

- **Methoden moderner Röntgenphysik I+II:
Struktur und Dynamik kondensierter Materie**

Vorlesung zum Haupt/Masterstudiengang Physik

WS 2010/11 und SS 2011

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Location: SemRm 4, Physik, Jungiusstrasse

Tuesdays 12.45 – 14.15

Thursdays 10.15 – 11.45

Methoden moderner Röntgenphysik I: Struktur und Dynamik kondensierter Materie

Hard X-Rays – Lecture 2

Gerhard Grübel (GG), Stephan Roth (SR), Alke Meents (AM), Oliver Seeck (OS)

19.10. Introduction (GG)

26.10. X-ray Scattering Primer, Sources of X-rays (GG)

2.11. Refraction and Reflexion, Kinematical Scattering (I) (GG)

9.11. Kinematical Scattering Theory (II) (GG)

18.11. Applications of KST and “perfect” crystals (SR)

25.11. Small Angle and Anomalous Scattering (SR)

2.12. - 6. 1. Modern Crystallography (AM)

13. 1. - 3. 2. Surfaces and Interfaces (OS)

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” crystal 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

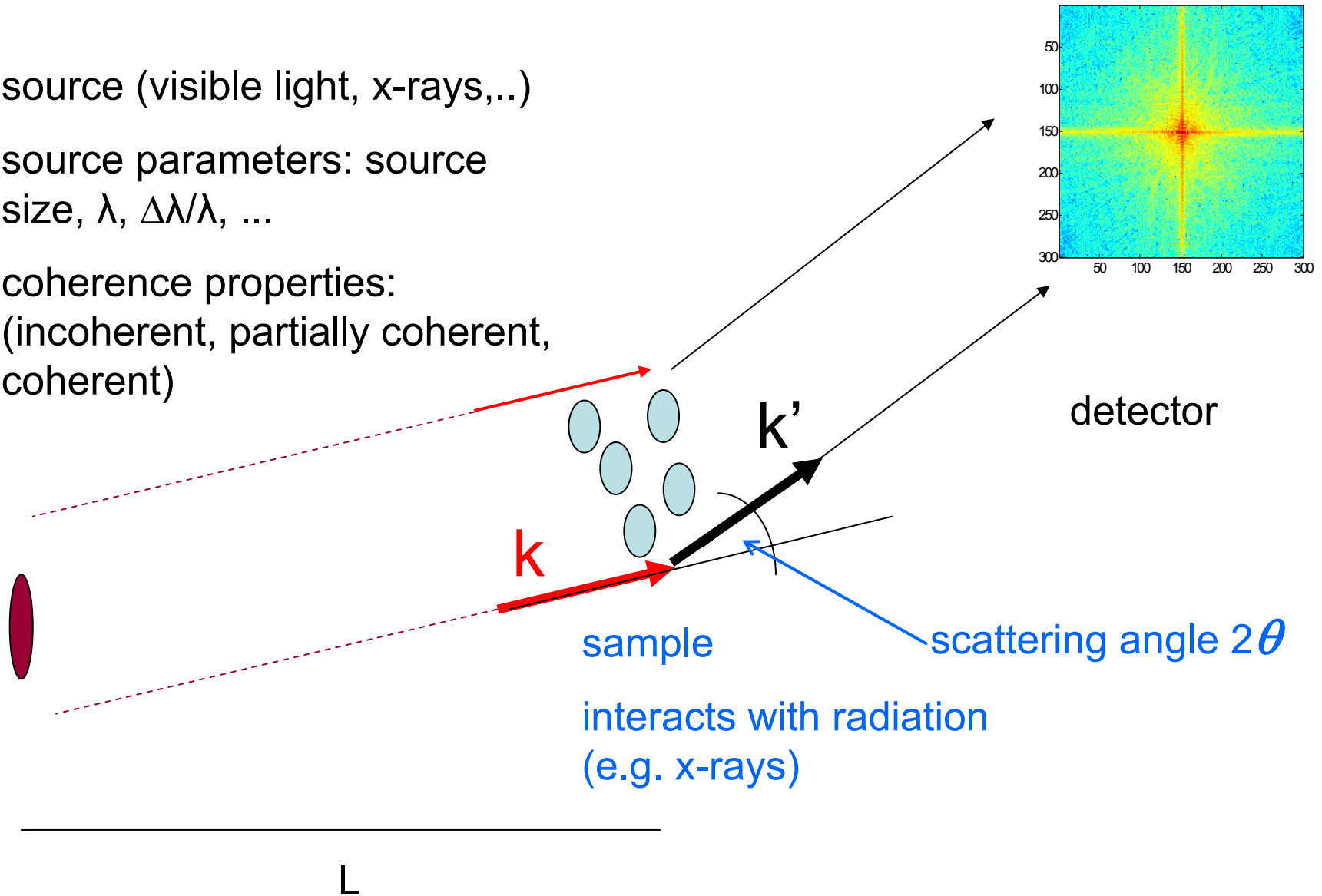
Coherence Properties

Set-Up for Scattering Experiments

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

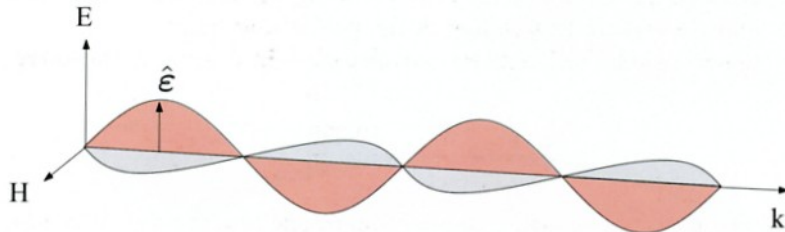
source parameters: source size, λ , $\Delta\lambda/\lambda$, ...

coherence properties: (incoherent, partially coherent, coherent)



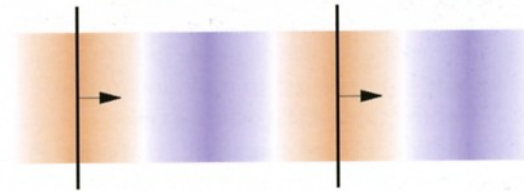
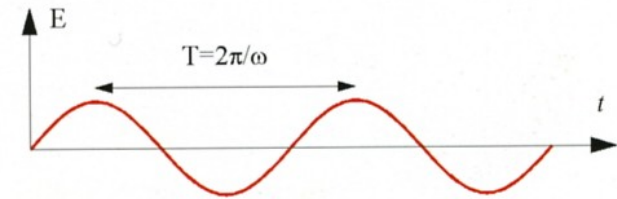
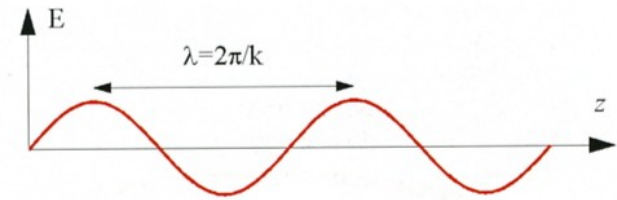
▪ X-rays: Electromagnetic waves and photons

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:

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



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

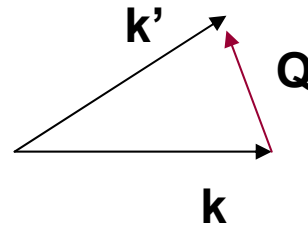
consider a monochromatic plane (electromagnetic) wave with wavevector k :

$$\mathbf{E}(\mathbf{r},t) = \epsilon E_0 \exp\{i(\mathbf{k}\mathbf{r}-\omega t)\}$$

elastic scattering:

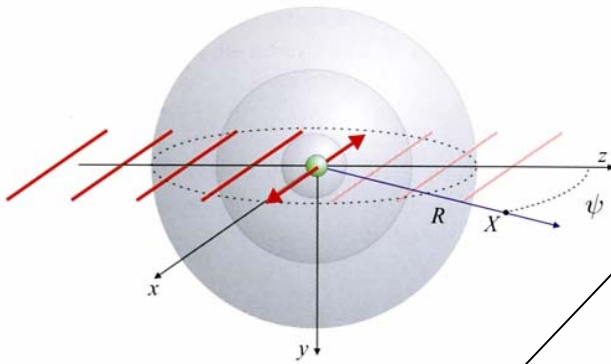
$$\hbar \mathbf{k}' = \hbar \mathbf{k} + \hbar \mathbf{Q}$$

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



Scattering by a single electron:

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



phase shift of π btw. incident and radiated field

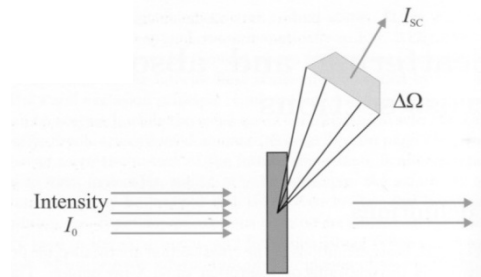
$$-\left(\frac{e^2}{4\pi\epsilon_0 mc^2}\right) \exp(ikR)/R \cos\psi$$

spherical wave

thomson scattering length r_0

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

■ scattered intensity:



$$I_s/I_0 = \frac{|E_{\text{rad}}|^2 R^2 \Delta\Omega}{|E_{\text{in}}|^2 A_0}$$

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

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

A_0 : incident beam size

$$I_s/I_0 = (d\sigma/d\Omega) (\Delta\Omega/A_0)$$

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)

$$(d\sigma/d\Omega) = r_0^2 P \quad P = \begin{cases} 1 & \text{vertical} \\ \cos^2\psi & \text{horizontal} \\ \frac{1}{2}(1+\cos^2\psi) & \text{unpolarized} \end{cases}$$

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

▪
scattering by a single atom:

scattering amplitude $A(Q) = -r_0 f(Q)$

≡ scattering amplitude by
an ensemble of electrons

$$-r_0 f^0(Q) = -r_0 \sum_{r_j} \overbrace{\exp(iQ \cdot r_j)}^{\text{phase factor}}$$

↑
(atomic) formfactor

↑
position of scatterers

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

form factor of an atom:

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

↑
dispersion corrections:

↑
level structure

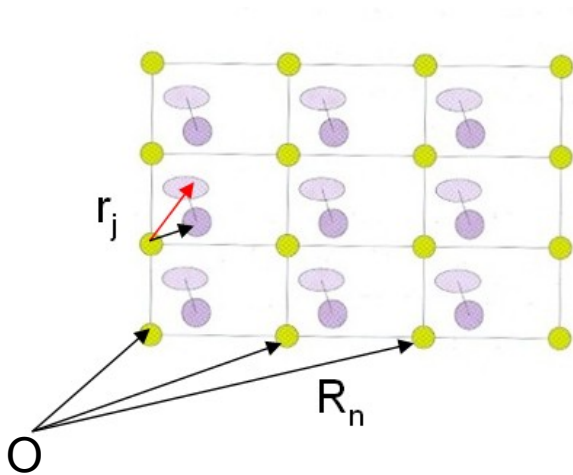
↑
absorption effects

scattering intensity:

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

■

scattering by a crystal:



$$r_j' = R_n + r_j$$

lattice vector + atomic position in lattice

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

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

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

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

unit cell structure factor:

$$\sum_{r_j} f_j(Q) \exp(iQr_j)$$

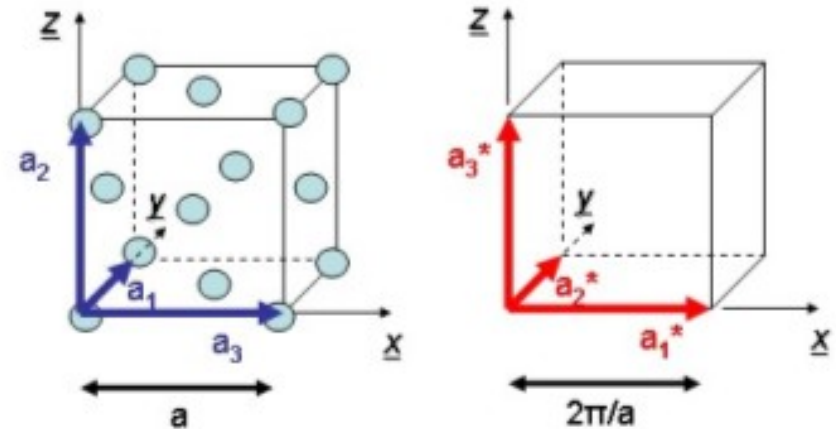
e.g. fcc lattice:

$$r_1 = 0$$

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

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

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



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

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

$$\text{with } Q = G = h a_1^* + k a_2^* + l a_3^*$$

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

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

Compton Scattering

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

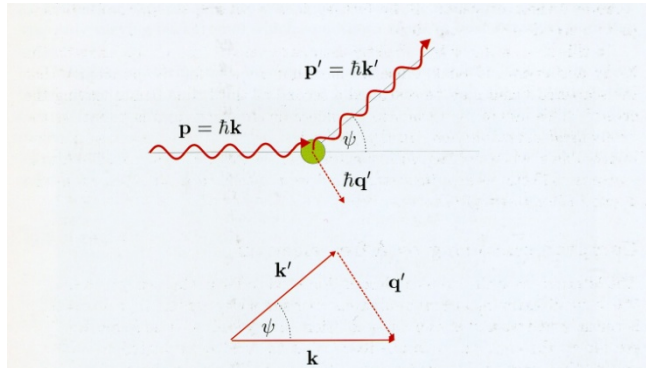
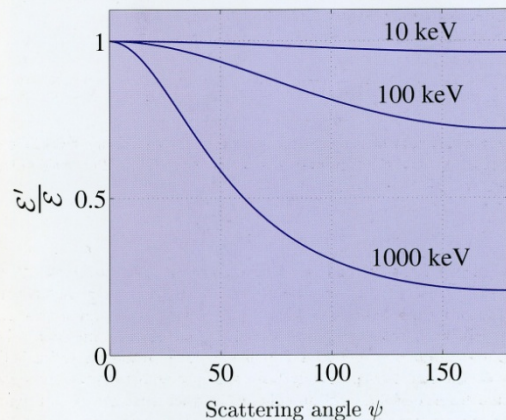


Figure 1.7: Compton scattering. A photon with energy $\mathcal{E} = \hbar ck$ and momentum $\hbar k$ scatters from an electron at rest with energy mc^2 . The electron recoils with a momentum $\hbar q' = \hbar(k - k')$ as indicated in the scattering triangle in the bottom half of the figure.



energy conservation:

$$m_0 c^2 + \hbar ck = \text{sqrt}\{(m_0 c^2)^2 + (\hbar cq')^2\} + \hbar ck'$$

with $\lambda_c = \hbar c / m_0 c^2$:compton wavelength

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

momentum conservation: $q' = k - k'$

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

$$(1) = (2)$$

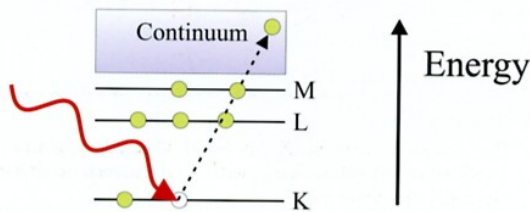
$$k/k' = 1 + \lambda_c k(1 - \cos \psi) = E/E' = \lambda'/\lambda$$

➔ origin of background

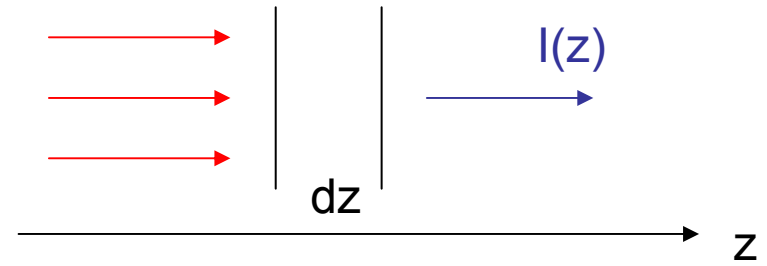
➔ determine electronic momentum distribution of materials

Photoelectric absorption

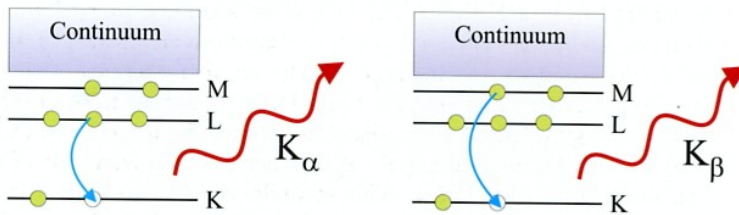
(a) Photoelectric absorption



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



(b) Fluorescent X-ray emission



$$I(z) = I_0 \exp(-\mu z)$$

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

ρ_a atomic number density

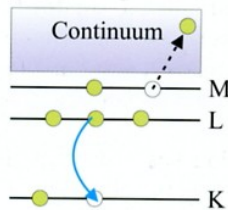
$\sigma_a = \sigma_a(E)$ absorption cross section

ρ_m mass density

N_A Avogadro's number

A atomic mass number

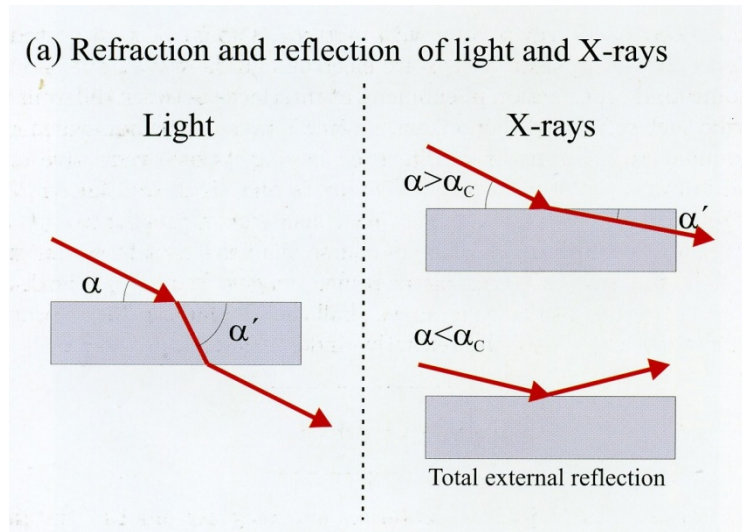
(c) Auger electron emission



Refraction

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

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



Snell's law:

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

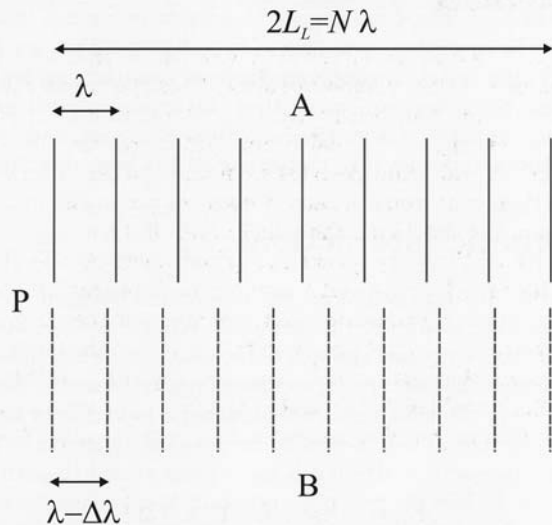
note: total external reflexion
for x-rays ($\alpha' = 0$)

$$n < 1$$

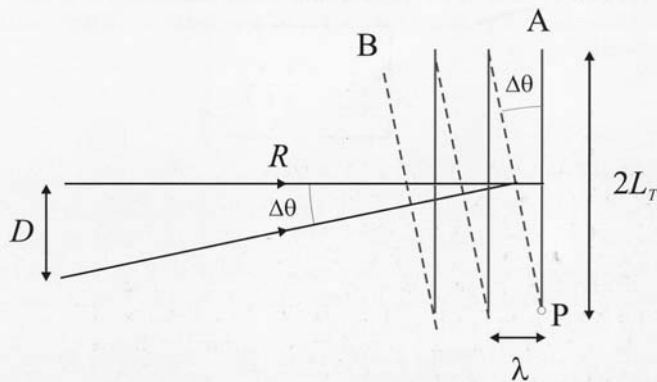
$$\alpha_c = \text{sqrt}(2\delta)$$

Coherence

(a) Longitudinal coherence length, L_L



(b) Transverse coherence length, L_T



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 :

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

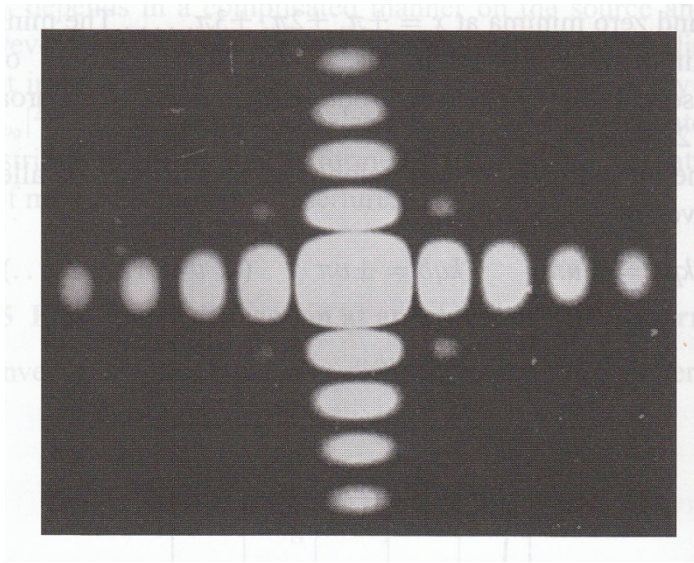
Transverse coherence:

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

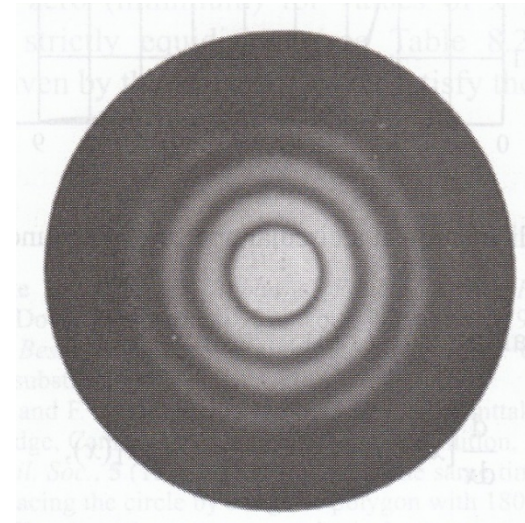
$$2\xi_t \Delta\theta = \lambda$$

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

▪ Fraunhofer Diffraction

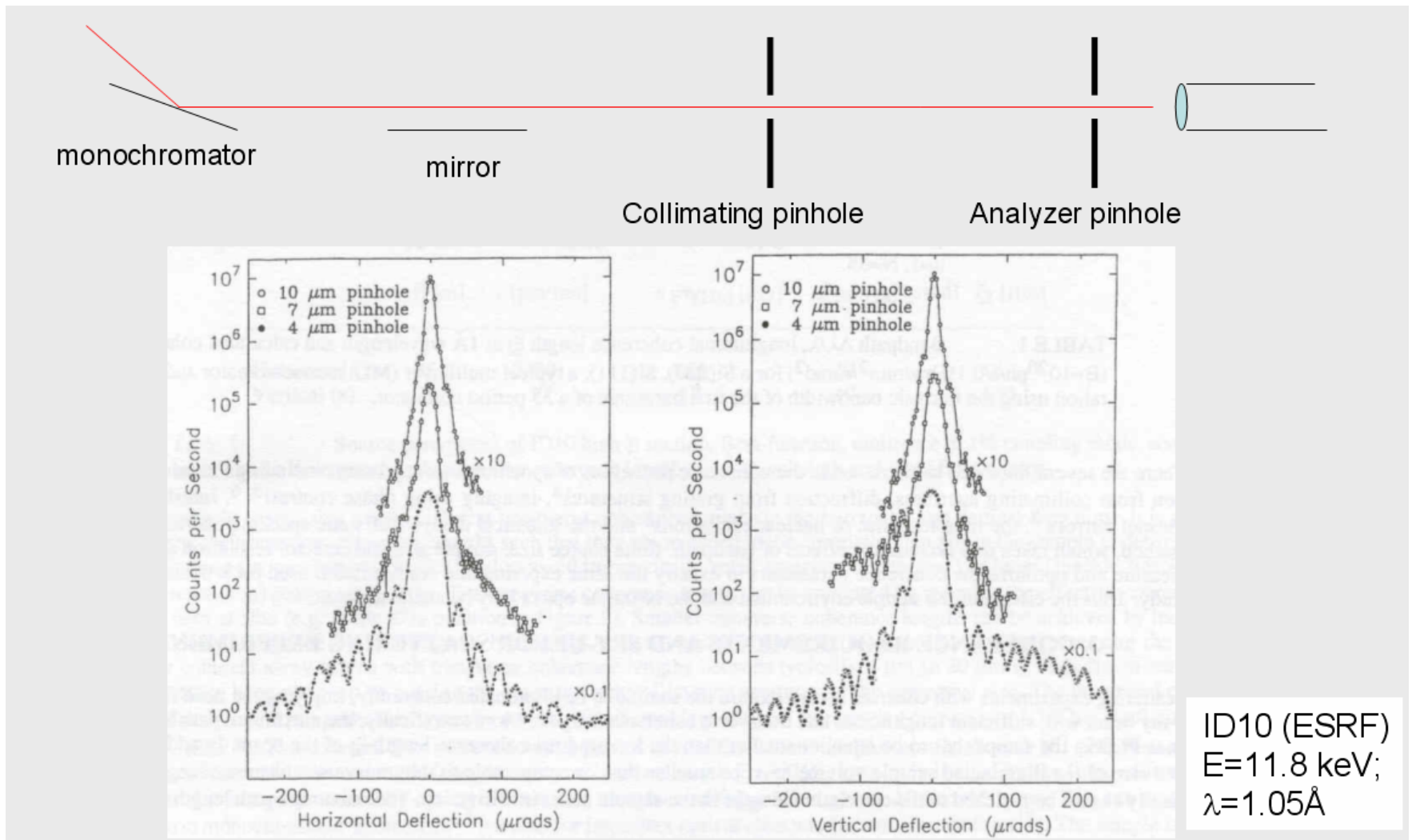


Fraunhofer diffraction of a rectangular aperture $8 \times 7 \text{ mm}^2$, taken with mercury light $\lambda=579\text{nm}$ (from Born&Wolf, chap. 8)

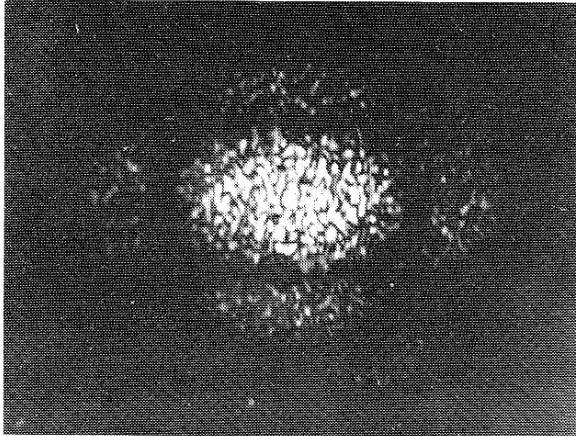


Fraunhofer diffraction of a circular aperture, taken with mercury light $\lambda=579\text{nm}$ (from Born&Wolf, chap. 8)

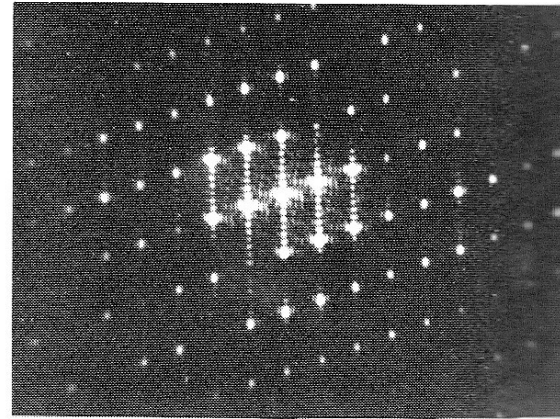
Fraunhofer Diffraction ($\lambda=0.1\text{nm}$)



- Speckle pattern



random arrangement of apertures: speckle



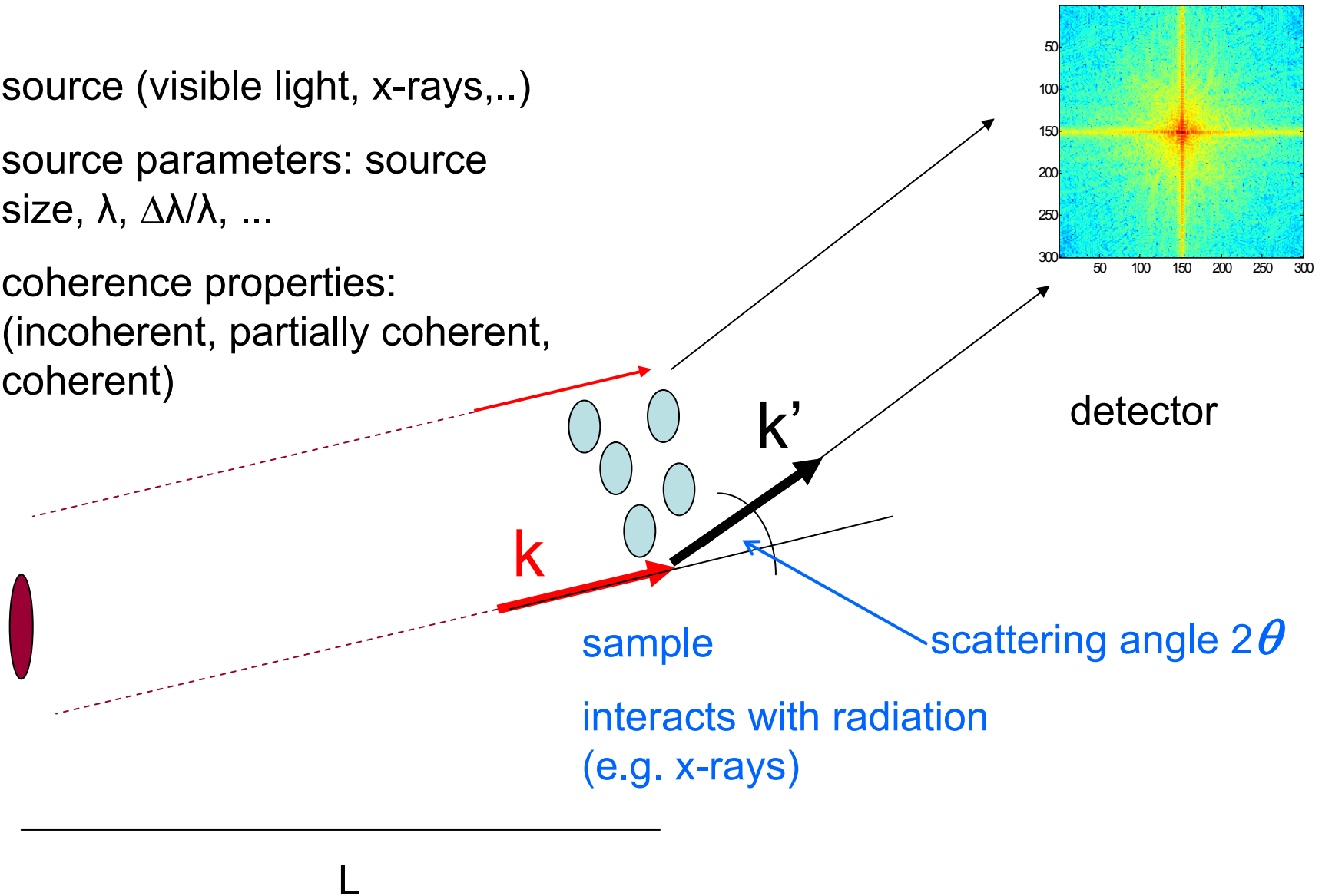
regular arrangement of apertures

Experimental Set-Up for Scattering Experiments

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

source parameters: source size, λ , $\Delta\lambda/\lambda$, ...

coherence properties:
(incoherent, partially coherent, coherent)

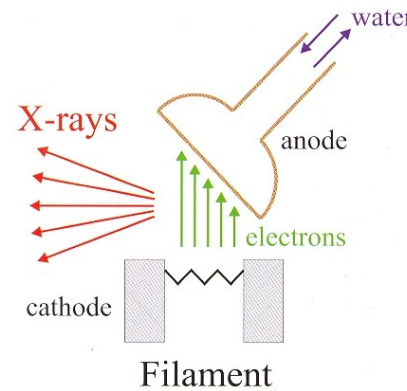


▪ Sources of X-Rays

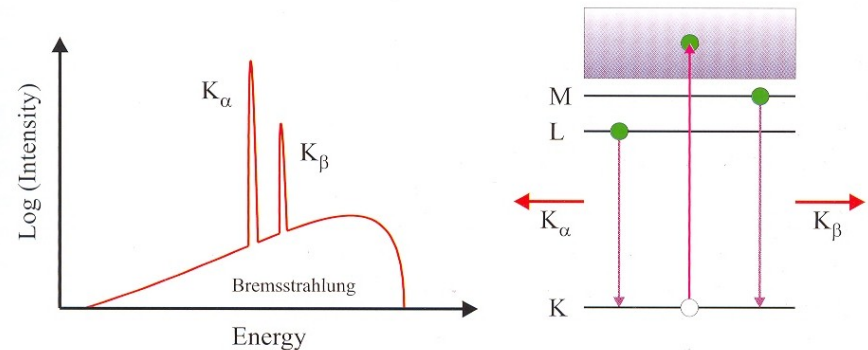
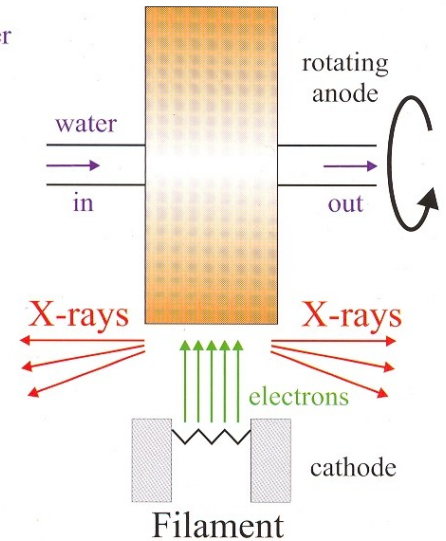
- 1895 discovered by W.C. Röntgen
- 1912 First diffraction experiment (v. Laue)
- 1912 Coolidge tube (W.D. Coolidge, GE)
- 1946 Radiation from electrons in a synchrotron, GE, Physical Review, 71,829(1947)



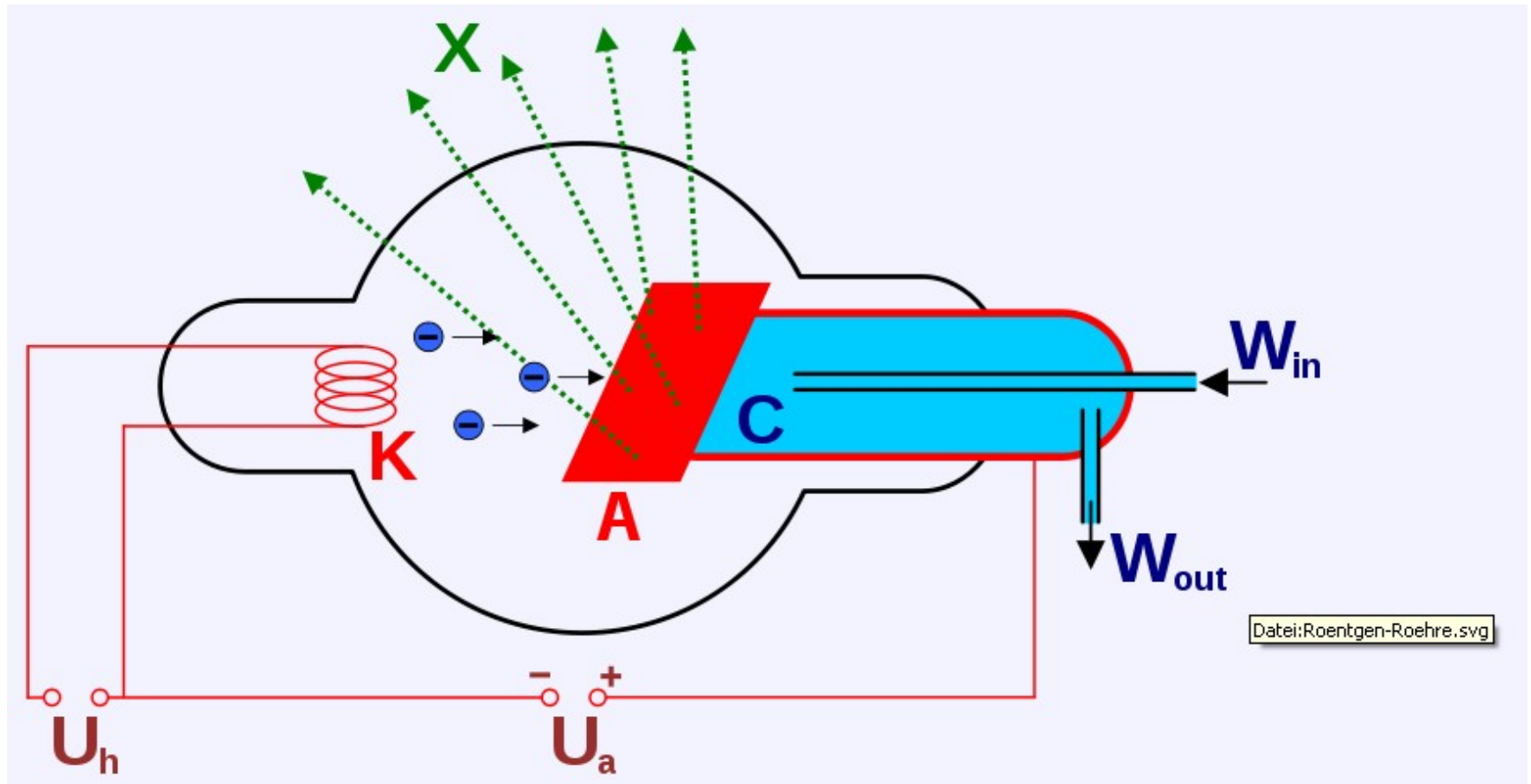
Coolidge Tube



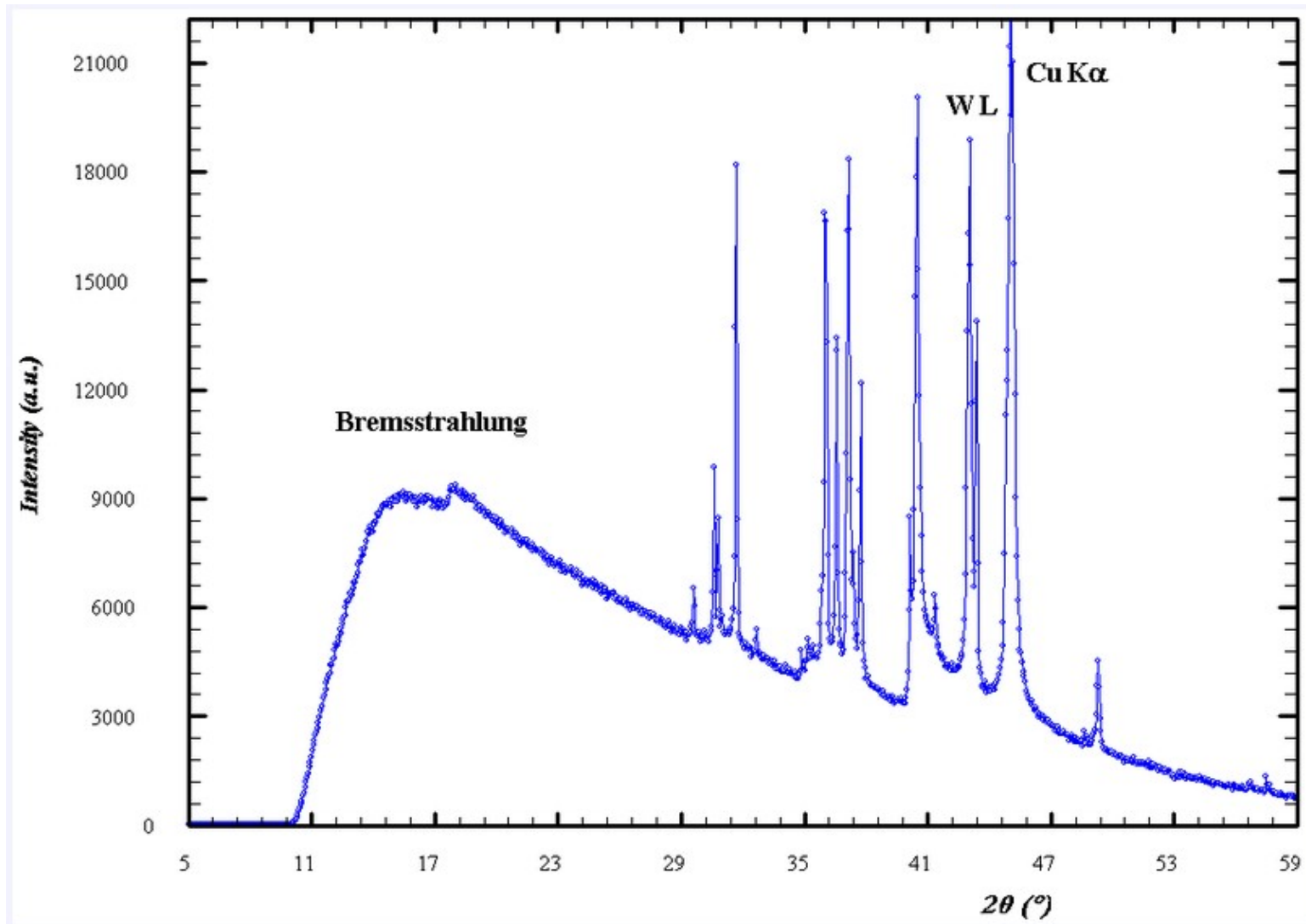
Rotating Anode



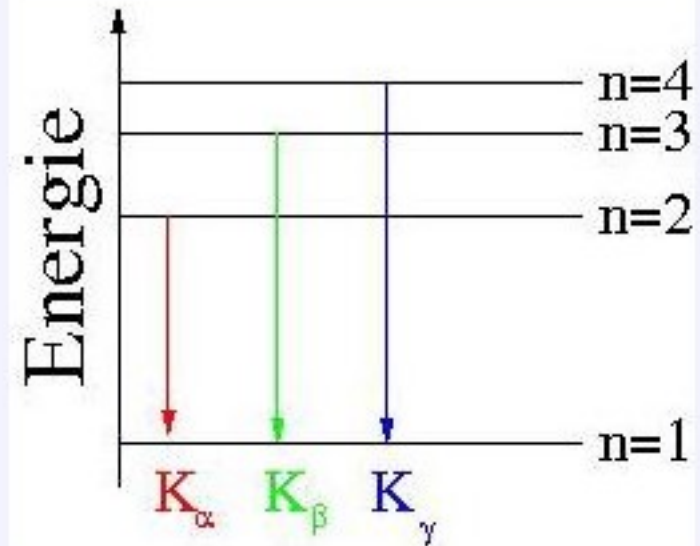
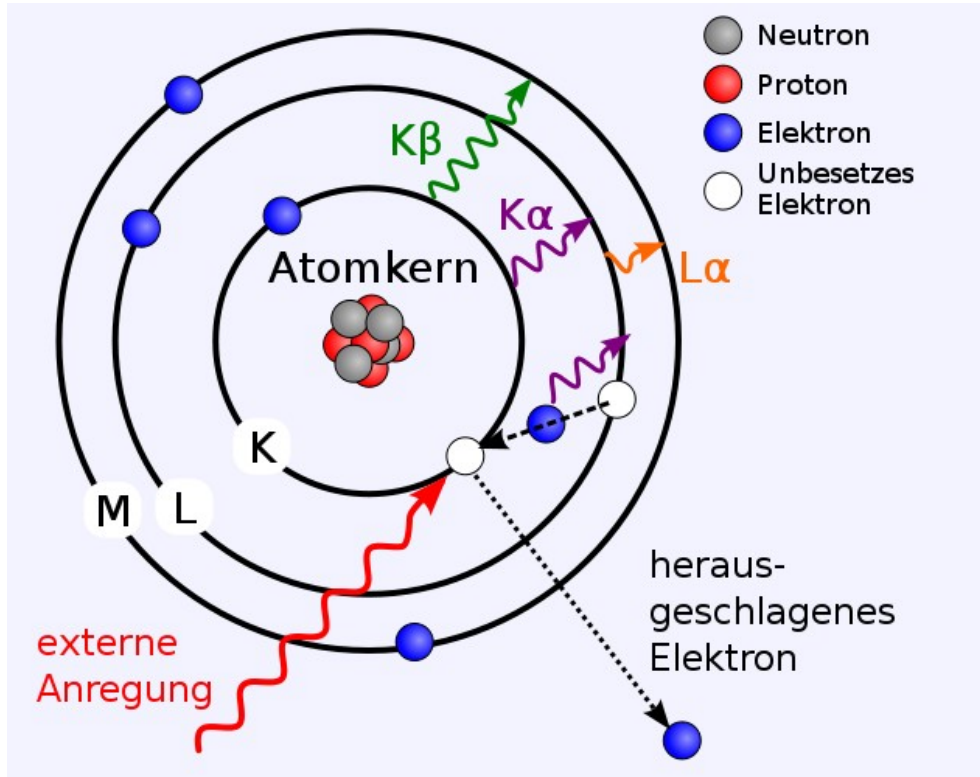
- X-ray Tube



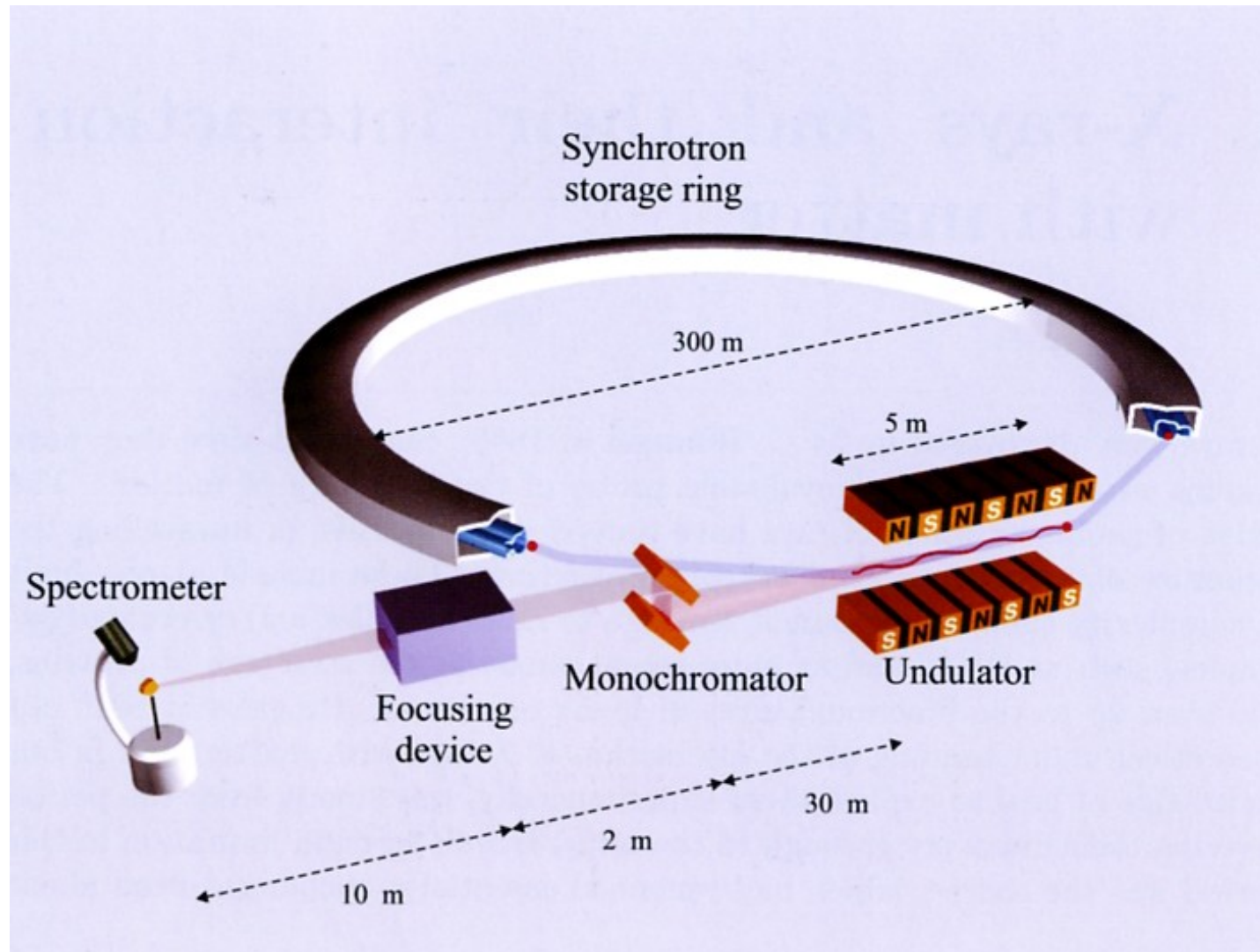
▪ X-ray Tube



▪ X-ray Tube



▪ Synchrotron Radiation Storage Ring



Photos machines

The three largest and most powerful synchrotrons in the world



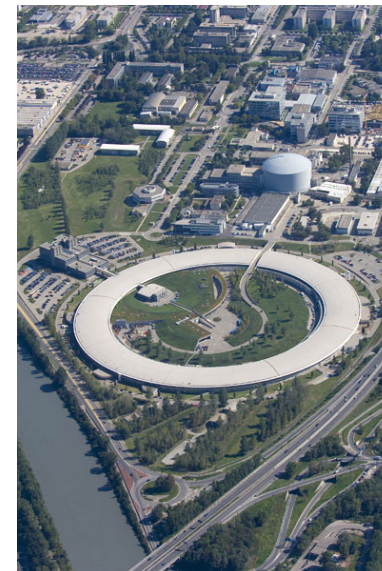
APS, USA



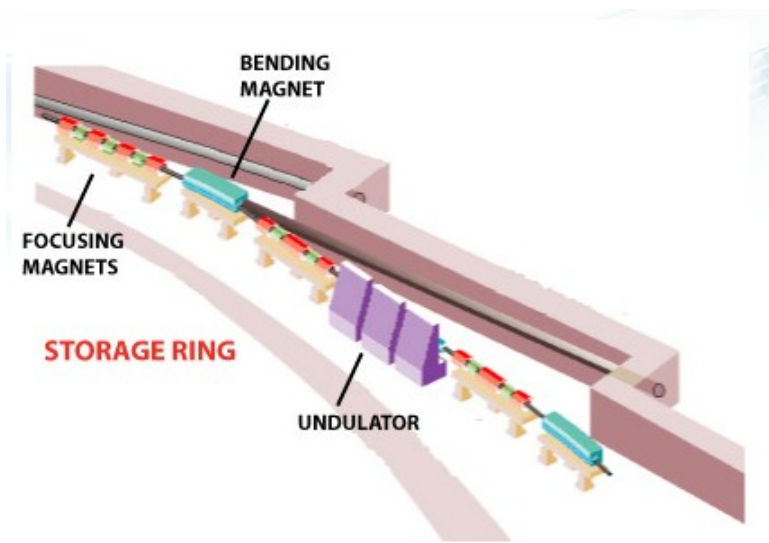
ESRF, Europe-France



Spring-8, Japan



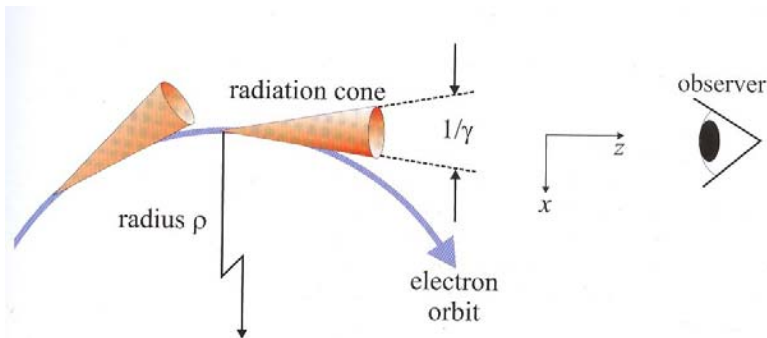
Synchrotron Radiation Primer



Energy E_e of an electron at speed v :

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

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



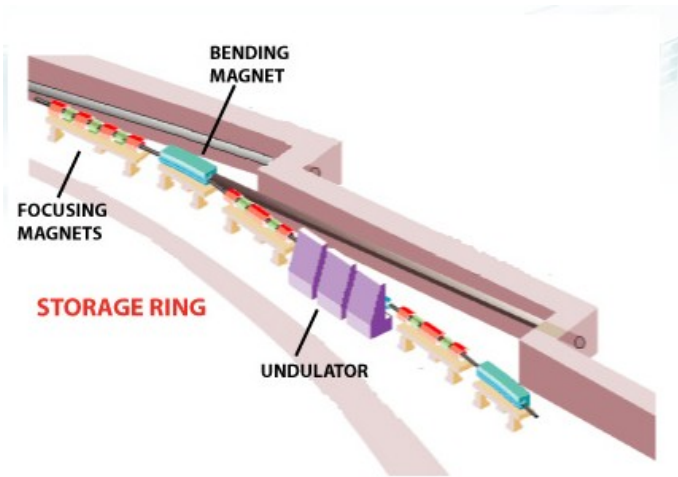
Centrifugal=Lorentz force yields for radius:

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

$$E_e \approx 6 \text{ GeV}, B = 0.8 \text{ T}$$

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

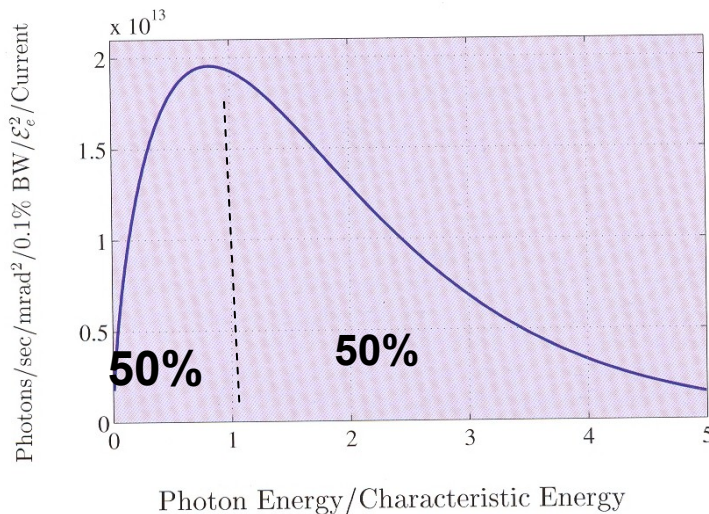
$$\Delta E [\text{keV}] = 88.5 E^4 [\text{GeV}] / \rho [\text{m}]$$

For 1 GeV and $\rho=3.33 \text{ m}$: $\Delta E = 26.6 \text{ keV/turn}$

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

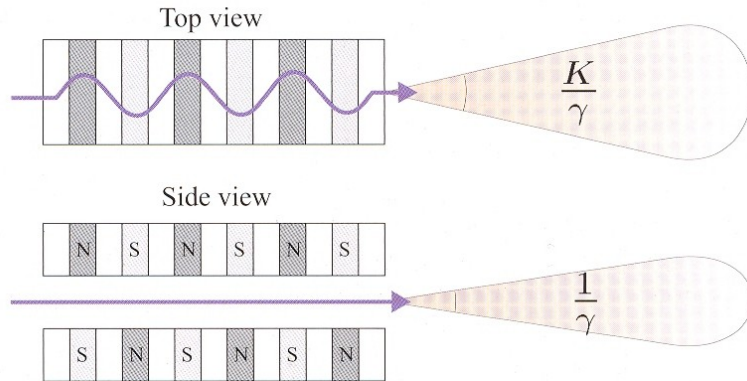
$$\rightarrow P = 0.5 \times 6.25 \times 10^{18} \text{ e}^-/\text{s} \times 26.6 \text{ keV}$$

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

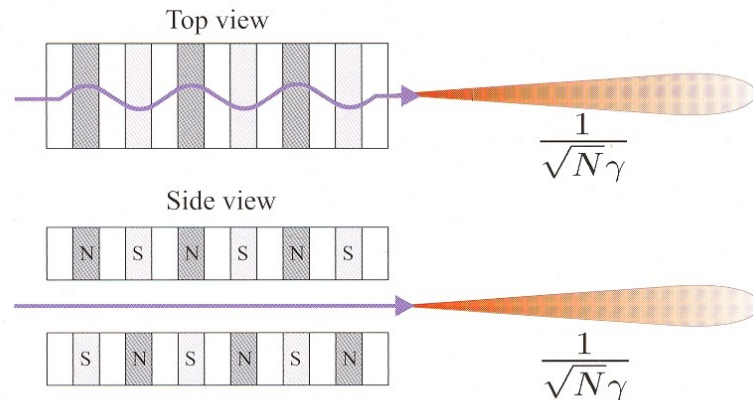


Insertion Devices (wigglers and undulators)

(a) Wiggler



(b) Undulator



Wiggler:

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

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

N: number poles

Undulator:

$$k = eB / mc \quad k_u = 0.934 \lambda_u [\text{cm}] B_0 [\text{T}]$$

with λ_u undulator period

undulator fundamental:

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

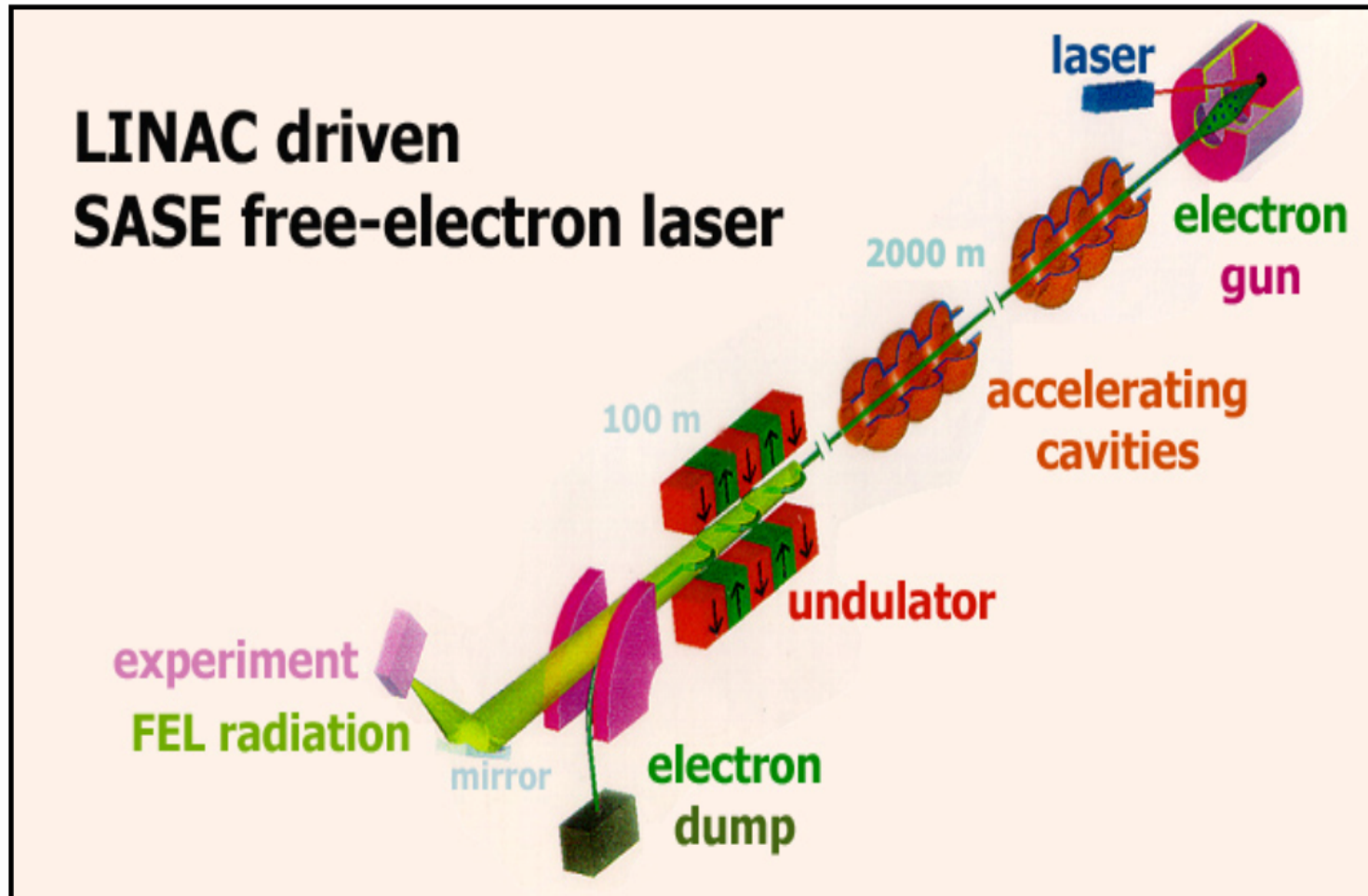
~~on axis~~

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

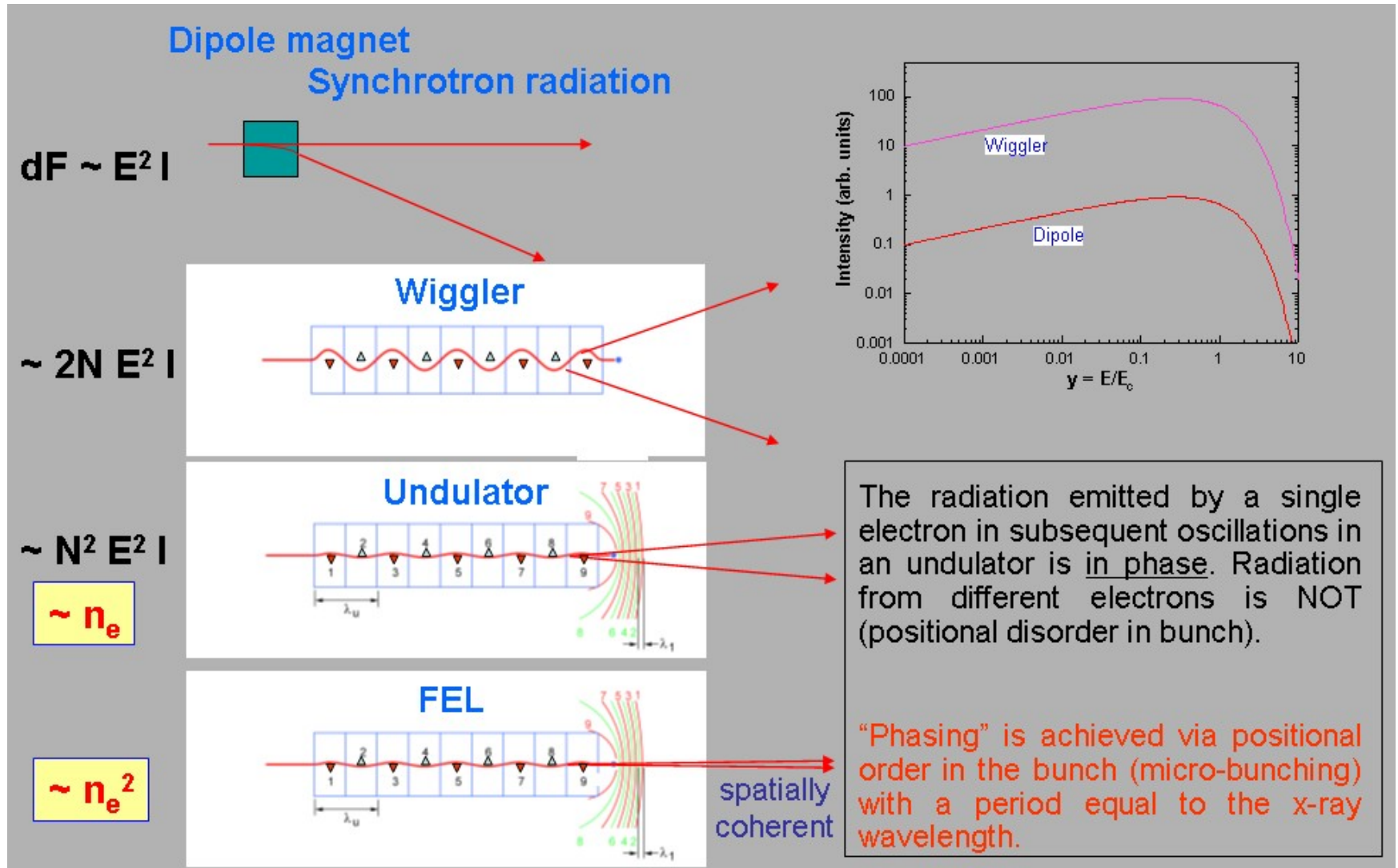
bandwidth:

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

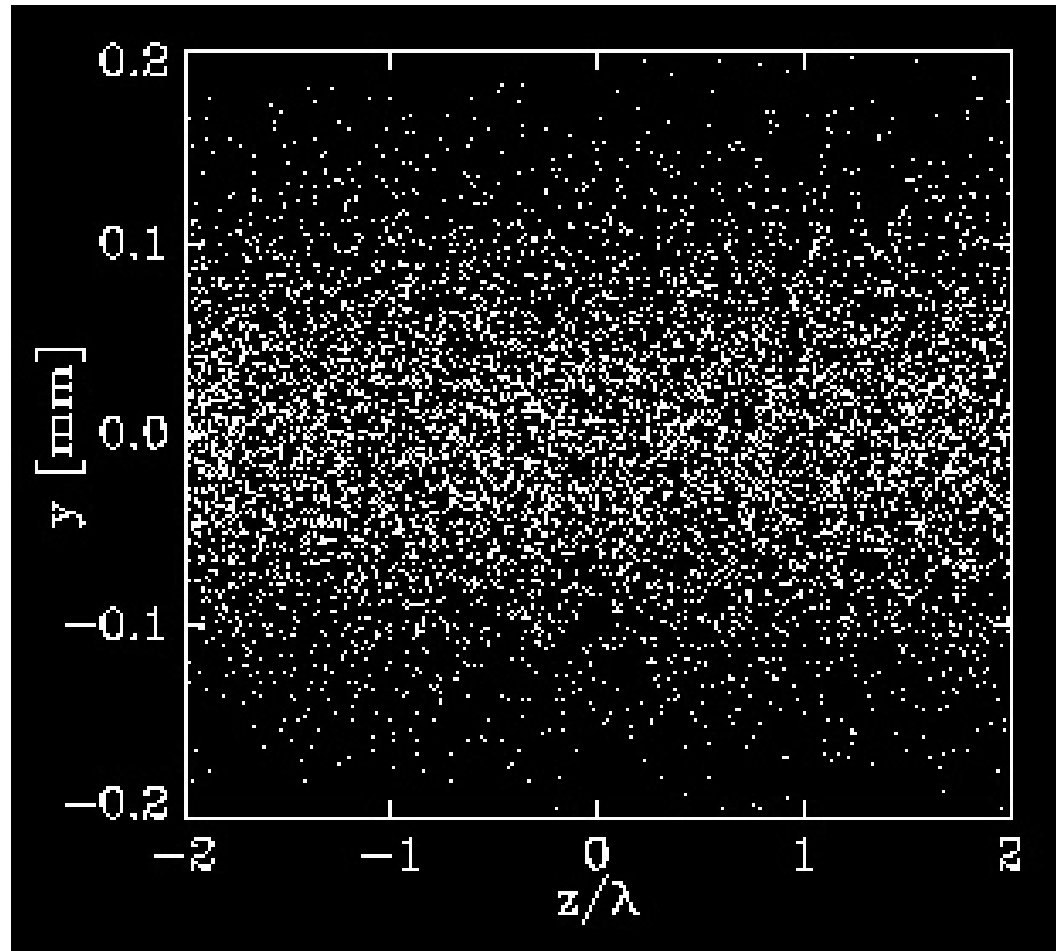
- Free Electron Lasers (FELs)



Synchrotron and FEL sources



- Electron bunching



GENESIS – simulation for TTF parameters

Courtesy Sven Reiche
(UCLA)

VUV and X-Ray FELs

