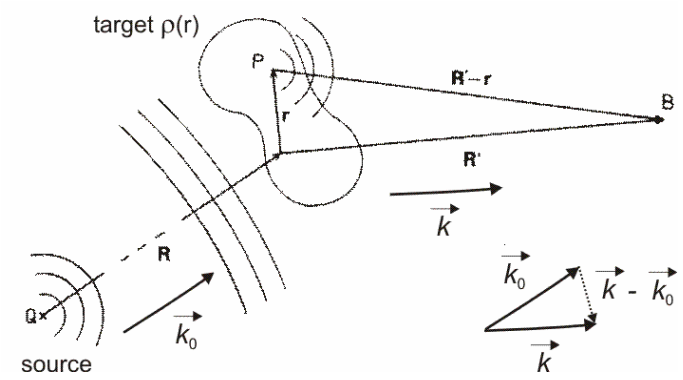
Scattering geometry



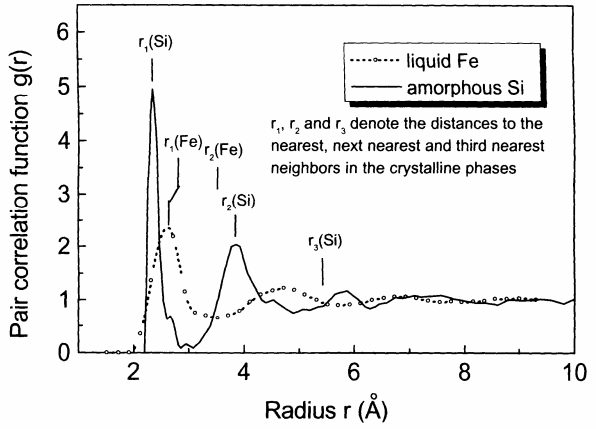
$$I = \int d^3r \rho(\vec{r}) e^{-i\vec{K}\vec{r}} \int d^3r' \rho^*(\vec{r'}) e^{i\vec{K}\vec{r'}} =$$
$$\int d^3r \rho(\vec{r}) e^{-i\vec{K}\vec{r}} \int d^3r' \rho(\vec{r'}+\vec{r}) e^{i\vec{K}(\vec{r'}+\vec{r})} =$$
$$\int d^3r' e^{-i\vec{K}\vec{r'}} \int d^3r \rho(\vec{r}) \rho(\vec{r'}+\vec{r})$$

$P(\vec{r}) = \int d^3r' \rho(\vec{r'}+\vec{r}) \rho(\vec{r'})$
autocorrelation function of scattering density

$P(\vec{r})$ has a maximum, if $\vec{r}$ corresponds to any spacing of scatterers

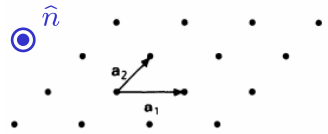
$P(\vec{r}) = \int d^3r' \rho(\vec{r'}+\vec{r}) \rho(\vec{r'})$
autocorrelation function of scattering density

$g(r) = P(|\vec{r}|)$ pair correlation

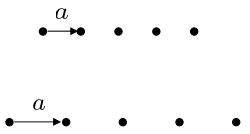


Real space lattice

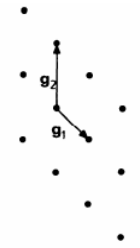
2d - lattice



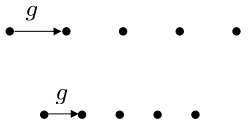
1d - chain



Reciprocal lattice



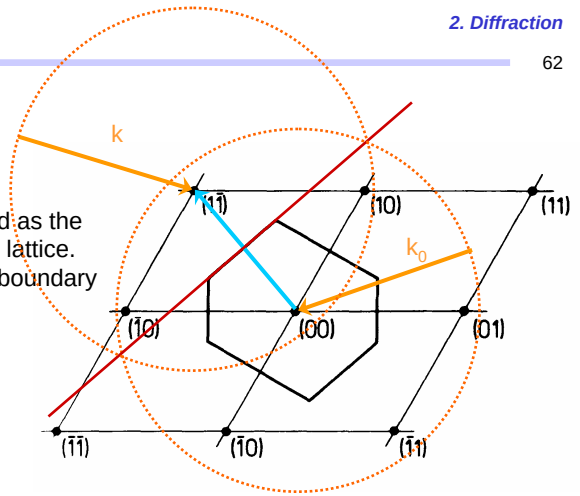
$\vec{g}_1 \perp \vec{a}_2, \vec{g}_1 \perp \hat{n}, \ \vec{g}_2 \perp \vec{a}_1, \vec{g}_2 \perp \hat{n}$



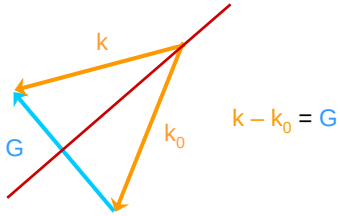
$g = 2\pi/a$

Brillouin zones

The **first Brillouin zone** is defined as the Wigner-Seitz cell of the reciprocal lattice. All **k** vectors at the Brillouin zone boundary fulfil the Laue condition.

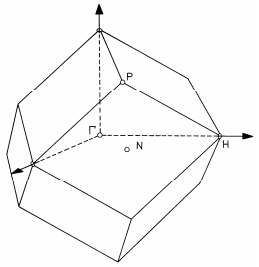


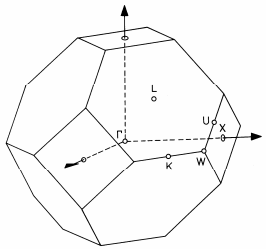
All $\mathbf{k}_0$, **k** satisfying the Laue condition lie on the bisecting plane perpendicular to $\mathbf{G}_{hkl}$

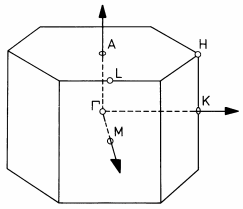


Brillouin zones

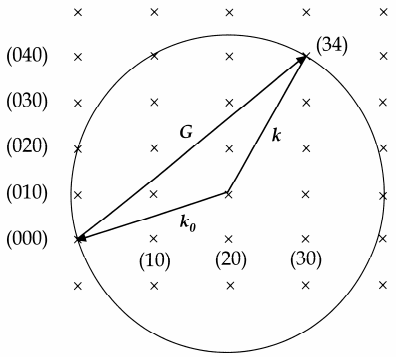
bcc **fcc** **hexagonal**







Ewald construction

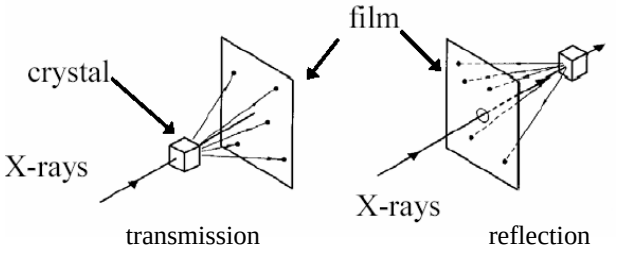


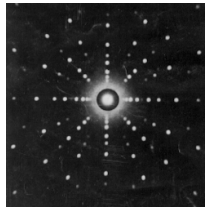
i) Die Richtung von k_0 ist durch das Experiment vorgegeben (einfallender Strahl).
ii) Zeichne k_0 so, dass die Spitze an einem Punkt des reziproken Gitters endet, hier (000).
iii) Zeichne einen Kreis (eine Kugeloberfläche) mit Radiusvektor k_0
iv) Für alle Punkte auf dem Kreis (der Kugeloberfläche) ist $\mathbf{G} = \mathbf{k} - \mathbf{k_0}$ erfüllt, hier **G** = (340) – (000) = (340).

Bemerkung: Der Anfang von k_0 liegt in der Abbildung nur zufällig nahe einem Punkt des reziproken Gitters.

X-ray diffraction

Laue method



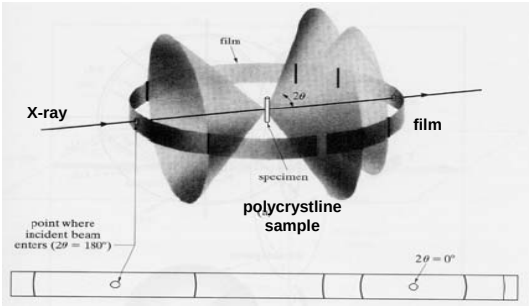


Diffraction of collimated, broadband X-ray beam at single crystal sample:

- $k' \leq k_0 \leq k''$
- analysis of crystal symmetry
- orientation of single crystals

X-ray diffraction

Debeye-Scherrer method

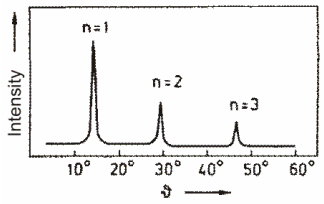


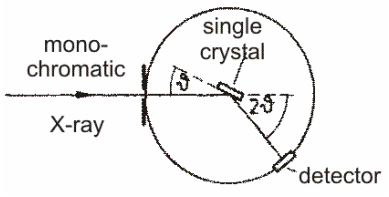
Monochromatic X-ray diffraction from polycrystalline powder sample

- Diffraction rings
- $0 \le 2\Theta \le 180 \Rightarrow G_{hkl} \le 2k_0$
- not verry precise, but lattice constant and crystal structure

X-ray diffraction

Rotating crystal method





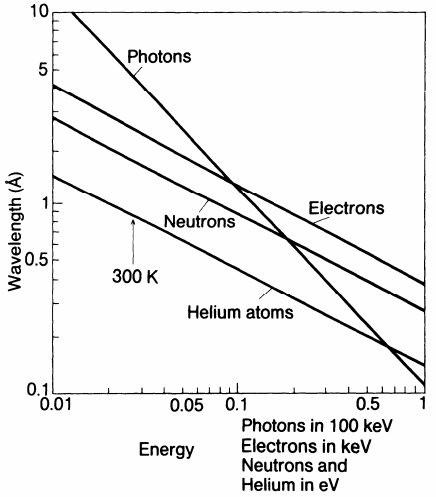
3-axis goniometer
(monochromator, sample, detector)

Monochromatic X-ray diffraction from single crystal

- simultaneous rotation: sample by ϑ, detector by 2ϑ
- resolution $\Delta\lambda / \lambda \approx 10^{-5}$ (X-rays or neutrons)

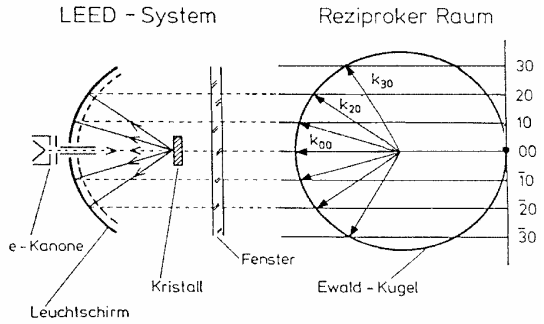
Photons, electrons, neutrons, He atoms

Wavelength $\lambda \approx$ lattice constant a



- photons: $\lambda(\text{Å}) \approx \frac{12{,}4}{E(\text{keV})}$ $12{,}4\text{keV} \triangleq 1\text{Å}$
- electrons: $\lambda(\text{Å}) \approx \frac{12{,}3}{\sqrt{E}(\sqrt{\text{eV}})}$ $100\text{ eV} \triangleq 1{,}23\text{Å}$
- neutrons: $\lambda(\text{Å}) \approx \frac{0{,}287}{\sqrt{E}(\sqrt{\text{eV}})}$ $10\text{ meV} \triangleq 2{,}87\text{Å}$
- He atoms: $\lambda(\text{Å}) \approx \frac{0{,}144}{\sqrt{E}(\sqrt{\text{eV}})}$ $10\text{ meV} \triangleq 1{,}44\text{Å}$

Low-energy electron diffraction

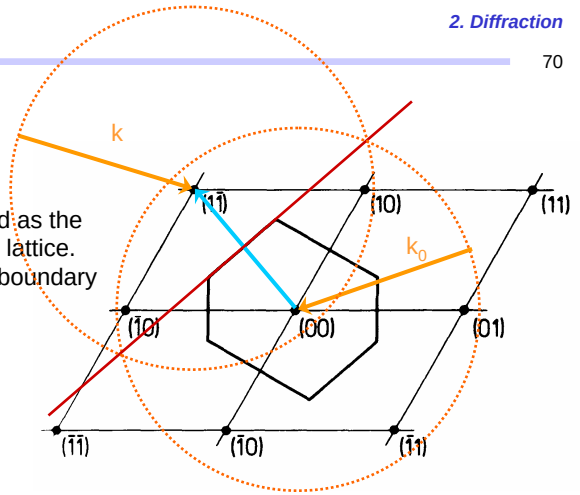


Electrons impinging on the crystal are elastically back-reflected and imaged by a phosphor screen.

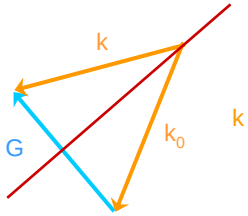
The short inelastic mean free path of electrons in conducting materials (only a few lattice planes) makes LEED a surface sensitive technique.

Brillouin zones

The **first Brillouin zone** is defined as the Wigner-Seitz cell of the reciprocal lattice. All **k** vectors at the Brillouin zone boundary fulfil the Laue condition.

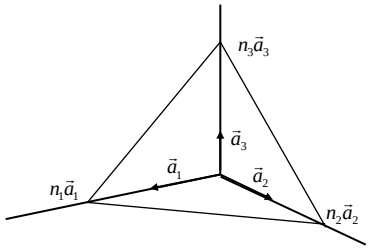


All $\mathbf{k}_0$, **k** satisfying the Laue condition lie on the bisecting plane perpendicular to $\mathbf{G}_{hkl}$



$k - k_0 = G$

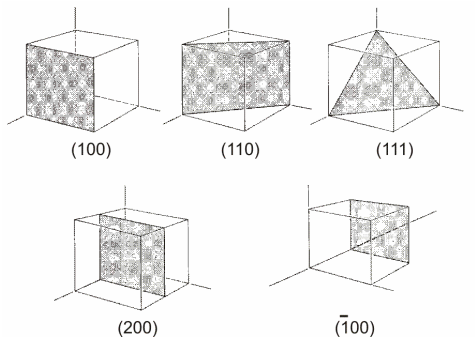
Miller indices



Lattice plane defined by 3 points:
$n_1\vec{a}_1, n_2\vec{a}_2, n_3\vec{a}_3$

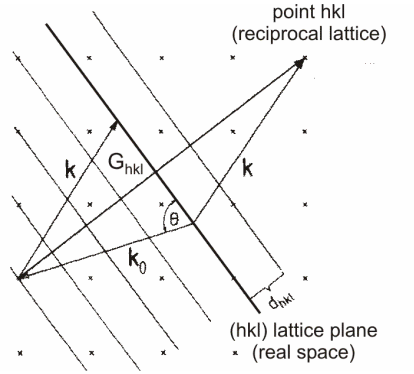
Miller indices:
$(h,k,l) = p \cdot (1/n_1, 1/n_2, 1/n_3)$

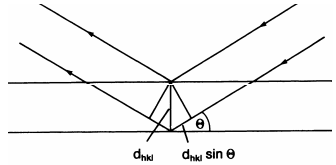
$G_{hkl} \perp$ lattice plane (hkl)



Some lattice planes and Miller indices of the cubic Bravais lattice

Laue condition and Bragg reflection

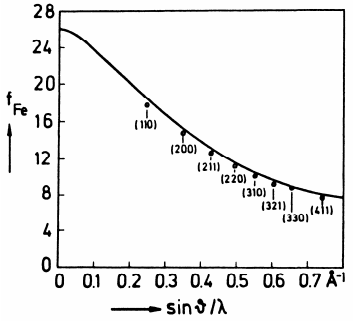


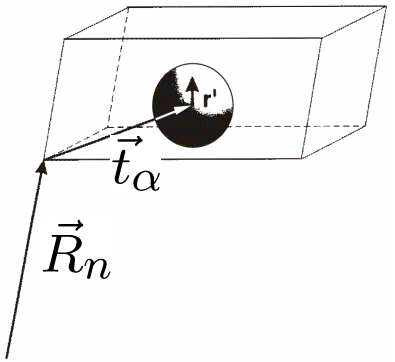


$$\vec{k} - \vec{k}_0 = \vec{G}_{hkl} \qquad n \cdot \lambda = 2 d_{hkl} \sin\vartheta$$

Structure factor and atomic form factor

Atomic form factor
f_{Fe} for iron





Structure factor

$$S_{hkl} = \sum_\alpha f_\alpha e^{-i\vec{G}_{hkl}t_\alpha}$$

Debye Waller factor

$$I_{hkl} \propto \exp[-\frac{1}{3}u^2 G_{hkl}^2]$$

Mean square displacement for harmonic oscillator :

$$\frac{1}{2}m\omega^2 u^2 = \frac{3}{2}kT$$

Debye-Waller factor:

$$I_{hkl} \propto \exp[-kT \cdot G_{hkl}^2/m\omega^2]$$

Intensity of X-ray diffraction (h00) spots from Al