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Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture 2

Vorlesung zum Haupt/Masterstudiengang Physik

SS 2013

G. Grübel, M. Martins, E. Weckert

Location: Hörs AP, Physik, Jungiusstrasse

Tuesdays 12.45 – 14.15

Thursdays 8:30 – 10.00

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Methoden moderner Röntgenphysik II: Streuung und Abbildung

Vorlesung: 4 SWS: Dienstag und Donnerstag
Übungen: 2 SWS: Dienstag (wenn vereinbart)
Proseminar: für Batchelor Studierende
8 Leistungspunkte für dieses Modul im Masterstudiengang

Tuesdays 12.45 – 14.15:
Thursdays 8.30 – 10.00: starting April 4, 2013

Tuesdays 14:30 – 16:00: *Tutorials/Übungen*
Organisation-1st meeting: April 9, 2013 in SemRm 4

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Gerhard Grübel (GG), Thomas Schneider (TS), Oliver Seeck (OS), Stephan Roth (SR), Hermann Franz (HF)

4.4. – 14.5.	Basics of X-ray physics	(GG)
16.5.	Site Visit	
28.5.-13.6.	Surfaces and Interfaces	(OS)
18.6.-27.6.	Biology	(TS)
2.7.-11.7.	Soft Matter	(SR)

Literature

Basic concepts: Elements of Modern X-Ray Physics
J. A. Nielsen and D. McMorrow, J. Wiley&Sons (2001)
X-Ray Diffraction
B.E. Warren, DOVER Publications Inc,, New York
Principles of Optics
M.Born and E. Wolf, Cambridge University Press, 7th. ed.
Soft X-rays and Extreme Ultraviolett Radiation
D. Attwood, Cambridge University Press (2000)
http://www.coe.berkeley.edu/AST/sxreuv/)
Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen
K. Wille, Teubner Studienbücher 1996

Lecture Notes

http://photon-science.desy.de/research/studentsteaching/lectures_seminars/ss13/roentgenphysik_streuung_und_abbildung/index_eng.html

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Introduction
Overview, Introduction to X-ray scattering

X-ray Scattering Primer
Elements of X-ray scattering

Sources of X-rays, Synchrotron Radiation
Laboratory sources, accelerator bases sources

Reflection and Refraction
Snell’s law, Fresnel equations,

Kinematical Diffraction (I)
Diffraction from an atom, molecule, liquids, glasses,..

Kinematical Diffraction (II)
Diffraction from a crystal, reciprocal lattice, structure factor,..

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Small Angle Scattering, and Soft Matter
Introduction, form factor, structure factor, applications, ..

Anomalous Diffraction
Introduction into anomalous scattering,..

Introduction into Coherence
Concept, First order coherence, ..

Coherent Scattering
Spatial coherence, second order coherence,..

Applications of coherent Scattering
Imaging and Correlation spectroscopy,..

X-ray Scattering: A Primer

Scattering from a single electron

Scattering from a single atom

Scattering from a crystal

Compton Scattering

Photoelectric Absorption

Absorption and Reflection

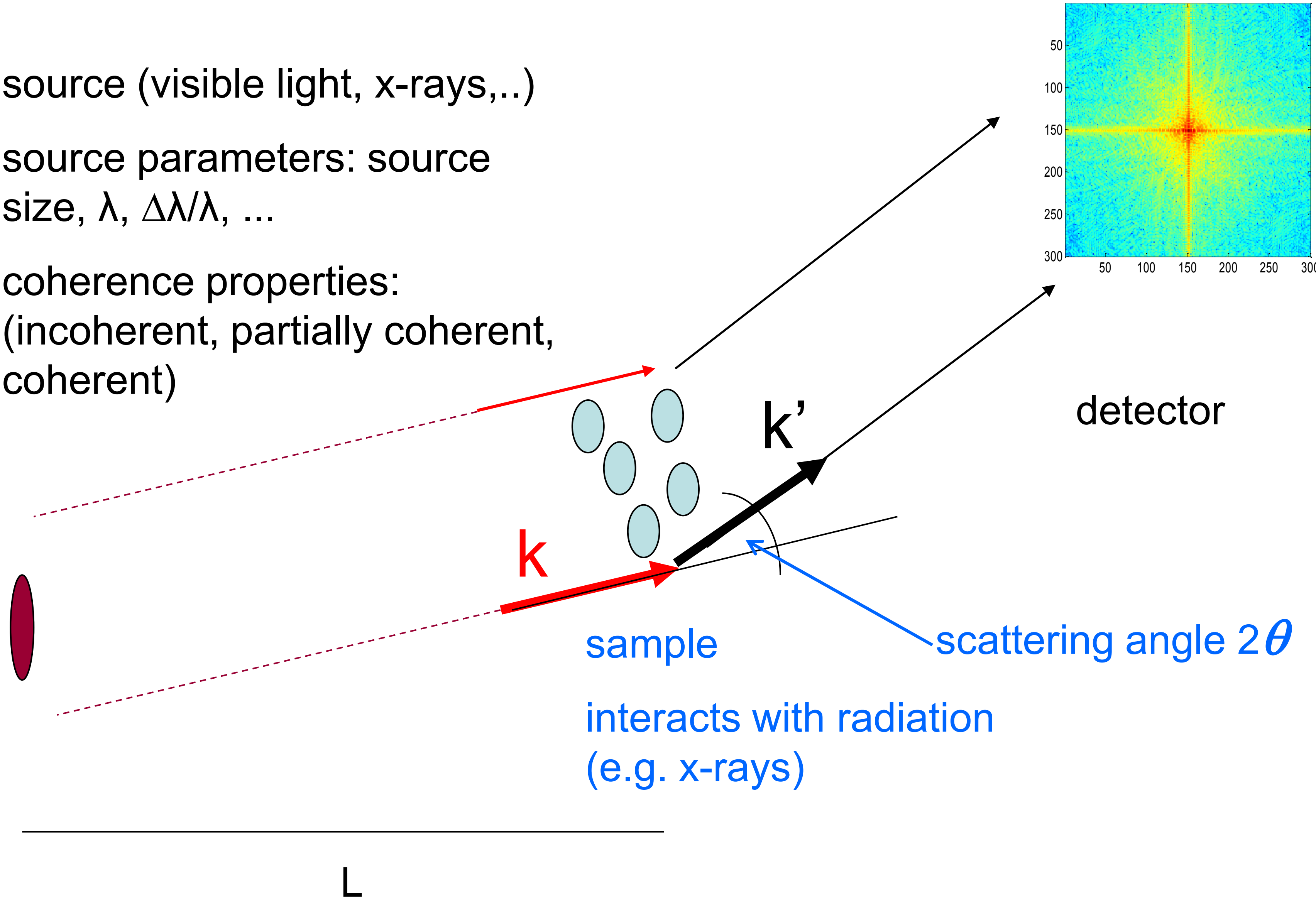
Coherence Properties

Set-Up for Scattering Experiments

source (visible light, x-rays,..)

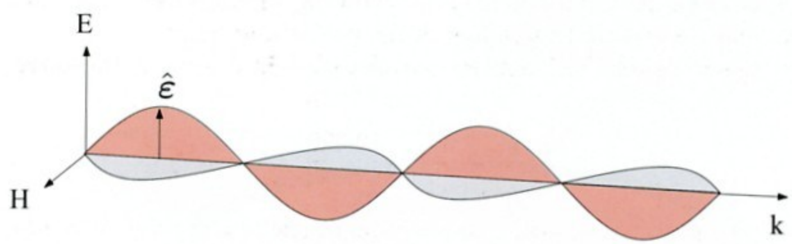
source parameters: source size, λ, Δλ/λ, ...

coherence properties: (incoherent, partially coherent, coherent)



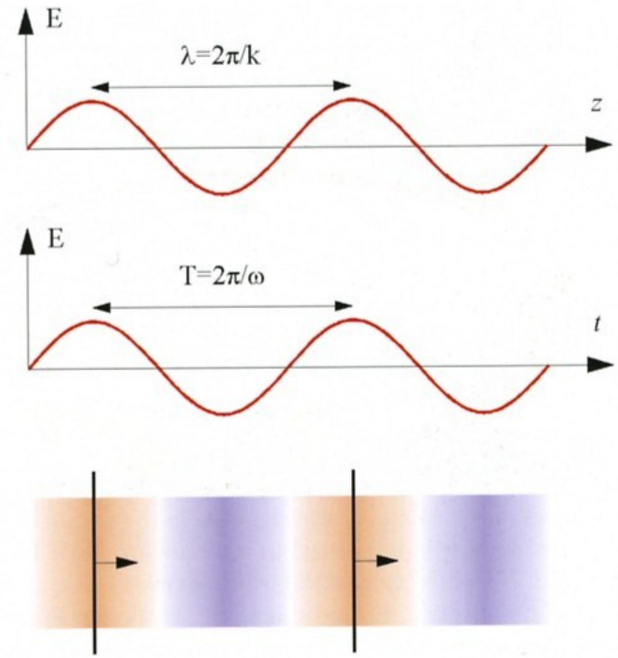
X-rays: Electromagnetic waves and photons

X-rays are electromagnetic waves with wavelengths in the region of Ångstroms (10^{-10} m). X-rays are transverse electromagnetic waves, where the electric and magnetic fields, **E** and **H**, are perpendicular to each other and to the propagation direction **k**.



Neglecting the H field one may write:

$$\mathbf{E}(\mathbf{r},t) = \boldsymbol{\varepsilon}\, E_o \exp\{i(\mathbf{kr}-\omega t)\}$$



with

ε: polarization vector

$|\mathbf{k}| = 2\pi/\lambda$; $E=h\nu = \hbar\omega = hc/\lambda$

$\lambda[\text{Å}] = hc/E = 12.398 / E[\text{keV}]$

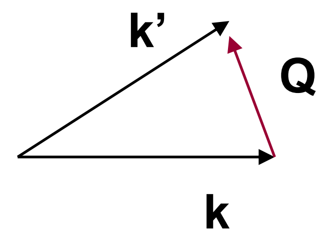
Scattering of X-rays

consider a monochromatic plane (electromagnetic) wave with wavevector k:

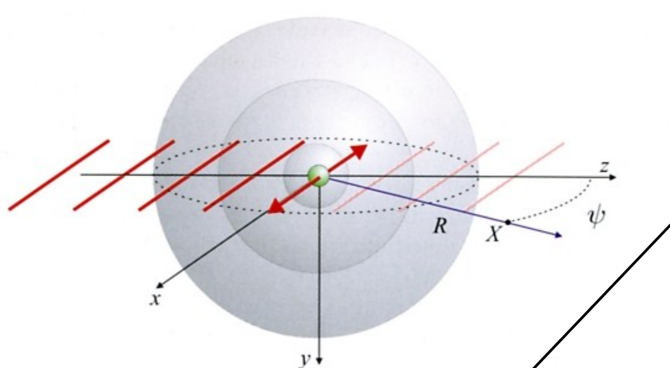
$\mathbf{E}(\mathbf{r},t) = \boldsymbol{\varepsilon}\, E_o \exp\{i(\mathbf{kr}-\omega t)\}$ with $|\mathbf{k}|=2\pi/\lambda$

elastic scattering:

$\hbar\, \mathbf{k'} = \hbar\, \mathbf{k} + \hbar \mathbf{Q}$



Scattering by a single electron:



$E_{rad}(R,t)/E_{in} =$

$-(e^2/4\pi\varepsilon_o mc^2)\exp(ikR)/R \cos\psi$

spherical wave

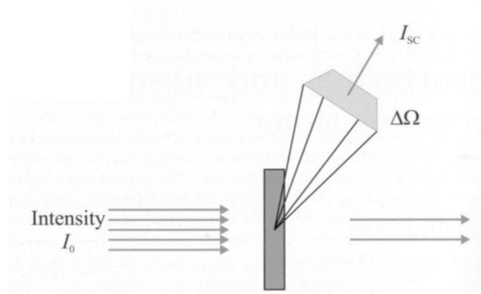
thomson scattering length r_o

($=2.82 \cdot 10^{-5}$ Å)

phase shift of π btw. incident and radiated field

▪

scattered intensity:



$$I_S/I_0 = \frac{|E_{rad}|^2 R^2 \Delta\Omega}{|E_{In}|^2 A_o}$$

$\Delta\Omega$: solid angle seen by detector

$R^2\Delta\Omega$: cross sectional area scattered beam

A_o: incident beam size

$$I_S/I_0 = (d\sigma/d\Omega)\,(\Delta\Omega/A_o)$$

with ($d\sigma/d\Omega$) being the differential cross section (for Thomson scattering):
(# photons scattered/s into $\Delta\Omega$: $Is/\Delta\Omega$ / incident flux: I_0/A_0)

$$(d\sigma/d\Omega) = r_o^2\, P \qquad P = \begin{cases} 1 & \text{vertical} \\ \cos^2\psi & \text{horizontal} \\ \tfrac{1}{2}(1+\cos^2\psi) & \text{unpolarized} \end{cases}$$

note: $\sigma_{total} = \int (d\sigma/d\Omega) = (8\pi/3)\, r_o^2$

▪

<u>scattering by a single atom:</u> scattering amplitude $A(Q) = -r_0 f(Q)$

$\equiv$ scattering amplitude by an ensemble of electrons

$$-r_o f^o(Q) = -r_o \sum_{r_j} \underbrace{\exp(iQ\cdot r_j)}_{\text{phase factor}}$$

↑ (atomic) formfactor ↑ position of scatterers

$$\{ f^o(Q \to 0) = Z, \quad f^o(Q \to \infty) = 0 \}$$

form factor of an atom:

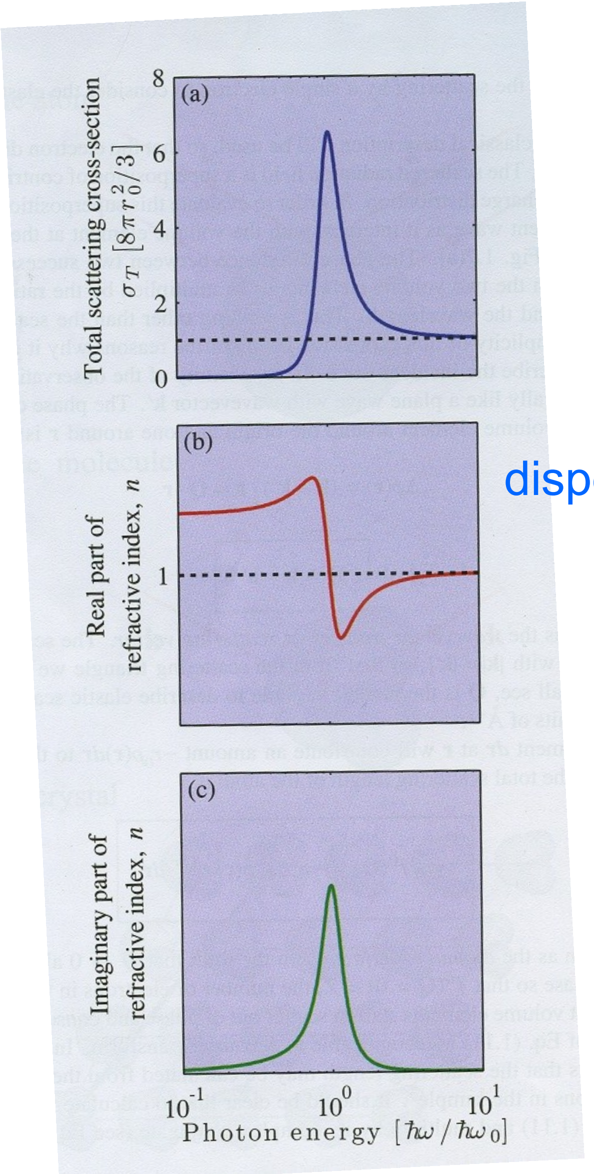
$$f(Q,\hbar\omega) = f^o(Q) + f'(\hbar\omega) + i f''(\hbar\omega)$$

dispersion corrections: level structure (f'), absorption effects (f'')

scattering intensity:

$$I_s = A(Q)A(Q)^* = r_o^2 f(Q) f^*(Q) P$$

▪ scattering by a single atom:



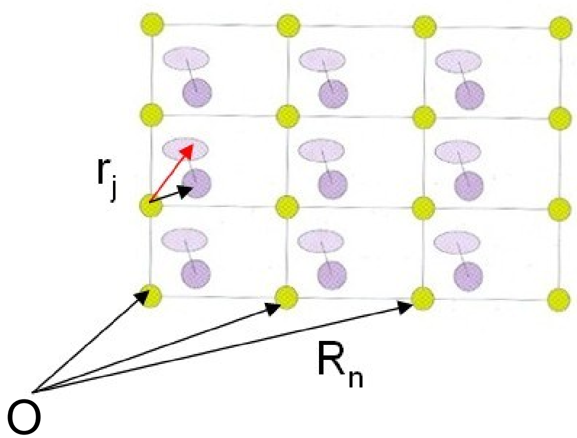
form factor of an atom:

$$f(Q,\hbar\omega) = f^o(Q) + f'(\hbar\omega) + i\,f''(\hbar\omega)$$

dispersion corrections: level structure absorption effects

▪

scattering by a crystal:



$r_{j'} = R_n + r_j$

lattice vector + atomic position in lattice

$$F^{crystal}(Q) = \underbrace{\Sigma_{rj}\, f_j(Q)\exp(iQr_j)}_{\text{unit cell structure factor}}\ \underbrace{\Sigma_{Rn}\exp(iQR_n)}_{\text{lattice sum}}$$

unit cell structure factor lattice sum

$$I_s = r_o^2\, F(Q)\, F^*(Q)\, P$$

lattice sum ≡ phase factor of order unity or N (number of unit cells) if

$$Q \bullet R_n = 2\pi \text{ x integer and } Q = G$$

▪

<u>unit cell structure factor:</u> $\Sigma_{rj}\, f_j(Q)\exp(iQr_j)$

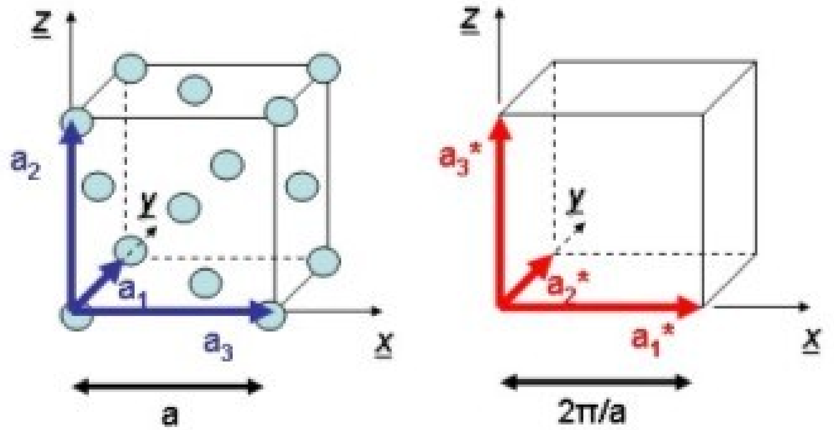
<u>e.g. fcc lattice:</u>

$r_1 = 0$

$r_2 = \frac{1}{2}(a_1+a_2)$

$r_3 = \frac{1}{2}(a_2+a_3)$

$r_4 = \frac{1}{2}(a_3+a_1)$



$a_1=a\underline{x}$; $a_2=a\underline{y}$; $a_3=a\underline{z}$; $v_c = a^3$; $a_1^*=(2\pi/a)\underline{x}$; $a_2^*=(2\pi/a)\underline{y}$; $a_3^*=(2\pi/a)\underline{z}$

$F_{hkl}^{fcc} = f(Q)\, \Sigma \exp(iQr_j)$ with $Q = G = h\, a_1^* + k\, a_2^* + l\, a_3^*$

$$= f(Q)\,\{1 + e^{i\pi(h+k)} + e^{i\pi(k+l)} + e^{i\pi(l+h)}\} \qquad (£)$$

$$= f(Q) \times \begin{cases} 4 & \text{if h,k,l are all even or odd} \\ 0 & \text{otherwise} \end{cases}$$

Compton Scattering

consider photon with momentum $p = \hbar$ **k** scattered by a electron, initially at rest

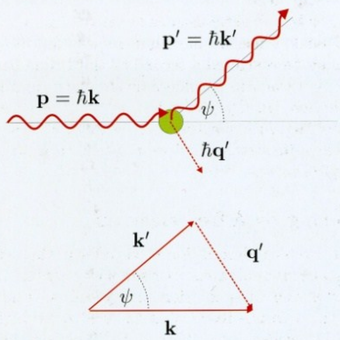
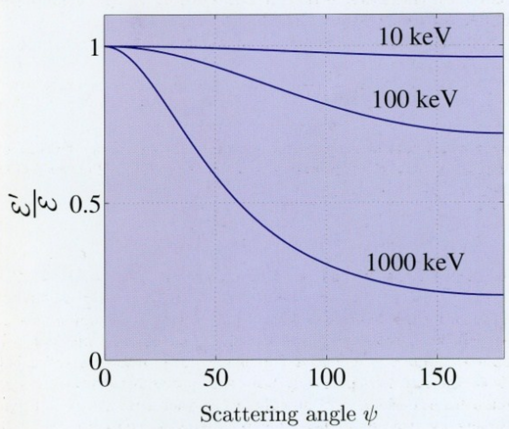


Figure 1.7: Compton scattering. A photon with energy $\mathcal{E} = \hbar ck$ and momentum $\hbar\mathbf{k}$ scatters from an electron at rest with energy mc^2. The electron recoils with a momentum $\hbar\mathbf{q}' = \hbar(\mathbf{k} - \mathbf{k}')$ as indicated in the scattering triangle in the bottom half of the figure.



<u>energy conservation:</u>

$m_0c^2 + \hbar ck = \mathrm{sqrt}\{(m_0c^2)^2 + (\hbar cq')^2\} + \hbar ck'$

with $\lambda_c = \hbar c / m_0c^2$:compton wavelength

$q'^2 = (k-k')^2 + 2(k-k')/\lambda_c q$ (1)

<u>momentum conservation</u>: $q' = k - k'$

$q' \cdot q' = q'2 = (k-k') \bullet (k-k') = k2 + k'^2 - 2kk'\cos\psi$ (2)

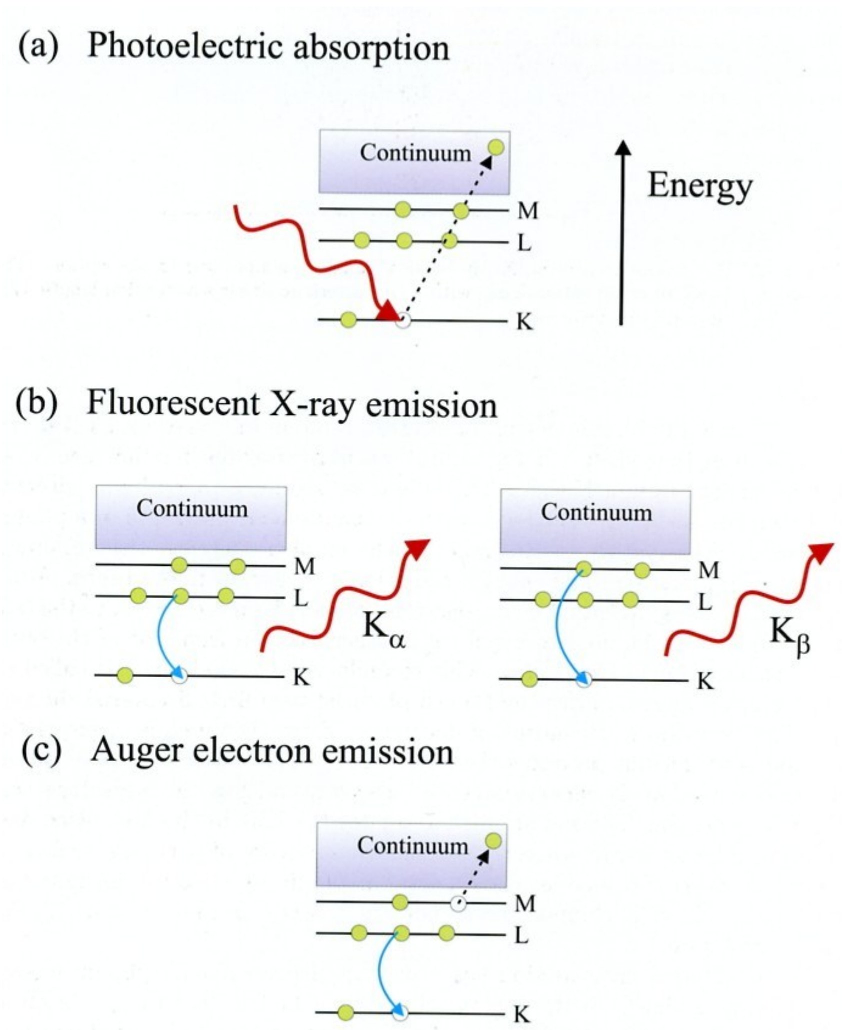
(1) = (2)

$k/k' = 1 + \lambda_c k(1-\cos\psi) = E/E' = \lambda'/\lambda$

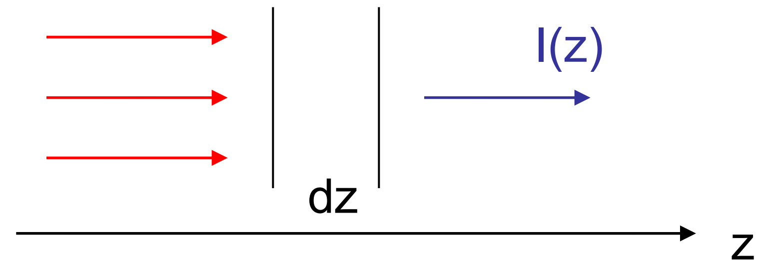
➔ origin of background

➔ determine electronic momentum distribution of materials

▪ Photoelectric absorption



$$-dI = I(z)\,\mu\,dz$$



$$I(z) = I_o \exp(-\mu z)$$

$$\mu = \rho_a \sigma_a = (\rho_m N_A / A)\,\sigma_a$$

ρ_a atomic number density

$\sigma_a = \sigma_a(E)$ absorption cross section

ρ_m mass density

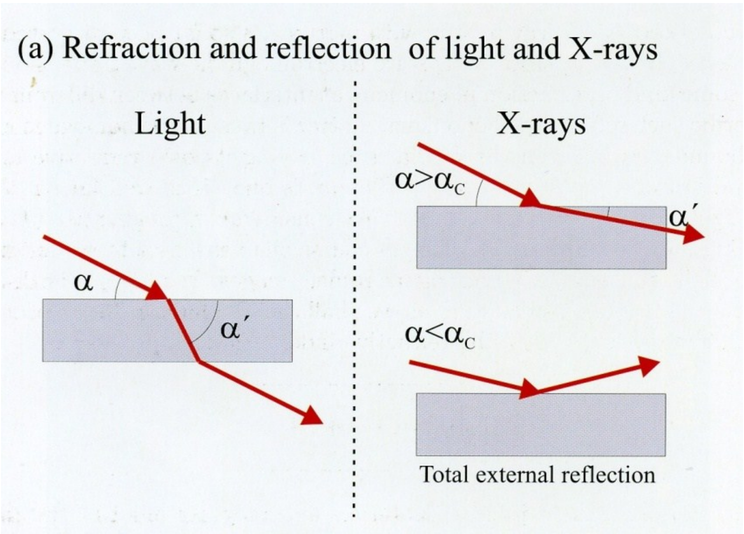
N_A Avogadro's number

A atomic mass number

Refraction

$$n = 1 - \delta + i\beta \qquad < 1$$

10^{-5} (δ) absorption ($<<\delta$) (β)



Snell's law:

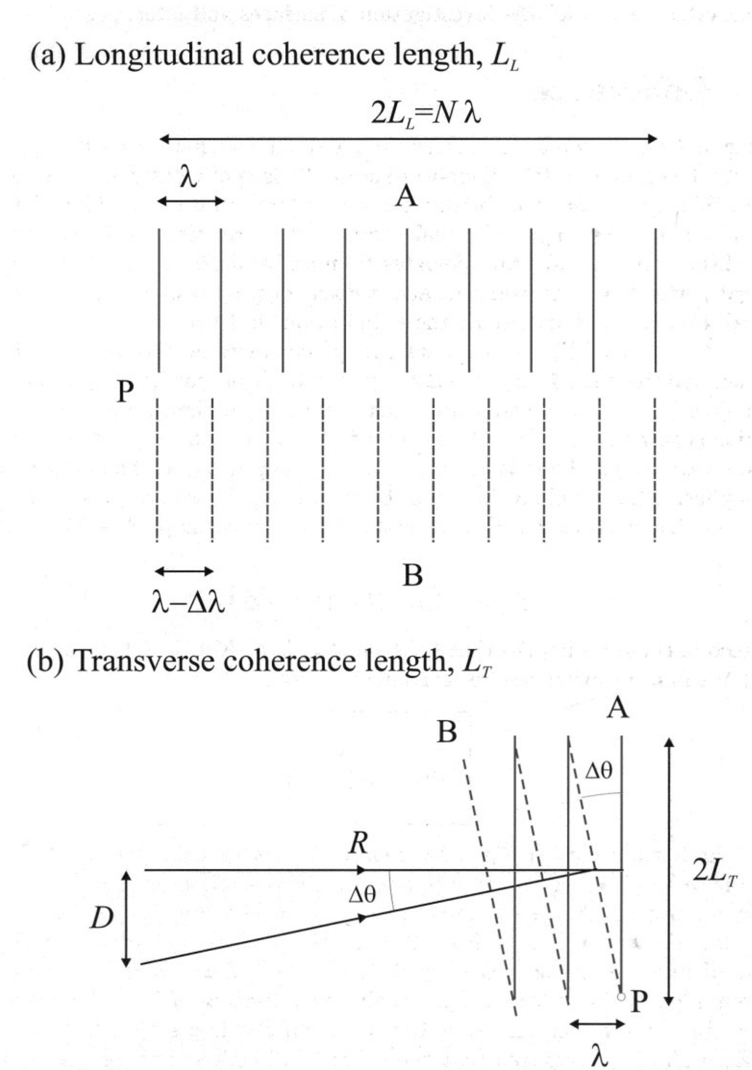
$\cos\alpha = n \cos\alpha'$

note: total external reflexion for x-rays ($\alpha' = 0$)

$n < 1$

$\alpha_c = \mathrm{sqrt}\,(2\delta)$

Coherence



Longitudinal coherence:

Two waves are in phase at point P. How far can one proceed until the two waves have a phase difference of π:

$$\xi_l = (\lambda/2)\,(\lambda/\Delta\lambda)$$

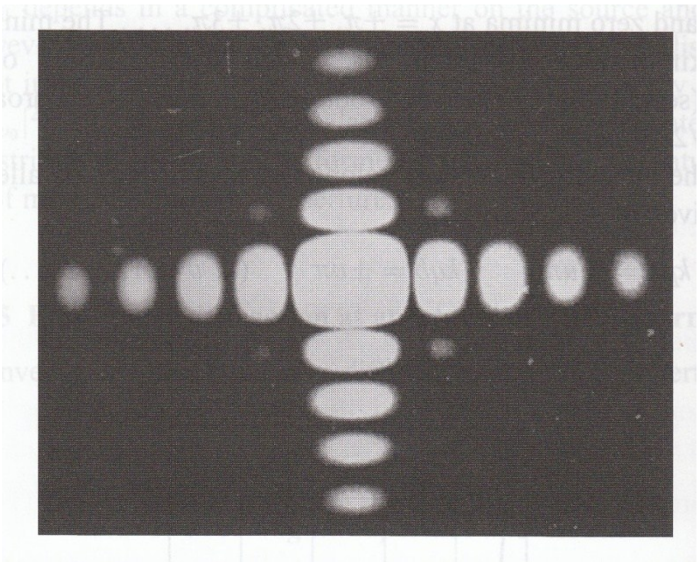
Transverse coherence:

Two waves are in phase at P. How far does one have to proceed along A to produce a phase difference of π:

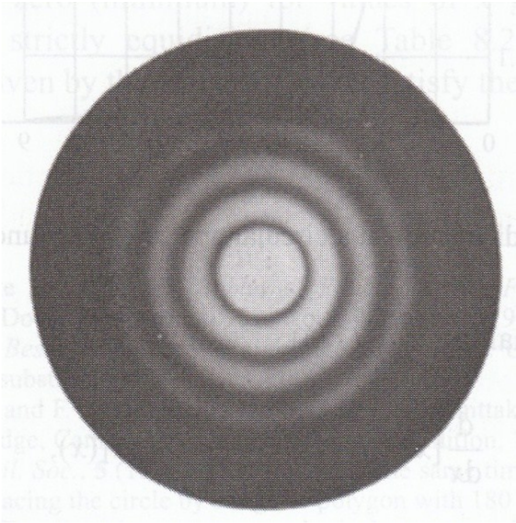
$$2\xi_t\,\Delta\theta = \lambda$$

$$\xi_t = (\lambda/2)\,(R/D)$$

Fraunhofer Diffraction

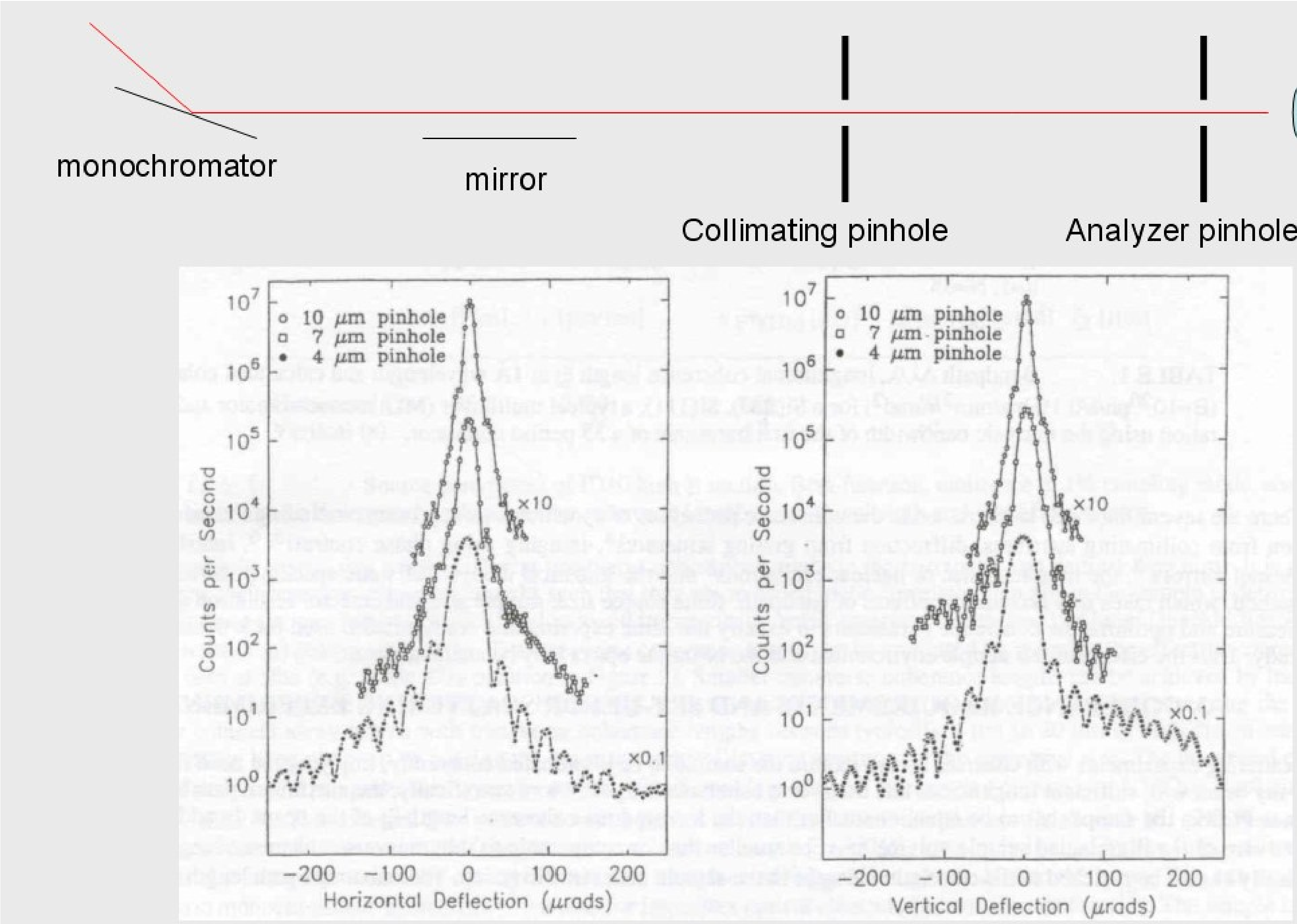


Fraunhofer diffraction of a rectangular aperture 8 x 7 mm^2, taken with mercury light λ=579nm
(from Born&Wolf, chap. 8)



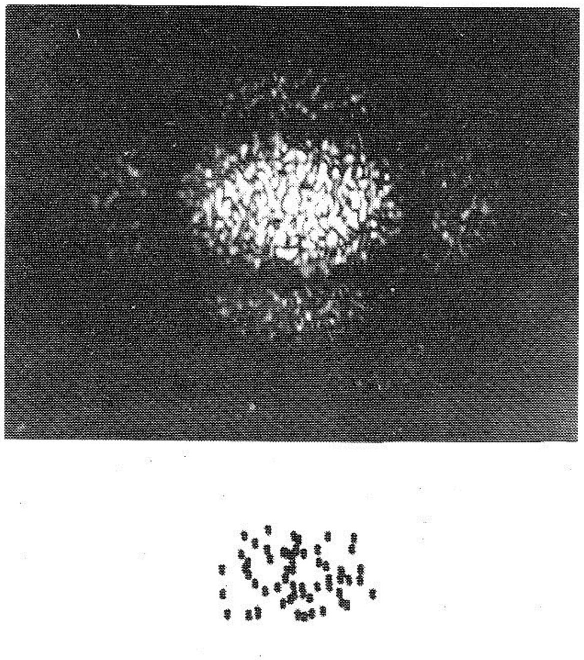
Fraunhofer diffraction of a circular aperture, taken with mercury light λ=579nm
(from Born&Wolf, chap. 8)

Fraunhofer Diffraction (λ=0.1nm)

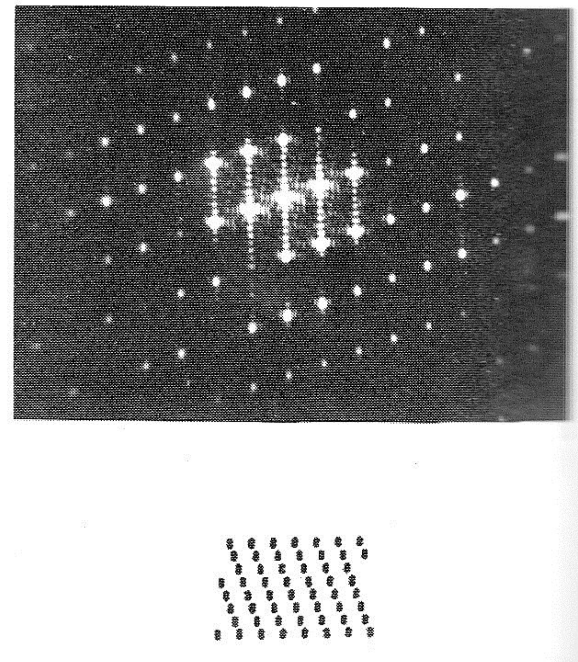


ID10 (ESRF)
E=11.8 keV;
λ=1.05Å

Speckle pattern



random arrangement of apertures: speckle



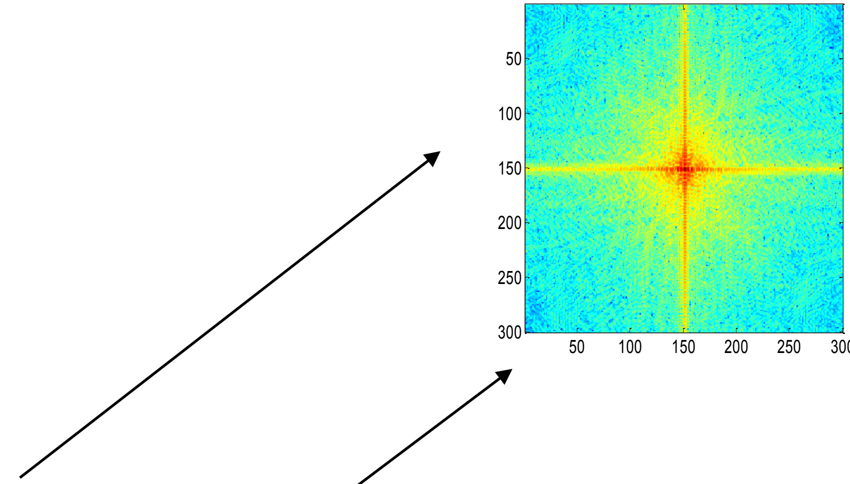
regular arrangement of apertures

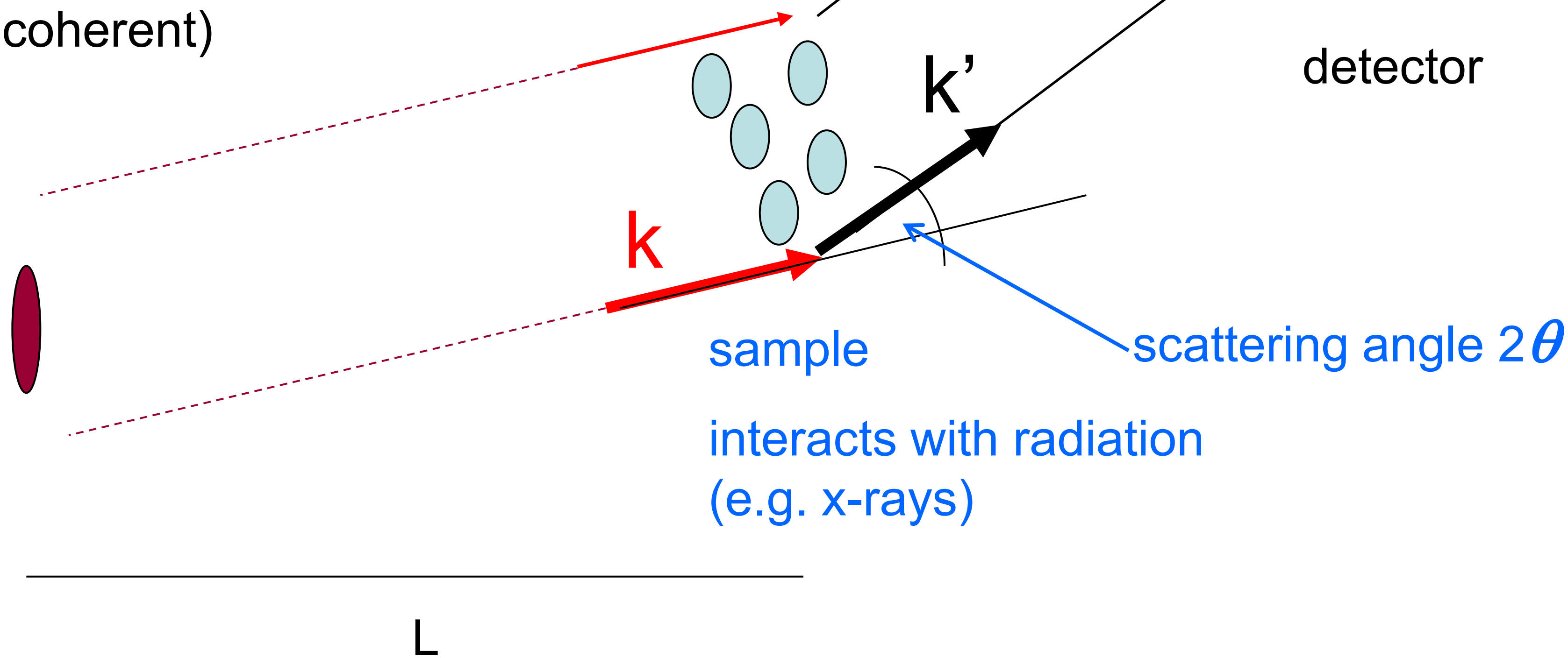
Experimental Set-Up for Scattering Experiments

source (visible light, x-rays,..)

source parameters: source size, λ, Δλ/λ, ...

coherence properties: (incoherent, partially coherent, coherent)





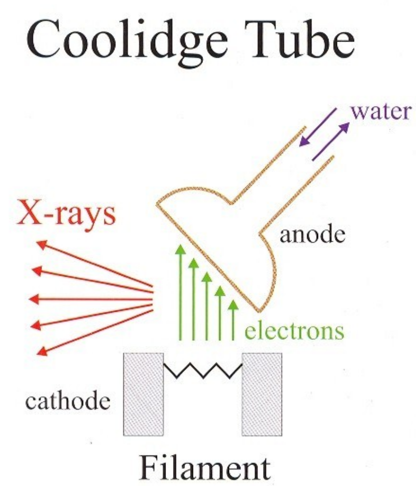
Sources of X-Rays

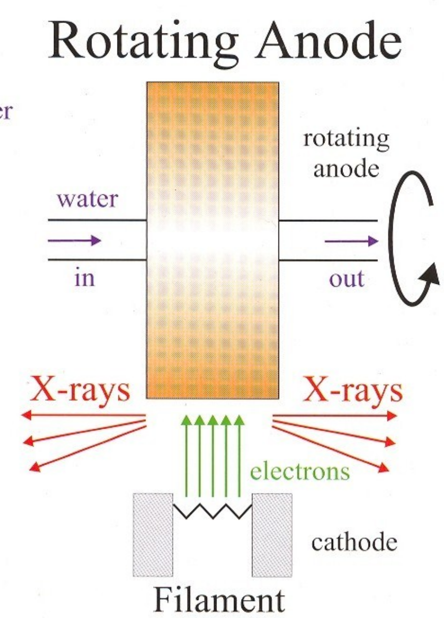
1895 discovered by W.C. Röntgen

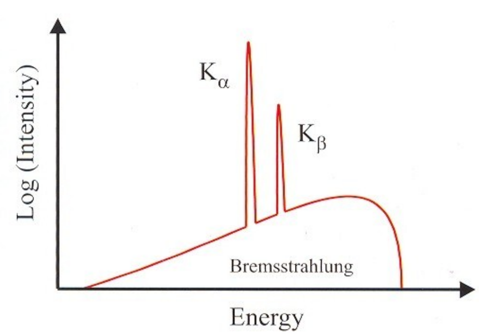
1912 First diffraction experiment (v. Laue)

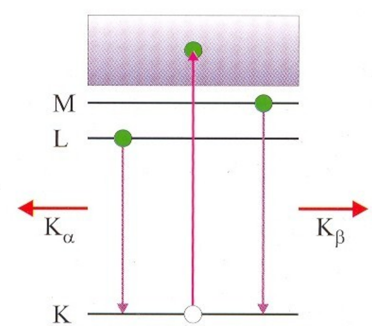
1912 Coolidge tube (W.D. Coolidge,GE)

1946 Radiation from electrons in a synchrotron, GE, Physical Review, 71,829(1947)

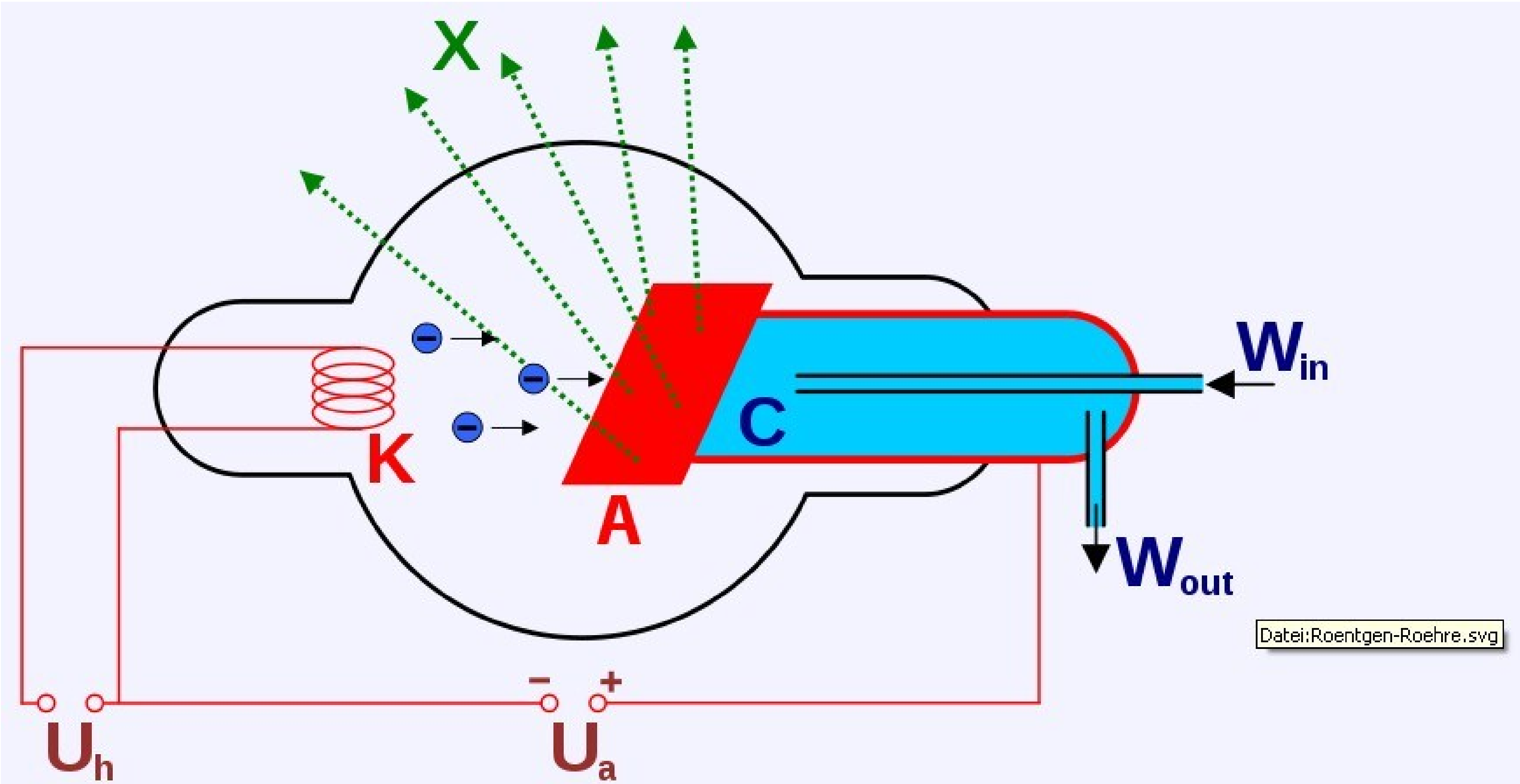






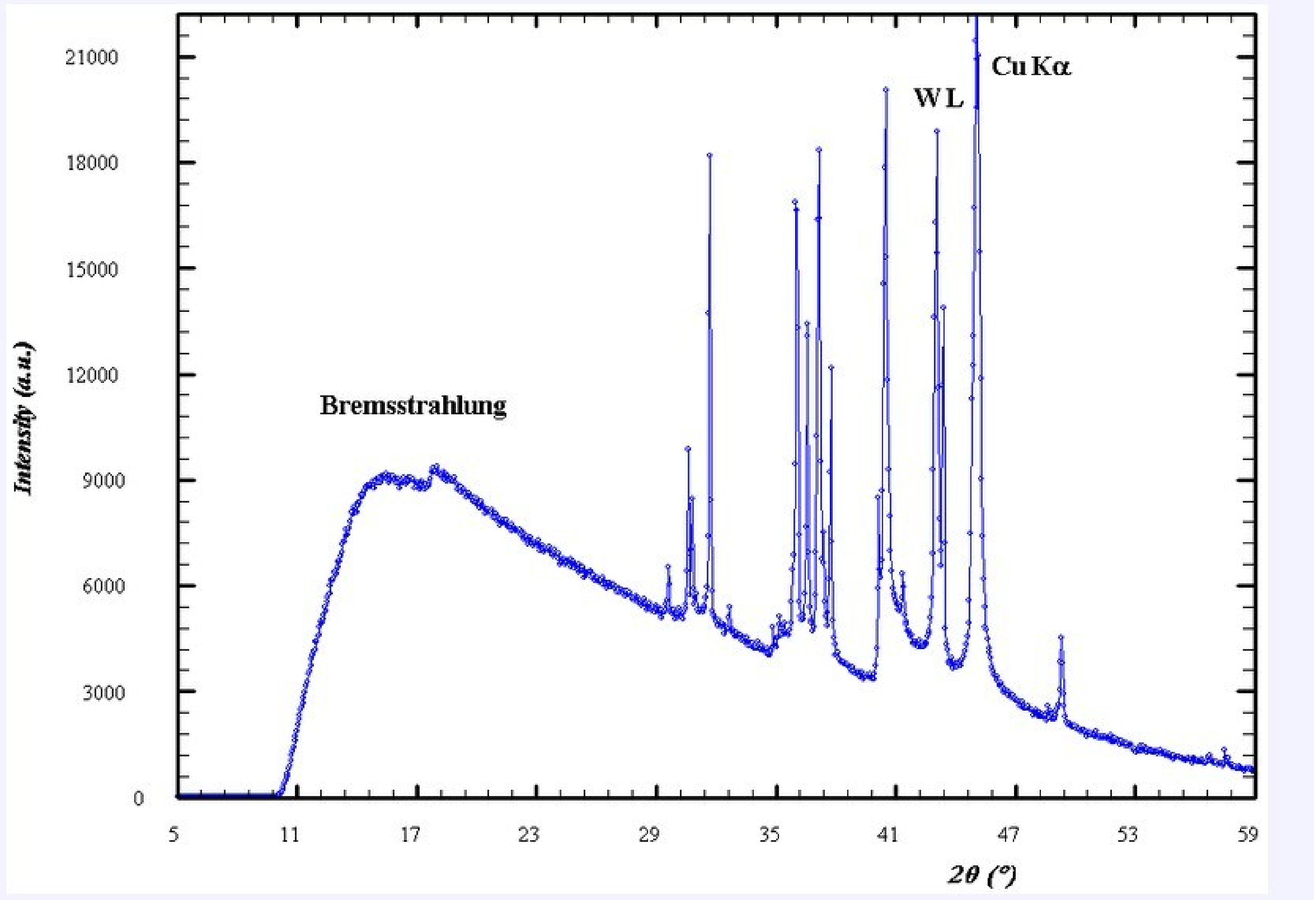


- # X-ray Tube



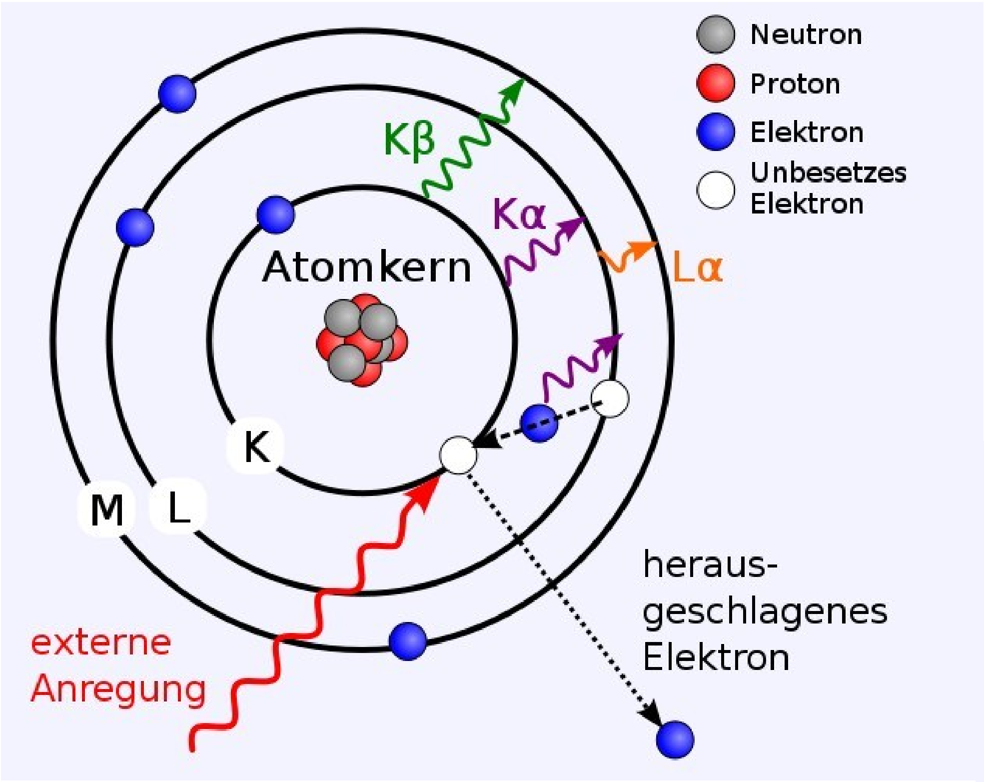
- # X-ray Tube

X-ray Tube

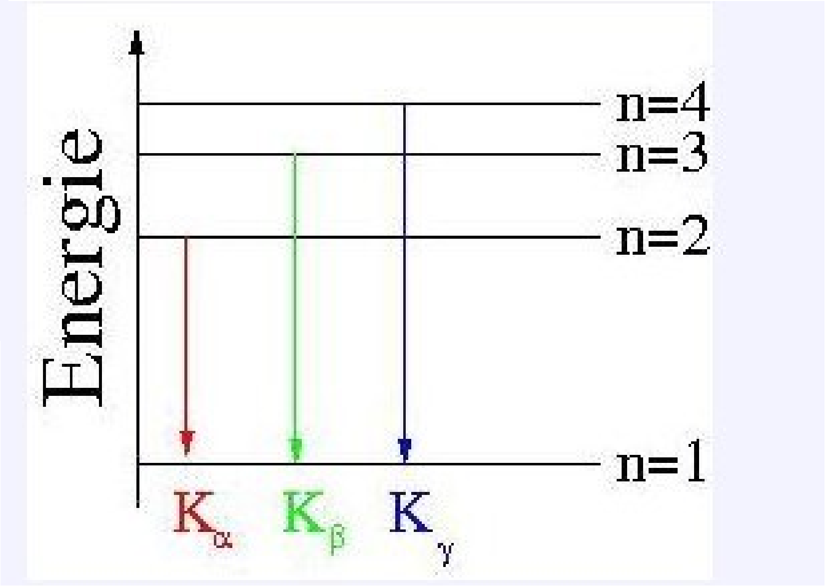


Cu Kα
W L
Bremsstrahlung
Intensity (a.u.)
21000
18000
15000
12000
9000
6000
3000
0
5
11
17
23
29
35
41
47
53
59
2θ (°)

- # X-ray Tube

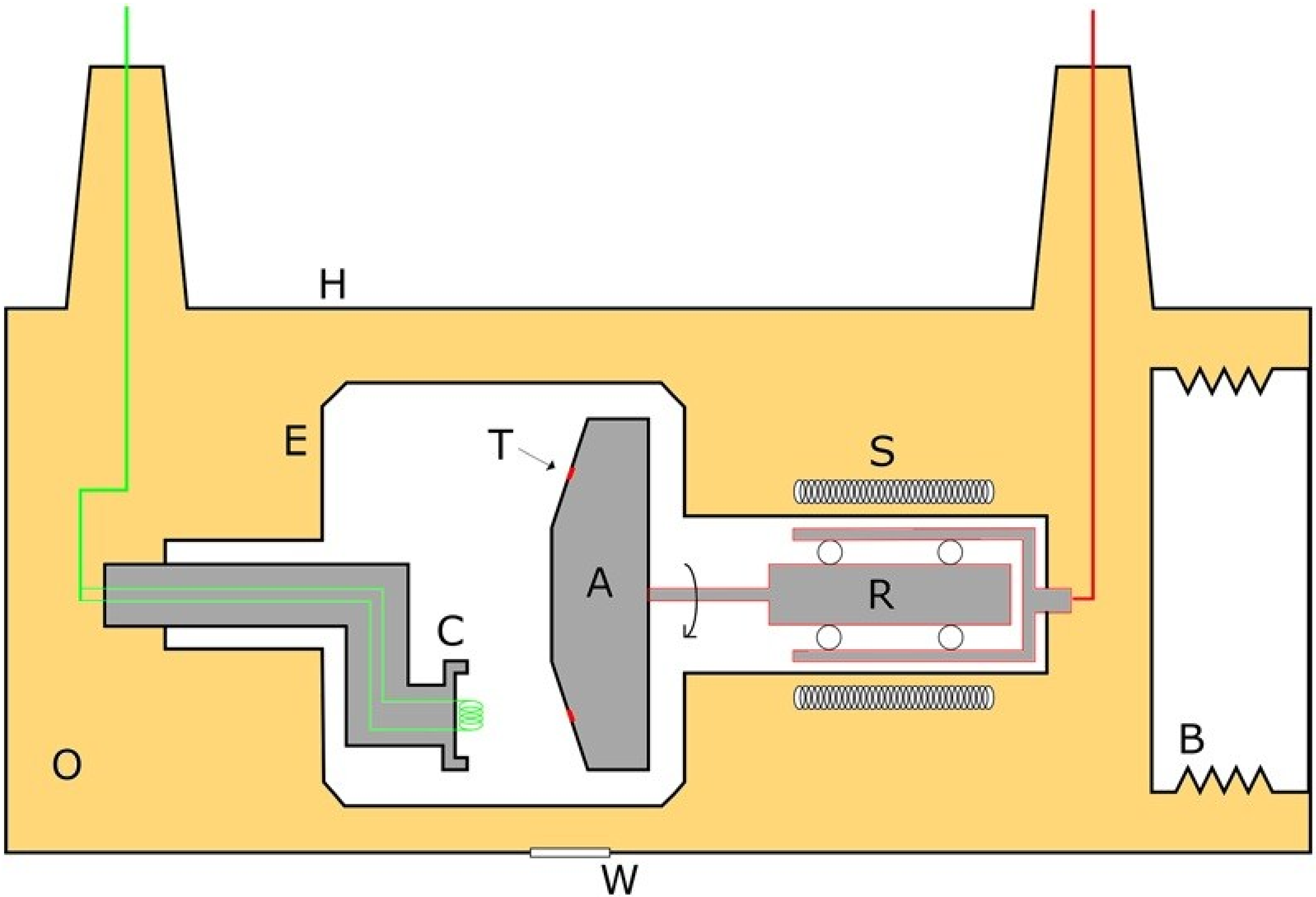


Neutron
Proton
Elektron
Unbesetzes Elektron
Kβ
Kα
Lα
Atomkern
K
L
M
externe Anregung
heraus-geschlagenes Elektron

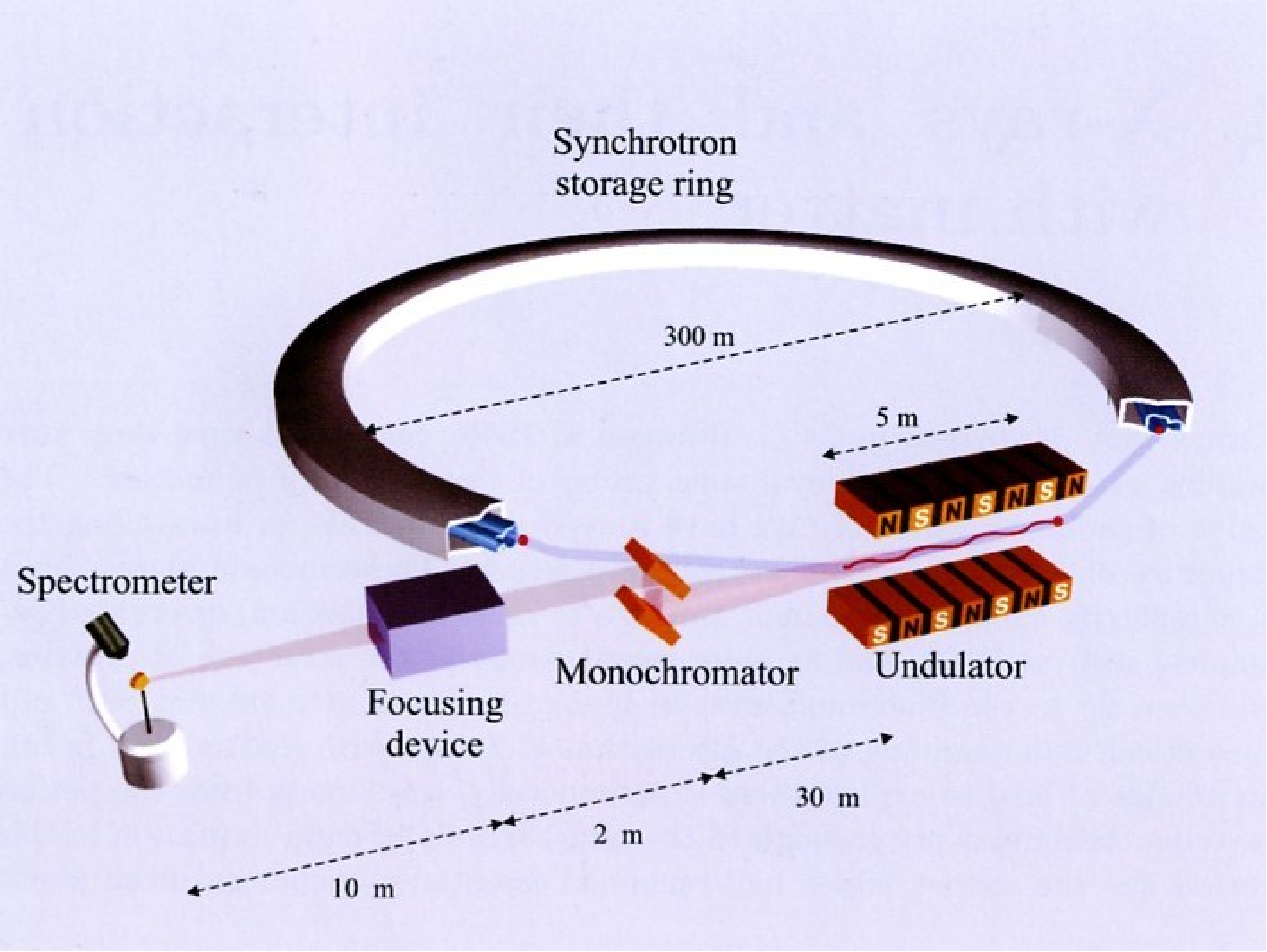


Energie
n=4
n=3
n=2
n=1
K_α
K_β
K_γ

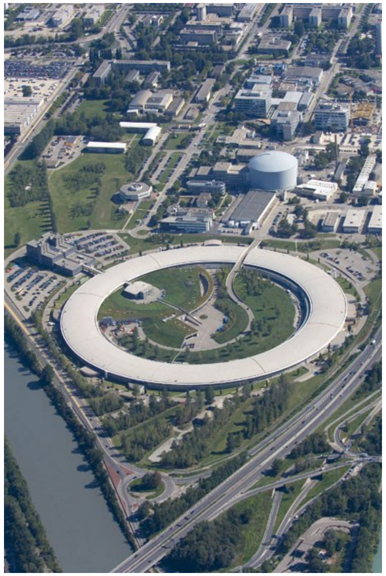
Rotating Anode



Synchrotron Radiation Storage Ring



▪ Photos machines



The most recent third generation machine:

Petra III at DESY/Hamburg