Diffraction

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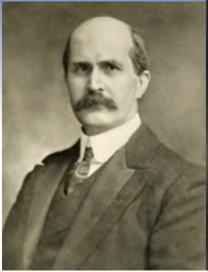
History of X-ray...

... starts in the German city of Würzburg, the 8 of November 1895, when Wilhelm Conrad RÃ¶ntgen working with a cathodic tube, observed a new radiation in a flurescent screen two meters from the tube and covered with black paper. Not knowing its nature, he called it X-rays.

History of X-ray...

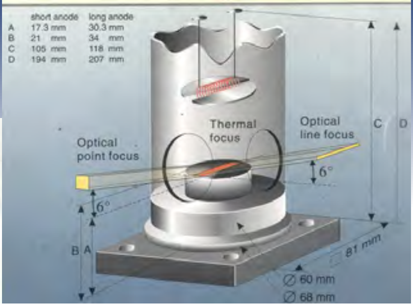
In 1912
... the german physicist Max von Laue at the University of Münich was listening to the young student P. P Ewald regarding his theoretical work on diffraction by 3D gratings. Laue came to realize that if x-rays where electromagnetic waves, and crystalline solids were made of periodic arrangement of atoms then, they should diffract X-rays.

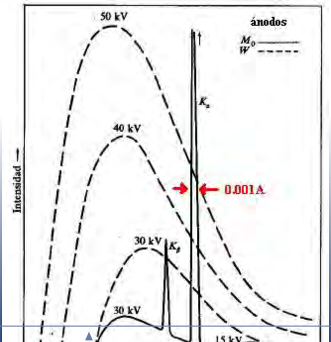
History of X-ray...



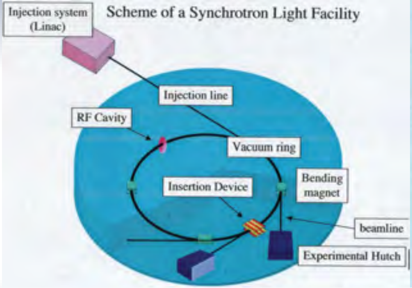
Bragg son and father realized that X-ray diffraction opened a new way of exploring the atomic arragement of atoms in a solid. They started analyzing the alakaline compunds KCl, KBr y NaCl and reported their structure to the Royal Socoety in June 1913. The paper was entitled ”The diffraction of Short Electromagnetic waves by a Crystal”.

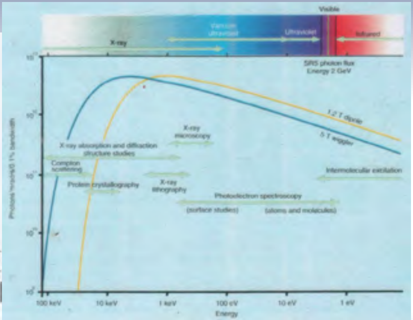
X-ray sources





X-ray sources





X-ray sources

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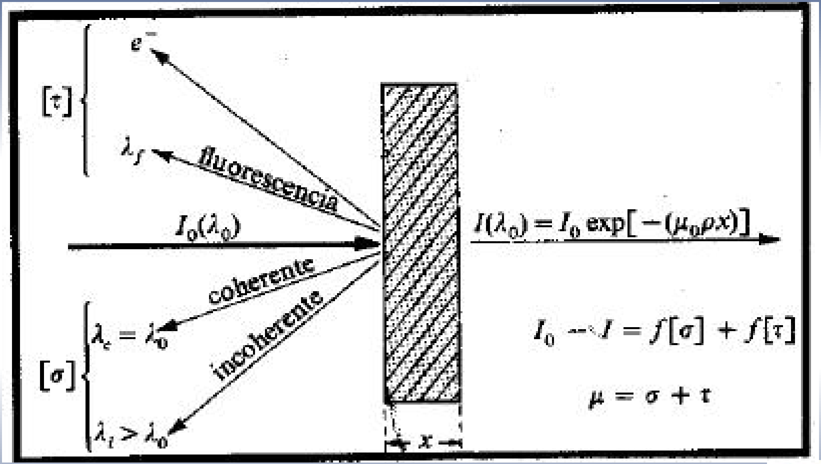
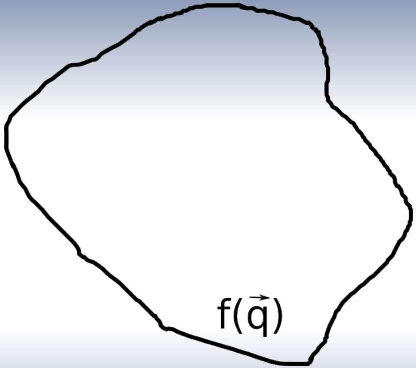


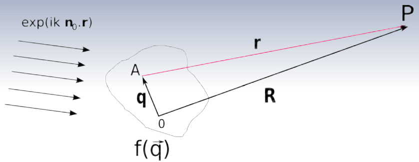
Diffraction in the Fraunhoffer aproximation



Let a three-dimensional object be characterized by a function $f(\vec{q})$ which represents the scattering power of the specimen.

Diffraction in the Fraunhoffer approximation

$$k = \frac{2\pi}{\lambda}$$



At point A a spherical wave is elastically scattered and at point P we have

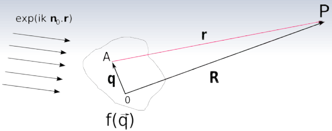
$$f(\vec{q}) \exp(ik\vec{n}_0 \cdot \vec{q}) \frac{\exp(ikr)}{kr}$$

where
$r = |\vec{R} - \vec{q}|$

then

$$\psi = \iiint_{-\infty}^{\infty} f(\vec{q}) \exp(ik\vec{n}_0 \cdot \vec{q}) \frac{\exp(ik|\vec{R} - \vec{q}|)}{k|\vec{R} - \vec{q}|} d^3\vec{q}$$

The Fraunhoffer aproximation

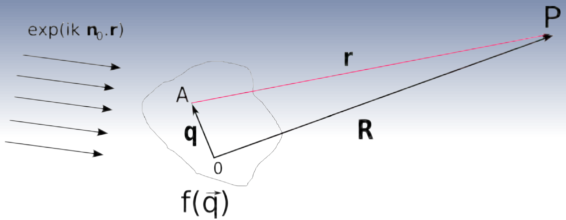


Definition (Fraunhoffer aproximation)

$$|\vec{q}| << |\vec{R}|$$

$$\frac{\exp\left(ik|\vec{R}-\vec{q}|\right)}{k|\vec{R}-\vec{q}|} \approx \frac{\exp\left(ik|\vec{R}|\right)}{k|\vec{R}|}\exp\left(-ik\vec{n}\cdot\vec{q}\right) \qquad \vec{n} = \frac{\vec{R}}{|\vec{R}|}$$

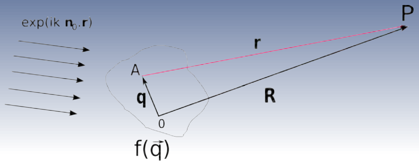
The Fraunhoffer aproximation



$$|\vec{R}-\vec{q}| = \sqrt{R^2 - 2\vec{R}\cdot\vec{q} + q^2} = \sqrt{1 - \frac{2\vec{R}\cdot\vec{q} - q^2}{R^2}} = R - \vec{n}\cdot\vec{q} + \varepsilon$$

$$\varepsilon \ll R$$

Diffraction in the Fraunhoffer approximation

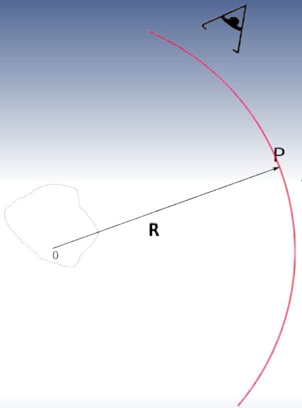


$$\psi(\vec{R},\vec{r^*}) = \frac{\exp(ikR)}{kR}\iiint_{-\infty}^{\infty} f(\vec{q})\exp(2i\pi(\vec{n}-\vec{n}_0)/\lambda\cdot\vec{q})d^3\vec{q} =$$

$$\frac{\exp(ikR)}{kR}\iiint_{-\infty}^{\infty} f(\vec{q})\exp(2i\pi\vec{r^*}\cdot\vec{q})d^3\vec{q}$$

$$\vec{r^*} = \frac{(\vec{n}-\vec{n}_0)}{\lambda}$$

Diffraction in the Fraunhoffer approximation

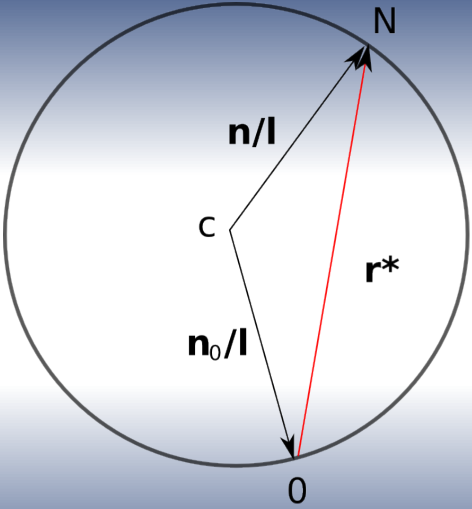


$$\psi(\vec{r^*}) = \left[\frac{\exp(ikR)}{kR}\right] \iiint_{-\infty}^{\infty} f(\vec{q}) \exp(2i\pi\vec{r^*}\cdot\vec{q}) d^3\vec{q}$$

$$C \iiint_{-\infty}^{\infty} f(\vec{q}) \exp(2i\pi\vec{r^*}\cdot\vec{q}) d^3\vec{q}$$

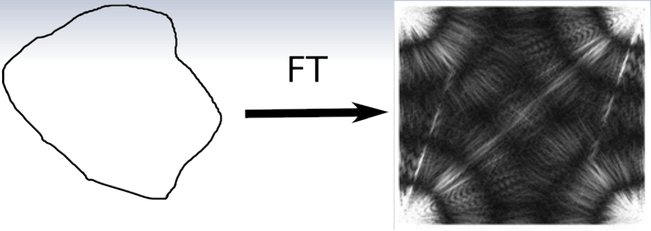
$$f(\vec{q}) = \frac{1}{C} \iiint_{-\infty}^{\infty} \psi(\vec{r^*}) \exp(-2i\pi\vec{r^*}\cdot\vec{q}) d^3\vec{r^*}$$

Ewald Sphere



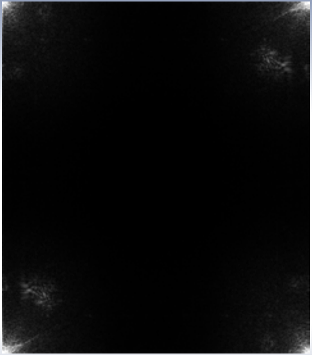
$$|\psi(\vec{R})|^2$$

Ewald Sphere

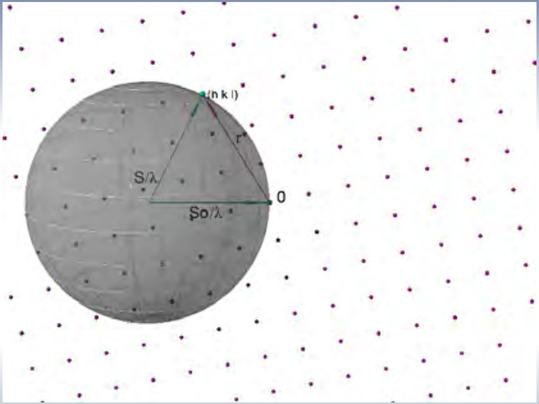


Diffraction

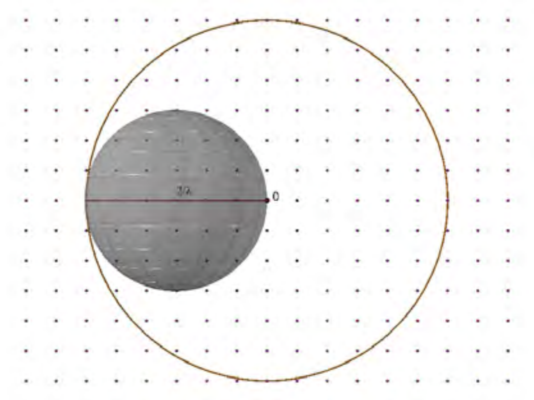
Fourier



Reciprocal lattice



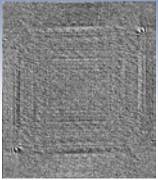
Reciprocal lattice



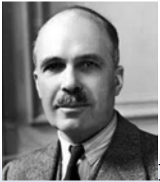
Diffraction in the Fraunhoffer approximation

Fourier

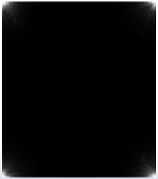
Fourier



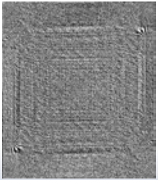
Γ^{-1}



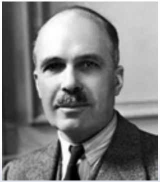
Bragg



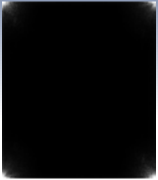
Bragg



Γ^{-1}

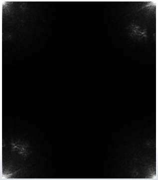


The phase problem

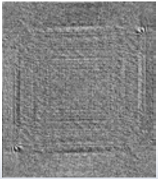


Bragg

Fourier



Fourier



Bragg

Fourier transform of real functions

Theorem (Γ of real functions)

The $f(\vec{r})$ is real only and only if $F(\vec{r^*})$ is hermitian

$$f(\vec{r}) = f^*(\vec{r}) \Longleftrightarrow F(\vec{r^*}) = F^*(-\vec{r}^*)$$

Friedel law

$$f(\vec{r}) = f^*(\vec{r}) \Rightarrow F(\vec{r^*})F^*(\vec{r^*}) = F^*(-\vec{r}^*)F(-\vec{r}^*)$$

Diffraction in the Fraunhoffer approximation

Friedel law

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