6.3(a) HW4.

Express HCP as simple hexagonal with a diatomic basis.

$$\vec{d_1}=0 \ \& \ \vec{d_2}=\frac{\vec{a_1}}{3}+\frac{\vec{a_2}}{3}+\frac{\vec{a_3}}{2} \quad \text{for } \vec{a_1}=a\hat{x},\ \vec{a_2}=\frac{a}{2}\hat{x}+\frac{\sqrt{3}a}{2}\hat{y},\ \vec{a_3}=c\hat{z}$$

$$\Rightarrow \vec{d_2}=\frac{a}{2}\hat{x}+\frac{\sqrt{3}}{6}a\hat{y}+\frac{c}{2}\hat{z}$$

The primitive vector of reciprocal lattice.

$$\vec{b_1}=\frac{2\pi}{a}(\hat{x}-\frac{1}{\sqrt{3}}\hat{y}),\quad \vec{b_2}=\frac{2\pi}{a}(\frac{2}{\sqrt{3}}\hat{y}),\quad \vec{b_3}=\frac{2\pi}{c}\hat{z}$$

let $\vec{K}=h\vec{b_1}+k\vec{b_2}+l\vec{b_3}$

$$S_{\vec{K}}=\sum_{j=1}^{n} f_j(\vec{K})\exp(i\vec{K}\cdot\vec{d_j})$$

$$= A\cdot(\exp(i\vec{K}\cdot\vec{d_1})+\exp(i\vec{K}\cdot\vec{d_2}))$$

$$= A\cdot(1+\exp(i\vec{K}\cdot\vec{d_2}))$$

$$\Rightarrow \vec{K}\cdot\vec{d_2}=(h\frac{2\pi}{a}(\hat{x}-\frac{1}{\sqrt{3}}\hat{y})+k\frac{2\pi}{a}\frac{2}{\sqrt{3}}\hat{y}+l\frac{2\pi}{c}\hat{z})\cdot(\frac{a}{2}\hat{x}+\frac{\sqrt{3}}{6}a\hat{y}+\frac{c}{2}\hat{z})$$

$$= h\cdot(\pi-\frac{\pi}{3})+k(\frac{2\pi}{3})+l\pi = \frac{\pi}{3}(2h+2k+3l).$$

$(h,k,l)=(1,1,1)\Rightarrow \pi/3$

$=(0,1,0)\ \&\ (1,0,0)\Rightarrow 2\pi/3$

$=(0,0,1)\Rightarrow \frac{3\pi}{3}$

$=(1,1,0)\Rightarrow \frac{4\pi}{3}$

$=(1,0,1)$ or $(0,1,1)\Rightarrow \frac{5}{3}\pi$

$=(0,0,0)\Rightarrow \frac{6}{3}\pi$

\#

①

6.3(b)

To make $S_K = 0$.

$\Rightarrow 1 + \exp(i\vec{k}\cdot\vec{d_2}) = 0 \Rightarrow \vec{k}\cdot\vec{d_2} = (2n+1)\pi$ (odd)

However, if $\vec{K}$ is on xy plane $\Rightarrow \vec{K}\cdot\vec{d_2} = \frac{2\pi}{3}(h+k)$ (even).

$\Rightarrow$ Base on above contradition, reciprocal lattice point always has nonvanishing structure factor on this case.

6.5(a).

$$S_K = S_{fcc}(f_+ \exp(i\vec{K}\cdot\vec{d_+}) + f_- \exp(i\vec{k}\cdot\vec{d_-})).$$

$$\vec{K} = \frac{4\pi}{a}(V_1\hat{x} + V_2\hat{y} + V_3\hat{z}).$$

$$\Rightarrow S_{\vec{K}} = S_{fcc}(f_+ + f_- \exp(i\frac{4\pi}{a}V_1\cdot\frac{a}{2})).$$

$$= S_{fcc}(f_+ + f_- \exp(iV_1\cdot 2\pi)) \Rightarrow \begin{cases} f_+ + f_-, & V_1 \in Z \\ f_+ - f_-, & V_1 = n + \frac{1}{2} \end{cases}$$

$n \in Z$

6.5(b)

$$S_K = f_+ \exp(i\vec{k}\cdot\vec{d_+}) + f_- \exp(i\vec{k}\cdot\vec{d_-}), \quad \vec{d_+} = 0, \quad \vec{d_-} = \frac{a}{4}(\hat{x}+\hat{y}+\hat{z}).$$

$$= f_+ + f_- \exp(i\frac{4\pi}{a}(V_1\hat{x} + V_2\hat{y} + V_3\hat{z})\cdot(\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})))$$

$$= f_+ + f_- \exp(\pi(V_1 + V_2 + V_3)).$$

if $V_i = n_i + \frac{1}{2} \Rightarrow V_1 + V_2 + V_3 = n\pi + \frac{1}{2} \Rightarrow S_K = f_+ \pm i f_-$.

if V_i are integer & $\sum_i V_i$ is even $\Rightarrow S_K = f_+ + f_-(\exp 2n\pi) = f_+ + f_-$.

if V_i are integer & $\sum_i V_i$ is odd $\Rightarrow S_K = f_+ + f_1(\exp(2n+1)\pi) = f_+ - f_-$