Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture 2	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2015 G. Grübel, M. Martins, E. Weckert	
Location	Lecture hall AP, Physics, Jungiusstraße	
Date	Tuesday Thursday	12:45 - 14:15 8:30 - 10:00

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture:	4 SWS	Tuesday and Thursday
Tutorial/Übungen:	2 SWS	Tuesday (if agreed on)

Proseminar: *For Bachelor students*
8 credits: For Master students

Fixed dates:	Tuesday	12:45 - 14:15
	Thursday	8:30 - 10:00
Organization meeting“Tutorial”:	Tuesday, April 7	14:30 - 16:00
Location:	Seminar room 4	

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecturers: Gerhard Grübel (GG), Thomas Schneider (TS), Oliver Seek (OS), Stephan Roth (SR),

Part I:	**Basics of X-ray Physics**	(GG)
Part II:	**Soft Matter**	(SR)
Part III:	**Surfaces and Interfaces**	(OS)
Part IV:	**Macromolecular Crystallography**	(TS)
	Site Visit	

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 Ultraviolet 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/ss15/index_eng.htm

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Part I:

Basics of X-ray Physics

by Gerhard Grübel (GG)

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 from Interfaces
Snell's Law, Fresnel Equations

Kinematical Diffraction (I)
Diffraction from an Atom, a Molecule, from 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 Scattering

Photoelectric Absorption

Absorption and Reflection

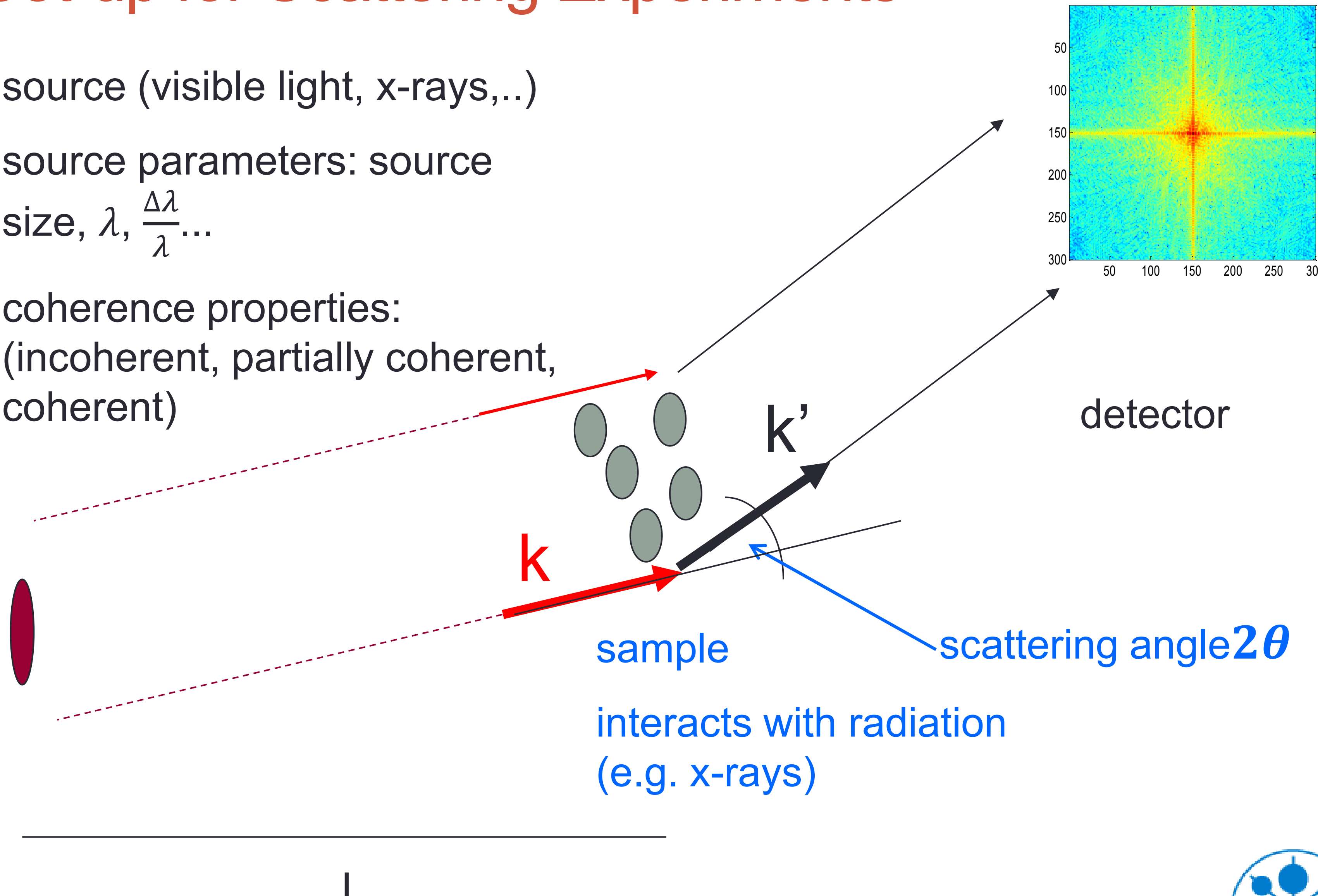
Coherence Properties

Set-up for Scattering Experiments

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

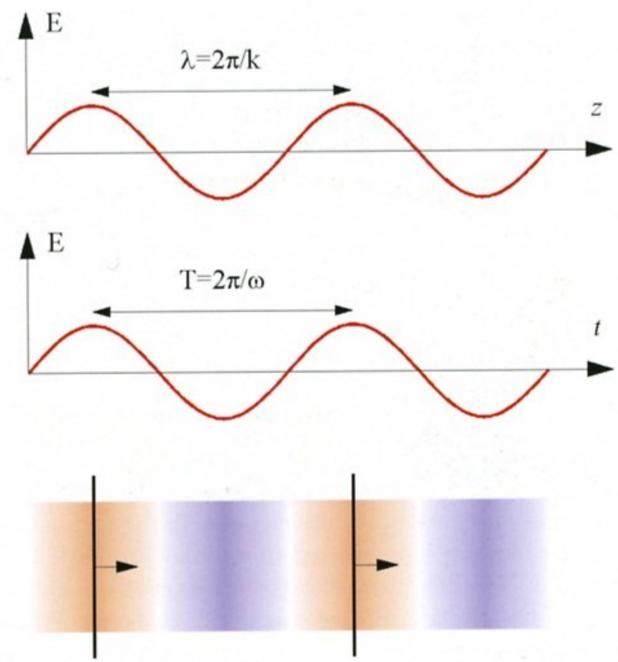
source parameters: source size, λ, $\frac{\Delta\lambda}{\lambda}$...

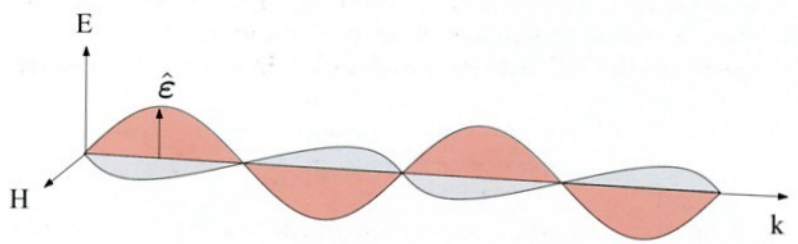
coherence properties: (incoherent, partially coherent, coherent)



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:

$$\mathbf{E}(\boldsymbol{r},t) = \boldsymbol{\varepsilon}\, \mathrm{E}_0 \mathrm{e}^{i(\mathbf{kr}-\omega t)}$$

with

ε: polarization vector

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

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

Scattering of X-rays

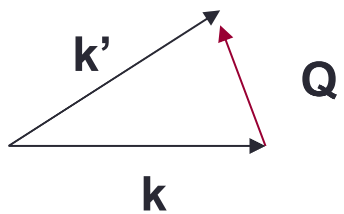
Consider a monochromatic plane (electromagnetic) wave with wave vector $\mathbf{k}$:

$$\mathbf{E}(\mathbf{r},t) = \boldsymbol{\varepsilon}\, \mathrm{E}_0 \mathrm{e}^{i(\mathbf{kr}-\omega t)}$$

with $|\mathbf{k}| = \frac{2\pi}{\lambda}$

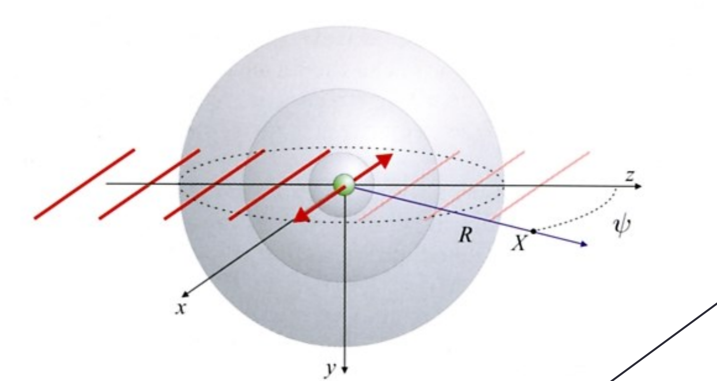
Elastic scattering:

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



Scattering by a Single Electron:

$$\frac{\mathrm{E_{rad}}(R,t)}{\mathrm{E_{in}}} = -\frac{e^2}{4\pi\varepsilon_0 mc^2}\frac{\mathrm{e}^{ikR}}{R}\cos\psi$$



spherical wave

Thomson scattering length r_0

$(= 2.82 \text{ x } 10^{-5}\text{Å})$

phase shift of π btw. incident and radiated field

Scattered intensity:

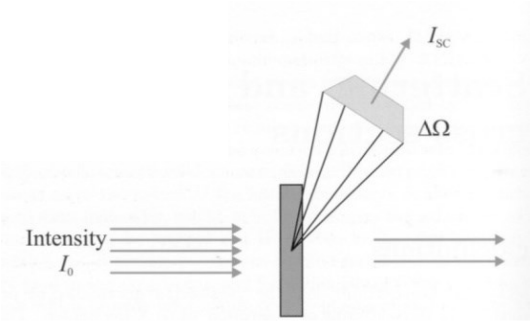
$$\frac{I_s}{I_0} = \frac{|E_{rad}|^2 R^2 \Delta\Omega}{|E_{in}|^2}$$

$$\frac{I_s}{I_0} = \left(\frac{d\sigma}{d\Omega}\right)\left(\frac{\Delta\Omega}{A_0}\right)$$

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

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

A_0: incident beam size



with (*dσ / dΩ*) being the differential cross section (for Thomson scattering):
(# photons scattered/s into $\Delta\Omega$: $I_s/\Delta\Omega$ / incident flux: I_0/A_0)

$$\left(\frac{d\sigma}{d\Omega}\right) = r_0^2 P$$

$$P = \begin{cases} 1 & \text{vertical} \\ \cos^2\psi & \text{horizontal} \\ \frac{1}{2}(1+\cos^2\psi) & \text{unpolarized} \end{cases}$$

Note: $\boldsymbol{\sigma_{total} = \int \left(\frac{d\sigma}{d\Omega}\right) = \left(\frac{8\pi}{3}\right) r_0^2}$

Scattering by a Single Atom: scattering amplitude $A(Q) = -r_0 f(Q)$

phase factor

- **scattering amplitude by an ensemble of electrons** $-r_0 f^0(Q) = -r_0 \sum_{rj} e^{i\,Q\,r_j}$

(atomic) form factor — position of scatterers

$$\{f^2(Q \to 0) = Z, \qquad f^2(Q \to \infty) = 0\}$$

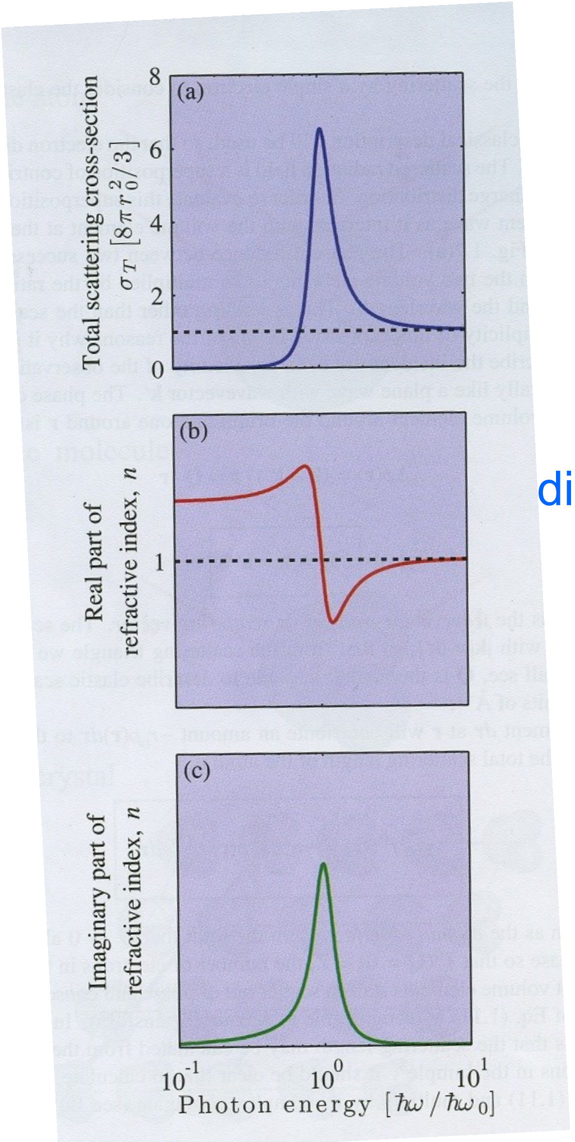
form factor of an atom: $f(Q, \hbar\omega) = f^0(Q) + f'(\hbar\omega) + i\, f''(\hbar\omega)$

dispersion corrections: level structure, absorption effects

scattering intensity: $I_s = A(Q)A(Q)^* = r_0^2 f(Q) f^*(Q) P$

DESY

Scattering by a Single Atom:

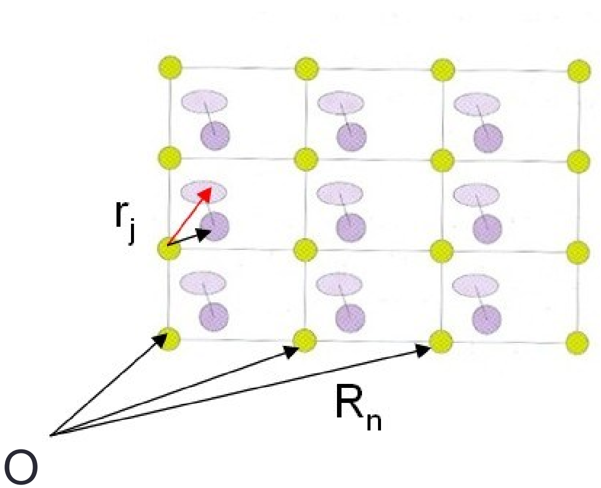


form factor of an atom:

$$f(Q,\hbar\omega) = f^0(Q) + f'(\hbar\omega) + i\, f''(\hbar\omega)$$

dispersion corrections: level structure absorption effects

Scattering by a Crystal:



$$r_j = R_n + r_j$$

lattice vector + atomic position in lattice

$$F^{crystal}(Q) = \underbrace{\sum_{r_j} f_j(Q) e^{iQr_j}}_{\text{unit cell structure factor}} \underbrace{\sum_{R_n} e^{iQR_n}}_{\text{lattice sum}}$$

unit cell structure factor   lattice sum

$$I_s = r_0^2 F(Q) F^*(Q) P$$

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

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

Unit cell structure factor:

$$\sum_{r_j} f_j(Q) e^{iQr_j}$$

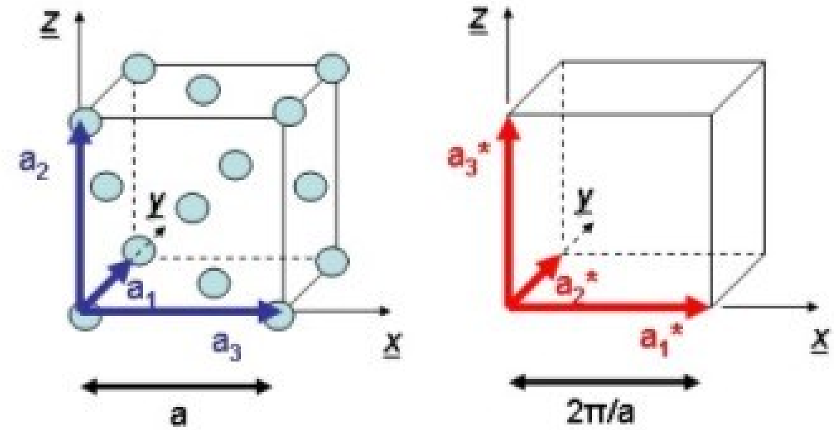
e.g. fcc lattice:

$$r_1 = 0$$

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

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

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



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

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

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

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

Compton Scattering

Consider photon with momentum initially at rest

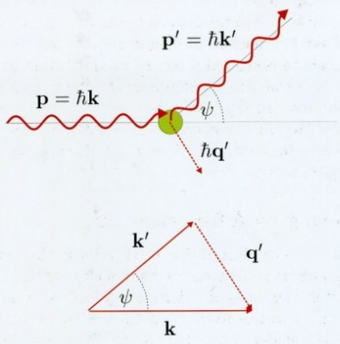
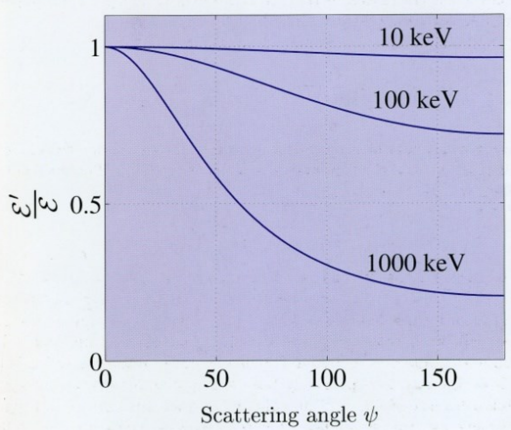


Figure 1.7: Compton scattering. A photon with energy $\mathcal{E} = \hbar ck$ and momentum $\hbar\mathbf{k}$ scatters from an electron at rest with energy mc^2. The electron recoils with a momentum $\hbar\mathbf{q}' = \hbar(\mathbf{k}-\mathbf{k}')$ as indicated in the scattering triangle in the bottom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



$p = \hbar\,\mathbf{k}$ scattered by a electron,

<u>Energy conservation:</u>

$$m_0c^2 + \hbar ck = \sqrt{\{(m_0c^2)^2 + (\hbar c q')^2\}} + \hbar ck'$$

with $\lambda_c = \dfrac{\hbar c}{m_0c^2}$: Compton wavelength

$$q'^2 = (k-k')^2 + 2\frac{(k-k')^2}{\lambda_c q} \qquad (1)$$

<u>Momentum conservation</u>: $p' = k - k'$

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

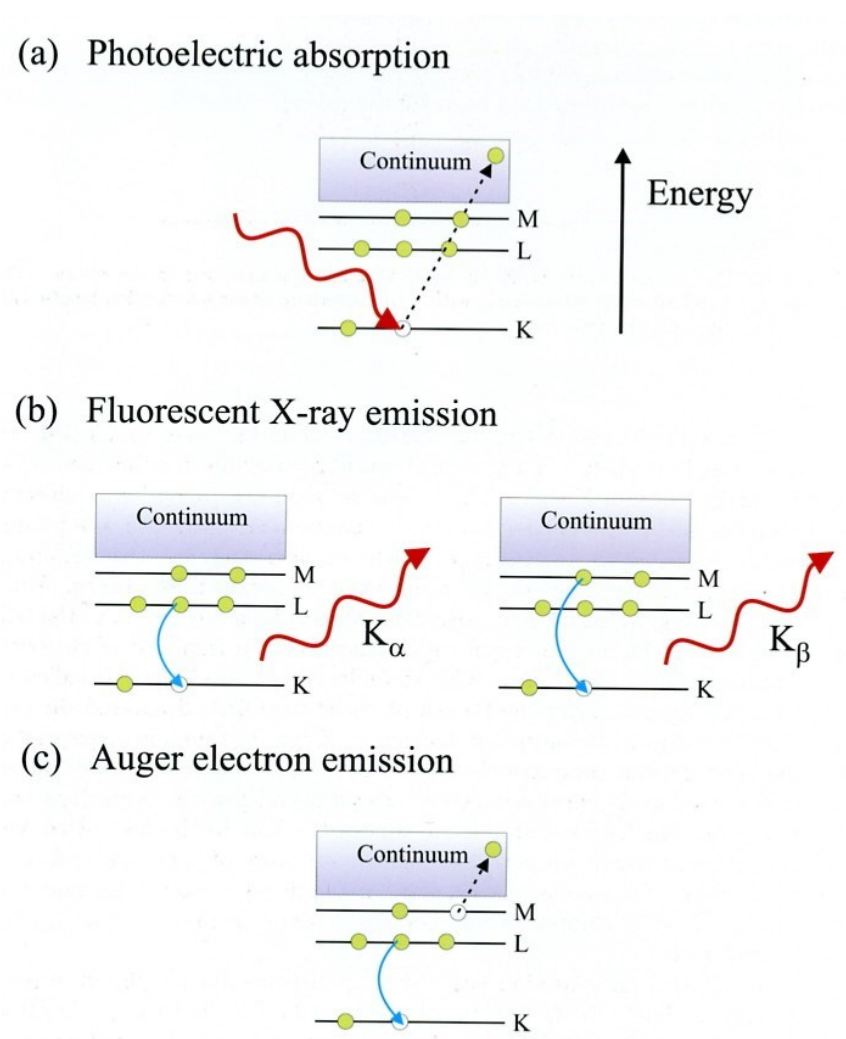
(1) = (2)

$$\frac{\mathbf{k}}{\mathbf{k}'} = \mathbf{1} + \boldsymbol{\lambda_c}\mathbf{k}(\mathbf{1} - \mathbf{cos}\,\boldsymbol{\psi}) = \frac{\boldsymbol{\varepsilon}}{\boldsymbol{\varepsilon}'} = \frac{\boldsymbol{\lambda}'}{\boldsymbol{\lambda}}$$

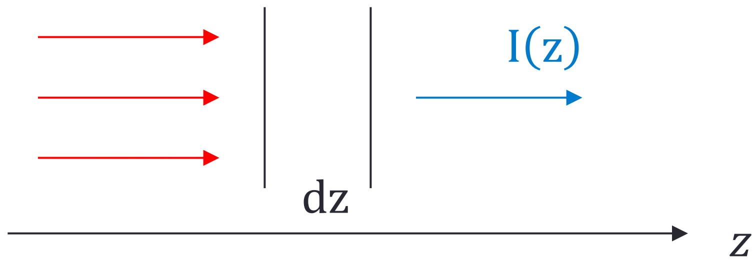
➔ origin of background

➔ determine electronic momentum distribution of materials

Photoelectric Absorption



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



$$I(z) = I_0 e^{-\mu z}$$

$$\mu = p_a \sigma_a = \left(\frac{p_m N_A}{A}\right) \sigma_a$$

p_a atomic number density

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

p_m mass density

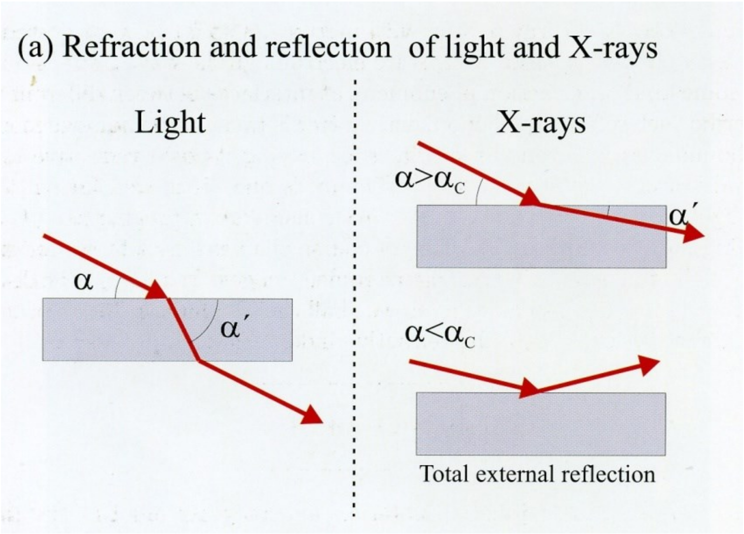
N_A Avogadro’s number

A atomic mass number

Refraction

$$\mathbf{n} = \mathbf{1} - \boldsymbol{\delta} + \mathbf{i}\boldsymbol{\beta} \qquad < 1$$

δ: 10^{-5} — β: absorption (<< δ)



Snell's law:

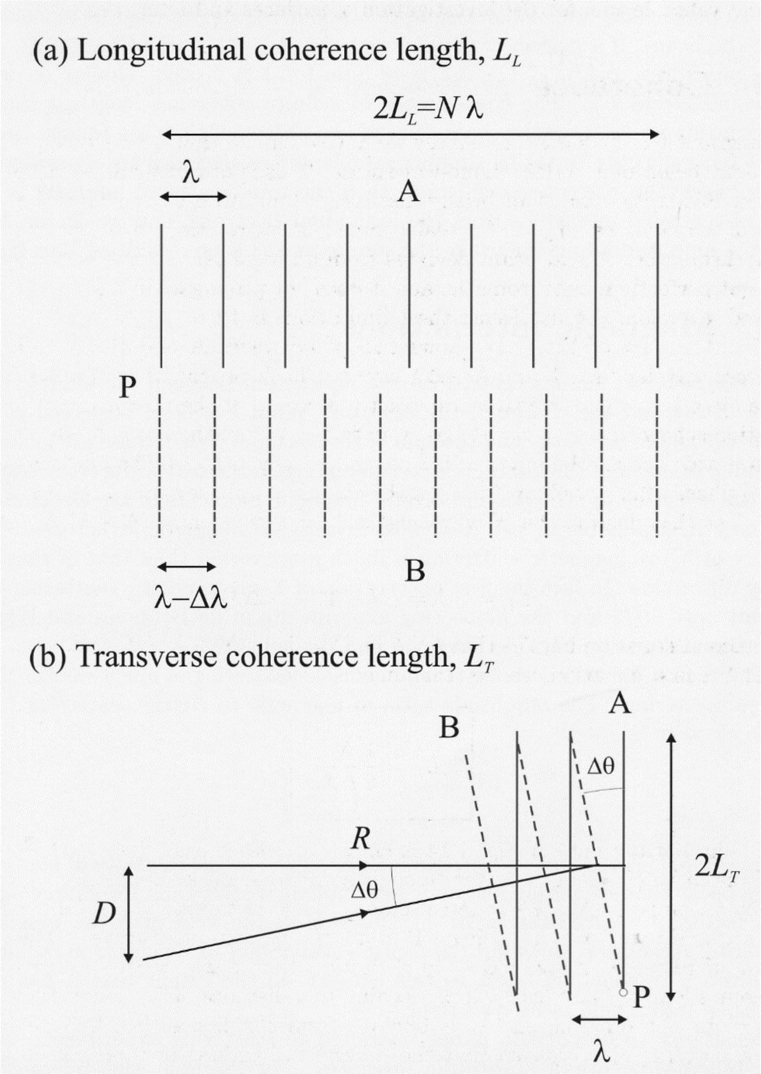
$\cos\alpha = \cos\alpha'$

Note: total external reflection for x-rays $(\alpha' = 0)$

n < 1

$\alpha_c = \sqrt{2\delta}$

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:

$$\xi_l = \frac{1}{2}\frac{\lambda^2}{\Delta\lambda}$$

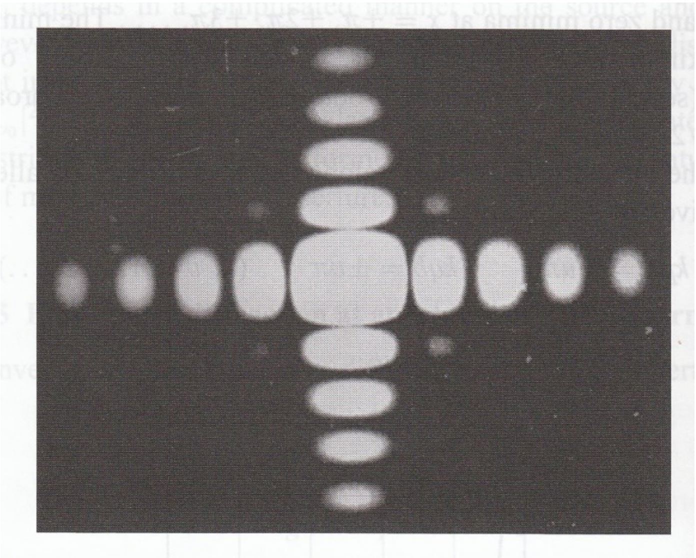
Transverse coherence:

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

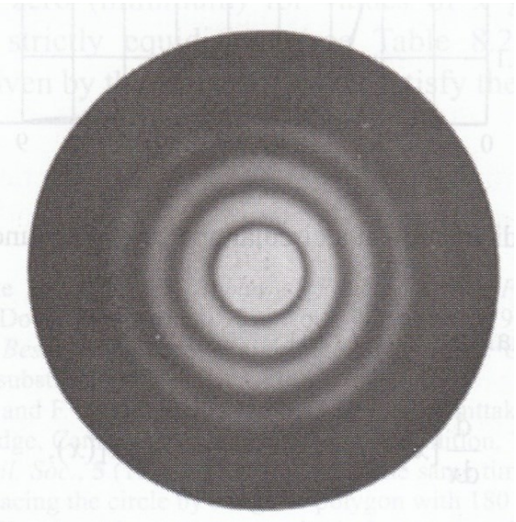
$$2\xi_t \, \Delta\theta = \lambda$$

$$\xi_t = \frac{\lambda}{2}\left(\frac{R}{D}\right)$$

Fraunhofer Diffraction

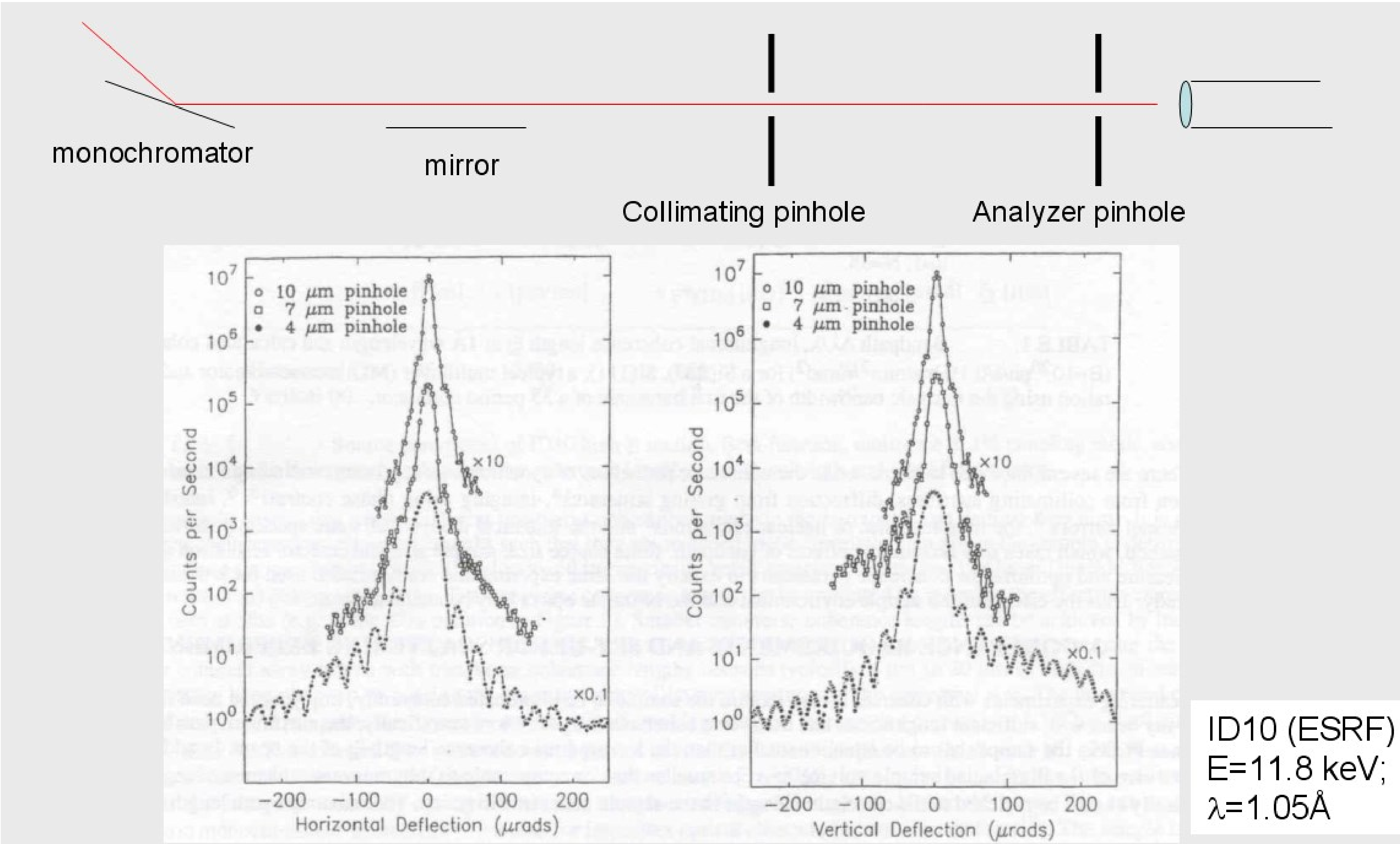


Fraunhofer diffraction of a rectangular aperture 8 x 7 mm^2, taken with mercury light λ=579nm (from Born&Wolf, chap. 8)

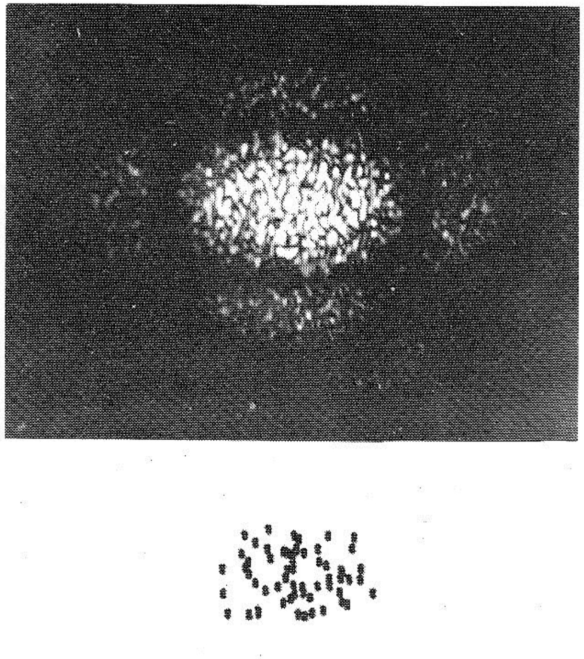


Fraunhofer diffraction of a circular aperture, taken with mercury light λ=579nm (from Born&Wolf, chap. 8)

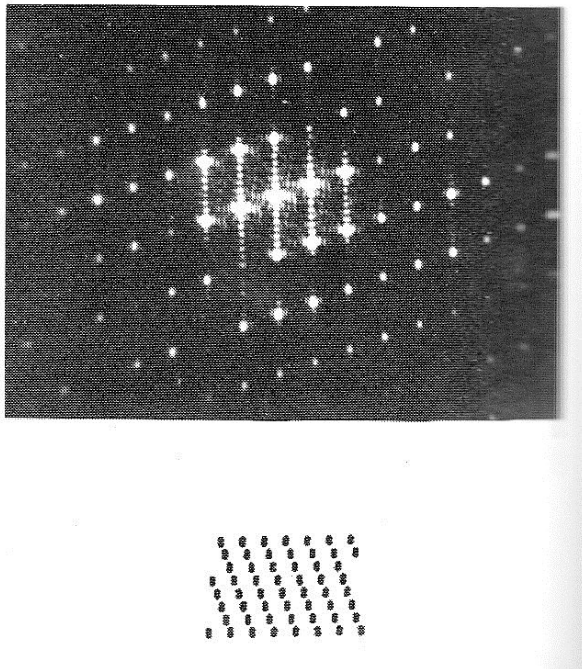
Fraunhofer Diffraction $(\lambda = 0.1nm)$



Speckle Pattern



random arrangement of apertures: speckle



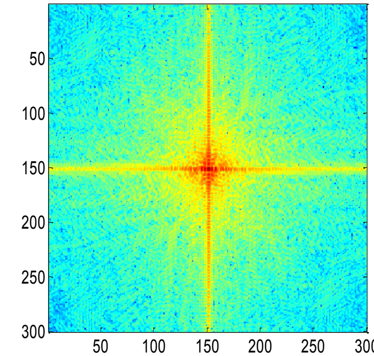
regular arrangement of apertures

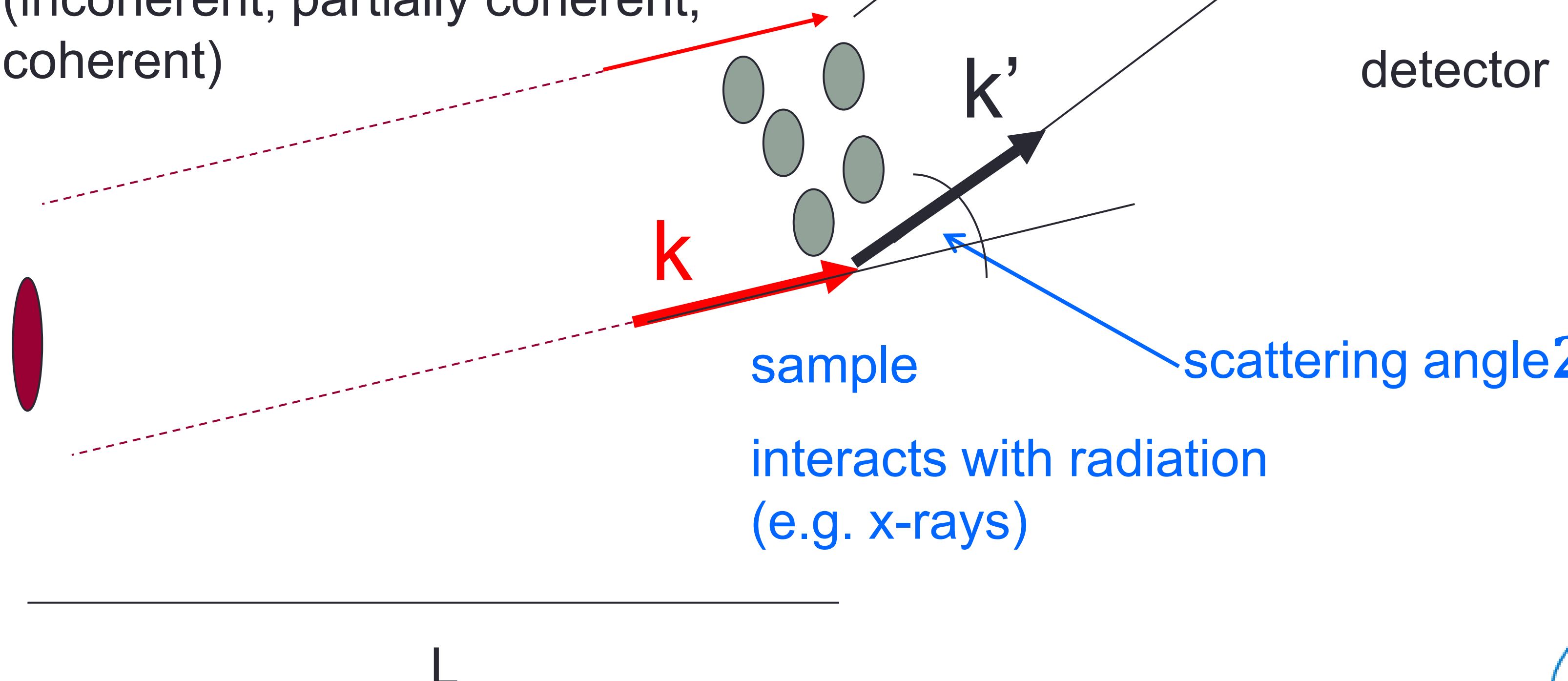
Experimental Set-up for Scattering Experiments

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

source parameters: source size, λ, $\frac{\Delta\lambda}{\lambda}$...

coherence properties: (incoherent, partially coherent, coherent)





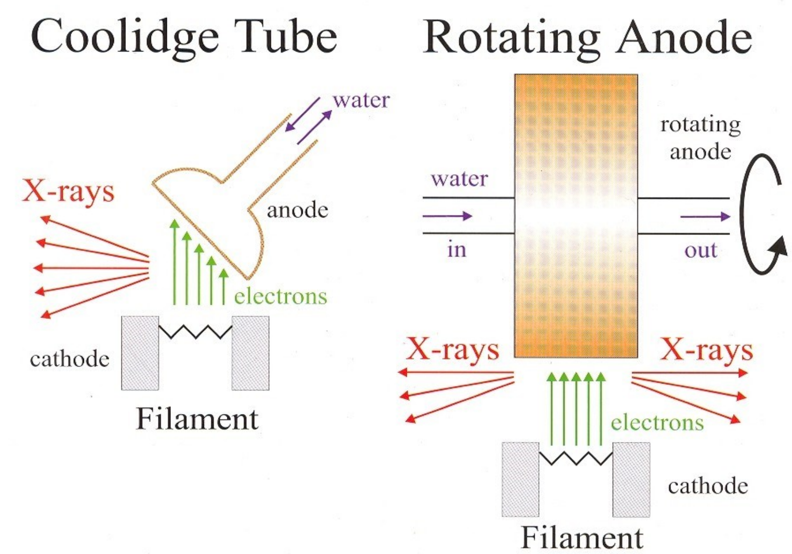
Source of X-Rays

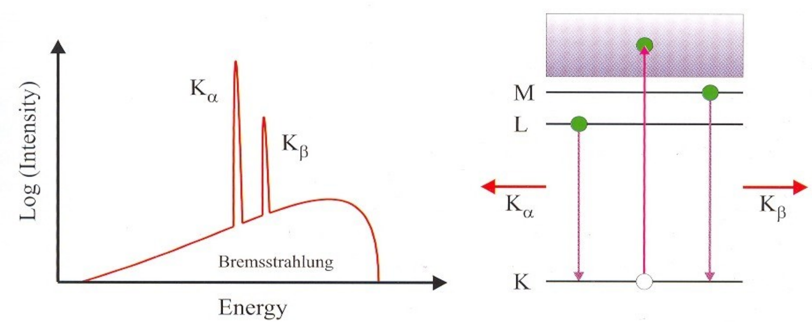
1895 Discovered by W.C. Röntgen

1912 First diffraction experiment (v. Laue)

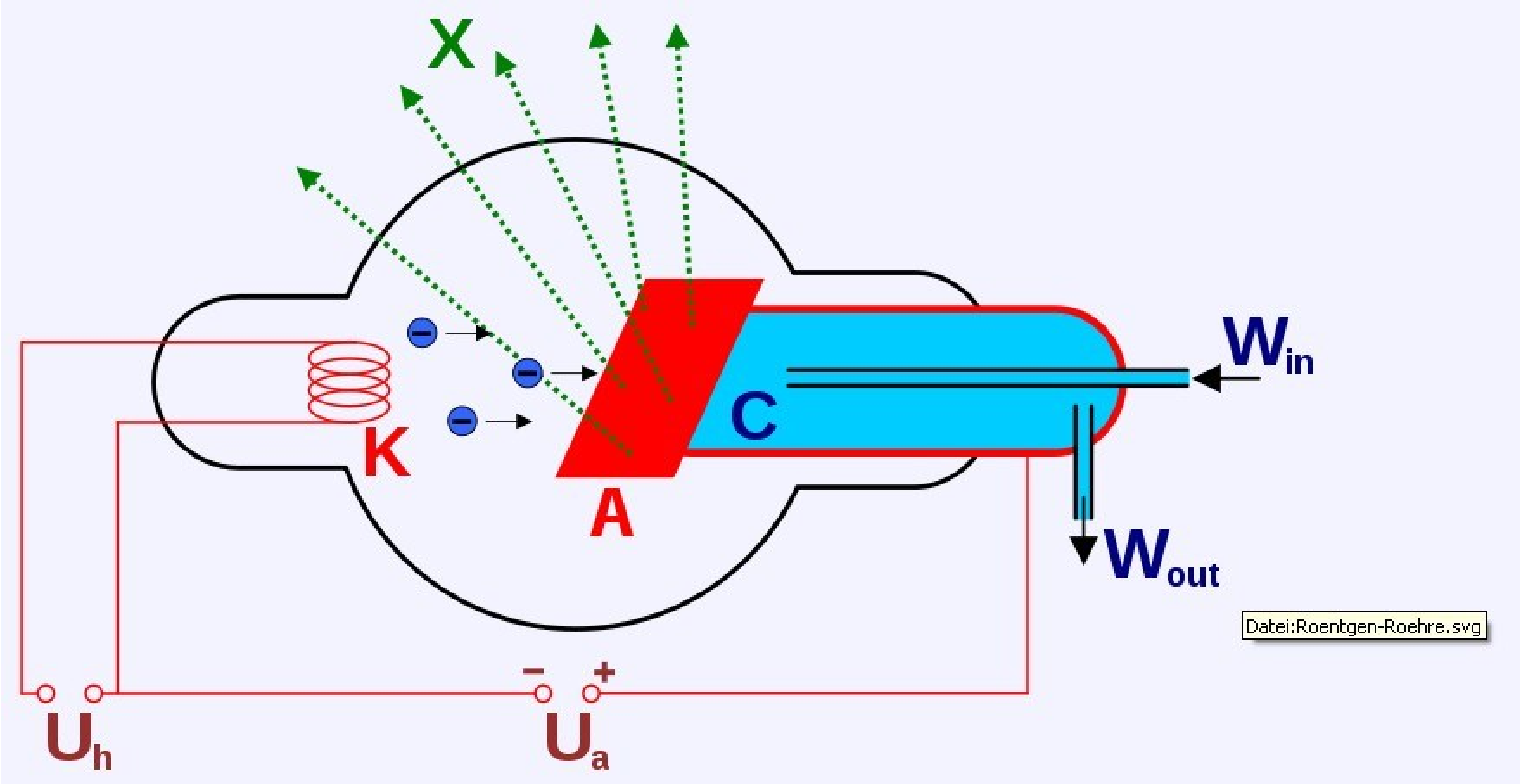
1912 Coolidge tube (W.D. Coolidge, GE)

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



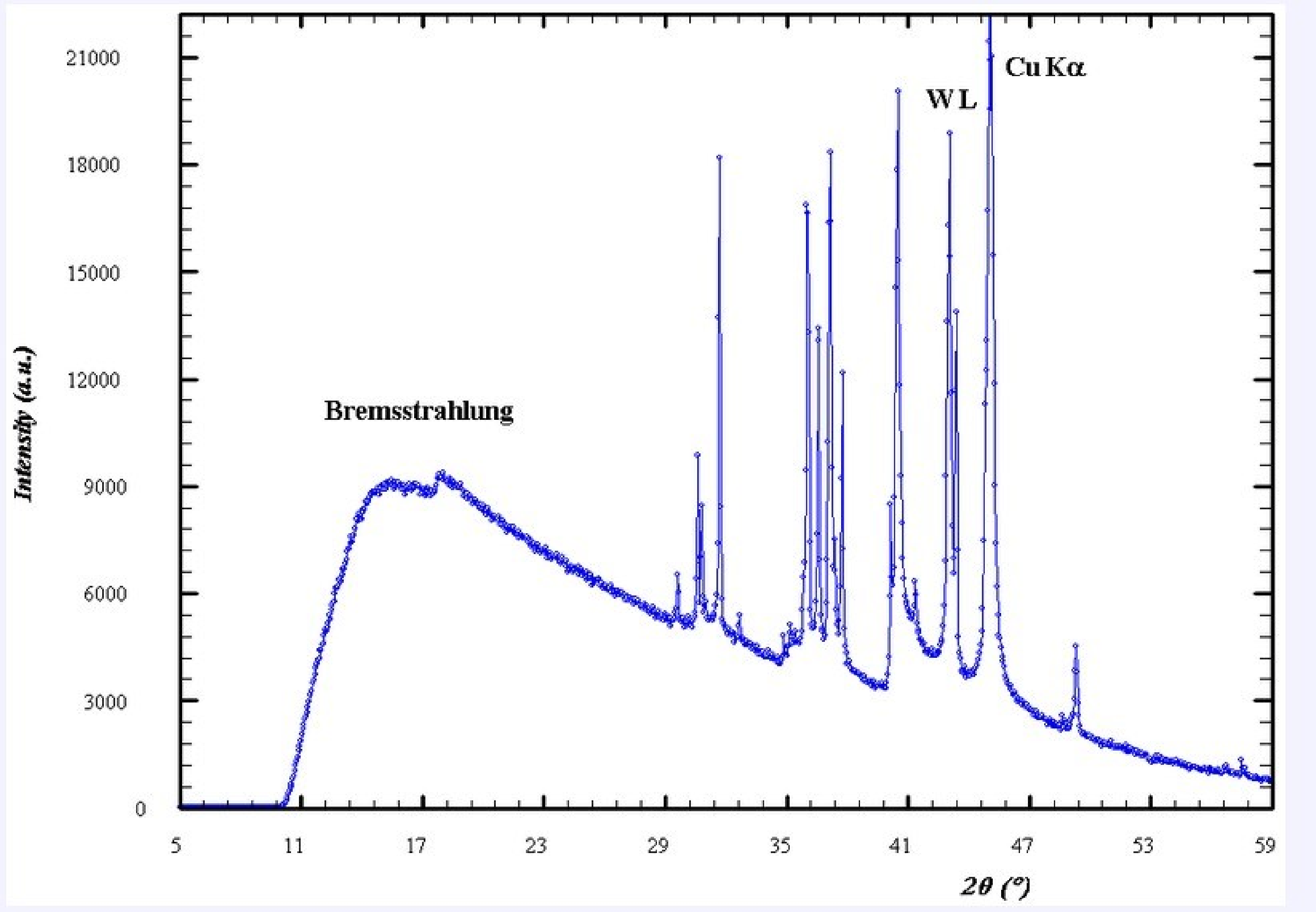


X-Ray Tube

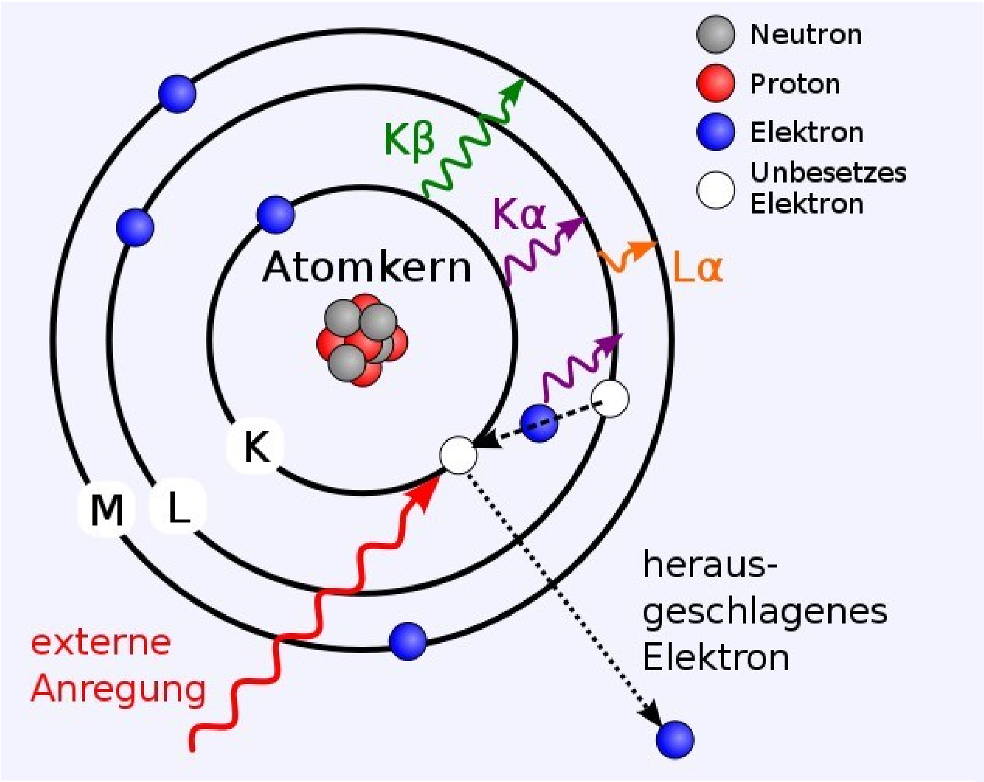


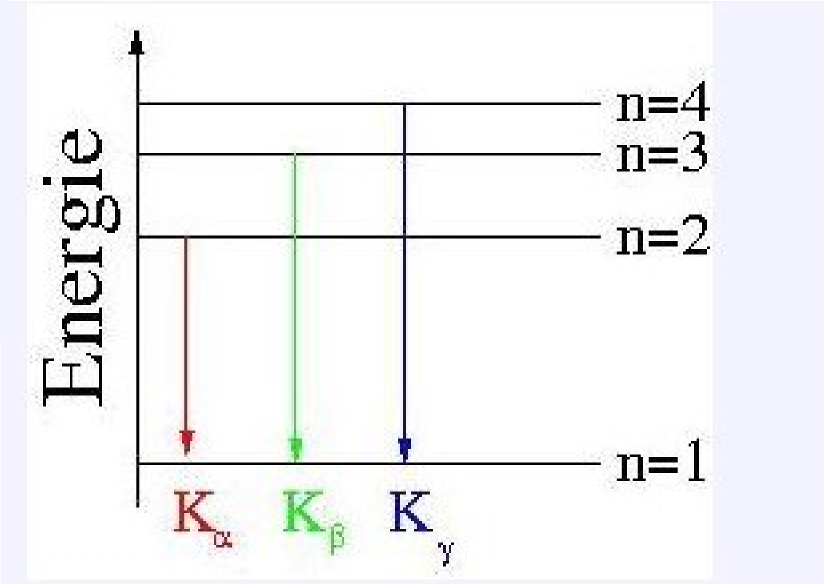
X-Ray Tube

X-Ray Tube

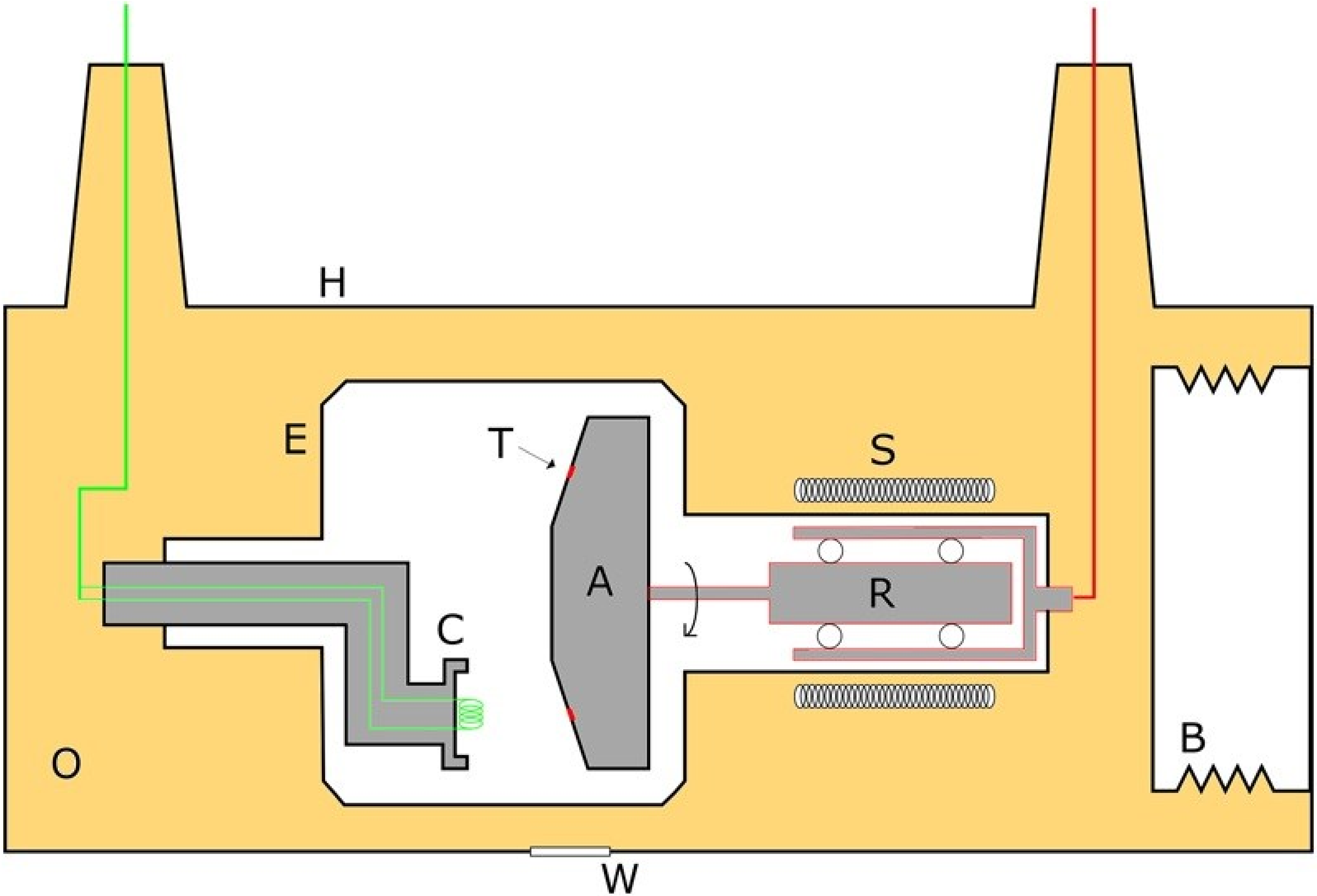

Cu Kα
W L
Bremsstrahlung
Intensity (a.u.)
21000
18000
15000
12000
9000
6000
3000
0
5
11
17
23
29
35
41
47
53
59
2θ (°)

X-Ray Tube

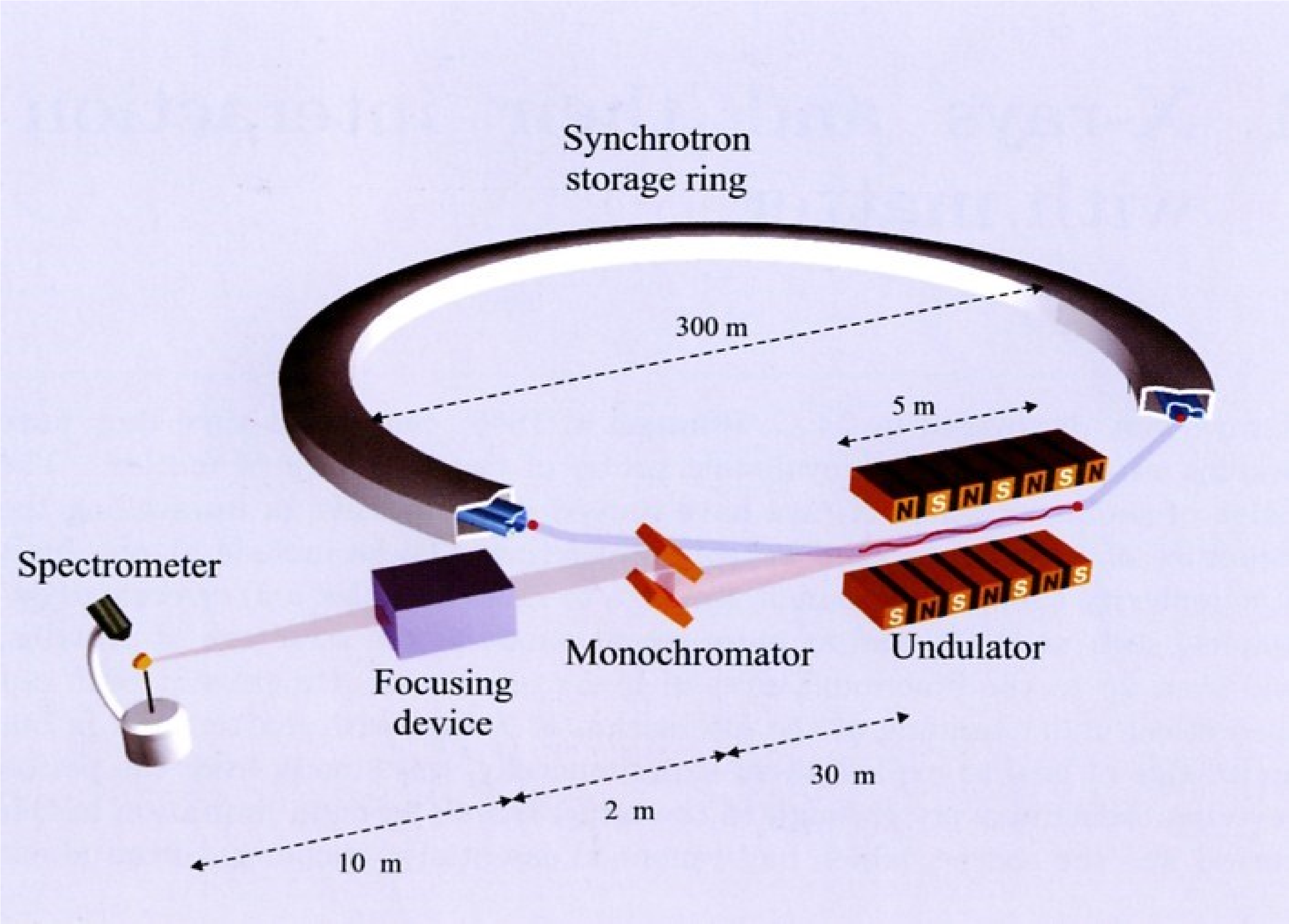

Neutron
Proton
Elektron
Unbesetzes Elektron
Kβ
Kα
Lα
Atomkern
K
M
L
heraus-
geschlagenes
Elektron
externe
Anregung


Energie
n=4
n=3
n=2
n=1
Kα
Kβ
Kγ

Rotating Anode



Synchrotron Radiation Storage Ring



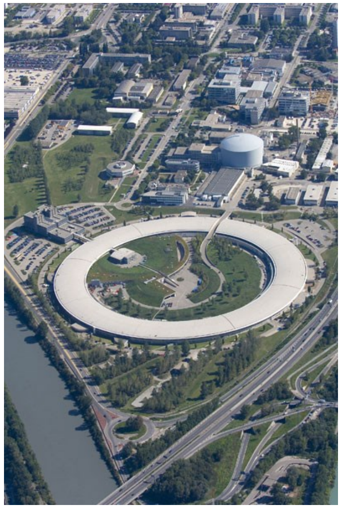
Photon Machines

The three largest and most powerful synchrotrons in the world

APS, USA

ESRF, Europe-France

Spring-8, Japan



The most recent third generation machine:

Petra III at DESY/Hamburg