HW#2.

1. Sodium chloride

FCC w/ 2 basis atoms $\begin{cases} (0,0,0) = \vec{r}_1 \\ (\frac{a}{2},0,0) = \vec{r}_2 \end{cases}$

Reciprocal vector of $\vec{G}$ of FCC

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

where $\vec{b}_1 = \frac{2\pi}{a}(-\hat{x}+\hat{y}+\hat{z})$

$\vec{b}_2 = \frac{2\pi}{a}(\hat{x}-\hat{y}+\hat{z})$

$\vec{b}_3 = \frac{2\pi}{a}(\hat{x}+\hat{y}-\hat{z})$

Thus,

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

$$= \frac{4\pi}{a}(\nu_1\hat{x} + \nu_2\hat{y} + \nu_3\hat{z})$$

where $\nu_1 = \frac{-h+k+l}{2}$, $\nu_2 = \frac{h-k+l}{2}$, $\nu_3 = \frac{h+k-l}{2}$

S_G is,

$$S_G = \sum_j f_j e^{-i(\vec{G}\cdot\vec{r})} \qquad \left(\begin{array}{l}\vec{r}_1 = (0,0,0) \\ \vec{r}_2 = (\frac{a}{2},0,0)\end{array}\right)$$

$$= f_1 + f_2 e^{-i2\pi\nu_1}$$

If, ν_1 is integer, $S_G = f_1 + f_2$

ν_1 is integer plus half, $S_G = f_1 - f_2$

If $f_1 = f_2$, constructive interference can occur when $-h+k+l$ is even

destructive interference can occur when $-h+k+l$ is odd.