$V_{sphere} = \frac{4}{3}\pi r^3$$

$$V_{cube} = (2r)^3 = 8r^3$$

$$f = \frac{V_{sphere}}{V_{cube}} = \frac{\frac{4}{3}\pi}{8} = \frac{\pi}{6} \simeq 0.524$$

b) <u>bcc</u>: Twice the sphere's diameter = cube body diagonal.

$$2d = \sqrt{3} \qquad d = \frac{\sqrt{3}}{2} \qquad r = \frac{\sqrt{3}}{4}$$

$$V_{sphere} = \frac{4\pi}{3} r^3 = \frac{\pi\sqrt{3}}{16}$$

There are two atoms per conventional unit cell of volume 1, so

$$f = \frac{\pi\sqrt{3}}{8} \cong 0.680$$

2c) <u>fcc</u>: Twice the sphere's diameter = face diagonal of cube.

$$2d = \sqrt{2} \qquad d = \frac{1}{\sqrt{2}} \qquad r = \frac{1}{2\sqrt{2}}$$

$$V_{sphere} = \frac{4}{3}\pi r^3 = \frac{\pi}{12\sqrt{2}}$$

There are 4 atoms in the conventional unit cell of volume 1, so

$$f = \frac{\pi}{3\sqrt{2}} \simeq 0.740$$

Physics 460 Homework # 4

Solutions (continued)

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3) a) The plane (hkl) intersects the axes $\vec{a}_1$, $\vec{a}_2$, & $\vec{a}_3$ at $kl\,\vec{a}_1$, $hl\,\vec{a}_2$, & $hk\,\vec{a}_3$.

The normal to the plane is the cross product

$$hkl\,\vec{n} = (hl\,\vec{a}_2 - kl\,\vec{a}_1) \times (hk\,\vec{a}_3 - kl\,\vec{a}_1)$$

$$\vec{n} = h(\vec{a}_2 \times \vec{a}_3) + k(\vec{a}_3 \times \vec{a}_1) + l(\vec{a}_1 \times \vec{a}_2)$$

Now $\vec{G} = \dfrac{2\pi\,\vec{n}}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$, thus

$\vec{G} \perp (hkl)$.

b) Let $\vec{r}_1$ and $\vec{r}_2$ be nearest points in two neighboring planes parallel to (hkl). $\vec{r}_1$ and $\vec{r}_2$ are points in the Bravais lattice, and so is

$$\vec{d} = \vec{r}_2 - \vec{r}_1 .$$

The distance between planes is

$$d = |\vec{d}| .$$

But $e^{i\vec{G}\cdot\vec{d}} = 1$ by the definition of a reciprocal lattice vector. Thus

$$\vec{G}\cdot\vec{d} = |\vec{G}|\, d \cos\theta = 2\pi n .$$

We showed that $\theta = 0$ in part (a). Thus $|\vec{G}|d = 2\pi n$.

The shortest reciprocal lattice vector in the direction $\hat{G}$ satisfies this relation with $n = 1$. Q.E.D.

c) In the s.c. lattice,

$$\vec{b}_1 = \frac{2\pi}{a}\hat{x}, \quad \vec{b}_2 = \frac{2\pi}{a}\hat{y}, \quad \vec{b}_3 = \frac{2\pi}{a}\hat{z}$$

$$\vec{G} = \frac{2\pi}{a}(h\hat{x} + k\hat{y} + l\hat{z})$$

$$|\vec{G}| = \frac{2\pi}{a}\sqrt{h^2+k^2+l^2}$$

$$d^2 = \frac{(2\pi)^2}{G^2} = \frac{a^2}{h^2+k^2+l^2}$$

Physics 460 HW 4
Solutions

4)

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

$$= \begin{vmatrix} \frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \\ -\frac{\sqrt{3}a}{2} & \frac{a}{2} & 0 \\ 0 & 0 & c \end{vmatrix}$$

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

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

$$= \frac{4\pi}{\sqrt{3}a^2c}\left(\frac{\sqrt{3}ac}{2}\hat{y} + \frac{ac}{2}\hat{x}\right)$$

$$= \frac{2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y}$$

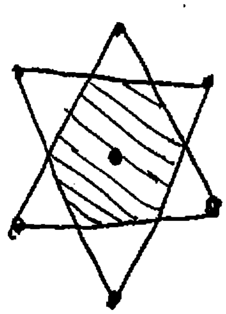
$$\vec{b}_2 = \frac{2\pi \, \vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{4\pi}{\sqrt{3}a^2 c}\left(\sqrt{3}\frac{ac}{2}\hat{y} - \frac{ac}{2}\hat{x}\right)$$

$$= -\frac{2\pi}{\sqrt{3}a}\hat{x} + \frac{2\pi}{a}\hat{y}$$

$$\vec{b}_3 = \frac{2\pi \, \vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{4\pi}{\sqrt{3}a^2 c}\left(\frac{\sqrt{3}a^2}{4}\hat{z} + \frac{\sqrt{3}a^2}{4}\hat{z}\right)$$

$$= \frac{2\pi}{c}\hat{z}$$

c) The 1st BZ extends from $-\frac{\pi}{c}\hat{z}$ to $\frac{\pi}{c}\hat{z}$. Its projection on the xy plane is a hexagon



bounded by the bisectors of $\pm\vec{b}_1$, $\pm\vec{b}_2$, $\pm(\vec{b}_1 - \vec{b}_2)$.

5)

$$V_{BZ} = \vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3)$$

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

$$= \frac{(2\pi)^3}{V_c^3} (\vec{a}_2 \times \vec{a}_3) \cdot \underbrace{[\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)]}_{V_c} \vec{a}_1$$

$$V_{BZ} = \frac{(2\pi)^3}{V_c^3} V_c^2 = \frac{(2\pi)^3}{V_c}$$

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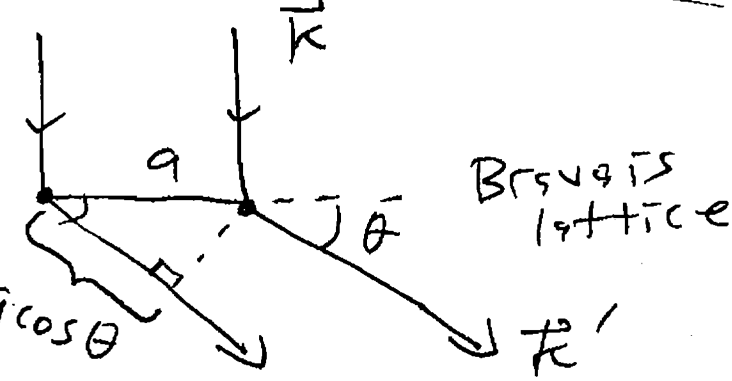
6)



a) The condition for constructive interference from neighboring cells of the Bravais lattice is

$$a \cos\theta = n\lambda .$$

b) The scattered amplitude from the two atoms in a unit cell is

$$S = f_1 + f_2 e^{-i \frac{a\cos\theta}{2} \frac{2\pi}{\lambda}}$$

$$= f_1 + f_2 e^{-i\pi \cos\theta \frac{a}{\lambda}}$$

But $\cos\theta = \frac{n\lambda}{a}$, so

$$S = f_1 + f_2 e^{-i\pi n}$$

$$= f_1 + f_2 (-1)^n.$$

c) If $f_1 = f_2$, the peaks for n odd disappear. The scattering condition is then $n = 2m$.

$a \cos\theta = 2m\lambda$ $\quad \frac{a}{2}\cos\theta = m\lambda$

$\Rightarrow$ lattice constant becomes $a/2$.