LECTURE #12

Note Title 2/9/2009

BRAVAIS / LATTICE WITH BASIS

RECIPROCAL LATTICE

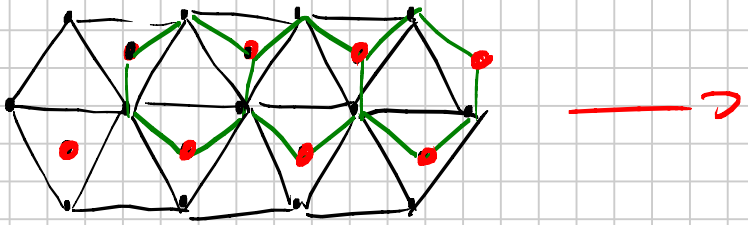
$\vec{a}_1, \vec{a}_2, \vec{a}_3 \longrightarrow \vec{b}_1, \vec{b}_2, \vec{b}_3$

(R) (K)

$\vec{b}_i \cdot \vec{a}_j = 2\pi \delta_{ij}$

WHAT IS RECIPROCAL LATTICE IF YOU HAVE A BASIS?

$\vec{a}_1 \ \vec{a}_2 \ \vec{a}_3$



2 HEXAGONAL REAL

$\vec{b}_1 \ \vec{b}_2 \ \vec{b}_3$

SAME AS FOR THE SIMPLE HEXAGONAL

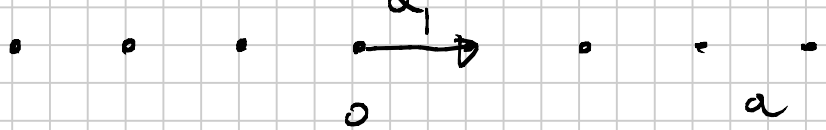
SAME AS IF YOU DID NOT HAVE A BASIS

BRILLOUIN ZONE ≡ WIGNER-SEITZ

UNIT CELL FOR THE RECIPROCAL LATTICE

1D

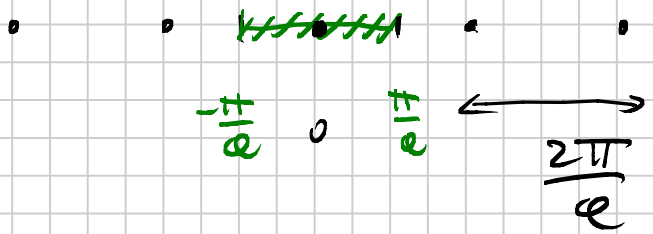
DIRECT



$a_1 \cdot b_1 = 2\pi$

$b_1 = \frac{2\pi}{a}$

RECIPROCAL

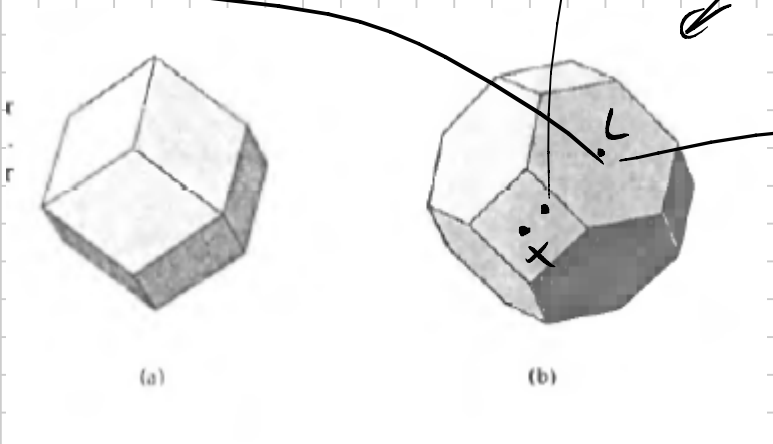


T POINT CENTER

DIAMOND FCC BCC REAL RECIPROCAL

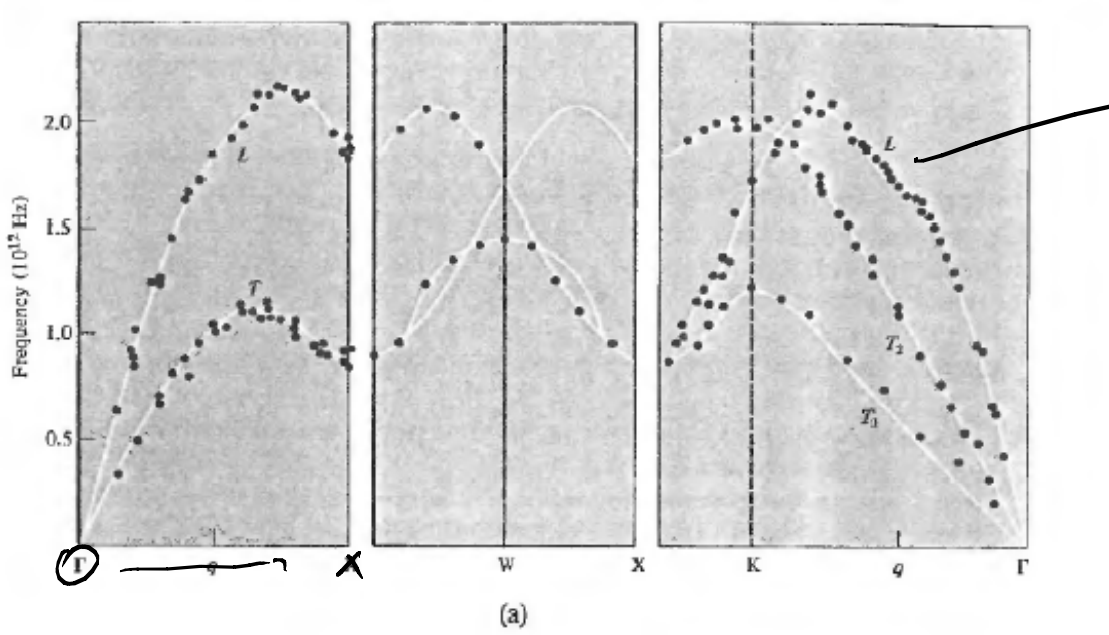
$L = \frac{\pi}{a}(1,1,1)$

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

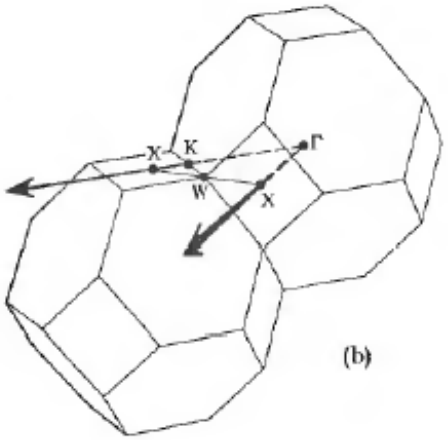


TRUNCATED OCTAHEDRON

8 NEIGHBORS IN THE REC LATTICE

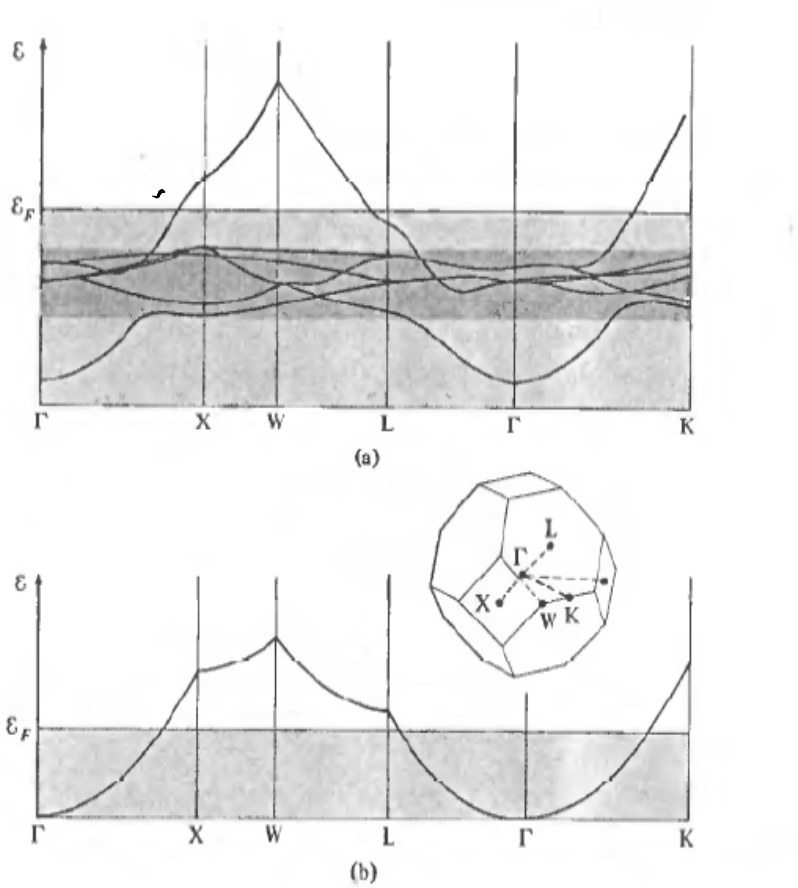


(a)



(b)

→ ENERGY OF PHONONS

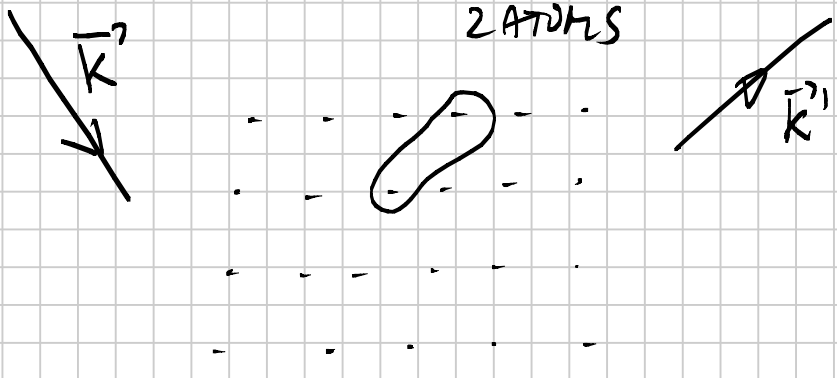


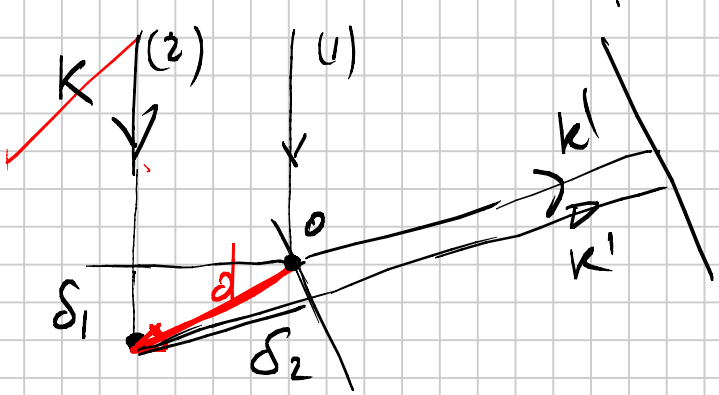
ELECTRONIC LEVELS

BRILLOUIN ZONE

SAME

WHY RECIPROCAL LATTICE?





δ = DIFFERENCE IN OPTICAL PATH

$$\delta = n\lambda$$

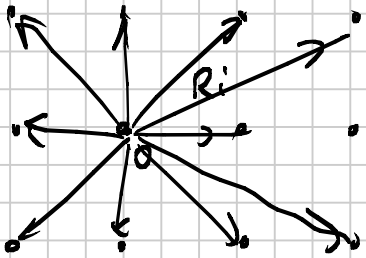
$$\lambda = \frac{2\pi}{|k|} = \text{WAVELENGTH}$$

$$\delta = \delta_1 + \delta_2 = \vec{d}\cdot\frac{\vec{k}}{|\vec{k}|} - \vec{d}\cdot\frac{\vec{k}'}{|\vec{k}'|} = n\frac{2\pi}{|k|}$$

ELASTIC SCATTERING

$$\frac{2\pi}{|k|} = \frac{2\pi}{|k'|}$$

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



$$\vec{R}_i\cdot(\vec{k}-\vec{k}') = 2\pi n \quad \forall\, \vec{R}_i$$

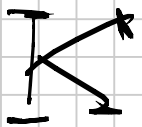
CONDITION FOR CONSTRUCTIVE INTERFERENCE FROM ALL ATOMS IN THE CRYSTAL

REC LATTICE $\{\vec{K}_J\}$ $\vec{K}_J \cdot \vec{R}_i^0 = 2\pi m$

DIFFRACTION PEAK EXISTS

$\Longrightarrow$

$\vec{K} - \vec{K}'$ IS A VECTOR OF THE RECIPROCAL LATTICE



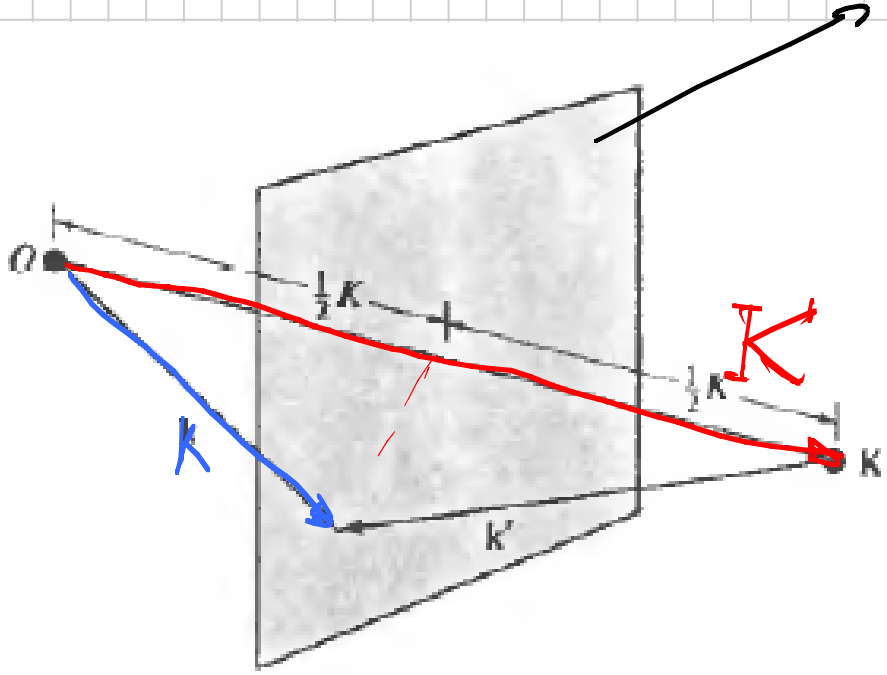
BRAGG PLANE

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

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

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

BRAGG PLANE

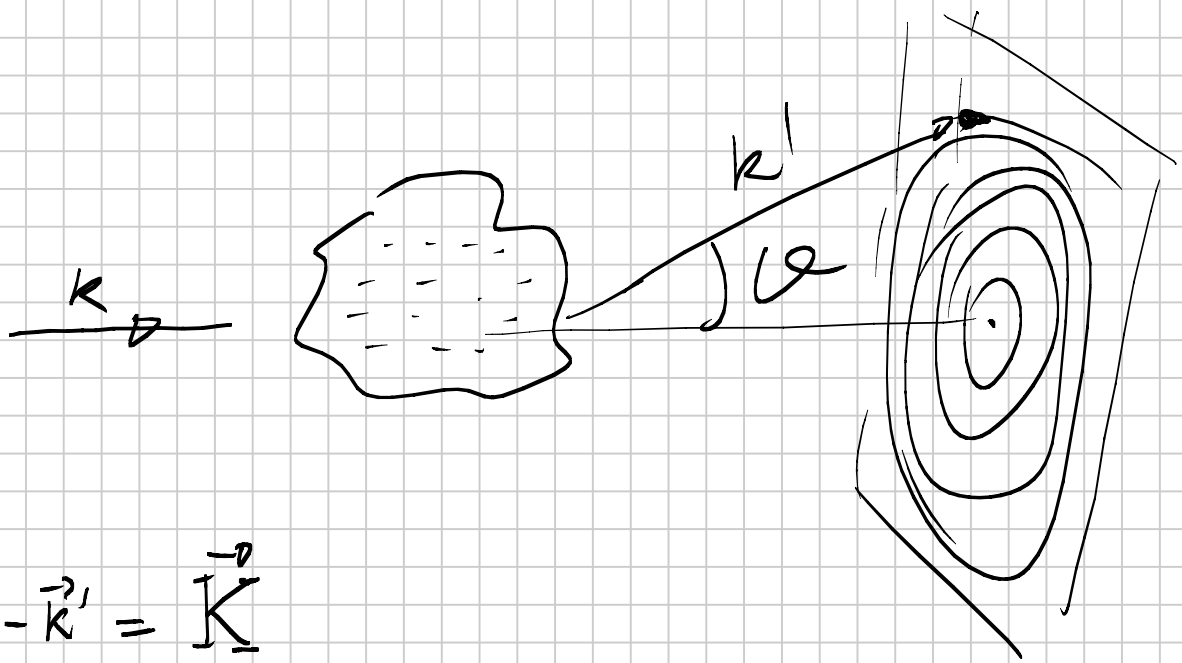


IF $K \in$ BRAGG PLANE

⇓

PEAK IN DIFFRACTION

BRILLOUIN ZONE BOUNDARIES ARE MADE OUT OF BRAGG PLANES



FROM ANGLES

θ_i

⇓

VALUES OF

$|\vec{K}_i|$

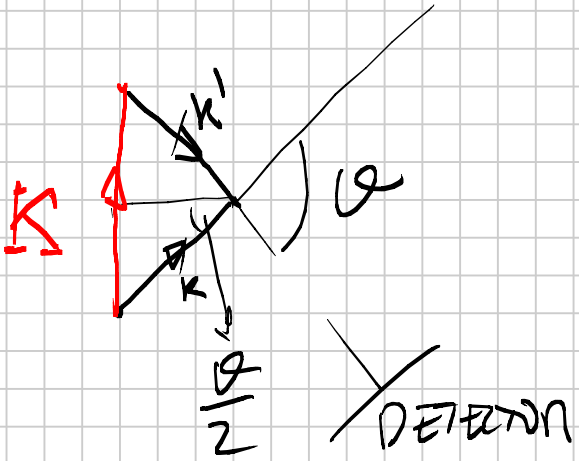
⇓

STRUCTURE OF RECIPROCAL LATTICE

⇓

STRUCTURE OF REAL LATTICE

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



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