Physics 431 - Homework 3

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1 Problem 1

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$$\begin{aligned} V_c &= \vec{a_1} \cdot \vec{a_2} \times \vec{a_3} \\ V_b &= \vec{b_1} \cdot \vec{b_2} \times \vec{b_3} \end{aligned} \tag{1}$$

Since the definition of our b vectors have the equation for V_c in the denominator, we can simply solve for our b vectors and then plug them into the equation for volume for V_b.

$$\begin{aligned} b_1 &= 2\pi \frac{\vec{a_2} \times \vec{a_3}}{\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}} = 2\pi \frac{\vec{a_2} \times \vec{a_3}}{V_c} \\ b_2 &= 2\pi \frac{\vec{a_3} \times \vec{a_1}}{\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}} = 2\pi \frac{\vec{a_3} \times \vec{a_1}}{V_c} \\ b_3 &= 2\pi \frac{\vec{a_1} \times \vec{a_2}}{\vec{a_1} \cdot \vec{a_2} \times \vec{a_3}} = 2\pi \frac{\vec{a_1} \times \vec{a_2}}{V_c} \end{aligned} \tag{2}$$

$$\begin{aligned} V_b &= \vec{b_1} \cdot \vec{b_2} \times \vec{b_3} \\ &= (2\pi \frac{\vec{a_2} \times \vec{a_3}}{V_c}) \cdot (2\pi \frac{\vec{a_3} \times \vec{a_1}}{V_c}) \times (2\pi \frac{\vec{a_1} \times \vec{a_2}}{V_c}) \\ &= \frac{(2\pi)^3}{{V_c}^3} (\vec{a_2} \times \vec{a_3}) \cdot (\vec{a_3} \times \vec{a_1}) \times (\vec{a_1} \times \vec{a_2}) \end{aligned}$$

Now we can use the vector identity in the problem

$$(c \times a) \times (a \times b) = (c \cdot a \times b)a$$

$$\begin{aligned} &= \frac{(2\pi)^3}{{V_c}^3} (\vec{a_2} \times \vec{a_3}) \cdot (\vec{a_3} \cdot \vec{a_1} \times \vec{a_2}) \vec{a_1} \\ &= \frac{(2\pi)^3}{{V_c}^3} \vec{a_1} (\vec{a_2} \times \vec{a_3}) \cdot (\vec{a_3} \cdot \vec{a_1} \times \vec{a_2}) \\ &= \frac{(2\pi)^3}{{V_c}^2} (\vec{a_3} \cdot \vec{a_1} \times \vec{a_2}) \\ &= \frac{(2\pi)^3}{V_c} \end{aligned} \tag{3}$$

2 Problem 2

2.1

$$
\begin{aligned}
|F|^2 = F^*F &= \frac{\sin^2 \frac{1}{2}M(a\cdot\triangle k)}{\sin^2 \frac{1}{2}(a\cdot\triangle k)} \\
F &= \sum_G \int dV n_G e^{i(G-\triangle K)\cdot r} \\
&= \sum e^{-ima\cdot\triangle K} \\
&= \frac{1-e^{-iM(a\cdot\triangle k)}}{1-e^{-i(a\cdot\triangle k)}} \\
F^* &= \frac{1-e^{iM(a\cdot\triangle k)}}{1-e^{i(a\cdot\triangle k)}}
\end{aligned}
$$

$$
\begin{aligned}
F^*F &= \frac{1-e^{iM(a\cdot\triangle k)}}{1-e^{i(a\cdot\triangle k)}}\frac{1-e^{-iM(a\cdot\triangle k)}}{1-e^{-i(a\cdot\triangle k)}} \\
&= \frac{1-e^{iM(a\cdot\triangle k)}-e^{-iM(a\cdot\triangle k)}+1}{1-e^{i(a\cdot\triangle k)}-e^{-i(a\cdot\triangle k)}}+1 \\
&= \frac{2-e^{iM(a\cdot\triangle k)}-e^{-iM(a\cdot\triangle k)}}{2-e^{i(a\cdot\triangle k)}-e^{-i(a\cdot\triangle k)}} \\
&= \frac{2-(\cos(M(a\cdot\triangle k))+i\sin(M(a\cdot\triangle k)))-(\cos(M(a\cdot\triangle k))-i\sin(M(a\cdot\triangle k)))}{2-(\cos(a\cdot\triangle k)+i\sin(a\cdot\triangle k))-(\cos(a\cdot\triangle k)-i\sin(a\cdot\triangle k))} \\
&= \frac{2-2\cos(M(a\cdot\triangle k))}{2-2\cos(a\cdot\triangle k)} \\
&= \frac{\sin^2 \frac{1}{2}M(a\cdot\triangle k)}{\sin^2 \frac{1}{2}(a\cdot\triangle k)}
\end{aligned}
\tag{4}
$$

2.2

$$
\begin{aligned}
a\cdot\triangle k &= 2\pi h \\
\text{At first 0 in our expansion} \\
a\cdot\triangle k &= 2\pi h+\epsilon \\
\epsilon &= \frac{2\pi}{M}
\end{aligned}
\tag{5}
$$

$$
\begin{aligned}
\sin^2\frac{1}{2}M(2\pi h+\epsilon) &= 0 \\
(M\pi h+\frac{1}{2}\epsilon) &= 0 \\
\epsilon &= -2M\pi h \\
&= \frac{2\pi}{M}
\end{aligned}
\tag{6}
$$

3 Problem 3

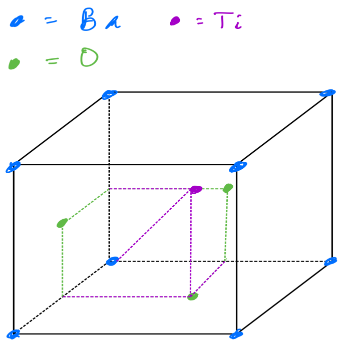
The Bragg and Von Laue conditions specify the scenario in which the incident waves have constructive interference. The waves which don't satisfy these conditions are experiences destructive interference and therefore you see a gradient distribution at spots of peak intensity as the interference transitions from constructive to destructive.

4 Problem 4

The diffractograms technically should not differ at all in the two cases. The reason for this presumption is from looking at the equation for intensity. The atoms are the same, so with the first and second case, we will have an $n(\vec{r})$ which remains the same. Second, the structure remains the same. Before the cooling, the structure is BCC, after the cooling, the structure is BCC, therefore as we integrate over all of our unit cells, there will be no difference in the intensity per unit cell once we average over the entire solid. The second case allows us to predict more reasonably what each unit cell will contribute to the intensity, as in the first case, you could have some cells that are all gold or all zinc. It is only when you integrate over the entire solid that you see these two structures are no different. At the core, they have the same structure and same atoms.

5 Problem 5

5.1



5.2

$$S(hkl) = \sum_j f_j e^{i\vec{u}_j \cdot \vec{G}}$$

$$\vec{G} \cdot \vec{u}_j = 2\pi(v_1 x_j + v_2 y_j + v_3 z_j)$$

$$S(hkl) = f_{Ba} + (-1)^l f_{Ti} + [1 + 2(-1)^l] f_O \tag{7}$$

$$\begin{aligned}
S(hkl) &= f_{Ba} e^{i(000)\cdot(hkl)} + [f_{Ti} e^{i(\frac{1}{2}\frac{1}{2}\frac{1}{2})\cdot(hkl)}] + f_O e^{i(\frac{1}{2}\frac{1}{2}0)\cdot(hkl)} + f_O e^{i(0\frac{1}{2}\frac{1}{2})\cdot(hkl)} + f_O e^{i(\frac{1}{2}0\frac{1}{2})\cdot(hkl)} \\
&= f_{Ba} e^0 + f_{Ti} e^{i\pi(hkl)} + (f_O e^{i\pi[h+k]}) + (f_O e^{i\pi[k+l]}) + (f_O e^{i\pi[h+l]}) \\
&= f_{Ba} + f_{Ti}(-1)^l + (f_O[1 + 2(-1)^l])
\end{aligned} \tag{8}$$

5.3