PAPER-A: CONDENSED MATTER PHYSICS
(B.Sc. Semester-V)

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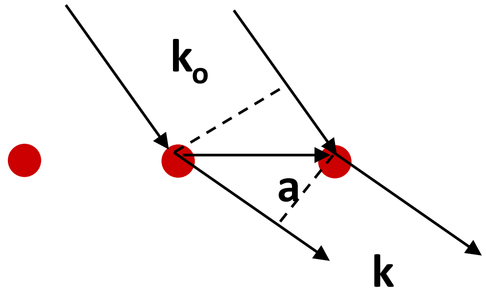
- ❑Laue equations,
- ❑Reciprocal lattices & its Properties

Laue conditions

$$\Psi(\vec{r}) = Ae^{2\pi i\vec{k}\cdot\vec{r}} \qquad k = \frac{1}{\lambda}$$

Scattering from a periodic distribution of scatters along the **a** axis



The scattered wave will be in phase and constructive interference
will occur if the phase difference is 2π.

$\Phi=2\pi\mathbf{a}\cdot(\mathbf{k}-\mathbf{k}_o)=2\pi\mathbf{a}\cdot\mathbf{g}= 2\pi h$, similar for **b** and **c**

$$\vec{g}_{hkl} = h\overrightarrow{a^*} + k\overrightarrow{b^*} + l\overrightarrow{c^*}$$

The Laue equations

The **Laue equations** give three conditions for incident waves to be diffracted by a crystal lattice

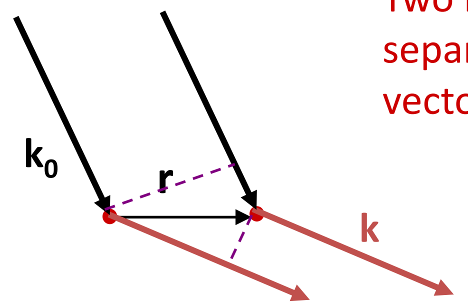
- Waves scattered from two lattice points separated by a vector **r** will have a path difference in a given direction.
- The scattered waves will be in phase and constructive interference will occur if the phase difference is 2π.
- The path difference is the difference between the projection of **r** on **k** and the projection of **r** on $\mathbf{k}_0$, $\boldsymbol{\phi} = 2\pi \mathbf{r} \cdot (\mathbf{k}-\mathbf{k}_0)$

If $(\mathbf{k}-\mathbf{k}_0) = \mathbf{r}^*$, then $\boldsymbol{\phi} = 2\pi n$

$\mathbf{r}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$

$\Delta = \mathbf{r} \cdot (\mathbf{k}-\mathbf{k}_0)$

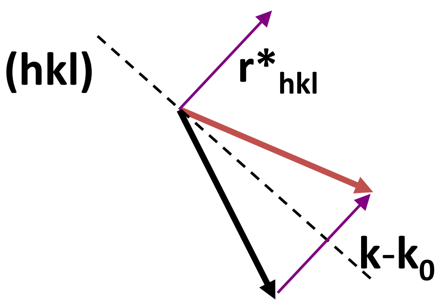
Two lattice points separated by a vector **r**



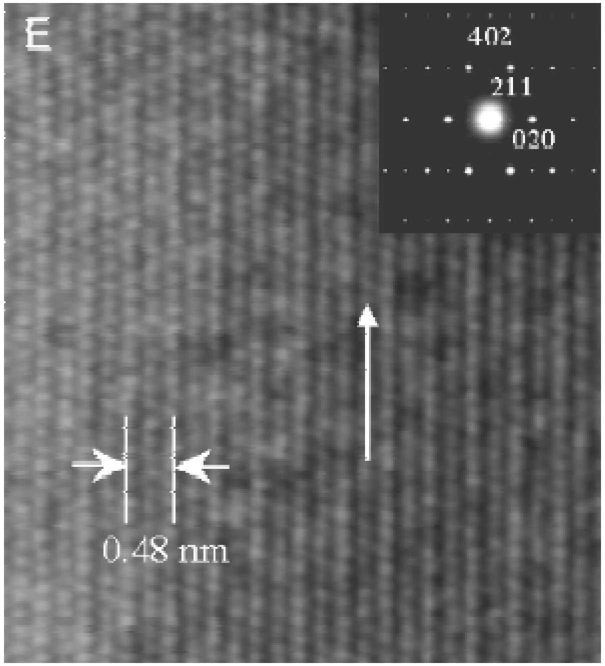
$\Delta = \mathbf{a} \cdot (\mathbf{k}-\mathbf{k}_o) = h$

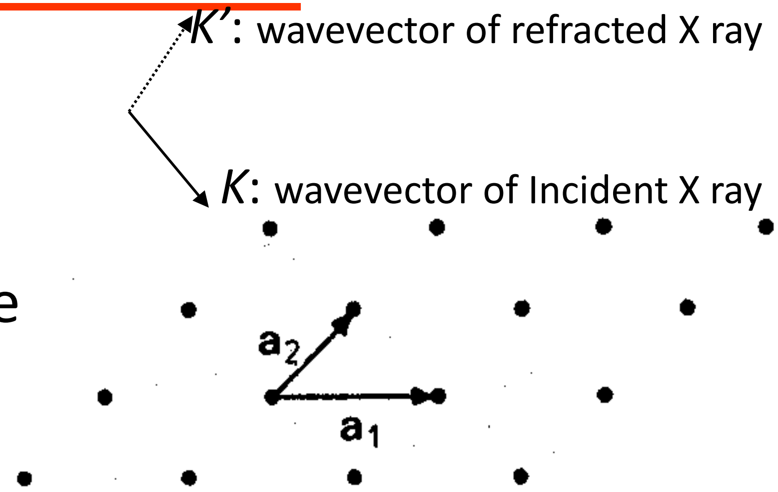
$\Delta = \mathbf{b} \cdot (\mathbf{k}-\mathbf{k}_o) = k$

$\Delta = \mathbf{c} \cdot (\mathbf{k}-\mathbf{k}_o) = l$



The Reciprocal Lattice

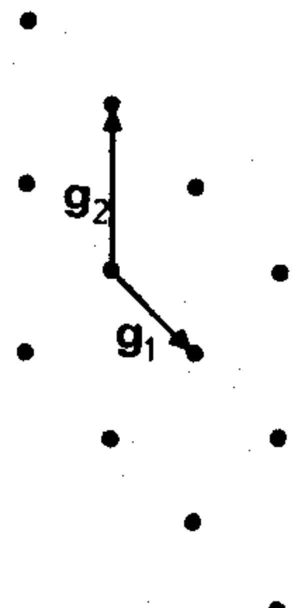




Real lattice

Construction refraction occurs only when $\Delta K \equiv K'-K=ng_1+mg_2$

Diffraction pattern or reciprocal lattice



- The X-ray diffraction pattern of a crystal is a map of the reciprocal lattice.
- It is a Fourier transform of the lattice in real space
- It is a representation of the lattice in the *K* space

The Reciprocal Lattice

- **g** is a vector normal to a set of planes, with length equal to the inverse spacing between them

$$\vec{g} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

- Reciprocal lattice vectors **a*,b*** and **c***

$$\vec{a}^* = 2\Pi \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})}, \vec{b}^* = 2\Pi \frac{\vec{c}\times\vec{a}}{\vec{b}\cdot(\vec{c}\times\vec{a})}, \vec{c}^* = 2\Pi \frac{\vec{a}\times\vec{b}}{\vec{c}\cdot(\vec{a}\times\vec{b})}$$

- These vectors define the reciprocal lattice
- All crystals have a real space lattice and a reciprocal lattice
- Diffraction techniques map the reciprocal lattice

Properties Of Reciprocal Lattice

Direct lattice is a lattice in ordinary space whereas the reciprocal lattice is a lattice in the Fourier space.

The primitive vectors in reciprocal lattice has the dimensions of (length)-1 whereas the primitive vectors of the direct lattice have the dimensions of length

A diffraction pattern of a crystal is a map of the reciprocal lattice of the crystal whereas a microscopic image is a map of direct lattice

When we rotate a crystal, both direct and reciprocal lattice rotates

Each point in the reciprocal lattice represents a set of parallel planes of the crystal lattice

If the coordinates of reciprocal vector G have no common factor, then G is inversely proportional to the spacing of the lattice planes normal to G

The volume of unit cell of the reciprocal lattice is inversely proportional to the volume of unit cell of the direct lattice

The direct lattice is the reciprocal of its own reciprocal lattice.

The unit cell of the reciprocal lattice need not be parallelopiped

3-D: the Fourier transform of a function *f*(*x*,*y*,*z*)

$$F(x,y,z) = \int\int\int_{-\infty}^{\infty} f(x,y,z)e^{-2\pi i(\underline{ux+vy+wz})}dxdydz$$

Note that $\vec{r} = x\hat{x} + y\hat{y} + z\hat{z}$ $\vec{u} = u\hat{u} + v\hat{v} + w\hat{w}$

ux+*vy*+*wz*: can be considered as a scalar product of $\vec{r}\cdot\vec{u}$

if the following conditions are met!

$$\hat{x}\cdot\hat{u} = 1;\ \hat{x}\cdot\hat{v} = 0;\ \hat{x}\cdot\hat{w} = 0$$

$$\hat{y}\cdot\hat{u} = 0;\ \hat{y}\cdot\hat{v} = 1;\ \hat{y}\cdot\hat{w} = 0 \rightarrow \vec{r}\cdot\vec{u} = ux + vy + wz$$

$$\hat{z}\cdot\hat{u} = 0;\ \hat{z}\cdot\hat{v} = 0;\ \hat{z}\cdot\hat{w} = 1$$

What is $\vec{r}$? Then what is $\vec{u}$?

Consider the requirements for the basic translation vectors of the "reciprocal lattice"

Say $\vec{a}^*$

$$\vec{a}\cdot\vec{a}^* = 1; \quad \underline{\vec{b}\cdot\vec{a}^* = 0; \quad \vec{c}\cdot\vec{a}^* = 0}$$

$$\text{i.e.} \quad \vec{a}^* \perp \vec{b}; \quad \vec{a}^* \perp \vec{c}$$

In other words, $\vec{a}^* \parallel \vec{b}\times\vec{c} \quad \rightarrow \vec{a}^* = k(\vec{b}\times\vec{c})$

$$\because \vec{a}\cdot\vec{a}^* = 1 \rightarrow \vec{a}\cdot\vec{a}^* = \vec{a}\cdot k(\vec{b}\times\vec{c}) = 1$$

$$\therefore k = \frac{1}{\vec{a}\cdot(\vec{b}\times\vec{c})} = \frac{1}{V}$$

$$\rightarrow \vec{a}^* = \frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})} = \frac{\vec{b}\times\vec{c}}{V}$$

Similarly, $\vec{b}^* = \dfrac{\vec{c}\times\vec{a}}{\vec{b}\cdot(\vec{c}\times\vec{a})} = \dfrac{\vec{c}\times\vec{a}}{V}$

$$\vec{c}^* = \frac{\vec{a}\times\vec{b}}{\vec{c}\cdot(\vec{a}\times\vec{b})} = \frac{\vec{a}\times\vec{b}}{V}$$

- **A translation vector in reciprocal lattice is called reciprocal lattice vector** $\vec{G}^*_{hkl}$

$$\vec{G}^*_{hkl} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

- **Orthogonality; Orthornormal Set**

$$\vec{a}\cdot\vec{a}^* = 1;\quad \vec{b}\cdot\vec{a}^* = 0;\quad \vec{c}\cdot\vec{a}^* = 0$$

$$\vec{a}\cdot\vec{b}^* = 0;\quad \vec{b}\cdot\vec{b}^* = 1;\quad \vec{c}\cdot\vec{b}^* = 0$$

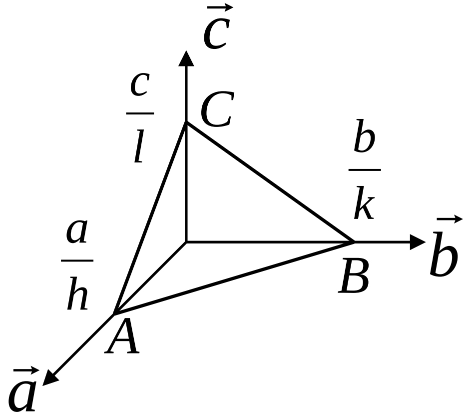
$$\vec{a}\cdot\vec{c}^* = 0;\quad \vec{b}\cdot\vec{c}^* = 0;\quad \vec{c}\cdot\vec{c}^* = 1$$

❑In orthorhombic, tetragonal and cubic systems,

$$\left|\vec{a}^*\right| = \left|\frac{1}{\vec{a}}\right| = \frac{1}{a} \qquad \left|\vec{b}^*\right| = \left|\frac{1}{\vec{b}}\right| = \frac{1}{b} \qquad \left|\vec{c}^*\right| = \left|\frac{1}{\vec{c}}\right| = \frac{1}{c}$$

❑ $\vec{G}^*_{hkl}$ is perpendicular to the plane (*h*, *k*, *l*) in real space

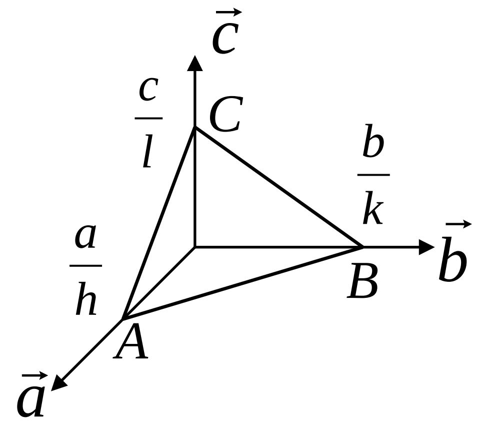
$$\overrightarrow{AB} = \frac{\vec{b}}{k} - \frac{\vec{a}}{h} \qquad \overrightarrow{AC} = \frac{\vec{c}}{l} - \frac{\vec{a}}{h}$$



The reciprocal lattice vector

$$\vec{G}^*_{hkl} = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*$$

$$\vec{G}^*_{hkl} \cdot \overrightarrow{AB} = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*) \cdot \left(\frac{\vec{b}}{k} - \frac{\vec{a}}{h}\right)$$



$$\vec{G}^*_{hkl} \cdot \overrightarrow{AB} = \left(h\vec{a}^* \cdot \frac{-\vec{a}}{h}\right) + \left(k\vec{b}^* \cdot \frac{\vec{b}}{k}\right) = 0$$

Similarly,

$$\vec{G}^*_{hkl} \cdot \overrightarrow{AC} = (h\vec{a}^* + k\vec{b}^* + l\vec{c}^*) \cdot \left(\frac{\vec{c}}{l} - \frac{\vec{a}}{h}\right)$$

$$\vec{G}^*_{hkl} \cdot \overrightarrow{AC} = \left(h\vec{a}^* \cdot \frac{-\vec{a}}{h}\right) + \left(l\vec{c}^* \cdot \frac{\vec{c}}{l}\right) = 0$$

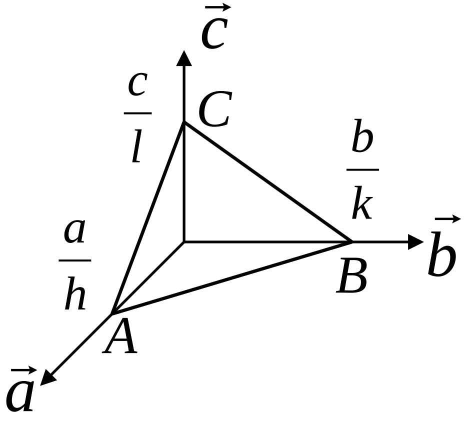
Therefore, $\vec{G}^*_{hkl} \perp \overrightarrow{AB}; \quad \vec{G}^*_{hkl} \perp \overrightarrow{AC}$

$\vec{G}^*_{hkl}$ is perpendicular to the plane (*h*, *k*, *l*)

Moreover, $\left|\vec{G}^{*}_{hkl}\right| = \dfrac{1}{d_{hkl}}$ ← **interplanar spacing of the plane (*h*, *k*, *l*)**

$$d_{hkl} = \frac{\vec{b}}{k}\cdot\frac{\vec{G}^{*}_{hkl}}{\left|\vec{G}^{*}_{hkl}\right|} = \frac{\vec{b}}{k}\cdot\frac{h\vec{a}^{*}+k\vec{b}^{*}+l\vec{c}^{*}}{\left|\vec{G}^{*}_{hkl}\right|}$$

$$= \frac{\vec{b}}{k}\cdot\frac{k\vec{b}^{*}}{\left|\vec{G}^{*}_{hkl}\right|} = \frac{1}{\left|\vec{G}^{*}_{hkl}\right|}$$



$$\text{or}\quad d_{hkl} = \frac{\vec{a}}{h}\cdot\frac{\vec{G}^{*}_{hkl}}{\left|\vec{G}^{*}_{hkl}\right|} = \frac{\vec{a}}{h}\cdot\frac{h\vec{a}^{*}+k\vec{b}^{*}+l\vec{c}^{*}}{\left|\vec{G}^{*}_{hkl}\right|} = \frac{1}{\left|\vec{G}^{*}_{hkl}\right|}$$

$$\text{or}\quad d_{hkl} = \frac{\vec{c}}{l}\cdot\frac{\vec{G}^{*}_{hkl}}{\left|\vec{G}^{*}_{hkl}\right|} = \frac{\vec{c}}{l}\cdot\frac{h\vec{a}^{*}+k\vec{b}^{*}+l\vec{c}^{*}}{\left|\vec{G}^{*}_{hkl}\right|} = \frac{1}{\left|\vec{G}^{*}_{hkl}\right|}$$

The relationship between real lattice and reciprocal lattice in cubic system

REAL SPACE	RECIPROCAL SPACE
SIMPLE CUBIC	SIMPLE CUBIC
BCC	FCC
FCC	BCC

REFERENCES

- Introduction To Solid State Physics- Kittle
- Elementary Solid state Physics- Omar
- Solid state Physics- S. O. Pillai

THANK YOU !