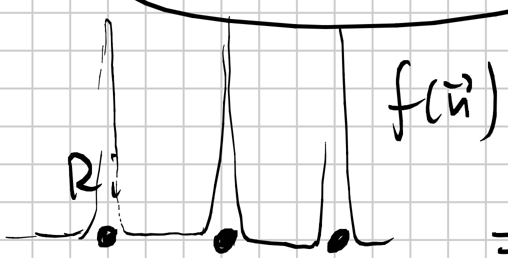
LECTURE # 10

Note Title 2/3/2010

REAL SPACE $\longleftrightarrow$ WAVE-VECTOR SPACE

DIRECT LATTICE $\longleftrightarrow$ RECIPROCAL LATTICE



$$\Rightarrow \quad f(\vec{r}) = \sum_i \delta(\vec{r} - \vec{R}_i)$$

$\{R_i\}$ IS A BRAVAIS LATTICE

$$\tilde{f}(\vec{k}) = \int e^{i\vec{k}\cdot\vec{r}} f(\vec{r})\, d\vec{r} = \int e^{i\vec{k}\cdot\vec{r}} \sum_{i \in \{R_i\}} \delta(\vec{r} - \vec{R}_i)\, d\vec{r} =$$

$$\sum_{i \in \{R_i\}} e^{ik\cdot\vec{R}_i}$$

$\rightarrow$ N (TOT # ATOMS) $\quad e^{i\vec{k}\cdot\vec{R}_i} = 1$ FOR ALL $\{R_i\}$

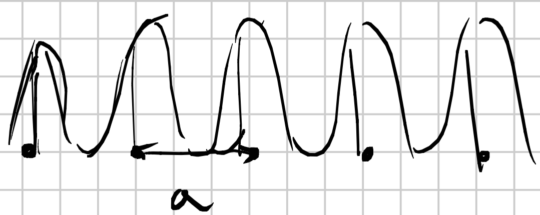
$\rightarrow$ 0 (SUM OF "NEARLY" RANDOM PHASES)

FIND $\vec{K}$ SUCH THAT $e^{i\vec{K}\cdot\vec{R}_i} = 1 \quad \forall\ \vec{R}_i$

$\{K_j\}$ MAKE A LATTICE IN WAVE-VECTOR SPACE

THIS IS THE RECIPROCAL LATTICE OF $\{\vec{R}_i\}$

$\{\vec{R}_i\}$ BRAVAIS $\Rightarrow$ $\{K_j\}$ ALSO MAKE A BRAVAIS



$e^{i\frac{2\pi}{a}ma} = 1 \qquad \frac{2\pi}{a} = K$

$\lambda = \frac{2\pi}{K}$

$\{R_i\} \Rightarrow e^{i\vec{K}_j\cdot\vec{R}_i} = 1 \Rightarrow \vec{K}_j\cdot\vec{R}_i = 2\pi m$

$m \in \mathbb{Z}$

$\{\vec{K}_J\}$ IS A BRAVAIS LATTICE $\Rightarrow$ I CAN FIND

$\vec{b}_1, \vec{b}_2, \vec{b}_3$ PRIMITIVE VECTORS

$$\vec{K}_J = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3 \qquad m_i \in \mathbb{Z}$$

GIVEN $\vec{a}_1, \vec{a}_2, \vec{a}_3 \Rightarrow$ HOW DO YOU FIND $\vec{b}_1, \vec{b}_2, \vec{b}_3$?

$$\vec{R}_i \cdot \vec{b}_1 = 2\pi m \qquad \forall \vec{R}_i$$

$$(m_1 \vec{a}_1 + \underbrace{m_2 \vec{a}_2}_{=0} + \underbrace{m_3 \vec{a}_3) \cdot \vec{b}_1}_{=0} = 2\pi m_1$$

$$\begin{cases} \vec{a}_1 \cdot \vec{b}_1 = 2\pi \\ \vec{b}_1 \perp \text{ TO } \vec{a}_2 \text{ AND } \vec{a}_3 \end{cases}$$

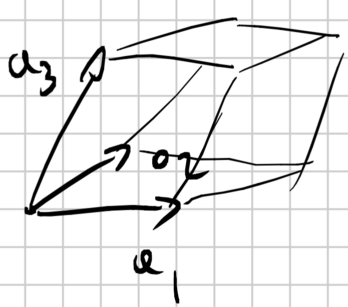
$$\vec{b}_1 = c \cdot \vec{a}_2 \times \vec{a}_3$$

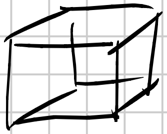
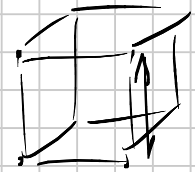
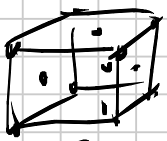
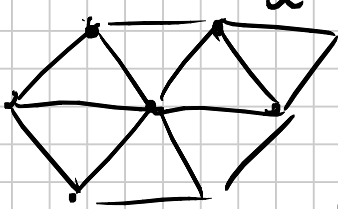
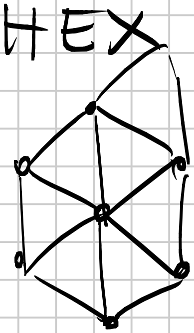
$$\vec{b}_1 \cdot \vec{a}_1 = 2\pi \quad \Rightarrow \quad c\,(\vec{a}_2 \times \vec{a}_3) \cdot \vec{a}_1 = 2\pi$$

$$c = \frac{2\pi}{|(\vec{a}_2 \times \vec{a}_3) \cdot \vec{a}_1|} \qquad \vec{b}_1 = \frac{2\pi}{|(\vec{a}_2 \times \vec{a}_3) \cdot \vec{a}_1|}\, \vec{a}_2 \times \vec{a}_3$$

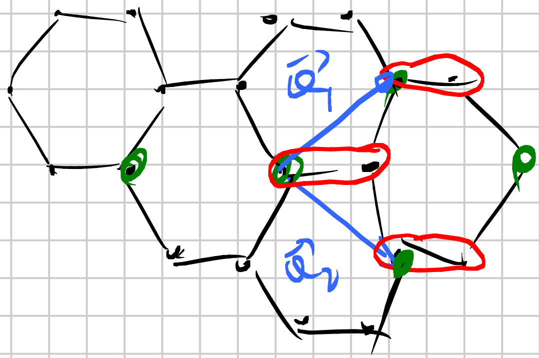
$$\vec{b}_i = \frac{2\pi}{|(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3|}\, \vec{a}_j \times \vec{a}_k \qquad i, j, k \in \{1, 2, 3\}$$

$|(\vec{a}_1 \times \vec{a}_2) \cdot \vec{a}_3| \rightarrow$ VOLUME OF PRIMITIVE CELL IN THE DIRECT LATTICE



DIRECT		RECIPROCAL LATTICE
SIMPLE CUBIC		SIMPLE CUBIC
 a		 $\frac{2\pi}{a}$
FCC	$\longrightarrow$	BCC
SIDE a		SIDE $\frac{4\pi}{a}$
 a		
BCC	$\longrightarrow$	FCC
SIDE a		SIDE $\frac{4\pi}{a}$
HEX	$\longrightarrow$	HEX
a  c DISTANT LAYERS		 $b = \frac{4\pi}{a\sqrt{3}}$ $\frac{2\pi}{c}$ SEPARATION LAYERS

WHAT HAPPENS IF YOU HAVE A BASIS

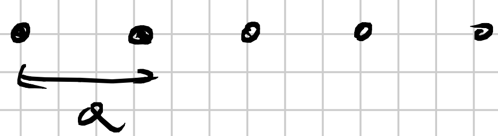


RECIPROCAL LATTICE IS DETERMINED BY $\vec{a}_1$ & $\vec{a}_2$

SAME AS IF YOU DID NOT HAVE A BASIS

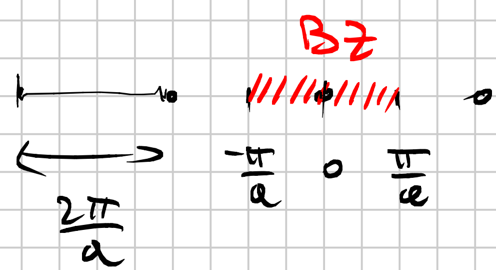
FIRST BRILLOUIN ZONE $\equiv$ WIGNER-SEITZ UNIT CELL FOR THE RECIPROCAL LATTICE

1D DIRECT

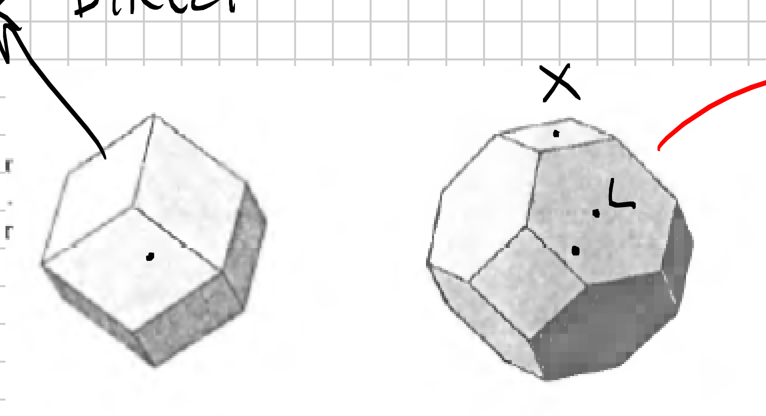


$\longrightarrow$

RECIPROCAL



BCC DIRECT



(a) (b)

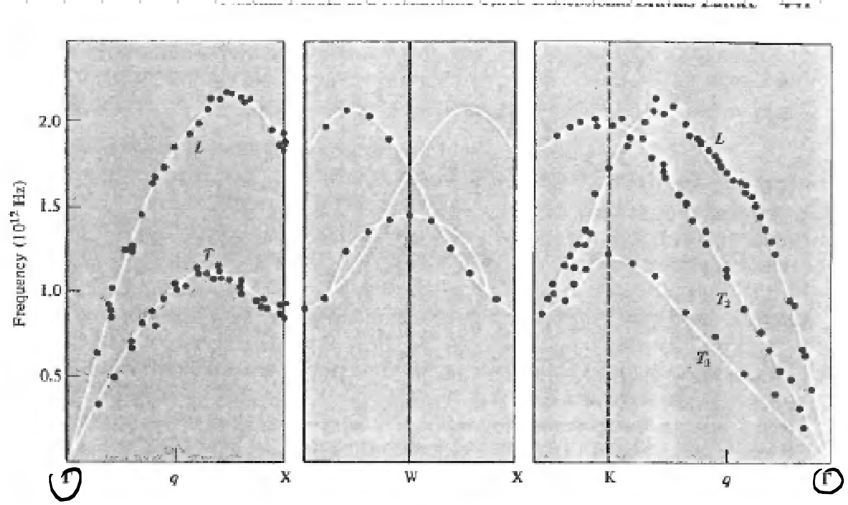
1° BZ FOR FCC REAL SPACE

CENTER OF BZ

Γ

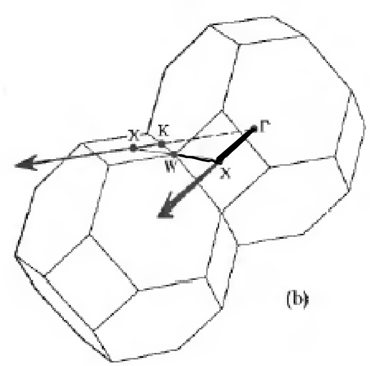
$$L = \frac{\pi}{a}(1,1,1)$$

$$X = \frac{2\pi}{a}(1,0,0)$$

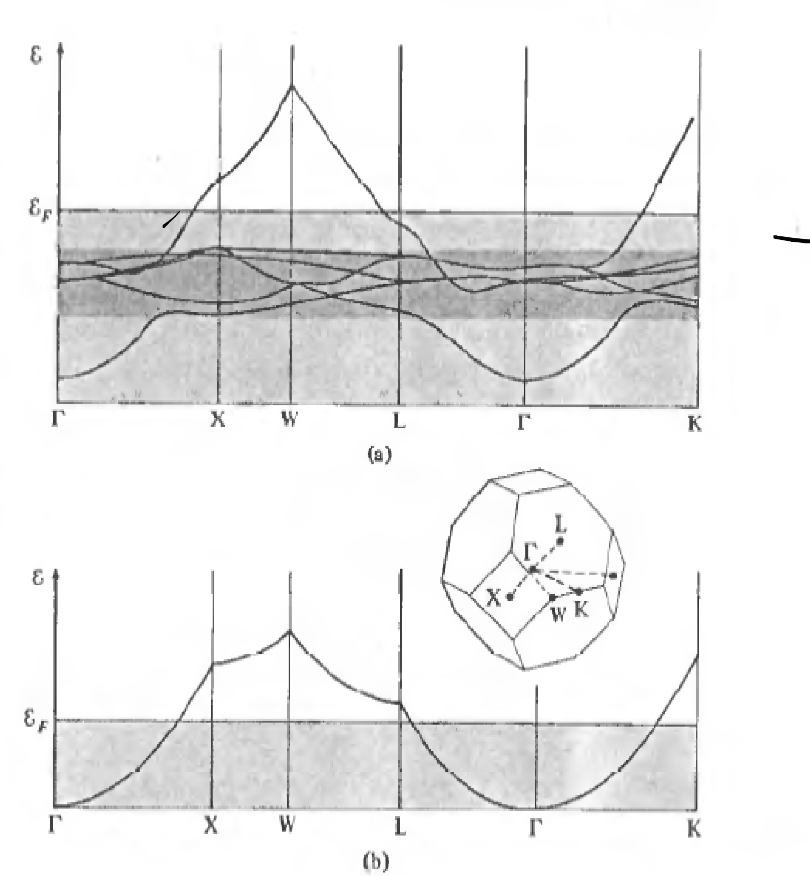


(a)

→ PHONONS



(b)

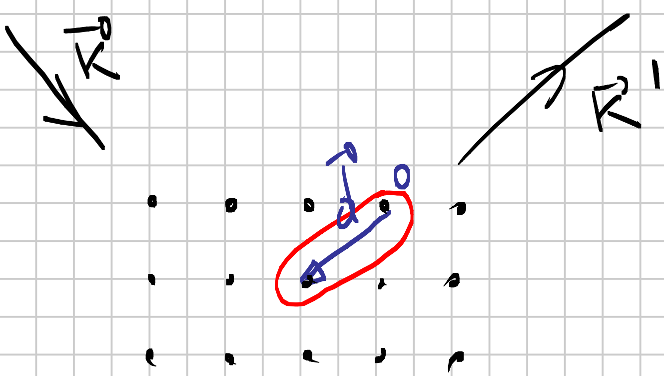


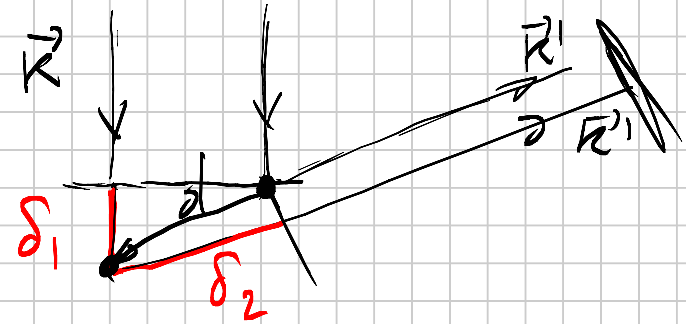
(a)

(b)

→ ELECTRONIC STATES

LINK OF RECIPROCAL LATTICE WITH SCATTERING





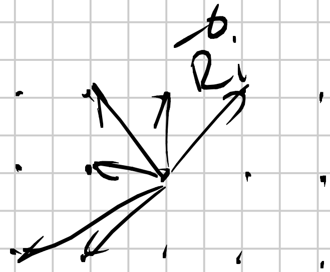
$\Delta = \delta_1 + \delta_2$ DIFFERENCE OPTICAL PATH $= \vec{d} \cdot \dfrac{\vec{k}}{|\vec{k}|} - \vec{d} \cdot \dfrac{\vec{k}'}{|\vec{k}'|}$

SCATTERING <u>ELASTIC</u> $\dfrac{2\pi}{|\vec{k}|} = \dfrac{2\pi}{|\vec{k}'|}$ $\quad |\vec{k}| = |\vec{k}'|$

CONSTRUCTIVE INTERFERENCE IF:

$$\Delta = m\lambda = m \cdot \frac{2\pi}{|\vec{k}|} \Rightarrow d \cdot \frac{\vec{k}}{\cancel{|\vec{k}|}} - \vec{d} \cdot \frac{\vec{k}'}{\cancel{|\vec{k}|}} = m \frac{2\pi}{\cancel{|\vec{k}|}}$$

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



$\Rightarrow$ CONSTRUCTIVE INTERF

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

$$\Rightarrow \boxed{\vec{k} - \vec{k}' \in \{\vec{K}_J\}}$$