



Anyagfizikája

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ELTE

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Szórési amplitúdó ($\underline{\kappa} = \underline{k}_i - \underline{k}_o$)

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

Periodikus rendszer

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

Így

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

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

Egyféle atom

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

Atomszórési tényező

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

Struktúra faktor

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

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

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

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

Ami számít

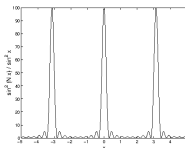
$$f(q) = \frac{\sin(\pi N q)}{\sin(\pi q)}$$

ha $q = \frac{l}{N}$ számláló 0
ha $q = m$ a nevező is 0
ekkor

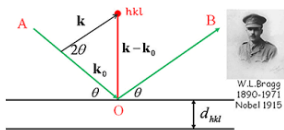
$$\frac{\sin(\pi N m)}{\sin(\pi m)} = N$$

Így

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



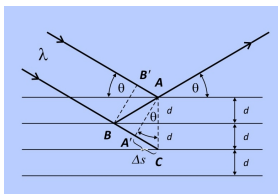
Bragg törvény



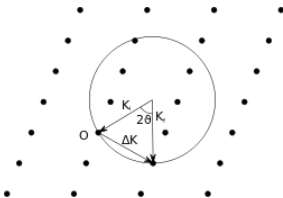
$$2|k| \sin(\Theta) = |G_{hkl}| = \frac{2\pi m}{d_{hkl}}$$

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

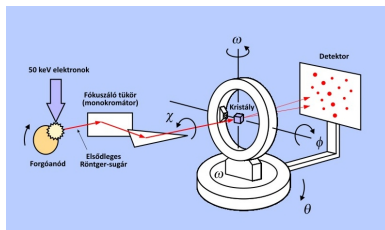
“Reflektálódás“



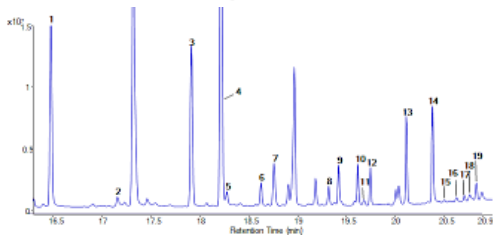
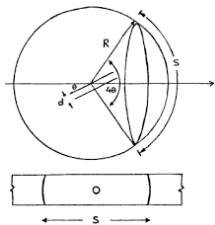
Ewald gömb



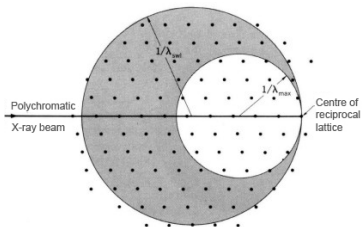
Diffraktométer



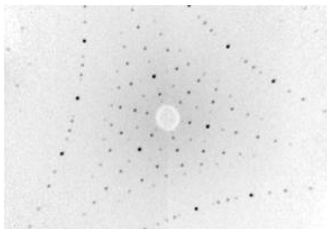
Pordiffrakció (Debye Scherrer felvétel)



Laue felvétel (folytonos fékezési sugárzás)



wolfram



Vonalprofil analízis

