Physics 431 - Homework 2

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1 Problem 1

$$
\begin{aligned}
&\text{FCC Primitive}\\
a_1 &= \frac{1}{2}a(\hat{y}+\hat{z})\\
a_2 &= \frac{1}{2}a(\hat{x}+\hat{z})\\
a_3 &= \frac{1}{2}a(\hat{x}+\hat{y})
\end{aligned} \tag{1}
$$

$$
\begin{aligned}
&\text{BCC Reciprocal Primitive}\\
b_1 &= \frac{2\pi}{a}(\hat{y}+\hat{z})\\
b_2 &= \frac{2\pi}{a}(\hat{x}+\hat{z})\\
b_3 &= \frac{2\pi}{a}(\hat{x}+\hat{y})
\end{aligned} \tag{2}
$$

To prove this is true we will use equation 13 in chapter 2 of Kittel. I went the wrong way on this, however, the relationship should still be proven since if FCC primitive is equivalent to BCC reciprocal primitive, then BCC primitive should be equivalent to FCC reciprocal primitive.

$b_1 = 2\pi\frac{a_2\times a_3}{a_1\cdot a_2\times a_3}$; $b_2 = 2\pi\frac{a_3\times a_1}{a_1\cdot a_2\times a_3}$; $b_3 = 2\pi\frac{a_1\times a_2}{a_1\cdot a_2\times a_3}$

$$
\begin{aligned}
a_1\cdot a_2\times a_3 =&\\
&= a_1\cdot(-\frac{a^2}{4},\frac{a^2}{4},\frac{a^2}{4})\\
&= a_1\cdot(-\frac{a^2}{4},\frac{a^2}{4},\frac{a^2}{4})\\
&= \frac{1}{4}a^3
\end{aligned} \tag{3}
$$

$$
\begin{aligned}
b_1 &= 2\pi\frac{a_2\times a_3}{\frac{1}{4}a^3}\\
&= \frac{2\pi}{\frac{1}{4}a^3}(-\frac{a^2}{4},\frac{a^2}{4},\frac{a^2}{4})\\
&= (-\frac{2\pi}{a},\frac{2\pi}{a},\frac{2\pi}{a})
\end{aligned} \tag{4}
$$

$$\begin{aligned} b_2 &= 2\pi \frac{a_3 \times a_1}{\frac{1}{4}a^3} \\ &= \frac{2\pi}{\frac{1}{4}a^3}(\frac{a^2}{4}, -\frac{a^2}{4}, \frac{a^2}{4}) \\ &= (\frac{2\pi}{a}, -\frac{2\pi}{a}, \frac{2\pi}{a}) \end{aligned} \tag{5}$$

$$\begin{aligned} b_3 &= 2\pi \frac{a_2 \times a_3}{\frac{1}{4}a^3} \\ &= \frac{2\pi}{\frac{1}{4}a^3}(\frac{a^2}{4}, \frac{a^2}{4}, -\frac{a^2}{4}) \\ &= (\frac{2\pi}{a}, \frac{2\pi}{a}, -\frac{2\pi}{a}) \end{aligned} \tag{6}$$

2 Problem 2

2.1

First we will define two vectors on the plane in the real space by subtracting the endpoints of the plane from each other.

$$v_1 = (\frac{a_1}{h}, -\frac{a_2}{k}, 0) \tag{7}$$

$$v_2 = (\frac{a_3}{l} - \frac{a_1}{h}) \tag{8}$$

Then we will take the dot product of G with each of both of these vectors to prove that G is perpendicular to this plane.

2.1.1

$$G \cdot v_1 \tag{9}$$

2.1.2

$$G \cdot v_2 \tag{10}$$

2.2

2.3

3 Problem 3

Generally this is a problem from Kittel so should not be bad

3.1

$$
\begin{aligned}
V &= a_1 \cdot a_2 \times a_3 \\
&= a_1 \cdot \begin{bmatrix} \frac{ac}{2} \\ \frac{\sqrt{3}ac}{2} \\ 0 \end{bmatrix} \\
&= \frac{\sqrt{3}}{2} a^2 c
\end{aligned} \tag{11}
$$

3.2

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3};\ b_2 = 2\pi \frac{a_3 \times a_1}{a_1 \cdot a_2 \times a_3};\ b_3 = 2\pi \frac{a_1 \times a_2}{a_1 \cdot a_2 \times a_3}$$

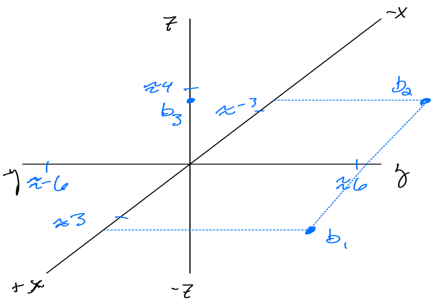
We know the answer to the bottom half of the equations for the primitive translations of the reciprocal lattice from part 1.

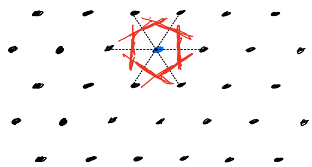
$$
\begin{aligned}
b_1 &= 2\pi \frac{a_2 \times a_3}{\frac{\sqrt{3}}{2} a^2 c} \\
&= \frac{2\pi}{\frac{\sqrt{3}}{2} a^2 c} \begin{bmatrix} \frac{ac}{2} \\ \frac{\sqrt{3}ac}{2} \\ 0 \end{bmatrix} \\
&= \begin{bmatrix} \frac{2\pi\sqrt{3}}{3a} \\ \frac{2\pi}{a} \\ 0 \end{bmatrix}
\end{aligned} \tag{12}
$$

$$
\begin{aligned}
b_2 &= 2\pi \frac{a_3 \times a_1}{\frac{\sqrt{3}}{2} a^2 c} \\
&= \frac{2\pi}{\frac{\sqrt{3}}{2} a^2 c} \begin{bmatrix} -\frac{ac}{2} \\ \frac{\sqrt{3}ac}{2} \\ 0 \end{bmatrix} \\
&= \begin{bmatrix} -\frac{2\pi\sqrt{3}}{3a} \\ \frac{2\pi}{a} \\ 0 \end{bmatrix}
\end{aligned} \tag{13}
$$

$$b_3 = 2\pi \frac{a_1 \times a_2}{\frac{\sqrt{3}}{2}a^2 c}$$
$$= \frac{2\pi}{\frac{\sqrt{3}}{2}a^2 c} \begin{bmatrix} 0 \\ 0 \\ \frac{\sqrt{3}a^2}{2} \end{bmatrix} \quad (14)$$
$$= \begin{bmatrix} 0 \\ 0 \\ \frac{2\pi}{c} \end{bmatrix}$$

3.3





4 Problem 4

4.1

$$Electron: \; 151eV$$

$$Neutron: \; 0.08eV$$
$$Photon: \; 12.4keV$$

4.2

The reason that the x-ray photons have a different slope compared to the neutrons and the electrons is due to the De Broglie wavelength, $\lambda_B = \frac{h}{p}$. Basically the difference in slope stems from the fact that photons have no mass, and their momentum is defined as $p = \frac{h}{\lambda}$, as compared to neutrons and electrons, where the momentum is defined by $p = mv$. Pretty interesting question to research so thank you.

4.3

Neutrons carry a spin and interact with magnetic moments. For this reason, you can measure the magnetic structure of the material in addition to the atomic crystal structure.

5 Problem 5

Structure	(hkl)	(hhl)	(hhh)	(0kl)	(0kk)	(00l)
Cubic	48	24	8	24	12	6
Tetragonal	16	8	8	8	8	2
Orthorhombic	8	8	8	4	8	2