

# Methoden moderner Röntgenphysik: Streuung und Abbildung

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Lecture 2	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2018 G. Grübel, A. Philippi-Kobs, O. Seeck, L. Frenzel, F. Lehmkuhler, M. Martins, W. Wurth		
Location	Lecture hall AP, Physics, Jungiusstraße		
Date	Tuesdays	13:00 - 14:30	(starting 3.4.)
	Thursdays	8:30 - 10:00	(until 12.7.)



# Methoden moderner Röntgenphysik: Streuung und Abbildung

## Part I:

### Basics of X-ray Physics

by Gerhard Grübel (GG)

- [ 3.4.] Organisation and Introduction
- [ 5.4.] X-ray Scattering Primer
- [10.4.] Sources of X-rays, Synchrotron Radiation
- [12.4.] Refraction and Reflection
- [17.4.] Kinematical Scattering Theory (I)
- [19.4.] Kinematical Scattering Theory (II), Applications
- [24.4.] Small Angle Scattering and Soft Matter
- [26.4.] Anomalous Scattering
- [ 3.5.] Introduction: Coherence I
- [ 8.5.] 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, 7<sup>th</sup> 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/students\\_\\_teaching/lectures\\_\\_seminars/ss18](http://photon-science.desy.de/research/students__teaching/lectures__seminars/ss18)



# Methoden moderner Röntgenphysik II: Streuung und Abbildung

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#### 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)

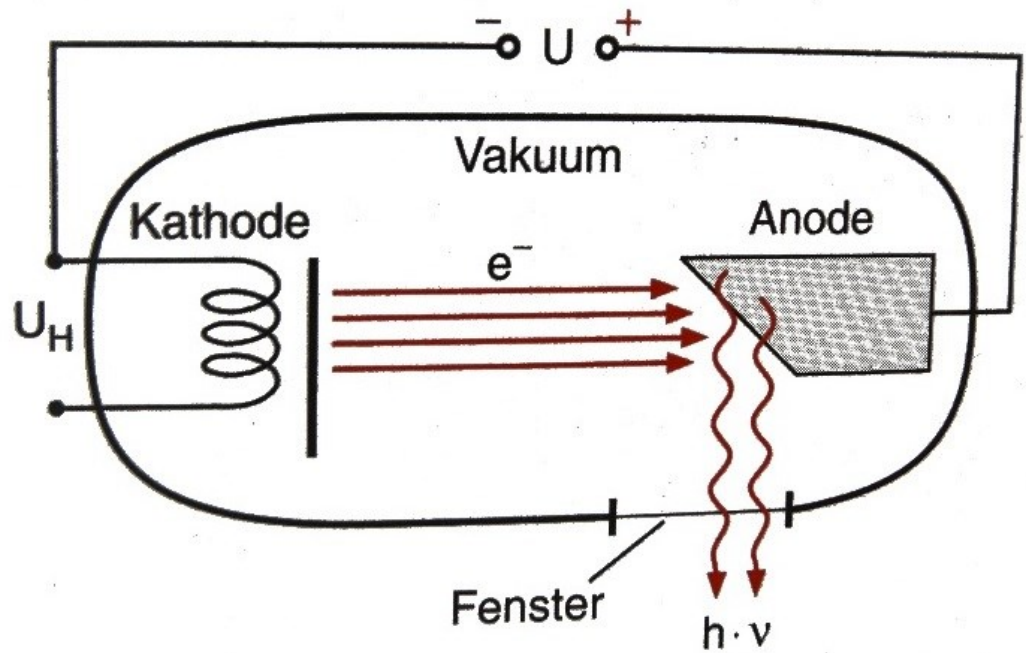
Diffraction from a Crystal, Reciprocal Lattice, Structure Factor, ...



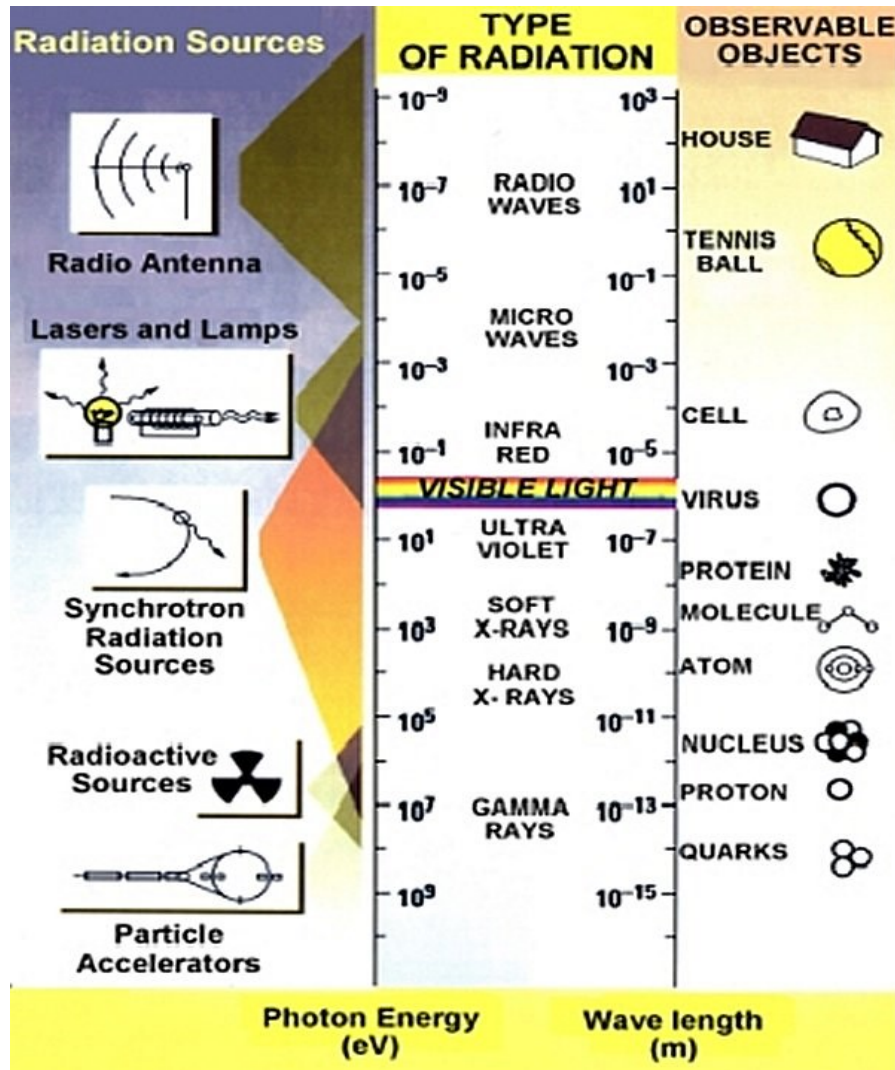
# Würzburg, 8. November 1895



Wilhelm C. Röntgen (1845 - 1923)



Klassische Röntgenröhre



X-rays

≡

Electromagnetic Radiation

≡

Wavelength

$$(\lambda[\text{\AA}] = \frac{12.398}{E[\text{keV}]})$$

≡

Object Size

≡

Angstroms

for Condensed  
Matter Research



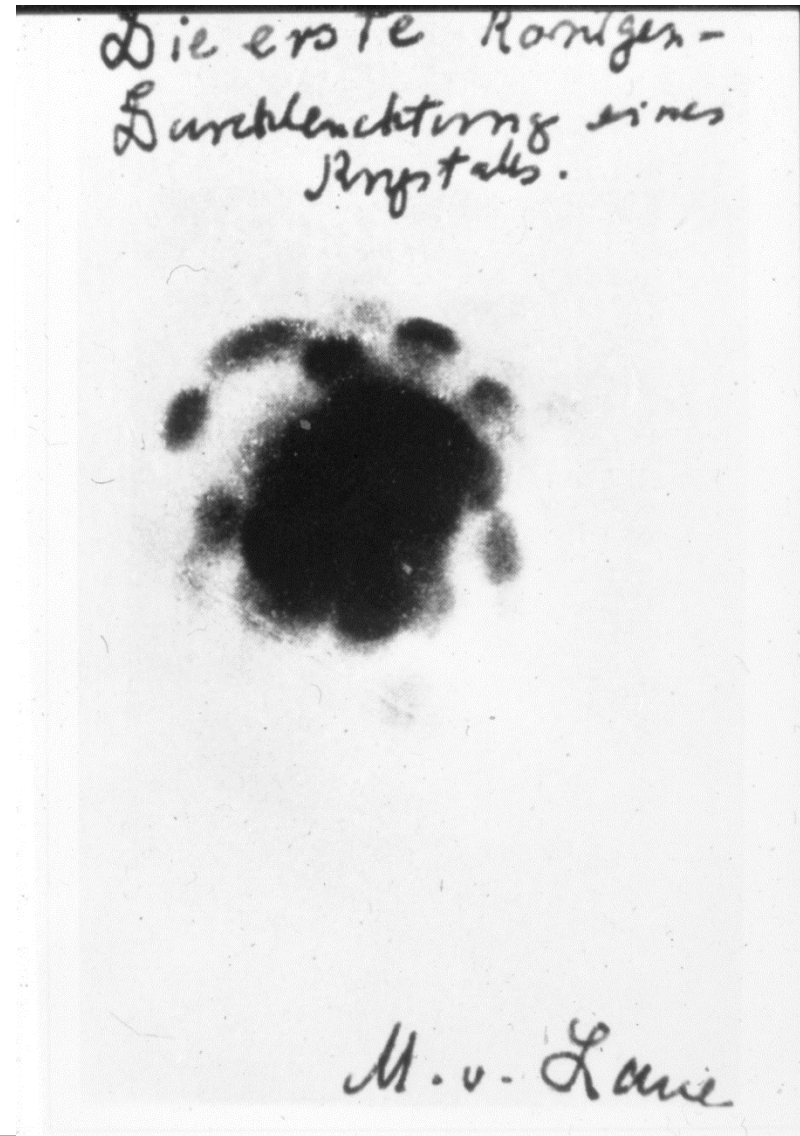
# Nobel Prices

- 1901 W.C. Röntgen in **Physik** für die **Entdeckung der Röntgenstrahlen**
- 1914 M. von Laue in **Physik** für **Röntgenbeugung an Kristallen**
- 1915 W.H. Bragg und W.L. Bragg in **Physik** für Bestimmung der **Kristallstruktur mit Röntgenbeugung**
- 1917 C.G. Barkla in **Physik** für die **charakteristische Strahlung der Elemente**
- 1924 K.M.G. Siegbahn in **Physik** für **Röntgenspektroskopie**
- 1927 A.H. Compton in **Physik** für **Streuung von Röntgenstrahlen durch Elektronen**
- 1936 P. Debye in **Chemie** für **Beugung von Röntgenstrahlen und Elektronen in Gasen**
- 1946 H.J. Muller in **Medizin** für die Entdeckung von **Mutationen durch Röntgenstrahlung**
- 1954 L. Pauling in **Chemie** für Entwicklungen in der **Strukturchemie**
- 1956 A.F. Cournand, W. Forssmann und D.W. Richards in **Medizin** für die **Entwicklung des Herzkatheters unter Röntgenkontrolle**
- 1962 J. Watson, M. Wilkins und F. Crick in **Medizin** für die **Strukturaufklärung des DNA-Moleküls**
- 1962 M. Perutz und J. Kendrew in **Chemie** für die **Strukturaufklärung von Hämoglobin**
- 1964 D.C. Hodgkin in **Chemie** für die **Röntgenstrukturanalyse von Penicillin** und wichtigen biochemischen Substanzen
- 1976 W.N. Lipscomb in **Chemie** für **Röntgenstrukturuntersuchungen an Boranen**
- 1979 A.M. Cormack und G.N. Hounsfield in **Medizin** für **Computertomographie**
- 1981 K.M. Siegbahn in **Physik** für **hochaufgelöste Elektronenspektroskopie**
- 1985 H.A. Hauptman und J. Karle in **Chemie** für die Entwicklung direkter Methoden zur **Bestimmung von Röntgenstrukturen**
- 1988 J. Deisenhofer, R. Huber und H. Michel in **Chemie** für die **Bestimmung der dreidimensionalen Struktur von Proteinen für die Photosynthese**
- 1997 P.D. Boyer, J.E. Walker und J.C. Skou in **Chemie** für **Aufklärung der Funktion des Enzyms ATP**
- 2002 R. Giacconi in **Physik** für die **Entwicklung der Röntgenastronomie**
- 2003 R. MacKinnon in **Chemie** für **Röntgenstrukturbestimmung von Ionenkanälen in Zellmembranen**
- 2009 V. Ramakrishnan, T. A. Steitz, A. E. Yonath in **Chemie** für **Studies of the Structure and Function of the Ribosome**

# v. Laue et. al.

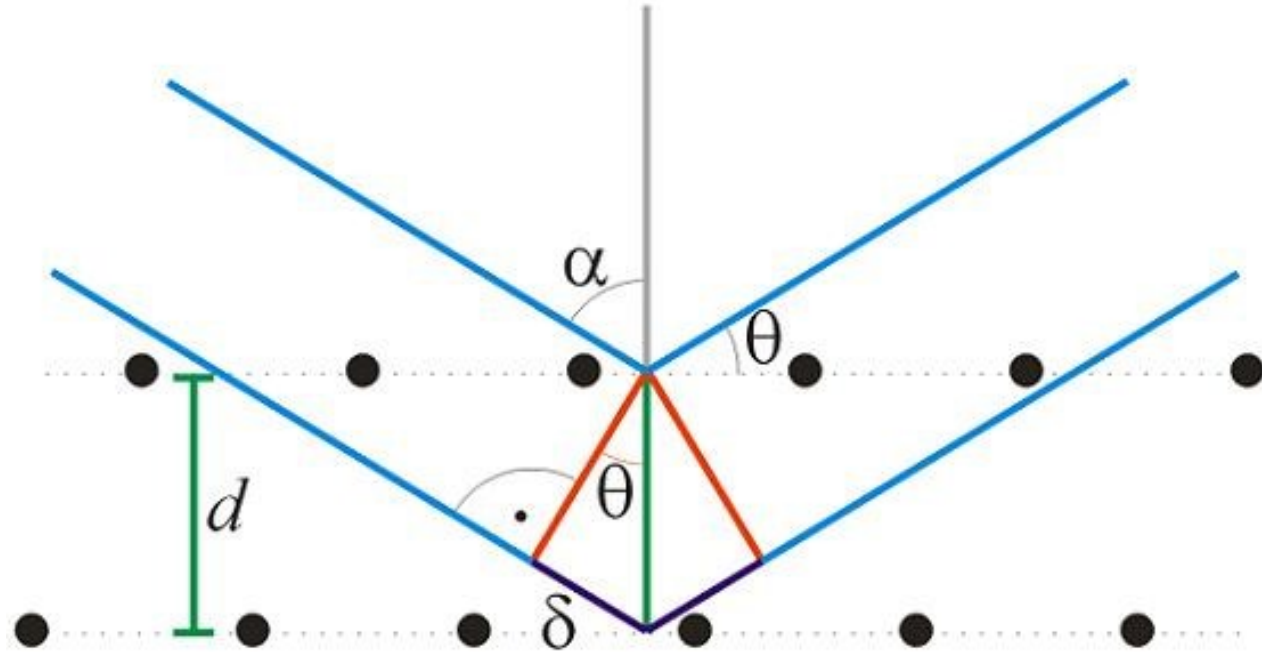
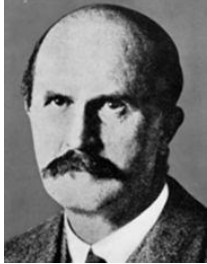
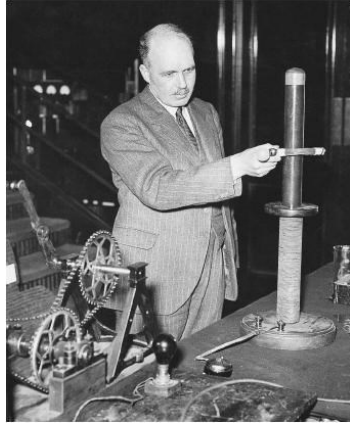
Interferenzen am Kristallgitter

Laue, Friedrich und Knipping 1912



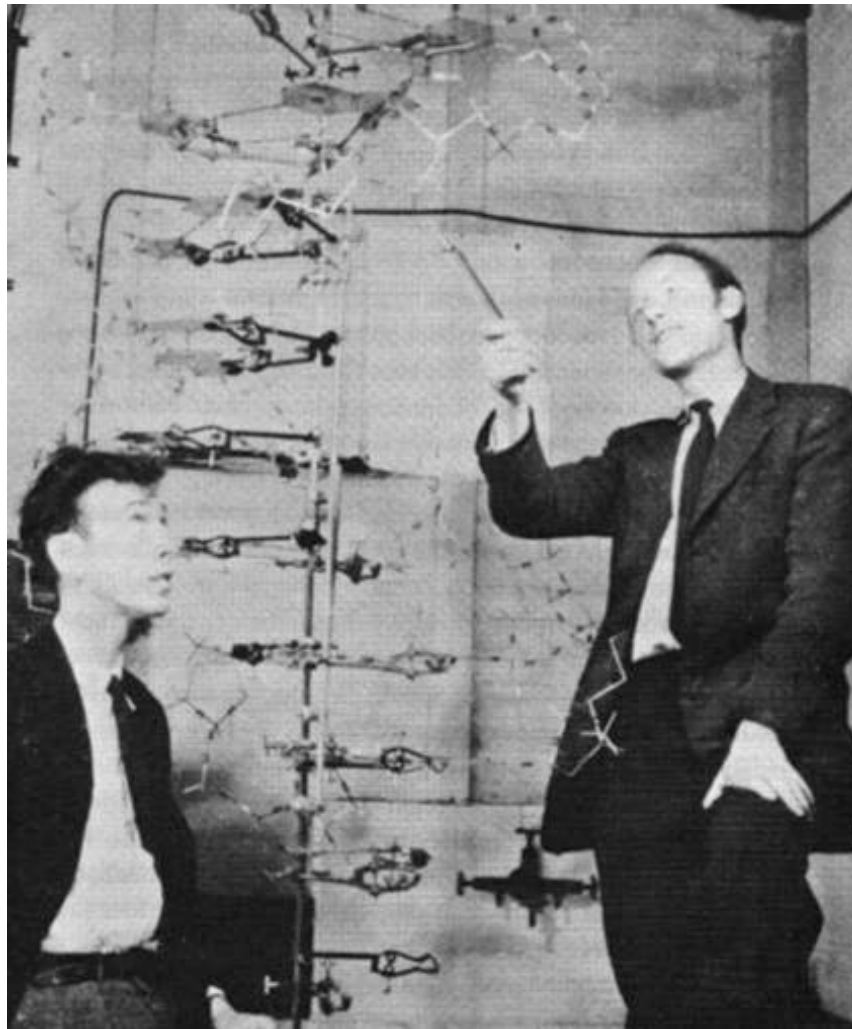


# Bragg's Law

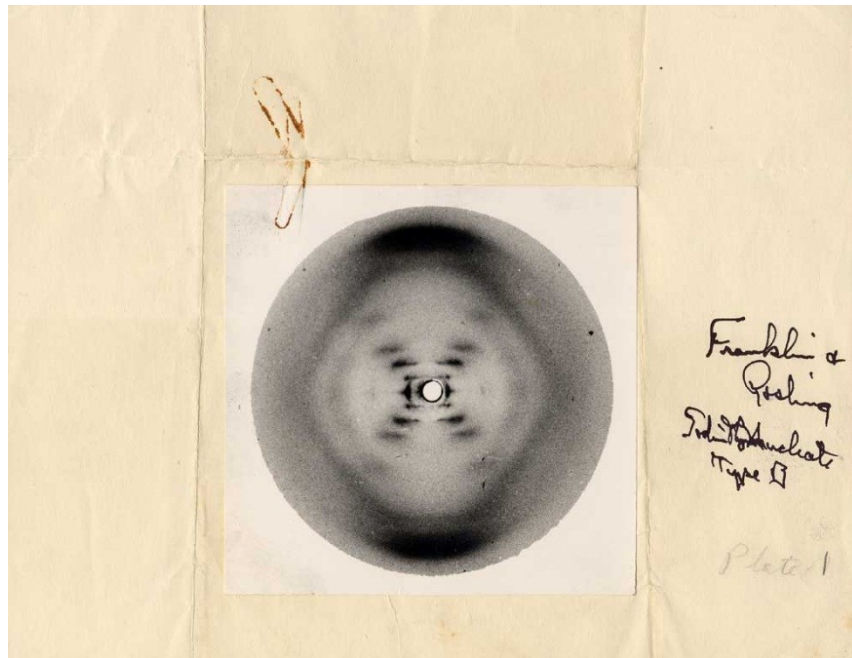
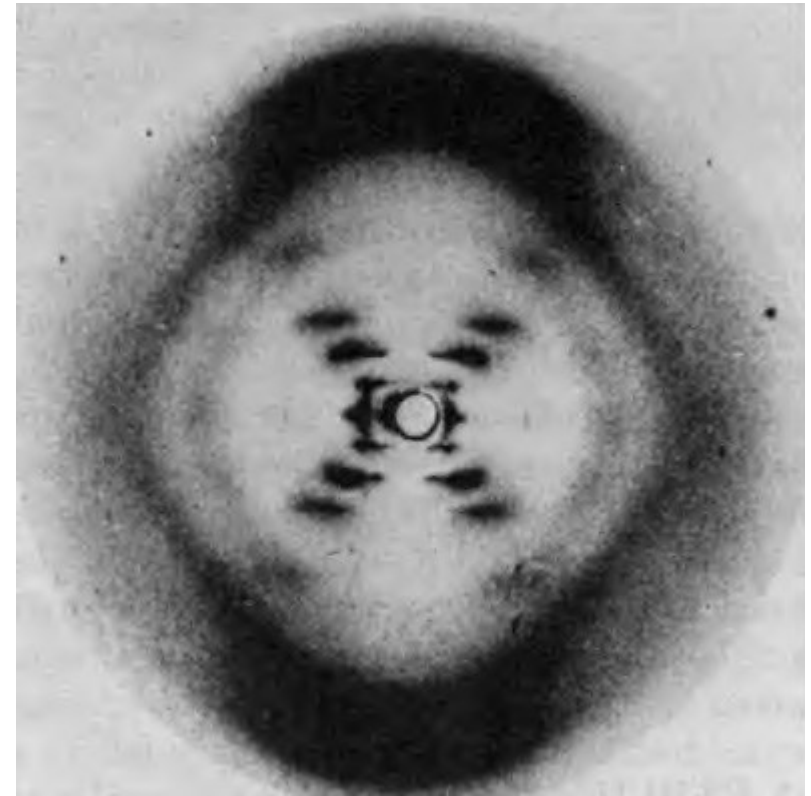


Scattering intensity only if:  $n\lambda = 2d \sin(\Theta)$

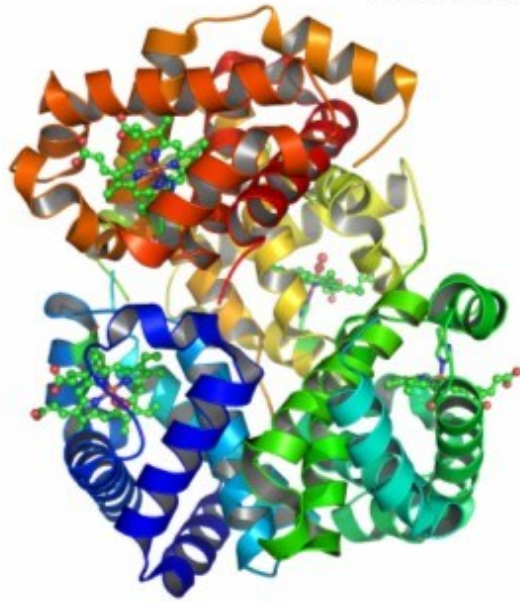
# Watson & Crick 1953



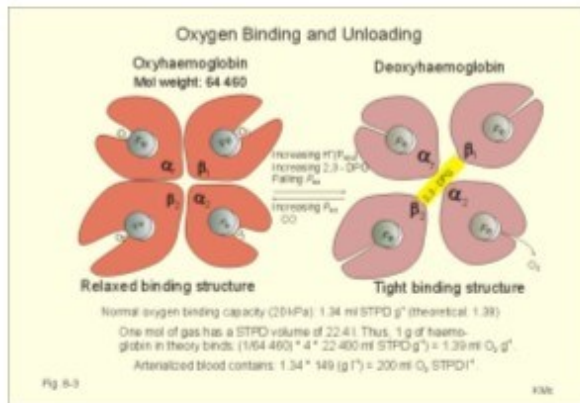
Rosalind Franklin's Famous X-ray that provided enough evidence to establish that DNA was a helix.



# Hämoglobin und Myoglobin Struktur mit Röntgenstrahlen

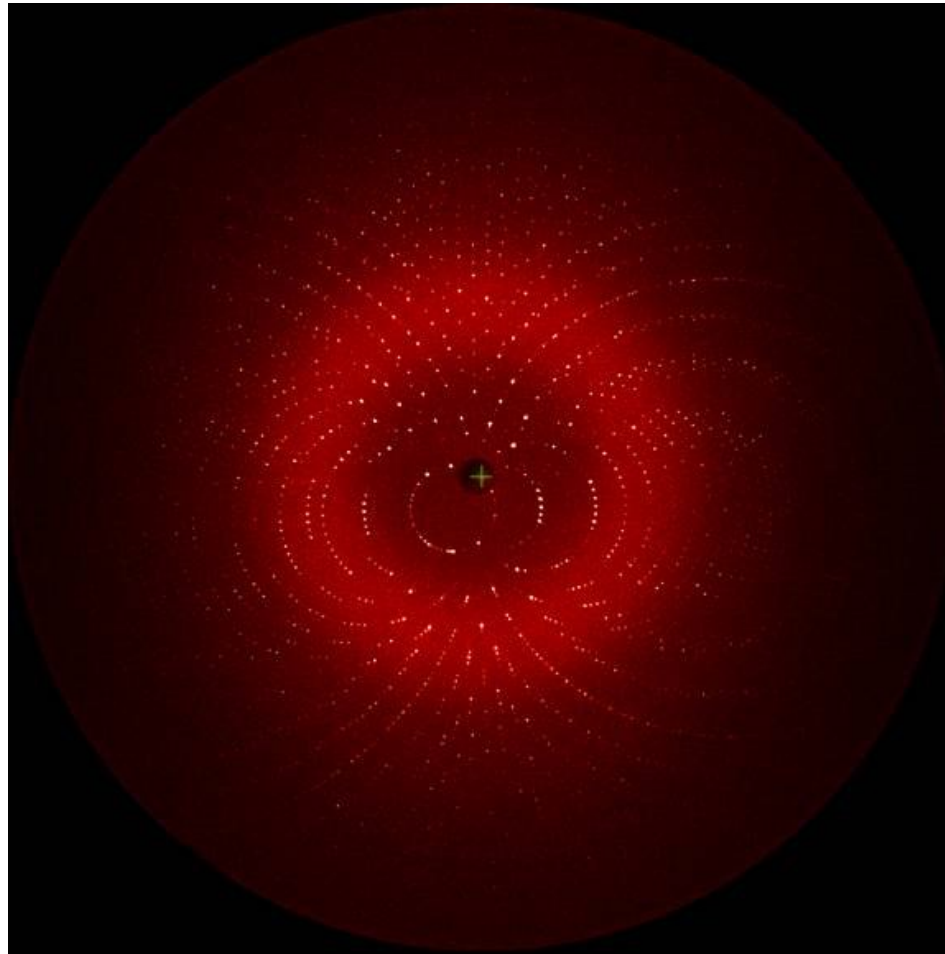


John Cowdery Kendrew  
 Max Perutz  
 Nobelpreis 1962



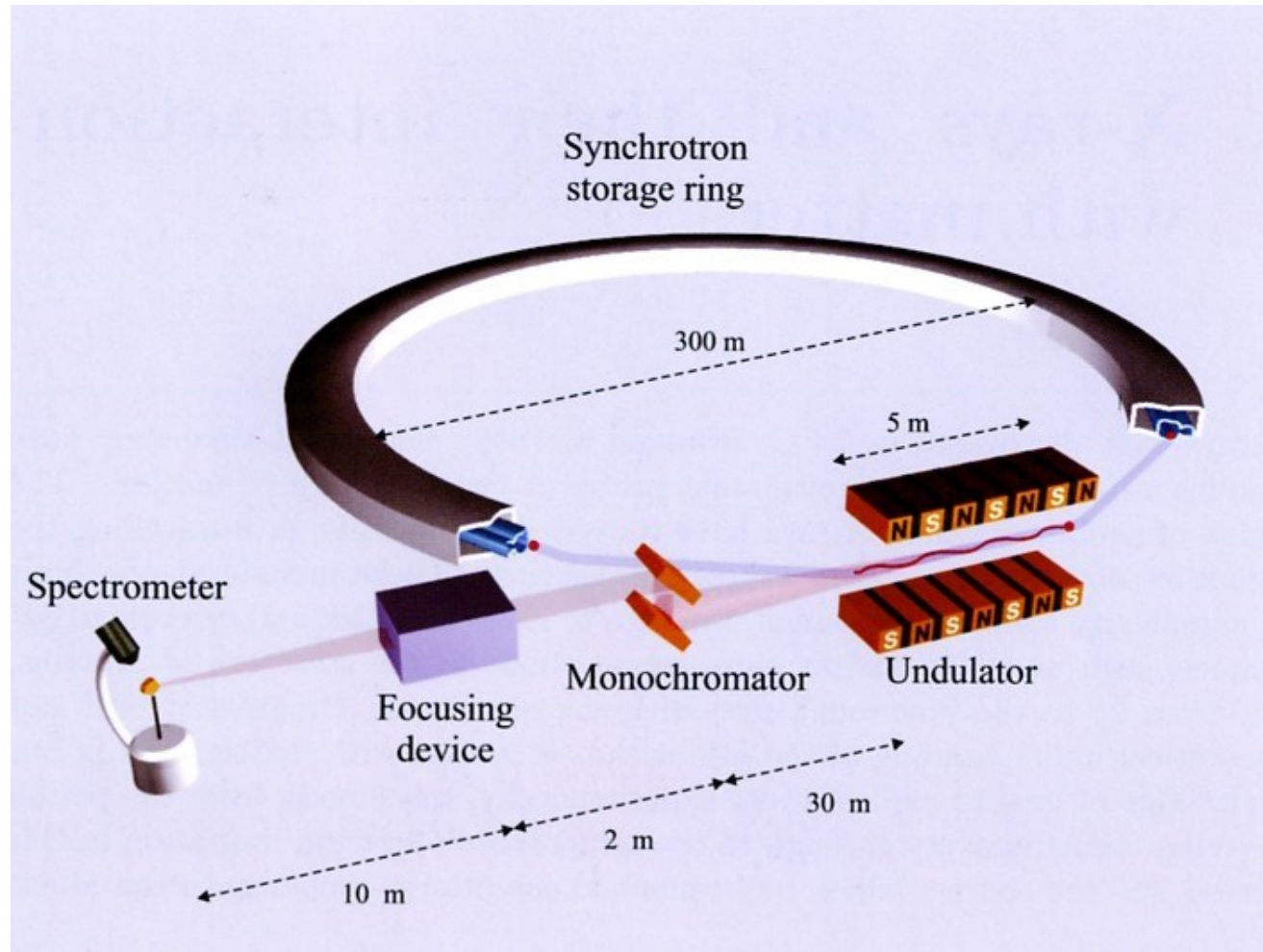
# X-ray Scattering Research Today

# Modern Protein Crystallography

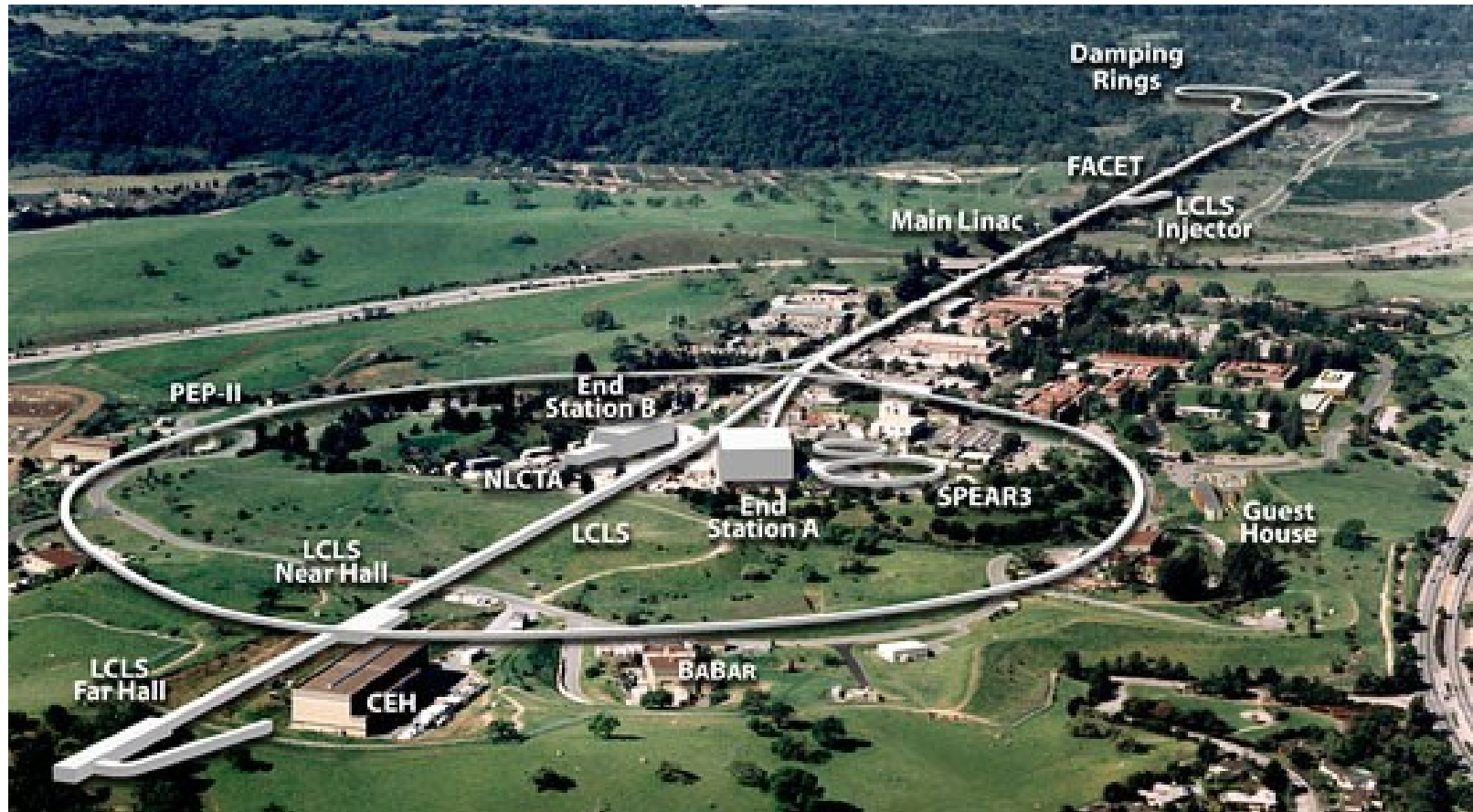


BioCARS 14-ID-B station of APS using an undulator with a gap of 25 mm from a crystal of the M37V mutant of CO-bound dimeric clam hemoglobin.

# Made Possible by Storage-Rings

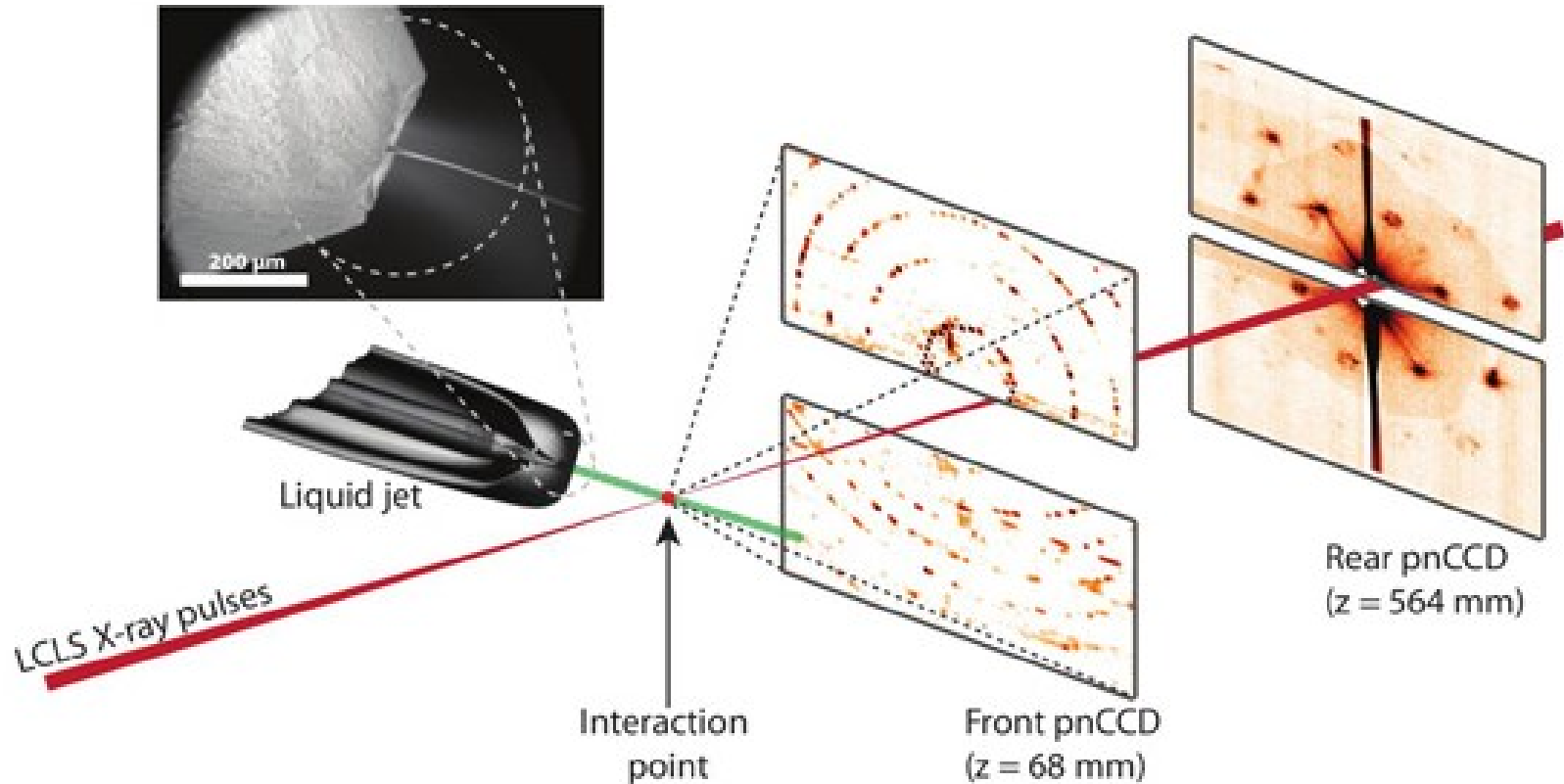


# LCLS – Linac Coherent Light Source - SLAC





# Serial Femtosecond Crystallography

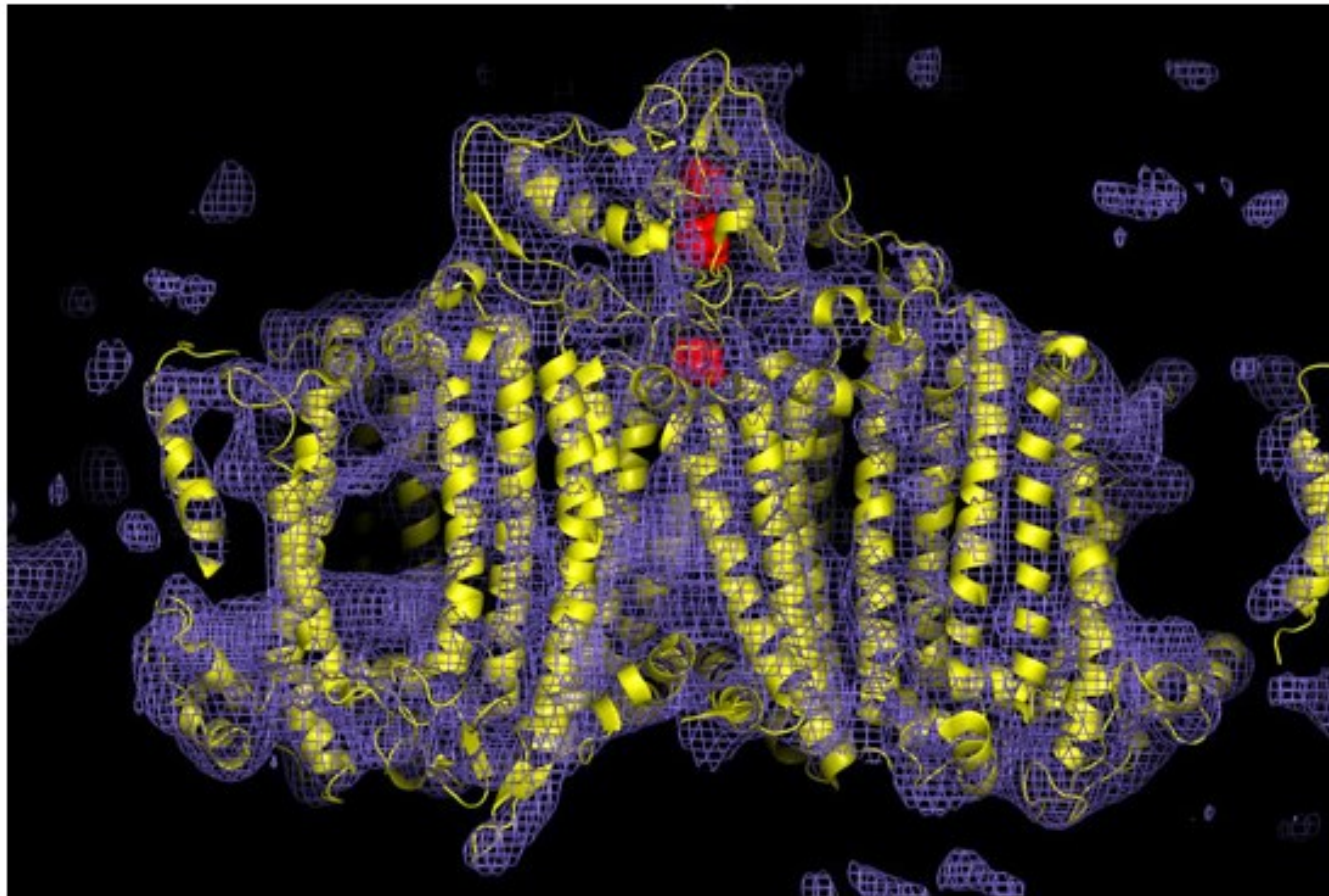


**Figure 1**

*Experimental set-up for serial femtosecond crystallography. First published in Nature 470, 73 – 78 (2011).*

Henry N. Chapman et al., NATURE 470, 73 (2011)

# Serial Femtosecond Crystallography



Extracted from 3 million diffraction patterns from photosystem I nanocrystals (200nm to 2 micron size)  
LCLS:30 Hz at 1.8 keV

**Figure 3**

*Electron density map of the photosystem I protein complex obtained from the LCLS diffraction data. First published in Nature 470, 73 – 78 (2011). Nanocrystals were grown by Petra Fromme of Arizona State University.*

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# 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**

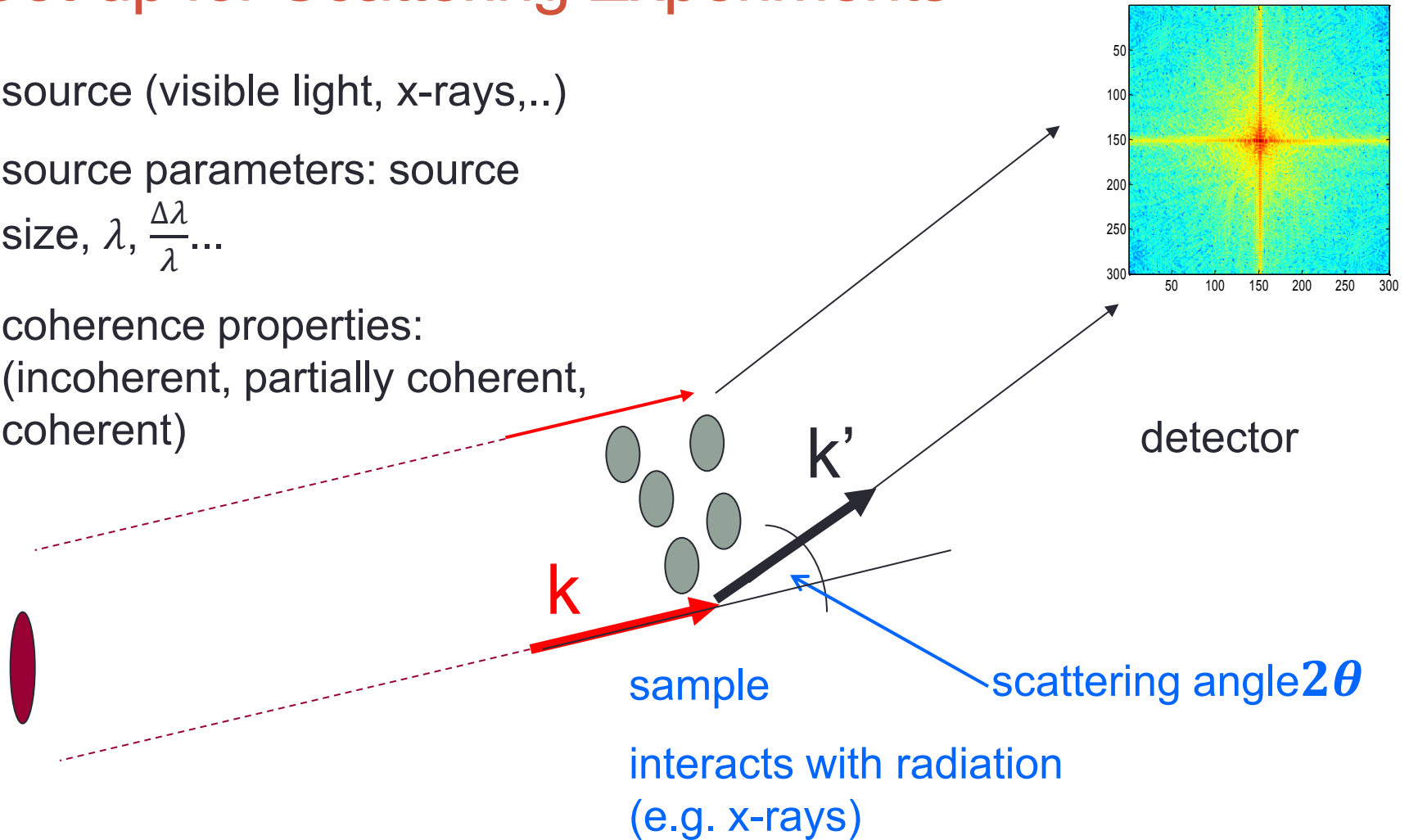
# Set-up for Scattering Experiments

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

source parameters: source

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

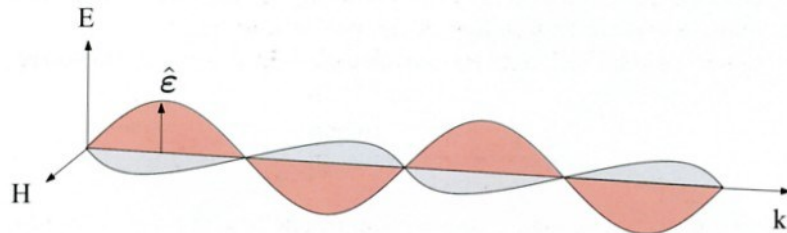
coherence properties:  
(incoherent, partially coherent,  
coherent)



L

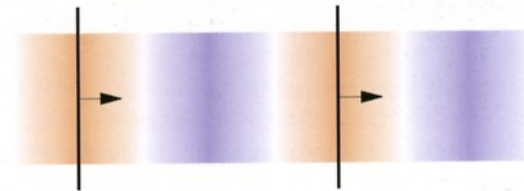
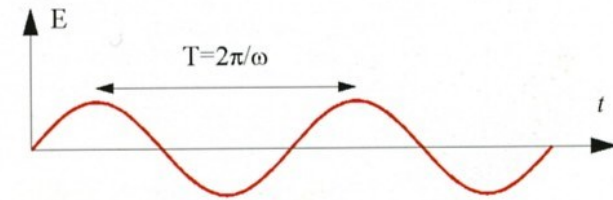
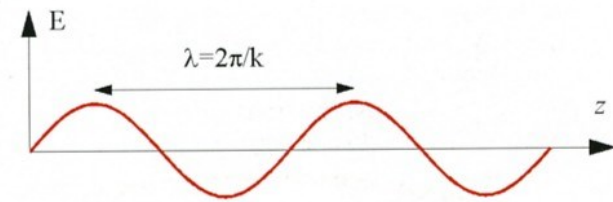
# X-rays: Electromagnetic Waves and Photons

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

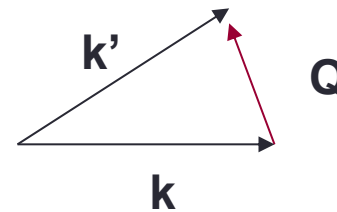
Consider a monochromatic plane (electromagnetic) wave with wave vector  $\mathbf{k}$ :

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

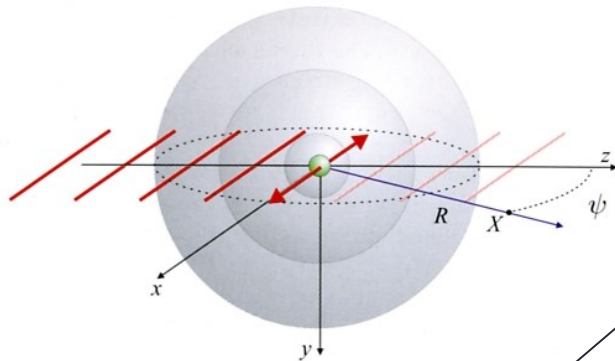
with  $|\mathbf{k}| = \frac{2\pi}{\lambda}$

Elastic scattering:

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



## Scattering by a Single Electron:



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

spherical wave

Thomson scattering length  $r_0$

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

phase shift of  $\pi$  btw. incident and radiated field



# Scattered intensity:

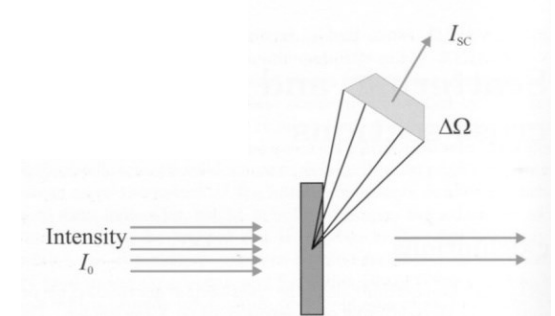
$$\frac{I_s}{I_0} = \frac{|E_{\text{rad}}|^2 R^2 \Delta\Omega}{|E_{\text{in}}|^2}$$

$\Delta\Omega$  : 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:

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



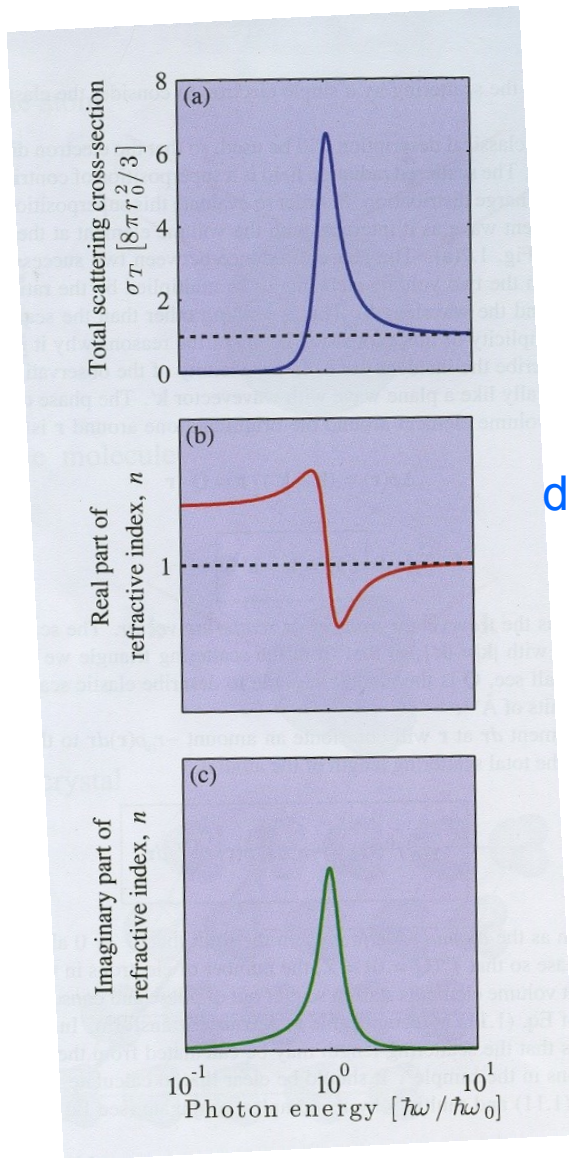
# Scattering by a Single Atom:

form factor of an atom:

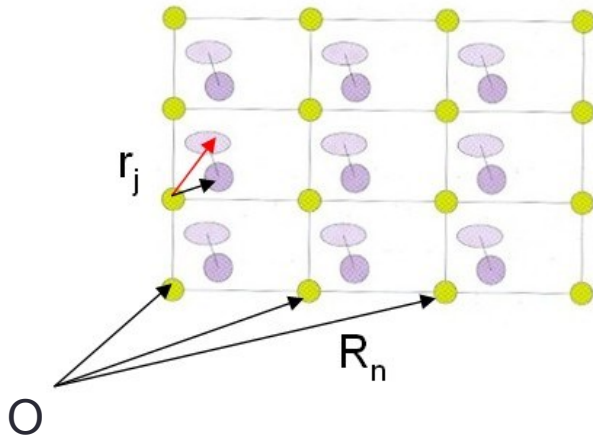
$$f(Q, \hbar\omega) = f^0(Q) + f'(\hbar\omega) + i f''(\hbar\omega)$$



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:

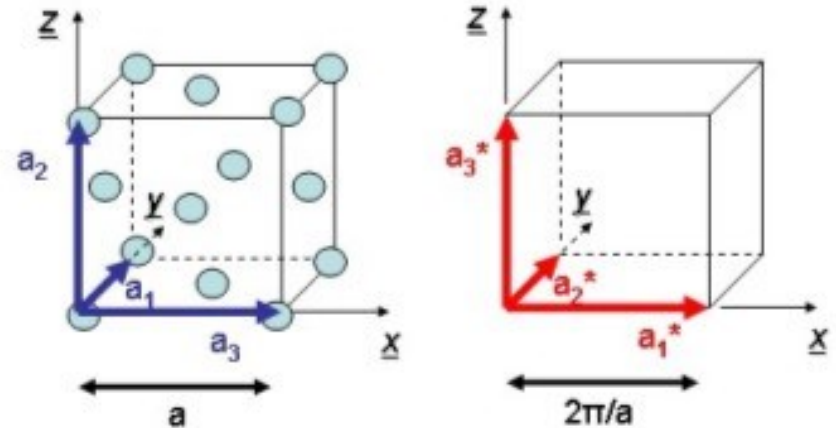
$$r_1 = 0$$

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

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

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

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



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

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

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

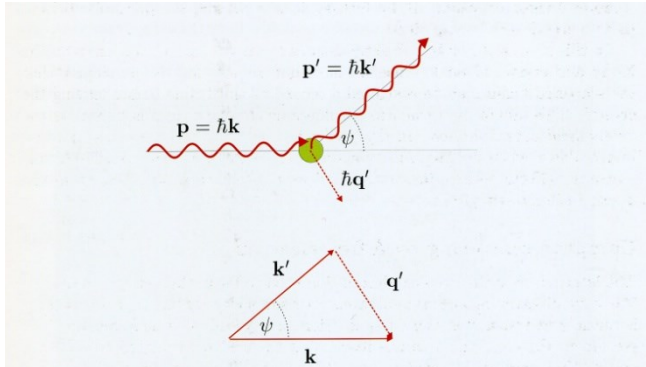
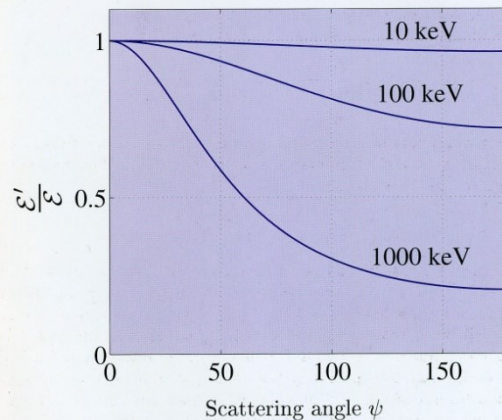
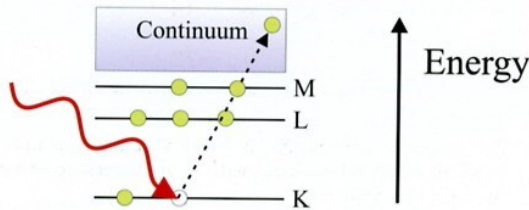


Figure 1.7: Compton scattering. A photon with energy  $\mathcal{E} = \hbar c k$  and momentum  $\hbar k$  scatters from an electron at rest with energy  $m c^2$ . The electron recoils with a momentum  $\hbar q' = \hbar(k - k')$  as indicated in the scattering triangle in the bottom half of the figure.

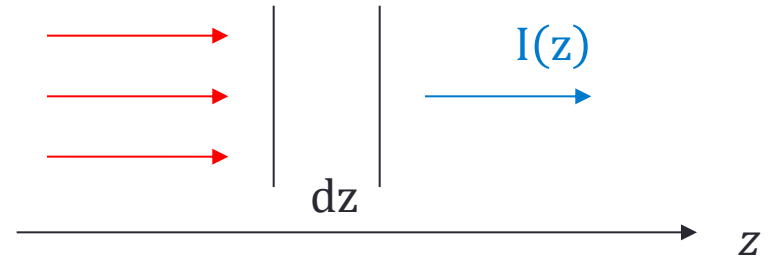


# Photoelectric Absorption

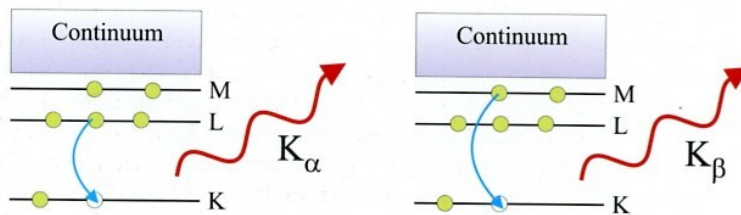
(a) Photoelectric absorption



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



(b) Fluorescent X-ray emission



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

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

$\rho_a$  atomic number density

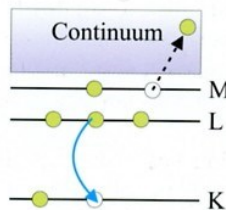
$\sigma_a = \sigma_a(E)$  absorption cross section

$\rho_m$  mass density

$N_A$  Avogadro's number

$A$  atomic mass number

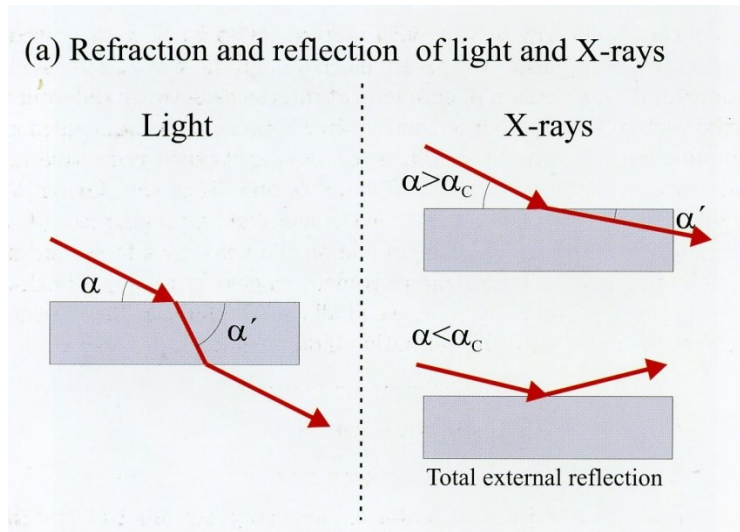
(c) Auger electron emission



# Refraction

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

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



## Snell's law:

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

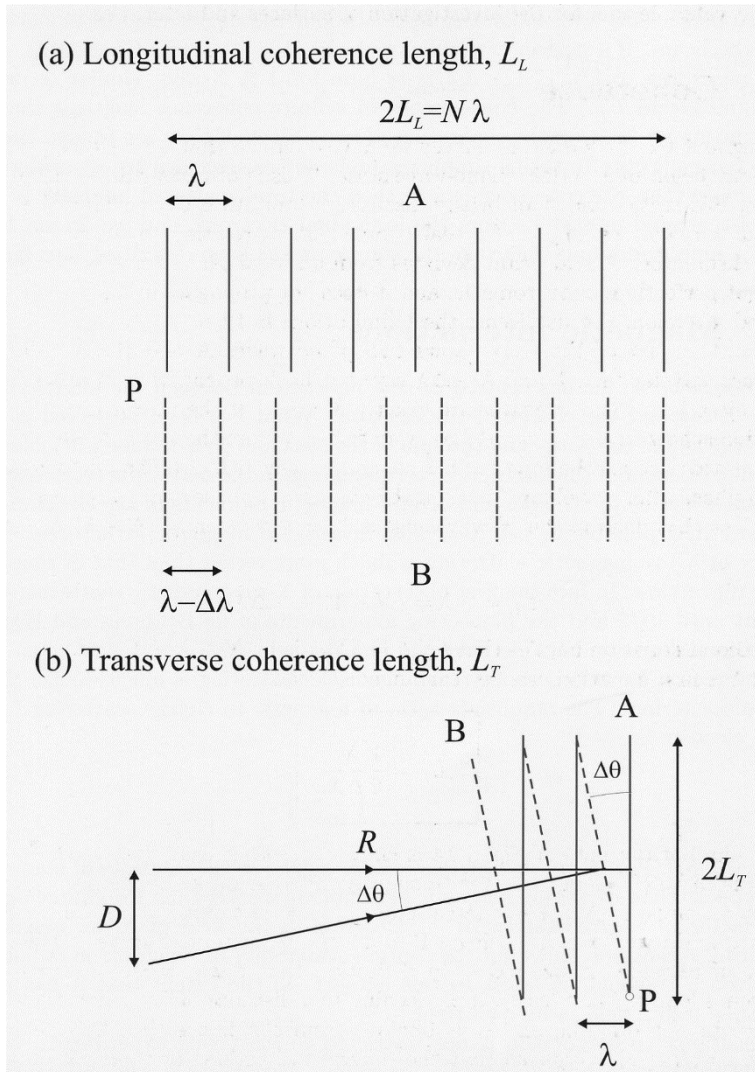
**Note:** total external reflection  
for x-rays ( $\alpha' = 0$ )

$$n < 1$$

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

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  $\pi$ :

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

## Transverse coherence:

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

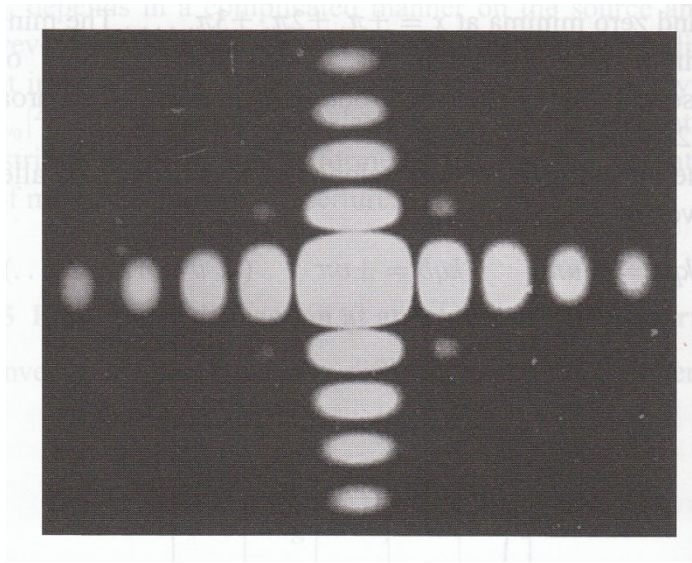
$$2\xi_t \Delta\theta = \lambda$$

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

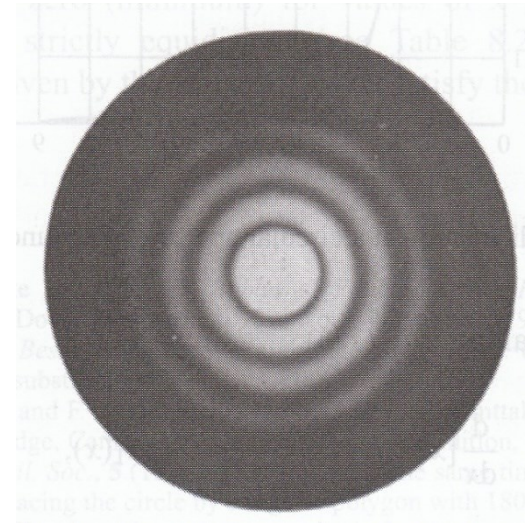




# Fraunhofer Diffraction

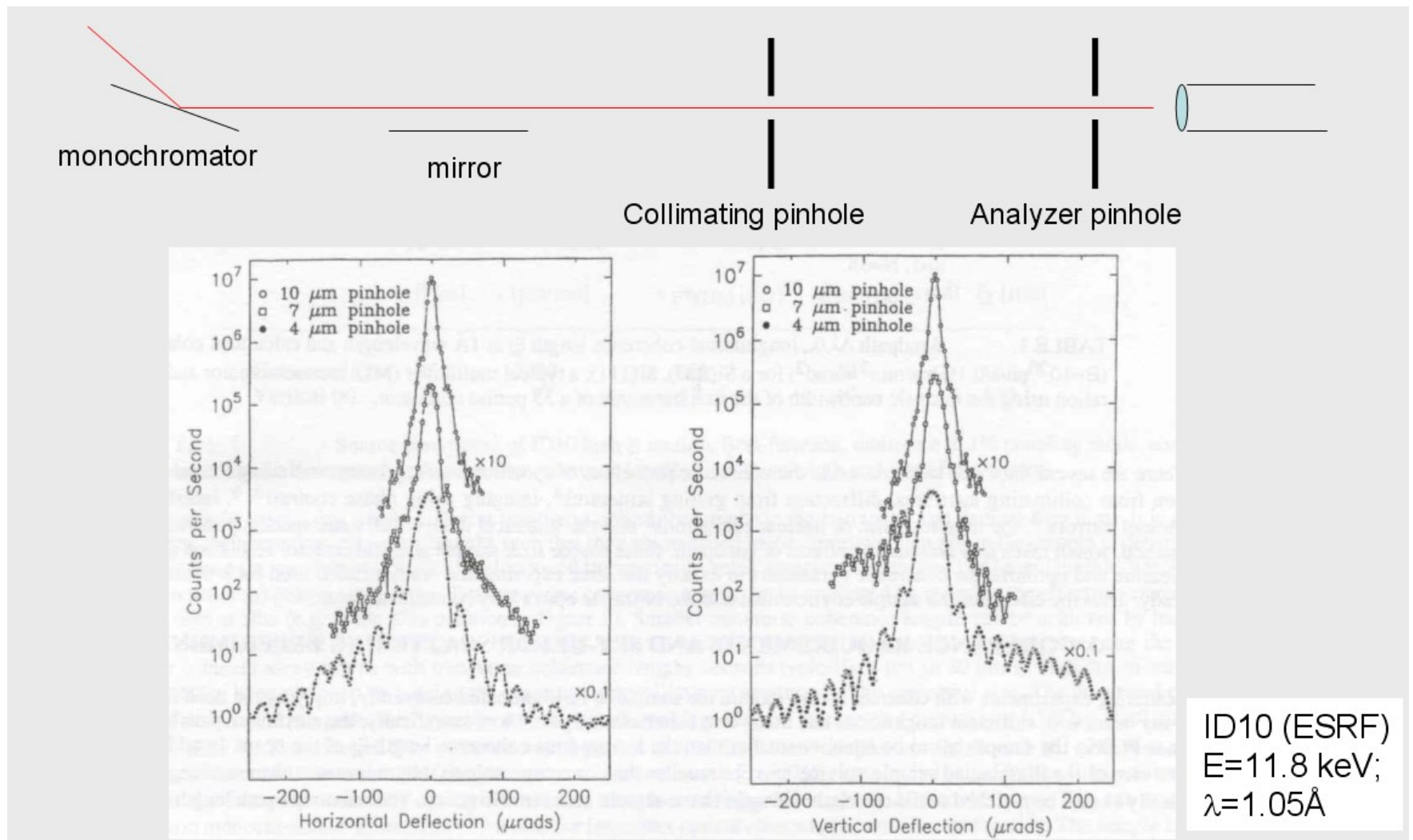


Fraunhofer diffraction of a rectangular aperture  $8 \times 7 \text{ mm}^2$ , taken with mercury light  $\lambda=579\text{nm}$  (from Born&Wolf, chap. 8)

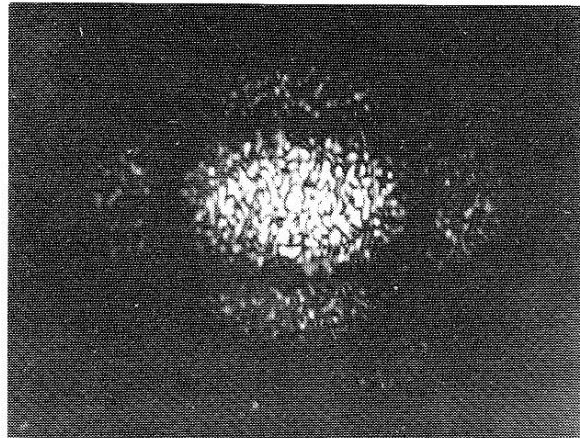


Fraunhofer diffraction of a circular aperture, taken with mercury light  $\lambda=579\text{nm}$  (from Born&Wolf, chap. 8)

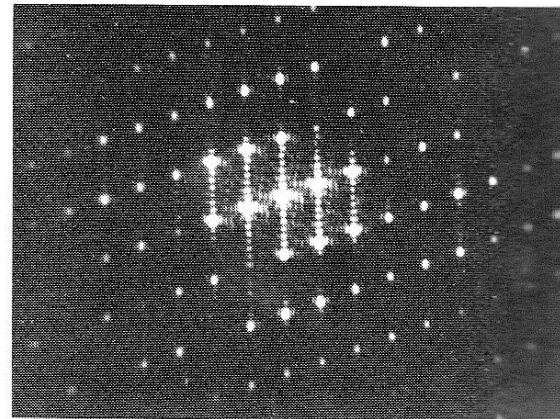
# Fraunhofer Diffraction ( $\lambda = 0.1nm$ )



# Speckle Pattern



random arrangement of apertures: speckle



regular arrangement of apertures

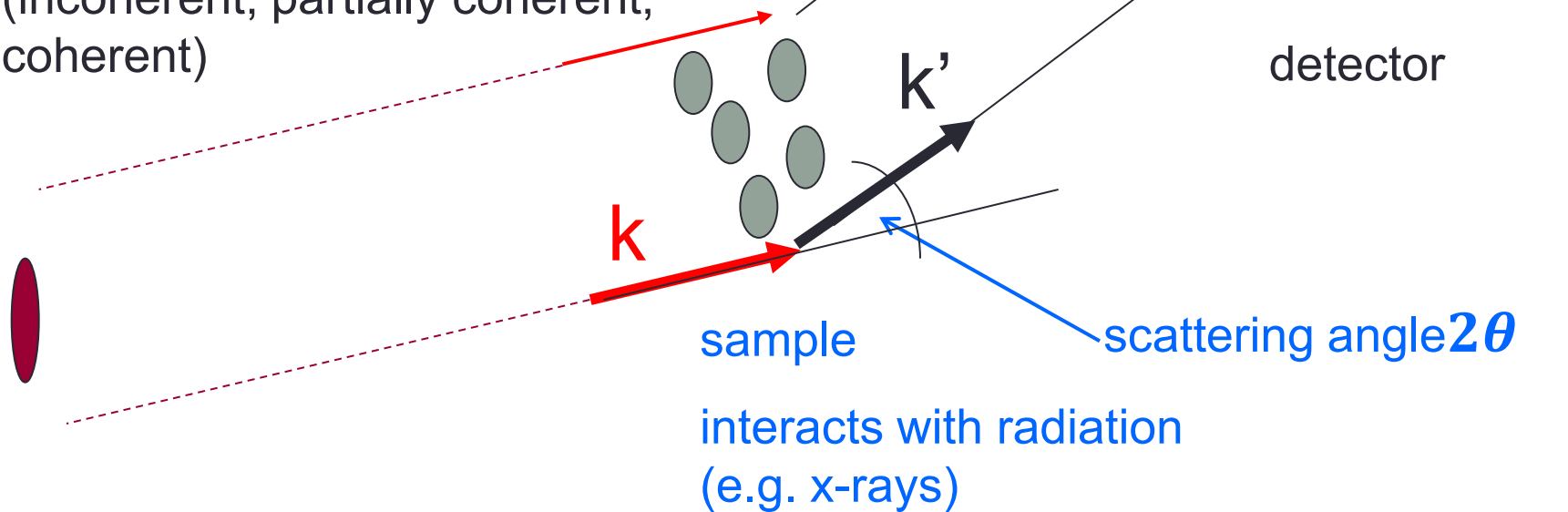
# Experimental Set-up for Scattering Experiments

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

source parameters: source

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

coherence properties:  
(incoherent, partially coherent,  
coherent)



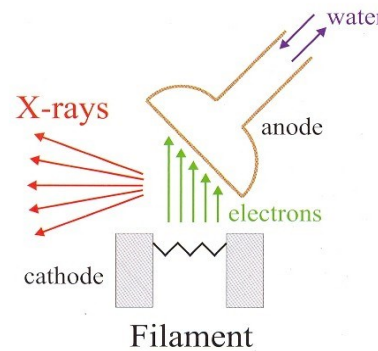
L

# Source of X-Rays

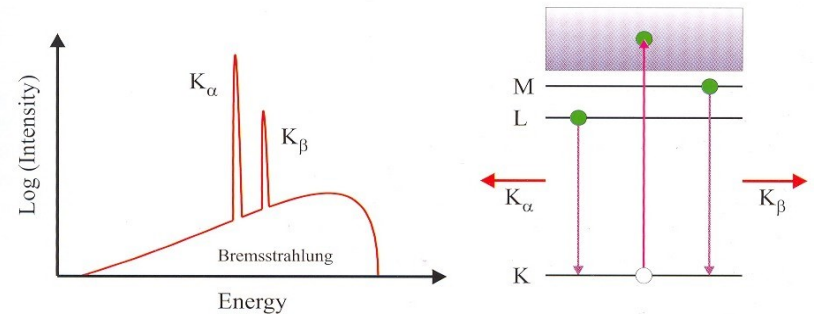
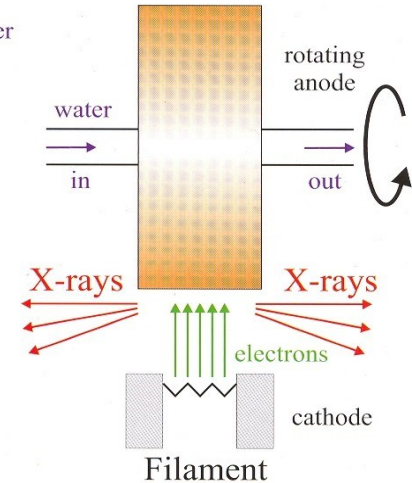
- 1895 Discovered by W.C. Röntgen
- 1912 First diffraction experiment (v. Laue)
- 1912 Coolidge tube (W.D. Coolidge, GE)
- 1946 Radiation from electrons in a synchrotron, GE, Physical Review, 71,829 (1947)



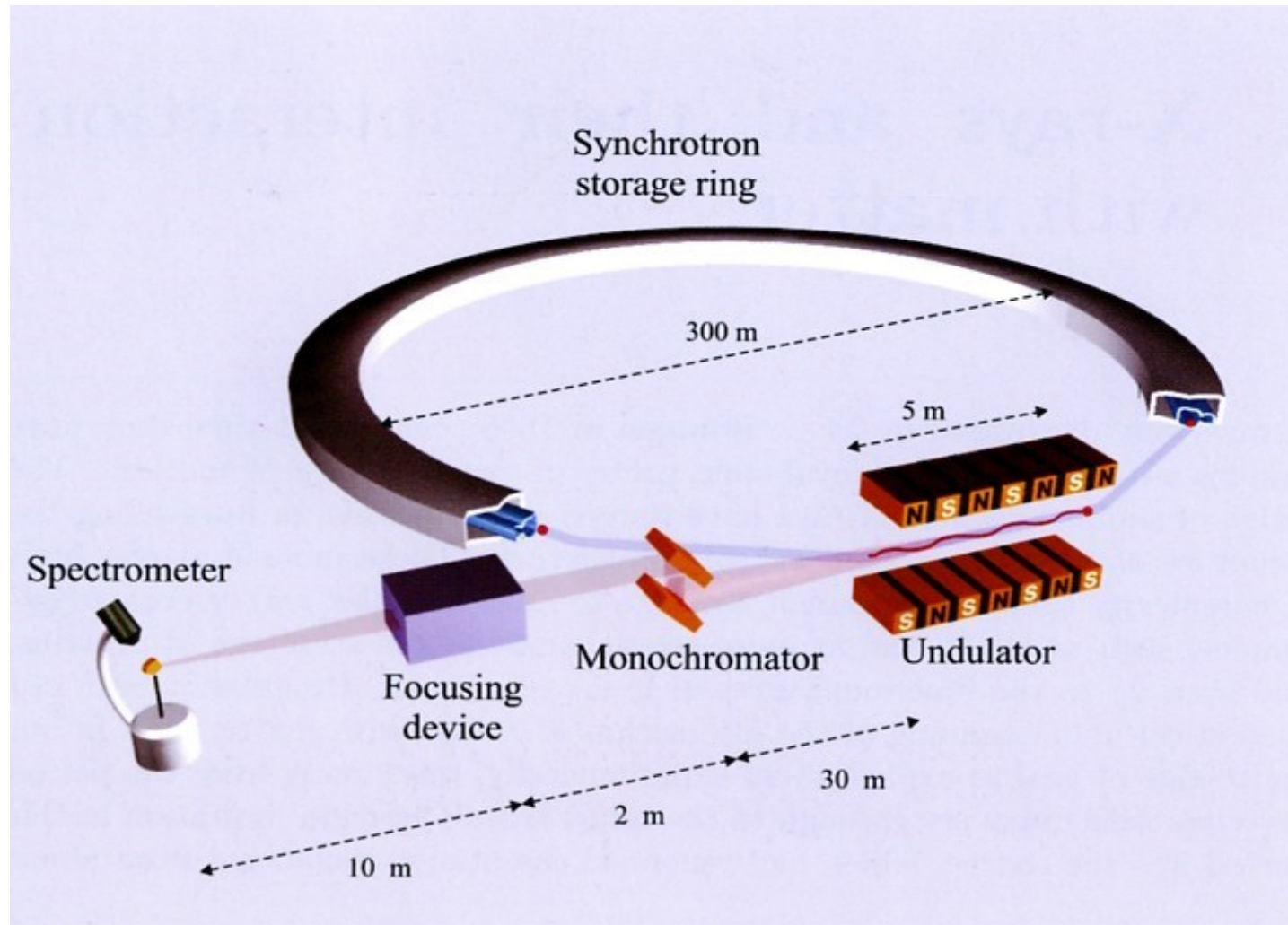
Coolidge Tube



Rotating Anode



# Synchrotron Radiation Storage Ring



# Photon Machines

The three largest and most powerful synchrotrons in the world



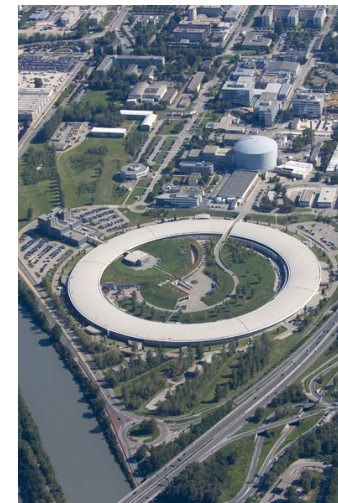
APS, USA



ESRF, Europe-France



Spring-8, Japan



# The most recent third generation machine:



**Petra III at DESY/Hamburg**