Methoden moderner Röntgenphysik I: Struktur und Dynamik kondensierter Materie

Vorlesung zum Haupt/Masterstudiengang Physik

WS 2009/10

G. Grübel, M. Martins, E. Weckert et al.

Location: SemRm 4, Physik, Jungiusstrasse

Thursdays 10.15 – 11.45

G.Grübel (GG), A.Meents (AM), C. Gutt (CG)

Methoden moderner Röntgenphysik I: Struktur und Dynamik kondensierter Materie

Hard X-Rays - **Introduction into X-ray physics - Lecture 2**

22.10.	Introduction	(GG)
29.10.	X-ray Scattering Primer, Sources of X-rays	(GG)
5.11.	Refraction and Reflexion, Kinematical Scattering (I)	(GG)
12.11.	Kinematical Scattering Theory (II)	(GG)
19.11.	Applications of KST and “perfect” crystals	(GG)
26.11.	Small Angle and Anomalous Scattering	(GG)
3.12. - 7. 1.	Modern Crystallography	(AM)
14. 1. - 4. 2.	Coherence base techniques	(CG)

Coherence of light and matter I: from basic concepts to modern applications

Introduction into X-ray physics: 22.10.-26.11.

Introduction
Overview, Introduction to X-ray scattering

X-ray Scattering Primer and Sources of X-rays
Elements of X-ray scattering, sources of X-rays

Reflection and Refraction, Kinematical Diffraction (I)
Snell's law, Fresnel equations, diffraction from an atom, molecule, crystal,…

Kinematical Diffraction (II)
Reciprocal lattice, structure factor,..

Applications of Kinematical Diffraction and "perfect" crystals
Quasiperiodic lattices, crystal truncation rods, lattice vibrations, Debye-Waller factor, "perfect" cystal theory

SAXS, Anomalous Diffraction
Introduction into small angle scattering and anomalous scattering

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

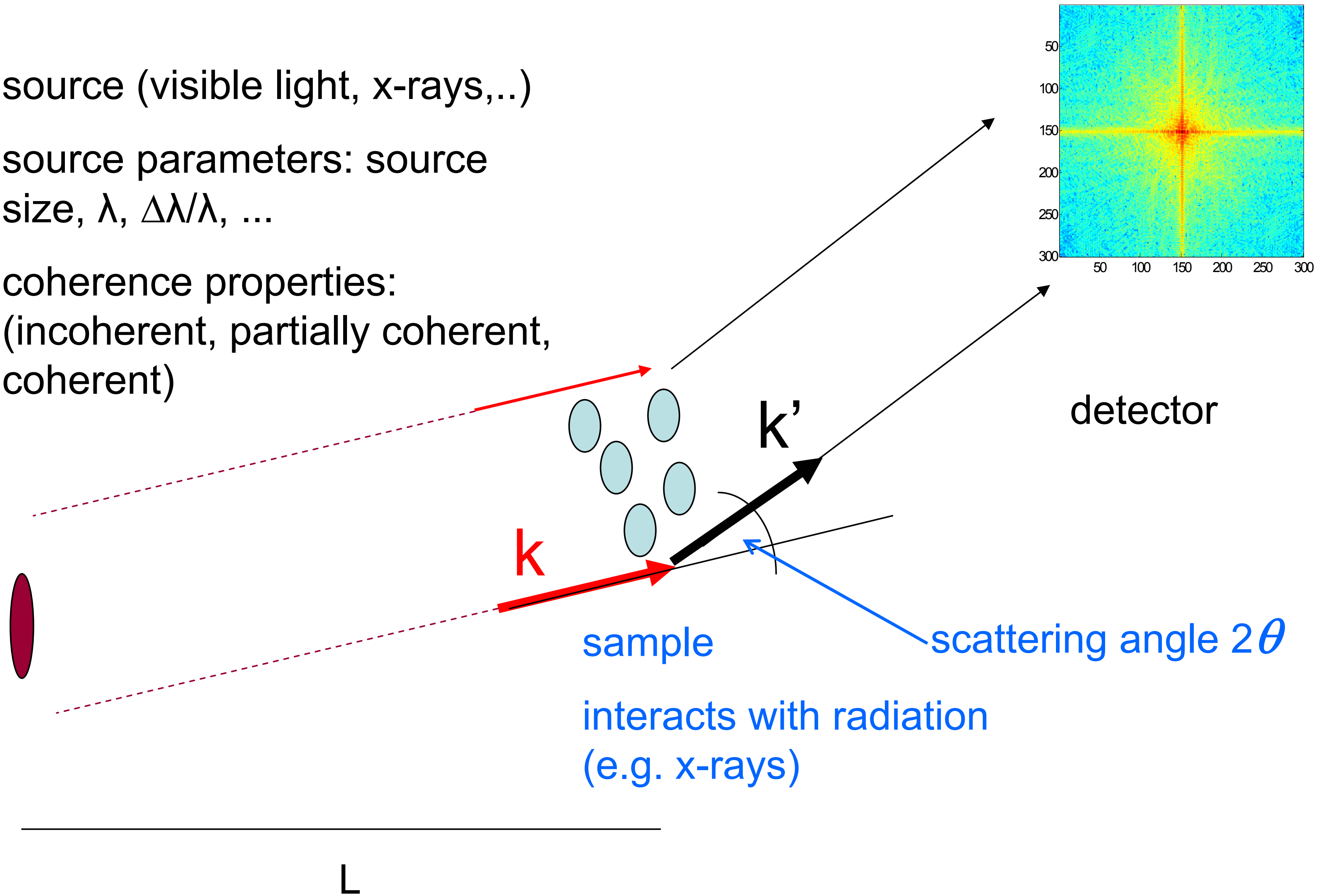
Coherence Properties

Set-Up for Scattering Experiments

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

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

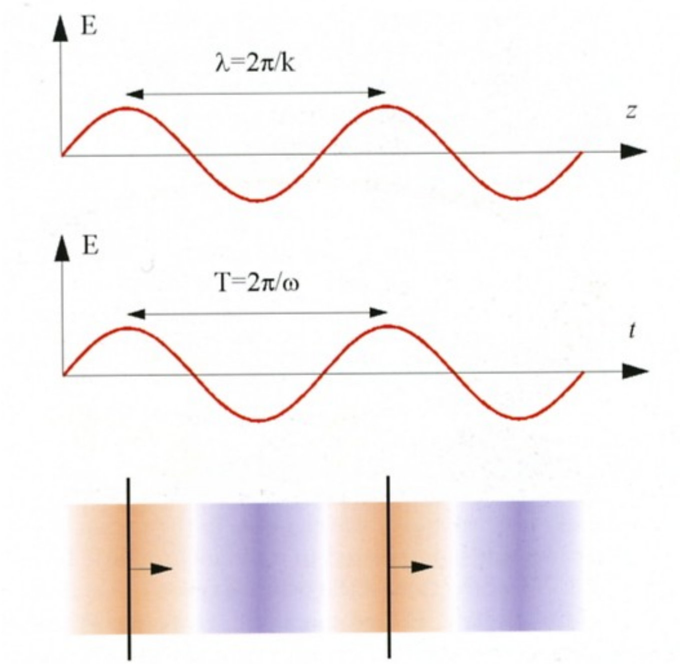
coherence properties: (incoherent, partially coherent, coherent)

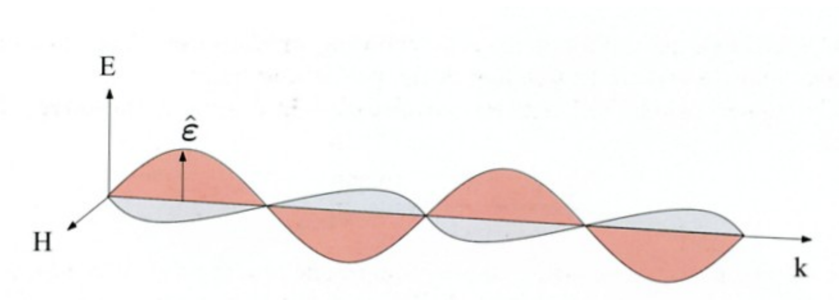


 Methoden moderner Roentgenphysik I - Vorlesung im Haupt/Masterstudiengang Physik, Universitaet Hamburg, WS 2008/9 G. Gruebel

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**.





Neglecting the H field one may write:

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

with

$\boldsymbol{\varepsilon}$: polarization vector

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

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

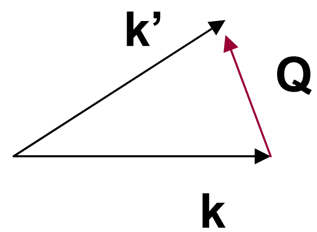
Scattering of X-rays

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

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

elastic scattering:

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



Scattering by a single electron:

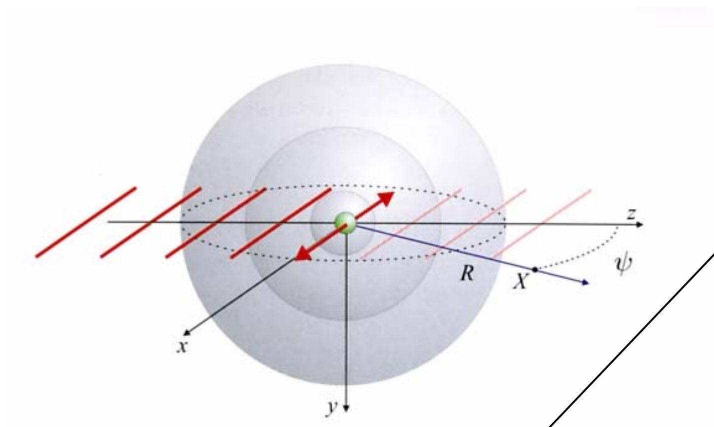
$E_{rad}(R,t)/E_{in} =$

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

spherical wave

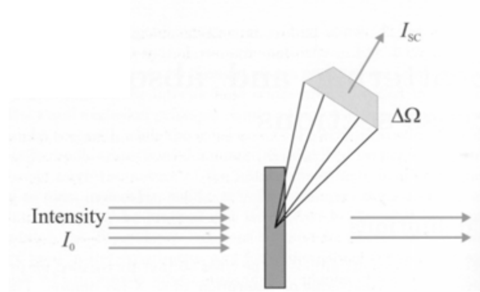
thomson scattering length r_o

($=2.82 \cdot 10^{-5}$ 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: $\sigma_{total} = \int (d\sigma/d\Omega) = (8\pi/3)\, r_o^2$

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

phase factor

≡ scattering amplitude by an ensemble of electrons

$$-r_o f^o(Q) = -r_o \sum_{rj} \exp(iQ \cdot r_j)$$

(atomic) formfactor ↑ position of scatterers ↑

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

form factor of an atom:

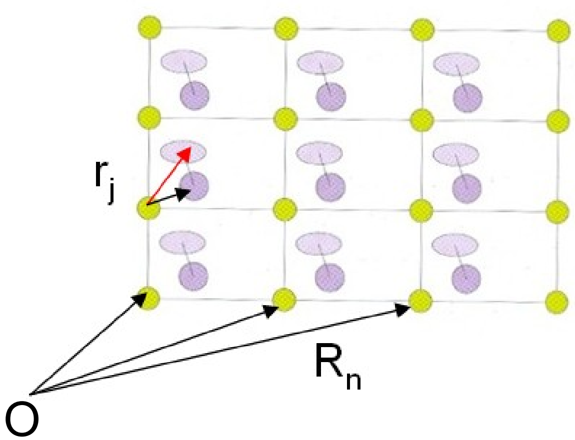
$$f(Q,\hbar\omega) = f^o(Q) + f'(\hbar\omega) + i f''(\hbar\omega)$$

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 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> $\Sigma_{rj}\, f_j(Q)\exp(iQr_j)$

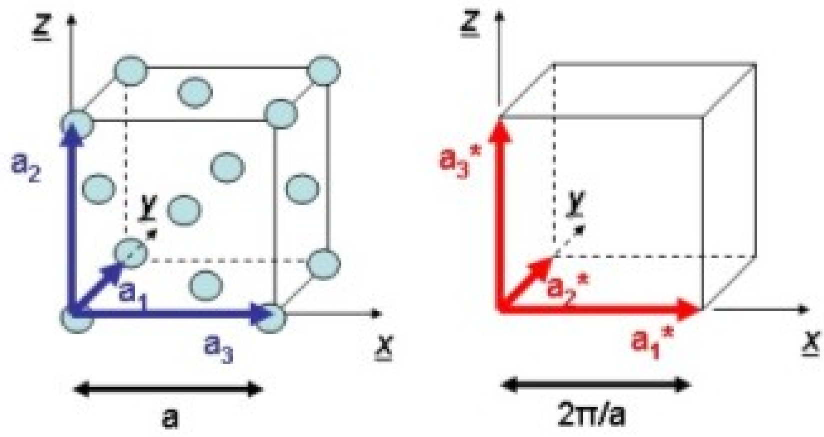
<u>e.g. fcc lattice:</u>

$r_1 = 0$

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

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

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



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

$F_{hkl}^{fcc} = f(Q)\, \Sigma\exp(iQr_j)$ 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 $p = \hbar \mathbf{k}$ scattered by a electron, initially at rest

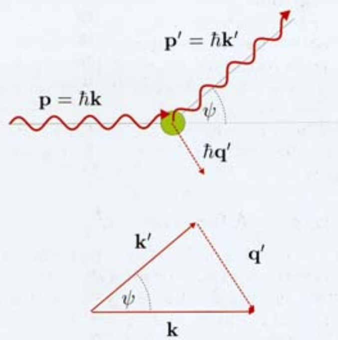
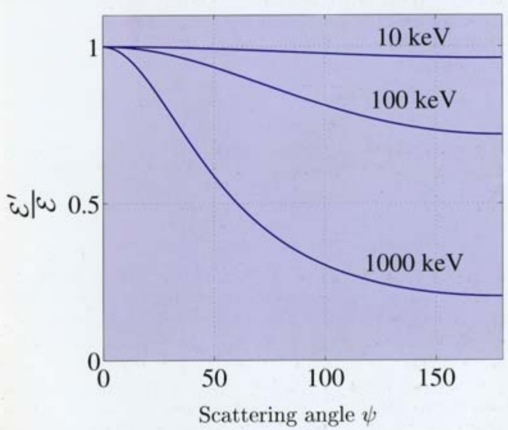


Figure 1.7: Compton scattering. A photon with energy $\mathcal{E} = \hbar ck$ and momentum $\hbar\mathbf{k}$ scatters from an electron at rest with energy mc^2. The electron recoils with a momentum $\hbar\mathbf{q}' = \hbar(\mathbf{k} - \mathbf{k}')$ as indicated in the scattering triangle in the bottom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



<u>energy conservation:</u>

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

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)

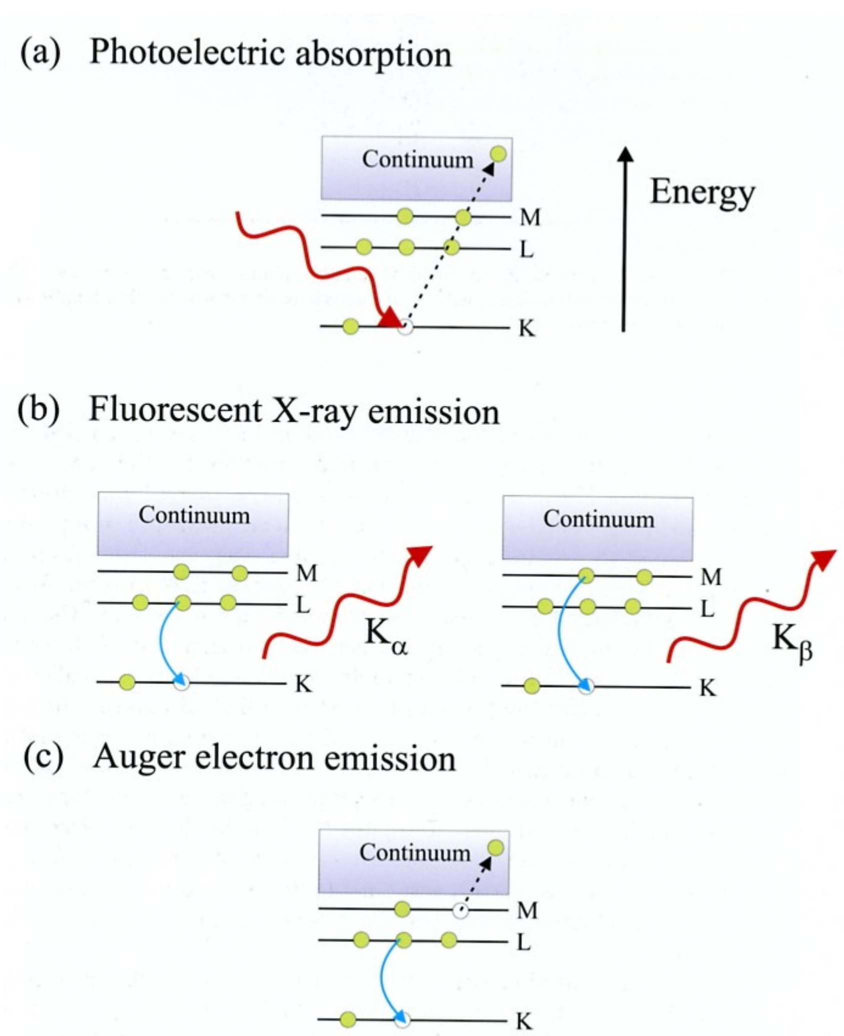
(1) = (2)

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

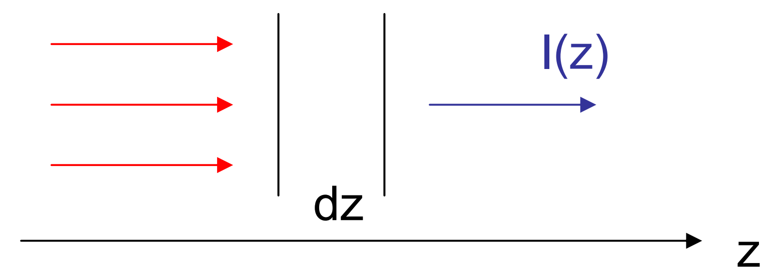
➔ origin of background

➔ 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

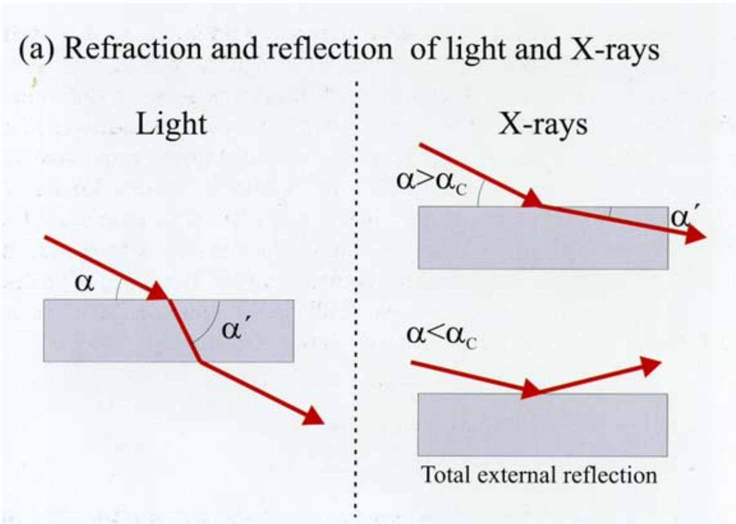
N_A Avogadro’s number

A atomic mass number

Refraction

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

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



Snell's law:

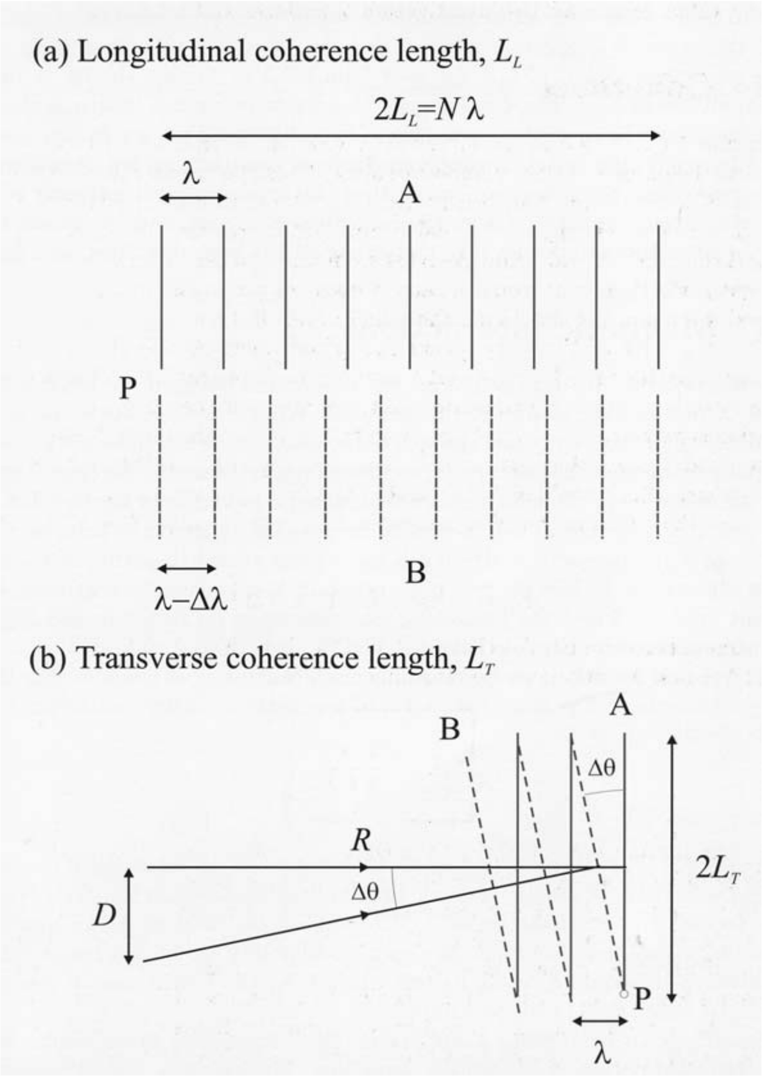
$\cos\alpha = n \cos\alpha'$

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

$n < 1$

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

Coherence



<u>Longitudinal coherence:</u>

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

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

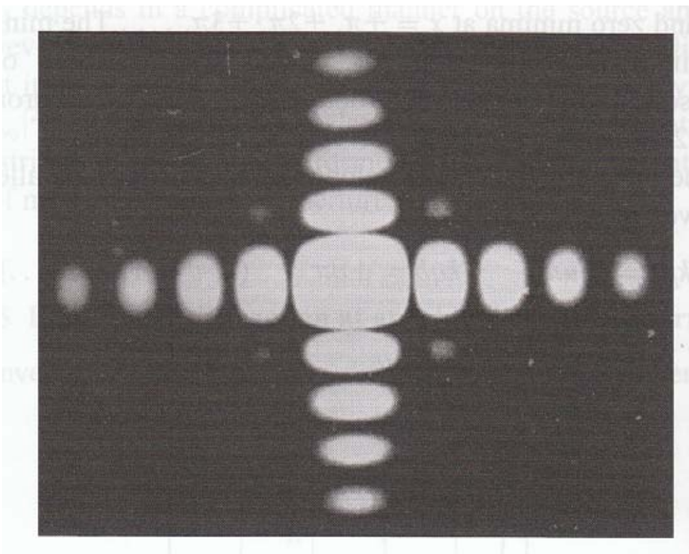
<u>Transverse coherence:</u>

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

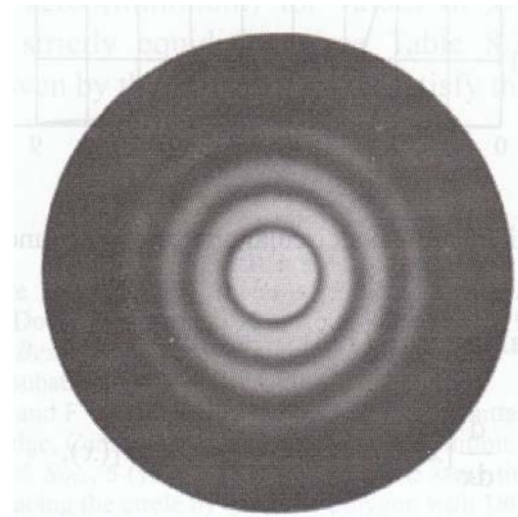
$$2\xi_t\,\Delta\theta = \lambda$$

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

Fraunhofer Diffraction

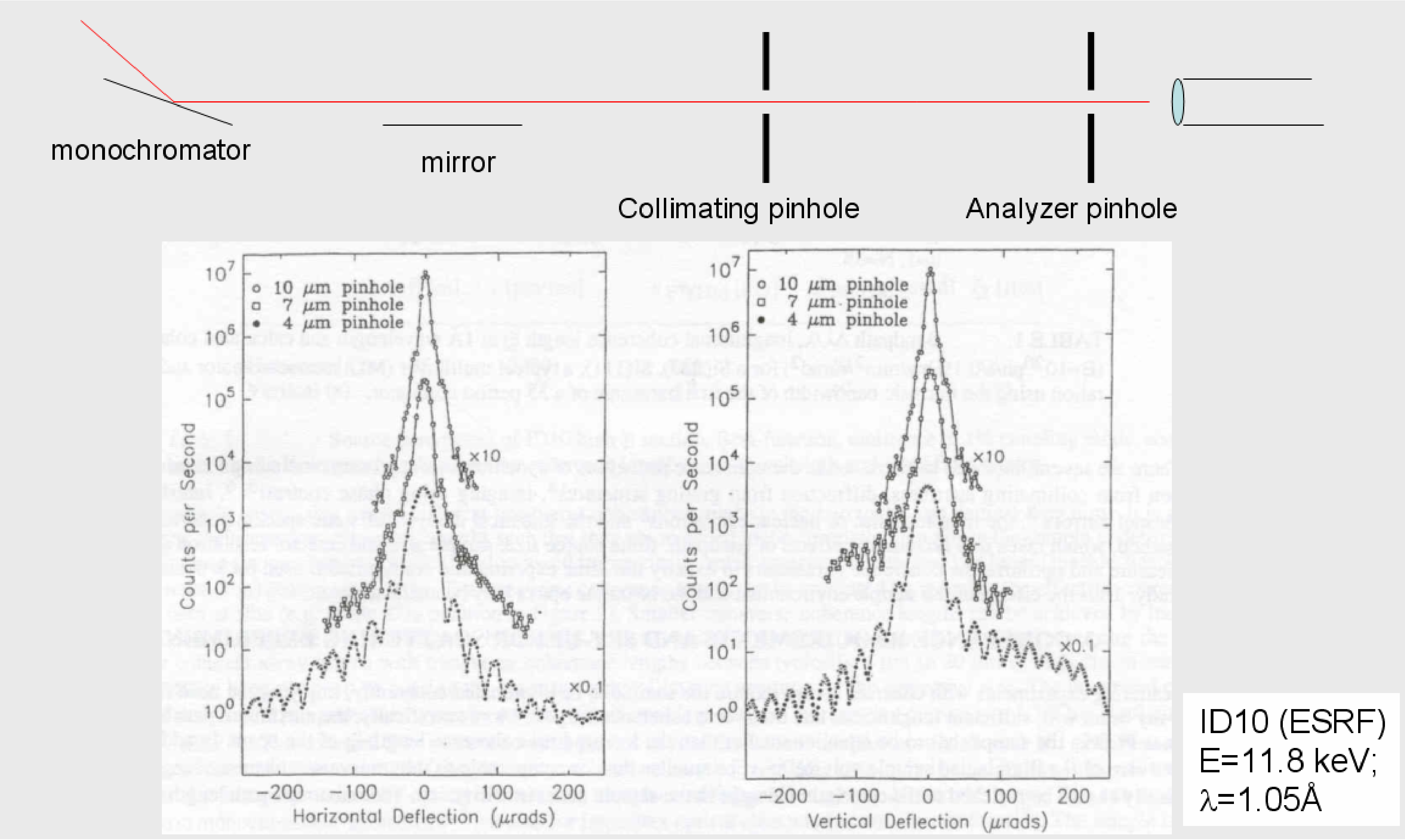


Fraunhofer diffraction of a rectangular aperture 8 x 7 mm^2, taken with mercury light λ=579nm
(from Born&Wolf, chap. 8)



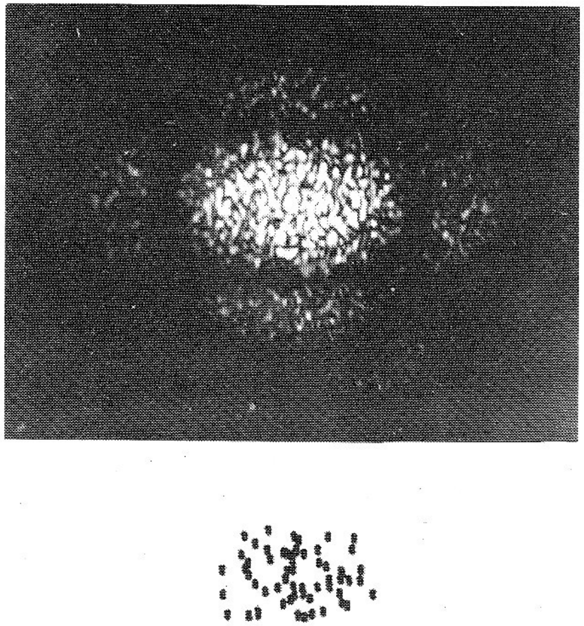
Fraunhofer diffraction of a circular aperture, taken with mercury light λ=579nm
(from Born&Wolf, chap. 8)

Fraunhofer Diffraction (λ=0.1nm)

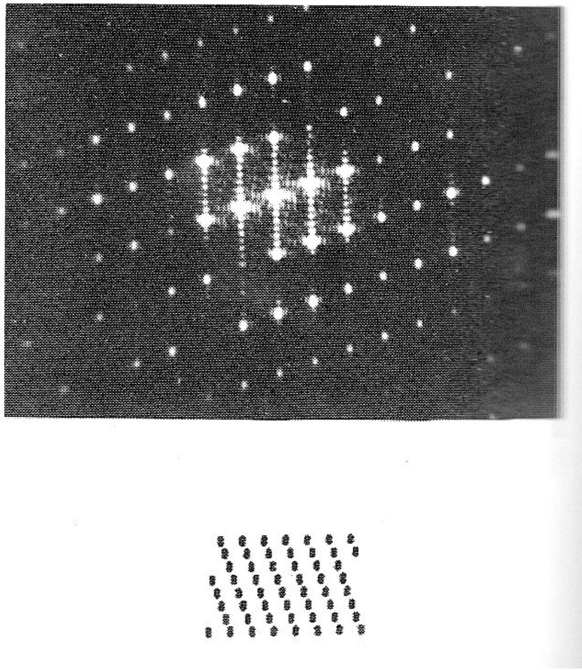


ID10 (ESRF)
E=11.8 keV;
λ=1.05Å

Speckle pattern



random arrangement of apertures: speckle



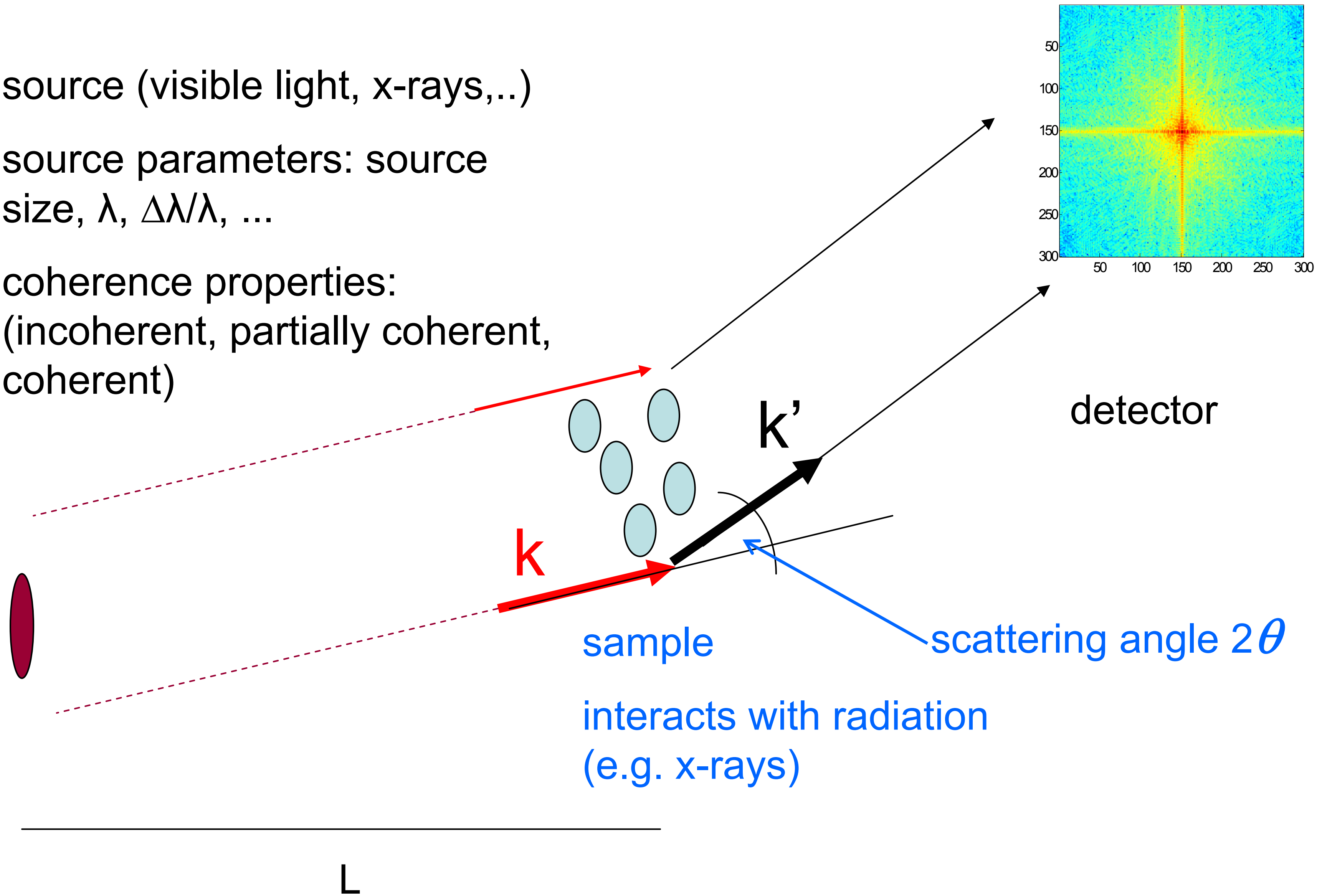
regular arrangement of apertures

Experimental Set-Up for Scattering Experiments

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

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

coherence properties: (incoherent, partially coherent, coherent)



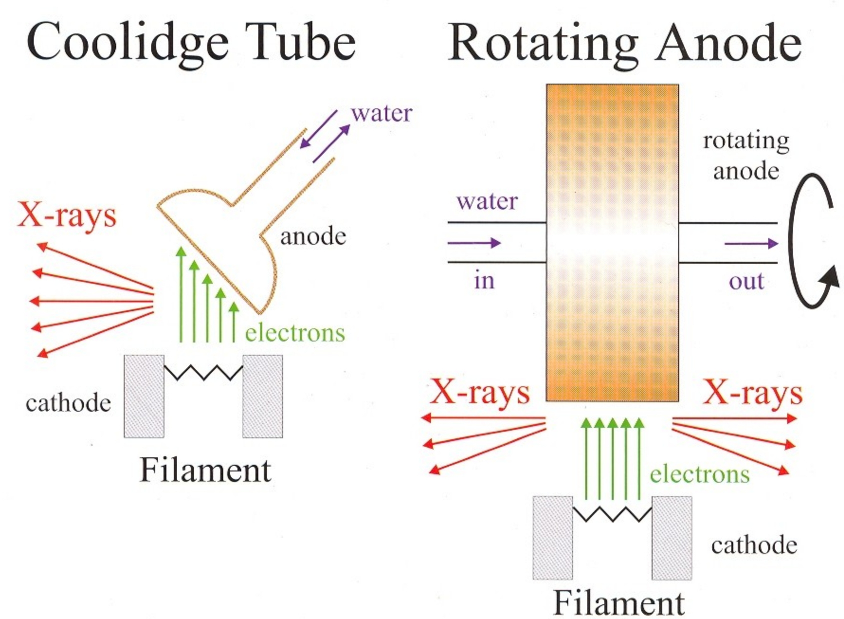
Sources of X-Rays

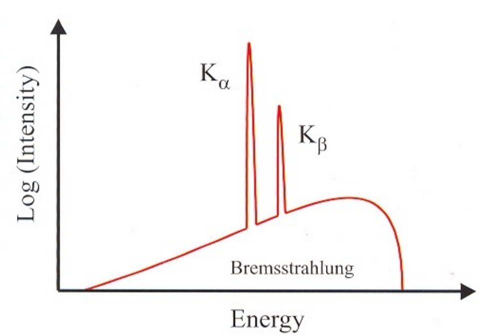
1895 discovered by W.C. Röntgen

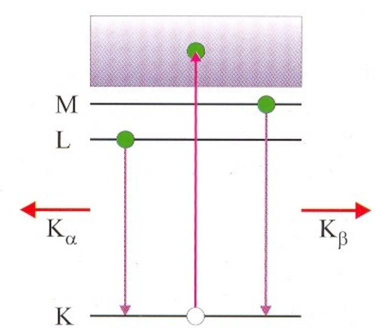
1912 First diffraction experiment (v. Laue)

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

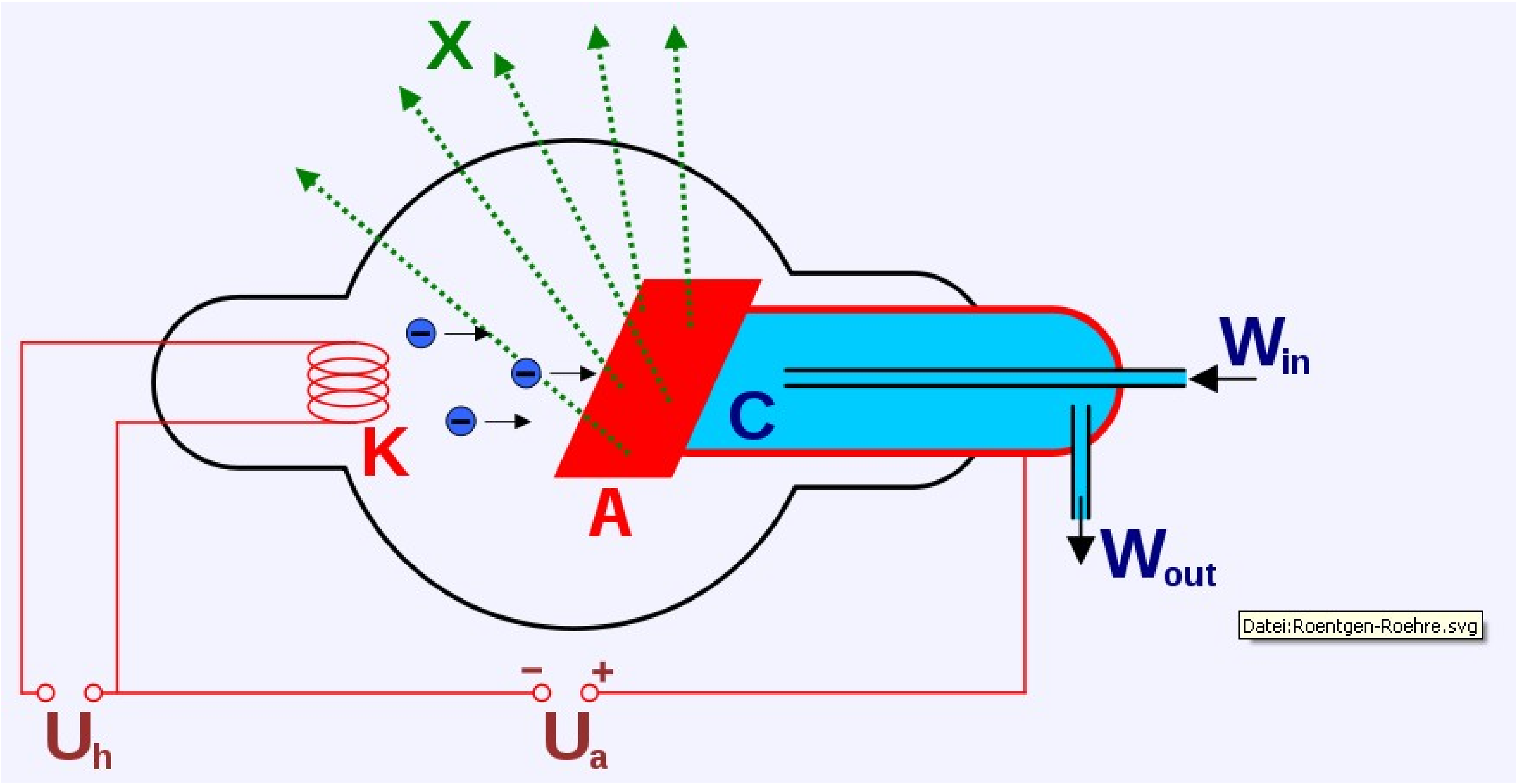
1946 Radiation from electrons in a synchrotron, GE, Physical Review, 71,829(1947)



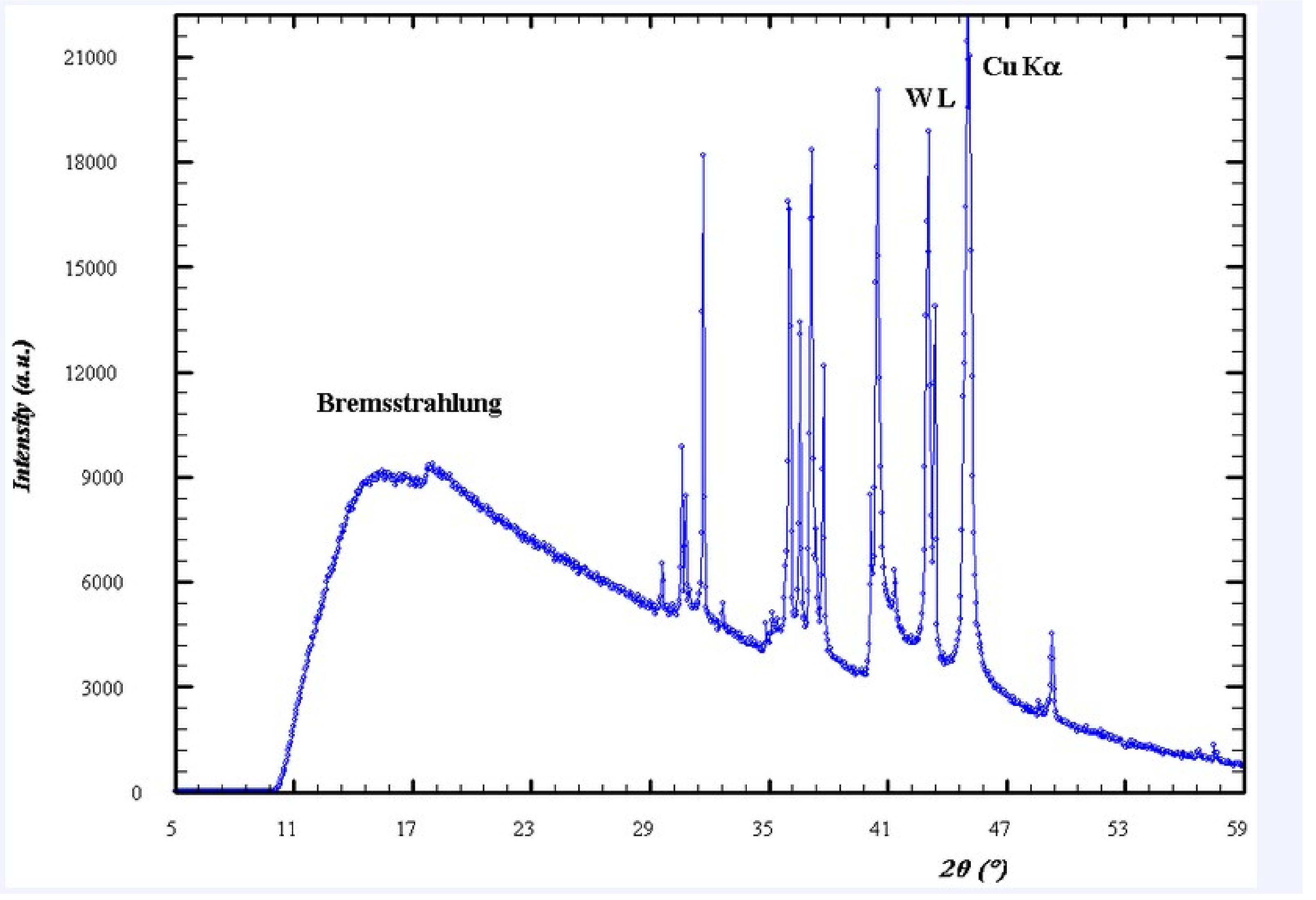




X-ray Tube

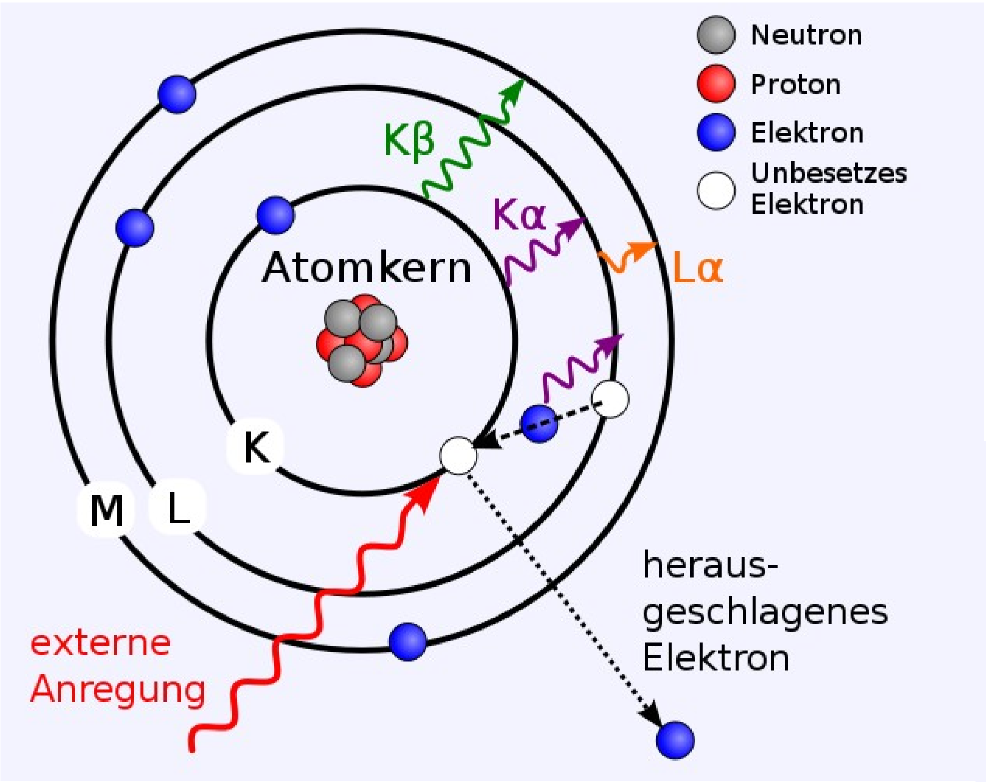


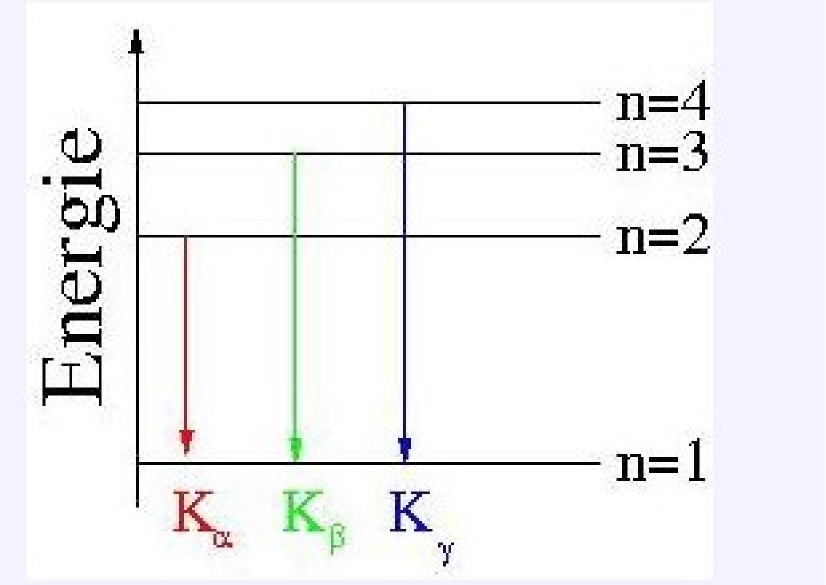
X-ray Tube



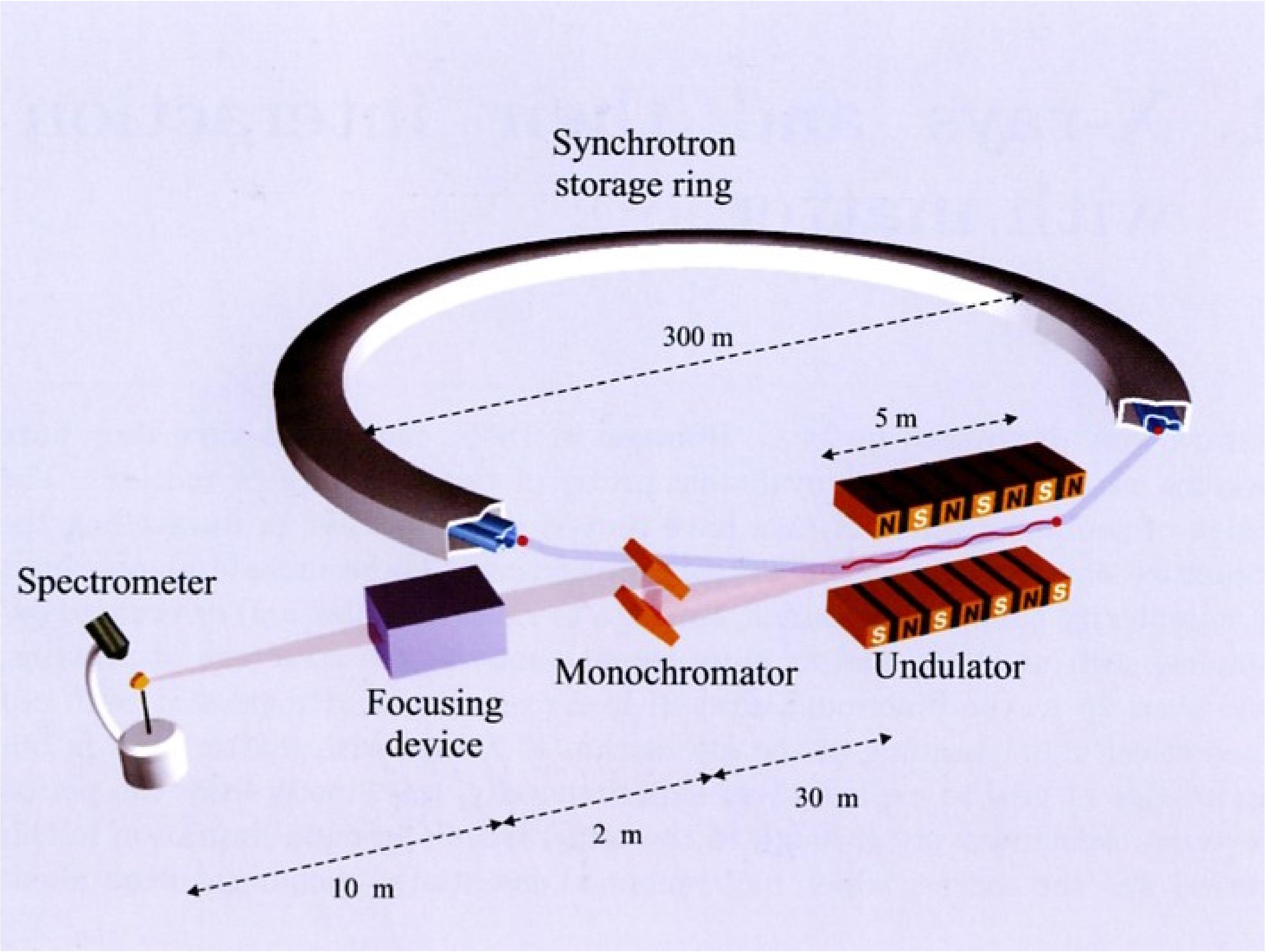
Cu Kα
W L
Bremsstrahlung
Intensity (a.u.)
21000
18000
15000
12000
9000
6000
3000
0
5
11
17
23
29
35
41
47
53
59
2θ (°)

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

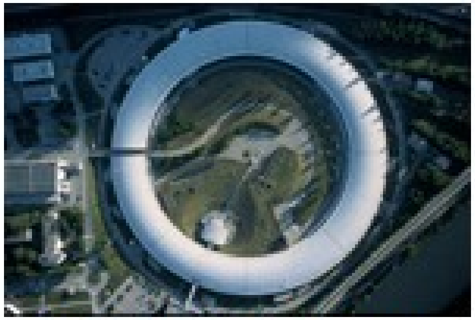
Synchrotron Radiation Storage Ring



Photos machines

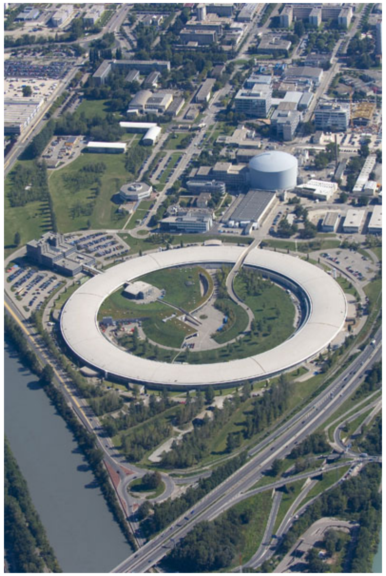
The three largest and most powerful synchrotrons in the world

APS, USA

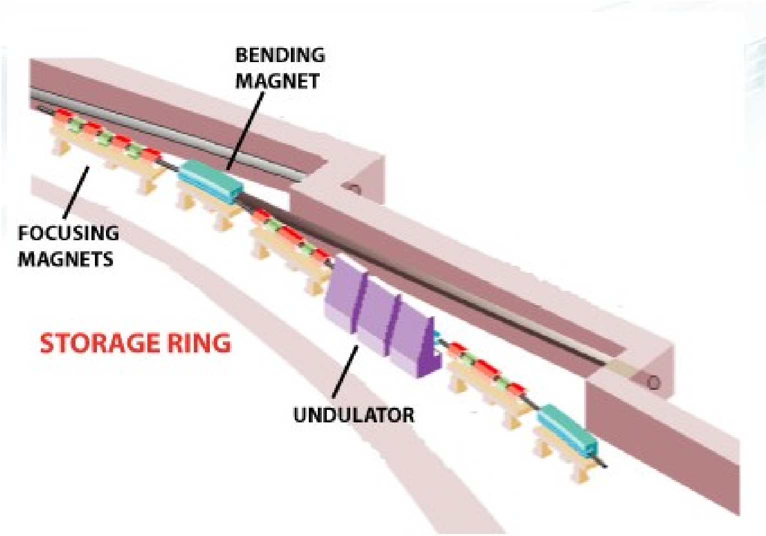


ESRF, Europe-France

Spring-8, Japan



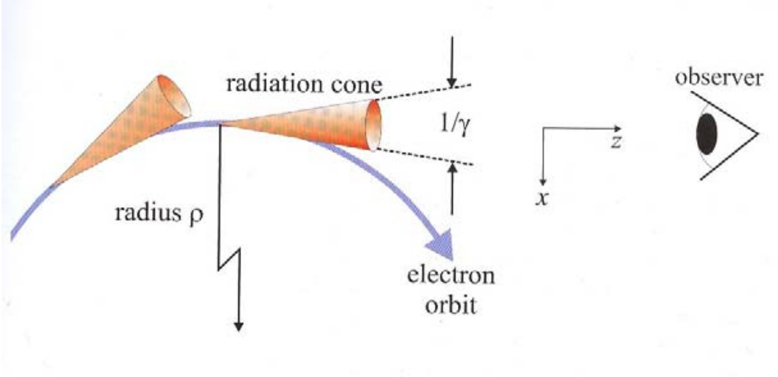
Synchrotron Radiation Primer



Energy E_e of an electron at speed v:

$$E_e = mc^2/\mathrm{sqrt}\{(1-(v/c)^2\} = \gamma\, mc^2$$

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



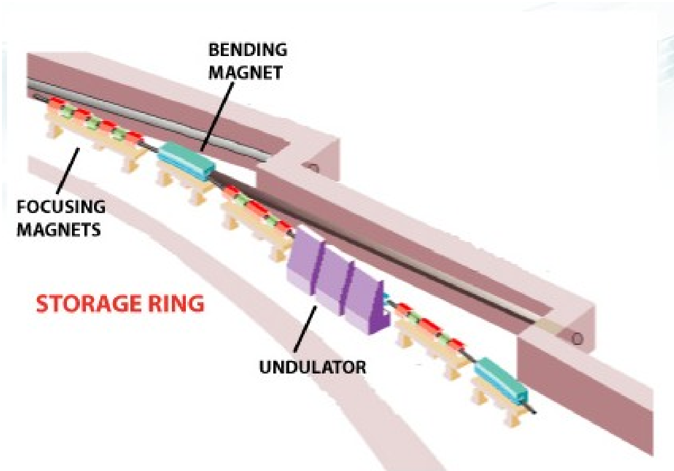
Centrifugal=Lorentz force yields for radius:

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

$E_e \approx 6$ GeV, B=0.8 T

Opening angle is of order $1/\gamma \approx 0.1$ mrad

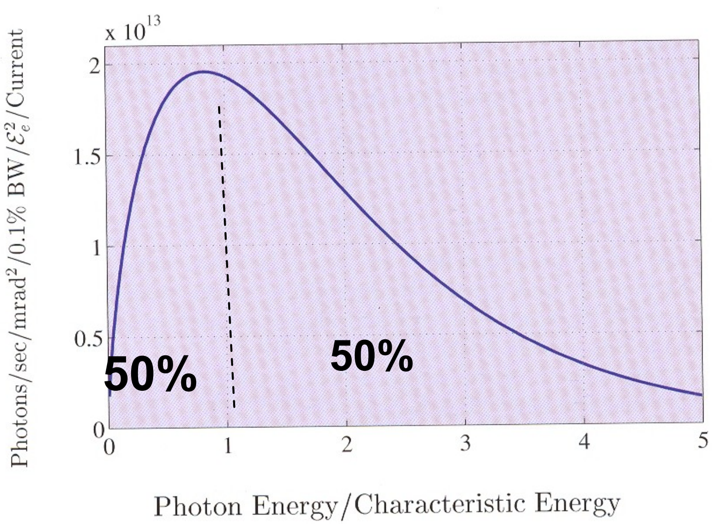
Bending magnets



<u>Characteristic energy $\hbar\omega_c$ for bend or wiggler:</u>

$\hbar\omega_c$ [keV] = 0.665 E_e^2[GeV] B(T) ≈20 keV

Flux ~ E^2



<u>Energy loss by synchrotron radiation per turn:</u>

ΔE [keV] = 88.5 E^4[GeV]/ρ[m]

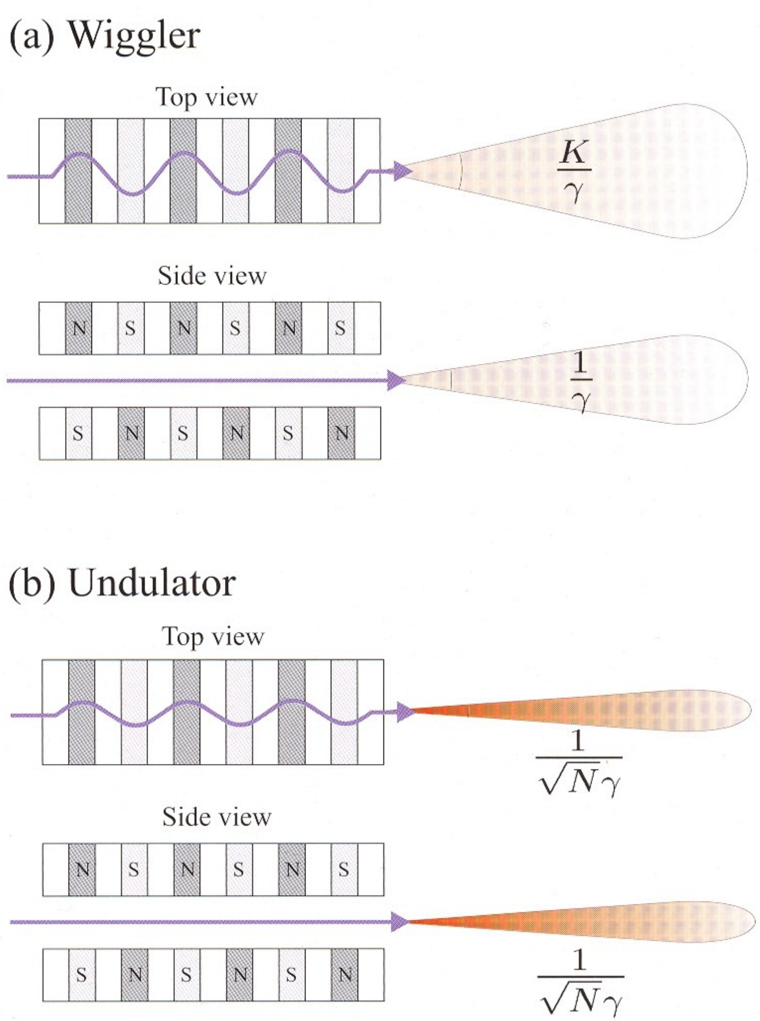
For 1 GeV and ρ=3.33 m: ΔE =26.6 keV/turn

For I=500 mA ≡ 0.5 Cb/s =0.5x6.25x10^{18} e^-/s

➔P= 0.5x6.25x10^{18} e^-/sx26.6 keV

=8.3125x10^{22}x1.6x10^{-19} = 13.3 KJ/s =13.3 KW

Insertion Devices (wigglers and undulators)



Wiggler:

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

Flux ~ $E^2 \times N$

N: number poles

Undulator:

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

with λ_u undulator period

undulator fundamental:

$\lambda_0 = \lambda_u/2\gamma^2 \{(1 + k^2/2 + (\gamma\theta)\}$

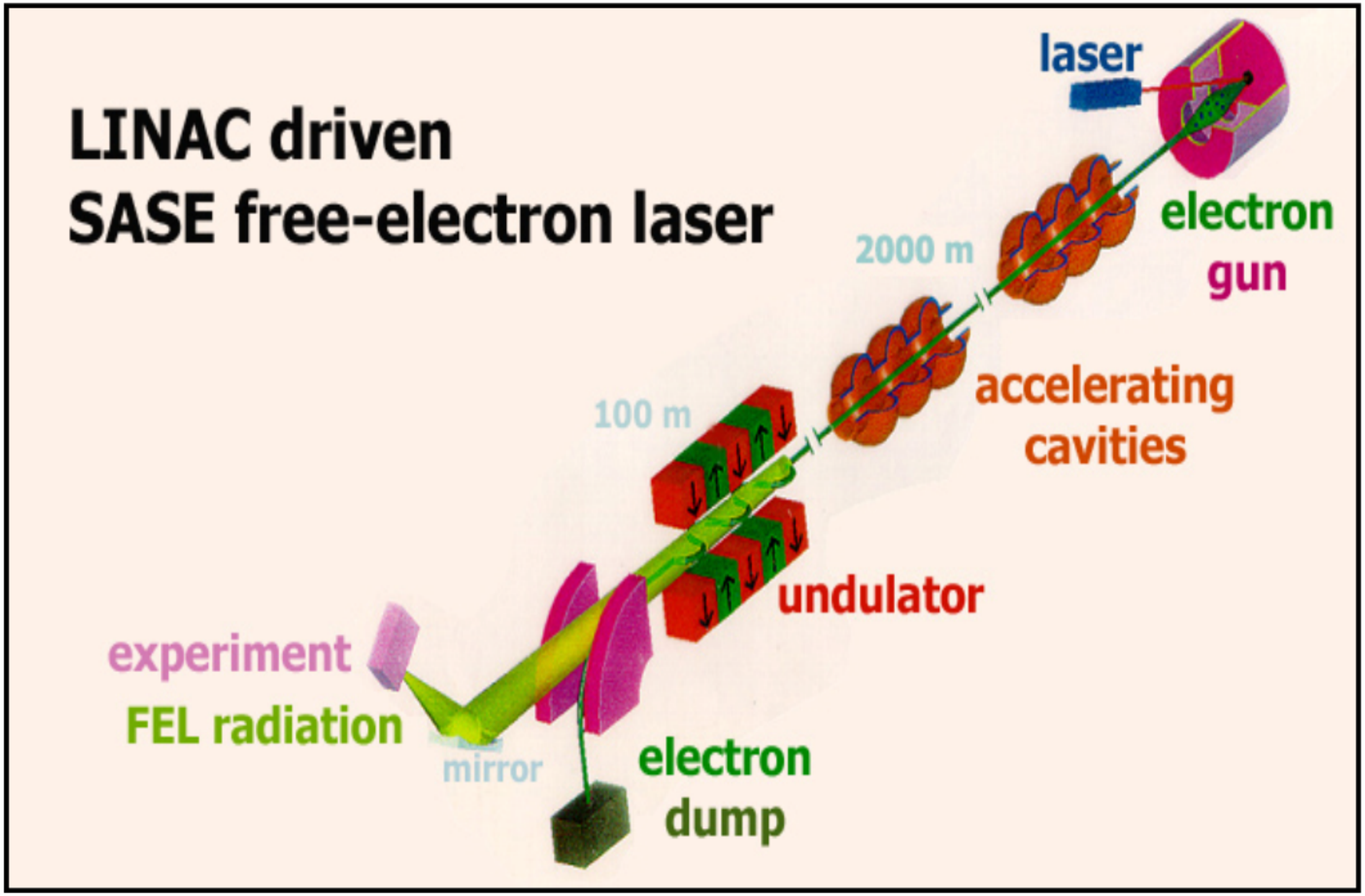
on axis

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

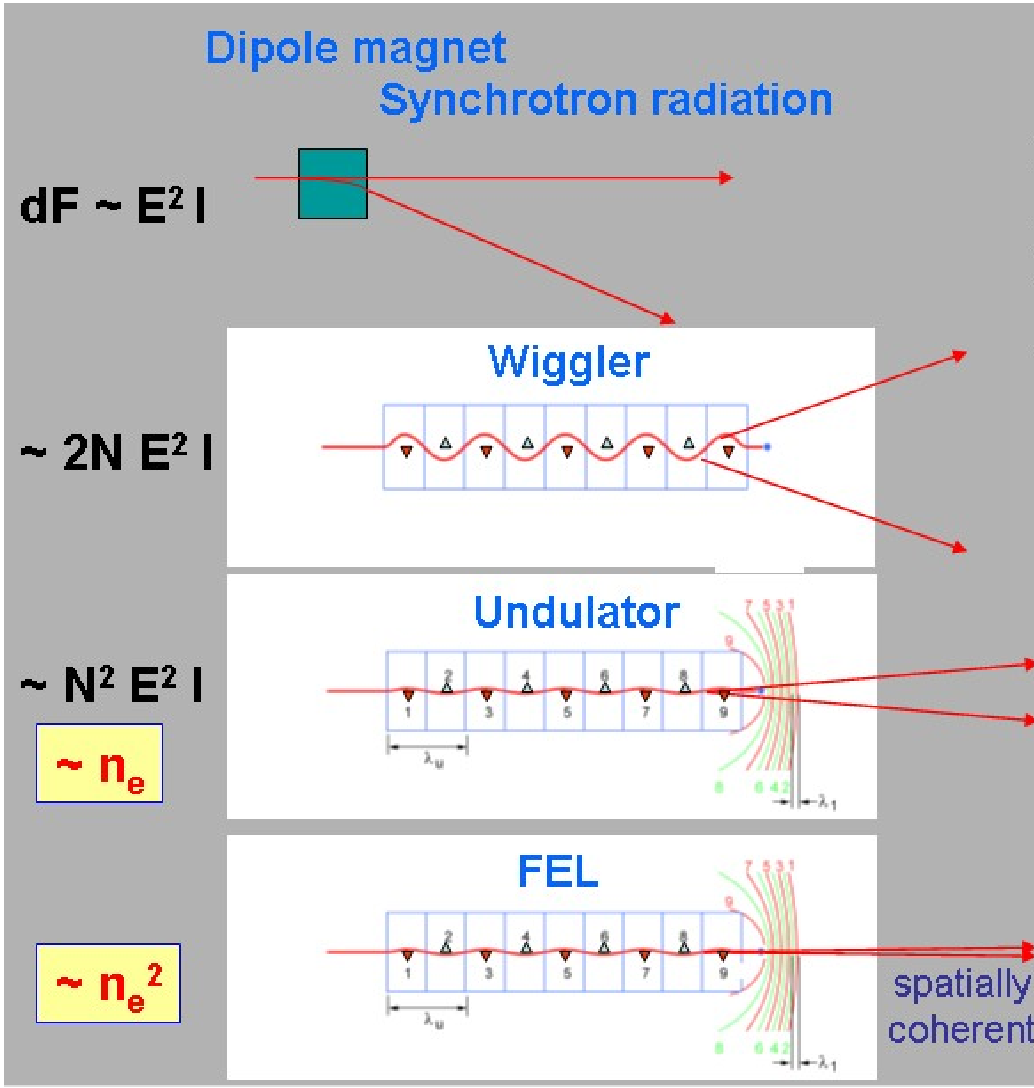
bandwidth:

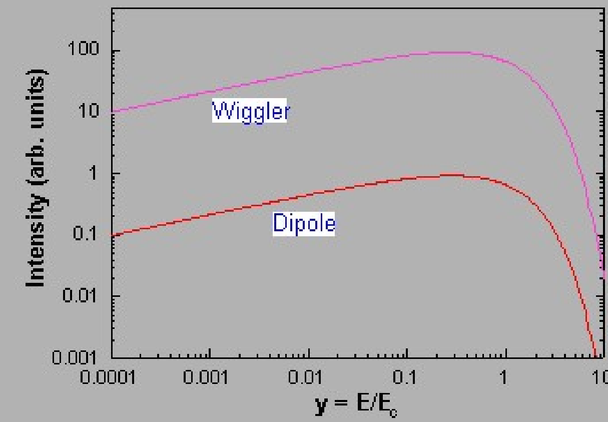
$\Delta\lambda/\lambda \sim 1/nN$

Free Electron Lasers (FELs)



Synchrotron and FEL sources

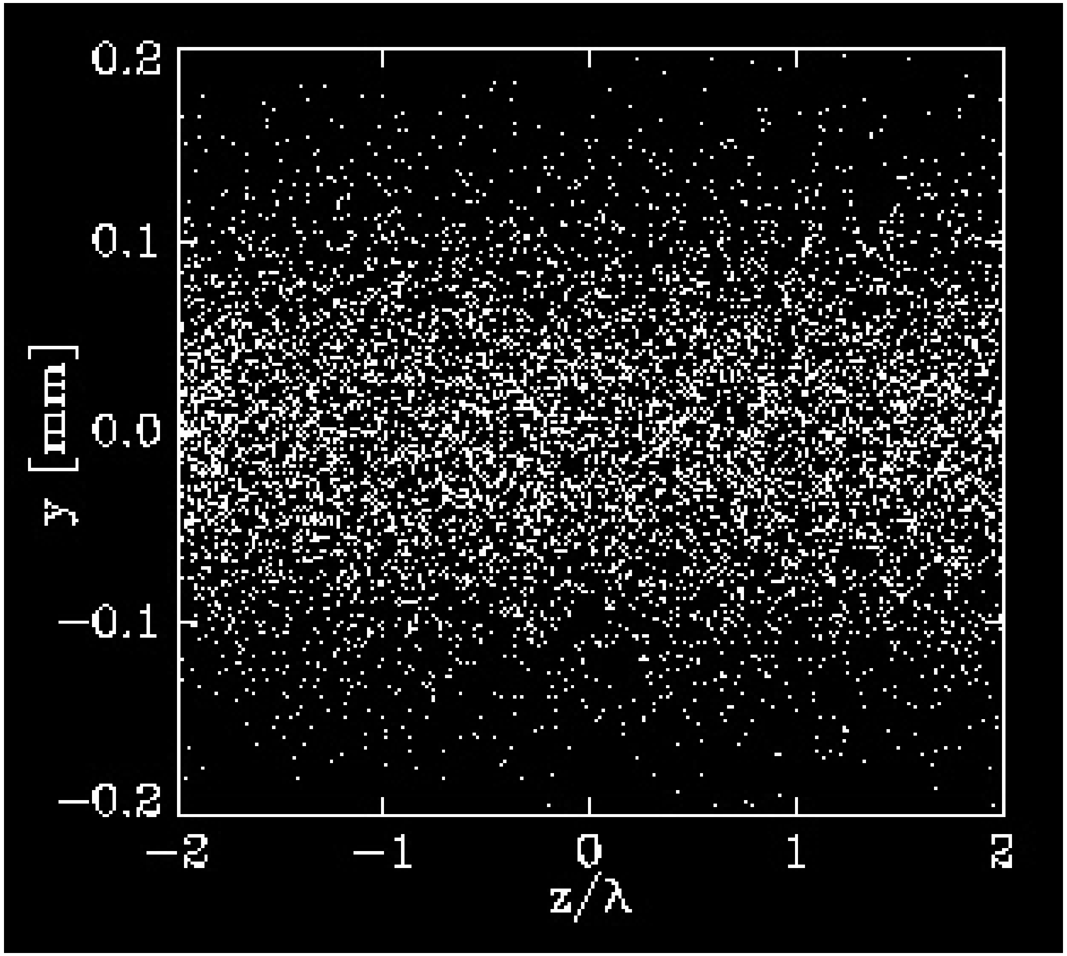




The radiation emitted by a single electron in subsequent oscillations in an undulator is in phase. Radiation from different electrons is NOT (positional disorder in bunch).

"Phasing" is achieved via positional order in the bunch (micro-bunching) with a period equal to the x-ray wavelength.

Electron bunching



GENESIS – simulation for TTF parameters

Courtesy Sven Reiche (UCLA)

VUV and X-Ray FELs