

3. hcp structure

(a) Use  $\vec{R}_1, \vec{R}_2, \vec{R}_3$  as the direct lattice vectors.

Reciprocal vectors  $\vec{G}_1 = 2\pi \frac{\vec{R}_2 \times \vec{R}_3}{\vec{R}_1 \cdot (\vec{R}_2 \times \vec{R}_3)}$

$\vec{G}_2 = 2\pi \frac{\vec{R}_3 \times \vec{R}_1}{\vec{R}_1 \cdot (\vec{R}_2 \times \vec{R}_3)}$

$\vec{G}_3 = 2\pi \frac{\vec{R}_1 \times \vec{R}_2}{\vec{R}_1 \cdot (\vec{R}_2 \times \vec{R}_3)}$

In HW2,  $\left\{ \begin{array}{l} \vec{R}_1 = a \left( \frac{\sqrt{3}}{2} \hat{x} + \frac{1}{2} \hat{y} \right) \\ \vec{R}_2 = a \left( -\frac{\sqrt{3}}{2} \hat{x} + \frac{1}{2} \hat{y} \right) \\ \vec{R}_3 = c \hat{z} \end{array} \right. \rightarrow \left\{ \begin{array}{l} \vec{G}_1 = \frac{4\pi}{\sqrt{3}a} \left( \frac{1}{2} \hat{x} + \frac{\sqrt{3}}{2} \hat{y} \right) \\ \vec{G}_2 = \frac{4\pi}{\sqrt{3}a} \left( -\frac{1}{2} \hat{x} + \frac{\sqrt{3}}{2} \hat{y} \right) \\ \vec{G}_3 = \frac{2\pi}{c} \hat{z} \end{array} \right.$

(b)  $\vec{G} = h \vec{G}_1 + k \vec{G}_2 + l \vec{G}_3$ , two atoms at  $(0,0,0), \left( \frac{2}{3} \vec{R}_1 + \frac{1}{3} \vec{R}_2 + \frac{1}{2} \vec{R}_3 \right)$

$\Rightarrow S_G = f \left[ 1 + \exp \left[ -i \left( \frac{2}{3} \vec{R}_1 + \frac{1}{3} \vec{R}_2 + \frac{1}{2} \vec{R}_3 \right) \cdot (h \vec{G}_1 + k \vec{G}_2 + l \vec{G}_3) \right] \right]$

$\vec{R}_1 \cdot \vec{G}_1 = 2\pi \frac{\vec{R}_1 \cdot (\vec{R}_2 \times \vec{R}_3)}{\vec{R}_1 \cdot (\vec{R}_2 \times \vec{R}_3)} = 2\pi$

$\vec{R}_2 \cdot \vec{G}_2 = \vec{R}_3 \cdot \vec{G}_3 = 2\pi$

$\vec{R}_1 \cdot \vec{G}_2 = \vec{R}_1 \cdot \vec{G}_3 = \vec{R}_2 \cdot \vec{G}_1 = \vec{R}_2 \cdot \vec{G}_3 = \vec{R}_3 \cdot \vec{G}_1 = \vec{R}_3 \cdot \vec{G}_2 = 0$

$\Rightarrow S_G = f \left[ 1 + \exp \left[ -i \left( \frac{2}{3} h \cdot 2\pi + \frac{1}{3} k \cdot 2\pi + \frac{1}{2} l \cdot 2\pi \right) \right] \right]$   
 $= f \left[ 1 + e^{-i\pi \left( \frac{4}{3} h + \frac{2}{3} k + l \right)} \right]$