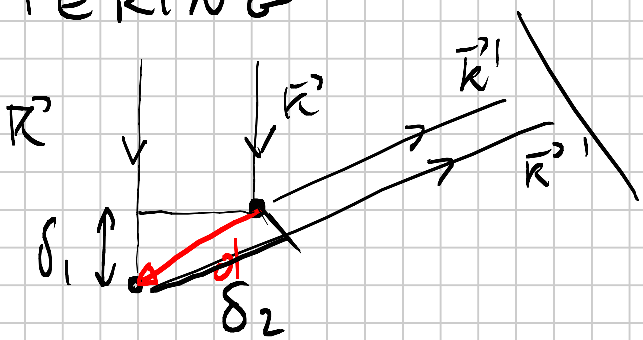
LECTURE # 12

Note Title 2/8/2010

LINK BETWEEN RECIPROCAL LATTICE AND X-RAY SCATTERING



δ = DIFFERENCE IN OPTICAL PATH

$$\delta = \delta_1 + \delta_2 = \frac{\vec{d} \cdot (\vec{k} - \vec{k}')}{|\vec{k}|}$$

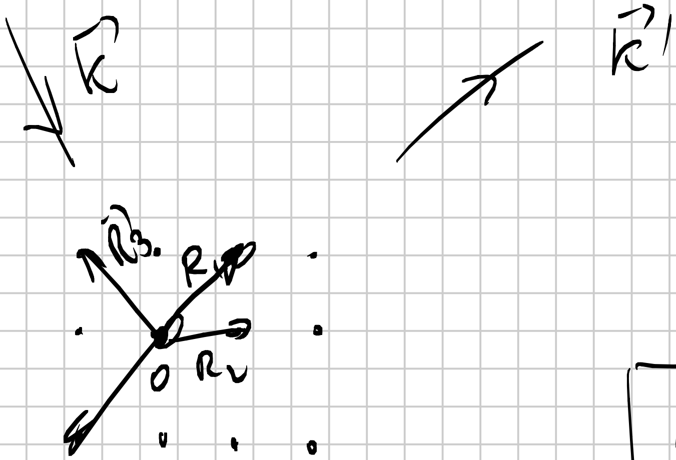
SCATTERING ELASTIC

$$|\vec{k}| = |\vec{k}'|$$

CONSTRUCTIVE INTERFERENCE

$$\delta = m\lambda$$

$$\vec{d} \cdot (\vec{k} - \vec{k}') = 2\pi m$$



$$\vec{R}_1 \cdot (\vec{k} - \vec{k}') = 2\pi m$$

$$\boxed{\vec{R}_i \cdot (\vec{k} - \vec{k}') = 2\pi m \qquad \forall \vec{R}_i}$$

CONDITION FOR CONSTRUCTIVE INTERFERENCE FROM <u>ALL</u> ATOMS IN A BRAVAIS LATTICE

$$(\vec{k} - \vec{k}') \cdot \vec{R}_i = 2\pi m \qquad \forall \vec{R}_i$$

$$\vec{K}_j \cdot \vec{R}_i = 2\pi m$$

DIFFRACTION PEAKS $\Longleftrightarrow$ $\vec{k} - \vec{k}'$ IS A VECTOR OF THE RECIPROCAL LATTICE

BRAGG PLANE

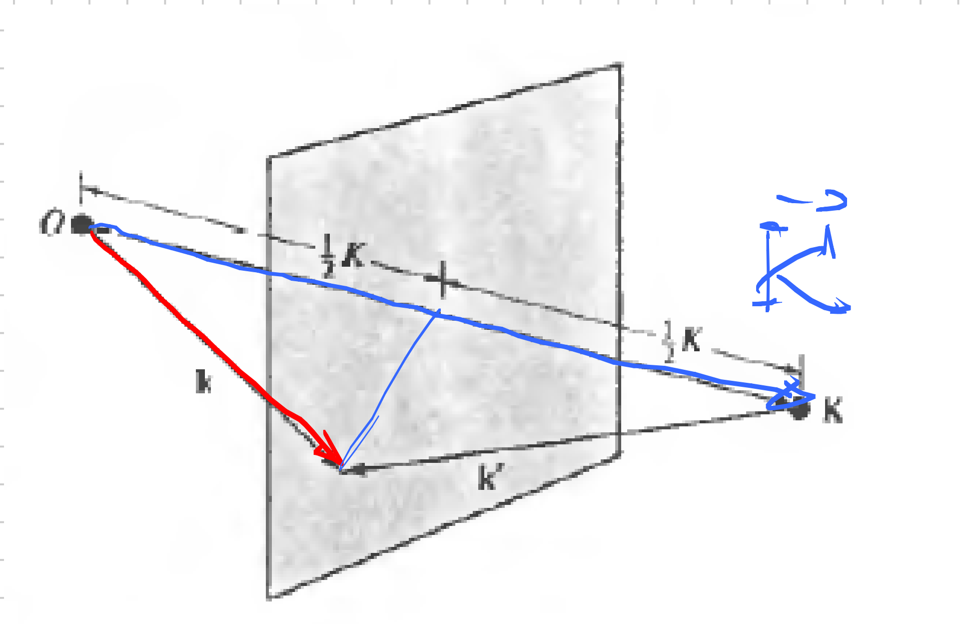
$$\vec{k} - \vec{k}' = \vec{K} \qquad |\vec{k}| = |\vec{k}'| \quad \text{ELASTIC}$$

$$|\vec{k}'| = |\vec{k} - \vec{K}| \rightarrow \cancel{|\vec{k}'|^2} = \cancel{|\vec{k}|^2} + |\vec{K}|^2 - 2\vec{k}\cdot\vec{K}$$

$$\boxed{\vec{k}\cdot\frac{\vec{K}}{|\vec{K}|} = \frac{|\vec{K}|}{2}}$$

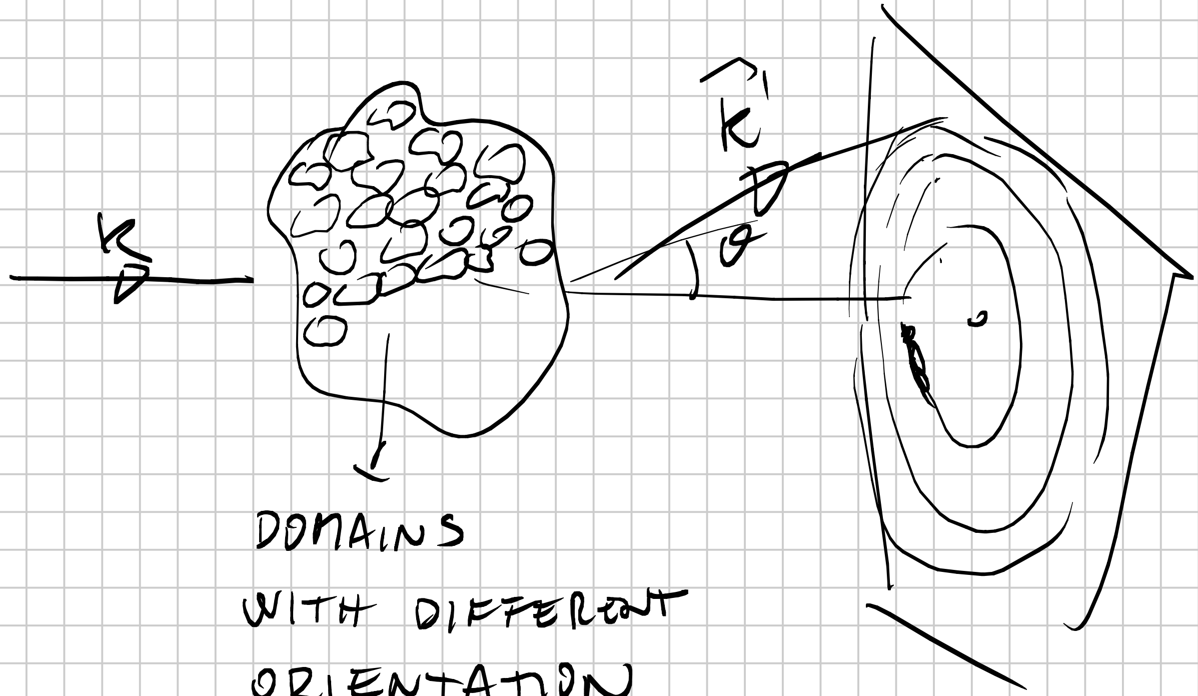
DEFINES A PLANE

BRAGG PLANE

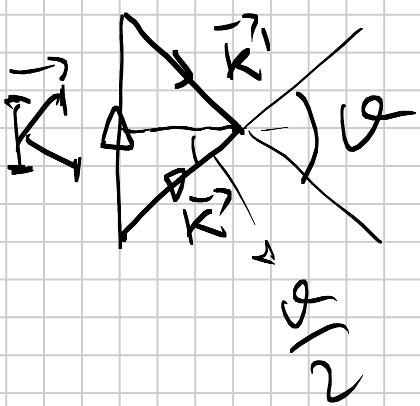


LINK 1° ST BRILLOUIN ZONE

1° BZ BOUNDARIES ARE DETERMINED BY BRAGG PLANES



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

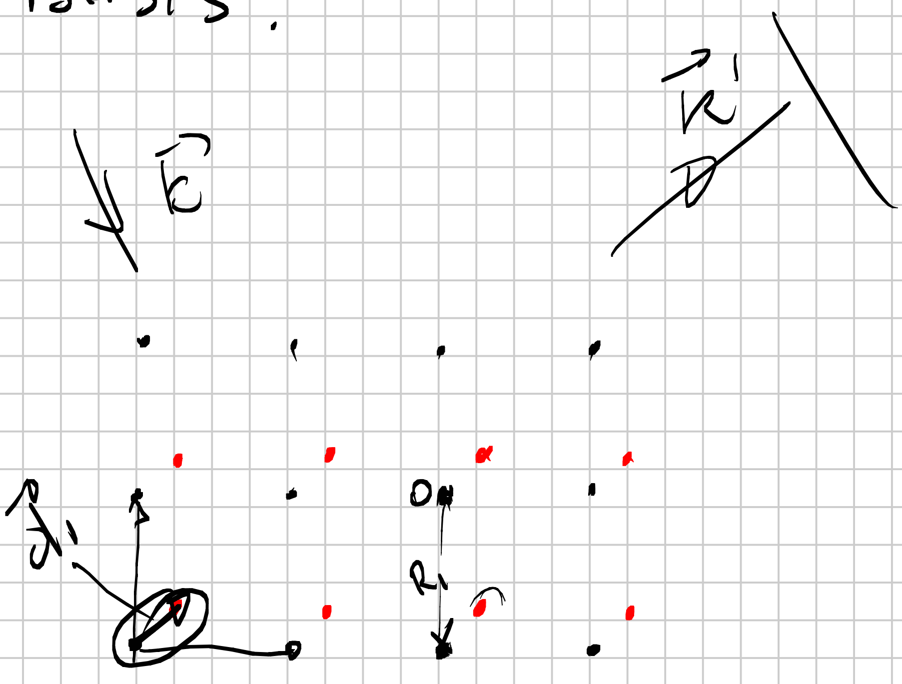


$$\underbrace{|\vec{k}|}_{\frac{2\pi}{\lambda}} \sin\frac{\theta}{2} = \frac{|\vec{K}|}{2}$$

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

$$\theta_i \to |\vec{K}|_i \to \text{IDENTIFY } |\vec{R}_i|$$

WHAT HAPPENS WHEN I HAVE A LATTICE WITH BASIS?



BASIS

$\vec{d} = 0$
$\vec{d} = \vec{d}_1$

$$A = e^{\overbrace{i(\vec{k}-\vec{k}')\cdot\vec{R}_1}^{\Delta \text{ OPTICAL PATH}}} +$$

$$+ e^{i(\vec{k}-\vec{k}')(\vec{R}+\vec{d}_1)}$$

ATOMIC STRUCTURE FACTOR

$$A = e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_1} \underbrace{\left(f_1 + f_2 e^{i(\vec{k}-\vec{k}')\cdot\vec{d}_1}\right)}_{S(\vec{k}-\vec{k}')}$$

$\downarrow$

STRUCTURE FACTOR

PEAK $\Rightarrow$ $e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_i} = 1 \quad \forall \vec{R}_i$

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

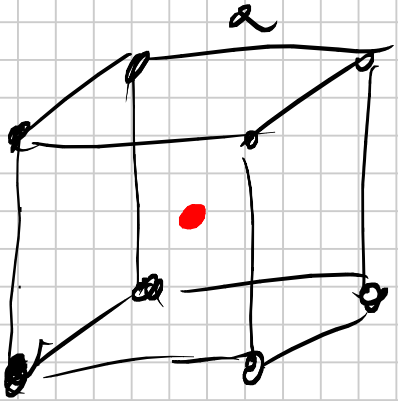
FOR EACH $\vec{K}$ I CAN HAVE DIFFERENT STRUCTURE FACTOR $S(\vec{K}) = f_1 + f_2 e^{i\vec{K}\cdot\vec{d}_1}$

ATOM $\bullet$ $\neq$ ATOM $\bullet$

WITH MANY ATOMS IN THE BASIS

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

SIMPLE CUBIC WITH 2 ATOM BASIS



$\vec{d}_B = 0$ $\qquad f_B$

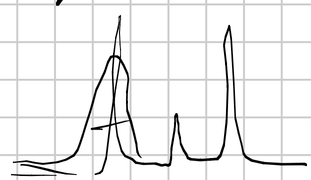
$\vec{d}_R = \frac{a}{2}(1,1,1)$ $\qquad f_R$

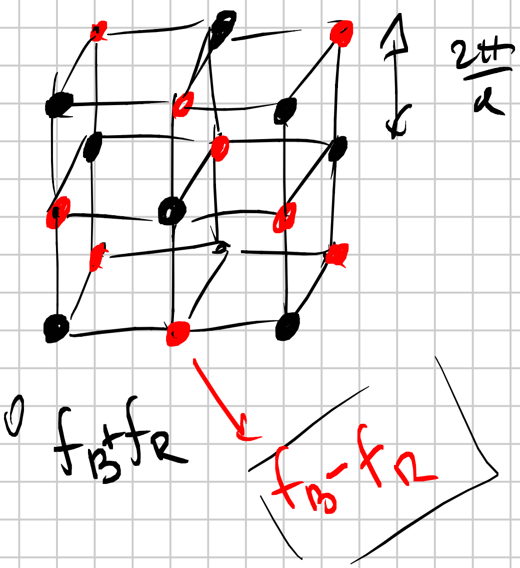
$$\vec{K} = m_1 \frac{2\pi}{a}\hat{x} + m_2 \frac{2\pi}{a}\hat{y} + m_3 \frac{2\pi}{a}\hat{z}$$

$$S(\vec{K}) = \left(f_B + f_R e^{i\vec{K}\cdot\vec{d}_R}\right) = \left(f_B + f_R e^{i\pi(m_1+m_2+m_3)}\right)$$

$\to f_B + f_R$ $\quad m_1+m_2+m_3$ EVEN

$\to f_B - f_R$ $\quad m_1+m_2+m_3$ ODD





LIMIT $\to$ $f_B = f_R$ $\to$ GET BCC

RED PEAKS DISAPPEAR

$\to$ REC LATTICE FCC OF SIDE $\frac{4\pi}{a}$

CHAP. 8

SYMMETRY LATTICE $\Longleftrightarrow$ ELECTRONIC STATES

BORN - OPPENHEIMER APPROX

e + IONS

SOLVE ELECTRONIC PROBLEM FOR IONS AT A FIXED POSITION

FIX POSITION OF IONS

NO e-e INTERACTION
(INDEPENDENT ELECTRON APPROX)

SINGLE e PROBLEM

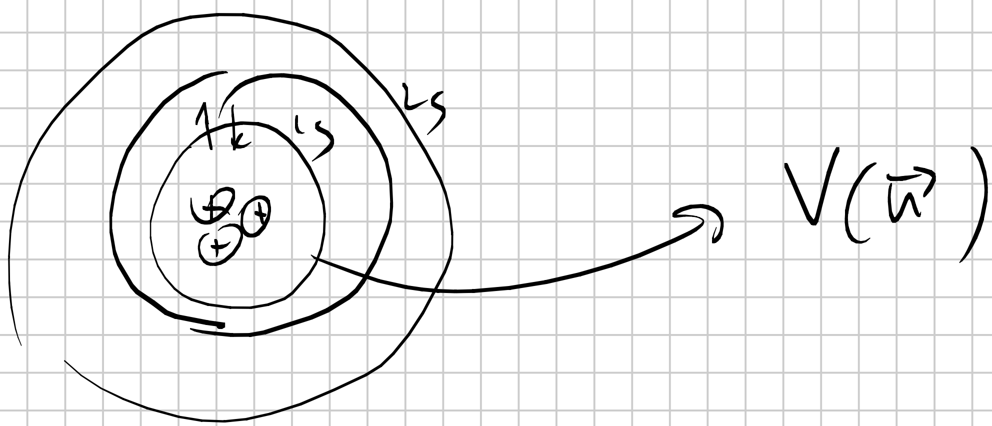
$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(\vec{r})\right)\psi_e(\vec{r}) = E\,\psi_e(\vec{r})$$

$V(\vec{r})$ HAS THE SYMMETRY OF THE LATTICE

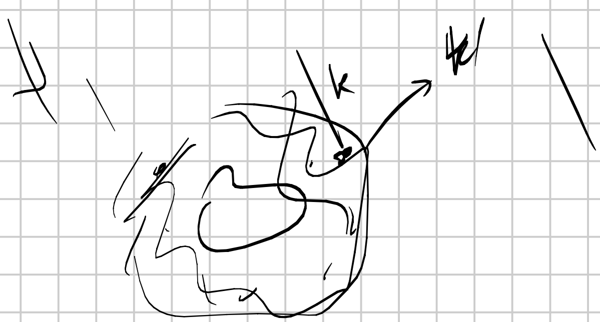
$$V(\vec{r}+\vec{R}_i) = V(\vec{r})$$

$V(\vec{r})$ EFFECTIVE POTENTIAL INCLUDING CORE ELECTRONS

Li $Z = 3$



$V(r)$ INCLUDE 2 ELECTRONS IN CLOSED SHELL



$$f(k) = \int dr\, \rho(r)\, e^{ikr}$$