

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture 2	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2017 G. Grübel, A. Philippi-Kobs, O. Seeck, T. Schneider, L. Frenzel, M. Martins, W. Wurth		
Location	Lecture hall AP, Physics, Jungiusstraße		
Date	Tuesday	12:30 - 14:00	(starting 4.4.)
	Thursday	8:30 - 10:00	(until 13.7.)



Methoden moderner Röntgenphysik II: Streuung und Abbildung

Part I:

Basics of X-ray Physics

by Gerhard Grübel (GG)

- [4.4.] Organisation and Introduction
- [6.4.] Introduction
- [11.4.] X-ray Scattering Primer
- [13.4.] Sources of X-rays, Synchrotron Radiation
- [18.4.] Refraction and Reflection
- [20.4.] Kinematical Scattering Theory (I)
- [25.4.] Kinematical Scattering Theory (II), Applications
- [27.4.] Small Angle Scattering and Soft Matter
- [2.5.] Anomalous Scattering
- [9.5.] Introduction: Coherence I
- [11.5.] Coherence II; Applications of Coherent X-ray Beams



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/ss17



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

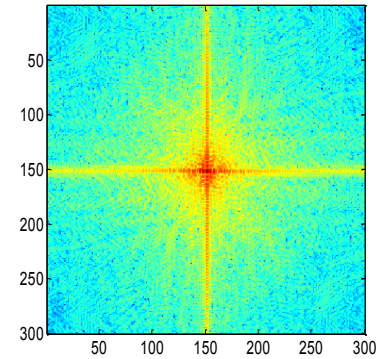
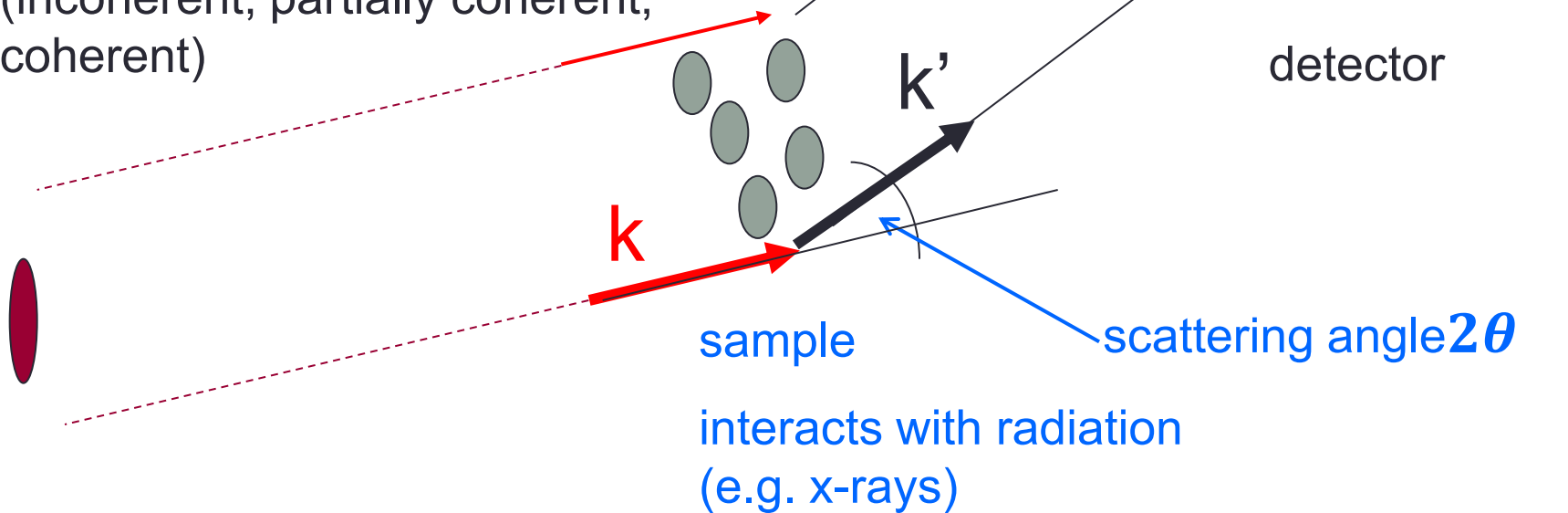
Set-up for Scattering Experiments

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

source parameters: source

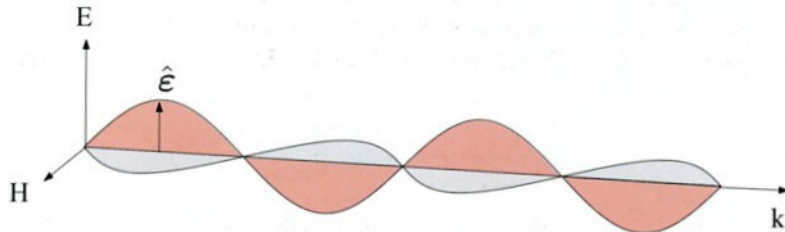
size, λ , $\frac{\Delta\lambda}{\lambda}$...

coherence properties:
(incoherent, partially coherent,
coherent)



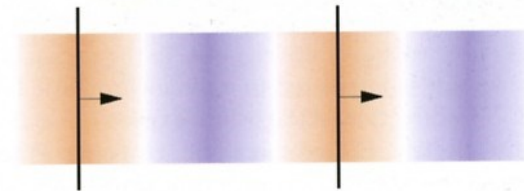
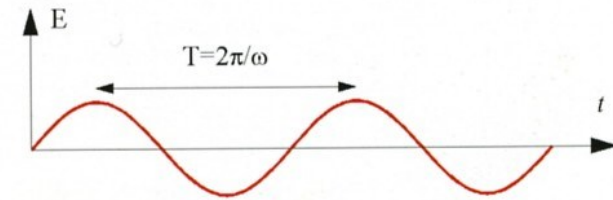
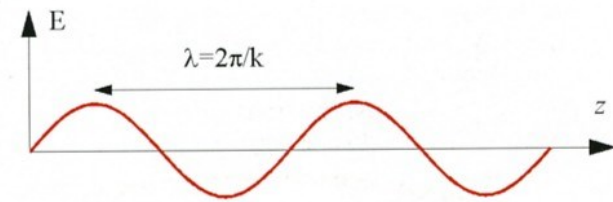
X-rays: Electromagnetic Waves and Photons

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 \mathbf{E} and \mathbf{H} are perpendicular to each other and to the propagation direction \mathbf{k} .



Neglecting the H field one may write:

$$\mathbf{E}(\mathbf{r}, t) = \boldsymbol{\varepsilon} E_0 e^{i(\mathbf{k}\mathbf{r} - \omega t)}$$



with

$\boldsymbol{\varepsilon}$: polarization vector

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

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



Scattering of X-rays

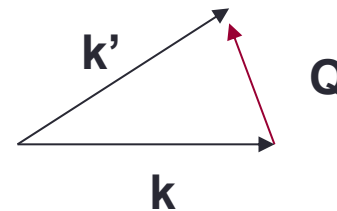
Consider a monochromatic plane (electromagnetic) wave with wave vector \mathbf{k} :

$$\mathbf{E}(\mathbf{r}, t) = \varepsilon E_0 e^{i(\mathbf{k}\mathbf{r} - \omega t)}$$

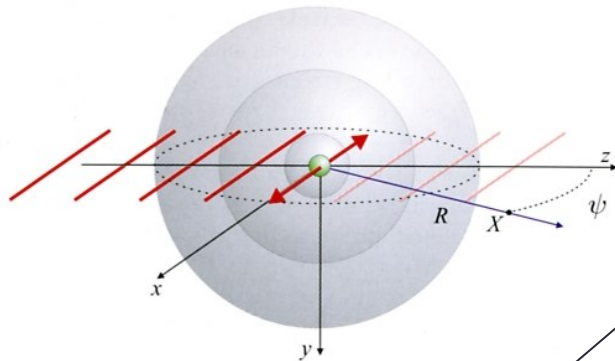
with $|\mathbf{k}| = \frac{2\pi}{\lambda}$

Elastic scattering:

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



Scattering by a Single Electron:



$$\frac{E_{\text{rad}}(R, t)}{E_{\text{in}}} = - \frac{e^2}{4\pi\epsilon_0 m c^2} \frac{e^{ikR}}{R} \cos \psi$$

spherical wave

Thomson scattering length r_0

$$(\approx 2.82 \times 10^{-5} \text{ \AA})$$

phase shift of π btw. incident and radiated field



Scattered intensity:

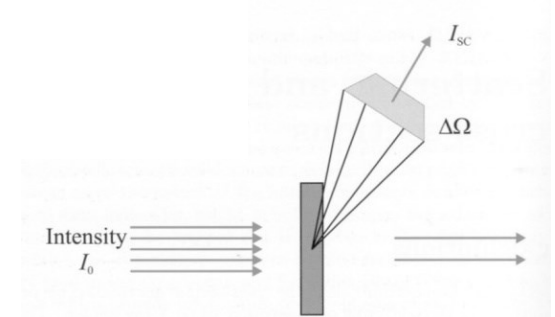
$$\frac{I_s}{I_0} = \frac{|E_{\text{rad}}|^2 R^2 \Delta\Omega}{|E_{\text{in}}|^2}$$

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

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

A_0 : incident beam size

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



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



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

≡ scattering amplitude by
 an ensemble of electrons

$$-r_0 f^0(Q) = -r_0 \sum_{r_j} e^{i Q r_j}$$



(atomic) form factor

position of scatterers

$$\{f^2(Q \rightarrow 0) = Z, \quad f^2(Q \rightarrow \infty) = 0\}$$

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:

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



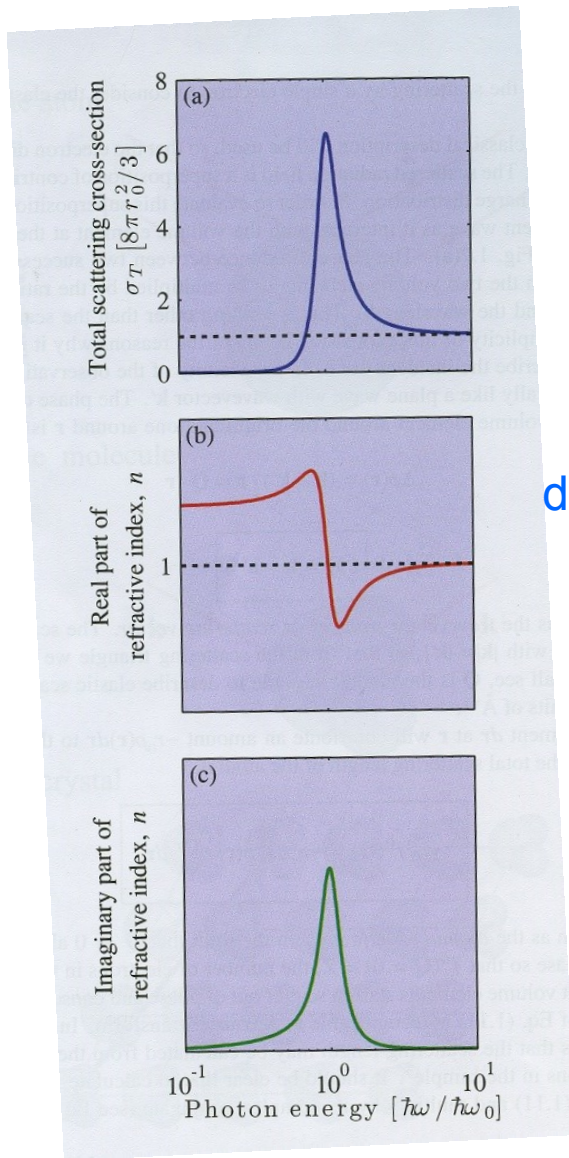
Scattering by a Single Atom:

form factor of an atom:

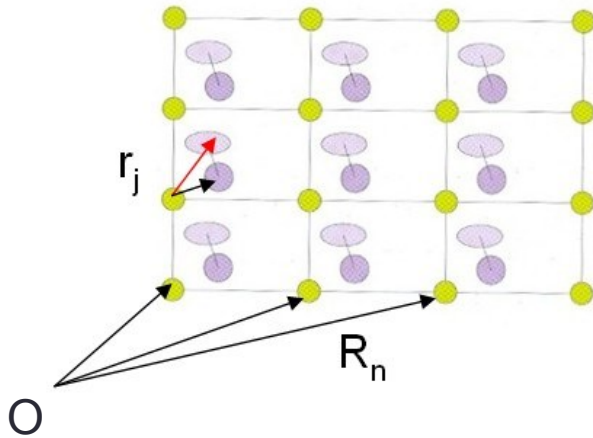
$$f(Q, \hbar\omega) = f^0(Q) + f'(\hbar\omega) + i f''(\hbar\omega)$$



dispersion corrections: level structure absorption effects



Scattering by a Crystal:



$$r_j' = R_n + r_j$$

lattice vector + atomic position in lattice

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

unit cell structure factor

lattice sum

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

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

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

Unit cell structure factor:

e.g. fcc lattice:

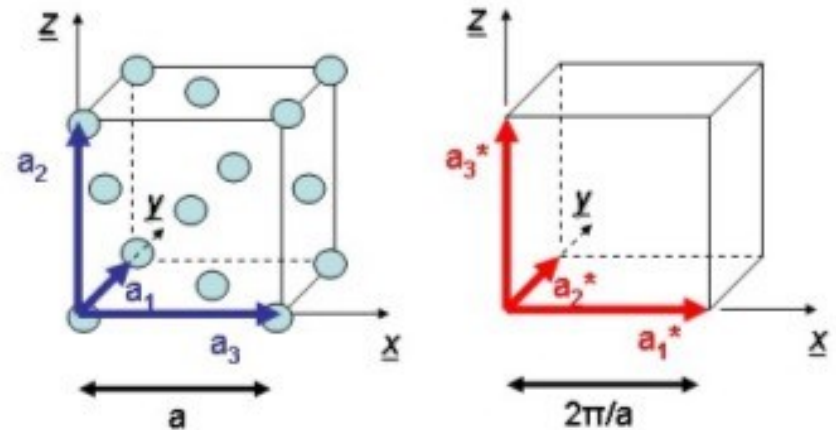
$$r_1 = 0$$

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

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

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

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



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

$$F_{hkl}^{fcc} = f(Q) \sum e^{iQr_j}$$

with $Q = G = h a_1^* + k a_2^* + l a_3^*$

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

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

Compton Scattering

Consider photon with momentum initially at rest

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

Energy conservation:

$$m_0 c^2 + \hbar c k = \sqrt{\{(m_0 c^2)^2 + (\hbar c q')^2\}} + \hbar c k'$$

with $\lambda_c = \frac{\hbar c}{m_0 c^2}$: Compton wavelength

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

Momentum conservation: $p' = k - k'$

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

$$(1) = (2)$$

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

➔ origin of background

➔ determine electronic momentum distribution of materials

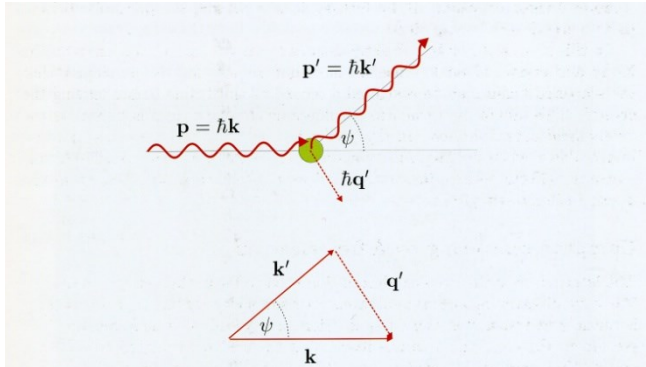
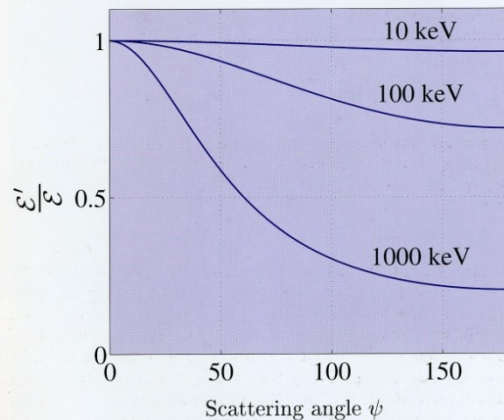
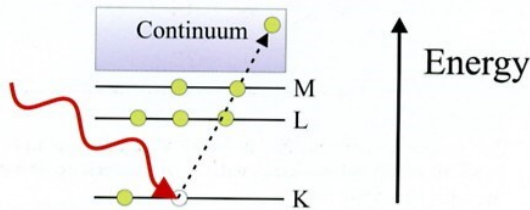


Figure 1.7: Compton scattering. A photon with energy $\mathcal{E} = \hbar c k$ and momentum $\hbar k$ scatters from an electron at rest with energy $m c^2$. The electron recoils with a momentum $\hbar q' = \hbar(k - k')$ as indicated in the scattering triangle in the bottom half of the figure.

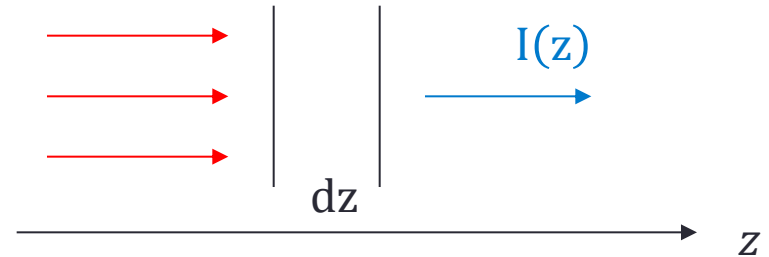


Photoelectric Absorption

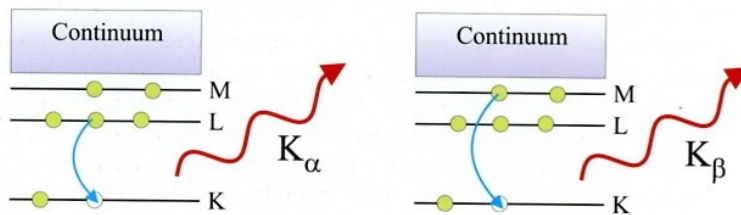
(a) Photoelectric absorption



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



(b) Fluorescent X-ray emission



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

$$\mu = \rho_a \sigma_a = \left(\frac{\rho_m N_A}{A} \right) \sigma_a$$

ρ_a atomic number density

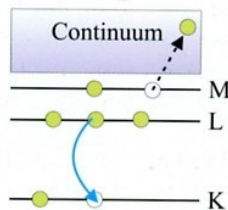
$\sigma_a = \sigma_a(E)$ absorption cross section

ρ_m mass density

N_A Avogadro's number

A atomic mass number

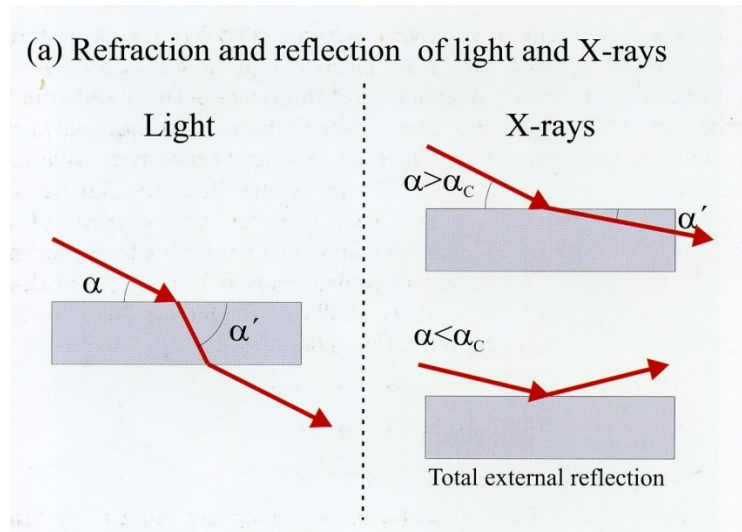
(c) Auger electron emission



Refraction

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

\uparrow \uparrow
 10^{-5} absorption ($\ll \delta$)



Snell's law:

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

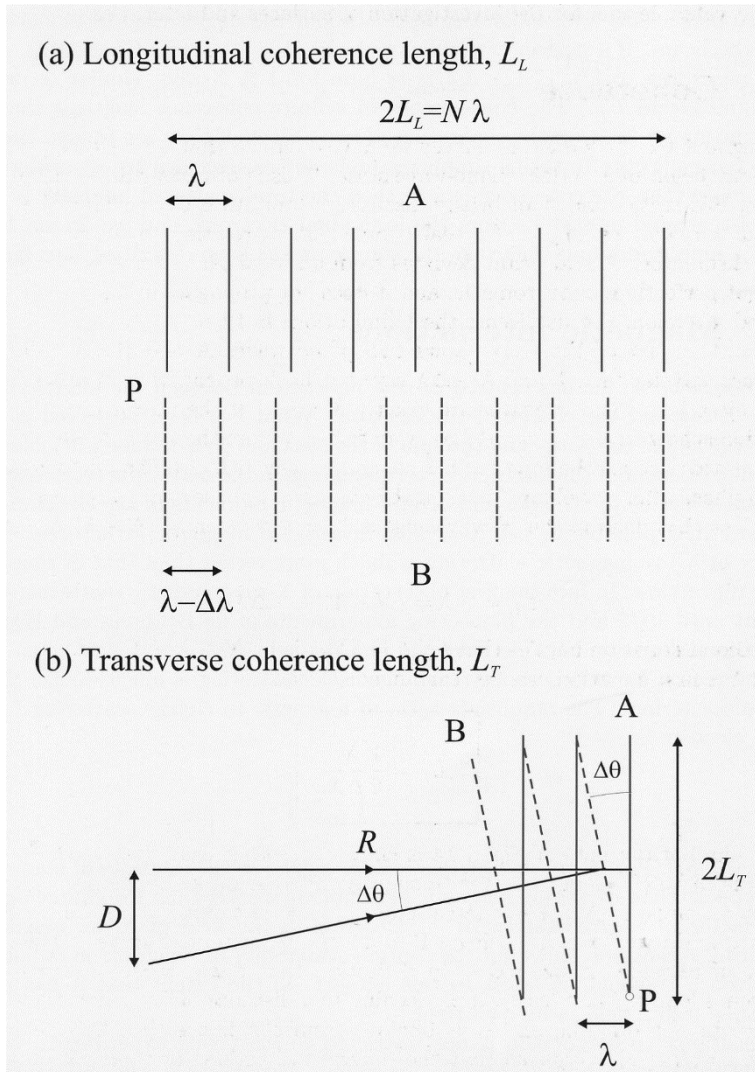
Note: total external reflection
for x-rays ($\alpha' = 0$)

$$n < 1$$

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

Note: $\cos z = 1 - z^2/2! + z^4/4! - z^6/6! \dots$

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 :

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

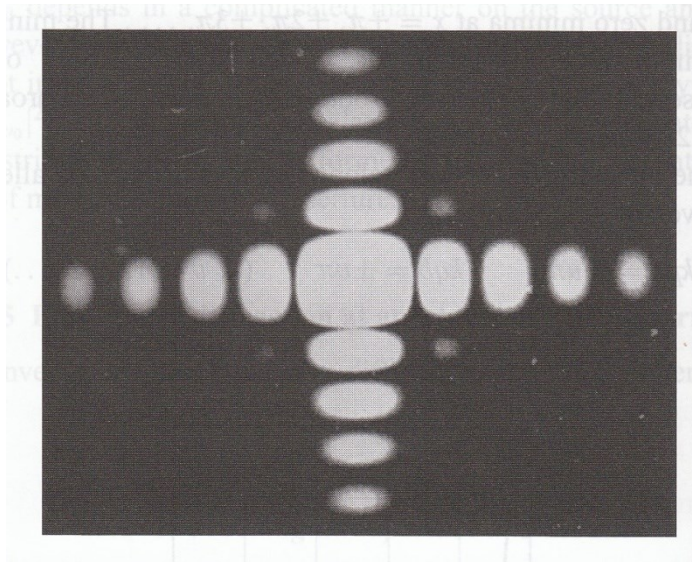
Transverse coherence:

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

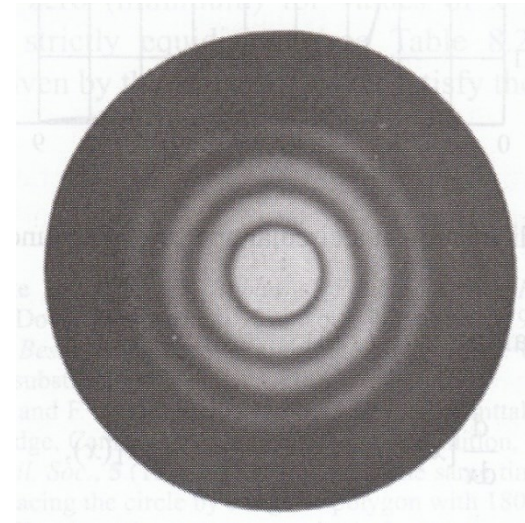
$$2\xi_t \Delta\theta = \lambda$$

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

Fraunhofer Diffraction

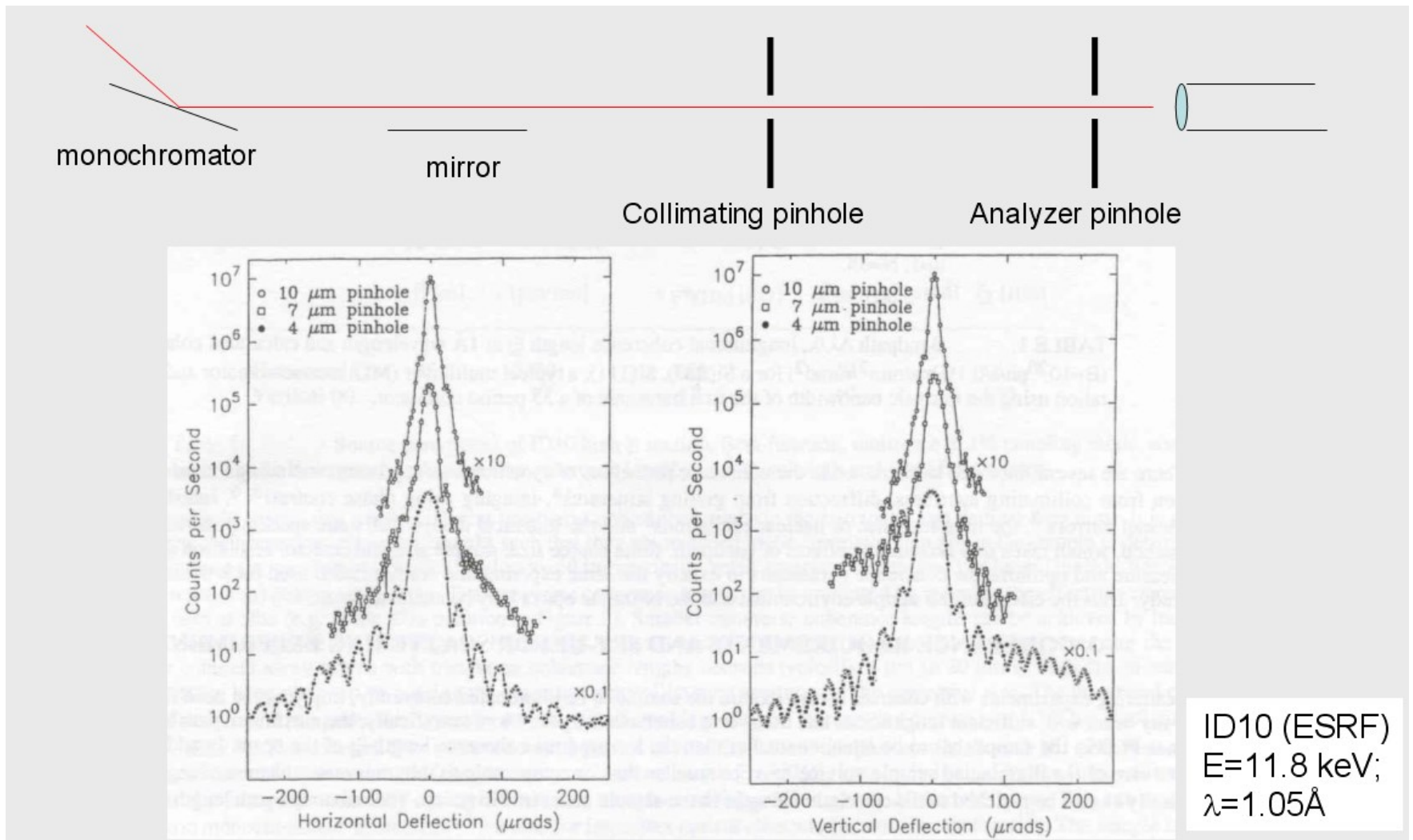


Fraunhofer diffraction of a rectangular aperture $8 \times 7 \text{ mm}^2$, taken with mercury light $\lambda=579\text{nm}$ (from Born&Wolf, chap. 8)

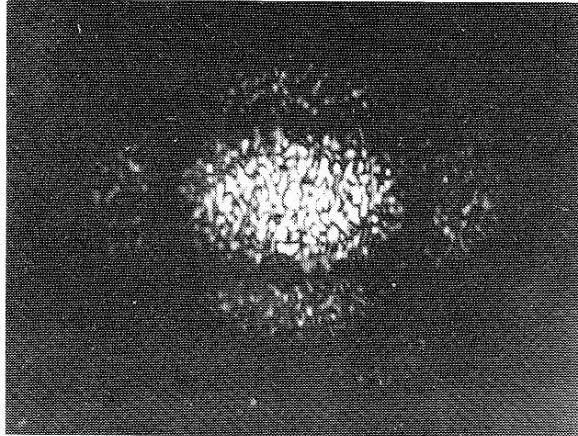


Fraunhofer diffraction of a circular aperture, taken with mercury light $\lambda=579\text{nm}$ (from Born&Wolf, chap. 8)

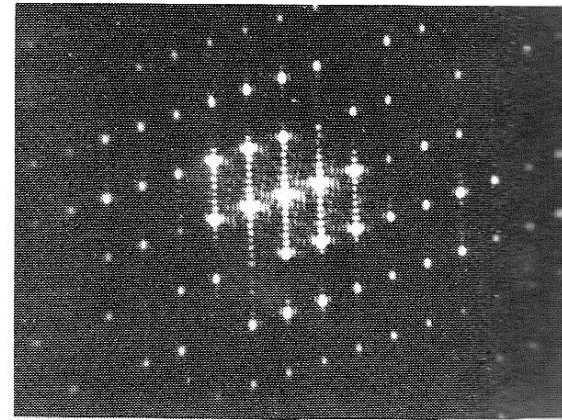
Fraunhofer Diffraction ($\lambda = 0.1nm$)



Speckle Pattern



random arrangement of apertures: speckle



regular arrangement of apertures

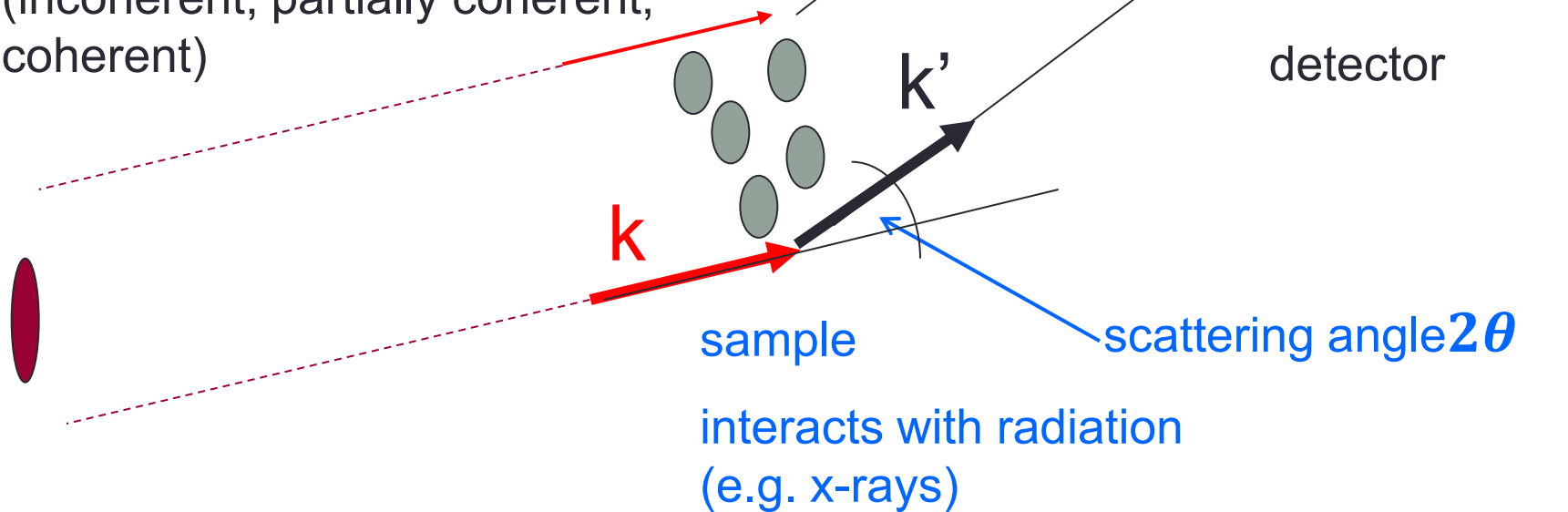
Experimental Set-up for Scattering Experiments

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

source parameters: source

size, λ , $\frac{\Delta\lambda}{\lambda}$...

coherence properties:
(incoherent, partially coherent,
coherent)

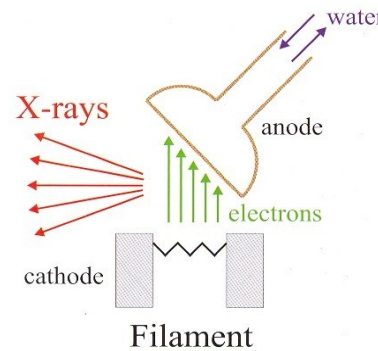


Source of X-Rays

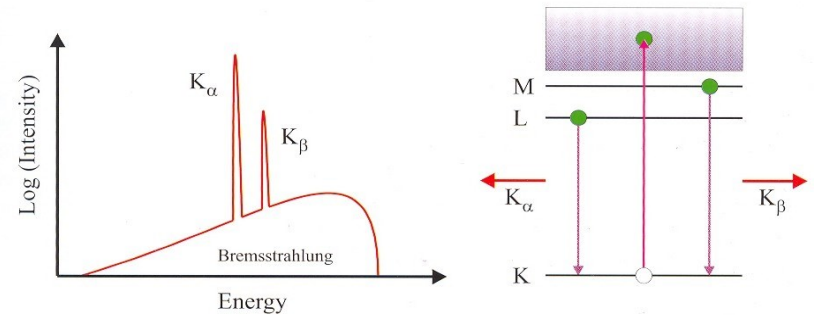
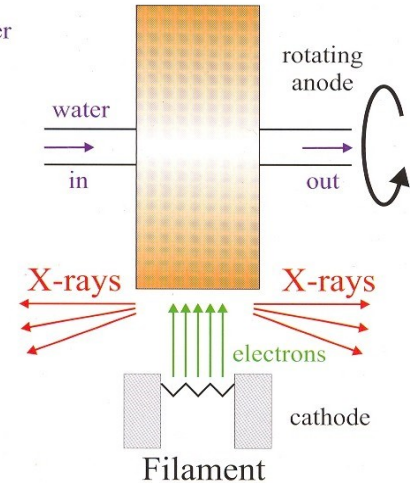
- 1895 Discovered by W.C. Röntgen
- 1912 First diffraction experiment (v. Laue)
- 1912 Coolidge tube (W.D. Coolidge, GE)
- 1946 Radiation from electrons in a synchrotron, GE, Physical Review, 71,829 (1947)



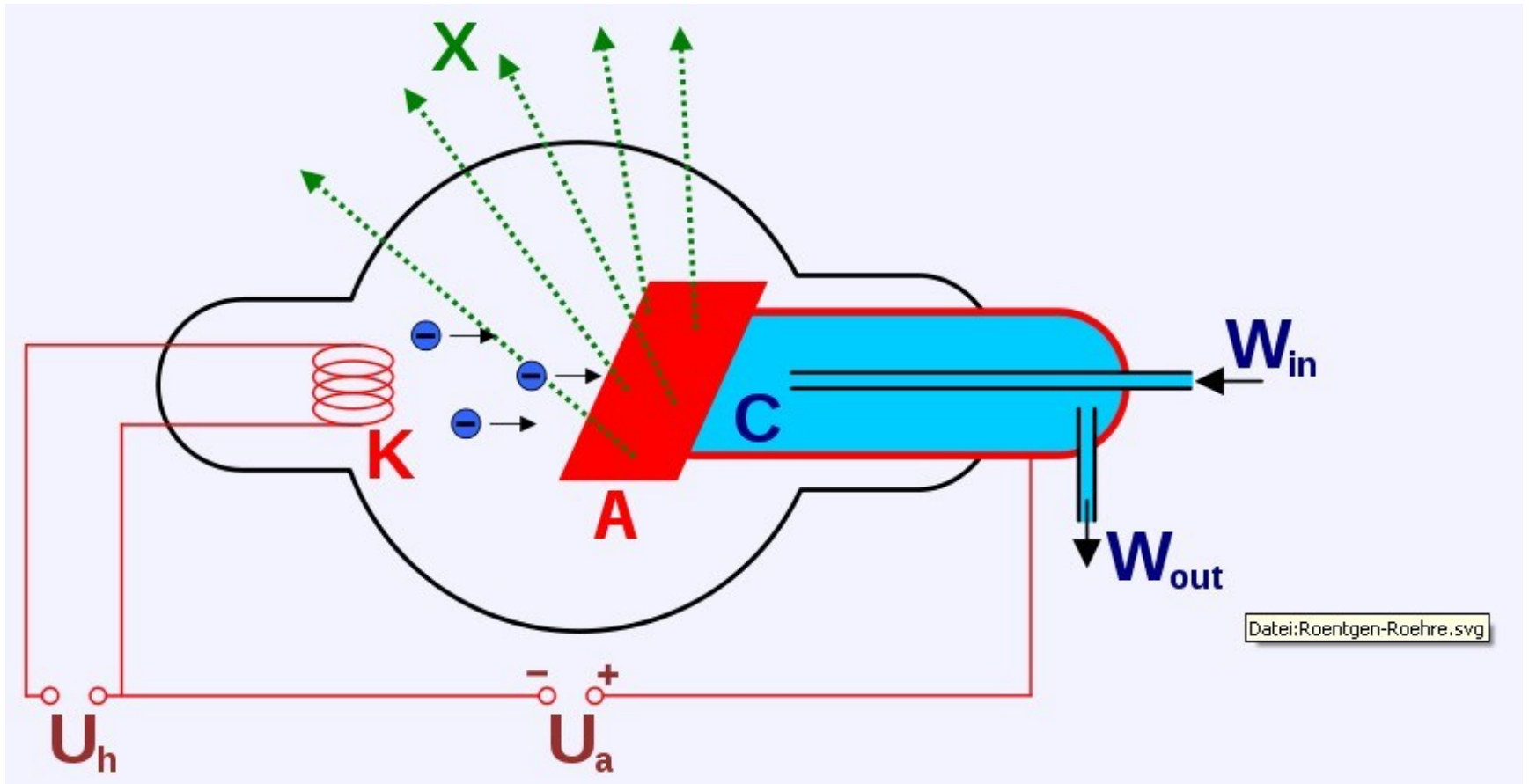
Coolidge Tube



Rotating Anode



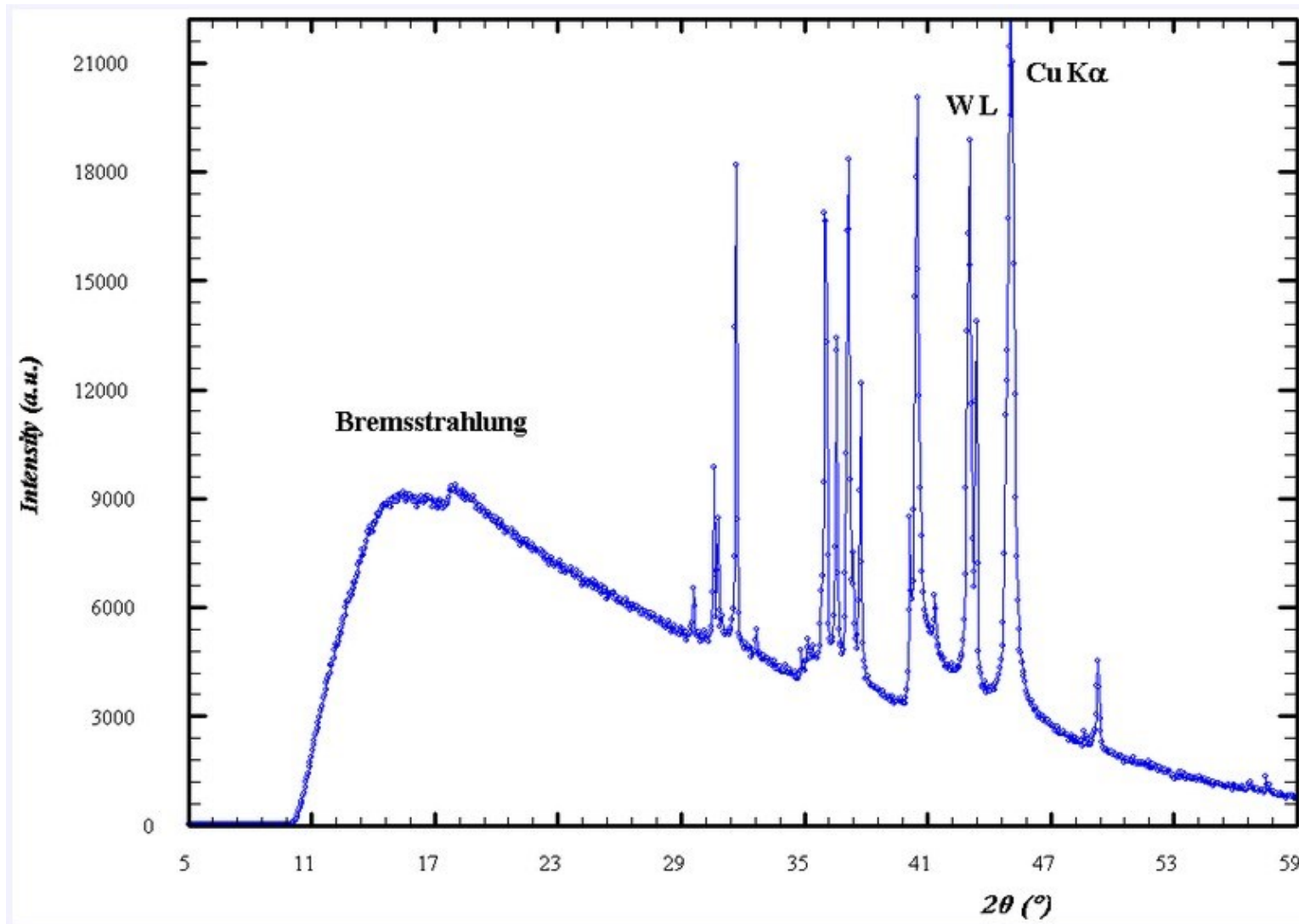
X-Ray Tube



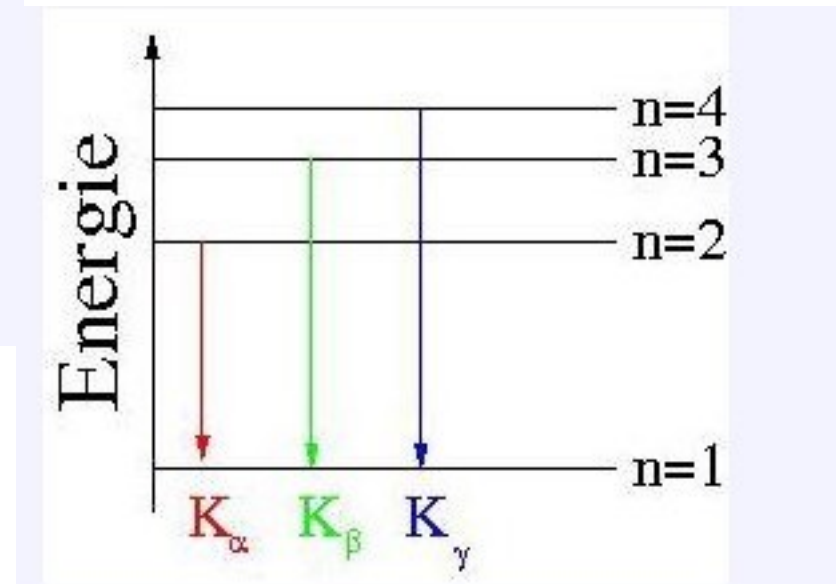
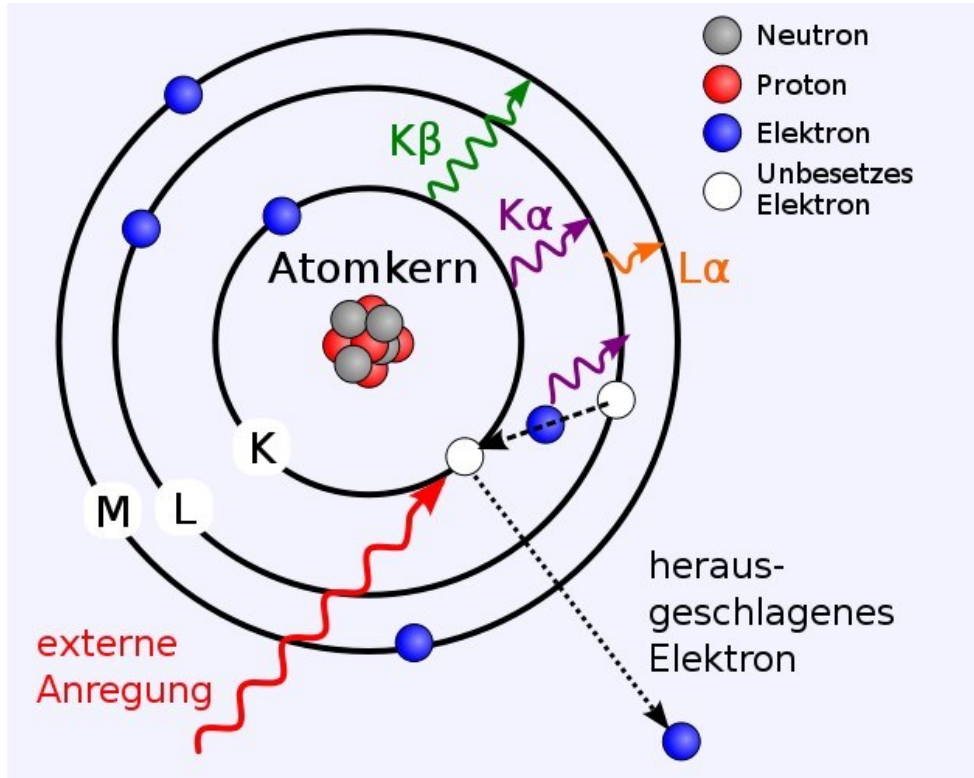
X-Ray Tube



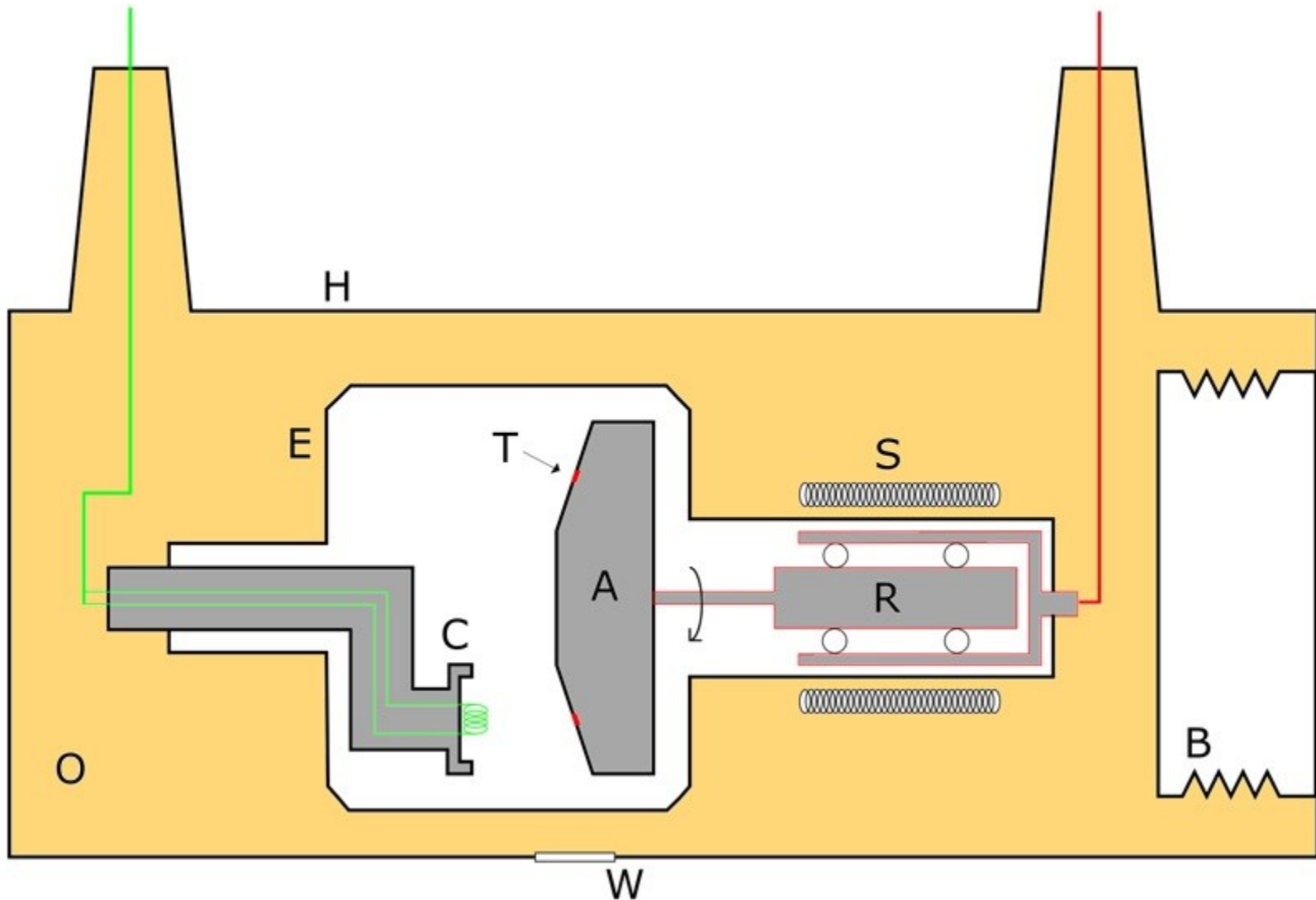
X-Ray Tube



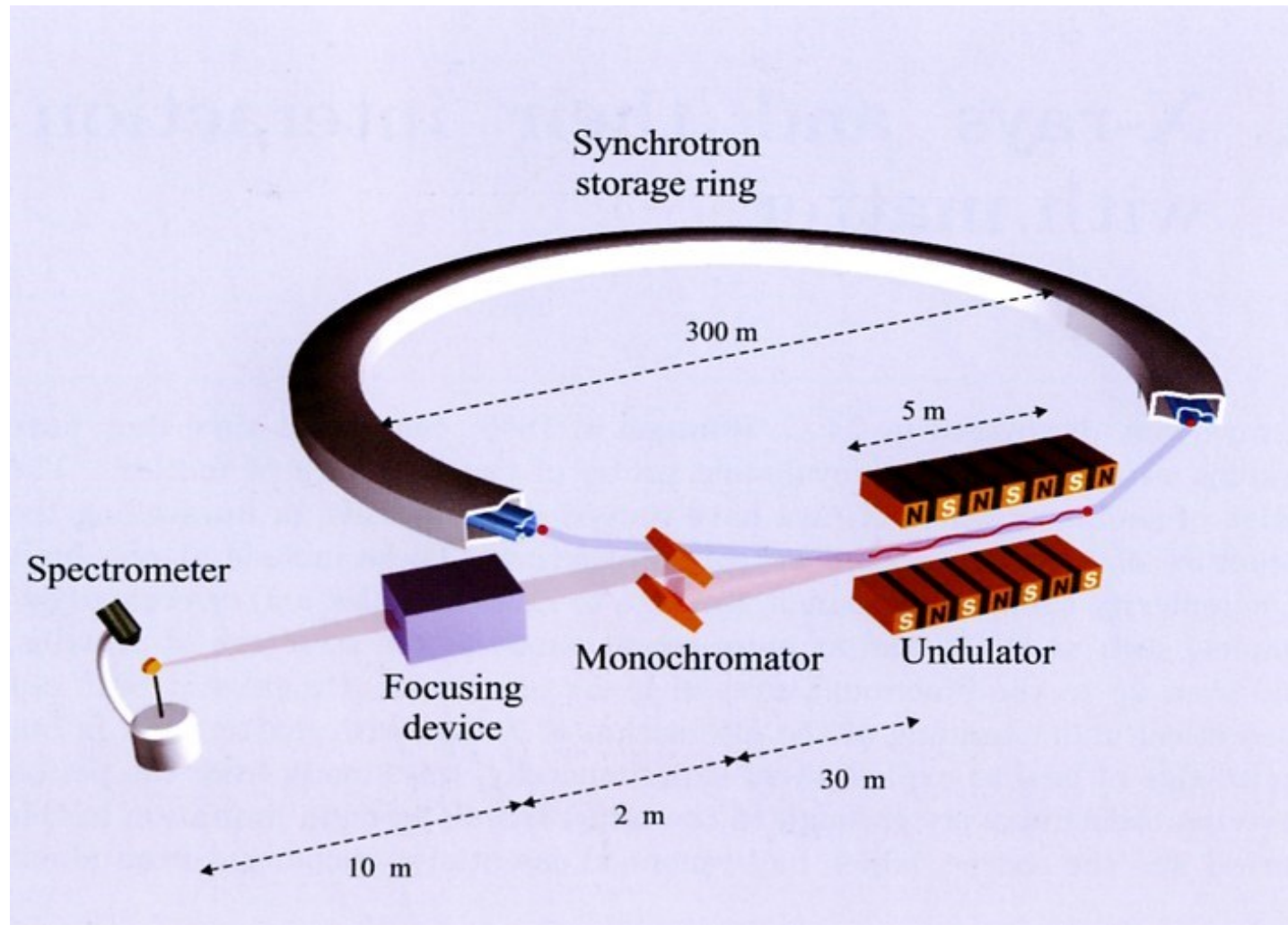
X-Ray Tube



Rotating Anode



Synchrotron Radiation Storage Ring



Photon Machines

The three largest and most powerful synchrotrons in the world



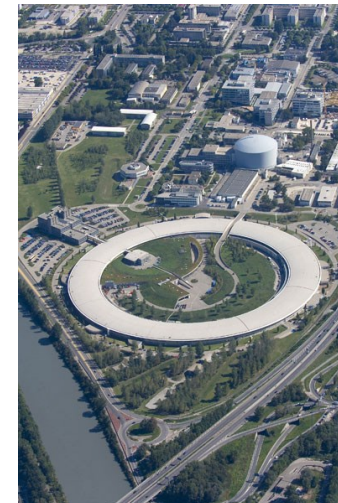
APS, USA



ESRF, Europe-France



Spring-8, Japan



The most recent third generation machine:



Petra III at DESY/Hamburg

The extension of PETRA III:



Petra III at DESY/Hamburg