Master Kurs im SS 2011

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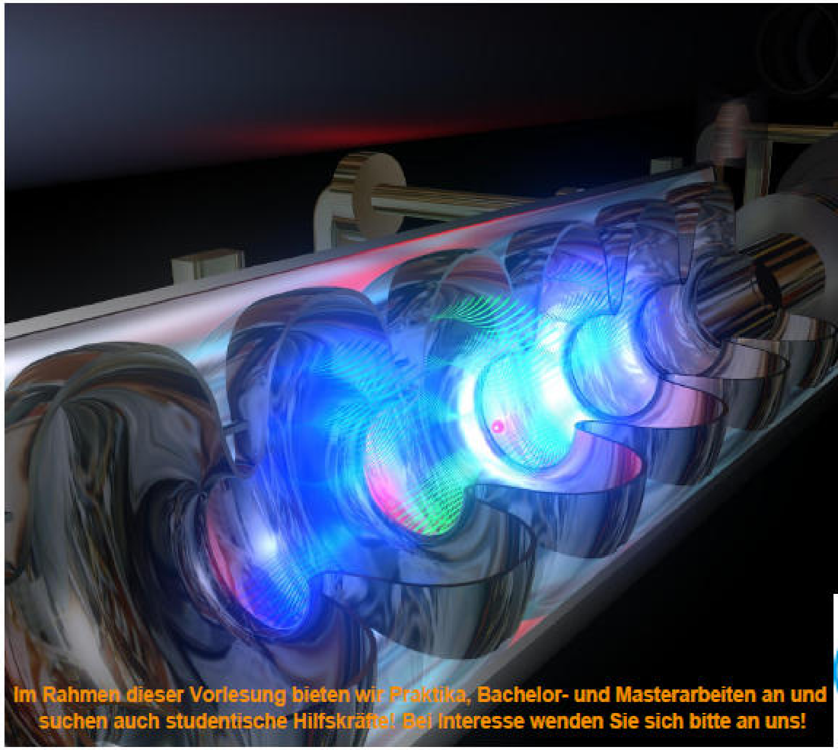
Methoden moderner Röntgenphysik II

Vierstündige Vorlesung mit Übungen und Proseminar
(Seminar Raum 3)

Di 14:00 – 15:30, Do 10:15 – 11:45
Beginn: 05.04.2011, 14:00



Im Rahmen dieser Vorlesung bieten wir Praktika, Bachelor- und Masterarbeiten an und suchen auch studentische Hilfskräfte! Bei Interesse wenden Sie sich bitte an uns!

Methoden moderner Röntgenphysik II

Vorlesungszeit: 4.4. – 16.7.

Ferien: 13.6 – 24.6.

66-360: Methoden moderner Roentgenphysik II

Di: 14:00-15:30 SemRm 3

Do: 10.15-11.45 „

Beginn: 5.4.

66-361: Uebungen

Di: 16:00-17.30 SemRm3 ab ????.

66-505: ProSeminar (for Batchelor students)

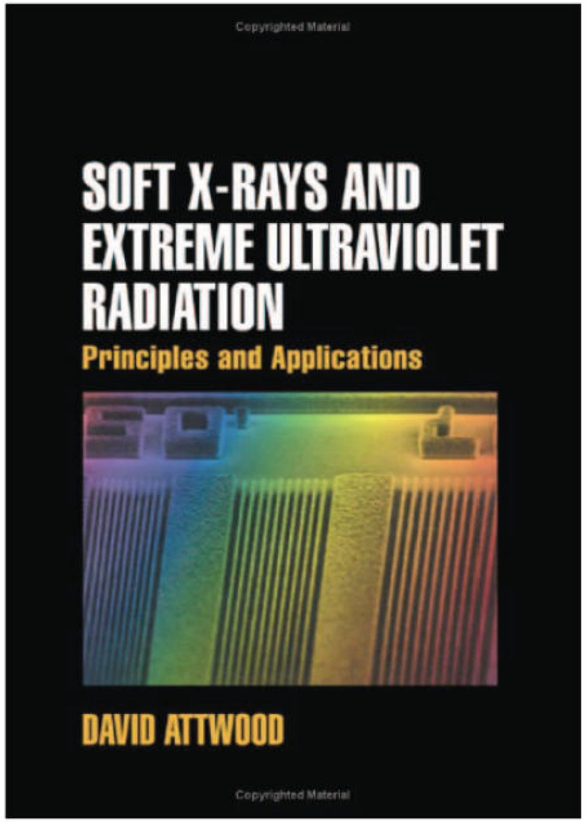
Vorbesprechung 5.4. 15:30 SemRm 3

Methoden moderner Röntgenphysik II

5.4. - 19.4. 2011	Wiederholung + Kohärenz	Christian Gutt
21.4. - 3.5. 2011	Weiche Materie	Stephan Roth
5. 5. 2011	Glass Physik	Hermann Franz
10.5. -12.5.2011	Magnetismus	Martin v. Zimmermann
17.5.- 14.7.2011	Festkörperspektroskopie	Wilfried Wurth
Im obigen Block	Inelastische Röntgenstreuung	Wolfgang Caliebe und Wolfgang Drube

Literature

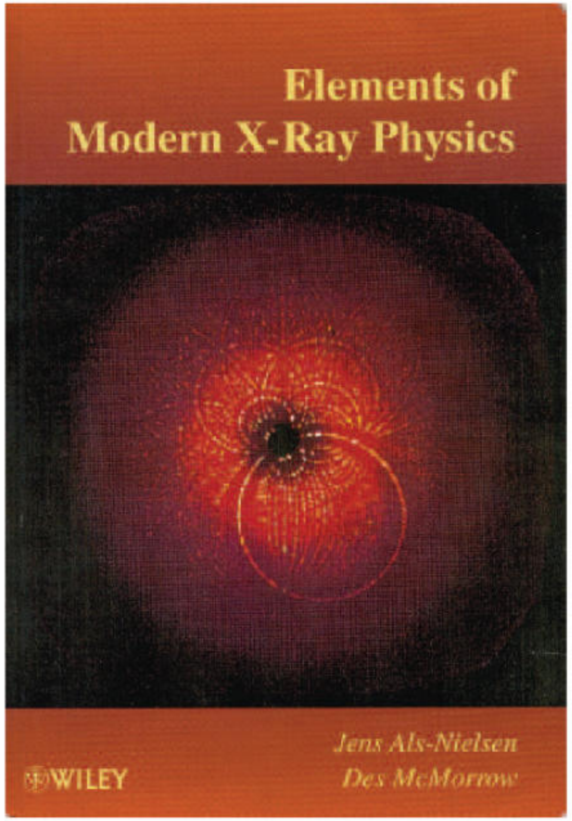
Basic concepts: Elements of Modern X-Ray Physics
J. A. Nielsen and D. McMorrow, J. Wiley&Sons (2001)
X-Ray Diffraction
B.E. Warren, DOVER Publications Inc,, New York
Principles of Optics
M.Born and E. Wolf, Cambridge University Press, 7th. ed.
Soft X-rays and Extreme Ultraviolett Radiation
D. Attwood, Cambridge University Press (2000)
http://www.coe.berkeley.edu/AST/sxreuv/)
Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen
K. Wille, Teubner Studienbücher 1996



SOFT X-RAYS AND EXTREME ULTRAVIOLET RADIATION

Principles and Applications

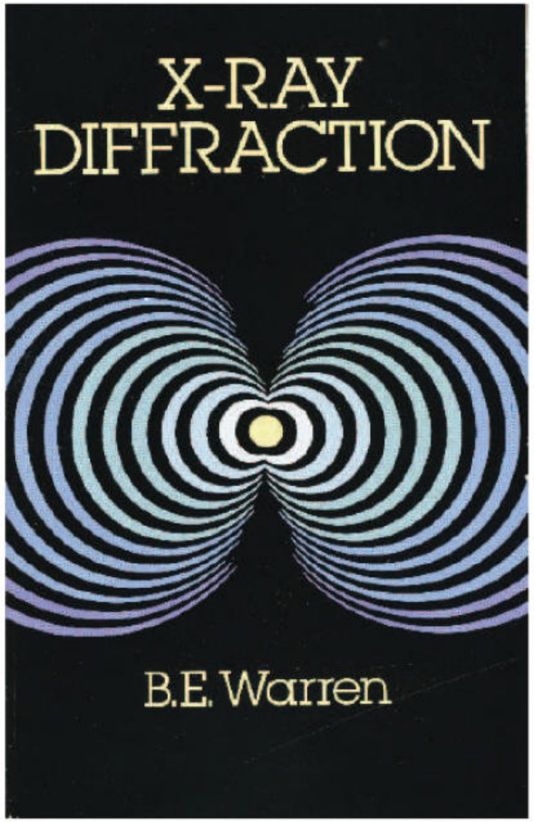
DAVID ATTWOOD



Elements of Modern X-Ray Physics

Jens Als-Nielsen
Des McMorrow

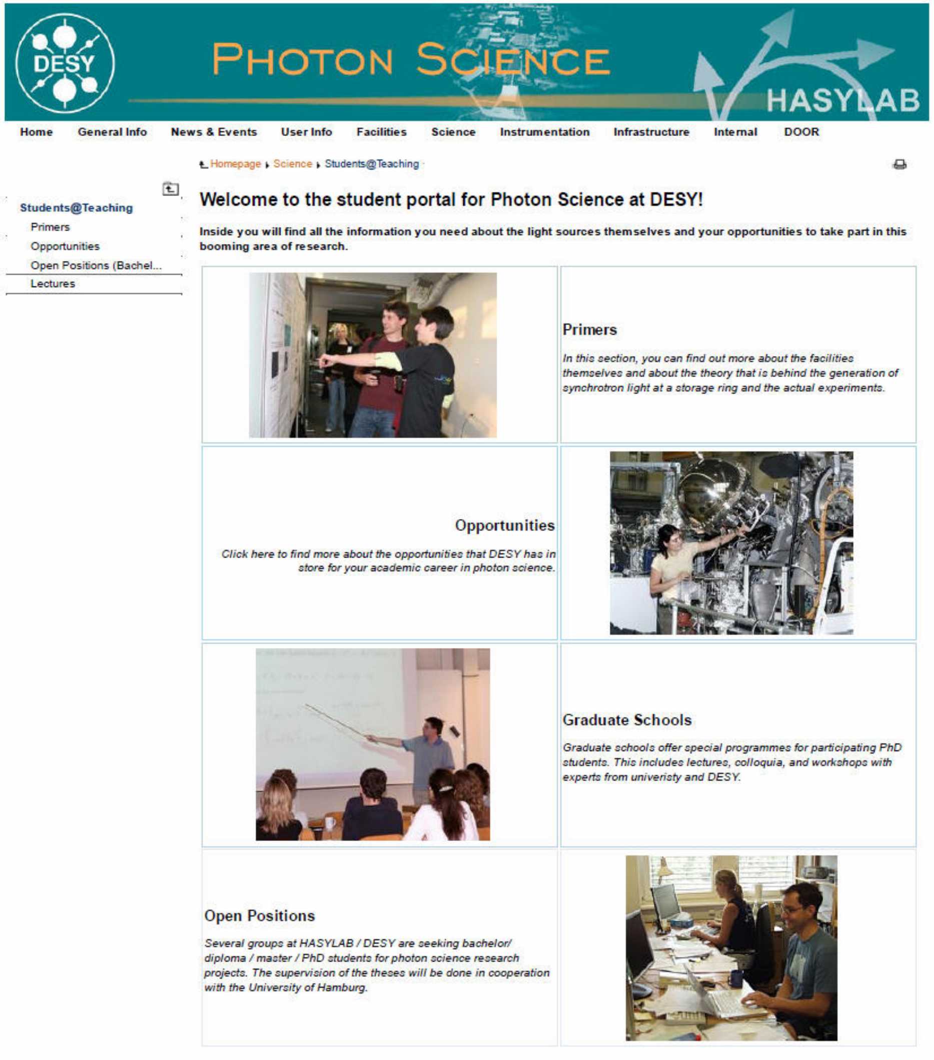
WILEY



X-RAY DIFFRACTION

B.E. Warren

http://hasylab.desy.de/science/studentsteaching/lectures/index_eng.html



Welcome to the student portal for Photon Science at DESY!

Inside you will find all the information you need about the light sources themselves and your opportunities to take part in this booming area of research.

Primers

In this section, you can find out more about the facilities themselves and about the theory that is behind the generation of synchrotron light at a storage ring and the actual experiments.

Opportunities

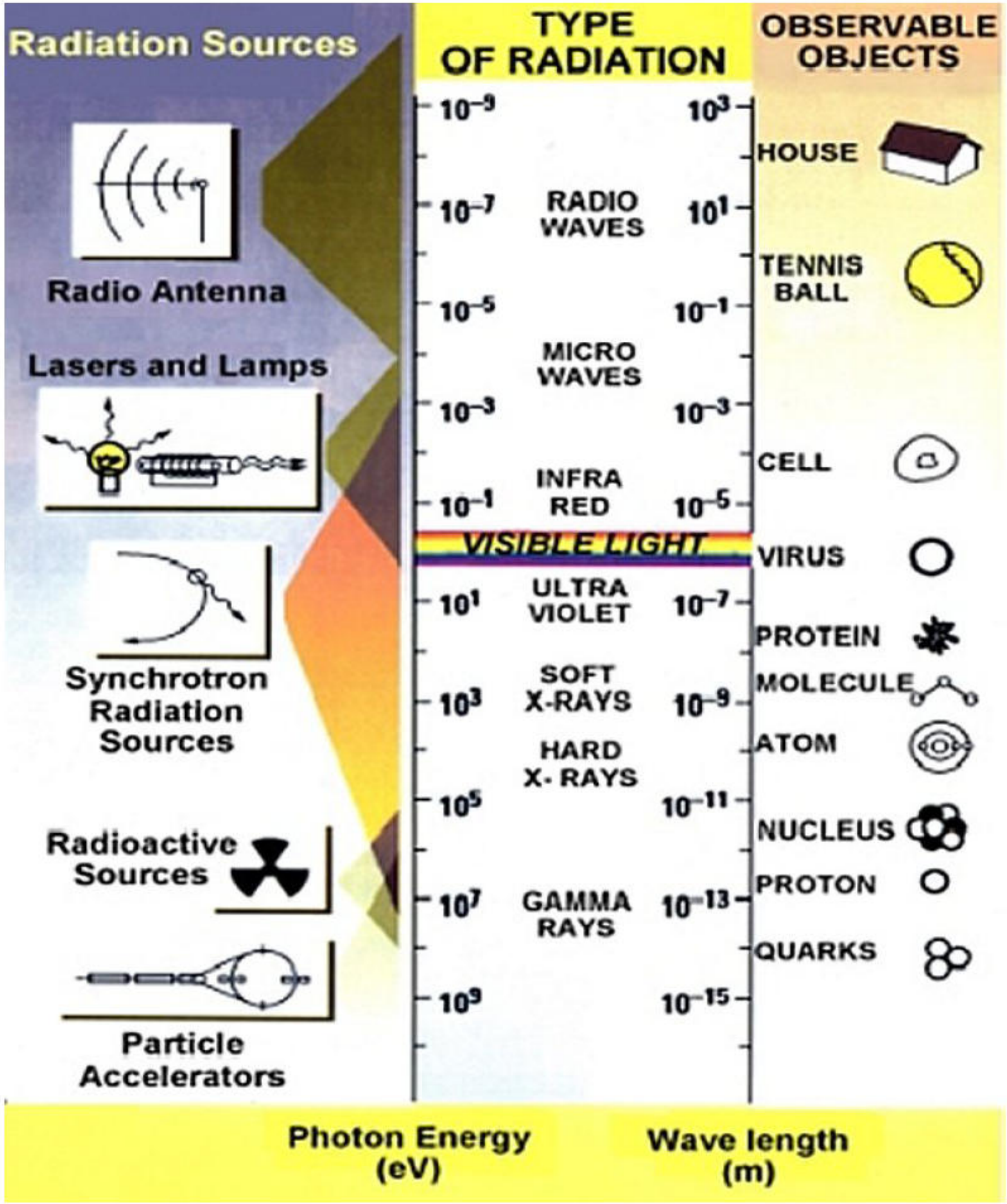
Click here to find more about the opportunities that DESY has in store for your academic career in photon science.

Graduate Schools

Graduate schools offer special programmes for participating PhD students. This includes lectures, colloquia, and workshops with experts from univeristy and DESY.

Open Positions

Several groups at HASYLAB / DESY are seeking bachelor/ diploma / master / PhD students for photon science research projects. The supervision of the theses will be done in cooperation with the University of Hamburg.



X-rays

≡

electromagnetic radiation

≡

Wavelength

(λ[Å]=12.398/E[keV])

≡

Object Size

≡

Ångstroms for Condensed Matter Research

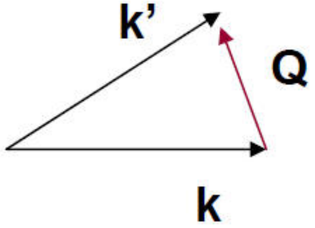
Scattering of X-rays

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

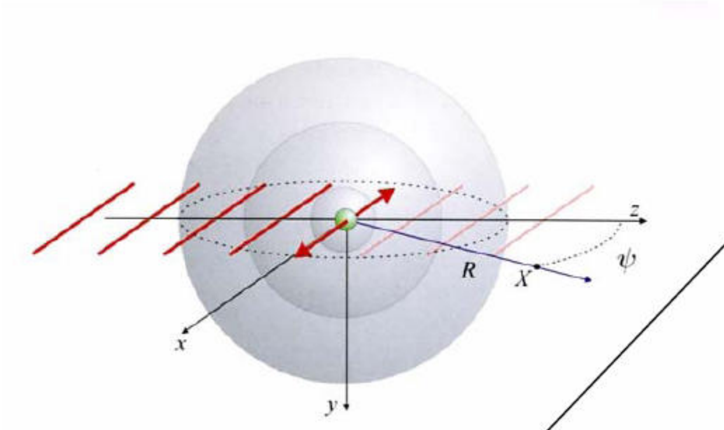
$\mathbf{E}(\mathbf{r},t) = \boldsymbol{\varepsilon}\, E_o \exp\{i(\mathbf{kr}-\omega t)\}$ with $|\mathbf{k}|=2\pi/\lambda$

elastic scattering:

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



Scattering by a single electron:



phase shift of π btw. incident and radiated field

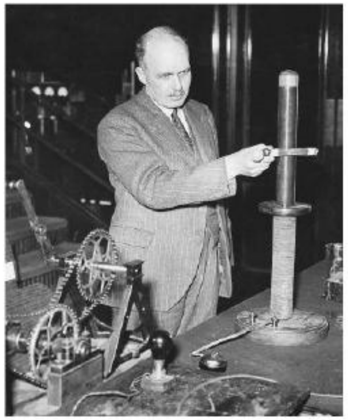
$E_{rad}(R,t)/E_{in} =$

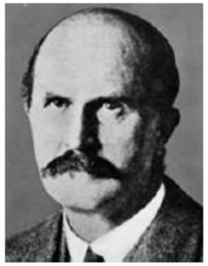
$-(e^2/4\pi\varepsilon_o mc^2)\underbrace{\exp(ikR)/R}_{\text{spherical wave}} \cos\psi$

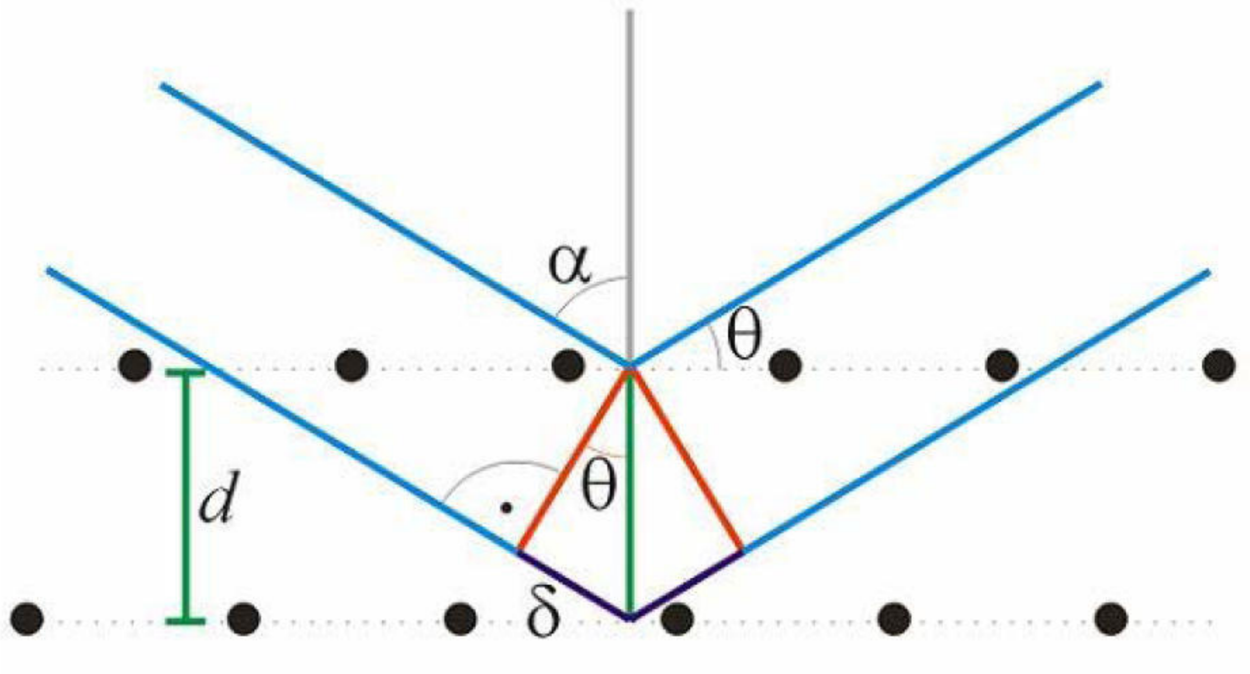
thomson scattering length r_o

(=2.82*10^{-5} Å)

Bragg's Law

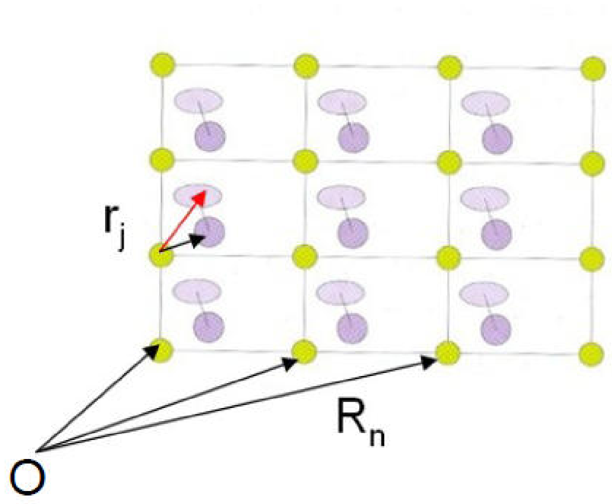






scattering intensity only if: $n\lambda = 2d\sin(\Theta)$

scattering by a crystal:



$$r_{j'} = R_n + r_j$$

lattice vector + atomic position in lattice

$$F^{crystal}(Q) = \underbrace{\Sigma_{rj}\, f_j(Q)\exp(iQr_j)}_{\text{unit cell structure factor}}\underbrace{\Sigma_{Rn}\exp(iQR_n)}_{\text{lattice sum}}$$

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

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

$$Q \bullet R_n = 2\pi \text{ x integer} \quad \text{and } Q = G$$

· Reciprocal Lattice

1-D: defined by (iia): $a_i \bullet a_j^* = 2\pi\, \delta_{ij}$

2-D and 3-D:

$$a_1^* = (2\pi/v_c)\, a_2 \times a_3$$

$$a_2^* = (2\pi/v_c)\, a_3 \times a_1$$

$$a_3^* = (2\pi/v_c)\, a_1 \times a_2$$

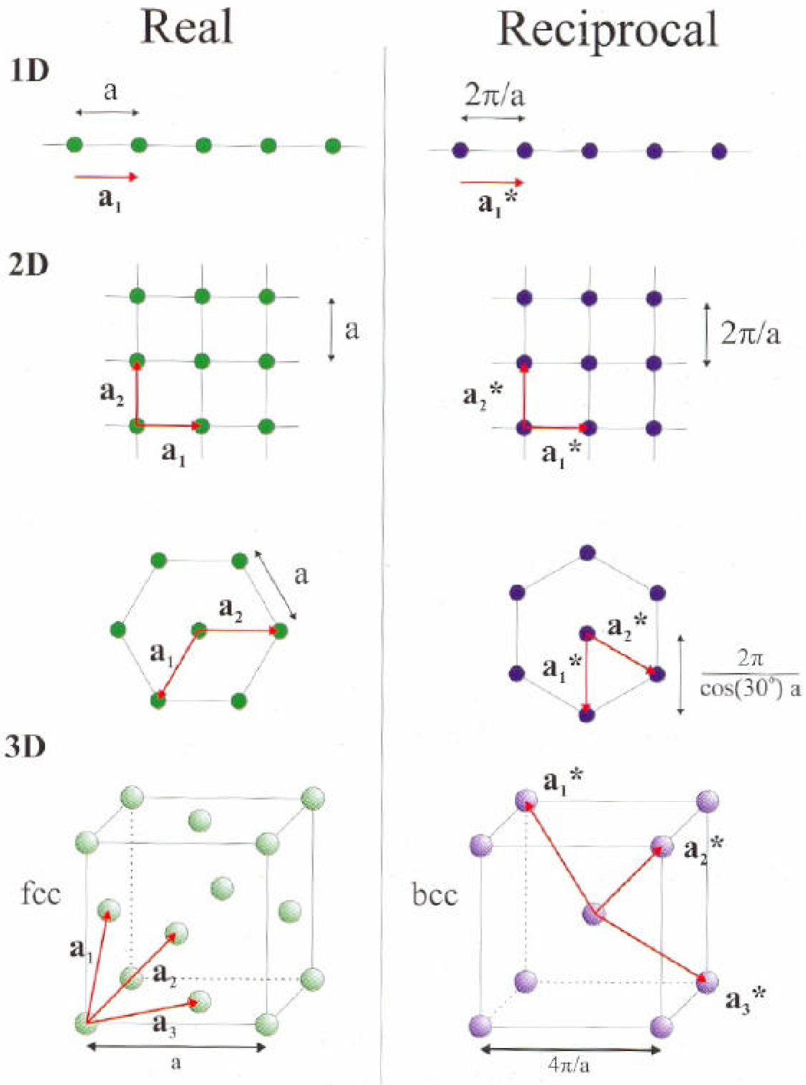
with $v_c = a_1 \bullet (a_2 \times a_3)$

note: in 2-D a_3 is chosen to be a unit vector normal to the 2-D plane spanned by a_1 and a_2.

Example: fcc lattice

$a_1=(a/2)(y'+z')$, $a_2=(a/2)(z'+x')$, $a_3=(a/2)(x'+y')$

$$a_1^* = (4\pi/a)\,(y/2+z/2-x/2)$$
$$a_2^* = (4\pi/a)\,(z/2+x/2-y/2)$$
$$a_3^* = (4\pi/a)\,(x/2+z/2-y/2)$$



The Ewald shere

Visualisation of diffraction effects in reciprocal space (a).

Laue condition requires Q = G = $ha_1^* + ka_2^*$

Design sphere with radius k pointing to origin (b).

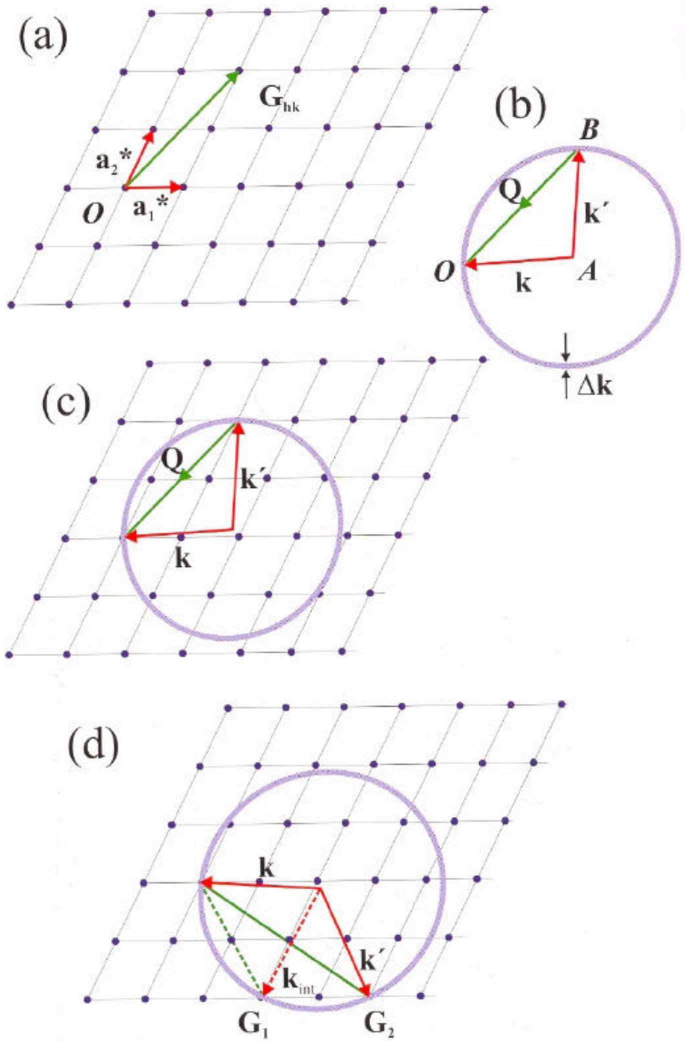
If any reciprocal lattice point falls on the circle then the Laue conditions is fulfilled (c).

Intensity is observed if the detector is placed in the direction of k’ (c).

A rotation about O corresponds to a rotation of the crystal.

<u>Note:</u> More than one reciprocal lattice point can lie on the sphere ≡ multiple scattering.

If the beam is not monochromatic the sphere adopts the corresponding width. In the white beam case all spots are ultimately detected.



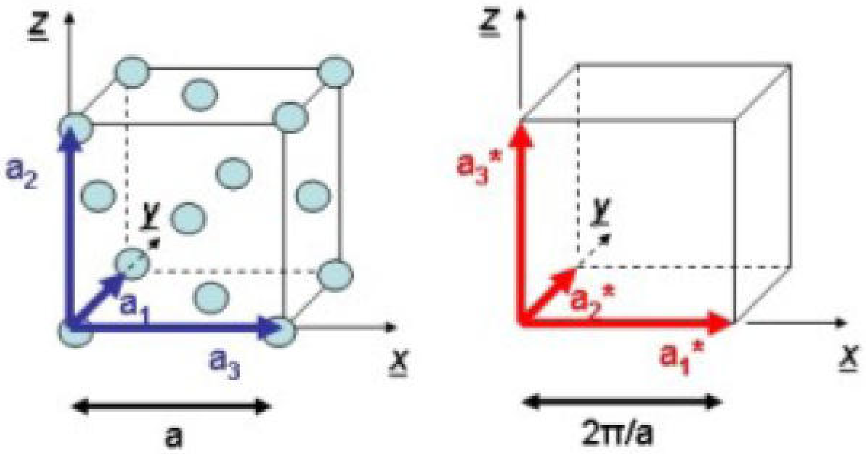
unit cell structure factor: $\Sigma_{r_j} f_j(Q)\exp(iQr_j)$

e.g. fcc lattice: $r_1 = 0$

$r_2 = ½\,(a_1+a_2)$

$r_3 = ½\,(a_2+a_3)$

$r_4 = ½\,(a_3+a_1)$



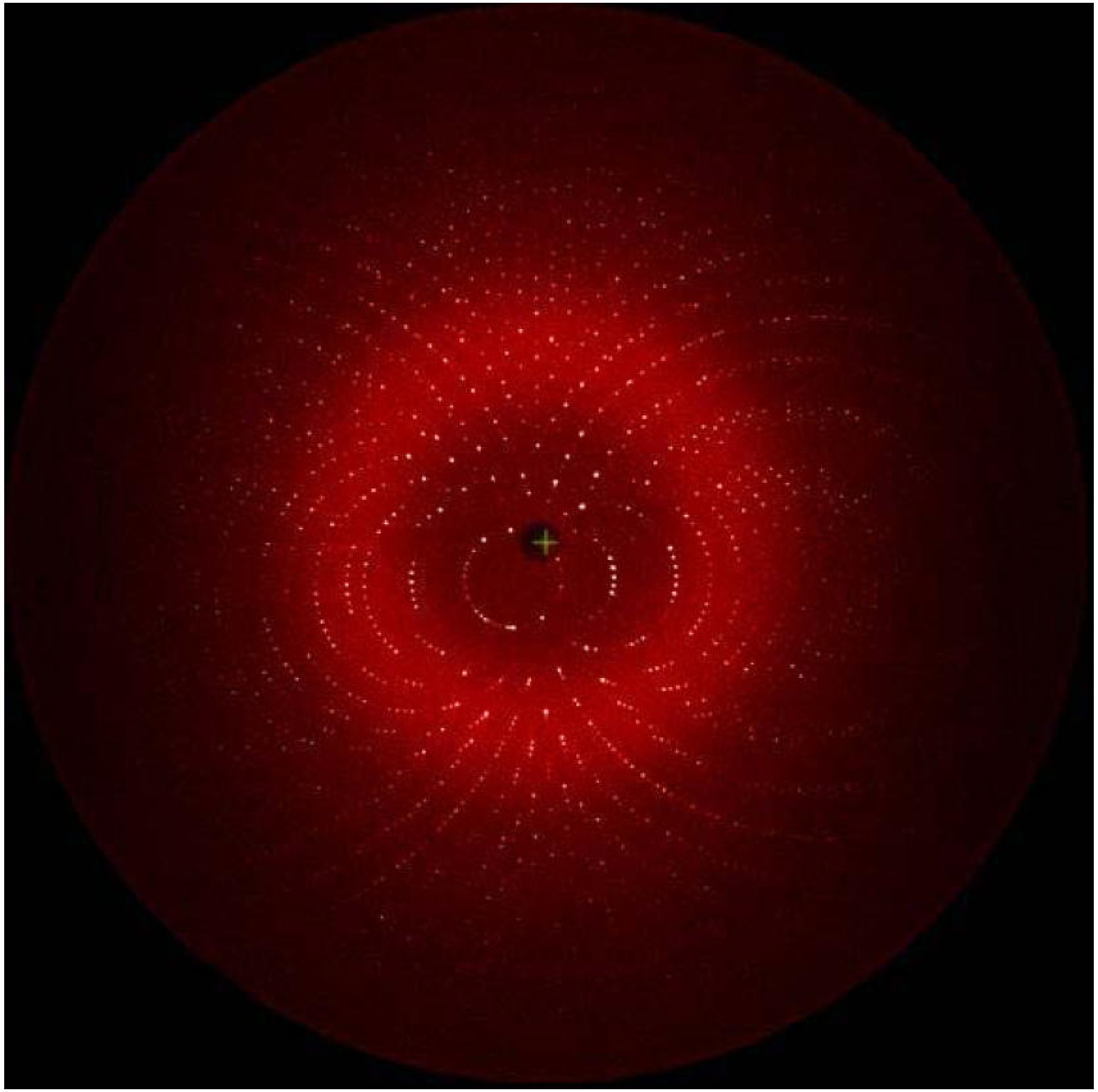
$a_1=a\underline{x}$; $a_2=a\underline{y}$; $a_3=a\underline{z}$; $v_c = a^3$; $a_1^*=(2\pi/a)\underline{x}$; $a_2^*=(2\pi/a)\underline{y}$; $a_3^*=(2\pi/a)\underline{z}$

$F_{hkl}^{fcc} = f(Q)\,\Sigma\exp(iQr_j)$ with $Q = G = h\,a_1^* + k\,a_2^* + l\,a_3^*$

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

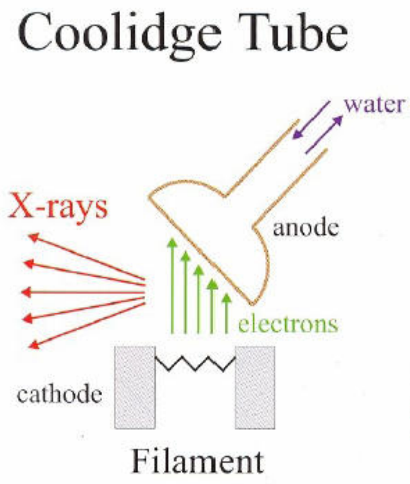
$$= f(Q) \times \begin{cases} 4 & \text{if h,k,l are all even or odd} \\ 0 & \text{otherwise} \end{cases}$$

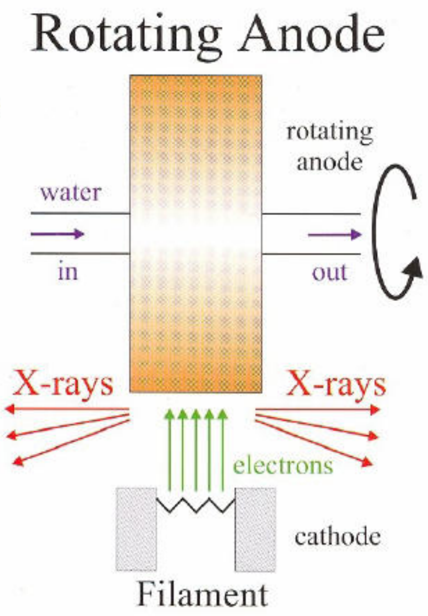
Modern Protein Crystallography

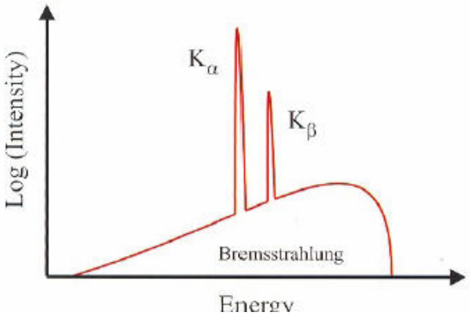


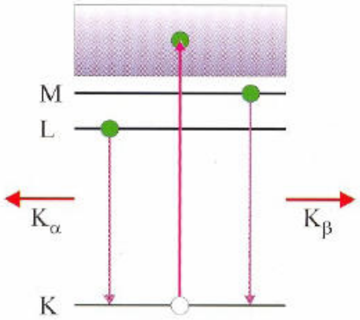
Sources of X-Rays

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)









HochleistungsRöntgenröhren

- Einfach zu handhaben
- Einsetzbar in fast jedem Labor
- Tpyisch nur zwei Anregungsenergien:
  Mg $K\alpha$ (1.2 keV) und Al $K\alpha$ (1.4 keV)
- Nicht durchstimmbar
- geringe Leistung
- schlechte Auflösung; ΔE 1-2 eV (natürliche Linienbreite der atomaren Übergänge)

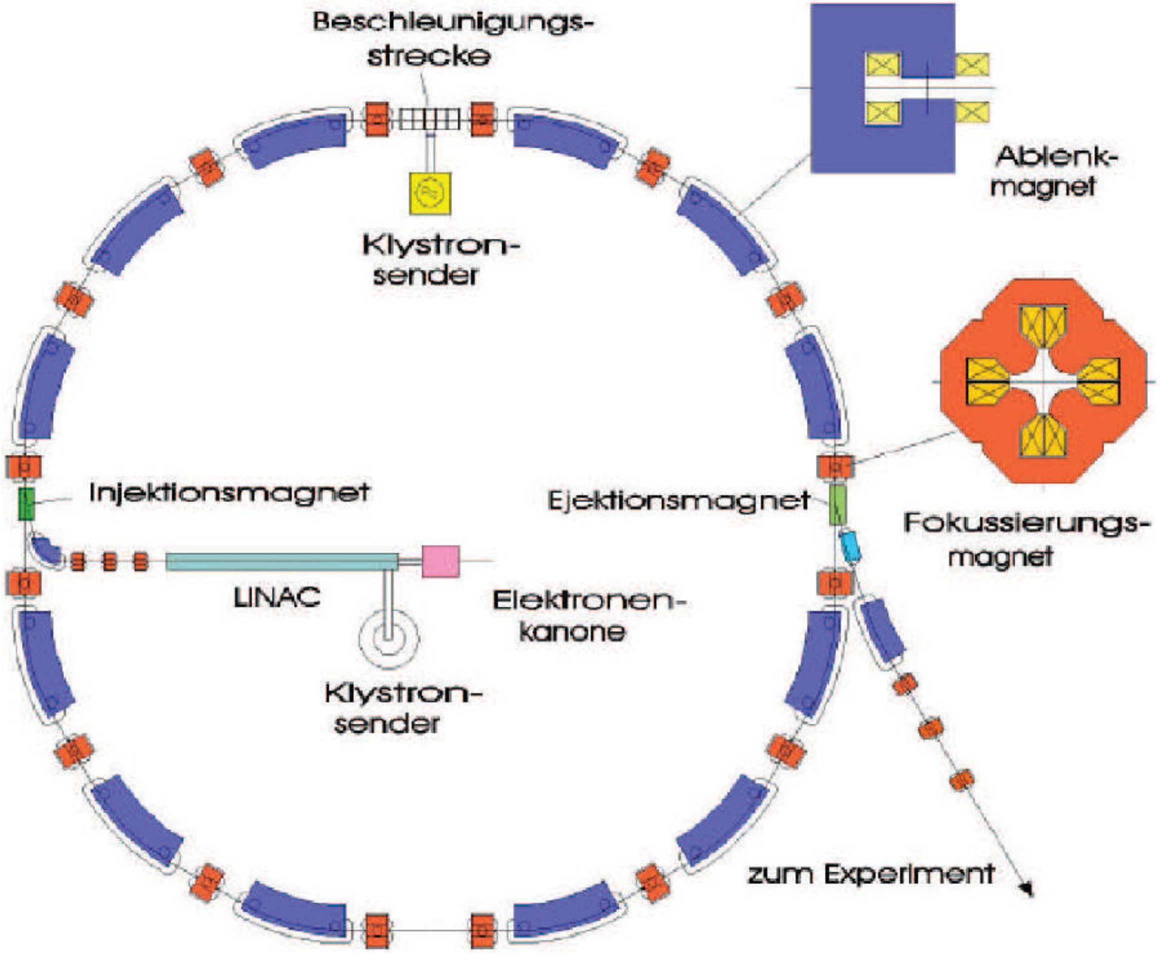
Synchrotronstrahlung

- Photonenenergie *frei* wählbar zwischen dem Infraroten (THz Strahlung) und harter Röntgenstrahlung ($>$100 keV)
- Sehr hohe Photonenzahlen
- Polarisation der Strahlung frei wählbar
- Großgerät

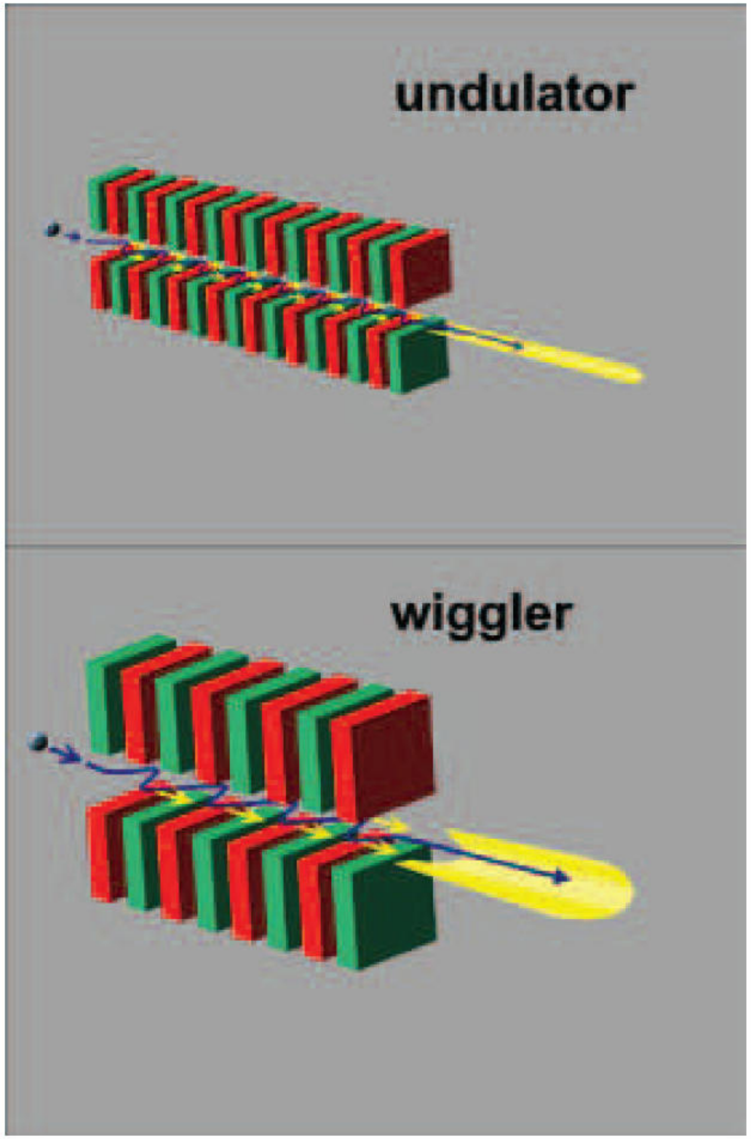
Freie Elektronen Laser (FEL)

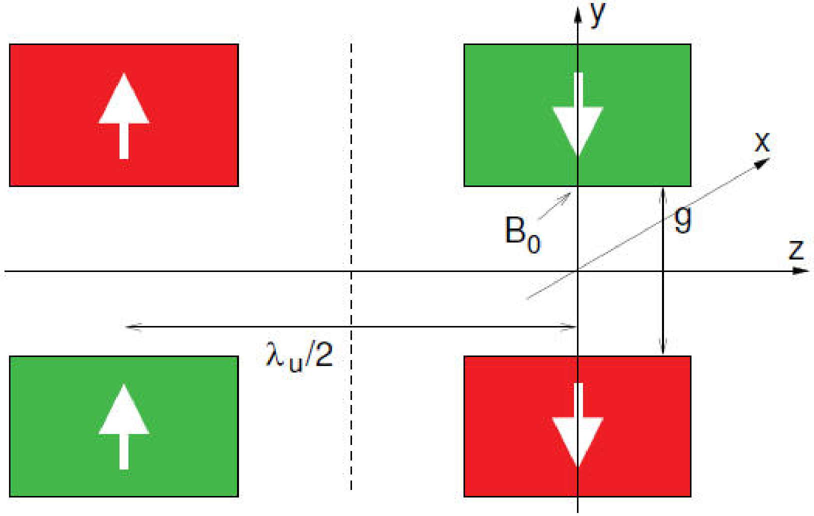
- Laserstrahlung im Röntgenbereich
- Extrem hohe Photonendichten
- Sehr kurze Lichtpulse (einige 10 fs)
- Photonenenergien in der Zukunft bis zu 14 keV

Aufbau eines Synchrotrons



Insertion Devices (IDs)





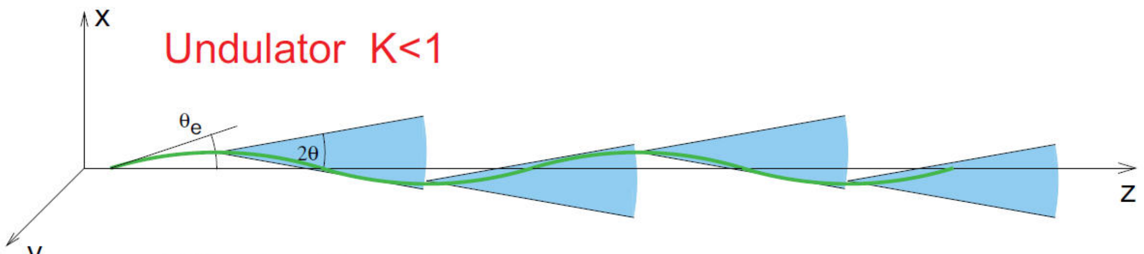
$$
\begin{aligned}
\bar{B} &= \frac{B_0}{\cosh \pi \frac{g}{\lambda_u}} \\
B_y(z) &= \bar{B} \cos \frac{2\pi}{\lambda_u} z
\end{aligned}
$$

$$v_x = \frac{Kc}{\gamma} \sin \frac{2\pi}{\lambda_u} z$$

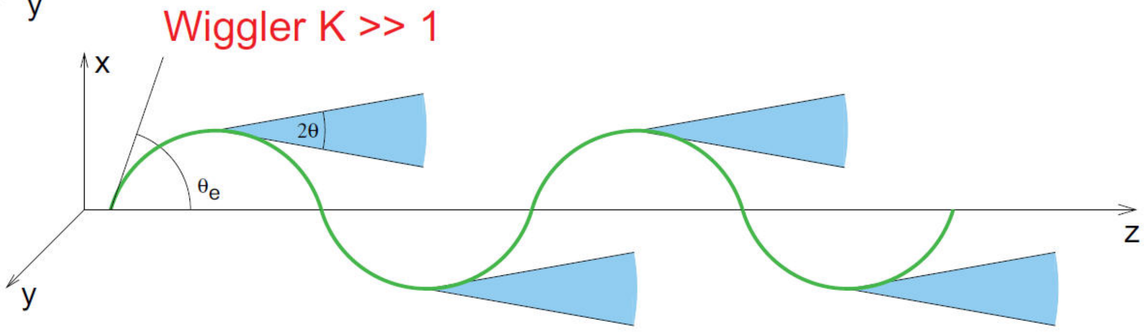
$$\text{mit} \quad K := \frac{e\bar{B}\lambda_u}{2\pi m_0 c}$$

$$|\theta_{e,max}| \approx \frac{K}{\gamma}$$

$$\gamma = \left(1 - \frac{v^2}{c^2}\right)^{-1/2}$$



Undulator K<1



Wiggler K >> 1

Undulator Parameter

Charakteristischer Abstrahlwinkel der SR: $\theta = 1/\gamma$, $\theta_e = K/\gamma$

$K \leq 1$ Undulator

Abstrahlkegel der einzelnen Magnetpole überlappen → kohärente Überlagerung → Interferenzeffekte

$K \gg 1$ Wiggler

Abstrahlkegel der einzelnen Magnetpole überlappen nicht → Nicht kohärente Überlagerung → Emittierte Strahlung entspricht weitgehend der eines Dipols, aber mit $2 \cdot N$ facher Intensität.

Wellenlänge λ der Undulatorstrahlung:

$$\lambda = \frac{\lambda_u}{2\gamma^{*2}}(1 + \gamma^{*2}\theta^2) = \frac{\lambda_u}{2\gamma^2}\left(1 + \frac{K^2}{2} + \gamma^2\theta^2\right) \tag{5}$$

Vergleich der verschiedenen Quellen

Dipol: P
Wiggler: $N \cdot P$
Undulator: $N^2 \cdot P$

Beim FEL werden wir sehen, daß für diesen dann

$$N^2 \cdot N_e^2$$

gilt

- Eine wichtige Größe zur Charakterisierung von Synchrotronstrahlung ist die Brillianz

$$B := \frac{\Delta P}{\Delta A \cdot \Delta \Omega}$$

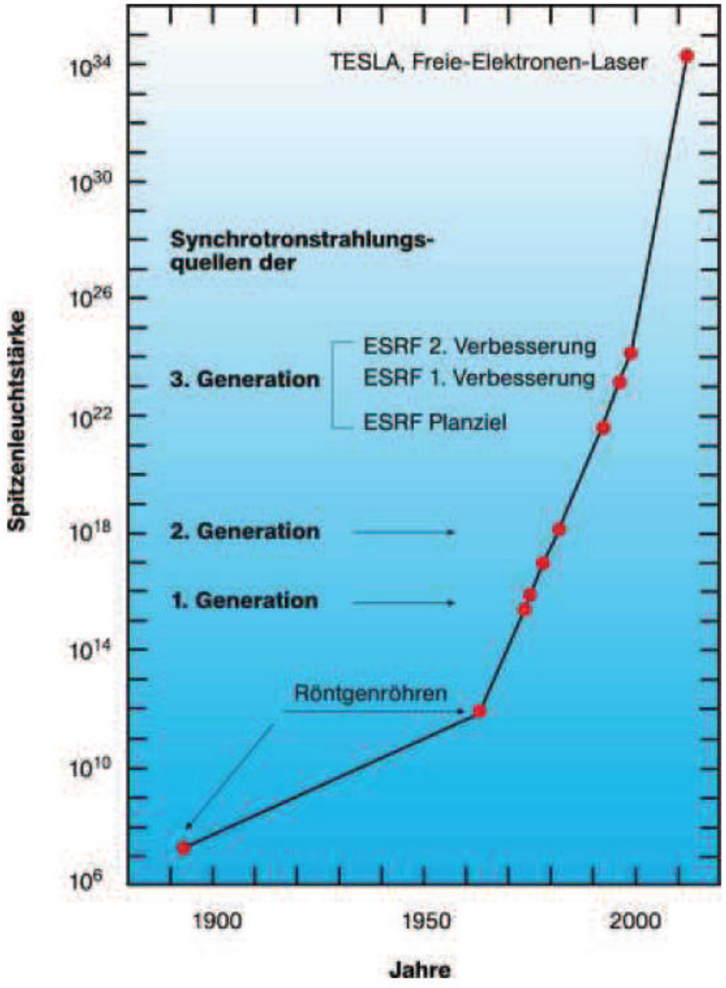
  Spektrale Brillianz

$$B_{\Delta\omega/\omega} := \frac{\Delta P}{\Delta A \cdot \Delta \Omega \cdot \Delta\omega/\omega}$$

- Dichte der Photonen im transversalen Phasenraum
- Um eine möglichst hohe Photonendichte am Ort des Experimentes zu erreichen, muß die Brillianz so groß wie möglich sein
- Größtmöglich Brillianz → Laser
- Einheit

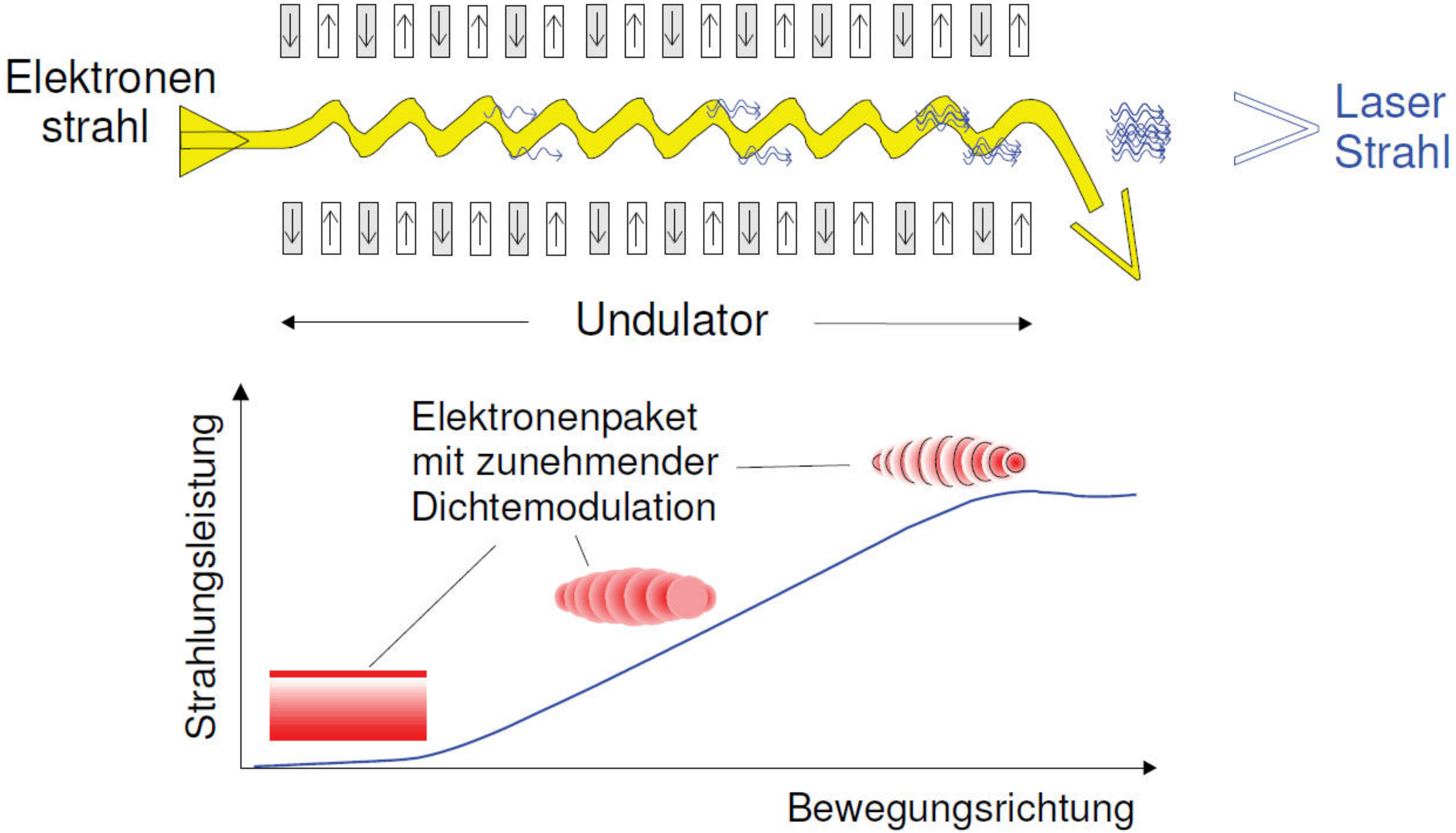
$$[B_{\Delta\omega/\omega}] = \frac{Photonen}{s \cdot mm^2 \cdot mrad^2 \cdot 0.1\%\mathrm{BW}}$$

Brillianz



- Entwicklung der Brillianz verschiedener Röntgenquellen mit der Zeit

Das FEL Prinzip



Elektronen strahl

Laser Strahl

Undulator

Strahlungsleistung

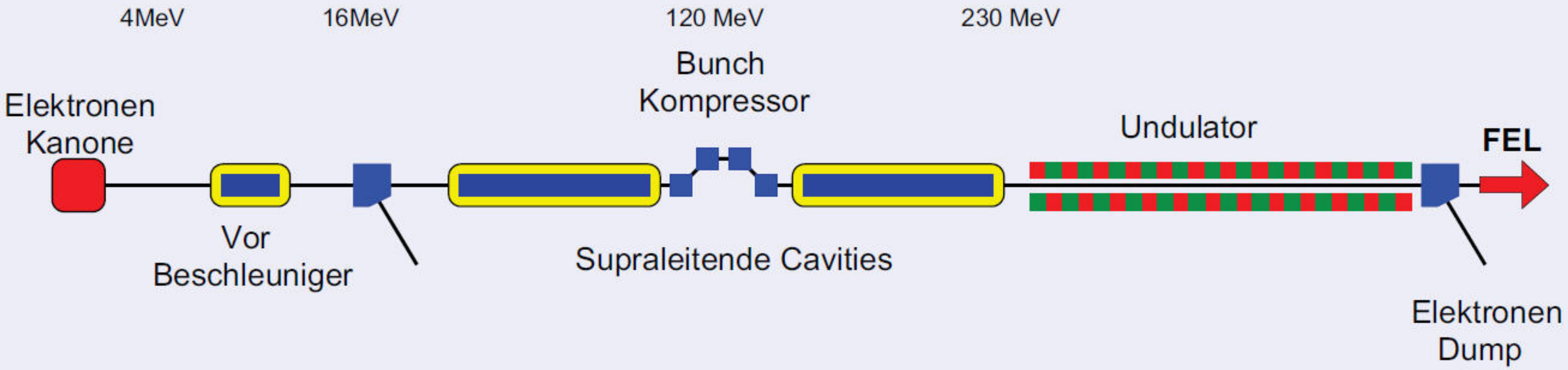
Elektronenpaket
mit zunehmender
Dichtemodulation

Bewegungsrichtung

Aufbau eines FEL

- Elektronenquelle: Erzeugung eines Elektronenbunches
- Beschleuniger: Beschleunigung auf relativistische Energien
- Magnetstruktur: Erzeugung der Röntgenstrahlung – Synchrotronstrahlung
- Röntgenoptik: Transport der FEL-Strahlung zum Experiment

Experiment



Realisierung eines FEL

Erster VUV-FEL

FLASH am Hasylab/DESY

Eigenschaften XFEL

- Typische Länge des Beschleunigers: 30-2000 m
- Länge der Magnetstruktur: 30-300 m
- Photonenenergiebereich 10 eV - 10 keV
- Pulslängen 10 – 100 *fs* (jetzt)

- Zahl der Photonen, die man an aktuellen Synchrotronquellen in 1 s bekommt, erzeugt ein FEL in 50 fs !