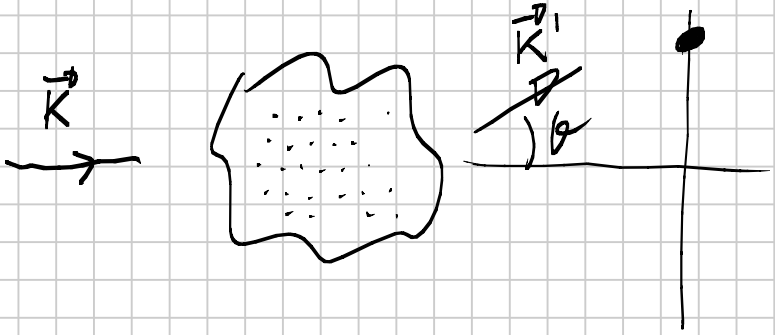
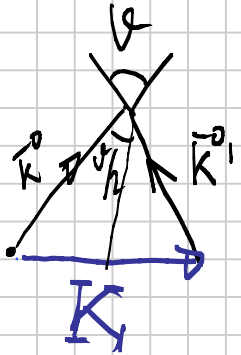
LECTURE # 15

Note Title 10/22/2008



PEAK $\Leftrightarrow$ $\vec{k} - \vec{k}' = \vec{K}$ IS A RECIPROCAL LATTICE VECTOR

$\vec{k} - \vec{k}'$



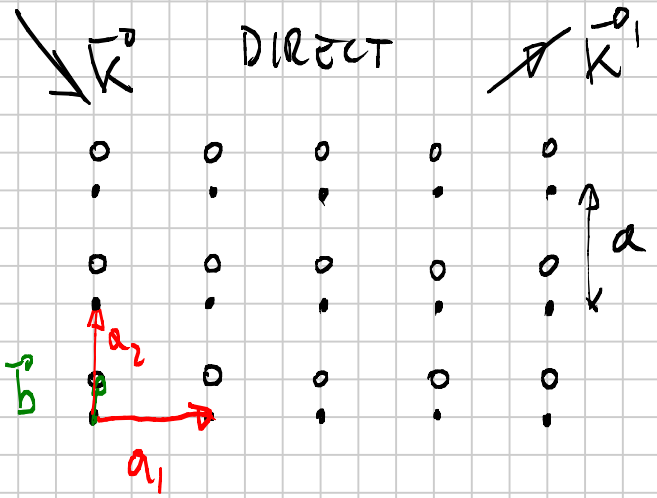
$$|\vec{K}| = 2|\vec{k}| \sin\frac{\theta}{2}$$

$|\vec{k}| = \frac{2\pi}{\lambda}$

DIFFERENT θ $\Rightarrow$ DIFFERENT $|\vec{K}|$ $\Rightarrow$ RECIPROCAL LATTICE

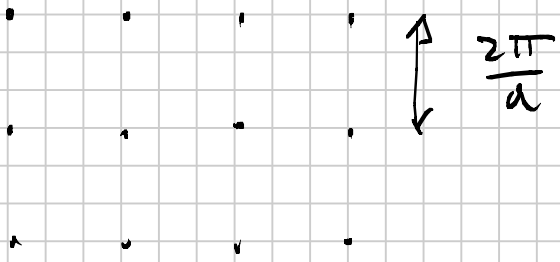
$\Rightarrow$ DIRECT LATTICE

WHAT HAPPENS IF WE HAVE A BASIS ?



- CONSTRUCTIVE INTERFERENCE BETWEEN ALL ●
- CONSTRUCTIVE INTERFERENCE BETWEEN ALL O

RECIPROCAL:



$\vec{K} - \vec{K}'$ HAS TO BE A POINT HERE

TOTAL SCATTERED LIGHT PROPORTIONAL TO :

$$\left(\begin{matrix} 1 \\ k \end{matrix} + e^{i(\vec{k}-\vec{k}')\cdot\vec{b}} \right) \longrightarrow S(\vec{k}-\vec{k}')$$

GEOMETRICAL STRUCTURE FACTOR

- ● ATOMS
- O ATOMS

(PHASE SHIFT DUE DIFFERENT OPTICAL PATH)

FOR EACH $\vec{K} = \vec{k} - \vec{k}'$

FOR UNIT CELLS WITH MANY ATOMS IN THE BASIS

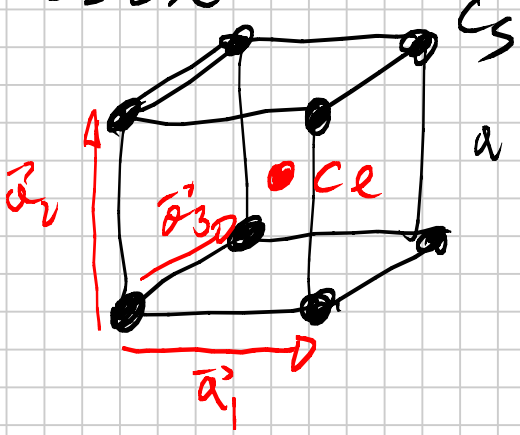
$$S(\vec{K}) = \sum_{i \in \text{BASIS}} e^{i\vec{K}\cdot\vec{b}_i}$$

FOR DIFFERENT ATOMS

$$S(K) = \sum_{i \in \text{BASIS}} f_i \, e^{i\vec{K}\cdot\vec{b}_i}$$

f_i: ATOMIC FORM FACTOR

CsCl



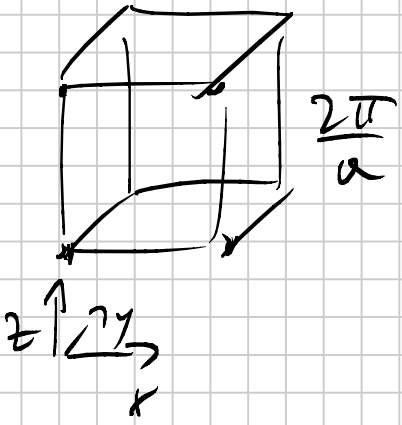
$\vec{b}_{Cs} = 0 \quad (f_1)$

$\vec{b}_{Cl} = \frac{a}{2}(111) \quad (f_2)$

$\vec{a}_1 = a(100)$

$\vec{a}_2 = a(010)$

$\vec{a}_3 = a(001)$



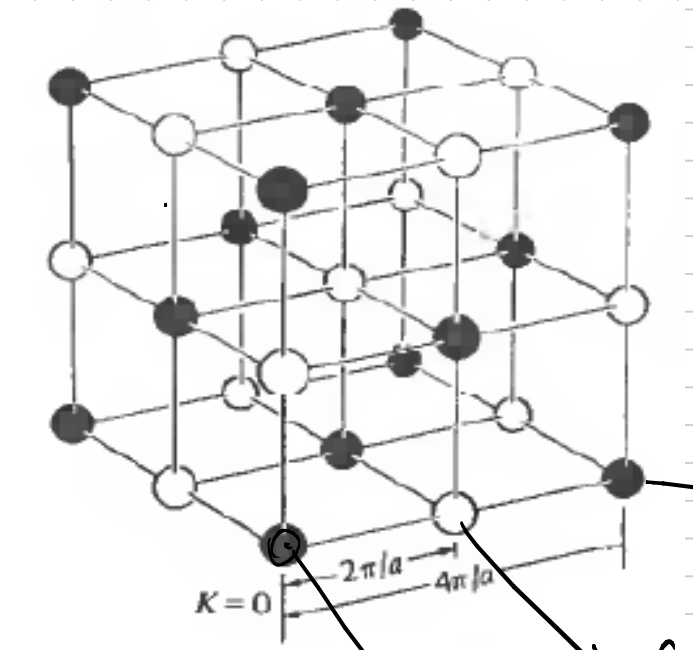
$$\vec{K} = \frac{2\pi}{a}\left(n_1\hat{x} + n_2\hat{y} + n_3\hat{z}\right)$$

$$S(\vec{K}) = \left(f_1 + f_2\, e^{i\vec{K}\cdot\vec{b}_{Cl}}\right) = f_1 + f_2\, e^{i\frac{2\pi}{a}\cdot\frac{a}{2}\cdot(n_1+n_2+n_3)}$$

$$S(\vec{K}) = f_1 + f_2\, e^{i\pi(n_1+n_2+n_3)}$$

$n_1+n_2+n_3$ ODD $\rightarrow f_1 - f_2$

$n_1+n_2+n_3$ EVEN $\rightarrow f_1 + f_2$



IF $f_1 = f_2$

THE RECIPROCAL

LATTICE FCC

THIS IS CONSISTENT

WITH BCC DIRECT.

LATTICE

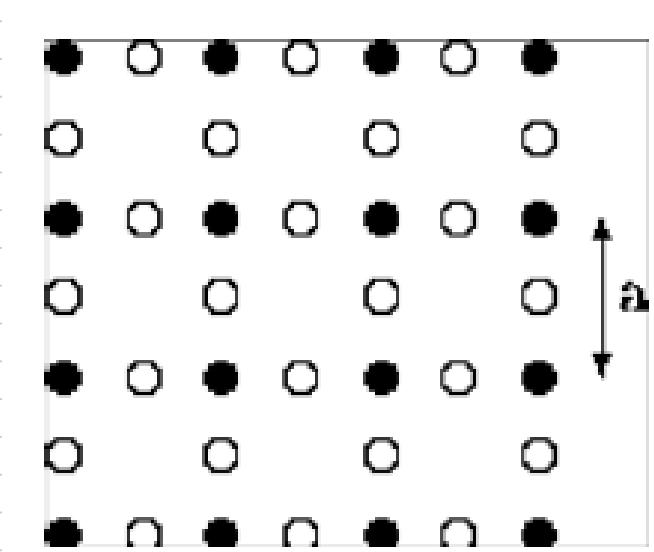


Figure 1.6: CuO_2 lattice

CuO_2

● Cu f_{Cu}

○ Oxygen f_O

$S(K)$