Methoden moderner Röntgenphysik: Streuung und Abbildung

Lecture 1	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2021		
	G. Grübel, O. Seeck, V. Markmann, F. Lehmkühler, Andre Philippi-Kobs, M. Martins		
Location	online		
Date	Tuesdays	12:30 - 14:00	(starting 6.4.)
	Thursdays	8:30 - 10:00	(until 8.7.)

Methoden moderner Röntgenphysik: Streuung und Abbildung

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

Proseminar: *For Bachelor students*

8 creditpoints For Master students

Fixed dates:	Tuesday	12:30 - 14:00
	Thursday	8:30 - 10:00
First meeting “Tutorial”:	Tuesday, April 13	14:15 - 15:45
Location:	online	

Methoden moderner Röntgenphysik: Online Info

Tuesday Zoom-Meeting
https://desy.zoom.us/j/92674682486
Meeting ID: 926 7468 2486
Passcode: 144456

Thursday Zoom-Meeting
https://desy.zoom.us/j/99738625981
Meeting ID: 997 3862 5981
Passcode: 841881

Tutorial Zoom-Meeting
https://desy.zoom.us/j/95288979489
Meeting ID: 952 8897 9489
Passcode: 832350

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.

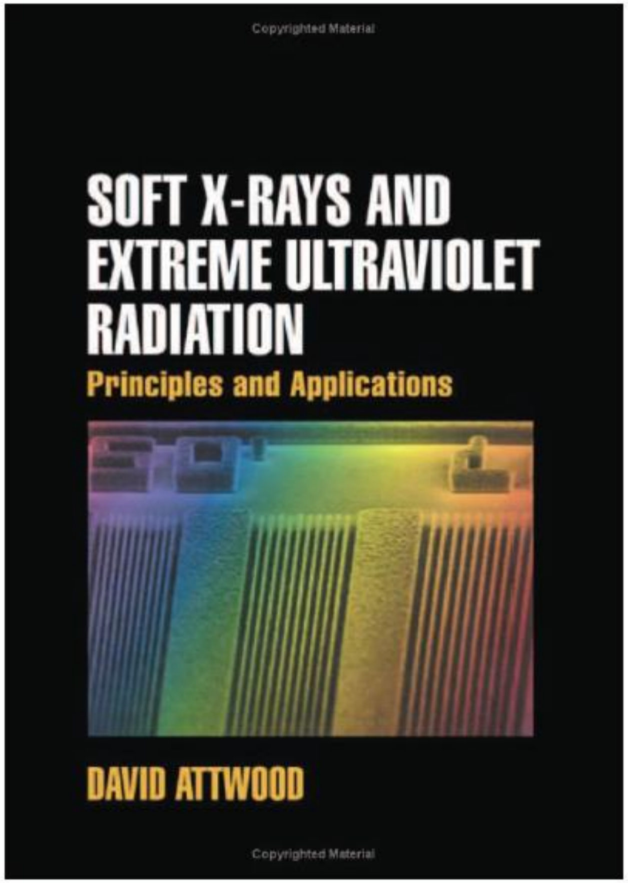
Soft X-rays and Extreme Ultraviolet Radiation
D. Attwood, Cambridge University Press (2000)
http://www.coe.berkeley.edu/AST/sxreuv/

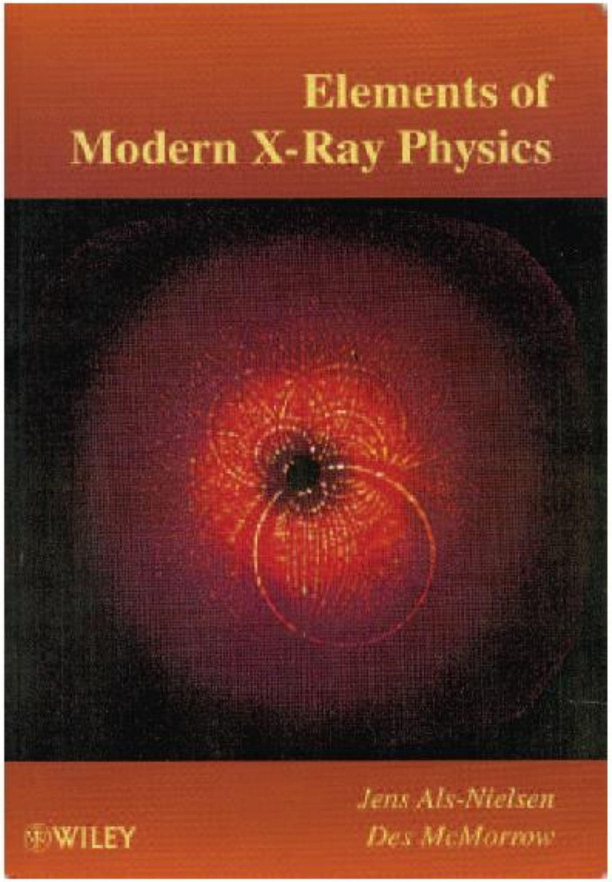
Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen
K. Wille, Teubner Studienbücher 1996

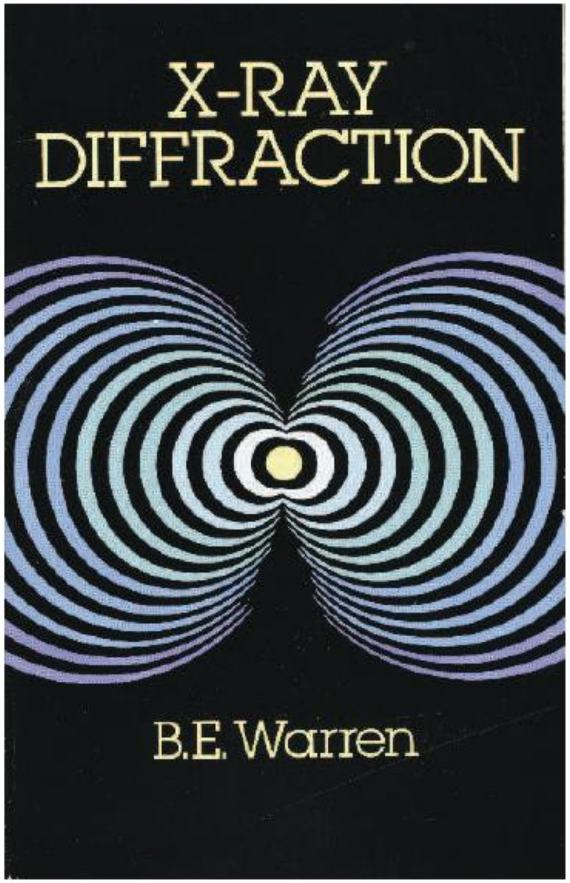
Lecture Notes

https://photon-science.desy.de/research/students__teaching/lectures__seminars/ss_20/index_eng.html

https://photon-science.desy.de/research/research_teams/coherent_x_ray_scattering/teaching/index_eng.html







*** some of the slides are courtesy of M. Tolan, C. Gutt and A. Hermmerich**

Methoden moderner Röntgenphysik: 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 & Sources of X-rays +Synchrotron Radiation
Elements of X-ray Scattering, 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: 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, Spatial Coherence, Second Order Coherence, ...

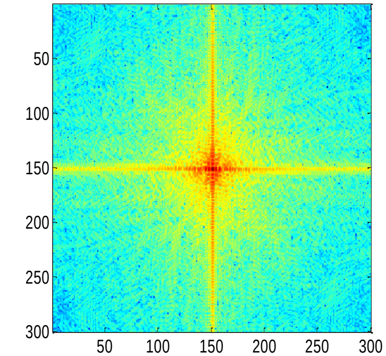
Coherent Scattering
Imaging and Correlation Spectroscopy, ...

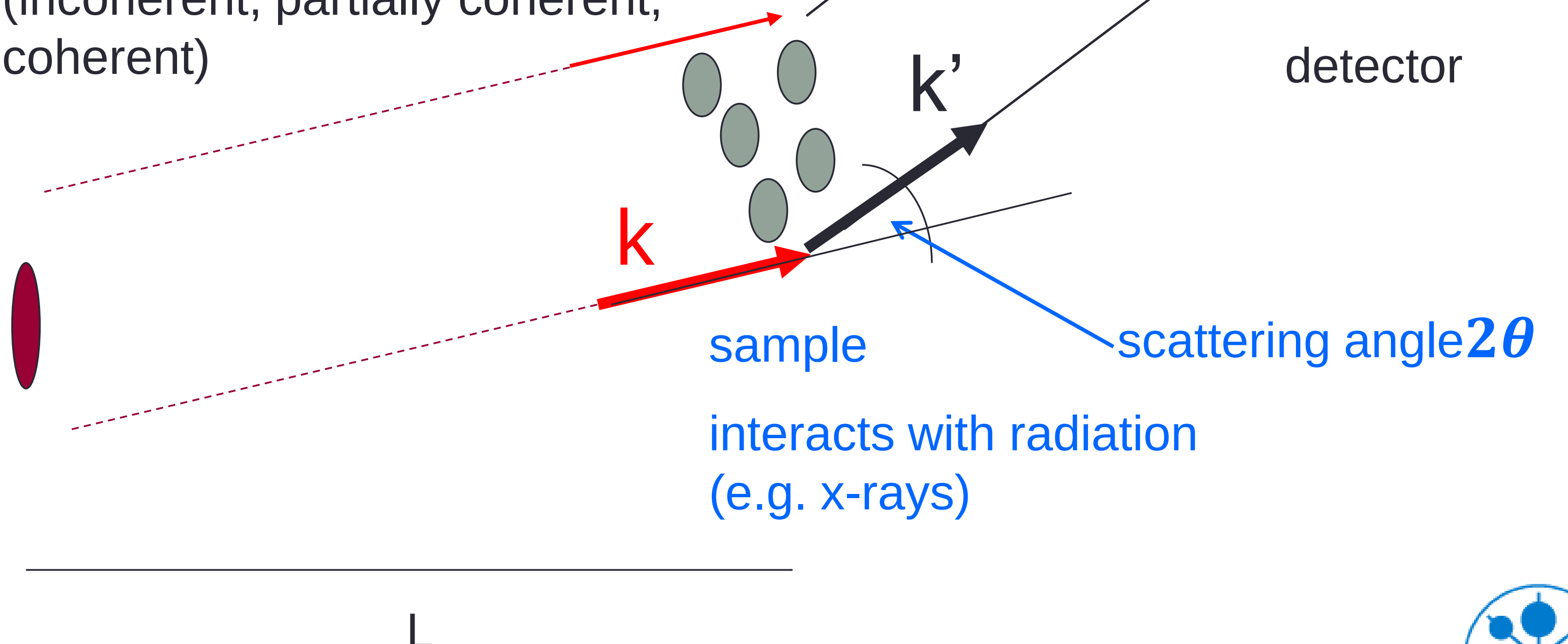
Set-up for Scattering Experiments

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

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

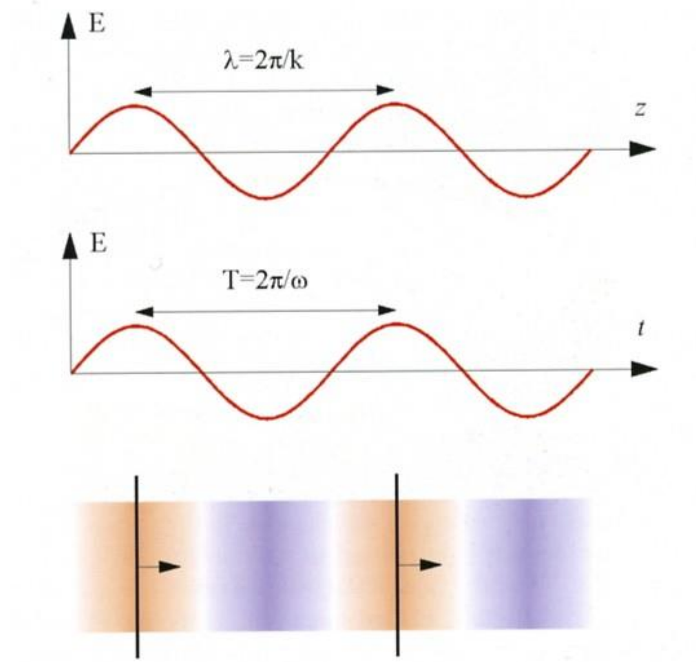
coherence properties: (incoherent, partially coherent, coherent)

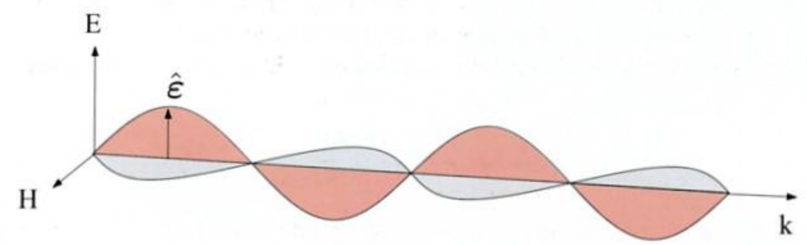




X-rays: Electromagnetic Waves and Photons

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





with

ε: polarization vector

Neglecting the H field one may write:

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

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

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

Scattering of X-rays

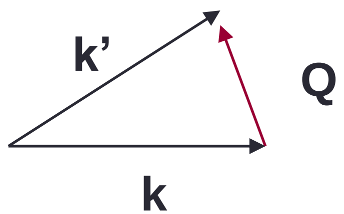
Consider a monochromatic plane (electromagnetic) wave with wave vector $\mathbf{k}$:

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

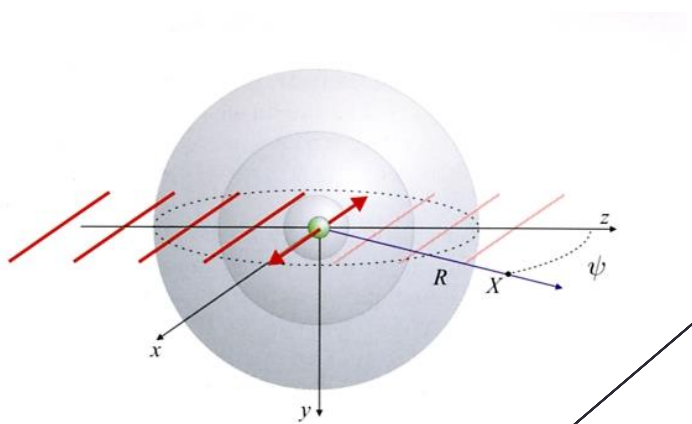
with $|\mathbf{k}| = \frac{2\pi}{\lambda}$

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:

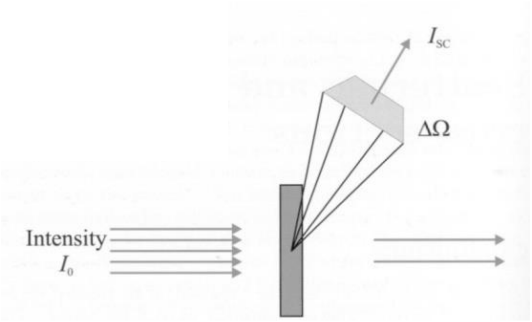
$$\frac{I_s}{I_0} = \frac{|E_{rad}|^2 R^2 \Delta\Omega}{|E_{in}|^2}$$

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

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

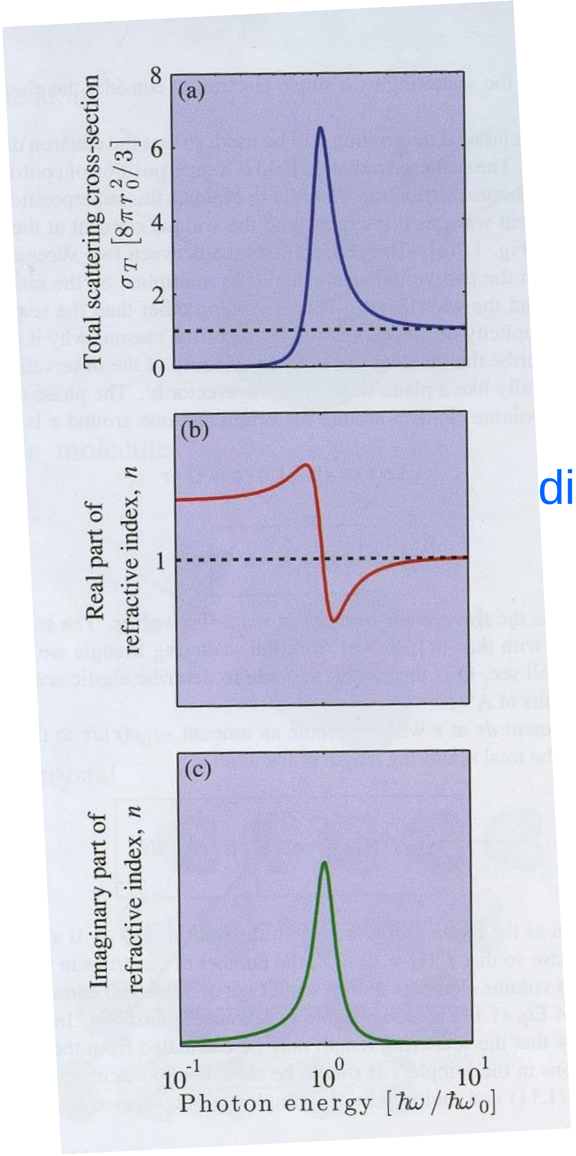
$$\{f^2(Q \to 0) = Z, \qquad f^2(Q \to \infty) = 0\}$$

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

Scattering by a Single Atom:

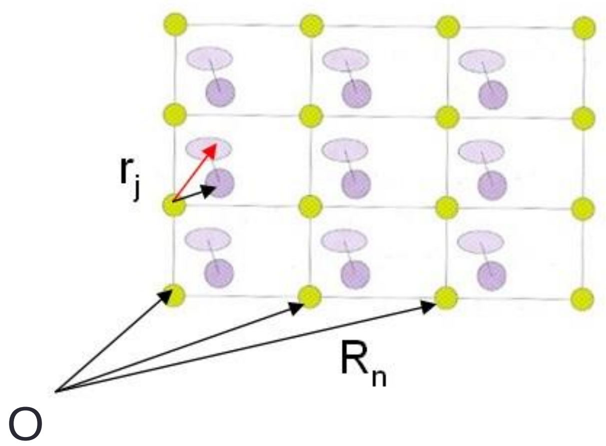


form factor of an atom:

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

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:

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

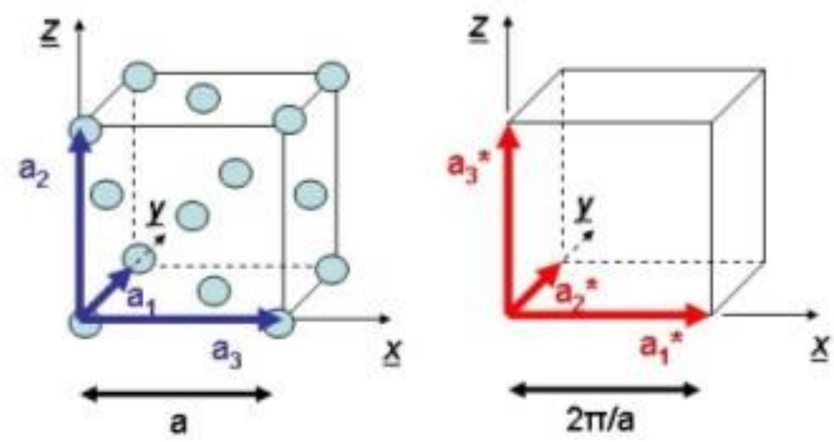
e.g. fcc lattice:

$$r_1 = 0$$

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

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

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



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

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

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

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

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

DESY

Compton Scattering

Consider photon with momentum initially at rest

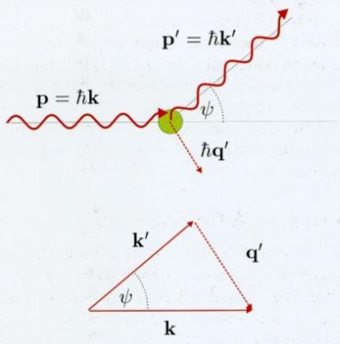
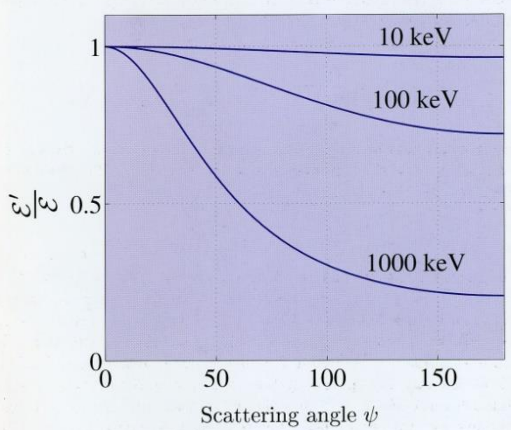


Figure 1.7: Compton scattering. A photon with energy $\mathcal{E} = \hbar ck$ and momentum $\hbar\mathbf{k}$ scatters from an electron at rest with energy mc^2. The electron recoils with a momentum $\hbar\mathbf{q}' = \hbar(\mathbf{k} - \mathbf{k}')$ as indicated in the scattering triangle in the bottom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



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

<u>Energy conservation:</u>

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

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

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

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

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

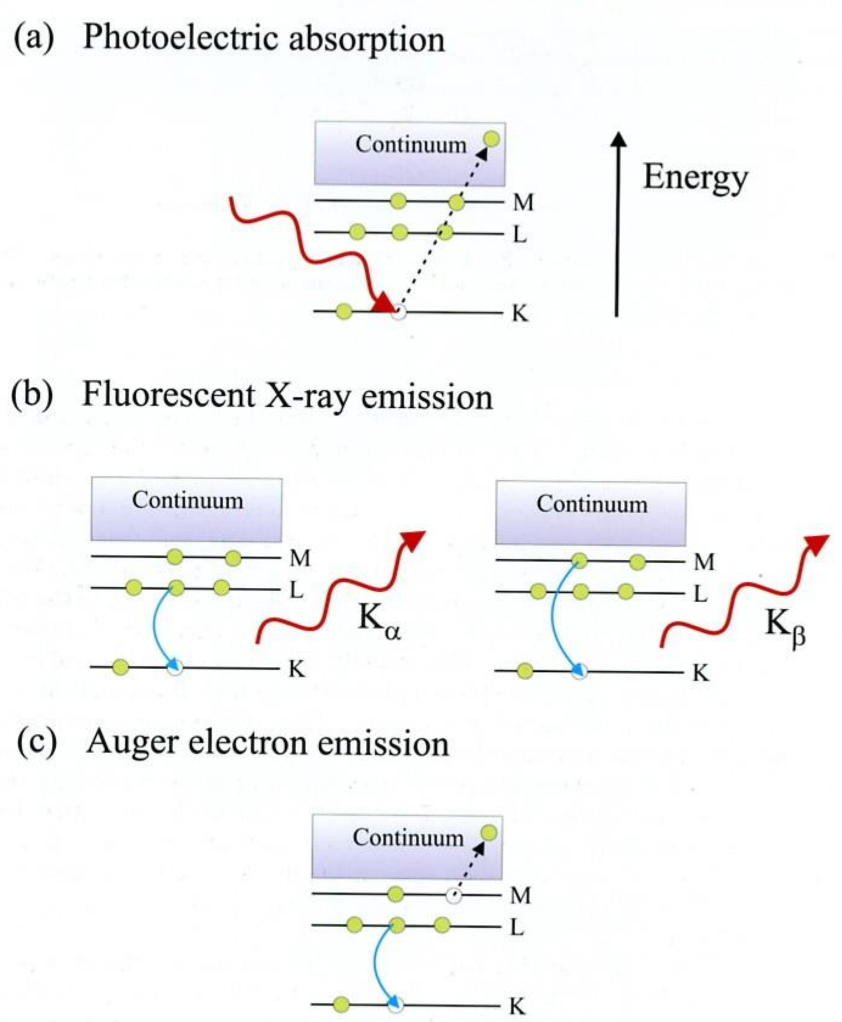
$(1) = (2)$

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

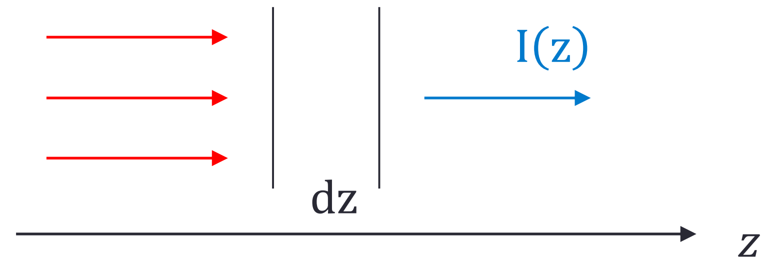
➔ origin of background

➔ 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

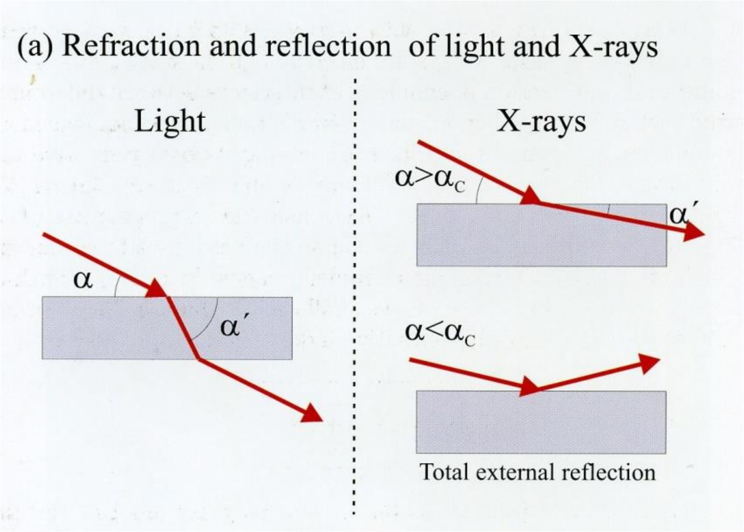
N_A Avogadro's number

A atomic mass number

Refraction

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

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



Snell's law:

$$\cos\alpha = \mathrm{n}\cos\alpha'$$

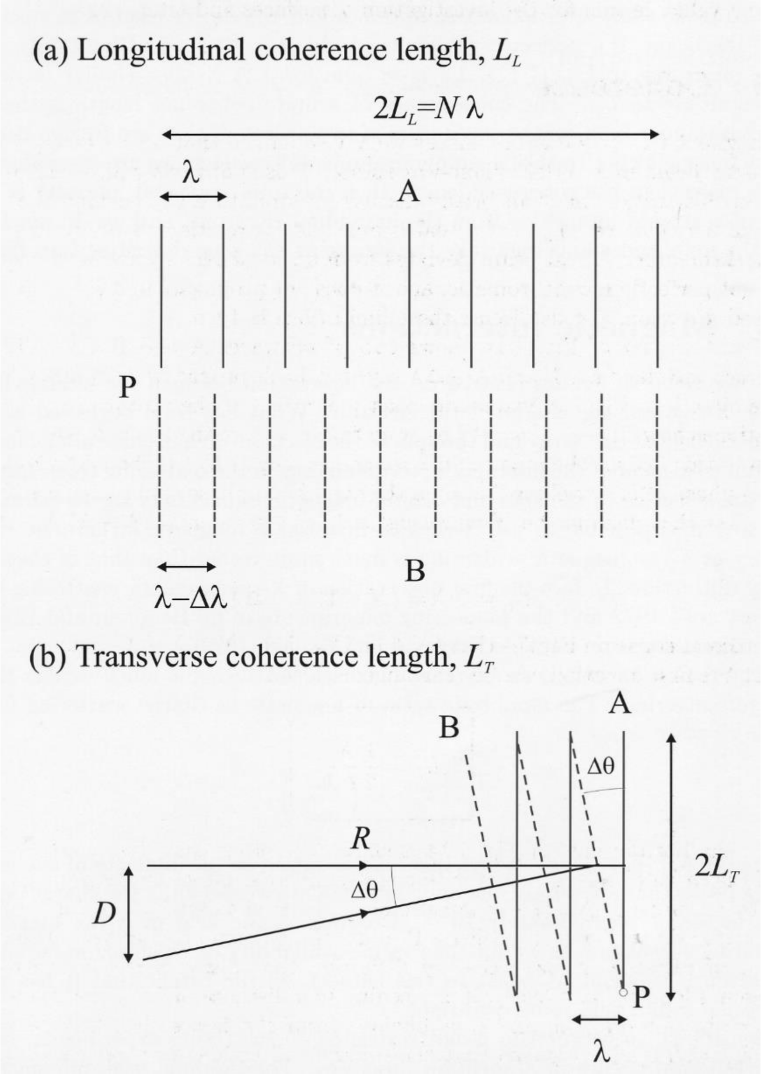
Note: total external reflection for x-rays ($\alpha' = 0$)

n < 1

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

Note: cos z = 1-z^2/2! +z^4/4! – z^6/6! …

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:

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

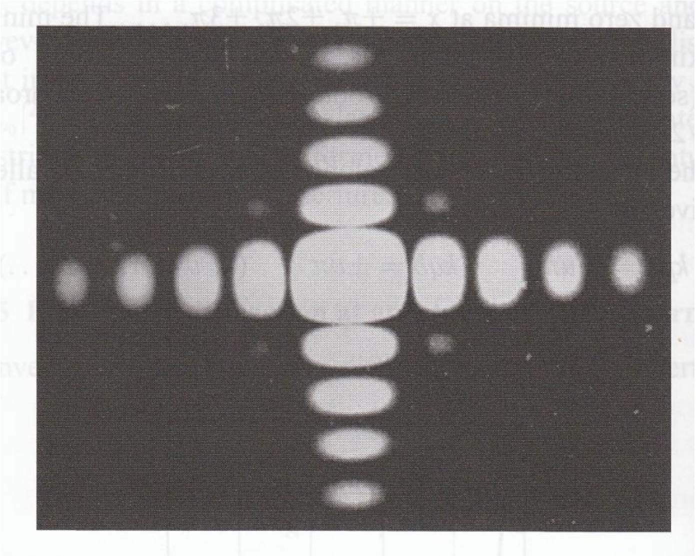
Transverse coherence:

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

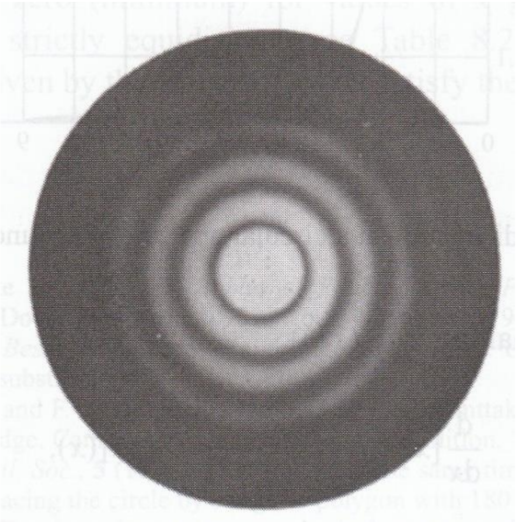
$$2\xi_t\,\Delta\theta = \lambda$$

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

Fraunhofer Diffraction

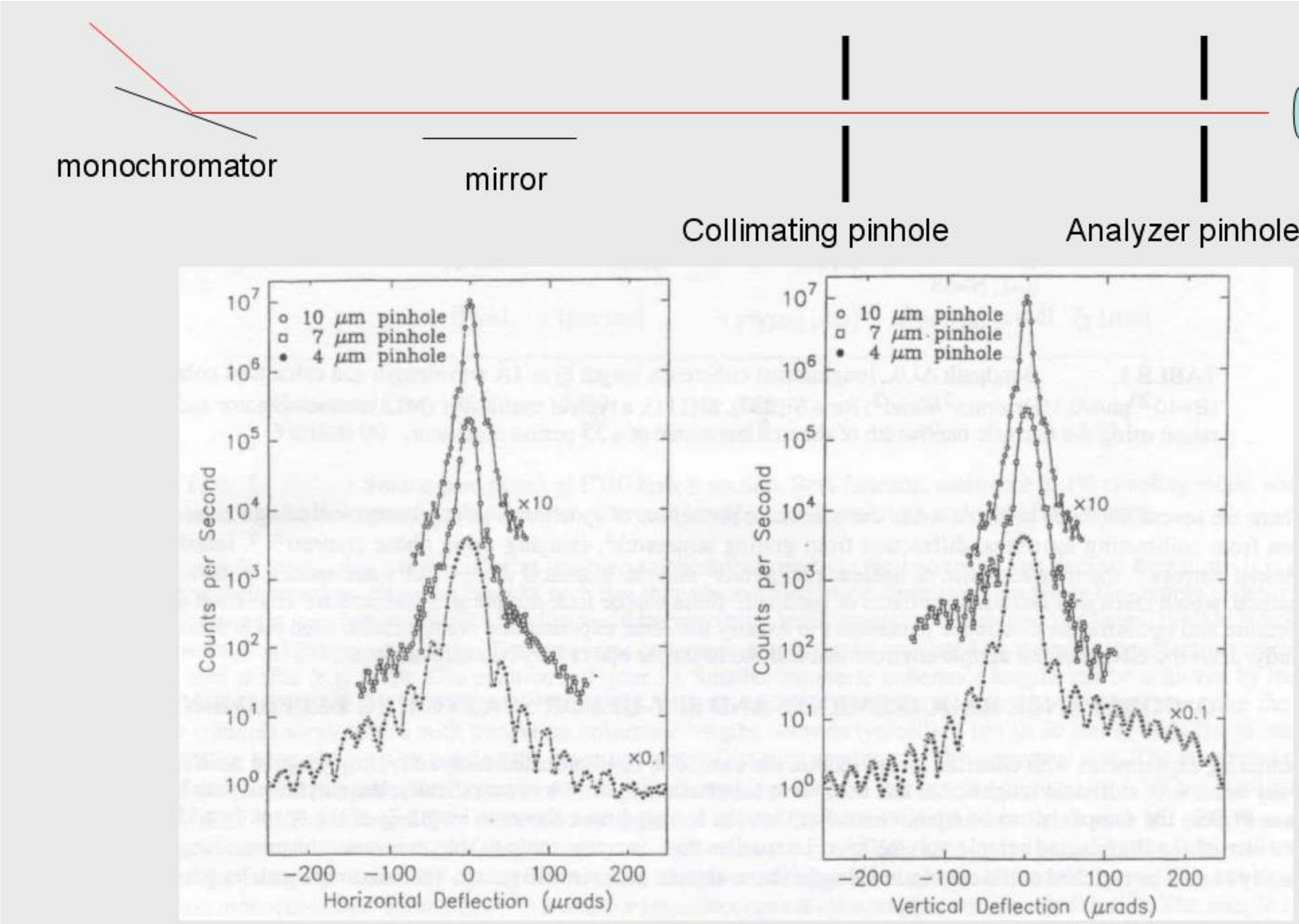


Fraunhofer diffraction of a rectangular aperture 8 x 7 mm^2, taken with mercury light λ=579nm
(from Born&Wolf, chap. 8)



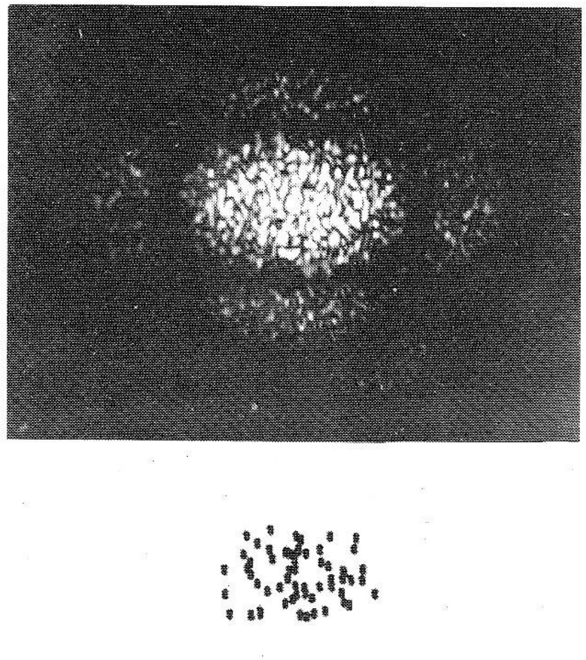
Fraunhofer diffraction of a circular aperture, taken with mercury light λ=579nm
(from Born&Wolf, chap. 8)

Fraunhofer Diffraction ($\lambda = 0.1nm$)

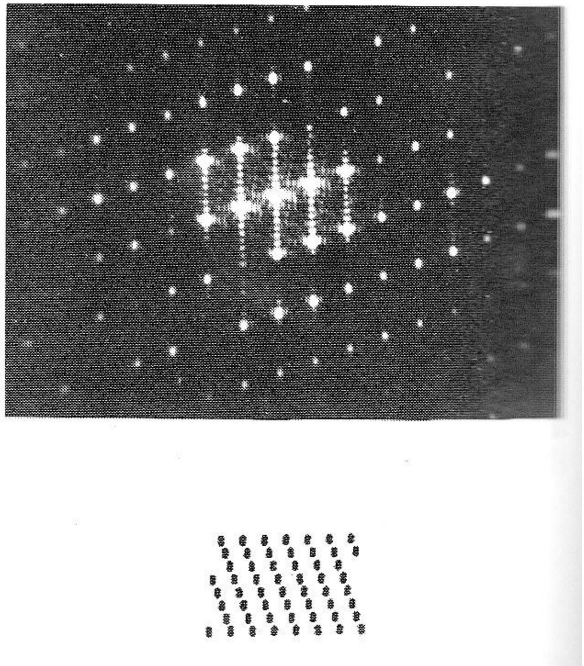


ID10 (ESRF)
E=11.8 keV;
λ=1.05Å

Speckle Pattern



random arrangement of apertures: speckle



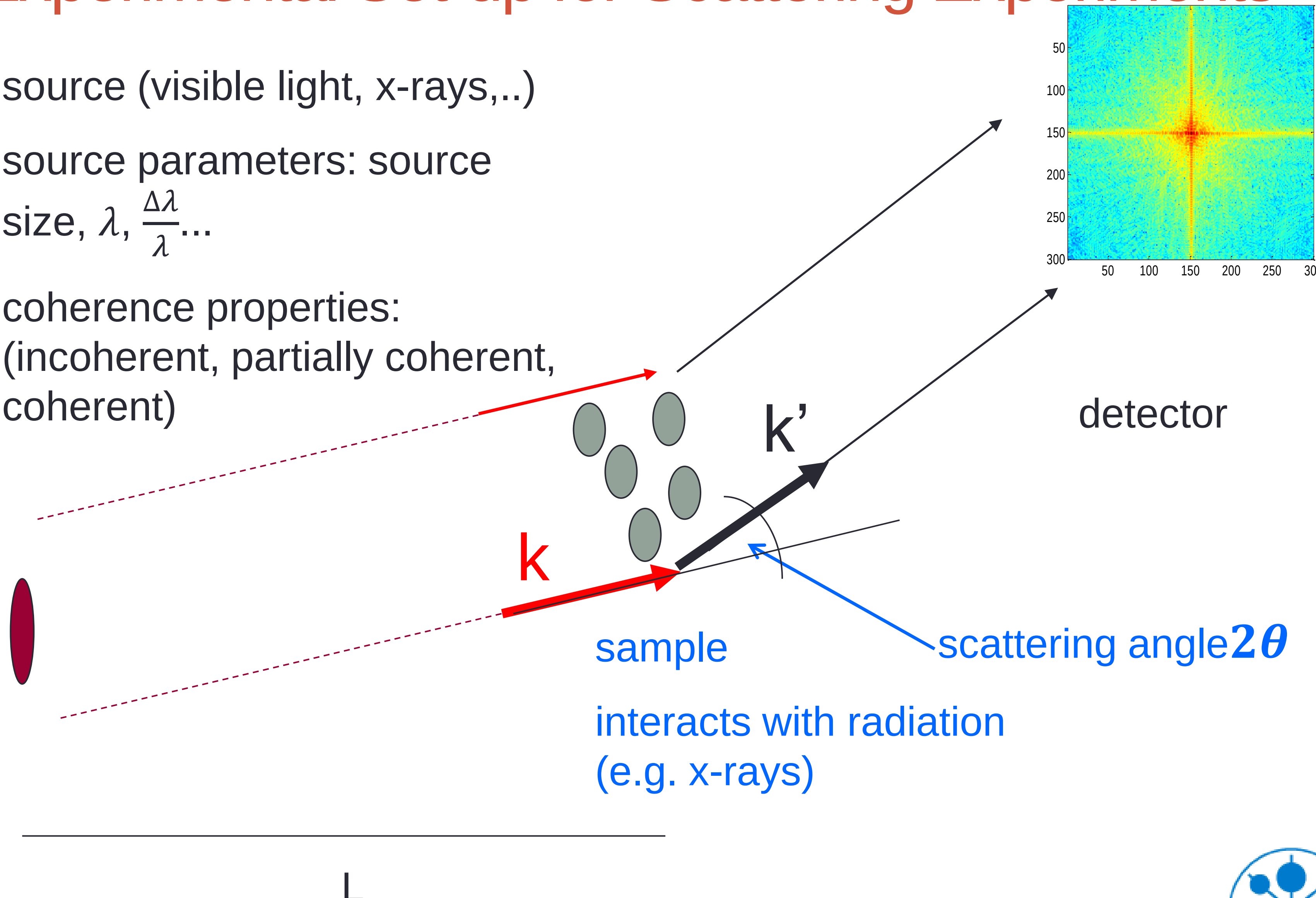
regular arrangement of apertures

Experimental Set-up for Scattering Experiments

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

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

coherence properties: (incoherent, partially coherent, coherent)



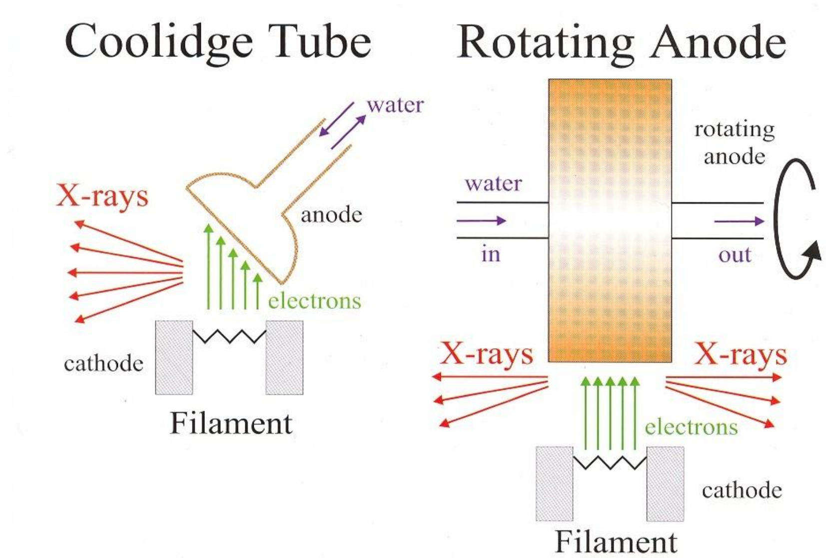
Source of X-Rays

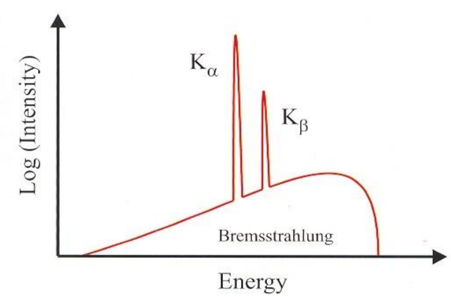
1895 Discovered by W.C. Röntgen

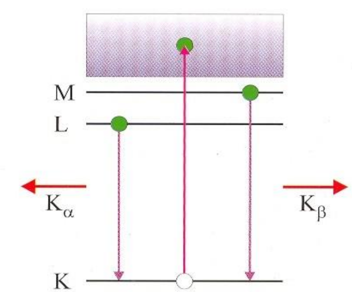
1912 First diffraction experiment (v. Laue)

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

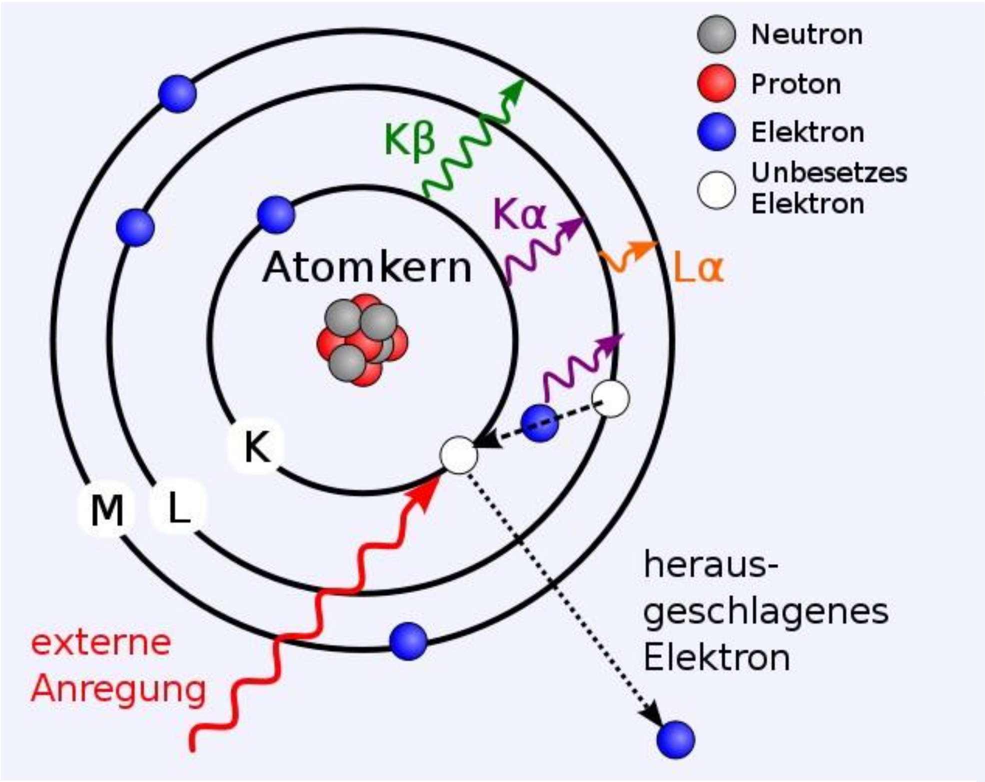
1946 Radiation from electrons in a synchrotron, GE, Physical Review, 71,829 (1947)

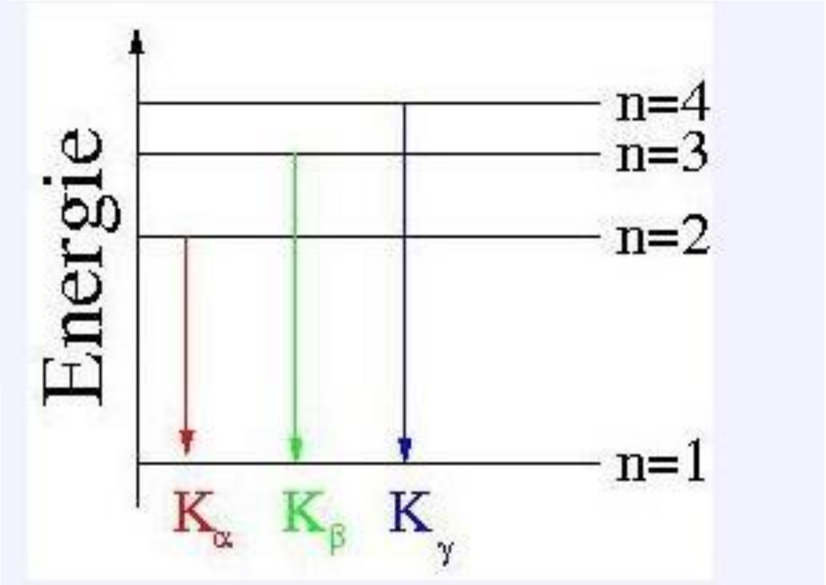




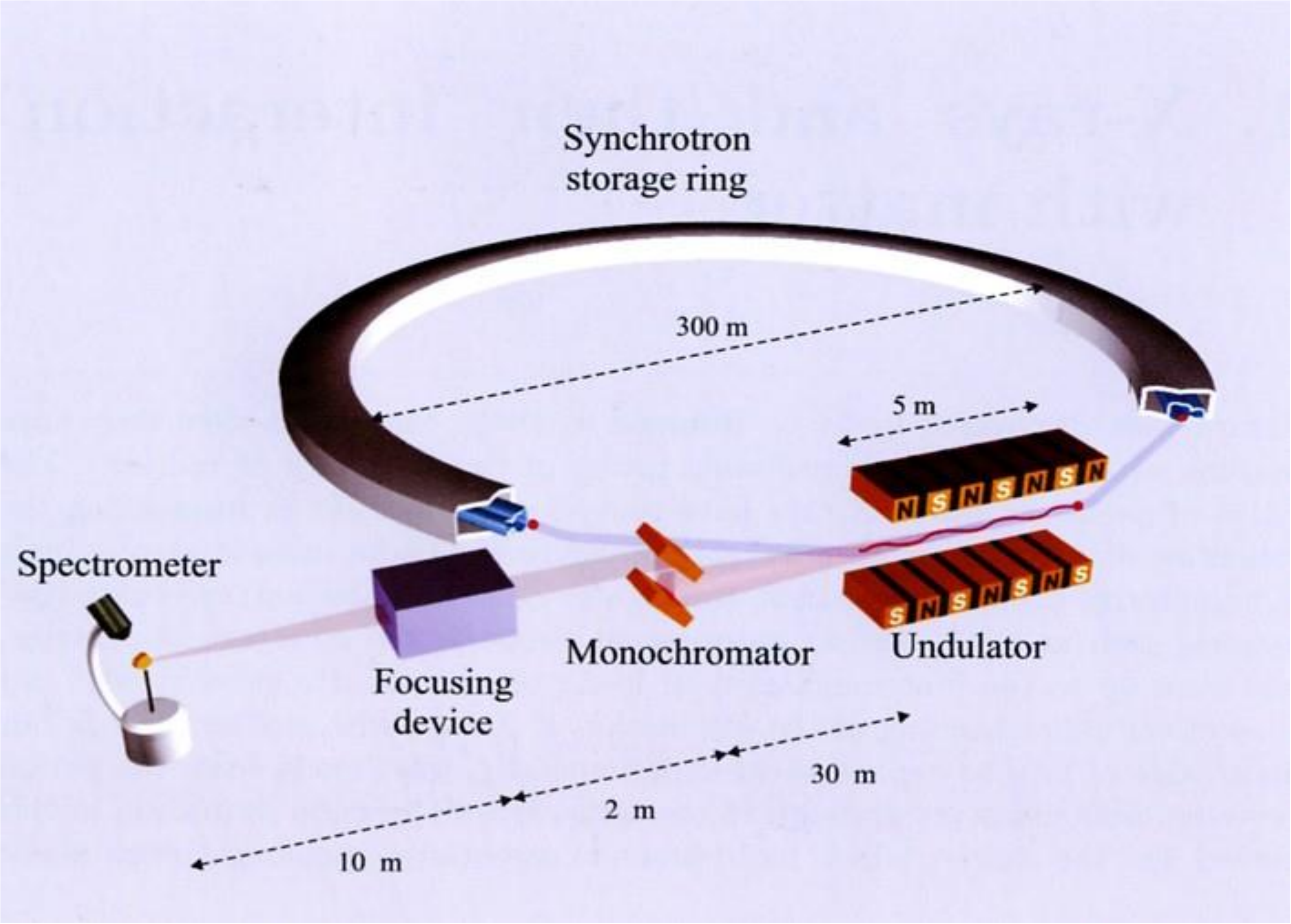


X-Ray Tube


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


Energie
n=4
n=3
n=2
n=1
Kα
Kβ
Kγ

Synchrotron Radiation Storage Ring



Circular Accelerators

Cyclotron
Microtron
Synchrotron
Storage Ring

Cyclotron

- Proposed in 1930 by E.O. Lawrence
- Electrons circulate in a homogeneous magnetic field B
- Frequency for one cycle is given by

$$\omega_c = \left(\frac{e}{m}\right) B_Z$$

- For non-relativistic electrons ω_c is independent of the velocity v

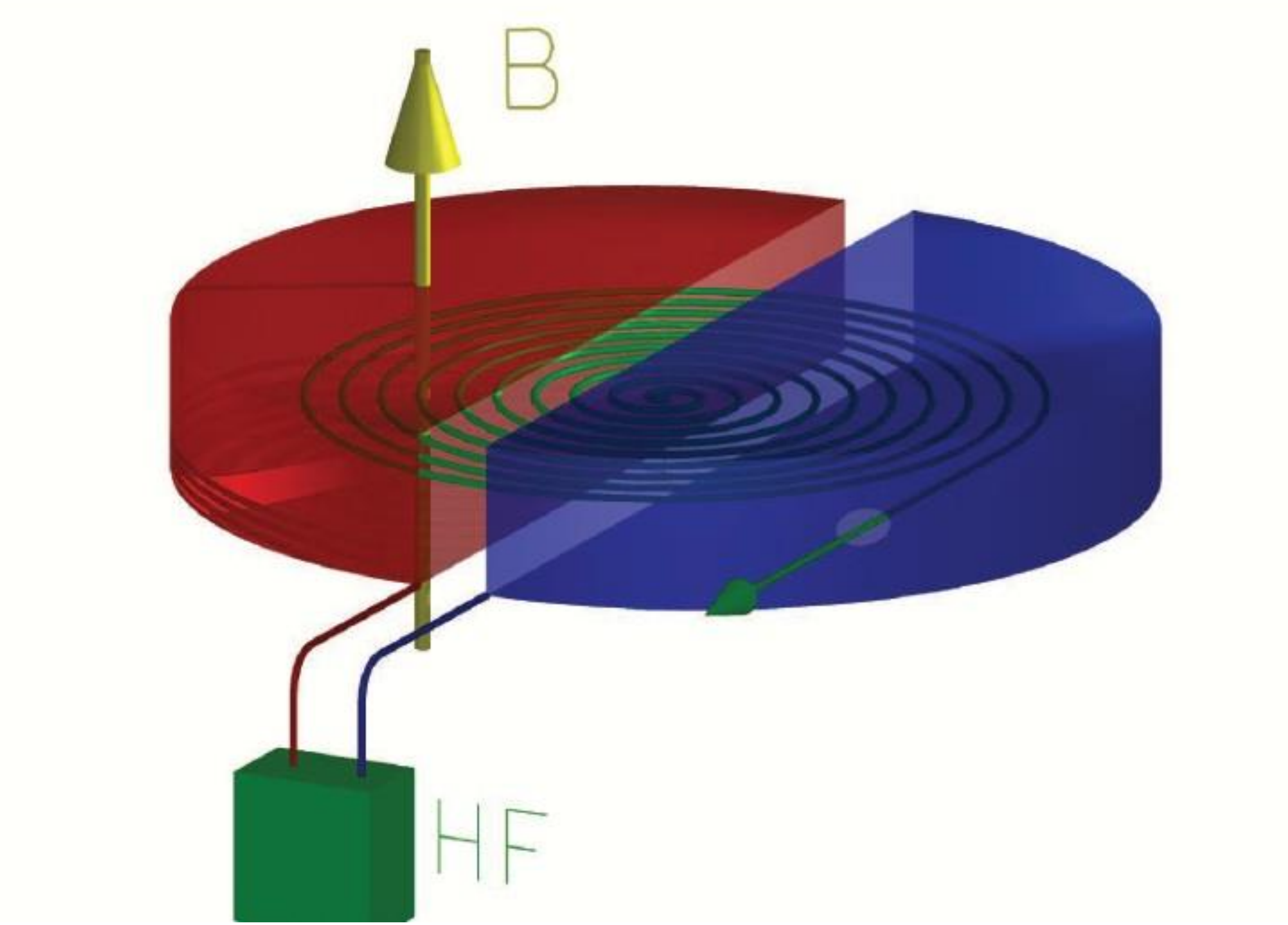
$$\left(\frac{v}{c} < 0.15\right)$$

- At high energies the mass changes and the frequency of the field needs to be adapted.

Example: $E_{kin} = 10\text{keV} = eU = m_e \frac{v_e 2}{2} \Rightarrow \frac{v_e}{c} = 0.2!$

- Electrons at $10\ \text{keV}$ are already relativistic!

Cyclotron



Cyclotron

Zyklotron der Uni Bonn

Synchrotron

- For relativistic particles $v \cong c$ in a B field, the radius is given by

$$R = \frac{E}{ecB}$$

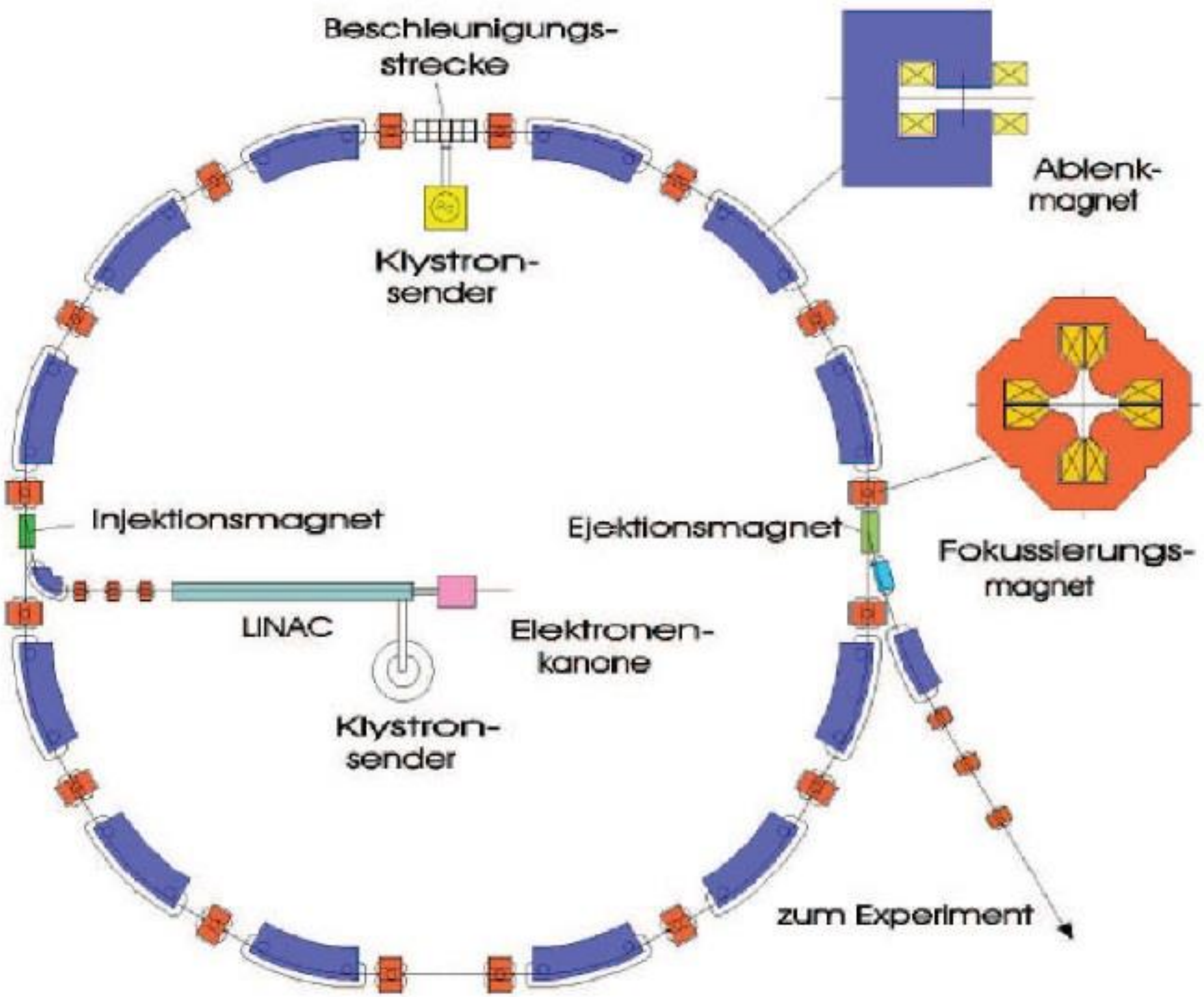
- For $E > 1\ \text{GeV and B} = 5\text{T} : R > \text{several meter}$
- Technically difficult
- Enforce trajectory with constant radius

  Bends in small , local magnets

  $\frac{E}{B} = \text{const.} \Rightarrow$ synchronous ramping of E and B

$\Rightarrow$ Synchrotron

Synchrotron



Synchrotron

- Modern synchrotron radiation sources are built as storage rings

- Synchrotron cannot operate at E=0 since it requires B=0.
  $\Rightarrow$ Use LINAC or Microtron as pre-accelerator
  Use synchrotron to reach the final energy E
  Use storage ring to keep electrons at energy

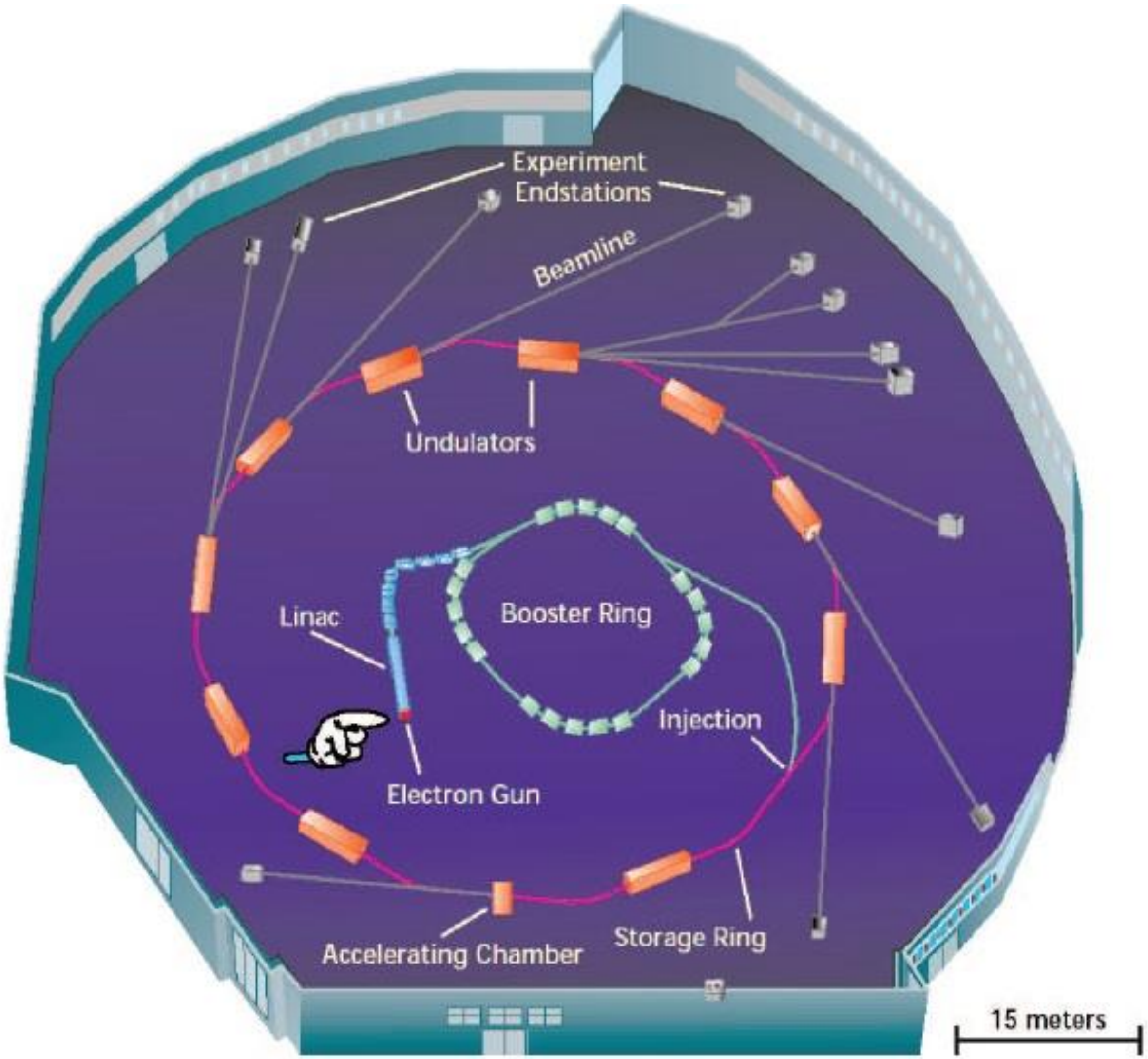
- The storage ring supplies the energy lost by radiation in each turn.

- Typical parameters: Lifetime: up to 30 h
  Current: 100 – 500 mA

- Current losses through interaction with residual gas $\Rightarrow$ UHV

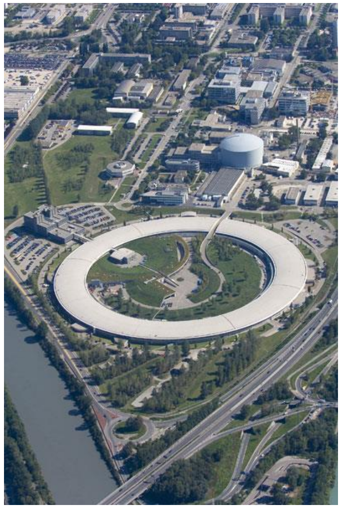
- Current supplied in bunches.

Storage Rings



Storage Rings

Photon Machines



Synchrotron Radiation Primer

Radiation of a non-relativistic, accelerated particle:

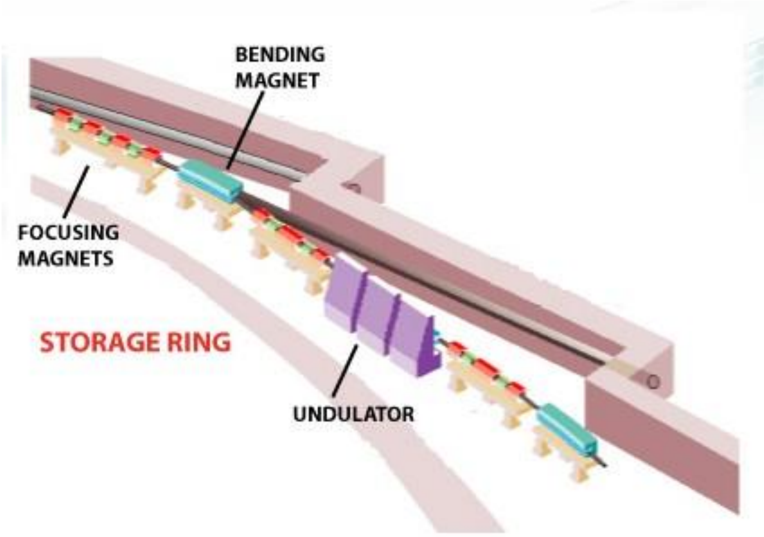
$$P = \left(\frac{e^2}{6\pi\varepsilon_0 m_{0^2} c^3}\right) \left(\frac{dp}{dt}\right)^2$$

Angular distribution resembles the one of a Hertz dipole:

$$\left(\frac{dP}{d\Omega}\right) = \left(\frac{e^2}{16\pi^2\varepsilon_0 m_{0^2} c^3}\right)\left(\frac{dp}{dt}\right)^2 \sin^2(\Psi)$$

Radiation is emitted (similar to the dipole) in the direction perpendicular to the acceleration

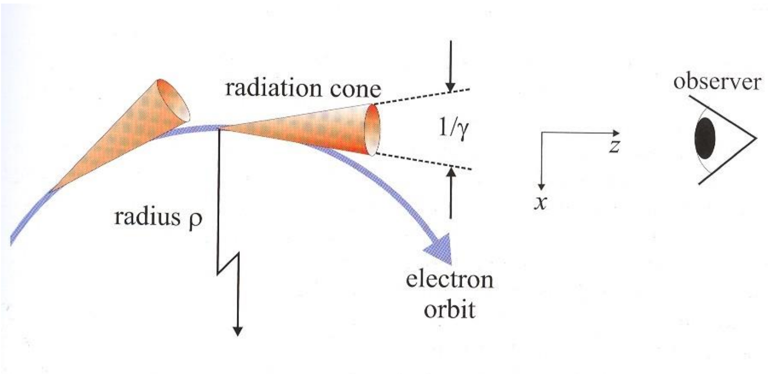
Synchrotron Radiation Primer



Energy E_e of an electron at speed v:

$$E_e = \frac{mc^2}{\sqrt{1-\left(\frac{v}{c}\right)^2}} = \gamma\, mc^2$$

For 5GeV and mc^2=0.511 MeV get $\gamma \approx 10^4$



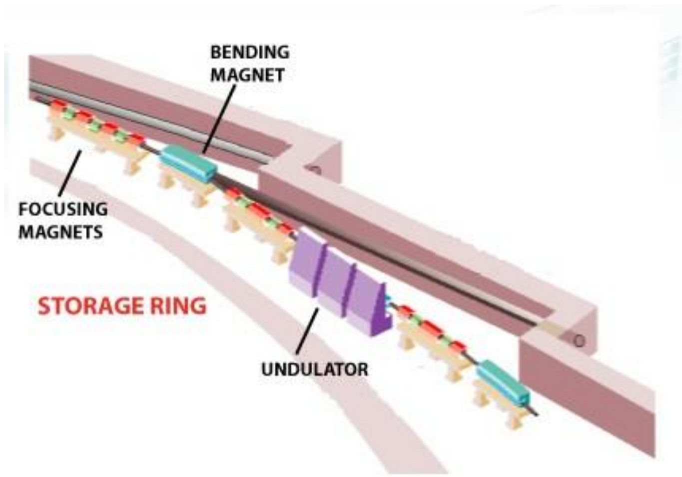
Centrifugal=Lorentz force yields for radius:

$$\rho = \frac{\gamma mc}{eB} = \frac{3.3\ E\ [\mathrm{GeV}]}{B[\mathrm{T}]} \approx 25\ \mathrm{m}$$

$$E_e = 6\ \mathrm{GeV}, \qquad B = 0.8\ \mathrm{T}$$

Opening angle is of order $\frac{1}{\gamma} \approx 0.1\ \mathrm{mrad}$

Bending Magnets



Characteristic energy $\hbar\omega_c$ for bend or wiggler:

$$\hbar\omega_c[\text{keV}] = 0.665 E_e^2\ [\text{GeV}] B(\text{T}) \approx 20\ \text{keV}$$

$$\text{Flux} \sim E^2$$

Energy loss by synchrotron radiation per turn:

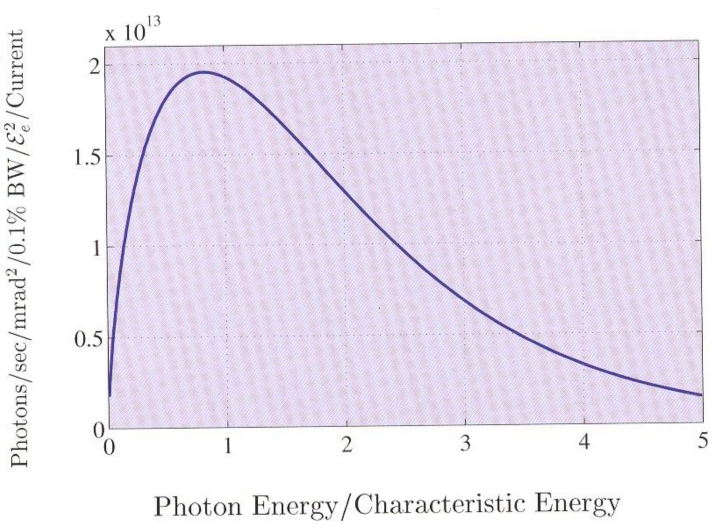
$$\Delta E[\text{keV}] = \frac{88.5\ E^4[\text{GeV}]}{\rho[\text{m}]}$$

For 1 GeV and $p = 3.33$ m: $\Delta E = 26.6$ keV/turn

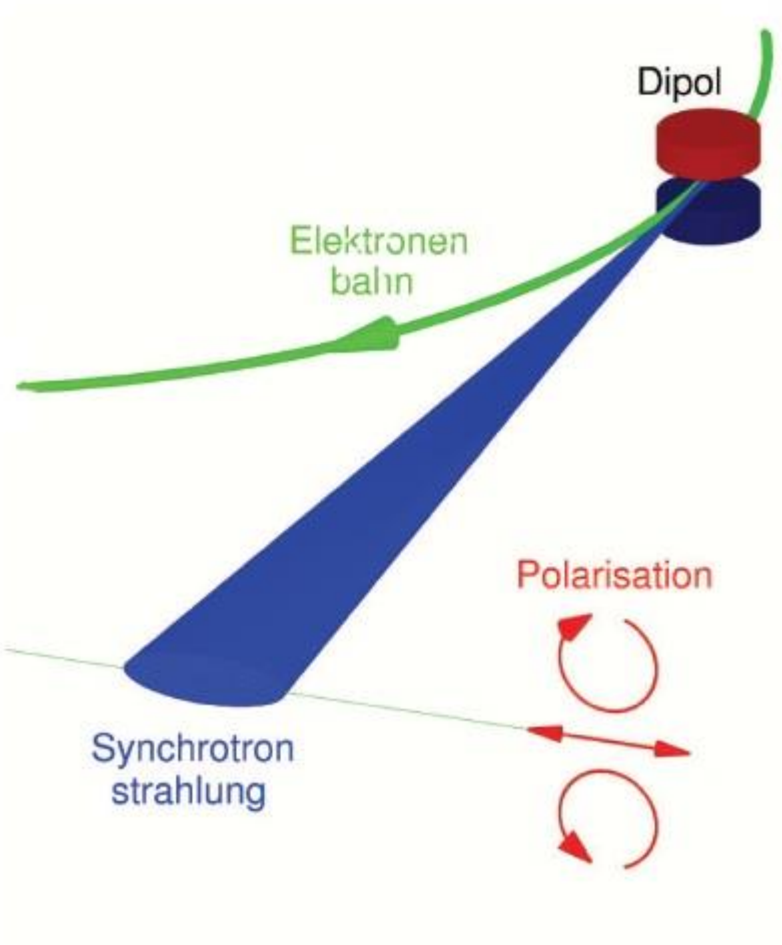
For $I = 500\text{mA} \equiv 0.5 \frac{\text{Cb}}{\text{s}} = 0.5 \times 6.25 \times 10^{18} \frac{e^-}{\text{s}}$

$$\rightarrow P = 0.5 \times 6.25 \times 10^{18} \frac{e^-}{s\ x\ 26.6\ \text{keV}}$$

$$= 8.3125 \times 10^{22} \times 1.6 \times 10^{-19} = 13.3 \frac{\text{kJ}}{\text{s}} = 13.3\ \text{KW}$$

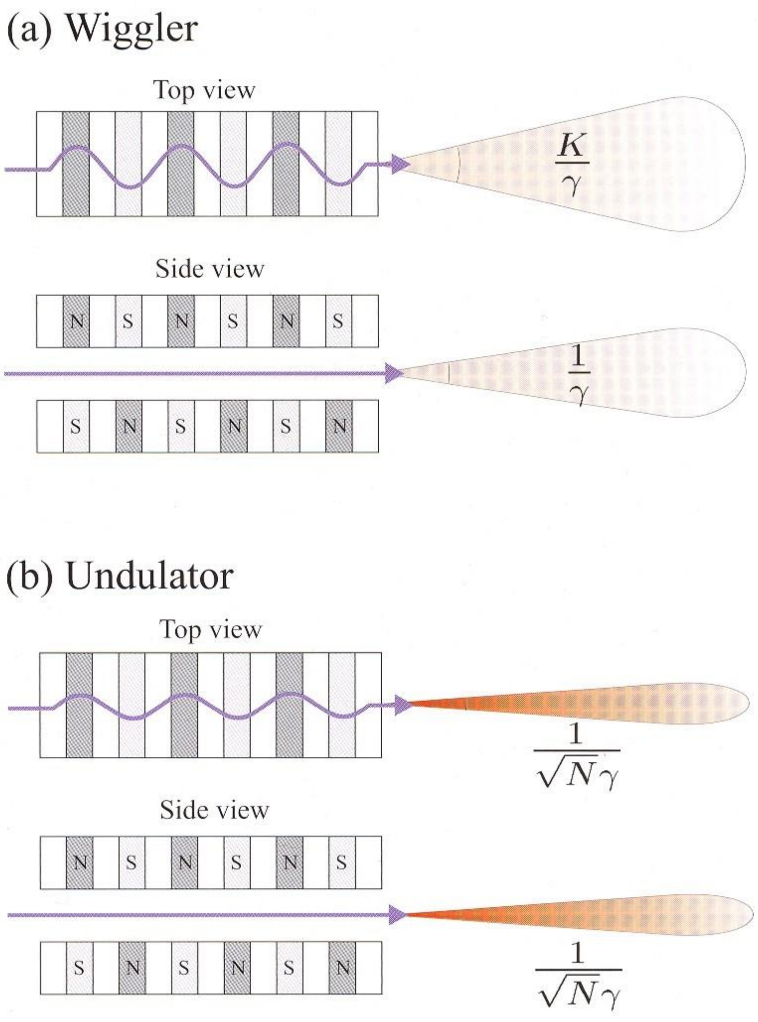


Polarization



- Synchrotron radiation is polarized linearly in the plane of the orbit
- Above and below the orbital plane of the polarization is circular
- Important applications for magnetic x-ray scattering

Insertion Devices (Wigglers and Undulators)



Wiggler:

$P[kW] = 0.633 E_e^2 [GeV]\, B^2[T]\ \ L[m]\ \ I[A]$

$Flux \sim E^2 \times N$

N: number poles

Undulator:

$k = eB / mc\ \ k_u = 0.934\ \lambda_u\ [cm]\ Bo[T]$

with λ_u undulator period

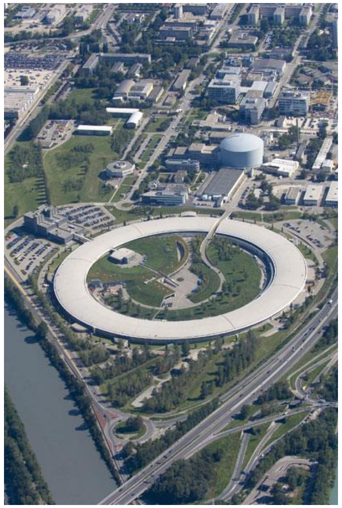
undulator fundamental:

$$\lambda_0 = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{k^2}{2} + \gamma\theta\right)$$ on axis

$Flux \sim E^2 \times N^2$

bandwidth: $\frac{\Delta\lambda}{\lambda} \sim \frac{1}{nN}$

Photon Machines



The most recent third generation machine:

Petra III at DESY/Hamburg