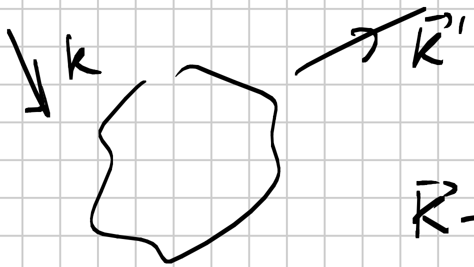
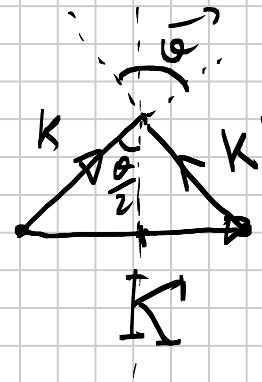
LECTURE #13

Note Title 10/22/2007

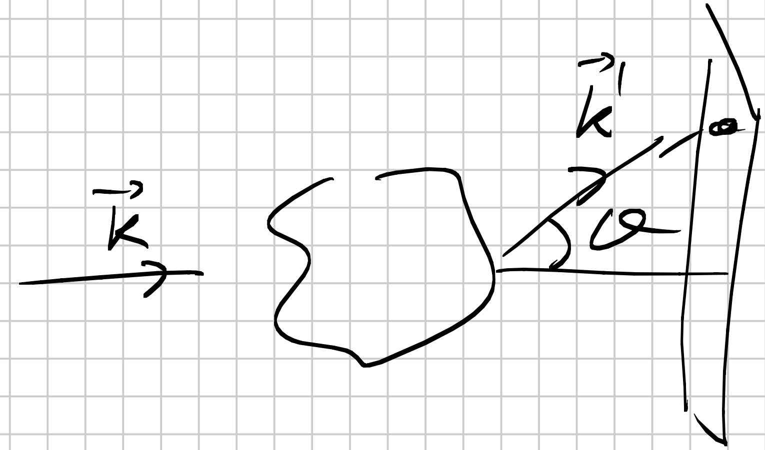
BRAGG PLANE



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



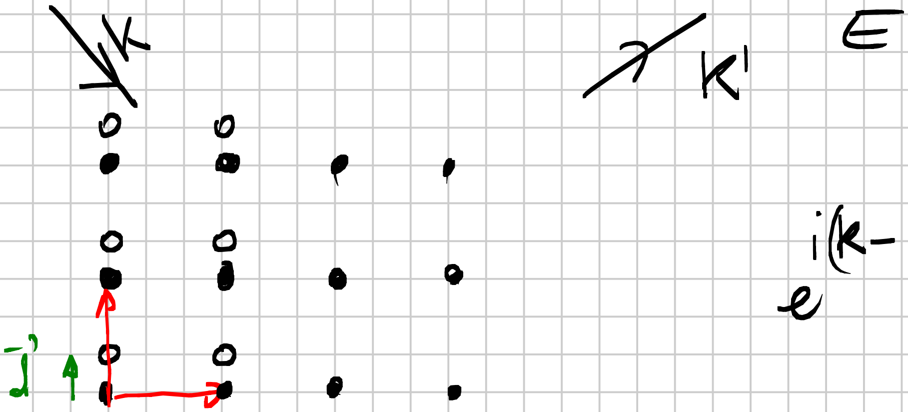
BRAGG PLANE



$$|k|\sin\frac{\theta}{2}=\frac{|\vec{K}_1|}{2}$$

$$|k|=\frac{2\pi}{\lambda} \rightarrow \theta_i \rightarrow |K_i| \rightarrow$$ Reciprocal lattice $\rightarrow$ Direct lattice

What happens if you have a basis?



$$e^{i(k-k')\cdot \vec{d}}$$

$$\left(1 + e^{i(k-k')\cdot \vec{d}}\right) = S(k-k')$$

GEOMETRICAL STRUCTURE FACTOR

1 FROM ●

$e^{i(k-k')\cdot \vec{d}}$ FROM ○

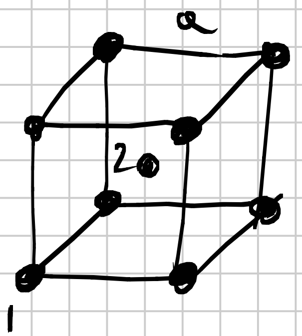
FOR EACH $\vec{K} = k - k'$

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

IF I HAVE DIFFERENT ATOMS

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

f_i = ATOMIC FORM FACTOR



f_1 $\qquad$ f_2

Simple cubic

$\vec{d}_1 = 0$

$\vec{d}_2 = \frac{a}{2}(111)$

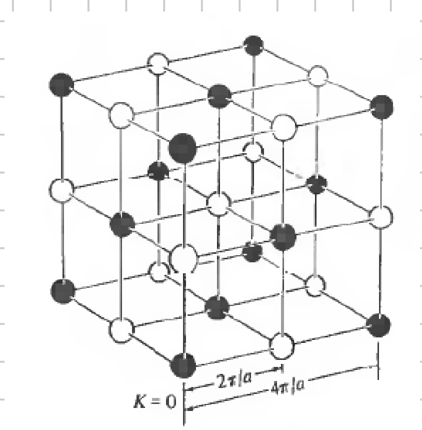
$$\vec{K} = \frac{2\pi}{a}\left(m_1\hat{x} + m_2\hat{y} + m_3\hat{z}\right)$$

$$S(\vec{K}) = f_1 + f_2\, e^{i\frac{\cancel{2}\pi}{\cancel{a}}\cdot\frac{\cancel{a}}{\cancel{2}}(m_1+m_2+m_3)}$$

$$S(\vec{K}) = f_1 + f_2\, e^{i\pi(m_1+m_2+m_3)}$$

$\nearrow$ $f_1 + f_2$ $\qquad$ $m_1+m_2+m_3$ even

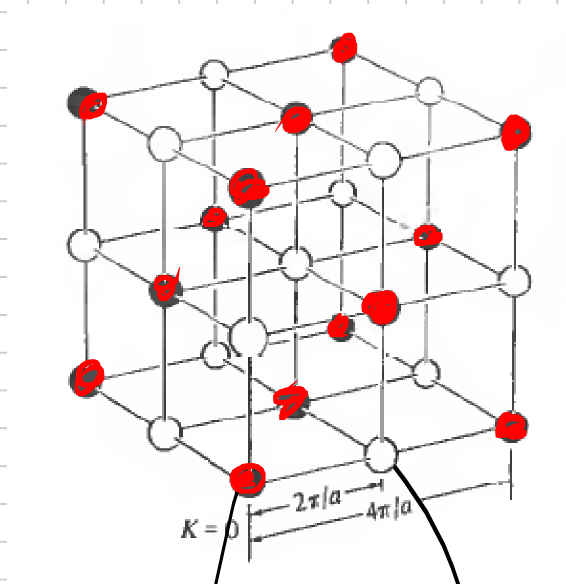
$\searrow$ $f_1 - f_2$ $\qquad$ $m_1+m_2+m_3$ odd



limit $f_1 = f_2$

$\downarrow$

FCC side $\frac{4\pi}{a}$



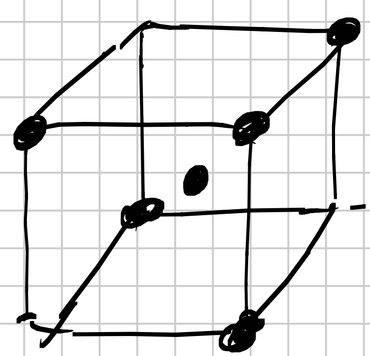
f_1+f_2 $\qquad$ f_1-f_2

DIAMOND

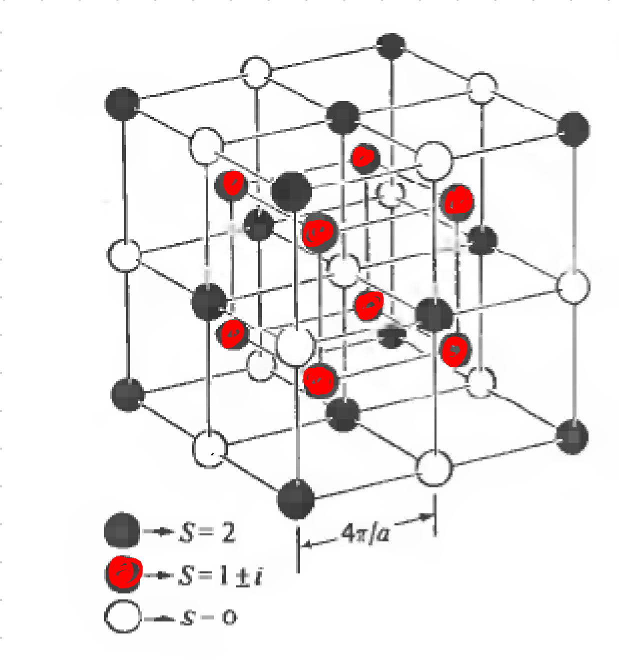
FCC side a
+
$d_1 = 0$
$d_2 = \frac{a}{4}(111)$

$\rightarrow$ BCC side $\frac{4\pi}{a}$

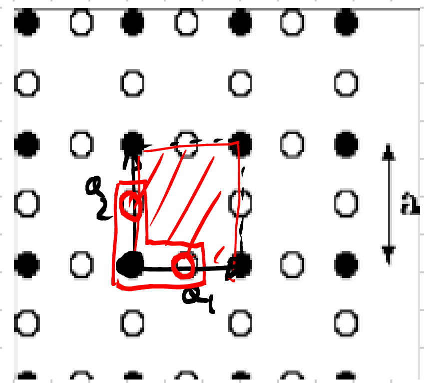
$S(K) \rightarrow 0$
$\rightarrow 1+i$
$\rightarrow 2$



0



CuO_2



$\vec{a}_1 = a(10)$

$\vec{a}_2 = a(01)$

$\vec{d} = 0 \qquad Cu$

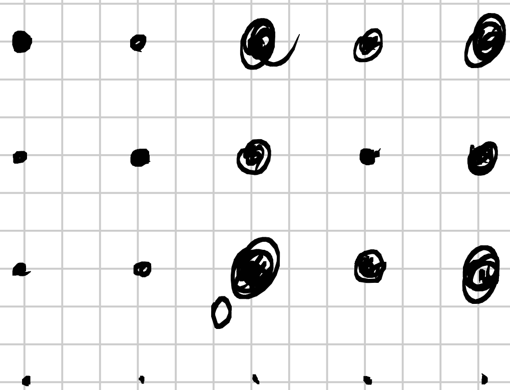
$\vec{d}_{O_1} = \frac{a}{2}(10)$

$\vec{d}_{O_2} = \frac{a}{2}(01)$

f_{Cu}

f_O

REC LATTICE



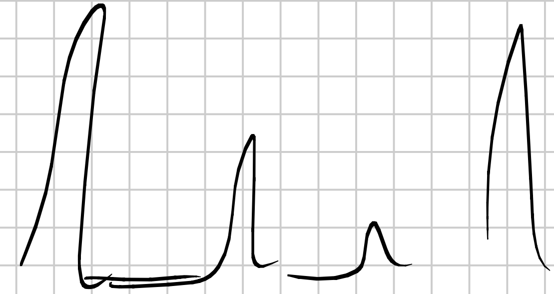
$$\vec{K} = \frac{2\pi}{a}(m_1 \hat{x} + m_2 \hat{y})$$

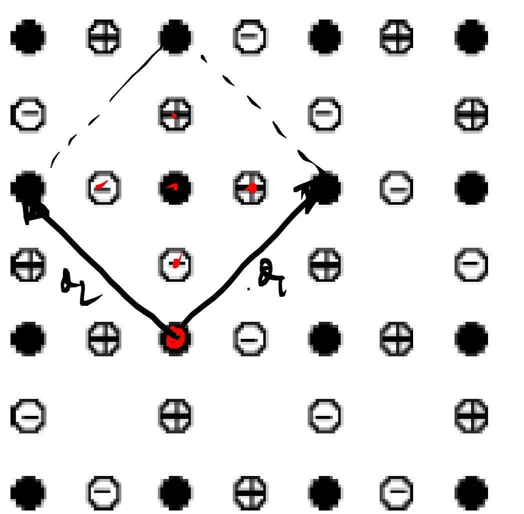
$$S(\vec{K}) = f_{Cu} + f_O\left(e^{i\pi m_1} + e^{i\pi m_2}\right)$$

$$\left.\begin{array}{l} m_1 = 1 \\ m_2 = 0 \end{array}\right\} \rightarrow \underline{\underline{f_{Cu}}}$$

n_1 & n_2 odd $\Big\}$ $f_{cu} - 2f_0$

n_1 & n_2 even $f_{cu} + 2f_0$



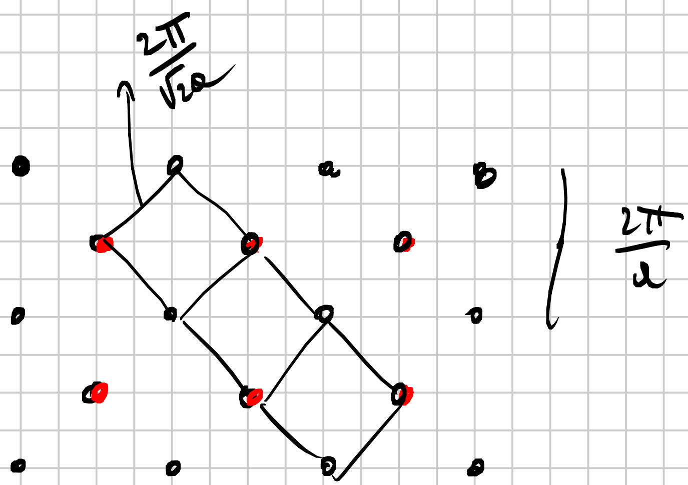


$\vec{a}_1 = a(1\,1)$ $\sqrt{2}\,a$

$\vec{a}_2 = a(-1\,1)$

6 ATOMS IN BASIS

SQUARE LATTICE



~~Chap 7~~

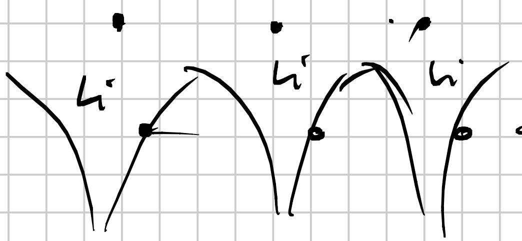
Chapt 8

Equilibrium position of nuclei → make lattice

ATOMS

Li → $(1s)^2 (2s)$ → last e^- moving in V_{ion} made out of $3p + 2e^-$ core

Li metal BCC lattice



→ $V_{ions}(\vec{r})$

↓

Problem of ONE electron

moving in V_{ion}

$$\left(-\frac{\hbar^2\nabla^2}{2m_e} - V_{ion}(\vec{r})\right)\psi(\vec{r}) = E\,\psi(\vec{r})$$

$$\boxed{V_{ion}(\vec{r}+\vec{R}_i) = V_{ion}(\vec{r})}$$

MOST IMPORTANT THEOREM IN SOLID STATE PHYSICS

BLOCH'S THEOREM

$$\begin{cases} \psi_{nk}(\vec{r}) = e^{ik\cdot\vec{r}}\,\underline{\underline{u_{nk}(\vec{r})}} & \text{with} \\ u_{nk}(\vec{r}+\vec{R}) = u_{nk}(\vec{r}) & \end{cases}$$

$\psi_{mk}(\vec{r})$ IS NOT PERIODIC

$$\boxed{\psi_{mk}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\,\psi_{mk}(\vec{r})}$$

What is $\vec{R}$

FREE ELECTRON $\frac{1}{\sqrt{V}}$

$$\boxed{L = Na}$$

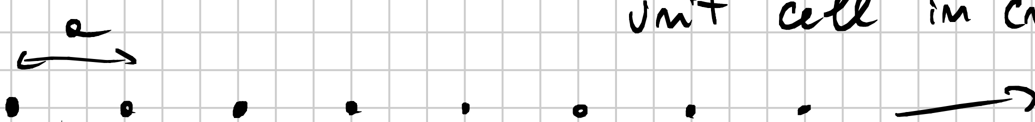
$K = m\frac{2\pi}{L}$

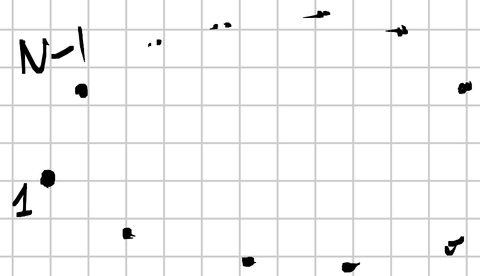
$e^{ik\cdot 0} = e^{iK\cdot L} = 1$

BORN-VON KARMANN
BOUNDARY CONDITION

1D

N total # of
unit cell in crystal





$$\psi_{nk}(x+Na) \equiv \psi_{nk}(x)$$

$$\psi_{nk}(x+Na) \overset{\text{Bloch}}{=} e^{iKNa}\,\psi_{nk}(x)$$

$$\Rightarrow e^{iKNa} = 1$$

Possible values for $k = \frac{2\pi}{Na} m$