

# LECTURE # 14

Note Title

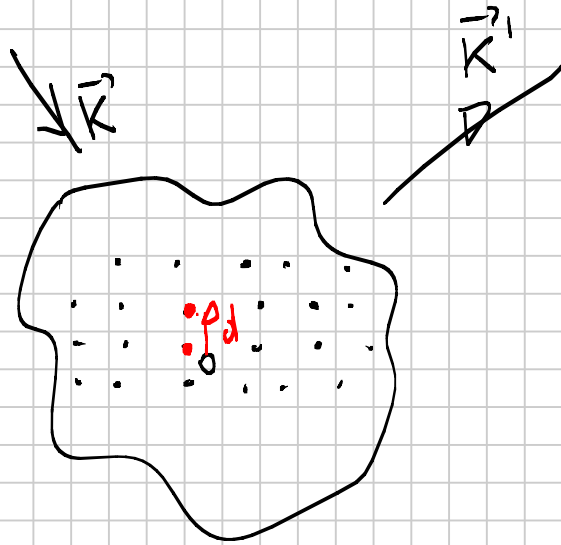
10/20/2008

Chapt 6

FOR 2 ATOMS, CONSTRUCTIVE INTERFERENCE IF

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

$\{\vec{R}_i\}$  GIVEN



FOR CRYSTAL, CONSTRUCTIVE INTERFERENCE FROM ALL ATOMS IF

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

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

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

$e^{i\vec{K} \cdot \vec{r}}$  WAVE WITH LATTICE SYMMETRY

$\{\vec{R}_i\}$  REAL SPACE

$\{\vec{K}_j\}$  WAVE-VECTOR SPACE

RECIPROCAL LATTICE CAN BE SEEN AS A

"FOURIER TRANSFORM" OF A DIRECT LATTICE



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

$$g(\vec{k}) = \int d^3\vec{r} e^{i\vec{k} \cdot \vec{r}} f(\vec{r}) = \int d^3\vec{r} e^{i\vec{k} \cdot \vec{r}} \sum_i \delta(\vec{r} - \vec{R}_i) =$$

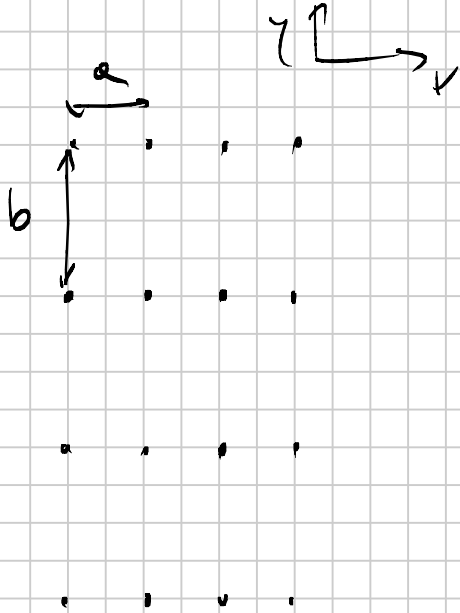
$$= \sum_i e^{i\vec{k} \cdot \vec{R}_i} \begin{cases} \infty & \text{IF } \vec{k} \cdot \vec{R}_i = 2\pi m \quad \forall R_i \\ 0 & \text{IF } \vec{k} \notin \text{RECIPROCAL LATTICE} \end{cases}$$

OTHERWISE

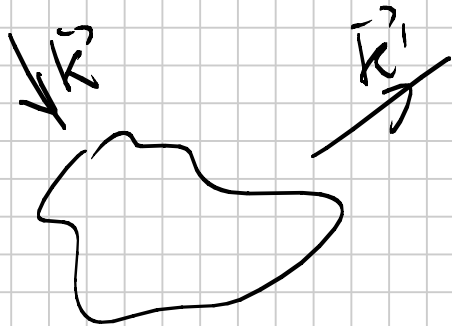
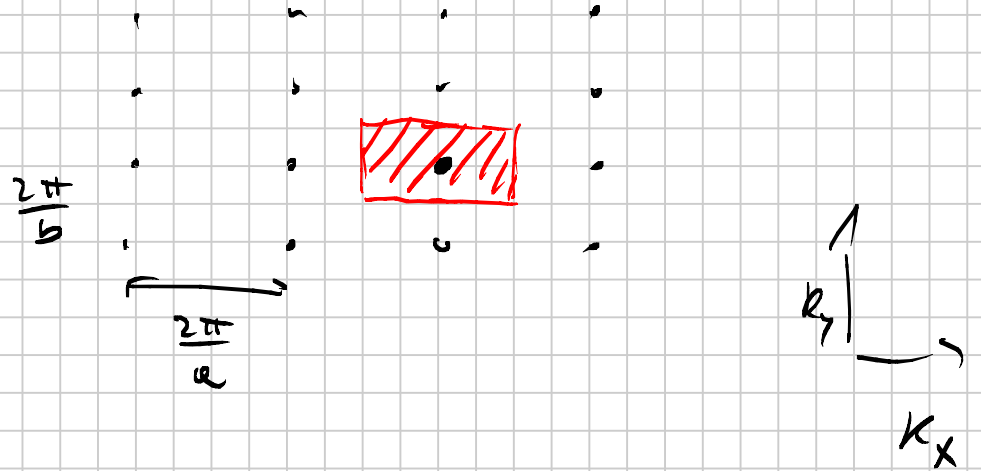
$$\Rightarrow g(\vec{k}) = \sum_J \delta(\vec{k} - \vec{K}_J) \quad \left\{ \vec{K}_J \right\} \text{ RECIPROCAL LATTICE}$$

# 1<sup>o</sup> BRILLOUIN ZONE

DIRECT LATTICE



REC LATTICE



ELASTIC SCATTERING

$$|\vec{K}| = |\vec{K}'| \quad \lambda = \lambda'$$

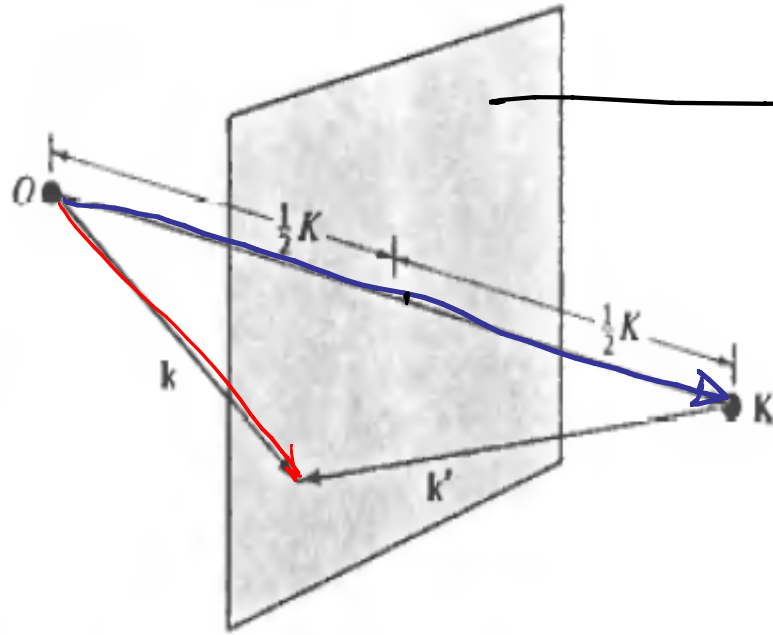
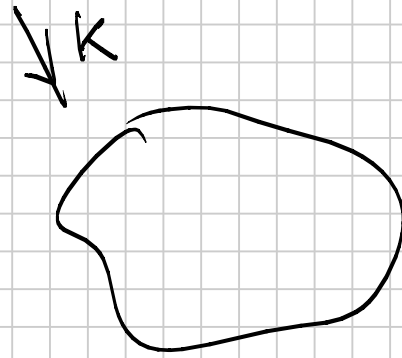
PEAK

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

$$\vec{k}' = \vec{k} - \vec{K} \quad \Rightarrow \quad |\vec{k}'|^2 = |\vec{k}|^2 + |\vec{K}|^2 - 2\vec{k} \cdot \vec{K}$$

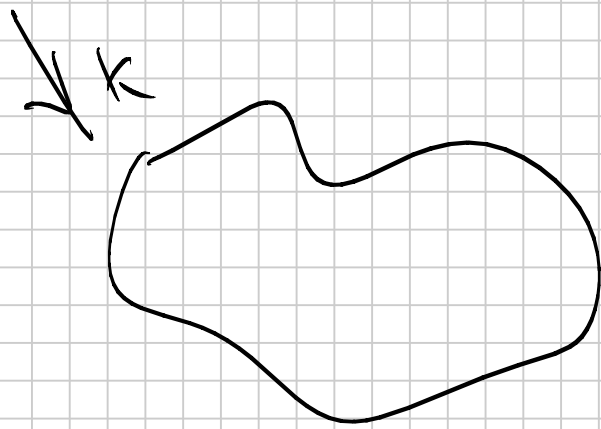
↓

$$\vec{k} \cdot \vec{k} = \frac{|\vec{k}|^2}{2}$$



BRAGG PLANE

k WILL GIVE  
PEAK ONLY IF  
k BELONGS TO  
A BRAGG PLANE



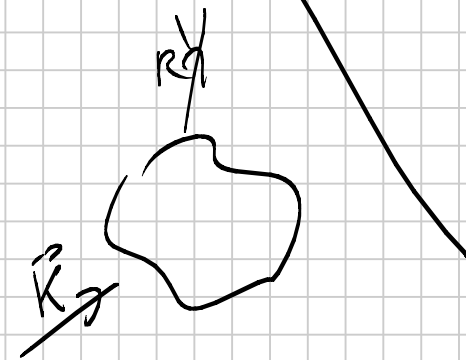
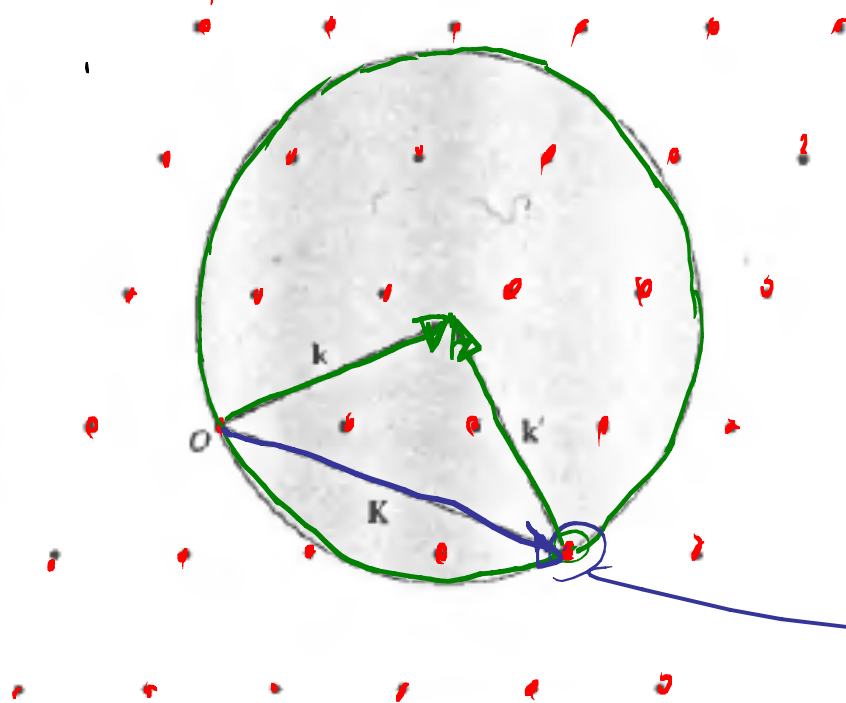
IN THE MOST GENERAL  
CASE  $\vec{k}$  IS NOT ON  
A BRAGG PLANE  
 $\Rightarrow$  NO PEAKS

HOW DO I LOOK FOR PEAKS?

- ① CHANGE  $\lambda$ , CHANGE  $|\vec{k}|$
- ② CHANGE ANGLE (ROTATE SAMPLE)

EWALD'S CONSTRUCTION

# RECIPROCAL LATTICE OF SAMPLE

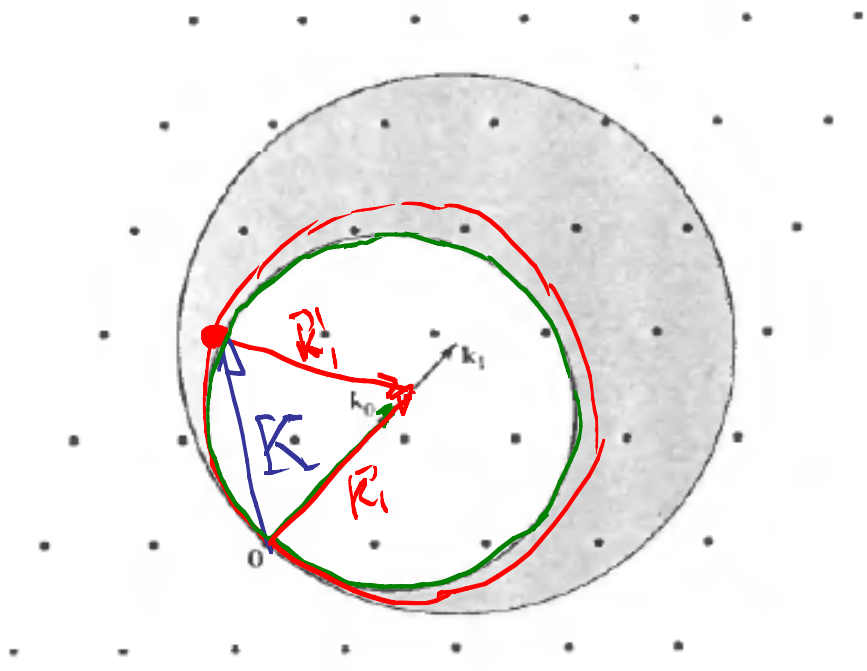


$$\vec{k} - \vec{k}' = \vec{K}$$

WILL GIVE A  
PEAK

VON-LAVE METHOD :

I CHANGE  $\lambda$

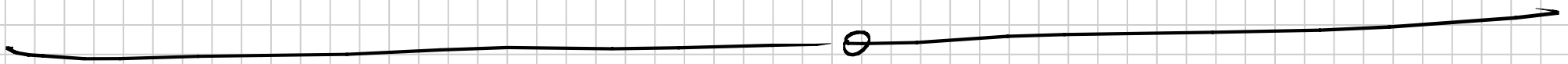


$k_0$  GIVES NO  
PEAK

SMALLER  $\lambda$

USE  $k_1'$

PEAK IN  $k_1'$



II ROTATE SAMPLE

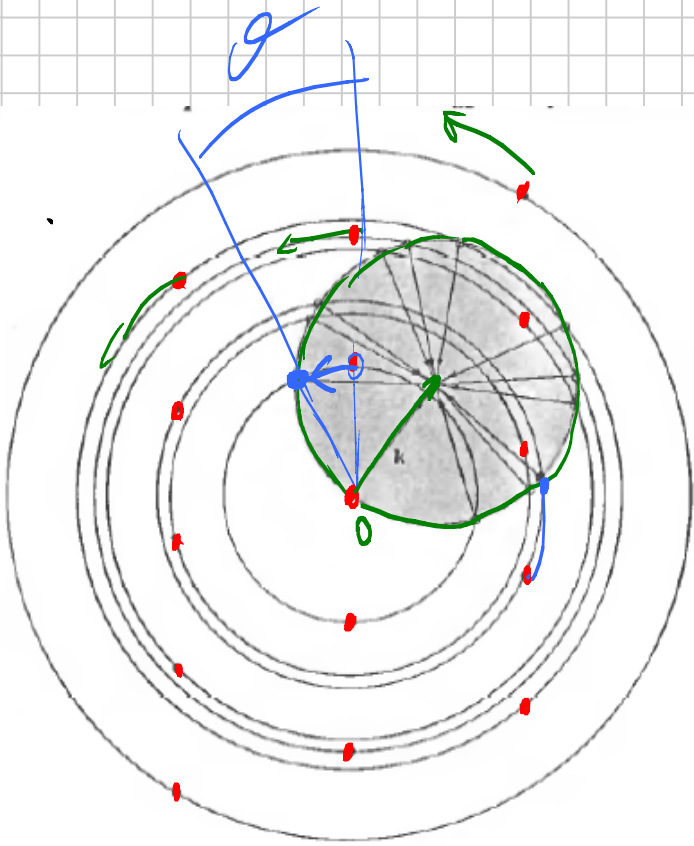
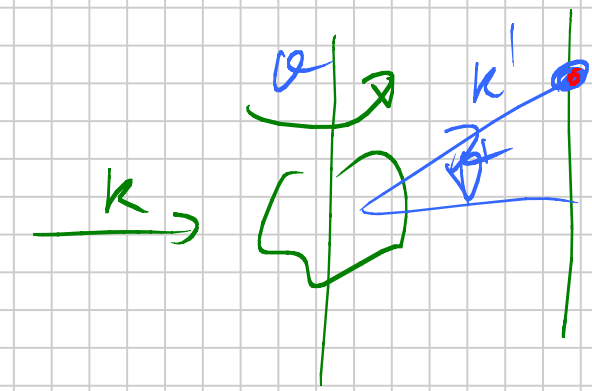
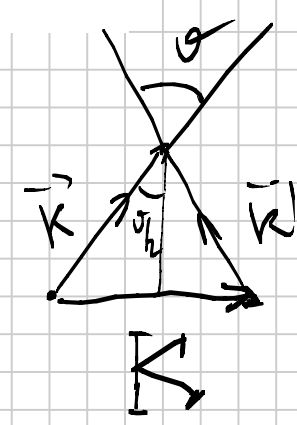


Figure 6.9

$\vec{k}$  FIXED  
NO PEAKS



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



$$|\vec{k}| \sin \frac{\varphi}{2} = \left| \frac{\vec{K}}{2} \right|$$

GIVEN  $\vec{k} \Rightarrow$  MEASURE  $\varphi_i \Rightarrow |\vec{K}_i| \Rightarrow$  STRUCTURE



# POLYCRYSTALLINE SAMPLE

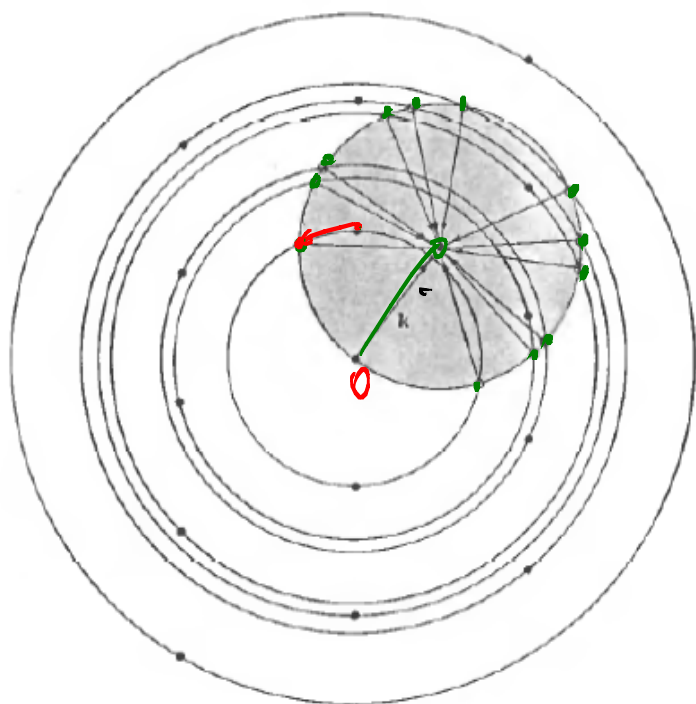
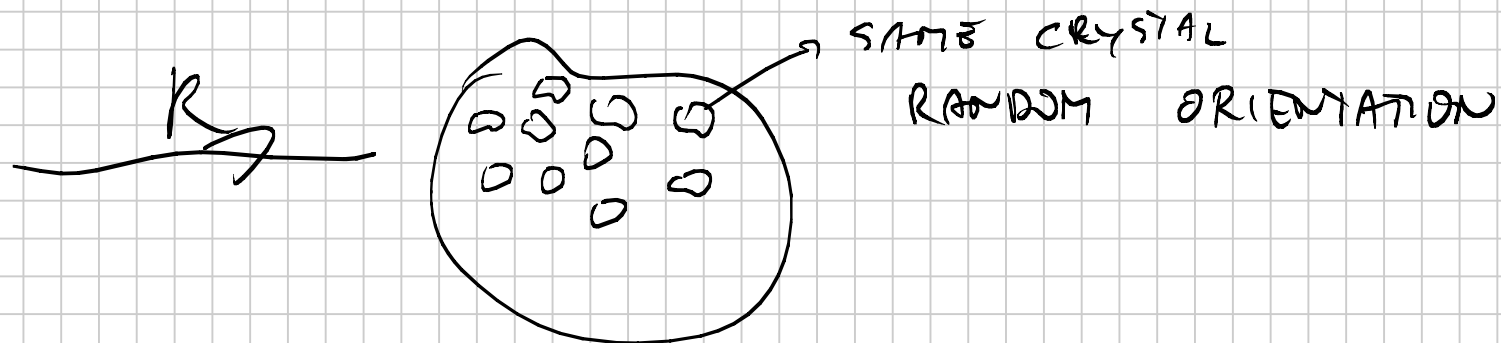
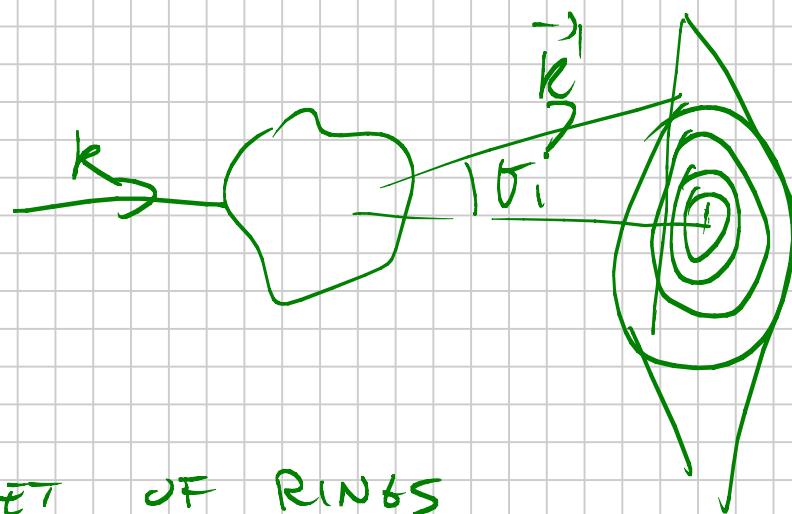


Figure 6.9

ALL POSSIBLE  
 $\vartheta$  AT THE SAME  
 TIME



SET OF RINGS

