Synchrotron Radiation

Illuminating the NanoCosmos

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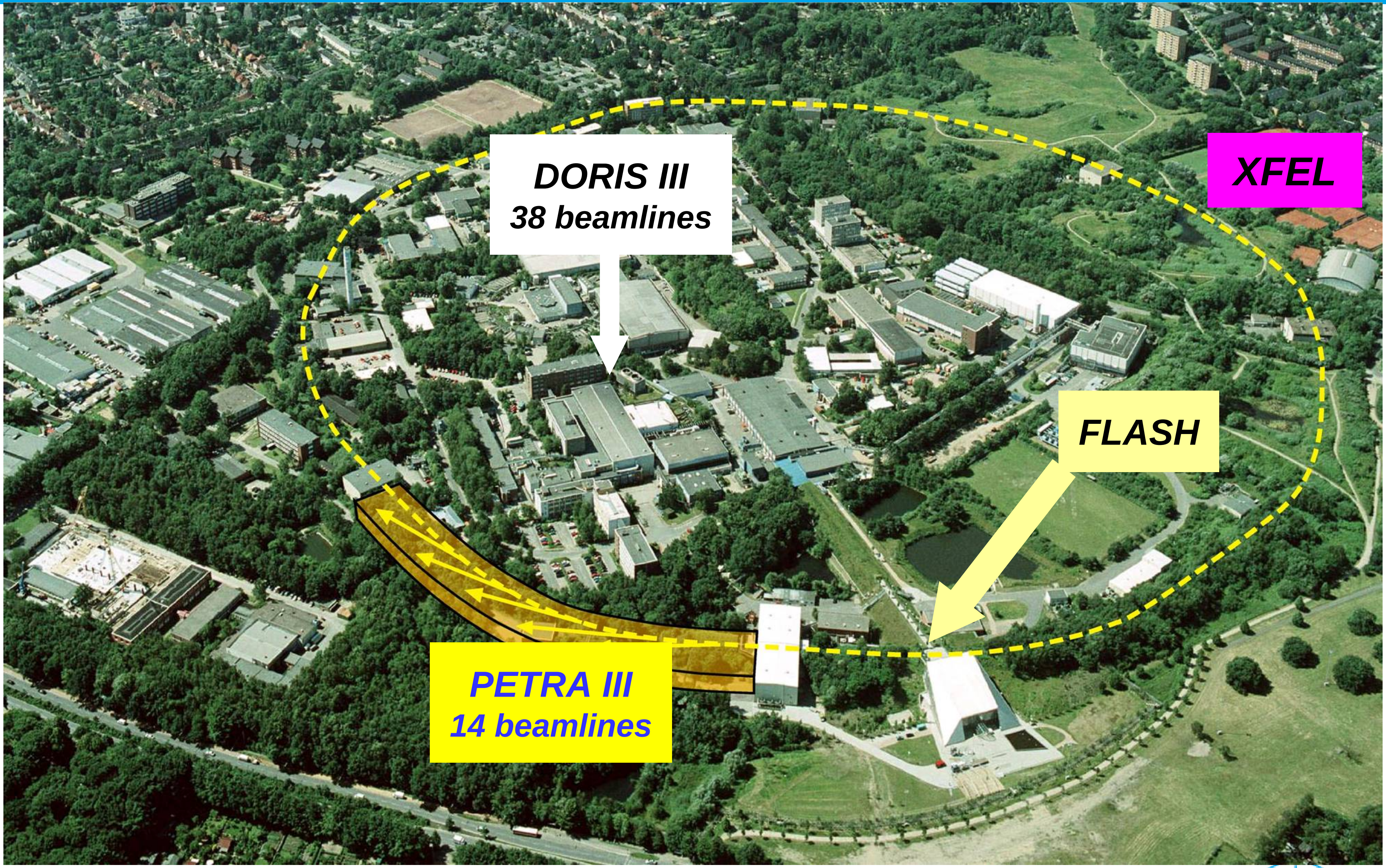
IX. Research Course on New X-Ray Sciences
17. February 2010

Outline

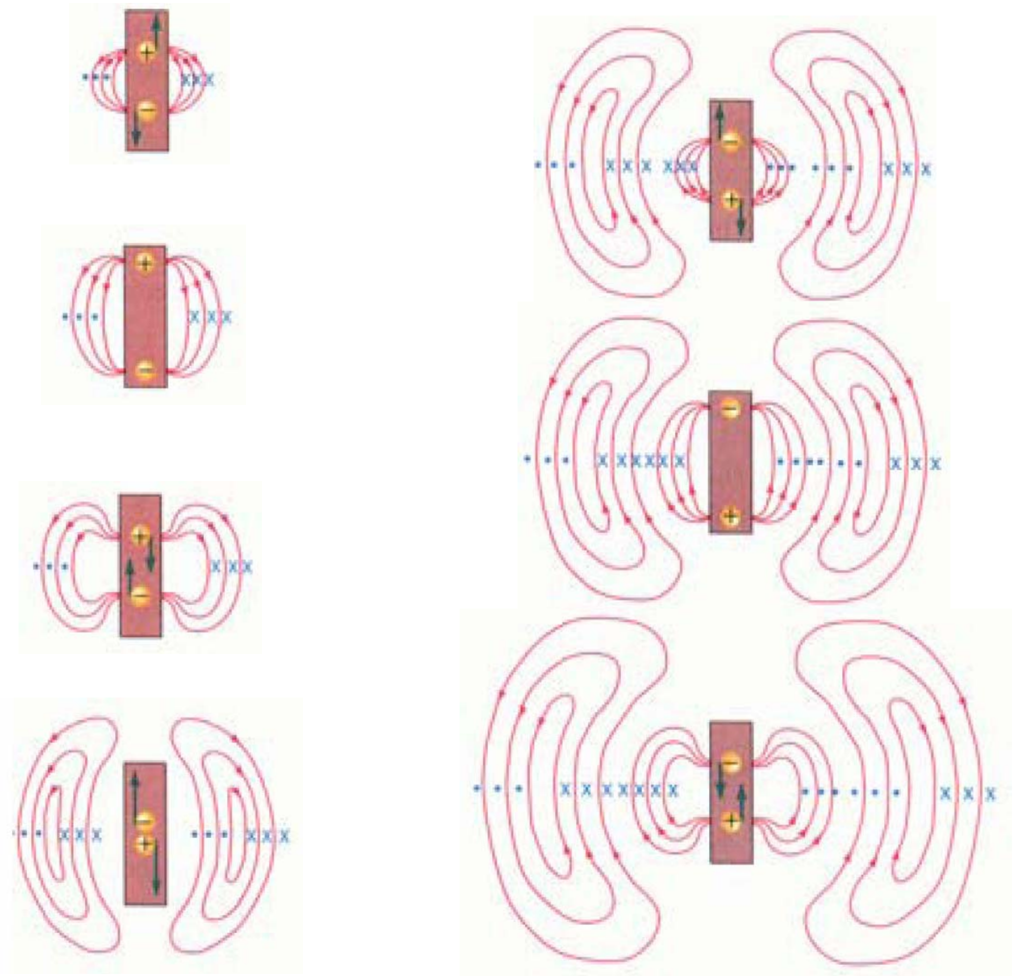
- Generation and Properties of Synchrotron Radiation
- Synchrotron Radiation Sources at DESY
- Research Examples
  - Protein Crystallography
  - Buried Interfaces

Photon Sources at DESY



The Electric Dipole (1)

Electric and magnetic fields around an oscillating electric dipole



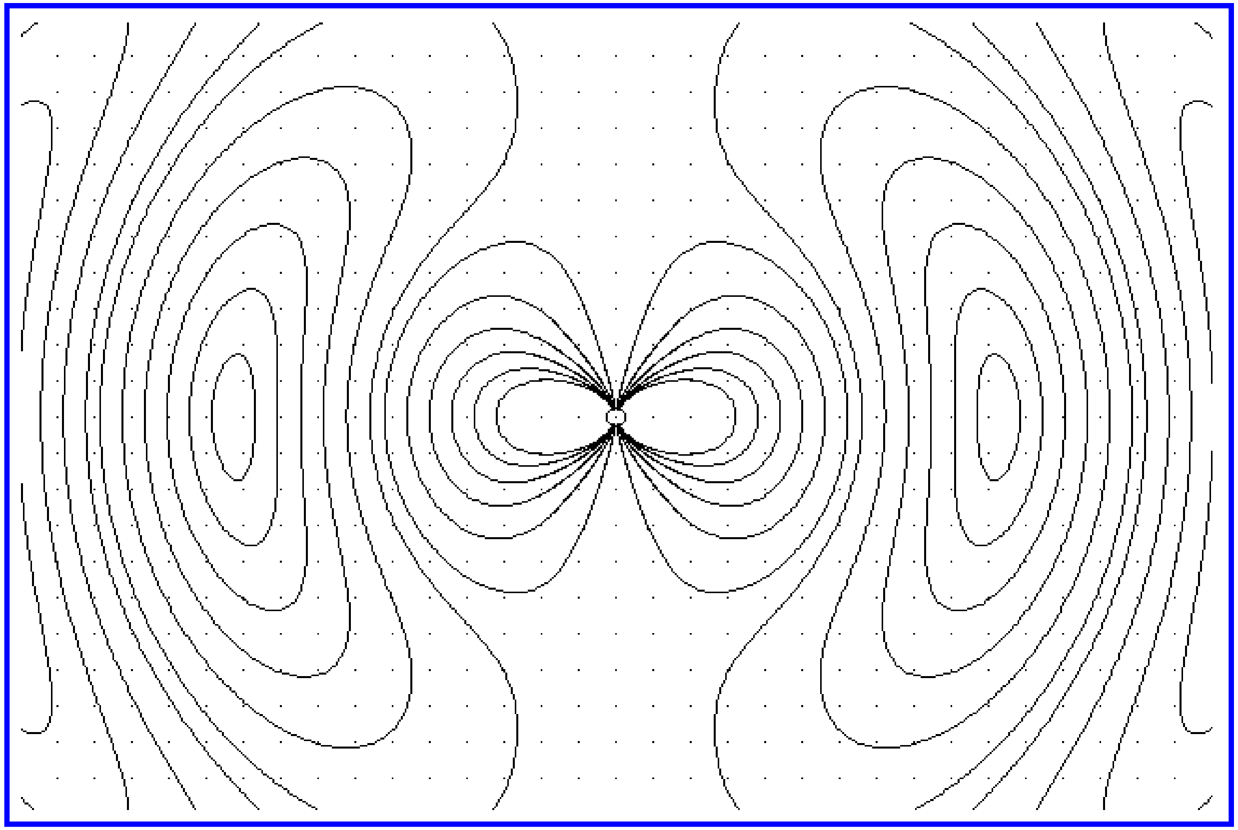
First Halfperiod:
E- and B-fields
propagate into space

Second Halfperiod:
Change of sign, the outer
fields decouple and
propagate freely.

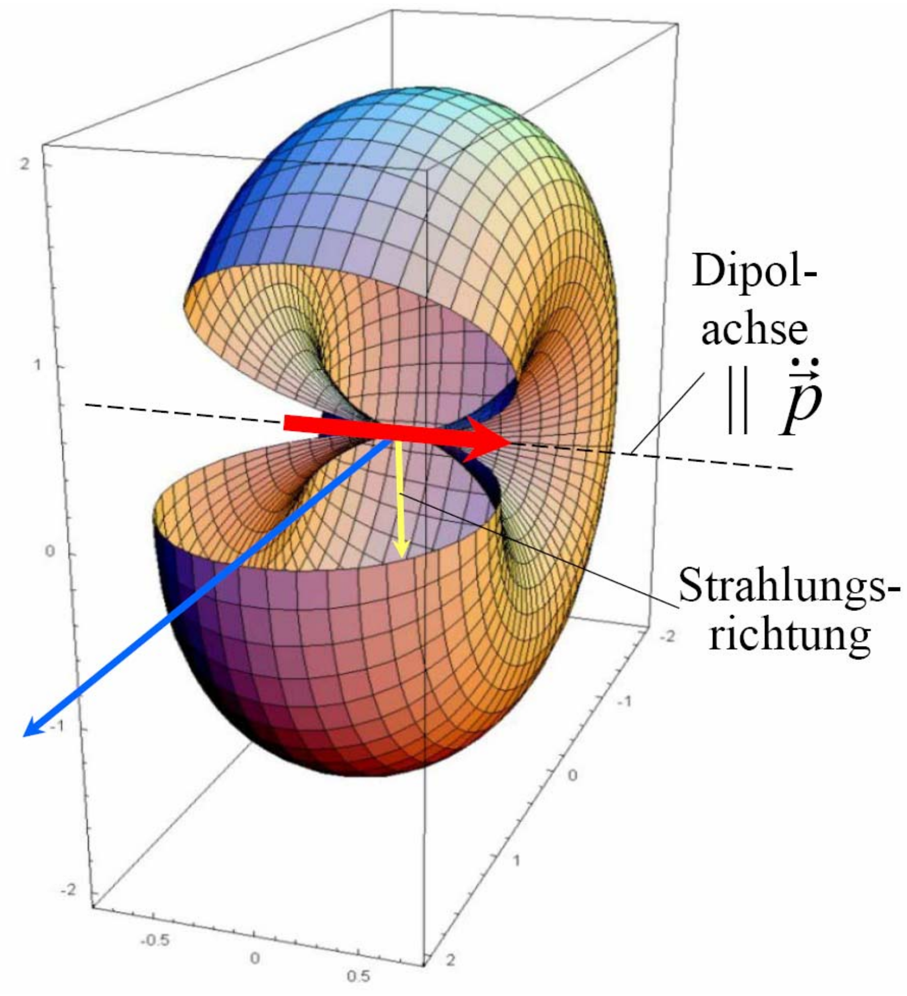
The Electric Dipole (2)

→ Generation of electromagnetic waves

→ Field lines around an oscillating electric dipole



Radiation characteristic of a Hertz dipole



Every accelerated charge radiates electromagnetic waves

Radiated power

$$P = \frac{e^2}{6\pi\varepsilon_0 m^2 c^3}\left(\frac{d\vec{p}}{dt}\right)^2$$

Larmor formula

Oscillatory motion:
No radiation in direction of the oscillation.

Maximum radiated power perpendicular to the oscillation direction:

Circular Acceleration: Synchrotron Radiation

Radiated power of an accelerated charged particle for nonrelativistic particles: Larmor formula

$$P_S = \frac{e^2}{6\pi\,\epsilon_0\,m_0^2\,c^3}\left|\frac{d\vec{p}}{dt}\right|^2$$

Lorentz transformation and application to circular acceleration:

$$\boxed{P_S = \frac{e^2 c}{6\pi\,\epsilon_0}\,\frac{1}{(m_0 c^2)^4}\,\frac{E^4}{R^2}}$$

E = particle energy
R = radius of curvature
m_0 = particle mass

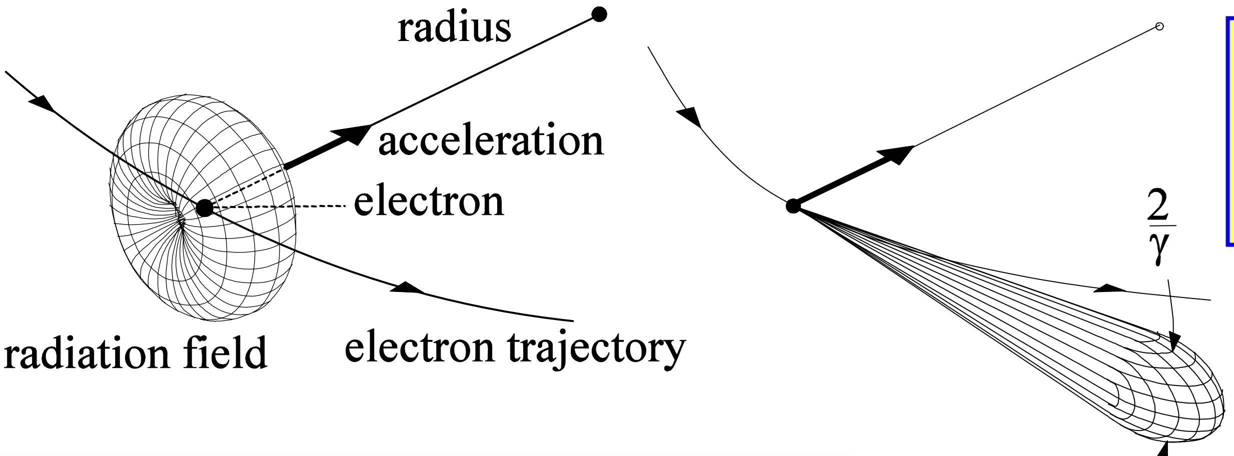
Dependence on particle mass:

$$\boxed{\frac{P_{S,e}}{P_{S,p}} = \left(\frac{m_p}{m_e}\right)^4 \approx 10^{13}}$$

Synchrotron radiation is sufficiently intense only for electrons/positrons !

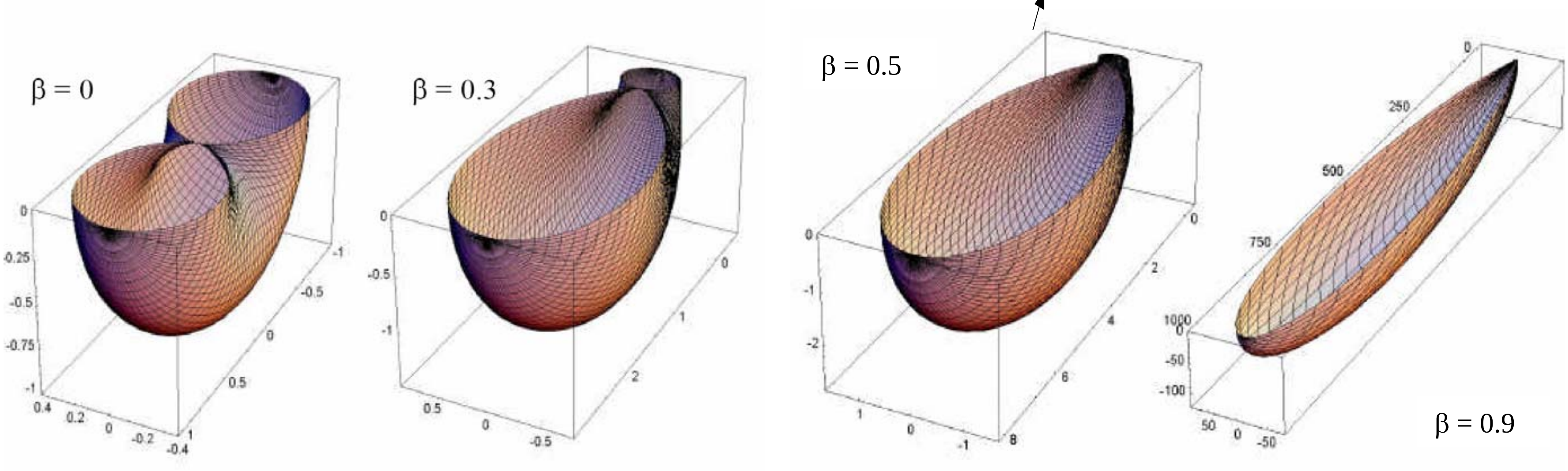
Emission pattern for circular acceleration

Rest frame $\xrightarrow{\text{Lorentz transformation}}$ Laboratory frame

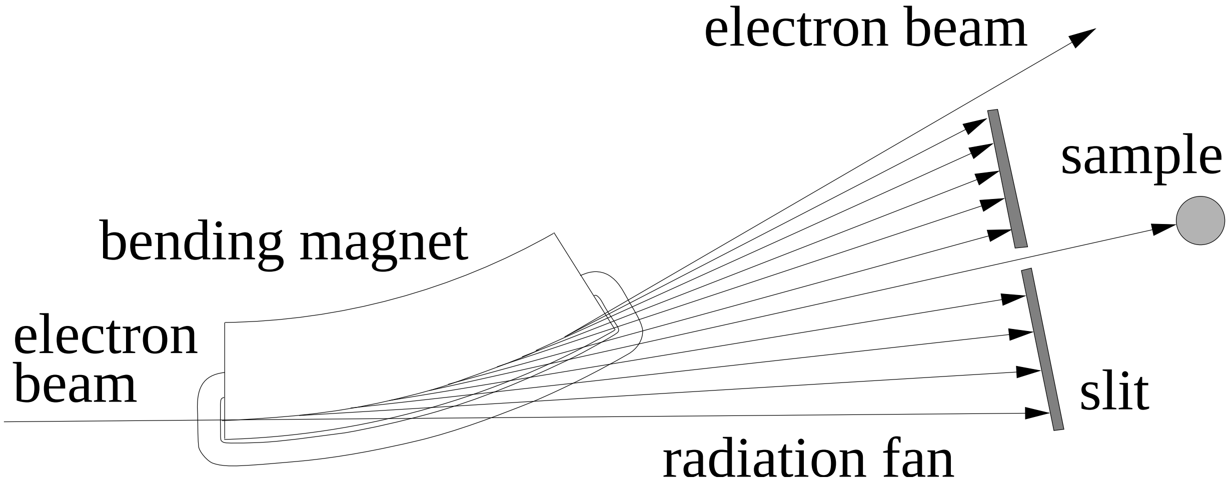


$$\gamma = \frac{1}{\sqrt{1-\left(\frac{v}{c}\right)^2}} = \frac{E}{m_0c^2}$$

Opening angle

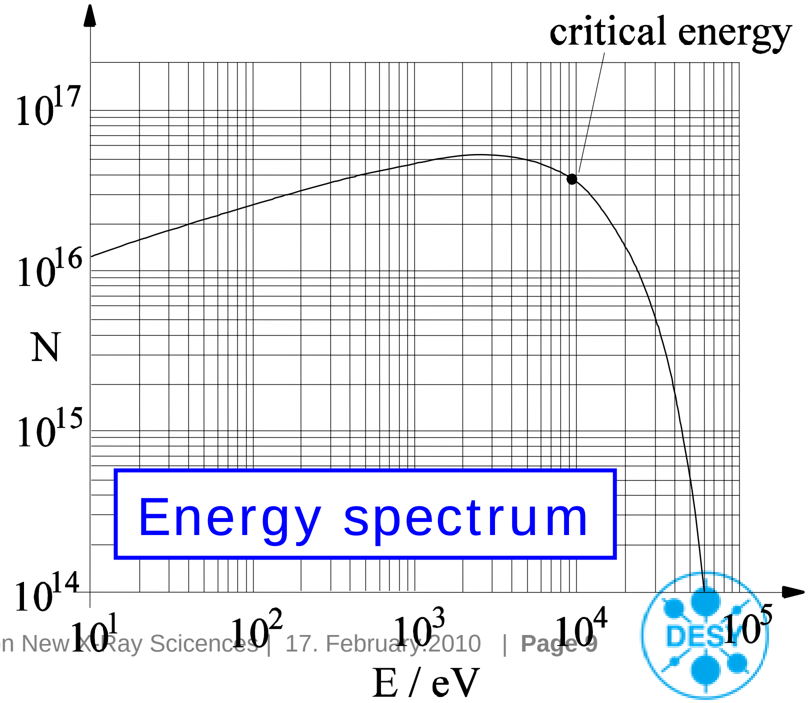


Radiation from a bending magnet



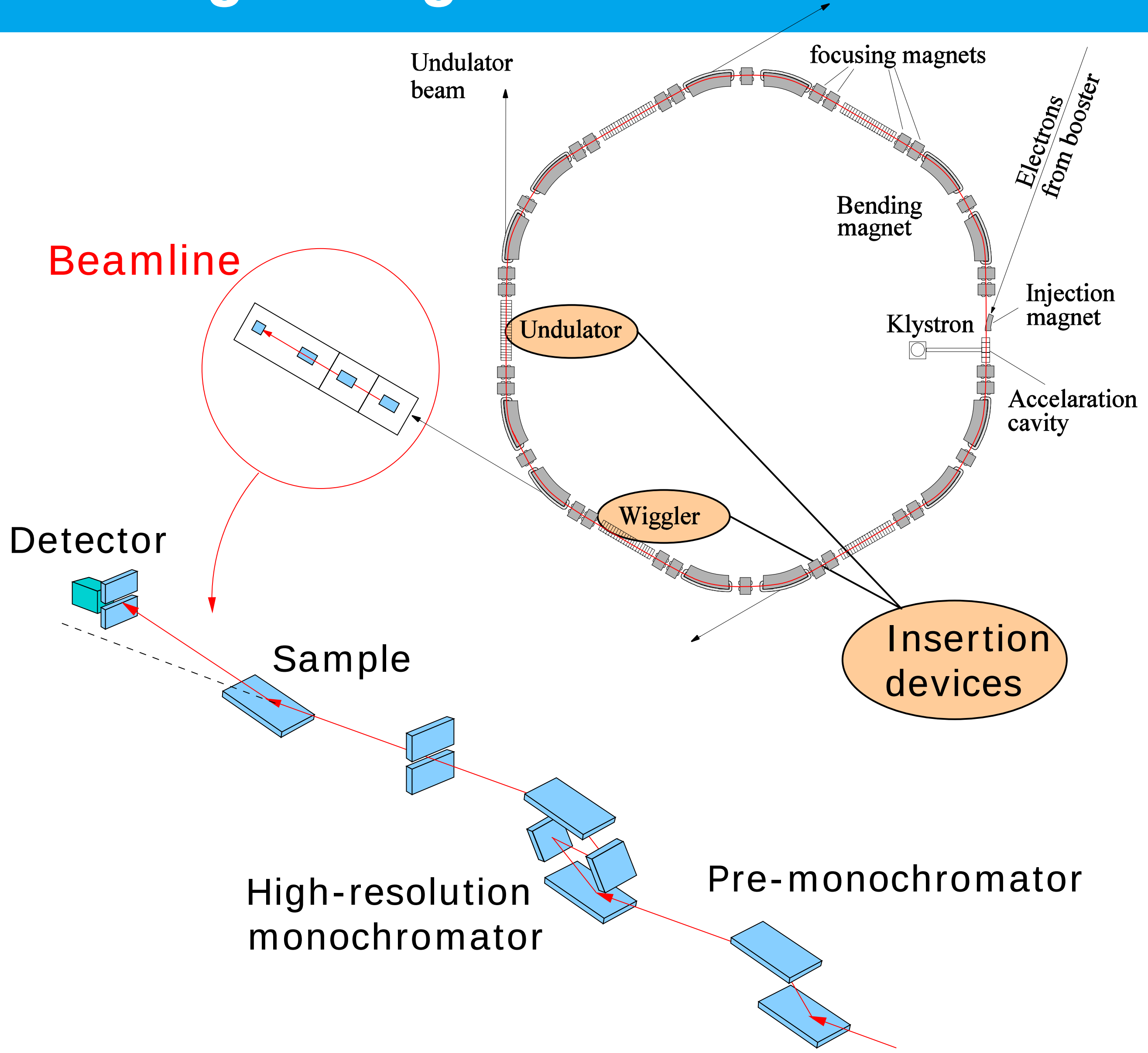
$$\begin{aligned} E &= 5\,\mathrm{GeV} \\ \Longrightarrow\ \gamma &= 10^4 \\ \Longrightarrow\ \Delta\Theta &= \frac{2}{\gamma} = 0.2\,\mathrm{mrad} \approx 40'' \end{aligned}$$

- The radiation is emitted in the plane of the orbiting particles
- The radiation is linearly polarized in the orbit plane

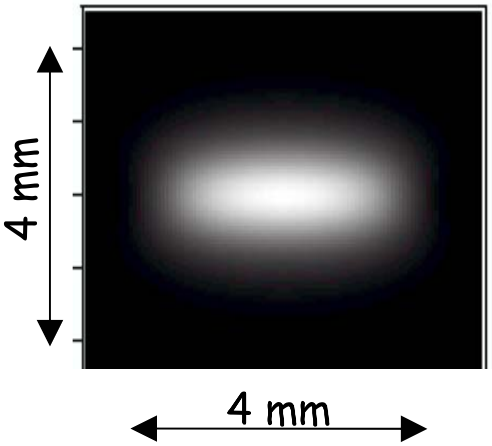


Energy spectrum

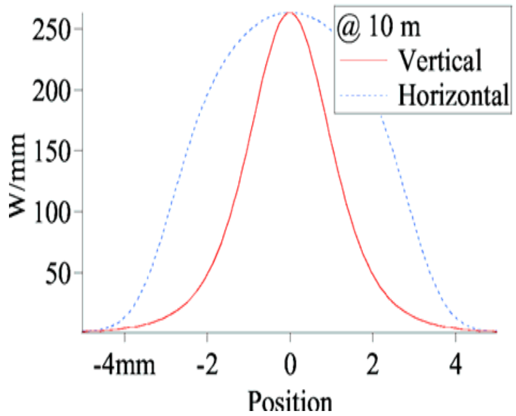
Storage Ring and Beamlines



Photon beam profile @ 10 m distance

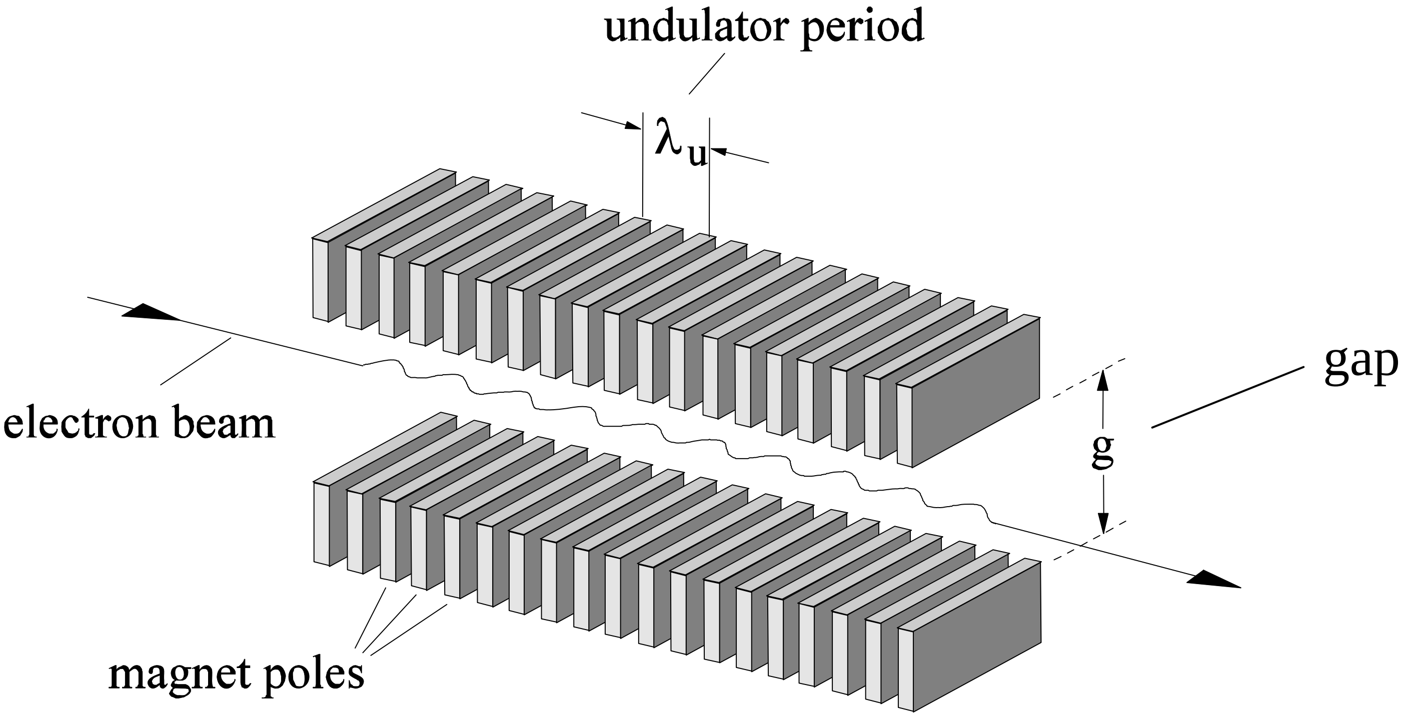


Power density



Insertion devices: Wigglers and undulators

Electrons travelling through periodic magnet structures (insertion devices) :

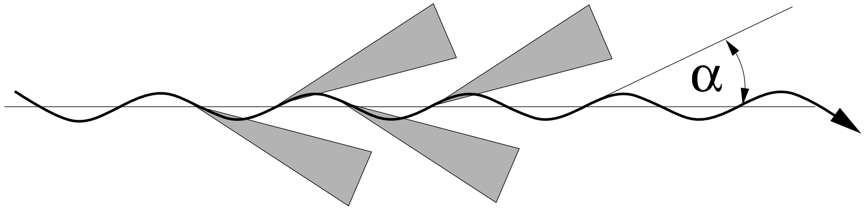


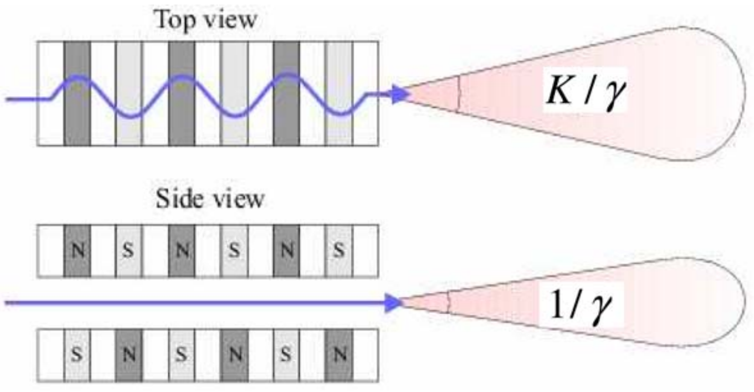
Undulator for PETRA III

Source: Babcock Noell, Würzburg

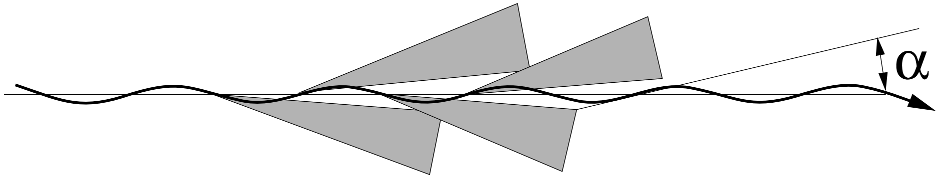
Insertion devices: Wigglers and Undulators (1)

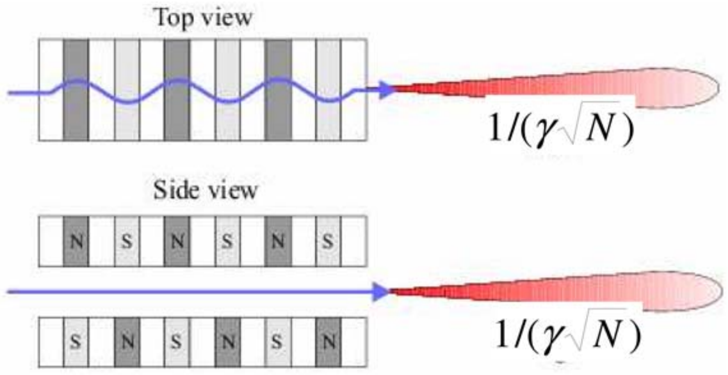
Wiggler regime: $\alpha > 1/\gamma$





Undulator regime: $\alpha < 1/\gamma$





In the undulator regime the radiation cones overlap and the wave trains can interfere constructively

Insertion devices: Wigglers and Undulators (2)

$$\alpha = \frac{K}{\gamma}$$

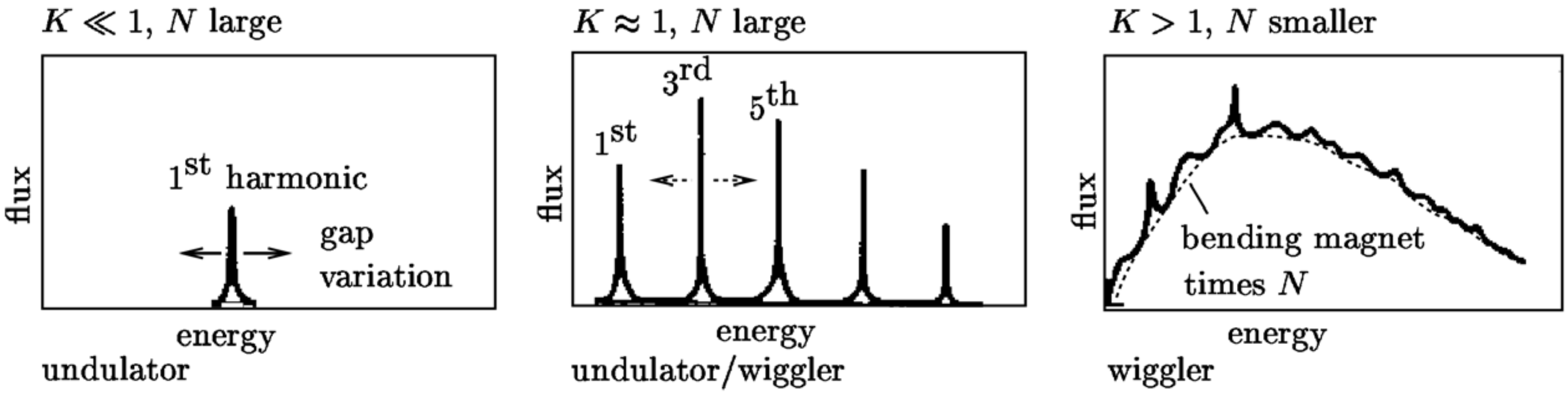
K : deflection parameter

$$\boxed{K = 0.934\,\lambda_u(\mathrm{cm})\,B_0(\mathrm{T})}$$

λ_u : magnetic period

B_0 : magnetic field at orbit

K determines the shape of the energy spectrum of an insertion device:



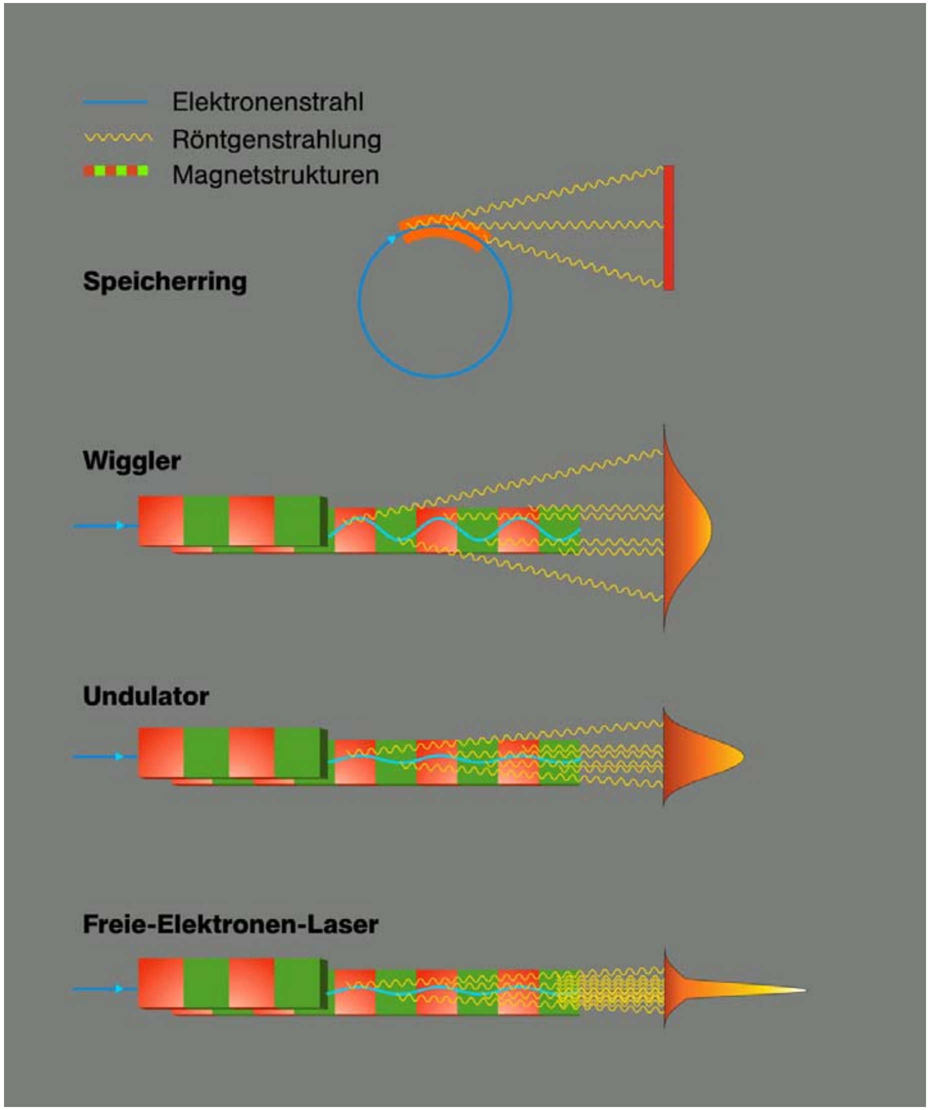
Energy of the n^{th} harmonic:

$$\boxed{E_n(\mathrm{keV}) = n\,\frac{0.95\,E^2(\mathrm{GeV})}{\lambda_u(\mathrm{cm})(1+K^2/2)}}$$

Angular width of n^{th} harmonic:

$$\boxed{\sigma = \frac{1}{\gamma}\sqrt{\frac{1+\frac{1}{2}K^2}{2Nn}}}$$

Intensity of the emitted radiation



N_p = Number of magnet poles

N_e = Number of electrons/bunch

Incoherent superposition

$$\boxed{I \sim N_e N_p}$$

Partially coherent superposition

$$\boxed{I \sim N_e N_p^2}$$

Fully coherent superposition

$$\boxed{I \sim N_e^2 N_p^2}$$

Self-Amplified Spontaneous Emission (SASE) → Talk by R. Treusch

Synchrotron Radiation: Units of Intensity

$$\text{Total flux} \equiv \frac{\text{Photons}}{\text{s}}$$

$$\text{Spectral flux} = \frac{\text{Total flux}}{0.1\%\text{bandwidth}} \quad \left[\frac{\text{Photons/s}}{0.1\%\text{bandwidth}}\right]$$

$$\text{Brightness} = \frac{\text{Total flux}}{\text{solid angle} \cdot 0.1\%\text{bandwidth}} \quad \left[\frac{\text{Photons/s}}{\text{mrad}^2 \cdot 0.1\%\text{bandwidth}}\right]$$

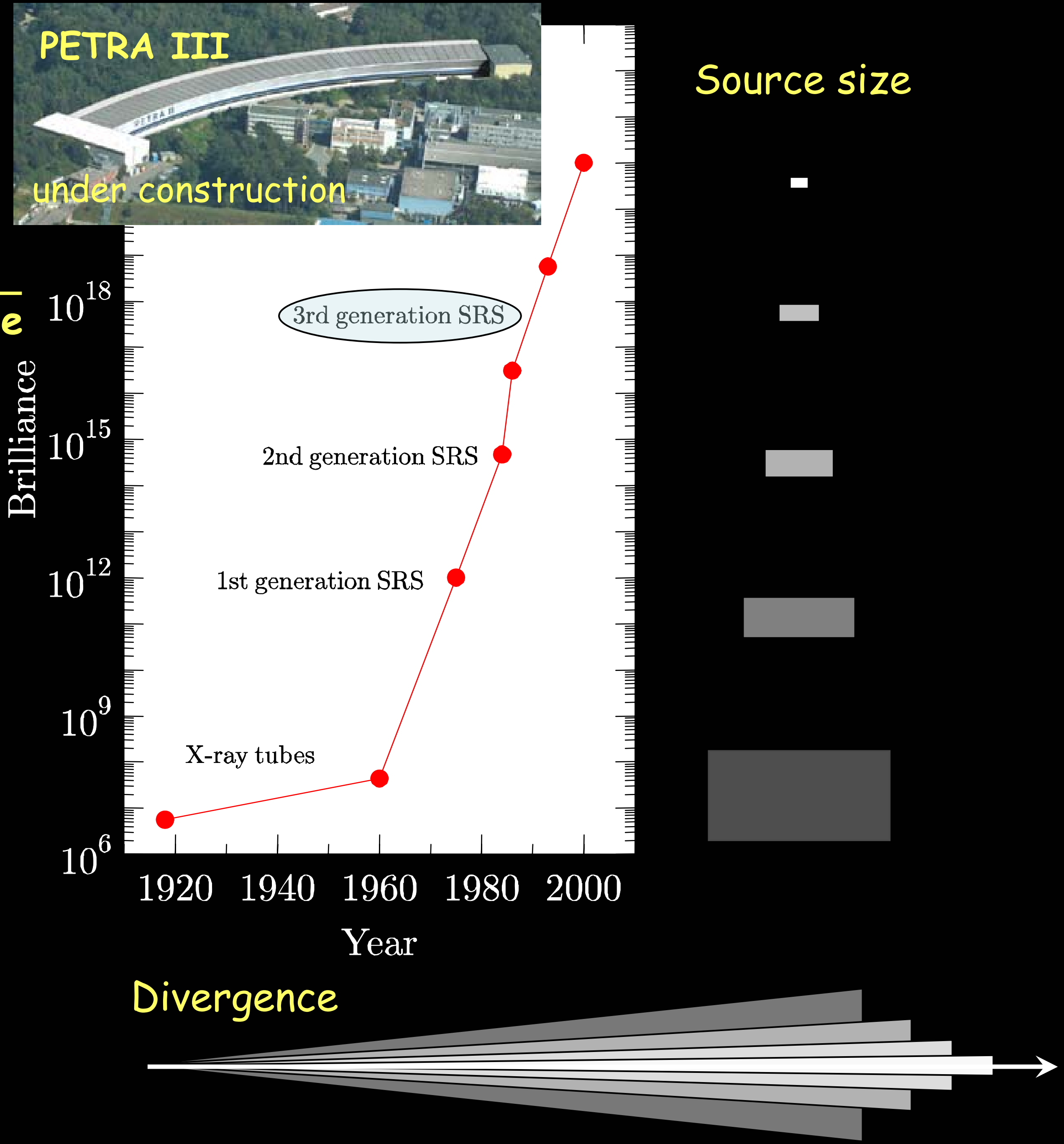
$$\text{Brilliance} = \frac{\text{Total flux}}{\text{solid angle} \cdot \text{source area} \cdot 0.1\%\text{bandwidth}}$$

$$\left[\frac{\text{Photons/s}}{\text{mrad}^2 \cdot \text{mm}^2 \cdot 0.1\%\text{bandwidth}}\right]$$

Brilliance is the figure of merit for the design of new synchrotron radiation sources

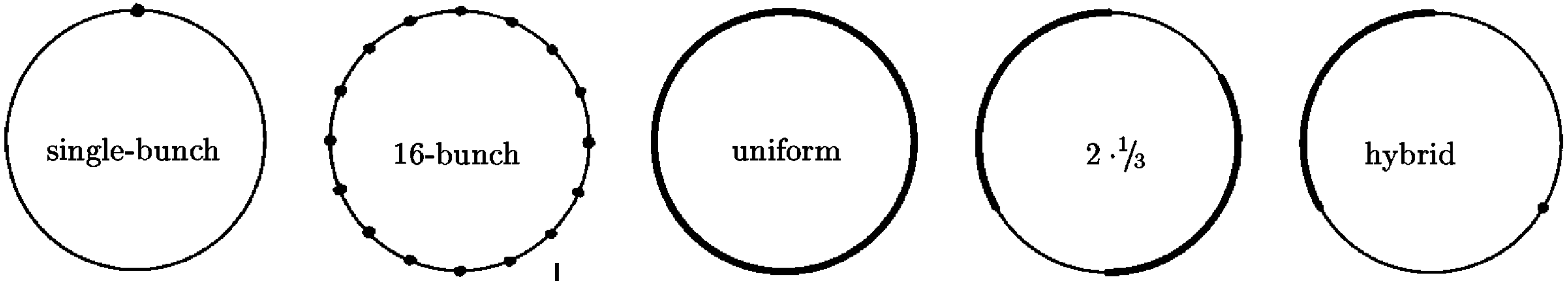
Evolution of Source Brilliance

$$\text{Brilliance} = \frac{\text{Spectral flux}}{\text{source area} \times \text{solid angle}}$$

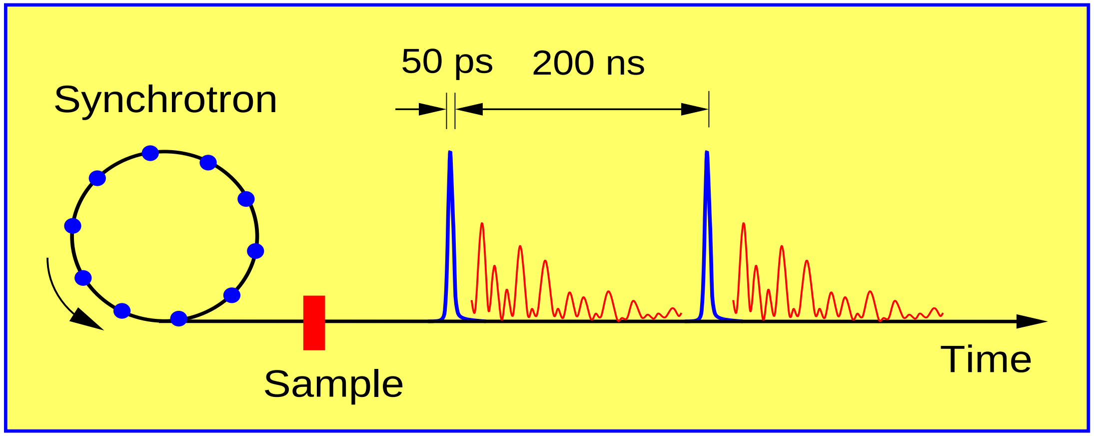


Time structure of synchrotron radiation (2)

Various filling modi can be realized depending on the experimental needs (example: ESRF)



$I_{max} = 16\,\mathrm{mA}$	$I_{max} = 90\,\mathrm{mA}$	$I_{max} = 200\,\mathrm{mA}$	$I_{max} = 200\,\mathrm{mA}$	$I_{max} = 193 + 7\,\mathrm{mA}$
lifetime = 8 h	lifetime = 10 h	lifetime = 60 h	lifetime = 55 h	lifetime = 40 / 7 h
2.81 μs gaps	176 ns gaps	2.839 ns gaps	2.839 ns & 0.94 μs	2.839 ns & 0.47 μs

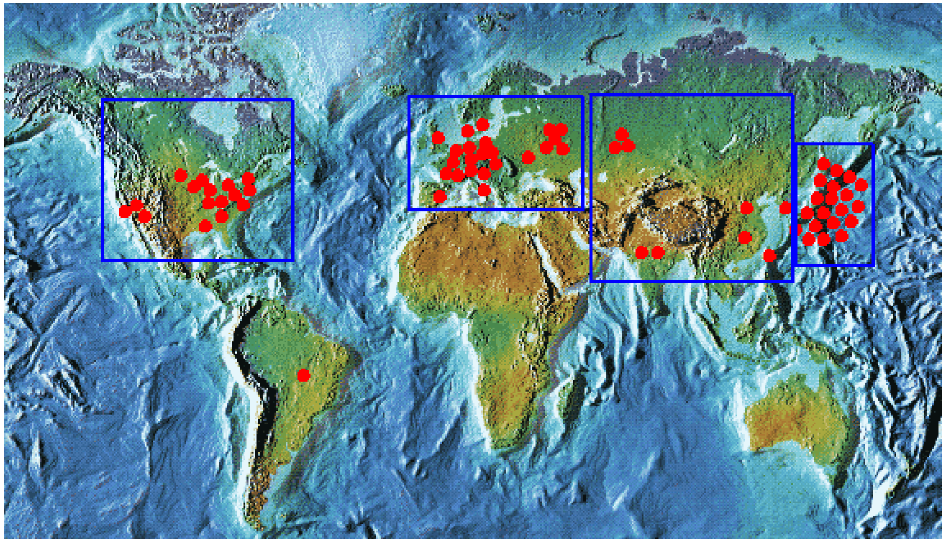


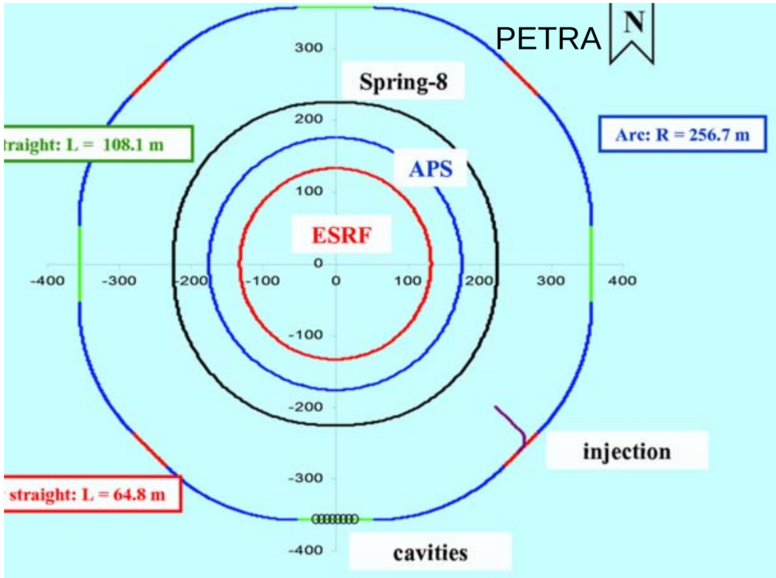
PETRA III:

950 bunches (8 ns)
40 bunches (190 ns)

Time-resolved measurements

Synchrotron radiation facilities around the world



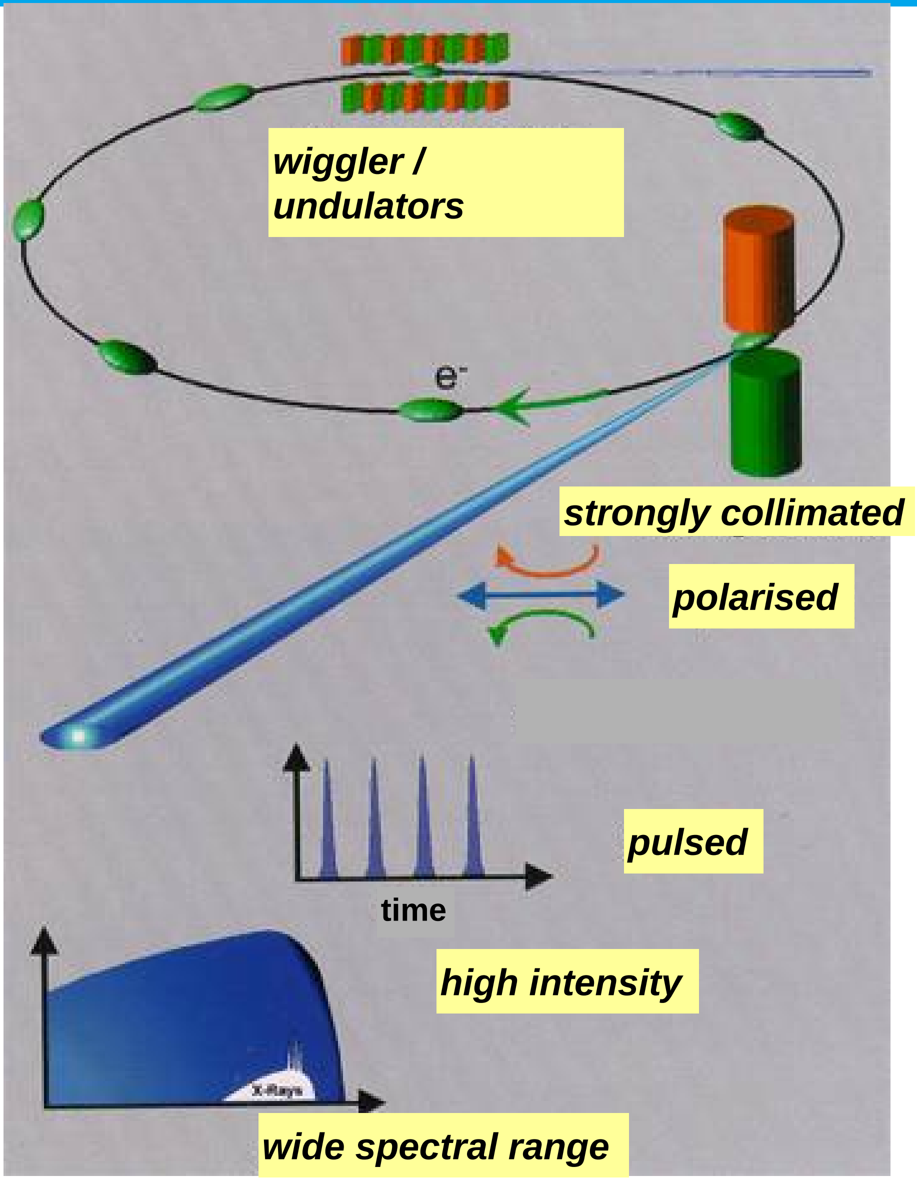


Parameters of selected facilities

Storage Ring, Location	Particle Energy [GeV]	Circum-ference [m]	Orbit Period [µs]	Bucket Separat. [ns]	Bunch Length [ps]
ESRF, Grenoble, France	6.0	844	2.816	2.84	70
APS, Argonne, USA	7.0	1104	3.683	2.84	60
SPring8, Japan	8.0	1436	4.790	1.97	100
PETRA II, Hamburg	12.0	2304	7.680	2.00	100

European Synchrotron Radiation Facility (ESRF), Grenoble,France

Summary: Properties of synchrotron radiation



Properties:

- high brilliance and flux
- infrared up to hard X-rays (>100keV)
- polarization
- time structure

Applications:

- spectroscopy
- diffraction/scattering
- imaging

Fields:

- solid state physics
- crystallography
- structural biology
- chemistry/catalysis
- geo-/environmental science
- materials science, nano science
- medical science
- atoms, molecules and clusters
- magnetism
- engineering science

Comparison of power densities

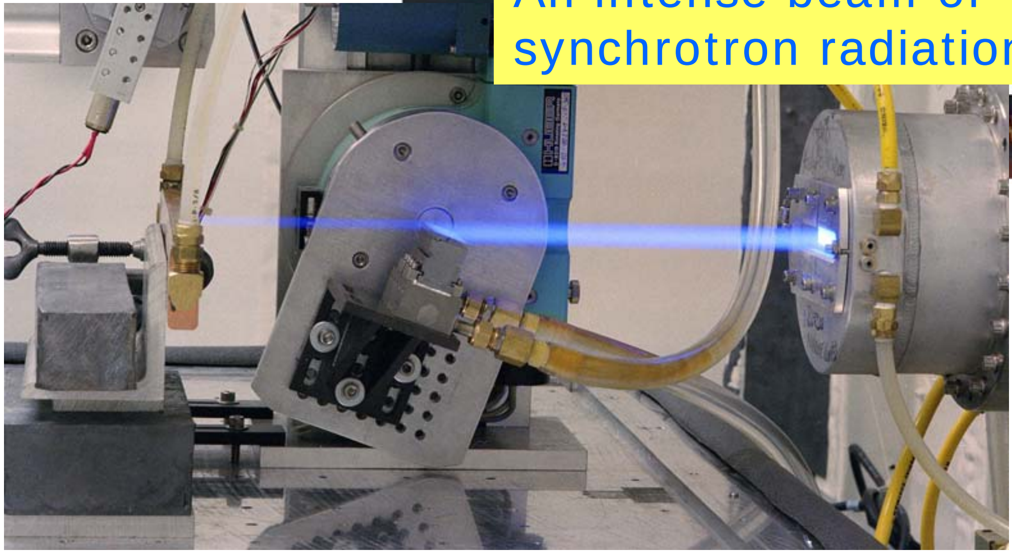
Sunlight on earth:

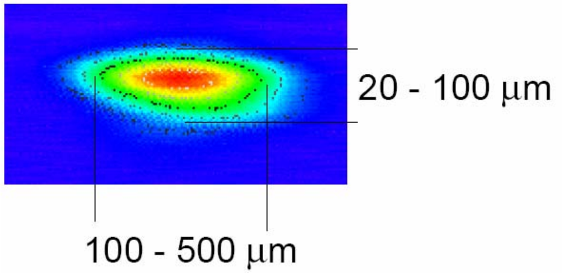
P_{sol} = 1 kW/m²

Synchrotron radiation behind undulator:

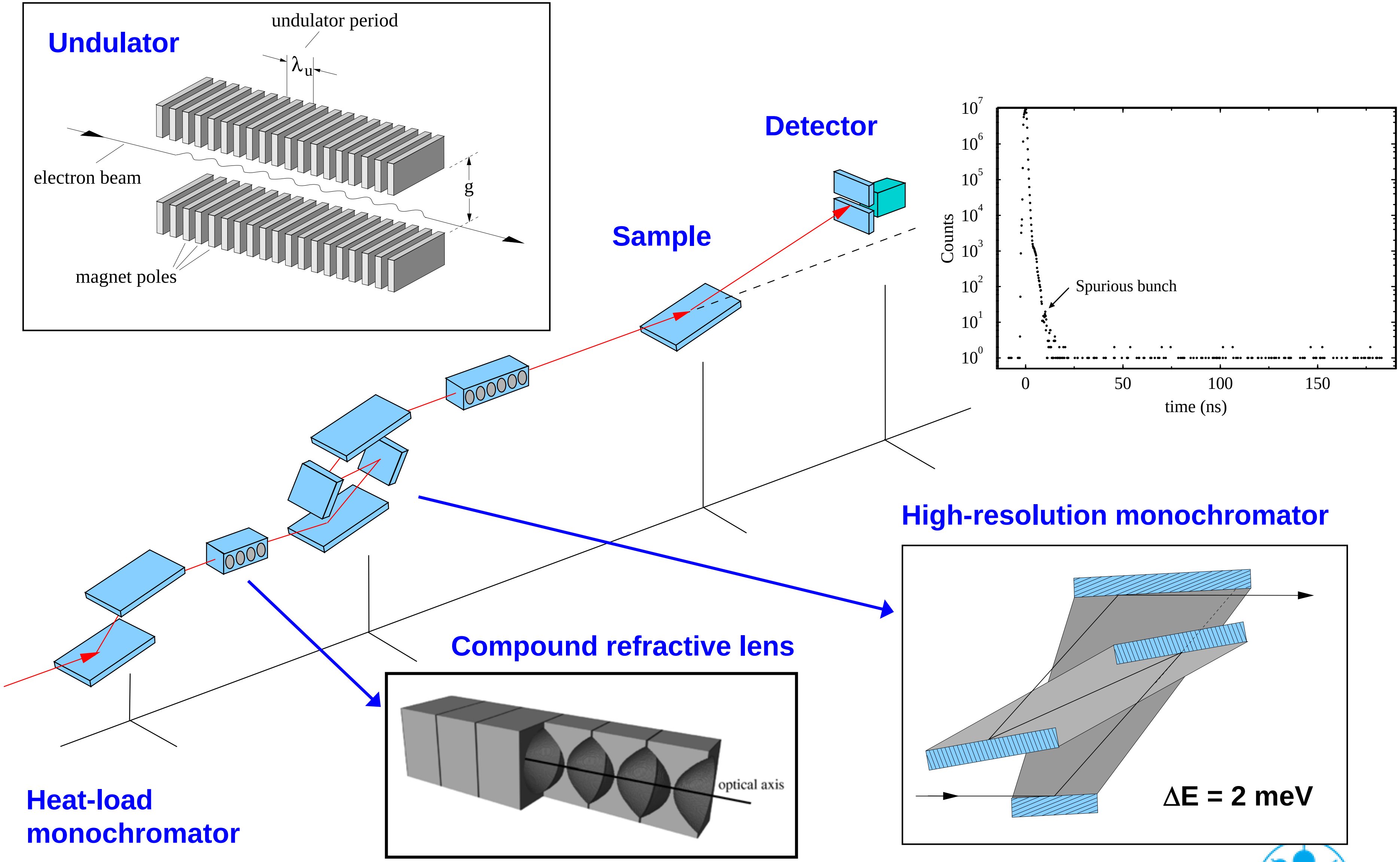
P_{SR} = 8000 MW/m²

An intense beam of synchrotron radiation in air





Handling of high-brilliance synchrotron radiation



Undulator

Detector

Sample

High-resolution monochromator

Compound refractive lens

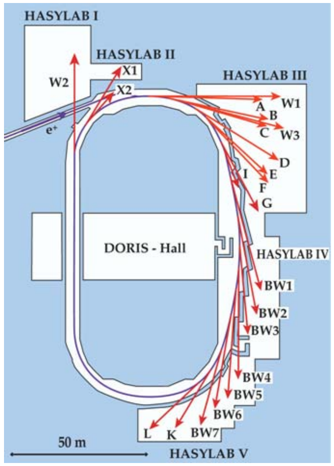
Heat-load monochromator

ΔE = 2 eV

ΔE = 2 meV

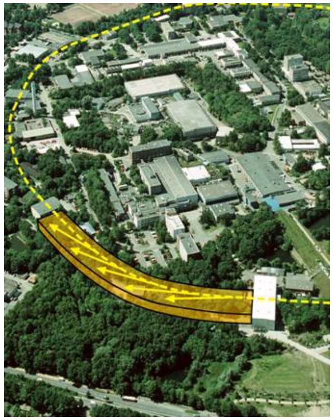
Photon Facilities at DESY

DORIS III

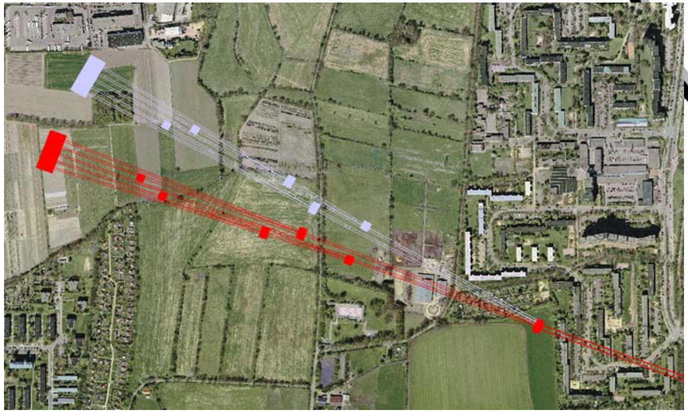


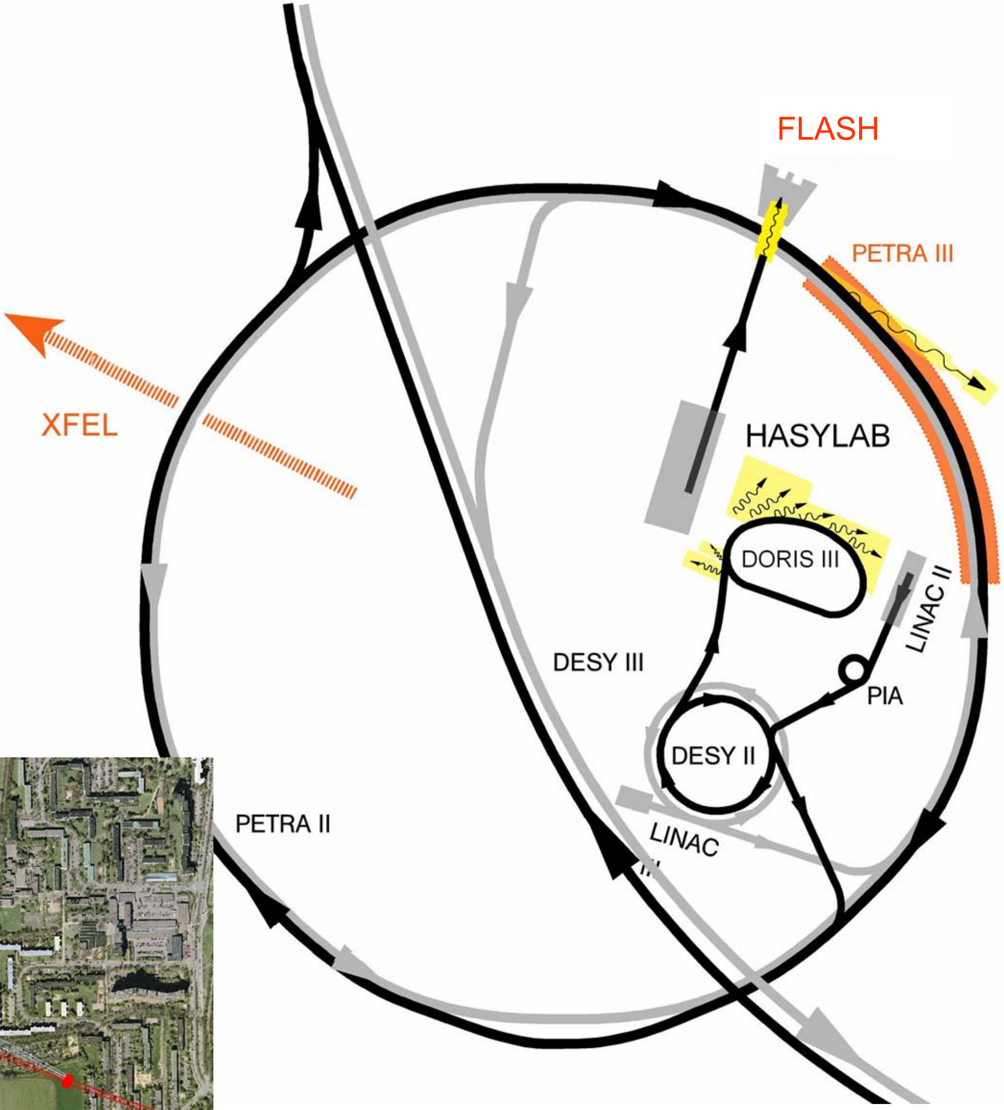
FLASH

PETRA II/III



XFEL





DORIS III

38 beamlines, 70 experimental stations

11 Stations operated by external organizations:

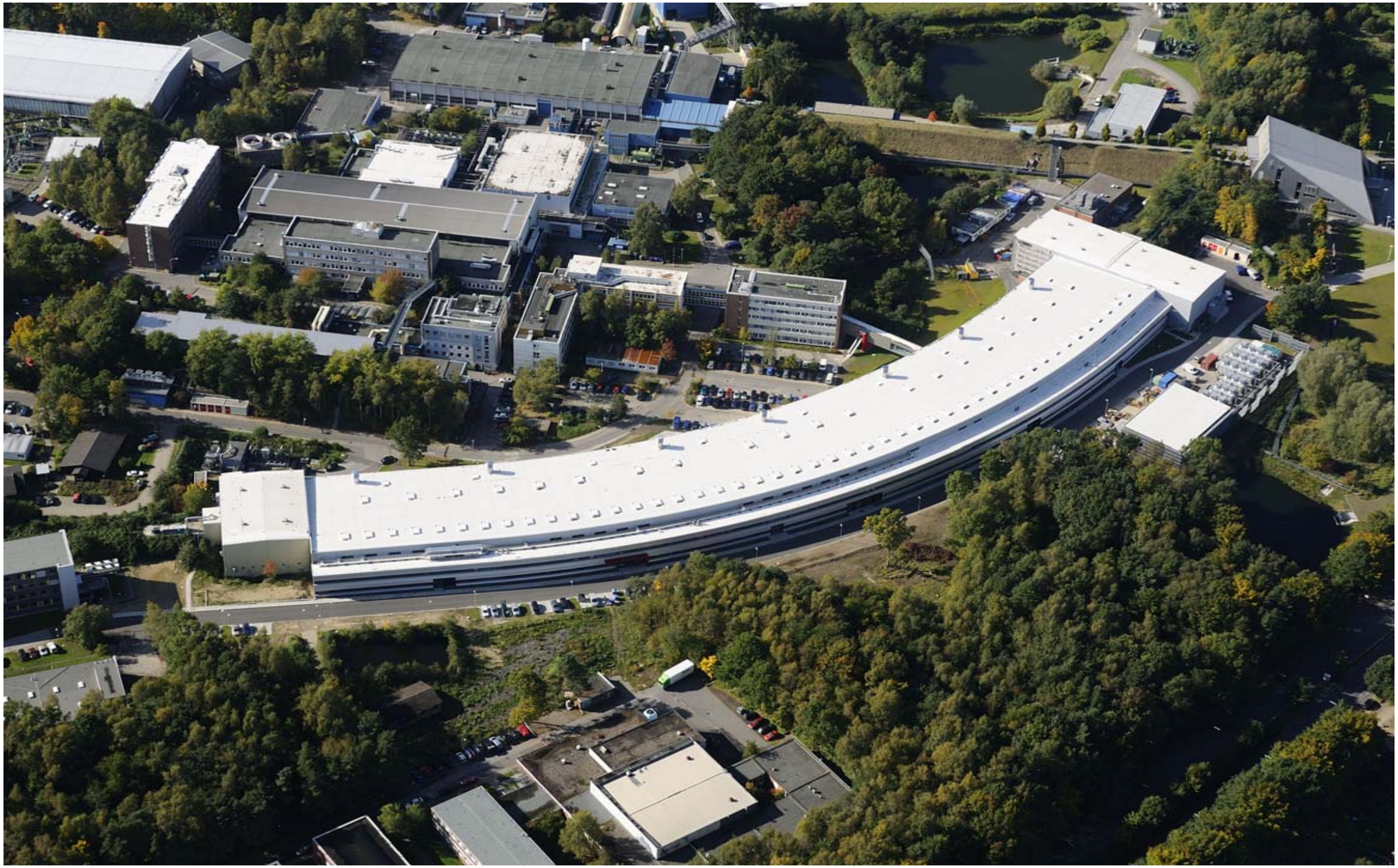
- EMBL: 7
- MPG: 1
- GKSS: 1
- GFZ: 2

16 stations operated with support from external institutions:

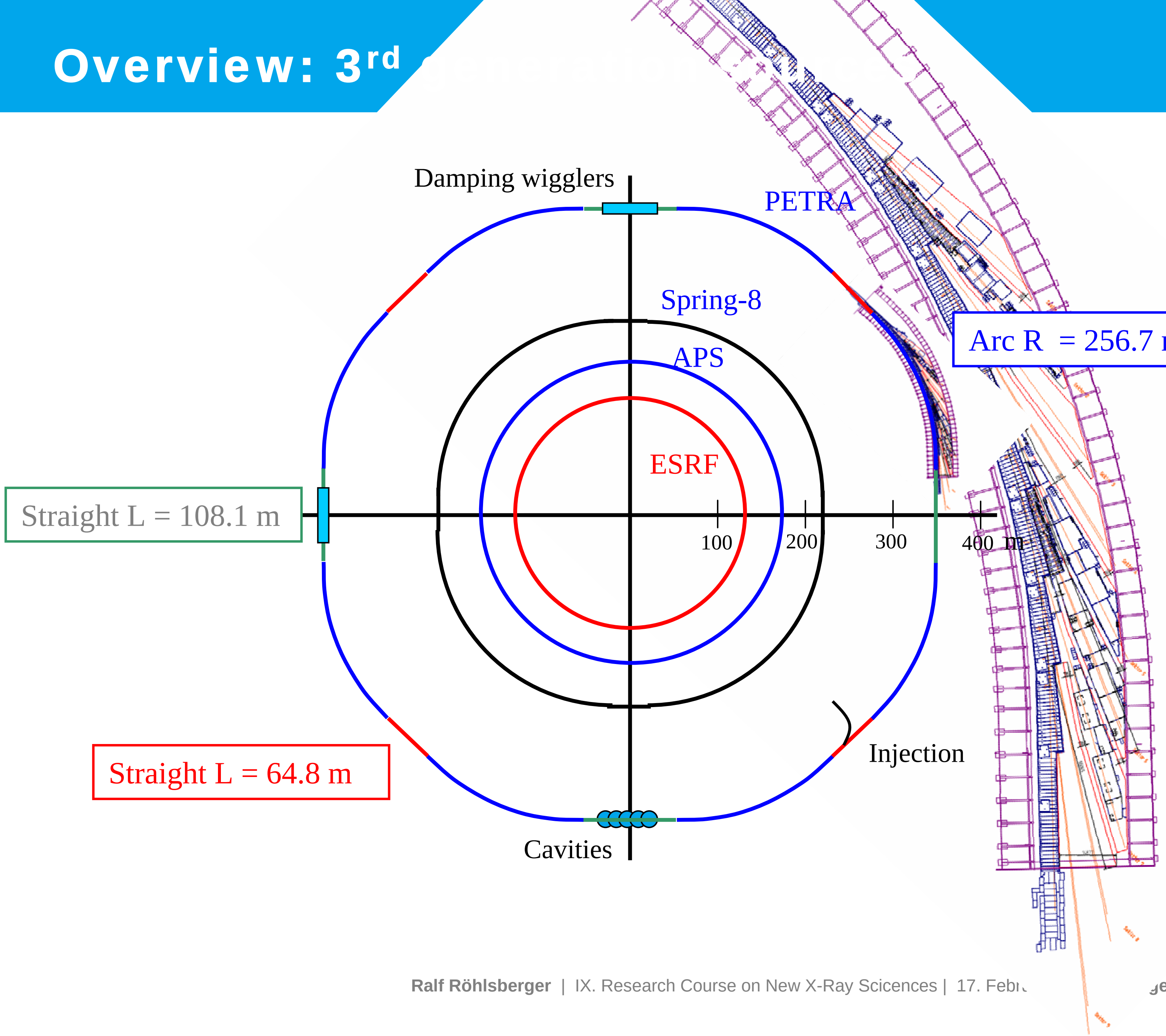
- BMBF-Verbundforschung
- FZ Jülich
- University Hamburg
- University Kiel
- University Aachen
- Debye Inst. Utrecht
- RISØ
- MPI Golm

PETRA III

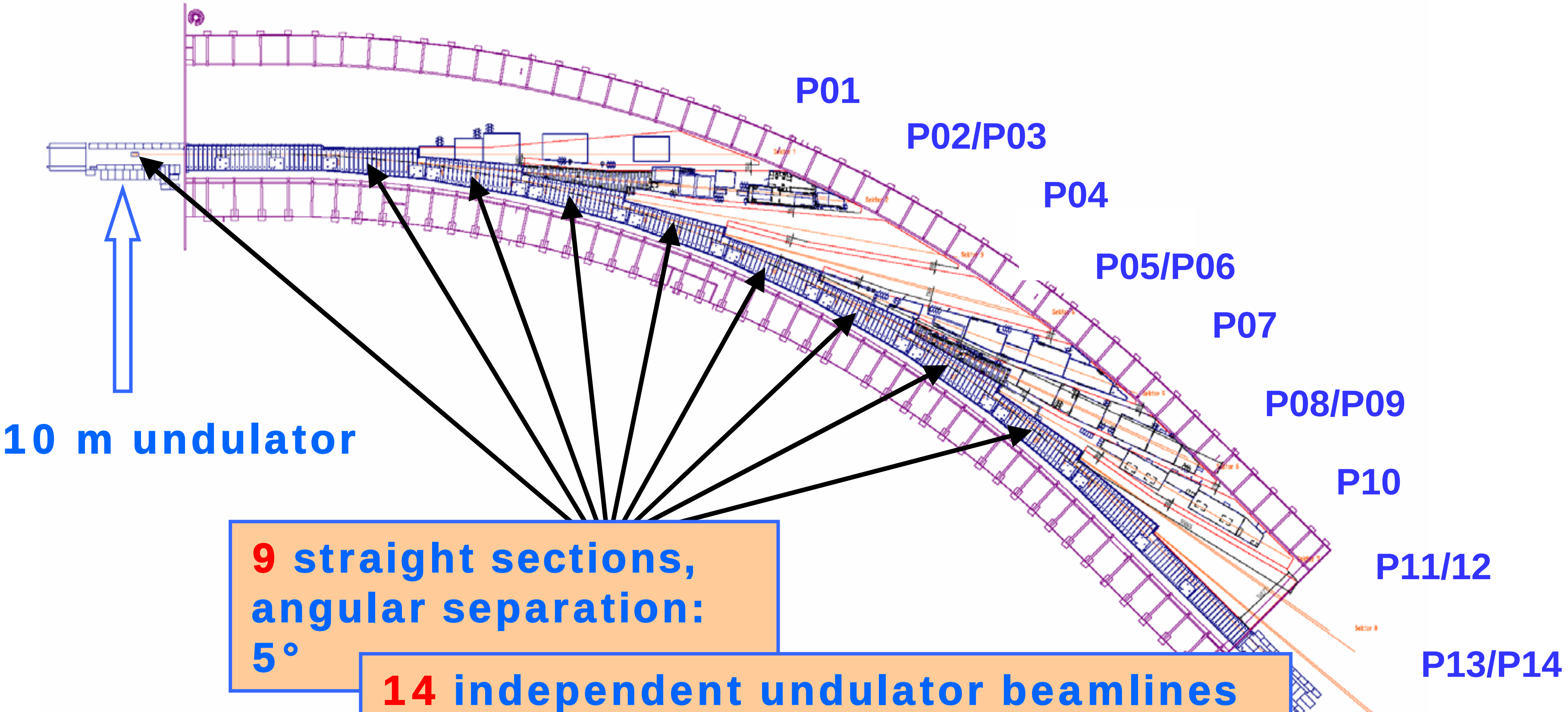
http://petra3.desy.de



Overview: 3rd generation sources

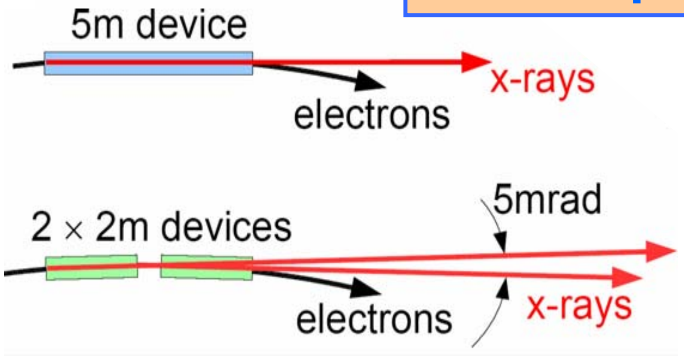


PETRA III: The experimental hall



9 straight sections, angular separation: 5°

14 independent undulator beamlines



Use of canted undulators (5 mrad, 2 m device length)

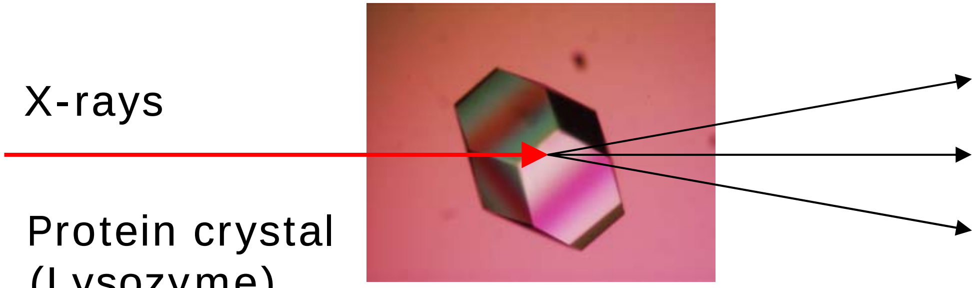
max. BL-length 103 m (from the source)

List of Beamlines at PETRA III

Number	Name	ID type	Energy range	Contact
P01	Dynamics beamline, IXS, NRS	10 m U32	5 - 40 keV	**H.C. Wille, DESY**
P02	Powder and extreme conditions	2 m U23	20 - 100 keV	**H. P. Liermann, DESY**
P03	Micro and Nano SAXS/WAXS	2 m U29	8 - 25 keV	**S. Roth, DESY**
P04	Variable Polarization XUV	5 m UE65 (APPLE)	0.2 - 3.0 keV	**J. Viefhaus, DESY**
P05	Micro- and nano-tomography	2 m U29	8 - 50 keV	**A. Haibel, GKSS**
P06	Hard X-ray nano probe, imaging	2 m U32	2.4 - 100 keV	**G. Falkenberg, DESY**
P07	High energy materials science	4 m U19 (IV)	50 - 300 keV	**N. Schell, GKSS**
P08	High resolution diffraction	2 m U29	5.4 - 30 keV	**O. Seeck, DESY**
P09	Resonant scattering/diffraction	2 m U32	2.4 - 50 keV	**J. Strempfer, DESY**
P10	Coherence applications	5 m U29	4 - 25 keV	**M. Sprung, DESY**
P11	Bio imaging/diffraction	2 m U32	8 - 35 keV	**A. Meents, MPG, HZI, DESY**
P12	BioSAXS	2 m U29	4 - 20 keV	**M. Rößle, EMBL**
P13	Macro molecular crystallography I	2 m U29	5 - 35 keV	**M. Cianci, EMBL**
P14	Macro molecular crystallography II	2 m U29	5 - 35 keV	**G. Bourenkov, EMBL**

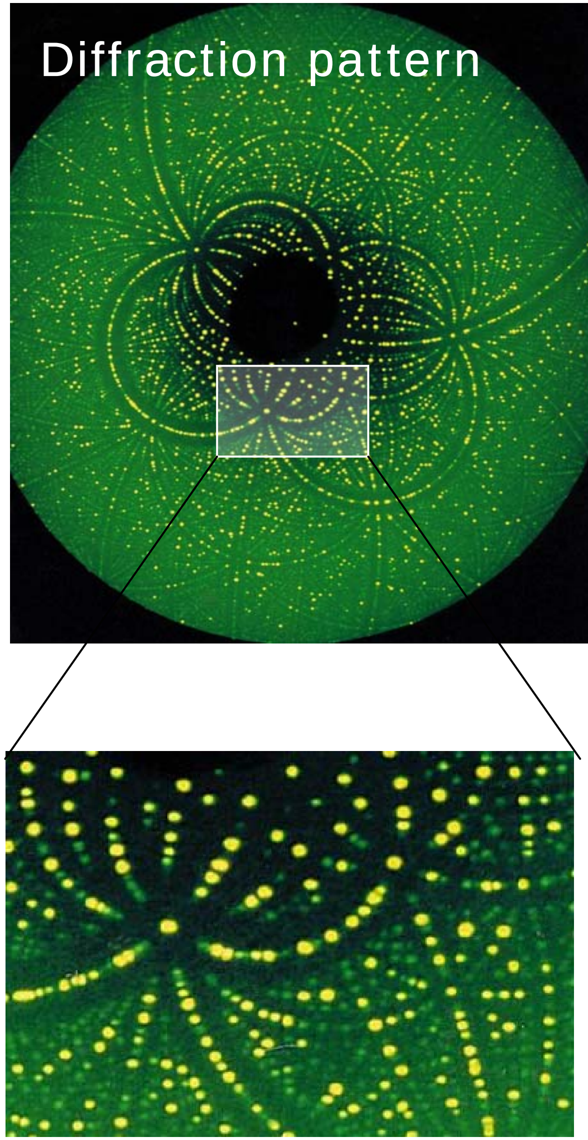
source size	
high beta section	**142 x 5 µm**
low beta section	**35 x 6 µm**

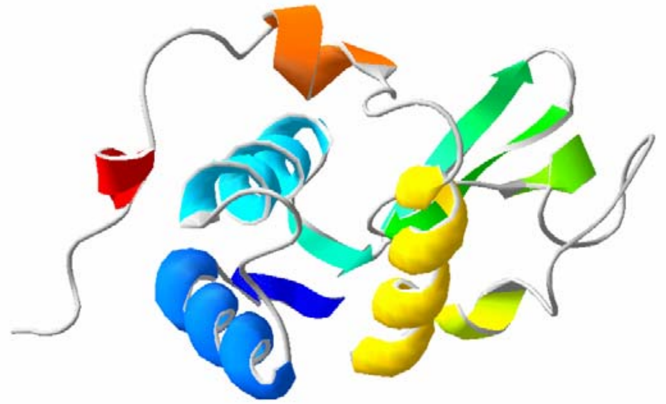
Protein crystallography



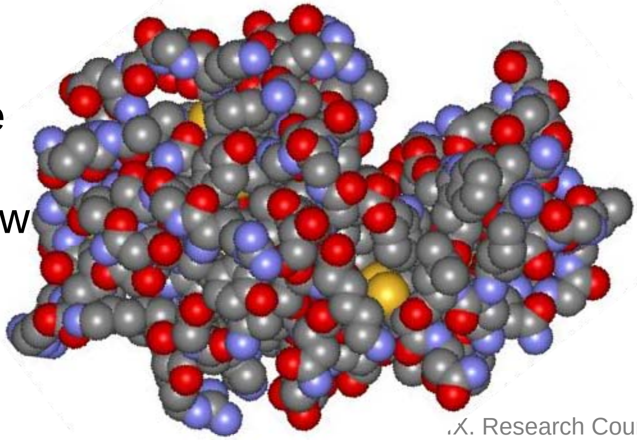
X-rays

Protein crystal
(Lysozyme)

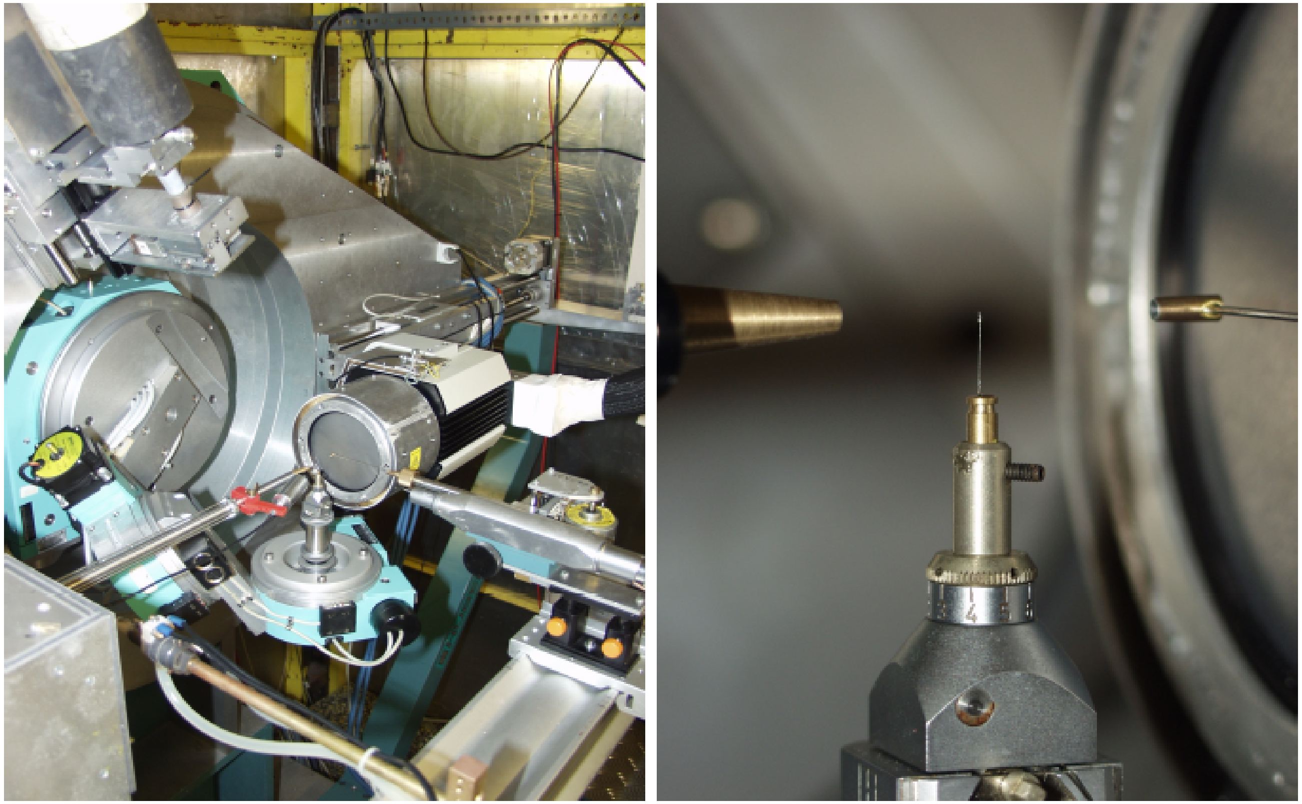




Carbon: Grey
Nitrogen: Blue
Oxygen: Red
Sulphur: Yellow



Experimental setup

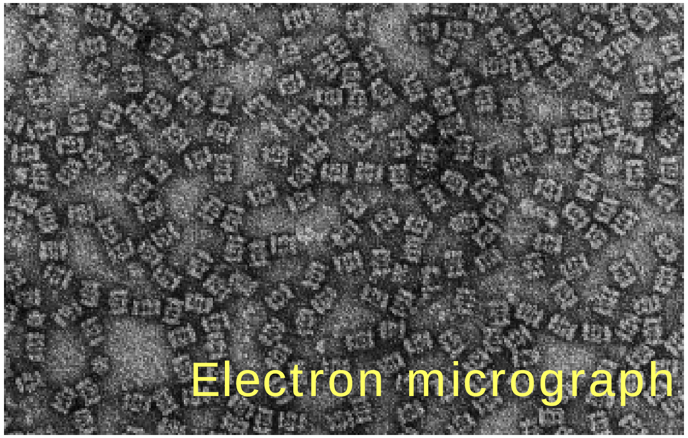


Single crystal diffractometer in κ-geometry with CCD and scintillation counter. Crystal mounted on a glass fiber. The κ-diffractometer has 3 rotations for the crystal and one for the detector.

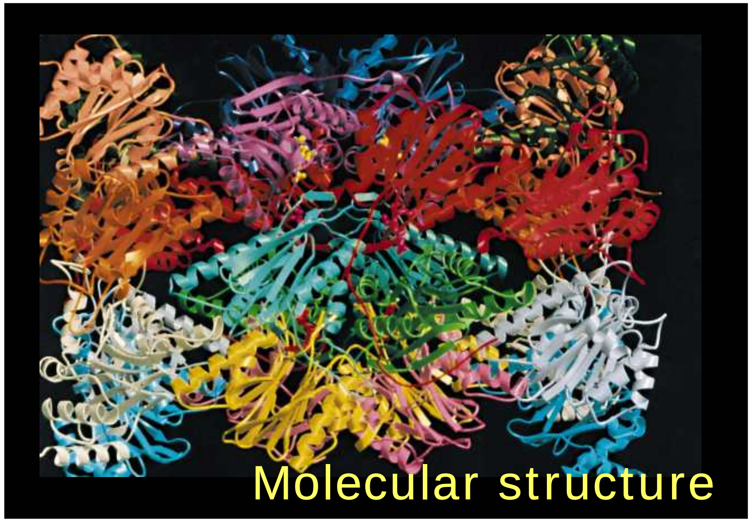
Protein Structure: Examples

The proteasome

(cuts proteins into peptides and amino acids)



Electron micrograph

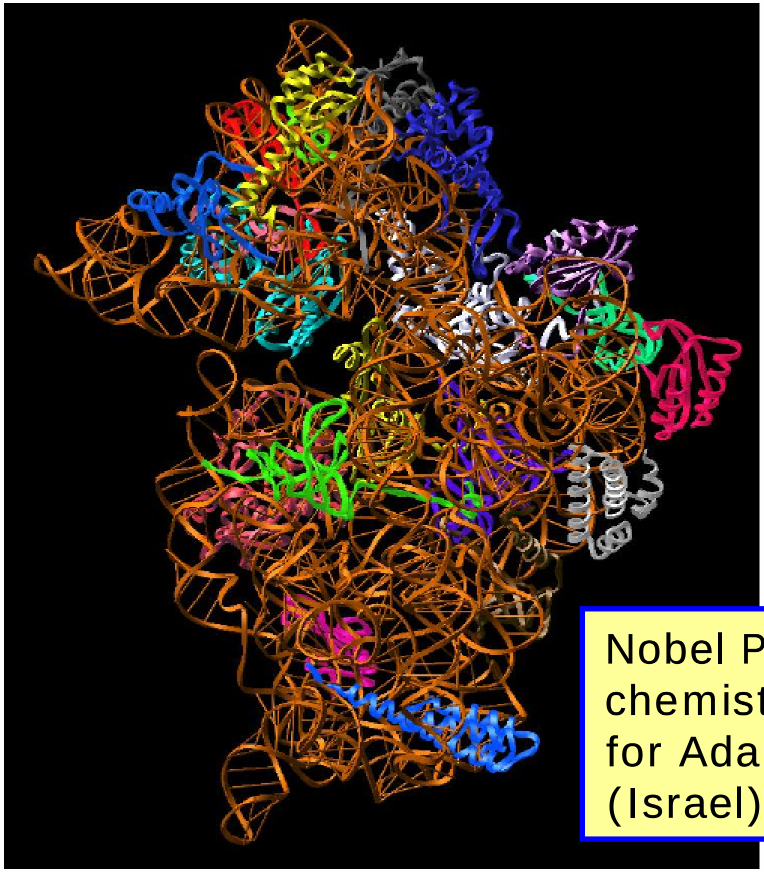


Molecular structure

The ribosome

(synthesis of proteins)

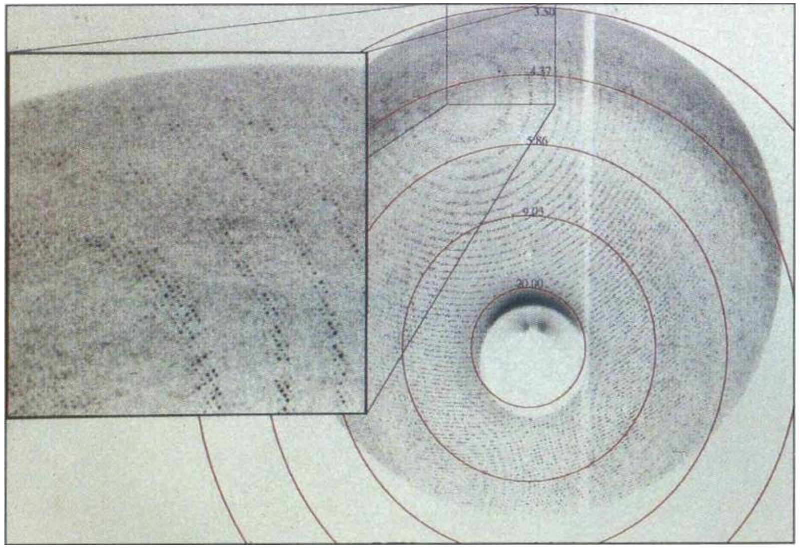
The 30S subunit of the ecoli ribosome



Nobel Prize in chemistry 2009 for Ada Yonath (Israel)

Extremely large complexes (e.g., viruses)

Example: Blue Tongue Virus



J.M. Grimes et al., Nature 395, 470-478 (1998)

X-ray reflection from surfaces

Index of refraction

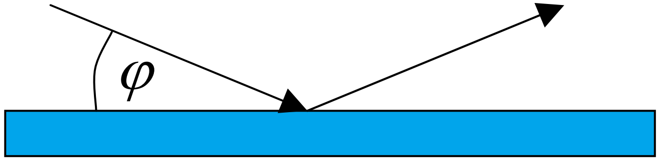
$$\boxed{n = 1 - \delta}$$

$$\delta = \frac{\rho_e \, r_0 \, \lambda^2}{4\pi}, \quad \rho_e \equiv \text{ electron density}$$

$$\approx 10^{-5} - 10^{-6} \quad \text{for} \quad \lambda = 0.1\,\text{nm}$$

For x-rays, every medium is optically thinner than vacuum !

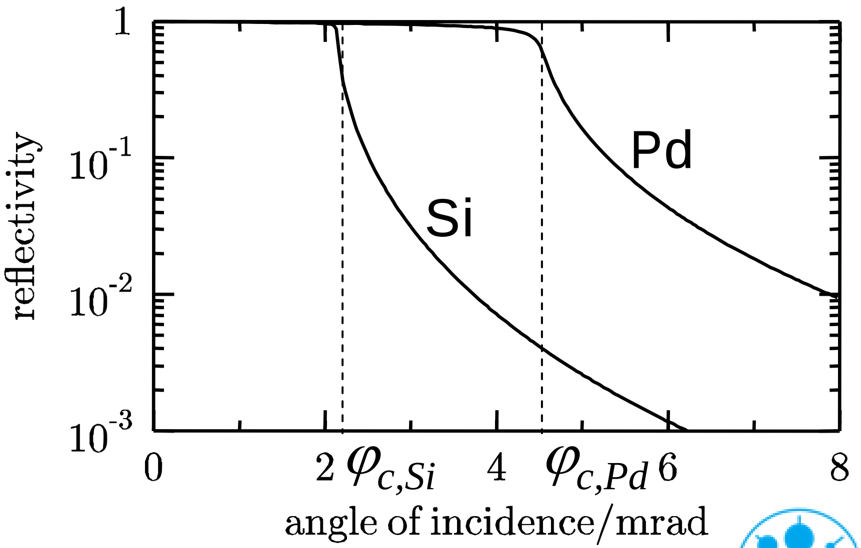
X-rays incident on a surface below the critical angle are totally reflected



Critical angle of total reflection

$$\boxed{\varphi_c = \sqrt{2\delta}}$$

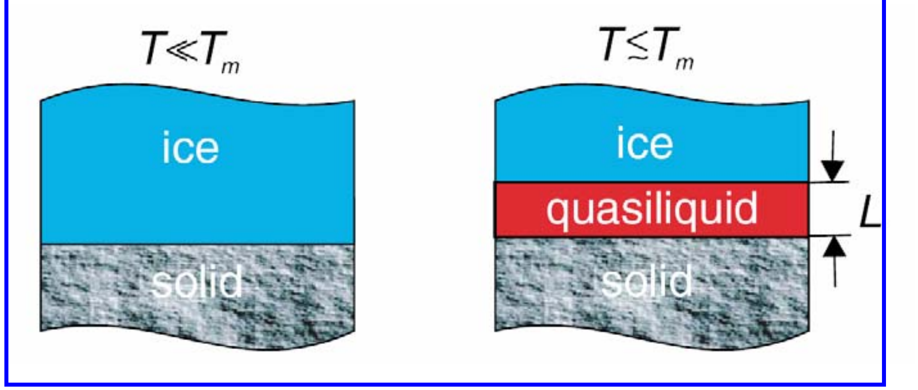
For angles $\varphi < \varphi_c$ the penetration depth of hard x-rays is only a few nm.



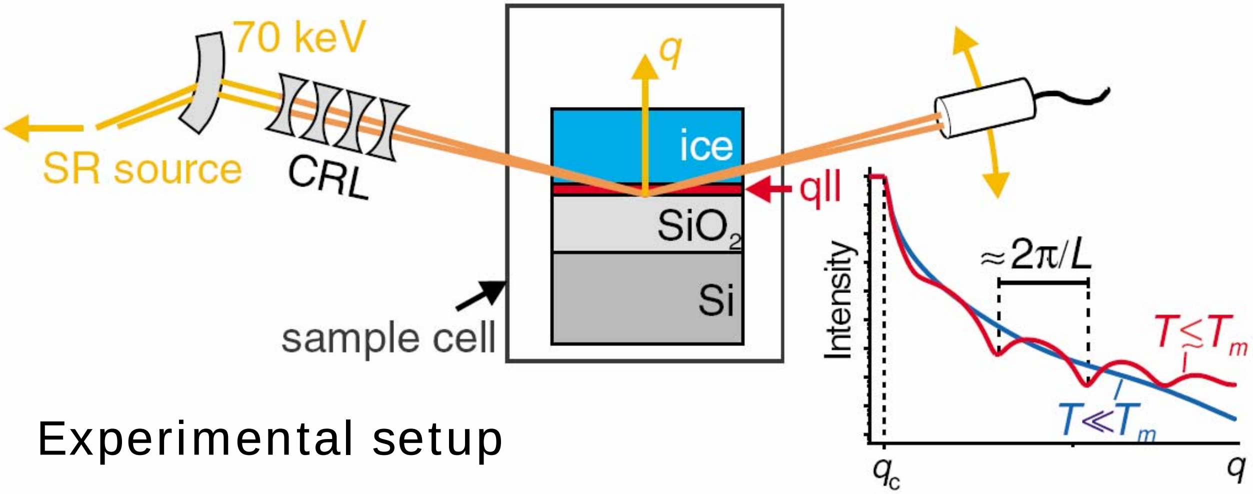
X-rays can be used for the study of structures at surfaces

Interfacial Melting of Ice in Contact with SiO_2

Hypothesis



S. Engemann et al.,
Phys. Rev. Lett. 92,
205701 (2004)



Experimental setup

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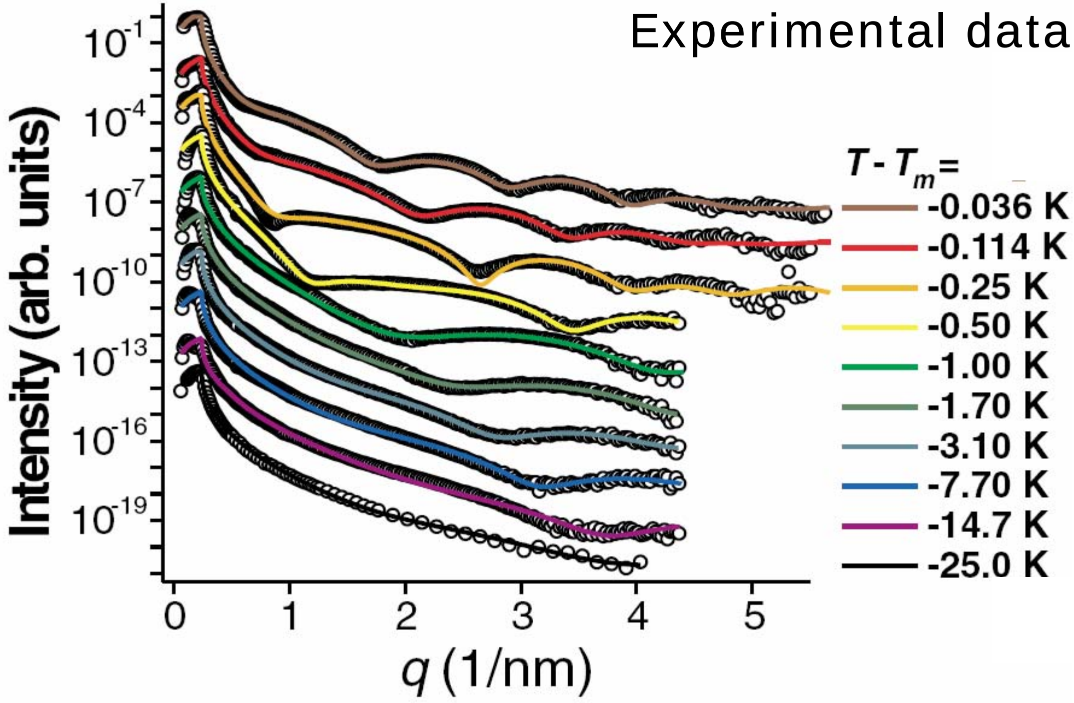
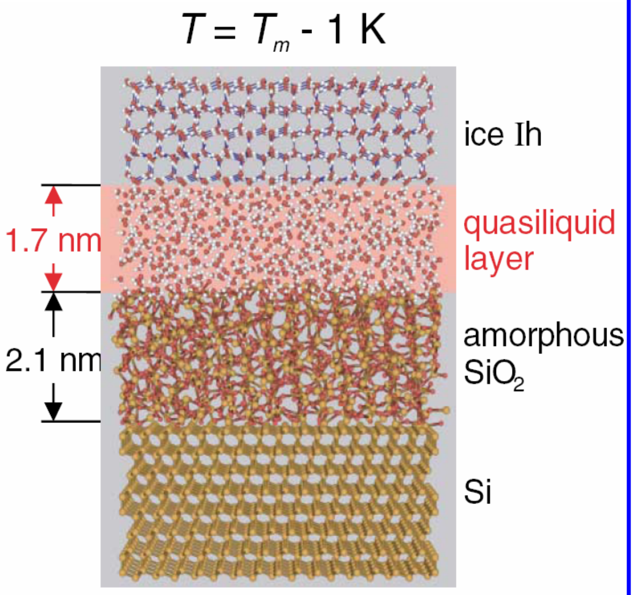
Experimental data



Structural model



S. Engemann et al., Phys. Rev. Lett. 92, 205701 (2004)