Last thoughts about Miller indices

Direction vectors

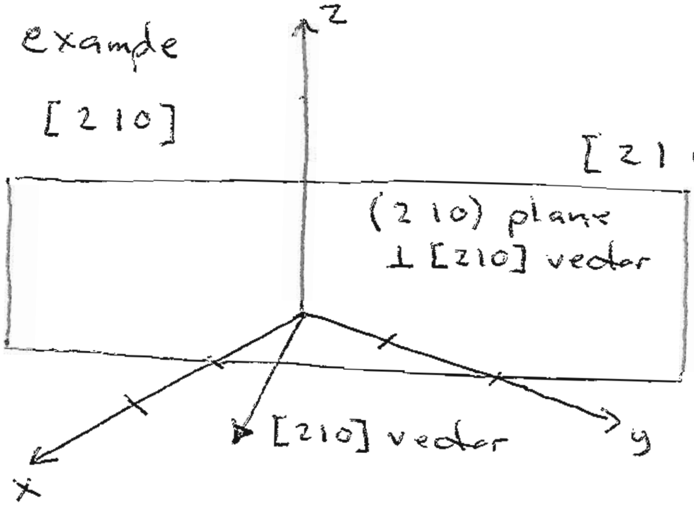
[h k l] a vector which is perpendicular to the set of planes (h, k, l)

For a conventional cube lattice vectors, (with $\hat{n}_i \cdot \hat{n}_j = \delta_{ij}$) [h k l] can be visualized as the vector pointing from the origin to the lattice point in <u>real</u> space

example

[2 1 0]

[2 1 0] $\perp$ (2 1 0)



plane (210) has intercepts along x, y, z of

$$\frac{1}{2} : \frac{1}{1} : \frac{1}{0}$$

$$= \underset{x}{1} : \underset{y}{2} : \underset{z}{\infty}$$

Chapter 6

Determination of Crystal Structures by X-ray Diffraction

using electromagnetic "probe" having $\lambda \sim 10^{-8}$ cm

$$\hbar\omega = \frac{hc}{\lambda} \cong 12.3 \times 10^{3}\,\text{eV}$$

$$\simeq 10^{4}\,\text{eV}$$

i.e. 10 keV

then we can get diffraction

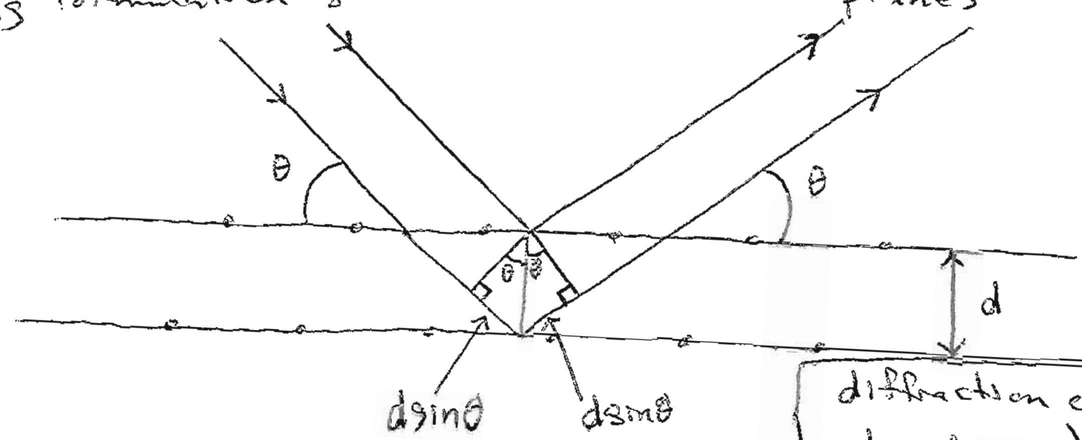
diffraction occurs upon interference between radiation scattered from sources located at the lattice points of a 3-dimensional lattice.

2 Equivalent Descriptions

A. Bragg formulation : diffraction from planes

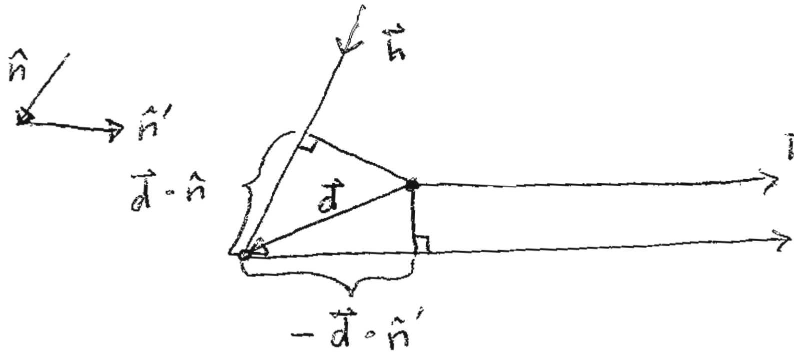
B. Von Laue formulation : diffraction from points

A. Bragg formulation : consider families of planes



$$\boxed{\text{diffraction condition: } 2d\sin\theta = n\lambda}$$

B. <u>Von Laue</u>: consider points of the lattice



$$\text{phase diff.} = \vec{d}\cdot\hat{n} + (-\vec{d}\cdot\hat{n}') = m\lambda$$

$$\Rightarrow \vec{d}\cdot(\hat{n}-\hat{n}') = m\lambda$$

$$\frac{2\pi}{\lambda}\,\vec{d}\cdot(\hat{n}-\hat{n}') = 2\pi m$$

$$\Rightarrow \vec{d}\cdot(\vec{k}-\vec{k}') = 2\pi m \qquad \vec{k} = \frac{2\pi}{\lambda}\hat{n}$$

$$\vec{k}' = \frac{2\pi}{\lambda}\hat{n}'$$

generally $\vec{d}$ can be any Bravais lattice vector $\vec{R}$

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

$$\Rightarrow e^{i(\vec{k}-\vec{k}')\cdot\vec{R}} = 1 \quad \text{for all } \vec{R}$$

which is the definition of the reciprocal lattice vectors $\vec{K}$

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

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

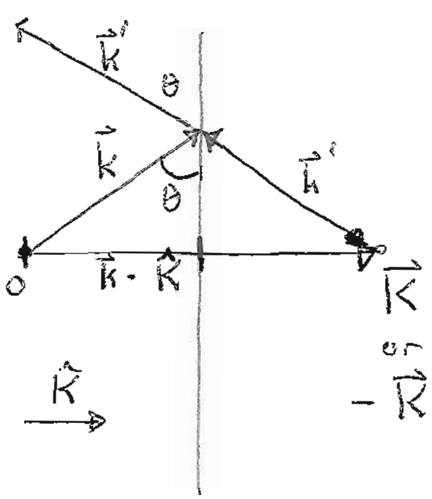
$$\left(\text{also } -\vec{K} = \vec{k} - \vec{k}'\right) \Rightarrow \vec{k} = \vec{k}' - \vec{K}$$

$$k^2 = |\vec{k} - \vec{K}|^2$$

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

$$\Rightarrow \quad \vec{k}\cdot\vec{K} = \tfrac{1}{2}K^2$$

$$\Rightarrow \quad \vec{k}\cdot\hat{K} = \tfrac{1}{2}K \quad , \quad \hat{K} = \frac{\vec{K}}{K}$$



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

$$\cancel{\vec{K}\cdot(\vec{k}-\vec{k}') = 2\pi n} \qquad K = 2k\sin\theta$$

$$\vec{k}\cdot\hat{K} = k\sin\theta = \frac{K}{2} = \frac{2\pi n}{d\,2} = \frac{\pi n}{d}$$

$$k = \frac{2\pi}{\lambda} \Rightarrow \frac{2\pi}{\lambda}\sin\theta = \frac{\pi n}{d}$$

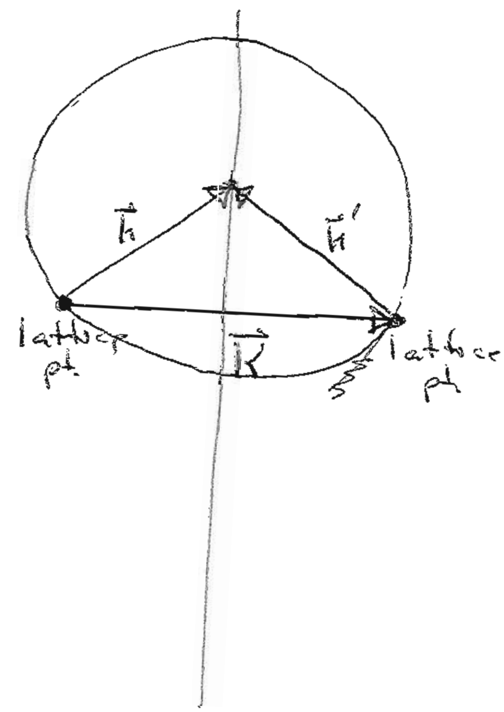
$$\Rightarrow \boxed{2d\sin\theta = n\lambda}$$

Thus $\boxed{\text{Von Laue} \Leftrightarrow \text{Bragg}}$

Expermental Realization

Ewald Construction ★ very important ★

- use Von Laue formulation



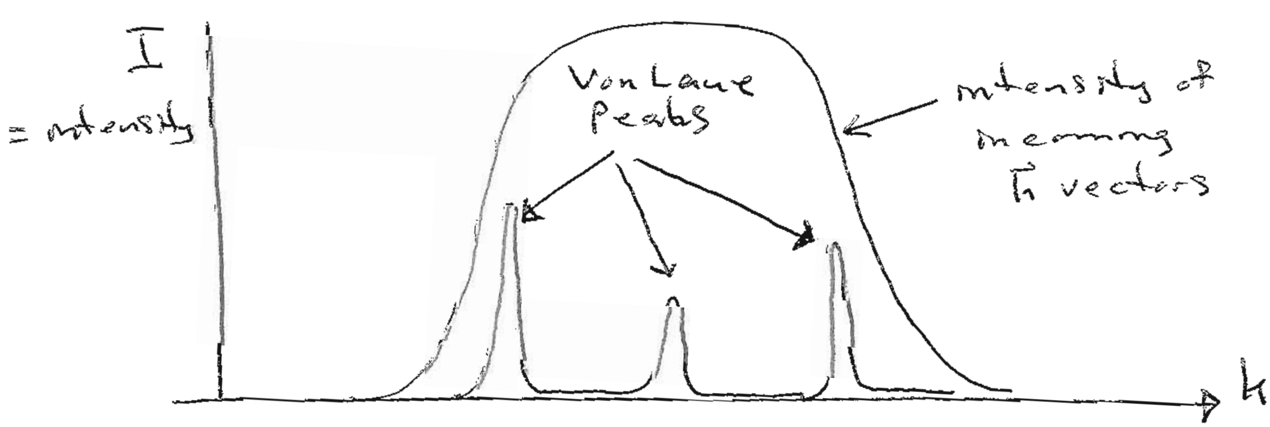
$|\vec{k}| = |\vec{k}'| = r$

= radius of Ewald sphere

Expermental Methods

1. Laue Method

vary the energy, and thus $|\vec{k}|$, using broad-spectrum (multi-wavelength) source



hold incident, scattering angles fixed

$$k = \frac{\sqrt{2mE}}{\hbar}$$

Finding a Von Laue peaks at

$$k = k_1, k_2, k_3, \ldots$$

then since angles (θ) are known,

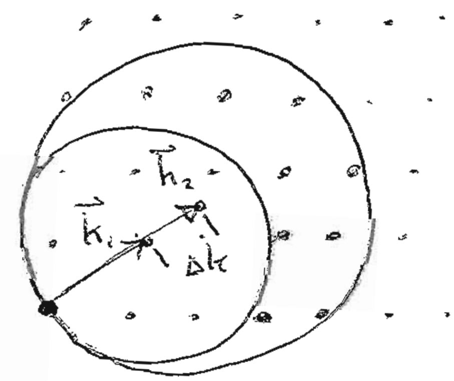
$$K_1 = 2k_1 \sin\theta_1$$

$$K_2 = 2k_2 \sin\theta_2$$

$\Rightarrow \{K_i\}$ set of reciprocal lattice vector magnitudes

2. Rotating crystal Method

- monochromatic x-rays
- vary the angle of incidence
- ~~Ewald sphere~~



$\Delta k = k_2 - k_1$

2. Powder or Debye-Scherrer method

- equivalent to rotating crystal method but allow rotation axis to vary over all possible rotation axes. (orientations)