Condensed Matter Physics

Diffraction

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October 8, 2018

Scattering amplitude

Scattering amplitude ($\underline{\kappa} = \underline{k}_i - \underline{k}_o$)

$$A(\underline{\kappa}) = \int \rho(\underline{r}) e^{i\underline{\kappa}\underline{r}} dV$$

Periodic system

$$\rho(\underline{r}) = \sum_{\underline{R}_n} \sum_{j=1}^{p} \rho_j(\underline{r} - \underline{R}_n - \underline{r}_j)$$

So,

$$A(\underline{\kappa}) = \int \sum_{\underline{R}_n} \sum_{j=1}^{p} \rho_j(\underline{r} - \underline{R}_n - \underline{r}_j) e^{i\underline{\kappa}\underline{r}} dV$$

$$A(\underline{\kappa}) = \int \sum_{\underline{R}_n} \sum_{j=1}^{p} \rho_j(\underline{r}') e^{i\underline{\kappa}(\underline{r}' + \underline{R}_n + \underline{r}_j)} dV'$$

Scattering amplitude

Uniform atom

$$A(\underline{\kappa}) = \left[\int \rho(\underline{r}')e^{i\underline{\kappa}\underline{r}'}\,dV'\right]\left[\sum_{j=1}^{p} e^{i\underline{\kappa}\underline{r}_j}\right]\left[\sum_{\underline{R}_n} e^{i\underline{\kappa}\underline{R}_n}\right]$$

Atomic scattering factor

$$f(\underline{\kappa}) = \int \rho(\underline{r}')e^{i\underline{\kappa}\underline{r}'}\,dV'$$

Structure factor

$$f_s(\underline{\kappa}) = \sum_{j=1}^{p} e^{i\underline{\kappa}\underline{r}_j}$$

$\kappa = q_i\underline{b}_i \quad \underline{R}_n = n_i\underline{a}_i \quad \kappa\underline{R}_n = 2\pi(q_i n_i)$

$$\sum_{\underline{R}_n} e^{i\underline{\kappa}\underline{R}_n} = \left(\sum_{n_1} e^{2\pi i q_1 n_1}\right)\left(\sum_{n_2} e^{2\pi i q_2 n_2}\right)\left(\sum_{n_3} e^{2\pi i q_3 n_3}\right)$$

Scattering amplitude

$$\sum_{n=0}^{N} e^{2\pi iqn} = \frac{e^{2\pi iqN} - 1}{e^{2\pi iq} - 1} = \frac{e^{\pi iqN}}{e^{\pi iq}} \frac{\sin(\pi Nq)}{\sin(\pi q)}$$

What matters

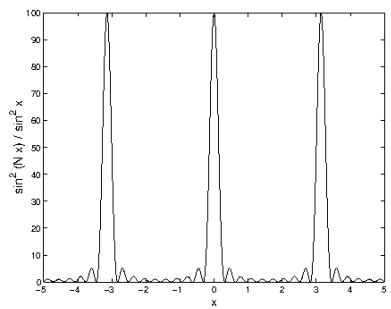
$$f(q) = \frac{\sin(\pi Nq)}{\sin(\pi q)}$$

if $q = \frac{l}{N}$ numerator 0
if $q = m$ the denominator is also 0
leads

$$\frac{\sin(\pi Nm)}{\sin(\pi m)} = N$$

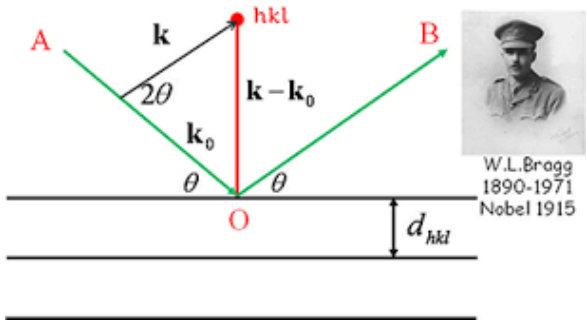
So,

$$\underline{\kappa} = \underline{G}_{hkl}$$



Methods

Bragg law

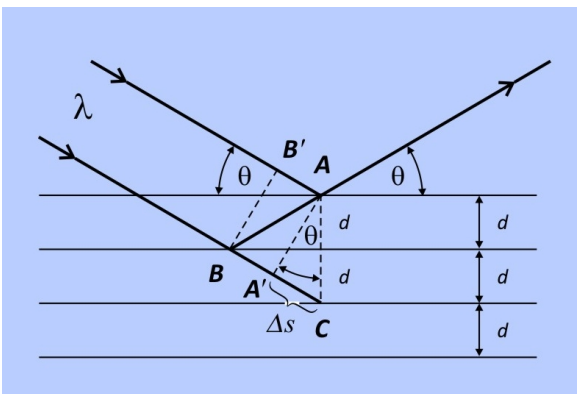


W.L.Bragg
1890-1971
Nobel 1915

$$2|\underline{k}|\sin(\Theta) = |\underline{G}_{hkl}| = \frac{2\pi m}{d_{hkl}}$$

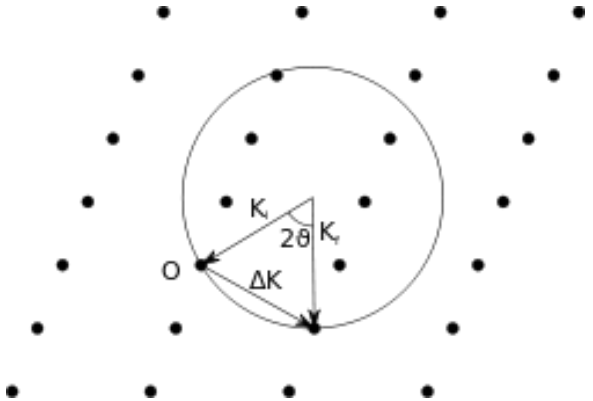
$$\frac{2}{\lambda}\sin(\Theta) = \frac{m}{d_{hkl}}$$

"Reflection"

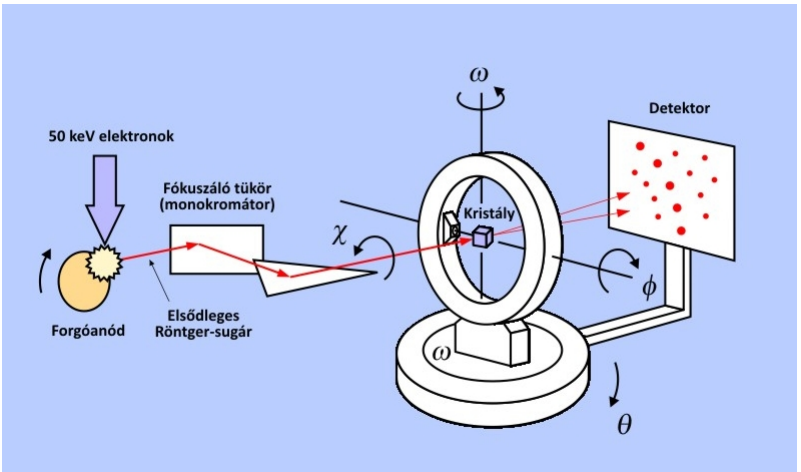


Methods

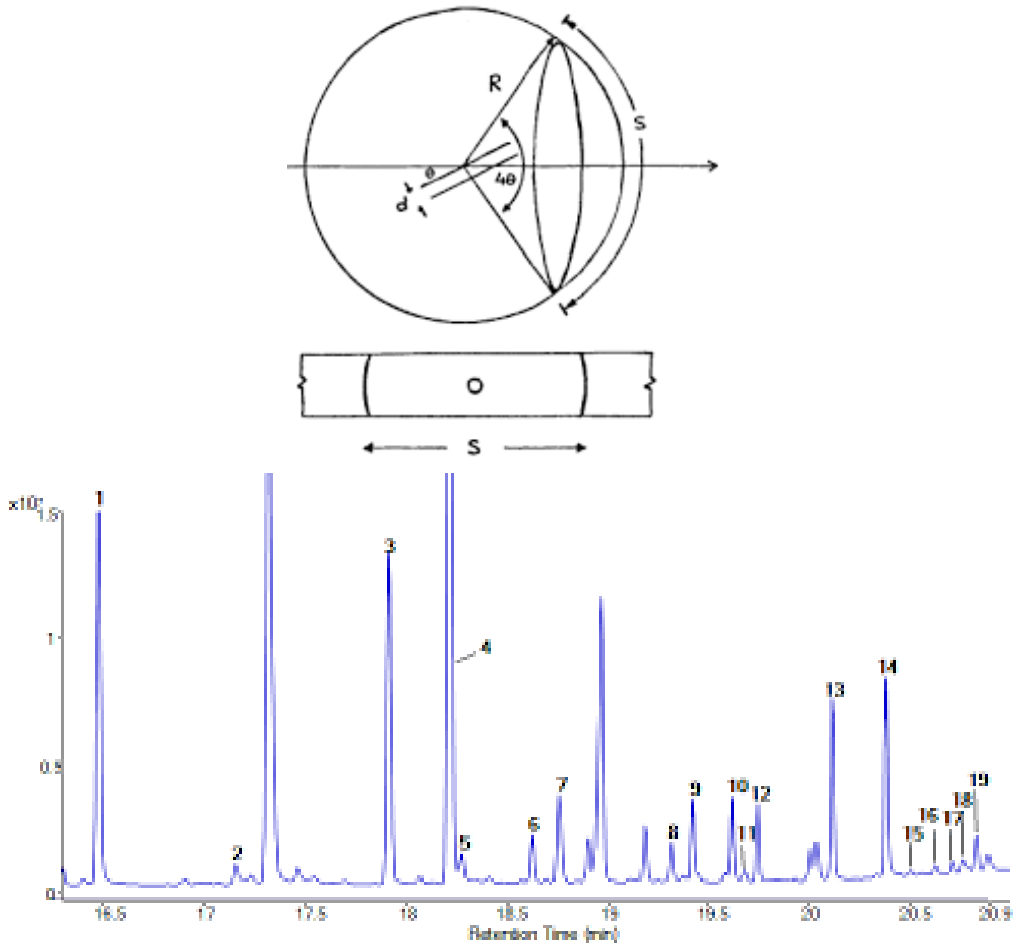
Ewald sphere



Diffractometer

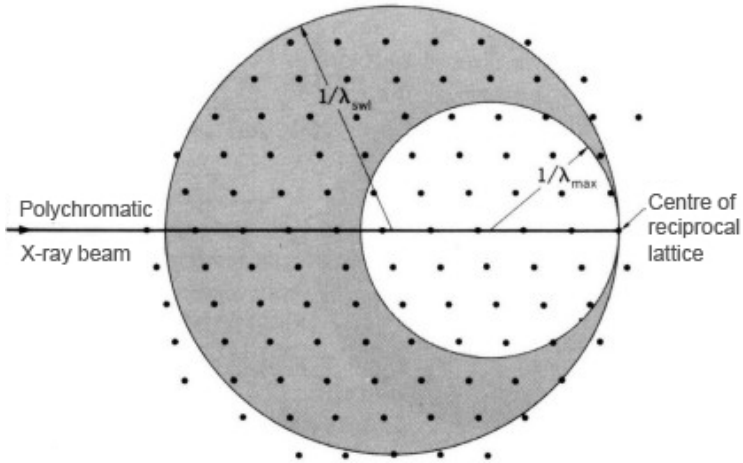


Powder diffraction (Debye Scherrer)

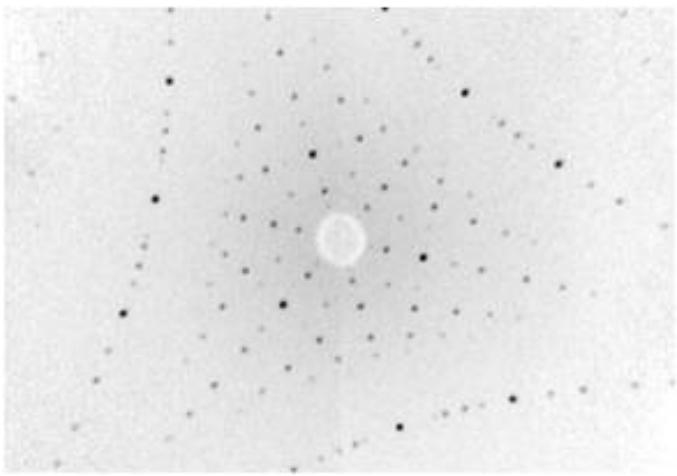


Methods

Laue method (continuous radiation)



wolfram



Methods

Line profile analysis