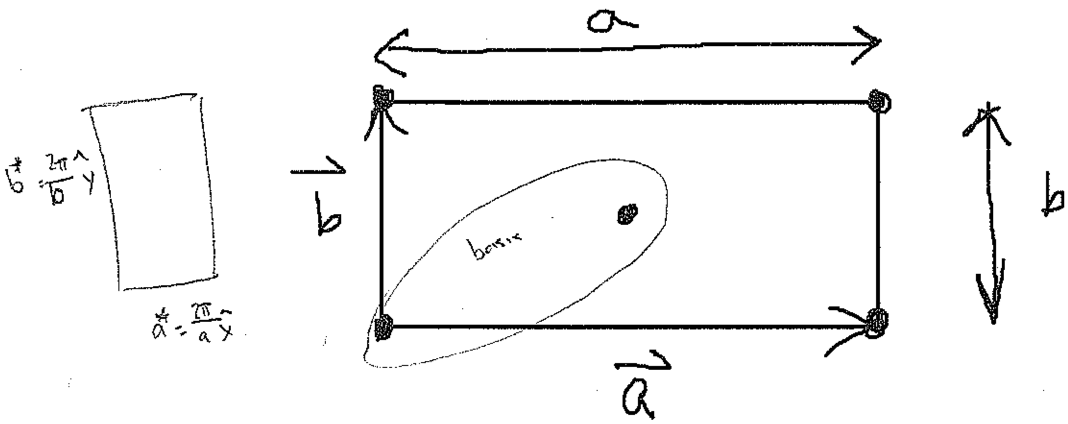
Let us assume that we have a centered rectangular BL with one atom per lattice point (each point below). A convenient way to represent such a crystal is to take a rectangular BL (= conventional BL) with sides a and b, and *two* atoms per basis (= a conventional basis). For this conventional BL, plot its reciprocal BL. Keep only those reciprocal BL points where the structural factor is non-zero (as you will find that for certain BL points the structure factor IS zero). These points constitute the reciprocal BL of the original centered rectangular BL (= primitive BL)!

I hope you will see that the use of a conventional BL and the structural factor is a nice way to calculate a reciprocal BL of a complicated BL (such as fcc, bcc)! [*Think in terms of the physical meaning of the reciprocal BL as spots on the pattern of an X-ray diffraction experiment, through the Bragg condition.*] So, looking at your results for this particular exercise, what is the reciprocal BL of the centered rectangular BL? Make sure the relation $VV^* = (2\pi)^D$ is indeed satisfied (both for the conventional BL and for the primitive BL). Set the atomic form factor to be 1 (the same for all dots).



$S_G = f_1 e^{-i\vec G\cdot\vec r_1} + f_2 e^{-i\vec G\cdot\vec r_2}$

$f_1 = f_2 = 1$ since atoms are identical

$S_G = e^{-i\vec G\cdot\vec r_1} + e^{-i\vec G\cdot\vec r_2}$

$\vec r_1$ = origin

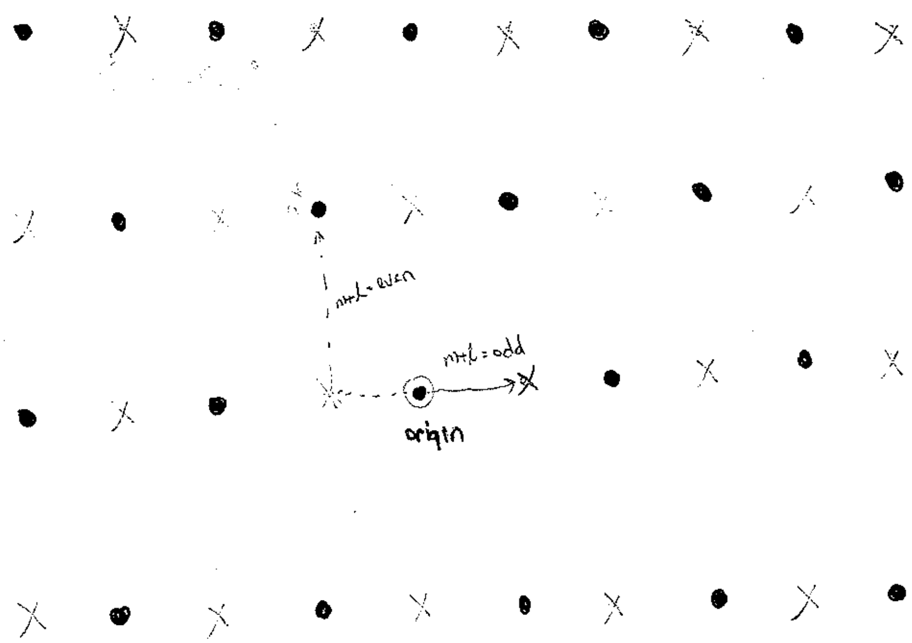
$S_G = 1 + e^{-iG\cdot\frac{1}{2}(a\hat x + b\hat y)}$

$G = \frac{2\pi}{a} l\hat x + \frac{2\pi}{b} m\hat y$

$S_G = 1 + e^{-i\left(\frac{2\pi}{a}l\cdot\frac{1}{2}a + \frac{2\pi}{b}m\frac{1}{2}b\right)}$

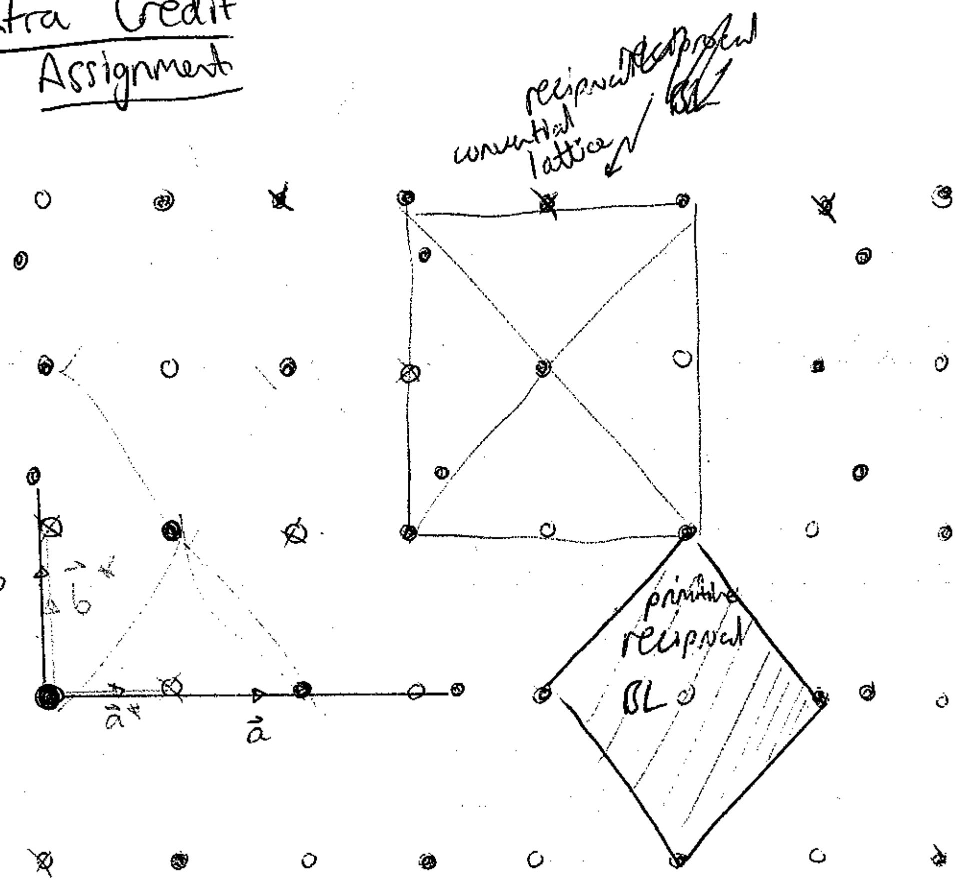
$S_G = 1 + e^{-i\pi(m+l)}$

$$\boxed{S_G = \begin{cases} 0 & \text{if } m+l = \text{odd} \\ 2 & \text{if } m+l = \text{even} \end{cases}}$$



great solution. Wish letters were bigger.

Extra Credit Assignment



Let $f_i = 1$ for all i. $r_0 = 0$, $r_1 = \frac{1}{2}\vec{a} + \frac{1}{2}\vec{b}$ basis atoms.

For $\vec{G} = 0$, $S_{\vec{G}} = \sum e^{-i(r_i \cdot \vec{G})} \neq 0$

$\vec{G} = \vec{a}^*$ $\quad S_G = e^{-i(\vec{r}_0 \cdot \vec{G})} + e^{-i(\vec{r}_1 \cdot \vec{G})} = e^0 + e^{-i(\frac{1}{2} \cdot \vec{a} \cdot \vec{a}^*)}$

$= 1 + e^{-i\pi} = 1 - 1 = 0$

$\vec{G} = 2\vec{a}^*$ $\quad S_G = 1 + e^{-i(\frac{1}{2} \cdot 2 \cdot 2\pi)} = 1 + 1 \neq 0$

$\vec{G} = \vec{b}^*$ $\quad S_G = 1 + e^{-i(\frac{1}{2}\vec{b} \cdot \vec{b}^*)} = 1 + e^{-i(\pi)} = 0$

$\vec{G} = \vec{a}^* + \vec{b}^*$ $\quad S_G = 1 + e^{-i(\pi + \pi)} \neq 0$

$\vec{G} = 2\vec{a}^* + \vec{b}^*$ $\quad S_G = 1 + e^{-i(2\pi + \pi)} = 0$

$\vec{G} = -\vec{b}^*$ $\quad S_G = 1 + e^{-i(-\pi)} \cancel{\neq 0} = 1 - 1 = 0$

$\vec{G} = \vec{a}^* - \vec{b}^*$ $\quad S_G = 1 + e^{-i(\pi - \pi)} \neq 0$

$G = 3\vec{a}^* + 2\vec{b}^*$ $\quad S_G = 1 + e^{-i(3\pi + 2\pi)} = 0$

Good solution

Could have been more general

$\vec{G} = l\vec{a}^* + m\vec{b}^*$

nice!

Conventional VV^*

$$V = \begin{vmatrix} a_1 & a_2 \\ b_1 & b_2 \end{vmatrix} = \begin{vmatrix} a & 0 \\ 0 & b \end{vmatrix} = ab \qquad V^* = \frac{2\pi}{a} \cdot \frac{2\pi}{b} = \frac{(2\pi)^2}{ab}$$

$\therefore VV^* = (2\pi)^2$ ie. $D = 2$

Primitive V^*

~~Conventional~~ $\vec{p}_1 = \frac{1}{2}\vec{a} + \frac{1}{2}\vec{b}$ (primitive Bravais vectors)

$\vec{p}_2 = \vec{b}$

so $\vec{p}_1 = \frac{a}{2}\hat{x} + \frac{b}{2}\hat{y}$

great!

$\vec{p}_2 = b\,\hat{y}$

$\therefore\ V = \begin{vmatrix} a/2 & b/2 \\ 0 & b \end{vmatrix} = \frac{ab}{2}$

Reciprocal vectors, $\vec{p}_1^{\,*} = \vec{a}^{\,*} - \vec{b}^{\,*}$

$\vec{p}_2 = \vec{a}^{\,*} + \vec{b}^{\,*}$

where $\vec{a}^{\,*} = \frac{2\pi}{a}\hat{x}$ and $\vec{b}^{\,*} = \frac{2\pi}{b}\hat{y}$

So $V^* = \begin{vmatrix} 2\pi/a & -2\pi/b \\ 2\pi/a & 2\pi/b \end{vmatrix} = \frac{(2\pi)^2}{ab} + \frac{(2\pi)^2}{ab} = 2\frac{(2\pi)^2}{ab}$

$\therefore\ V V^* = \frac{\cancel{ab}}{\cancel{2}} \cdot \cancel{2} \frac{(2\pi)^2}{\cancel{ab}} = (2\pi)^D$

$D=2$

Nice!

But could have simplified this part by noting that

$V \rightarrow \frac{1}{2}V$
$V^* \rightarrow 2V^*$ } when going from conventional → primitive.

← obvious from figures