

Introduction to Photon Science

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Sadia Bari

DESY Ukraine Winter School 2023

Content

- **PART I:**
 - History of X-ray Sources
 - Principle of Synchrotrons
 - Principle of Free-Electron Lasers
- **PART II:**
 - Science at Synchrotron facilities
 - Science at FEL facilities

Introduction to Photon Science

Part I: Basics of synchrotrons and free-electron lasers

A short history of X-ray sources

Generation of X-rays: X-ray tube

From discovery to first application

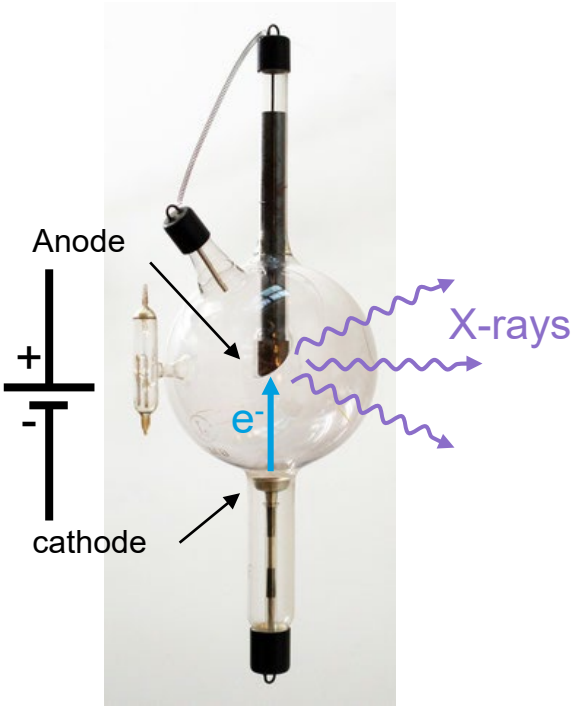
1895: Discovery of X-rays by Wilhelm Conrad Röntgen

"It seemed at first a new kind of invisible light. It was clearly something new, something unrecorded."

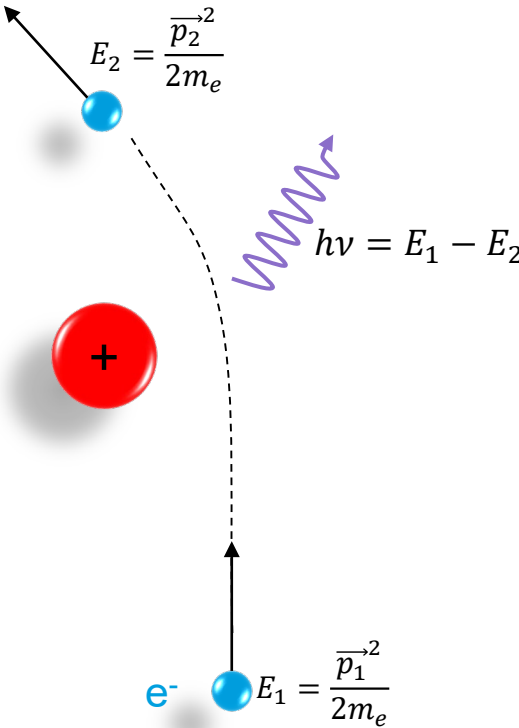


Wilhelm Conrad Röntgen
(1845 – 1923)
Nobel Prize 1901

Crookes tube



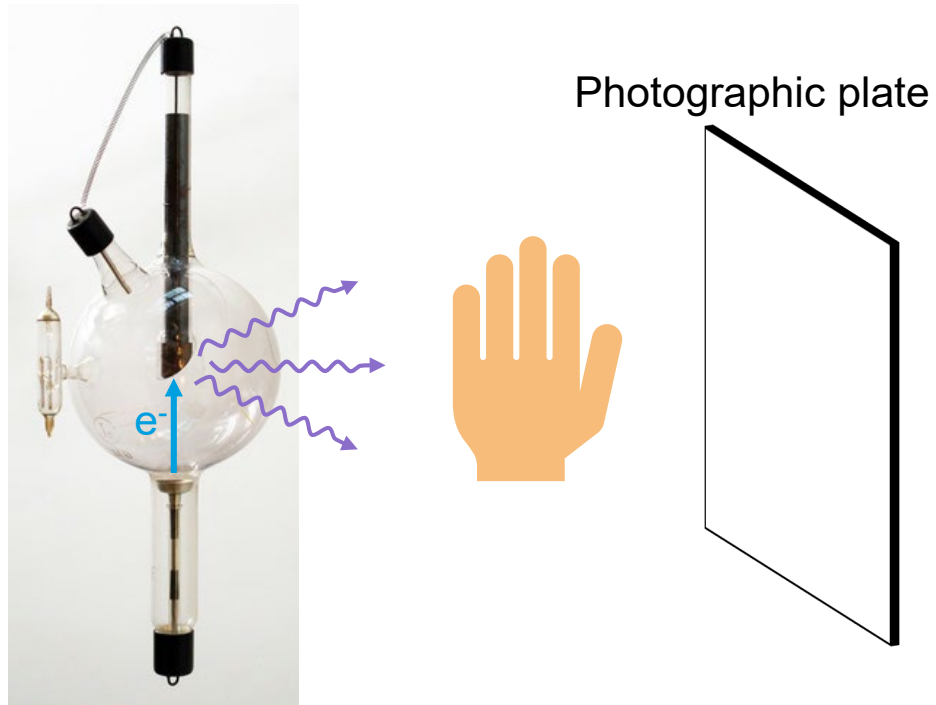
General principle for generation of X-rays: Bremsstrahlung



Generation of X-rays: X-ray tube

From discovery to first application

1 month later: first X-ray image



30-150 kV

25 min exposure time



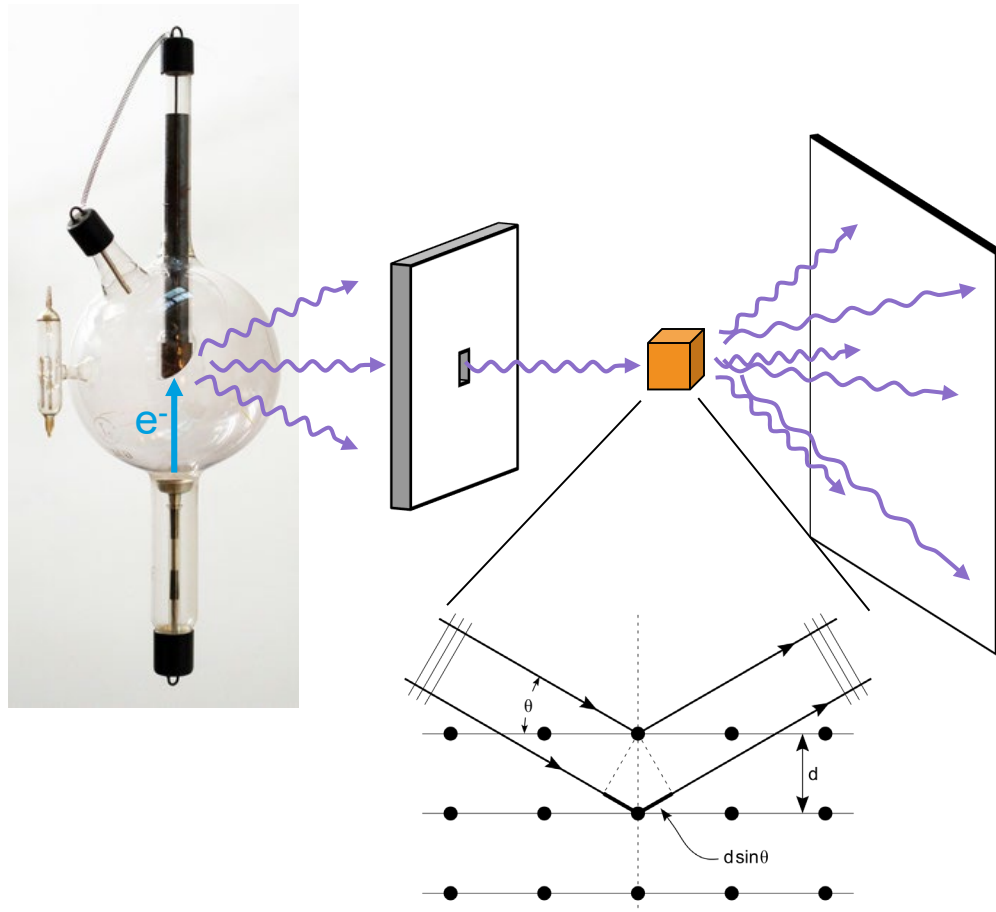
Röntgen's wife hand

Generation of X-rays: X-ray tubes

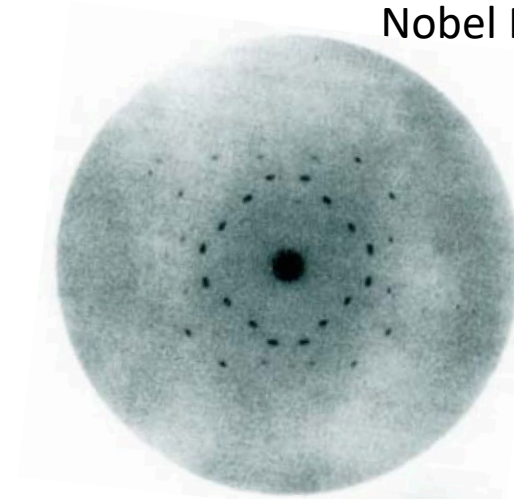
X-ray diffraction from crystalline structures

First diffraction patterns obtained by Max von Laue in 1912

W. Friedrich *et al.* *Annalen der Physik* **346**, 971–988 (1913)



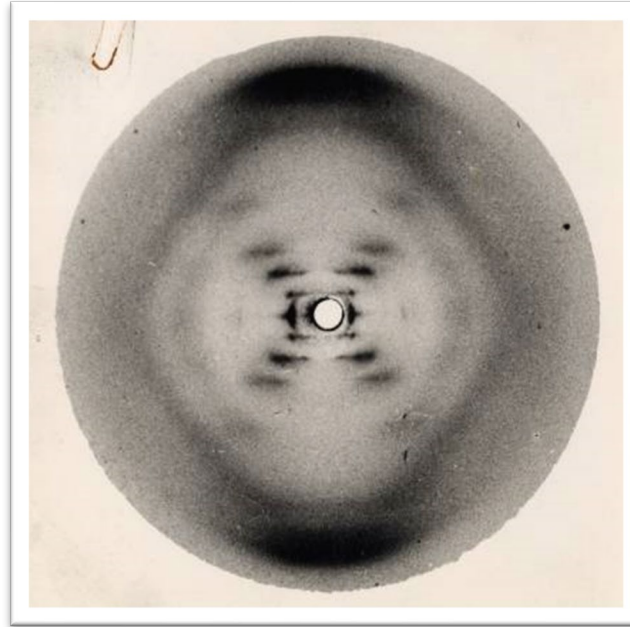
Max von Laue
(1879 – 1960)
Nobel Prize 1914



ZnS crystal

Generation of X-rays: X-ray tubes

X-ray diffraction from crystalline structures



1952: The first X-ray diffraction pattern of DNA
62 hours exposure time !



Rosalind Franklin
(1920 – 1958)
~~Nobel Prize 1962~~



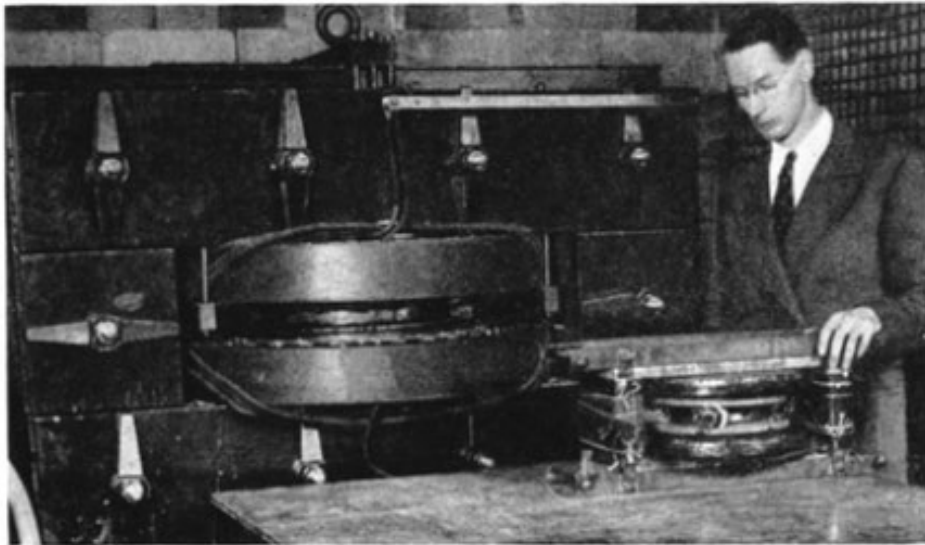
The **Nobel Prize in Physiology or Medicine 1962** was awarded jointly to Francis Harry Compton Crick, James Dewey Watson and Maurice Hugh Frederick Wilkins "**for their discoveries concerning the molecular structure of nucleic acids and its significance for information transfer in living material**"

Generation of X-rays: Betatron

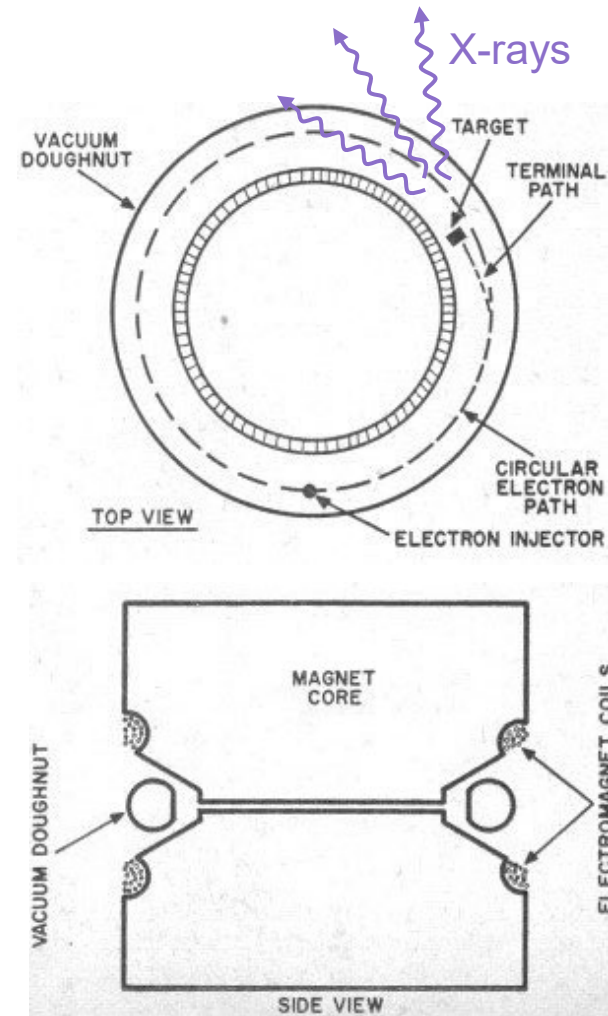
Acceleration in a magnetic field

The Betatron

World's Most Powerful X-Ray Machine Holds Vast Possibilities for Medicine, Industry, Research



Professor Donald W. Kerst with the first betatron, having 2.5-million volts output energy, on the table and the 20-million-volt machine alongside. The circular vacuum tube of the large unit can be seen in place in the center of the betatron, between the pole faces of the 3½-ton magnet. The larger betatron is only three feet high



Scientific American, Vol. 168, No. 5 (MAY · 1943), pp. 207-209

Generation of X-rays : Synchrotron

First observation of synchrotron radiation



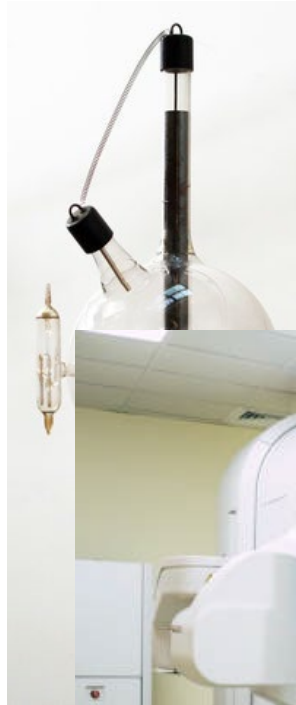
late 1970s → planning began
for special accelerators to
generate synchrotron radiation

April 24, 1947: First observation of SR at General Electric 70 MeV synchrotron
(Langmuir, Elder, Gurewitch, Charlton, Pollock)

→ relativistic speed

Generation of X-rays : and now?

Linac and 3rd generation synchrotron

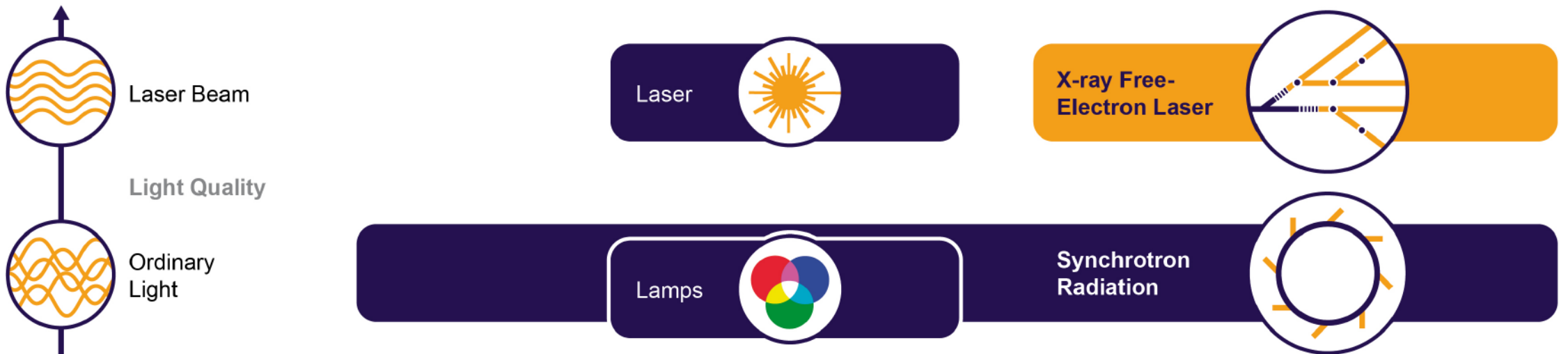
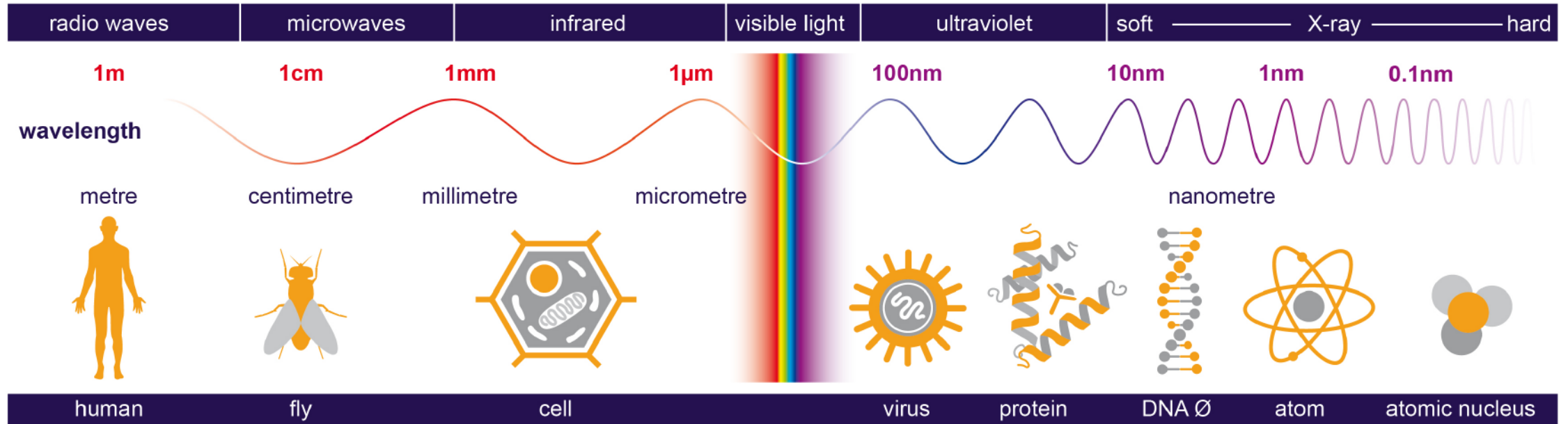


few MeV radiotherapy linac



ESRF (Grenoble, FR), 6 GeV synchrotron

Big facilities for studying tiny objects...



Synchrotron radiation facilities worldwide

ALBA
MAXIV
 PAUL SCHERRER INSTITUT
PSI
diamond
DESY
Elettra Sincrotrone Trieste
SOLEIL SYNCHROTRON
ESRF
 The European Synchrotron
SESAME
NSRRC
HZB Helmholtz Zentrum Berlin
PAL
 POHANG ACCELERATOR LABORATORY
SPring-8
Photon Factory
 Institute of Materials Structure Science
 High Energy Accelerator Research Organization, KEK
SYNCHROTRON THAILAND
Canadian Light Source
Argonne NATIONAL LABORATORY
ALS
 ADVANCED LIGHT SOURCE
BROOKHAVEN NATIONAL LABORATORY
SLAC
 NATIONAL ACCELERATOR LABORATORY
CHESS
 CORNELL HIGH ENERGY SYNCHROTRON SOURCE
LNLS

Australian Synchrotron

Free-electron lasers

European XFEL
SLAC
 NATIONAL ACCELERATOR LABORATORY
PAL
 POHANG ACCELERATOR LABORATORY
PSI
 PAUL SCHERRER INSTITUT
Elettra Sincrotrone Trieste
SPring-8

Synchrotron radiation facilities in Europe



DESY machine history

2000 Employees, 3000 International Guests
(100 apprentice, 100 undergraduate, 350 PHD, 300 Postdoc)
Annual Budget: 230 M€

DESY founded 1959 as an Electron Synchrotron Facility for Elementary Particle Research

1964 DESY (Synchrotron) e- 7.4 GeV
1974 DORIS (Storage Ring) 300m e+/e- 3.5 GeV (later 5 GeV)

1980 HASYLAB@DORIS
1984 Upgrade with 7 Wiggler/Undulator Beamlines
1993 Dedicated SR Source at 4.5 GeV

1978 PETRA (Storage Ring) 2.3km e+/e- 19 GeV
1990 HERA (Storage Ring) 6.3km p+/e- 920 GeV / 27.5 GeV (using PETRA as Booster)

1997 FLASH (Free Electron Laser)
2005 Dedicated User Facility

2007 Shutdown of HERA and Reconstruction of PETRA → PETRA III

2009 PETRA III Dedicated SR Source at 6 GeV (presently most brilliant SR source worldwide)

2012 Shutdown of DORIS
2014 FLASH II (Extension of FLASH)

Participation in the European XFEL project (operation since 2017)

Basics of Synchrotrons

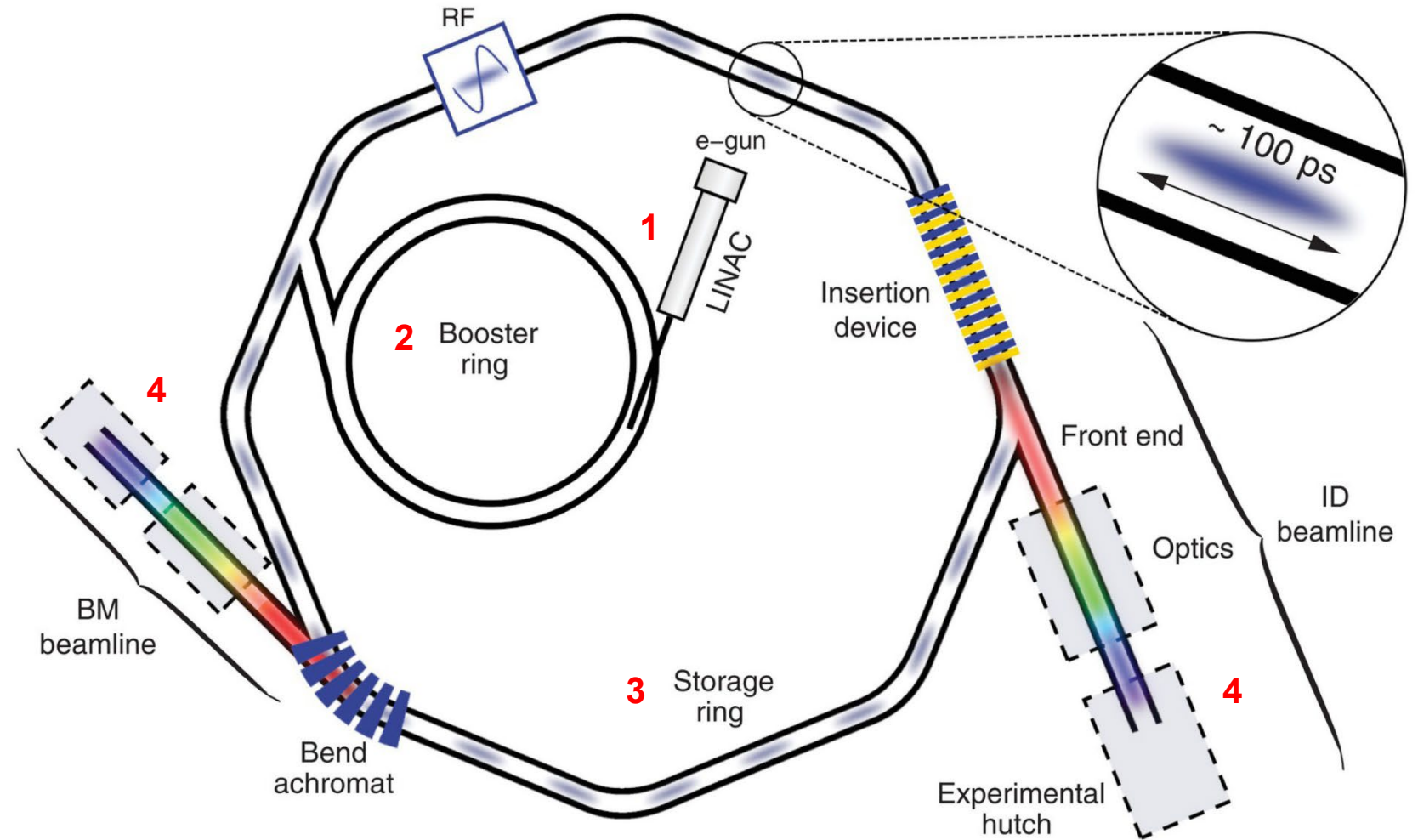
Synchrotrons and free-electron lasers (FELs)



Synchrotron

Principal structures

1. e^- are produced and accelerated in a LINAC
2. e^- are accelerated to nominal energy (GeV) in the booster accelerator
3. e^- bunches travel in the storage ring in a wide circular path, emitting light as they change directions
4. X-ray light, emitted towards “beamlines”
→ experiments



An Introduction to Synchrotron Radiation: Techniques and Applications, 2nd edition, P. Willmott, 2019, Wiley

Synchrotron Radiation (SR) is a relativistic effect

γ the relativistic Lorentz factor

Many features can be understood in terms of two processes:

- Lorentz contraction
- Doppler shift

When a relativistic charged particle is travelling through a periodic magnetic field, in the particles rest frame it sees a magnetic field rushing towards it.

In our rest frame the magnet period is λ_u

$$\gamma = \frac{E}{E_0}$$

$$\beta = \frac{v}{c}$$

$$\beta = \sqrt{1 - \frac{1}{\gamma^2}}$$

c is the velocity of light in free space

v is the velocity of the electron

β is the relative velocity of the electron

E is the electron energy

E_0 is the electron rest energy (0.511 MeV)

This γ factor turns up again and again in SR !

Synchrotron Radiation (SR) is a relativistic effect

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This γ factor turns up again and again in SR !

- What is γ at PETRA III ?
- What wavelength does the particle emit?
- What wavelength do we observe?

Synchrotron Radiation (SR) is a relativistic effect

γ the relativistic Lorentz factor

Many features can be understood in terms of two processes:

- Lorentz contraction
- Doppler shift

When a relativistic charged particle is travelling through a periodic magnetic field, in the particles rest frame it sees a magnetic field rushing towards it.

In our rest frame the magnet period is λ_u because of Lorentz contraction the electron sees it as λ_u / γ
 γ is the relativistic **Lorentz factor**

$$\gamma = \frac{E}{E_0}$$

$$\beta = \frac{v}{c}$$

$$\beta = \sqrt{1 - \frac{1}{\gamma^2}}$$

c is the velocity of light in free space

v is the velocity of the electron

β is the relative velocity of the electron

E is the electron energy (6 GeV @ PETRA III)

E_0 is the electron rest energy (0.511 MeV)

This γ factor turns up again and again in SR !

($\approx 12\,000$ @ PETRA III)

The particle emits light of wavelength λ_u / γ

Since it is travelling towards us this wavelength is due to the Doppler effect further reduced to $\sim \lambda_u / 2\gamma^2$

Radiation by acceleration of a charged particle

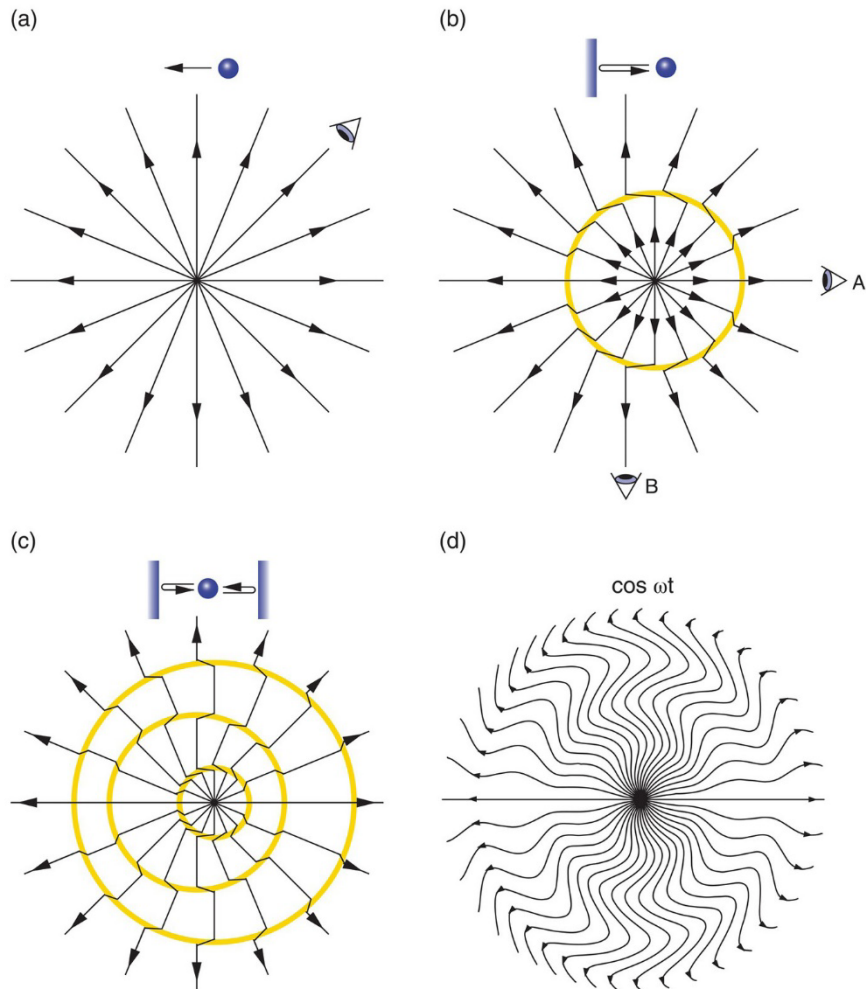
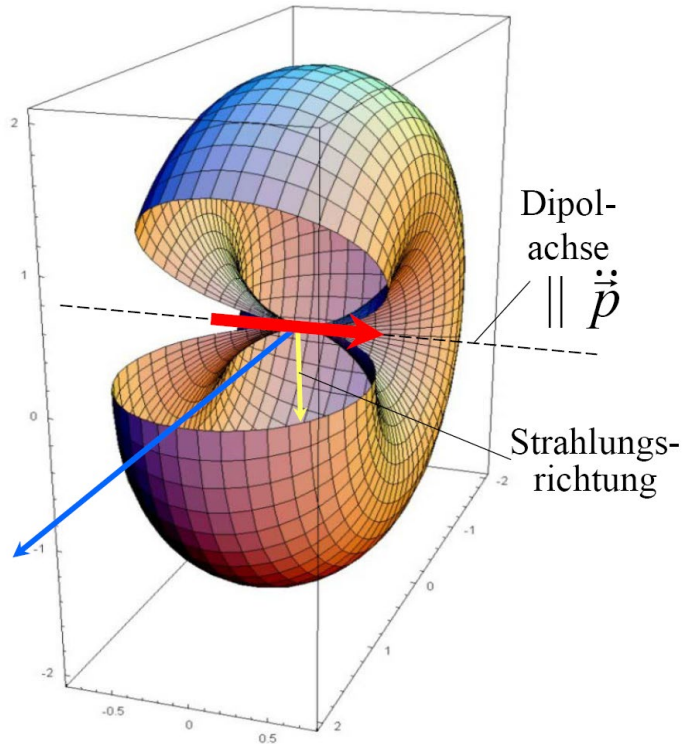


Figure 3.3 Generation of electromagnetic radiation by acceleration of a charged particle. (a) A charged particle at rest or moving at uniform speed will not emit light, as any observer of the particle detects no lateral component of the electric-field lines. (b) If, however, the particle undergoes acceleration, an observer positioned anywhere other than along the axis of that acceleration (position A), will see a shift in the position and direction of the electric-field lines as the event horizon washes over them at the speed of light (for example, at position B). (c) A charged particle bouncing between two boundaries will generate a corresponding set of pulses of electromagnetic radiation at regular intervals. (d) A simple-harmonic driving force will generate radiation at the same frequency.

An Introduction to Synchrotron Radiation: Techniques and Applications, 2nd edition, P. Willmott, 2019, Wiley

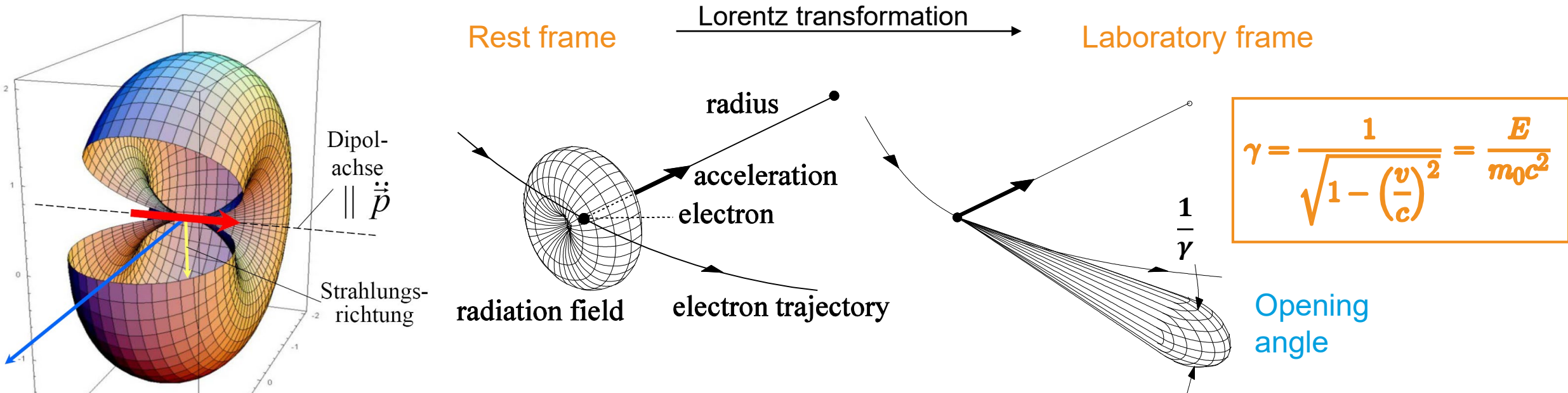
Emission pattern for circular acceleration



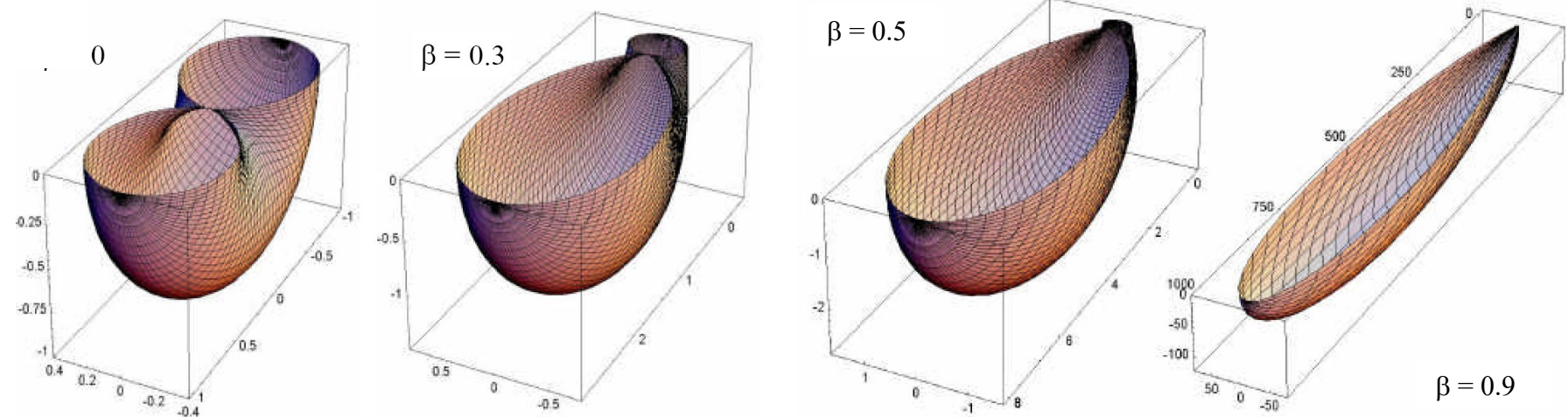
Hertzian Dipole

- Every accelerated charge radiates electromagnetic waves
- Oscillatory motion: No radiation in direction of the oscillation
- The maximum radiated power is observed perpendicular to the oscillation direction

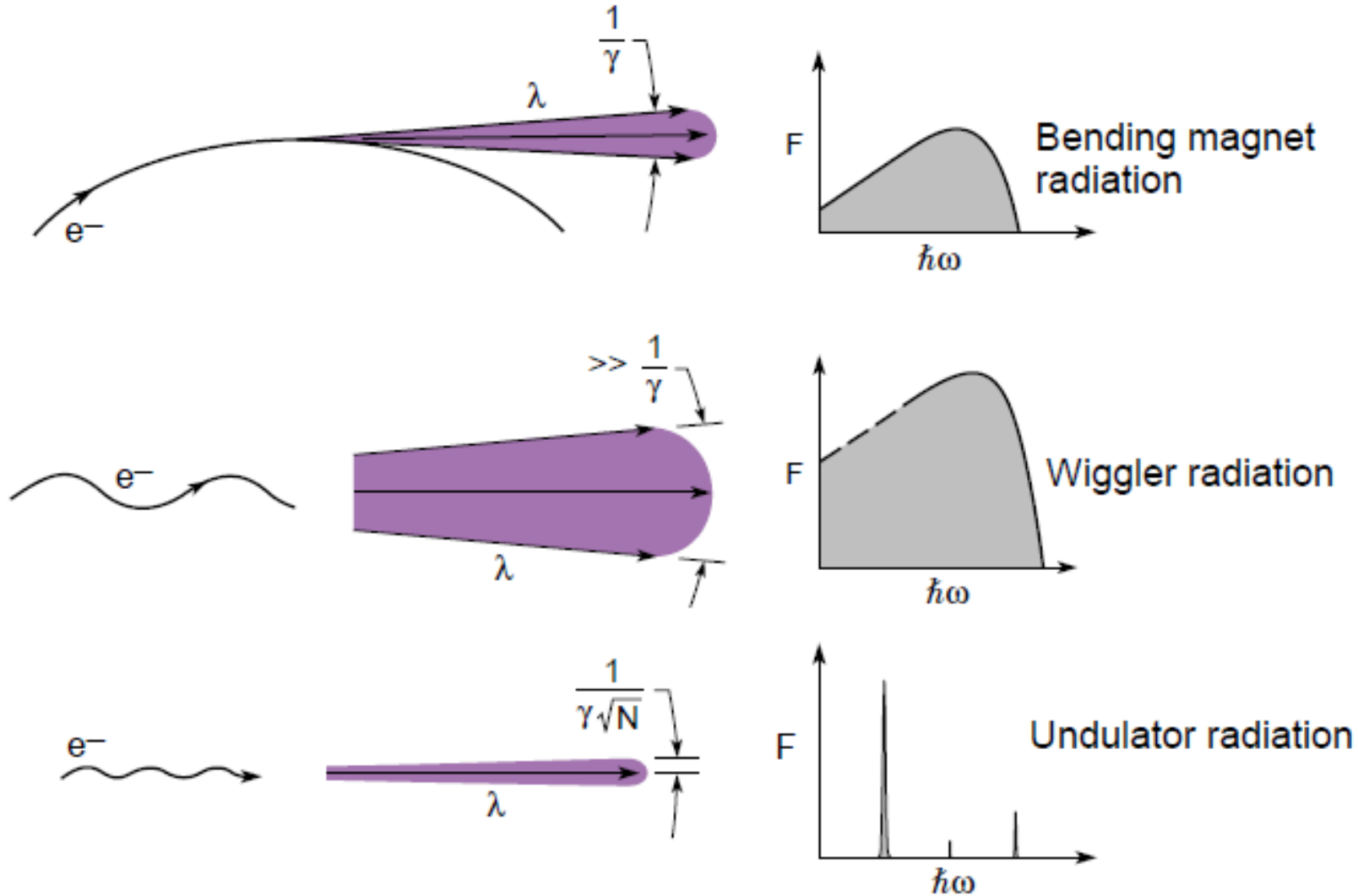
Emission pattern for circular acceleration



Hertzian Dipole

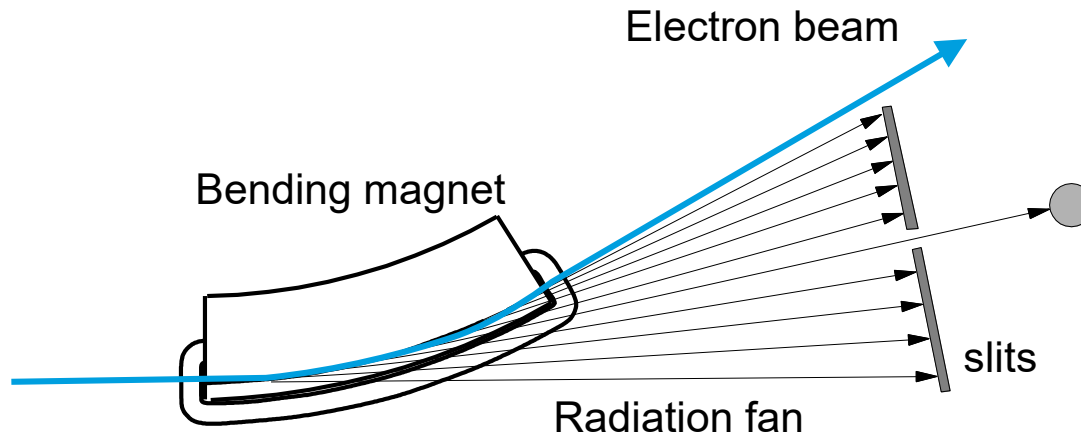


„Three types“ of radiation



Radiation from a bending magnet

Radiation spectrum and critical energy



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

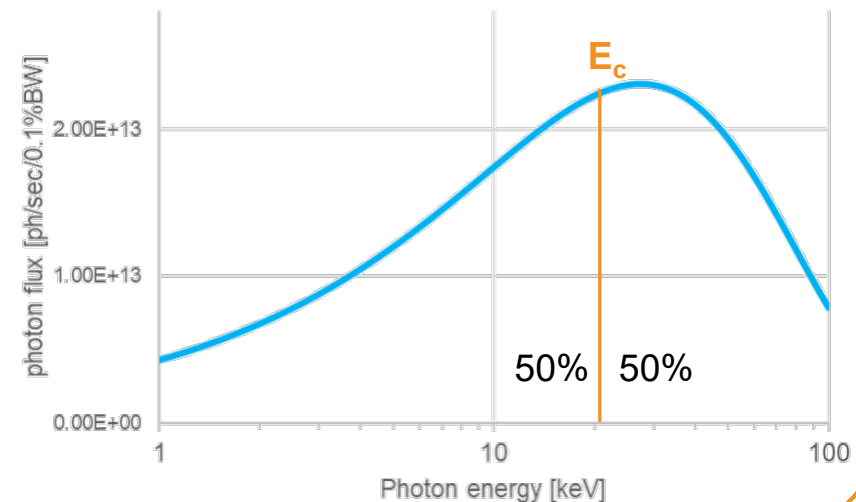
- Critical energy of bending magnet:

$$E_c = \frac{3}{2} \cdot \frac{\hbar c}{E_0^3} \cdot \frac{E^3}{r} = \frac{3}{2} \cdot \frac{\hbar c^2}{E_0^3} \cdot B \cdot E^2$$

$$E_c[\text{keV}] = 0.665 \times B[\text{T}] \times E[\text{GeV}]^2$$

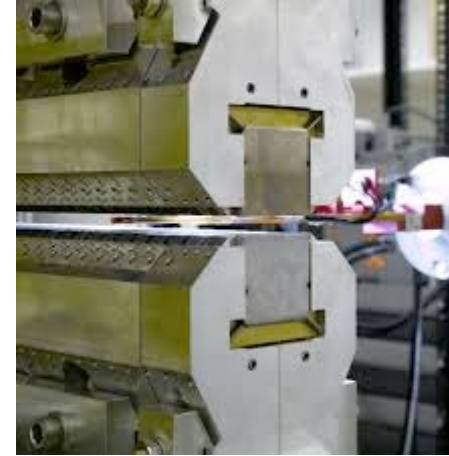
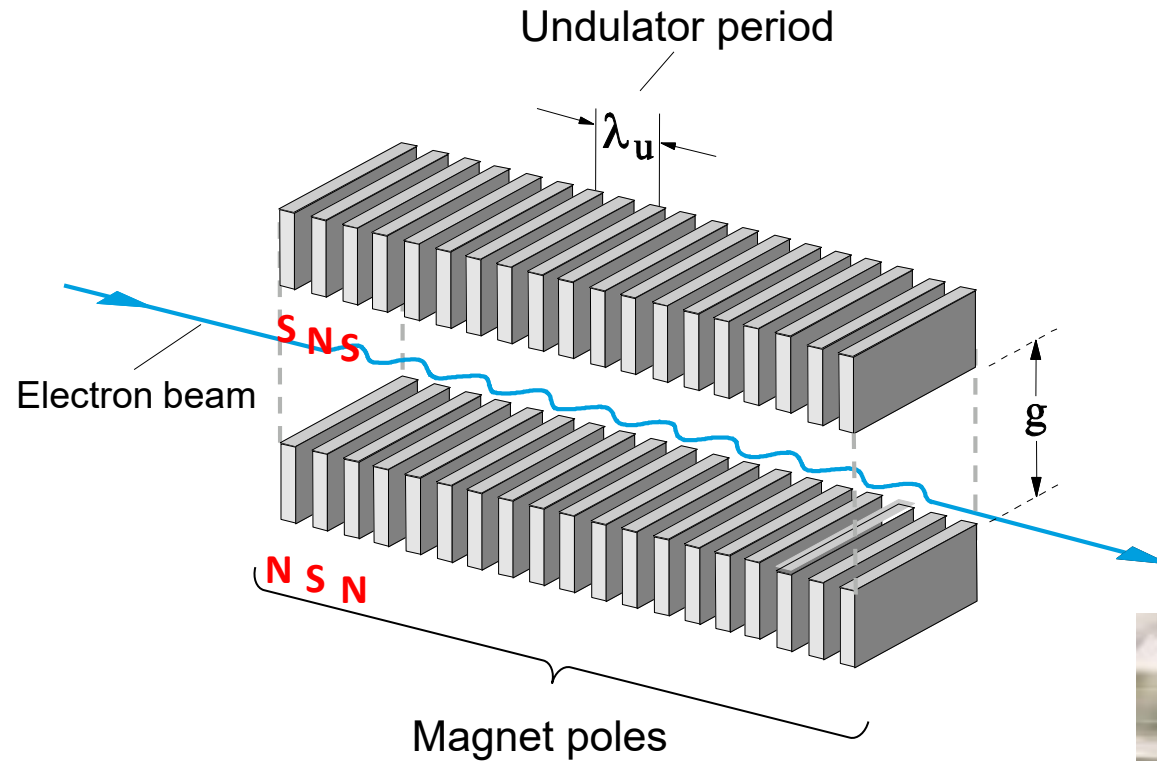
Example PETRA III bending magnet:
E = 6 GeV, B = 0.87 T (R = 22.9 m)

→ **$E_c = 20.9 \text{ keV}$**



Insertion devices: W wigglers and Undulators

Undulation motion



- Multiplication of the radiation intensity by periodically repeated magnet structures

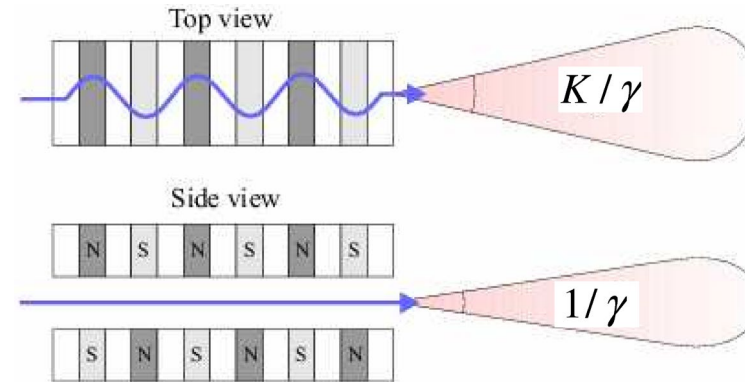
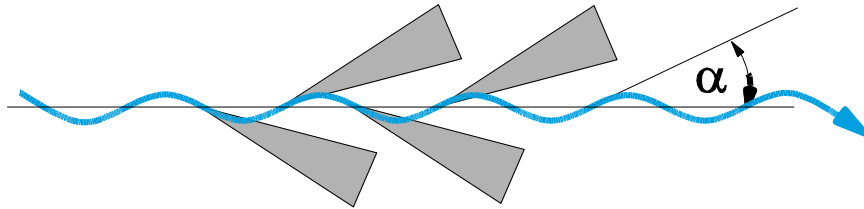
$$\text{Undulator strength parameter } K = \frac{eB\lambda_u}{2\pi m_e c}$$



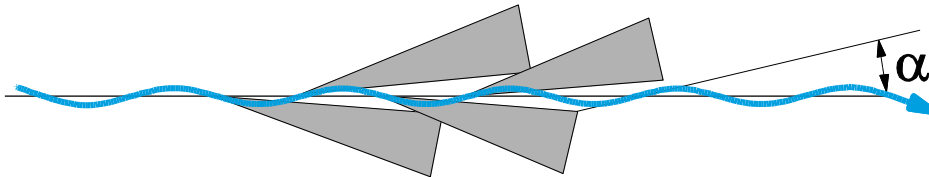
Insertion devices: Wigglers and Undulators

Energy and direction of radiation emission

$K \gg 1 \rightarrow$ Wiggler regime: $\alpha > 1/\gamma$
broad photon energy range



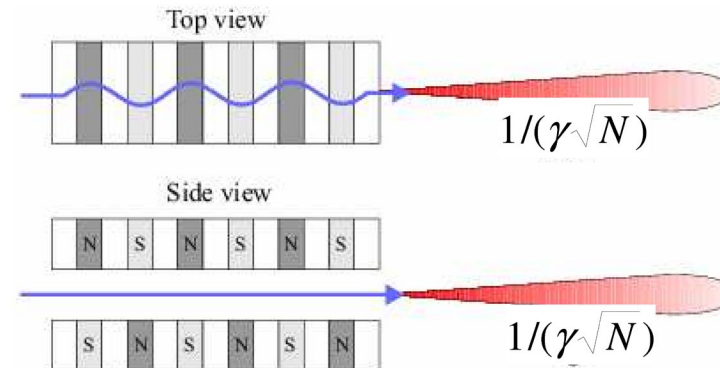
$K \leq 1 \rightarrow$ Undulator regime: $\alpha < 1/\gamma$



$$\lambda \approx \frac{\lambda_u}{2\gamma^2} \left(1 + \frac{K^2}{2} \right)$$

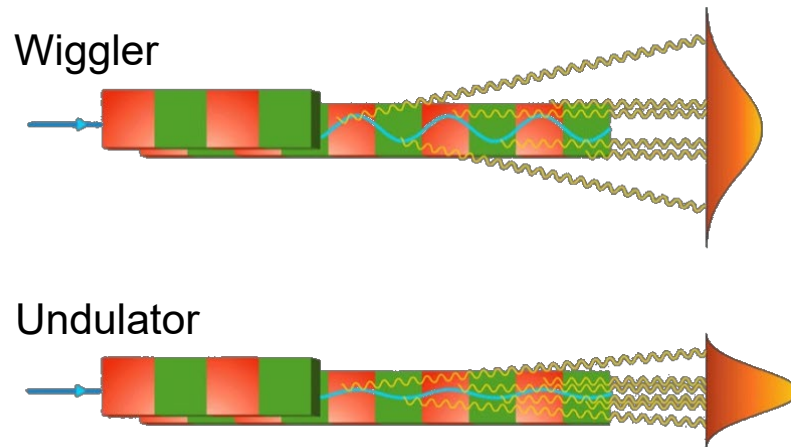
and $\frac{\Delta\lambda}{\lambda} \approx \frac{1}{N}$ with $N = \#$ periods of undulator

- In the undulator regime the radiation cones overlap and the wave trains can interfere constructively \rightarrow increase of intensity



Insertion devices: W wigglers and Undulators

intensity of the emitted radiation



N_p = Number of magnet poles

N_e = Number of electrons/bunch

Incoherent superposition

$$I \sim N_e N_p$$

Partially coherent superposition

$$I \sim N_e N_p^2$$

Photon intensities delivered by different source types

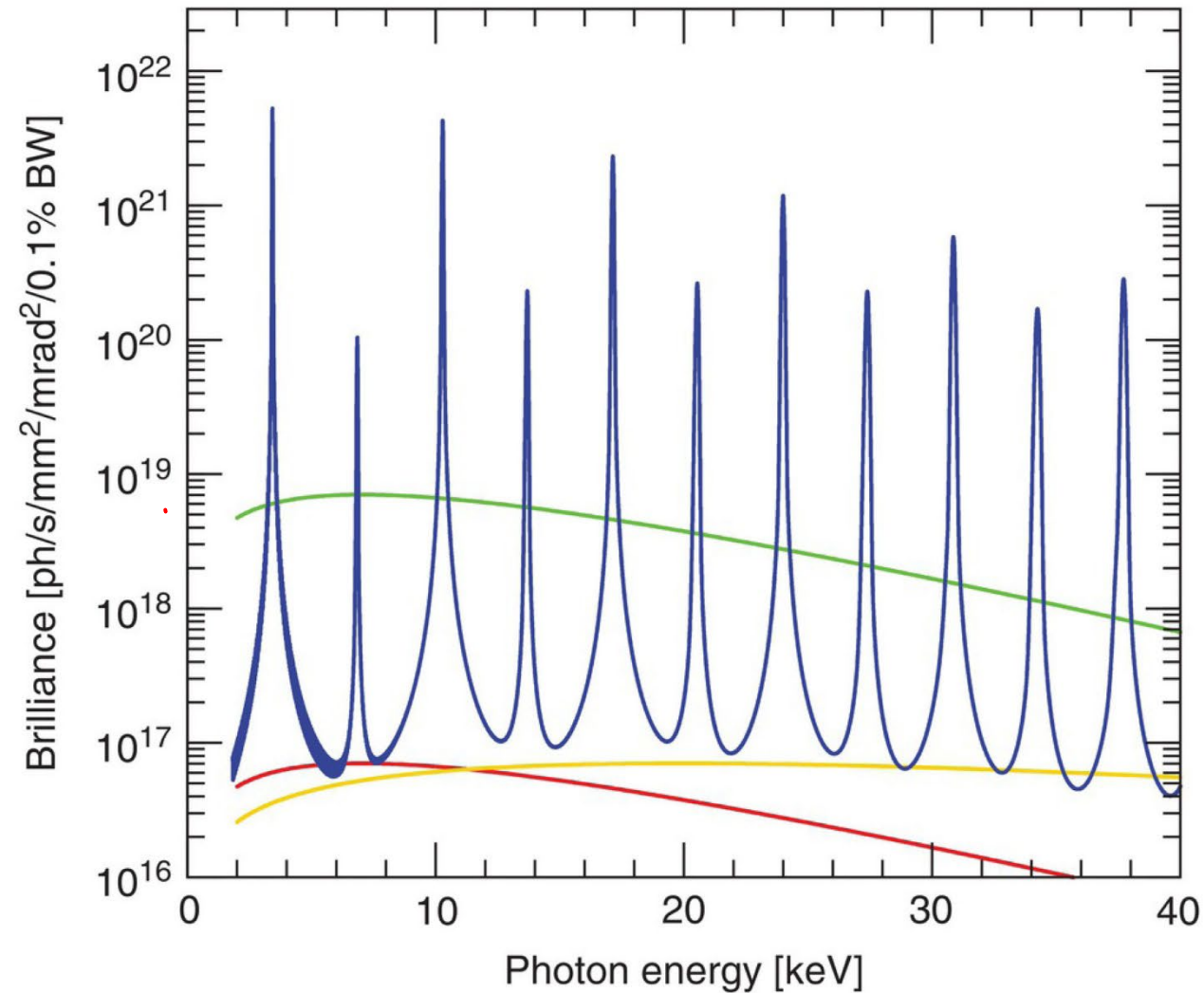


Figure 3.35 Comparison of brilliances at a 3 GeV DLSR running at 400 mA between a U14 undulator with $K = 1.6$ (blue), a bending magnet with $B = 1.41$ T (red), a superbend with $B = 4$ T (yellow), and a wiggler with the same field strength as the bending magnet and 100 periods (green).

An Introduction to Synchrotron Radiation: Techniques and Applications, 2nd edition, P. Willmott, 2019, Wiley

Quantities to describe photon intensity

Total Flux F

number of photons
per time and energy interval

$$[F_{tot}] = \frac{\text{Number of photons}}{s}$$

Spectral Flux

number of photons
per time, and energy bandwidth (BW)

$$[F] = \frac{\text{Number of photons}}{s \cdot 0.1\% BW}$$

Brilliance B

number of photons
per time, source area, solid angle
and energy bandwidth (BW)

$$[B] = \frac{\text{Number of photons}}{s \cdot \text{mm}^2 \cdot \text{mrad}^2 \cdot 0.1\% BW}$$

$$\begin{aligned} \text{Emittance} &= \text{size} \times \text{divergence} \\ \text{Brilliance} &= \frac{\text{Flux}}{\text{Emittance}} \end{aligned}$$

Peak brilliance B^{peak}

brilliance scaled to pulse duration τ

$$B^{peak} = \frac{B}{\tau \times f}$$

Degree (fraction) of lateral **coherence**

$$\frac{4\lambda^2}{\text{Emittance}} \leq 1 \quad \Rightarrow$$

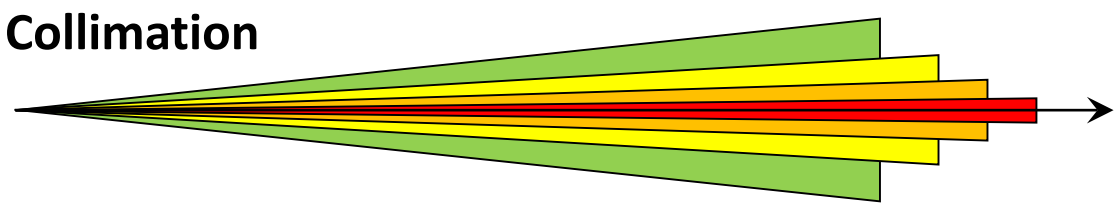
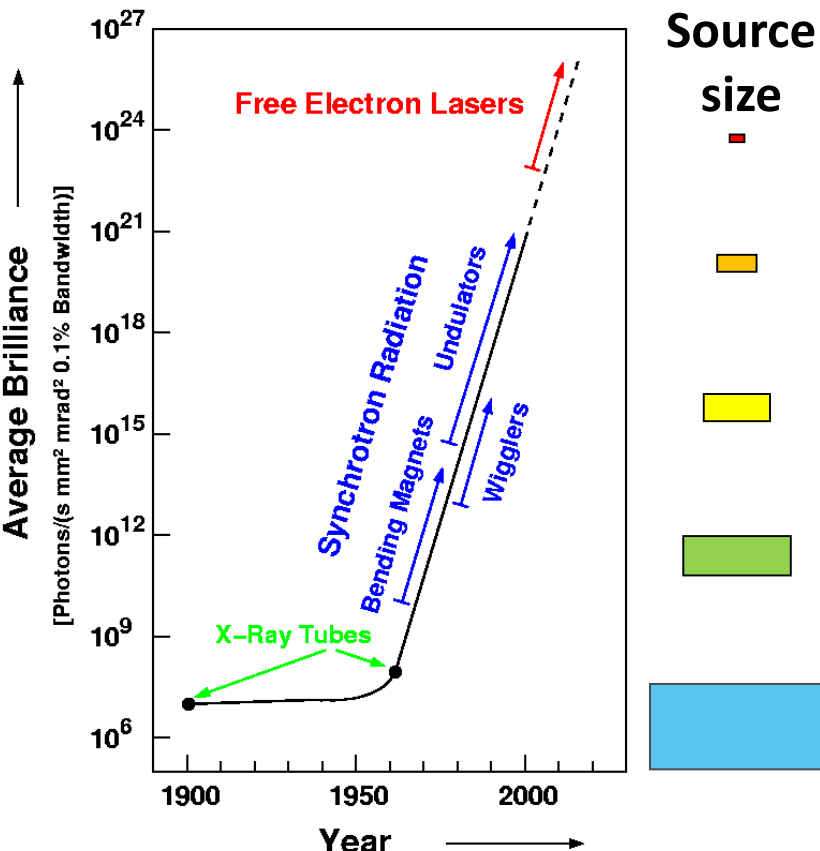
Emittance has a lower (diffraction) limit, at which the source becomes fully lateral coherent

Evolution of synchrotron radiation sources

Smaller, brighter!

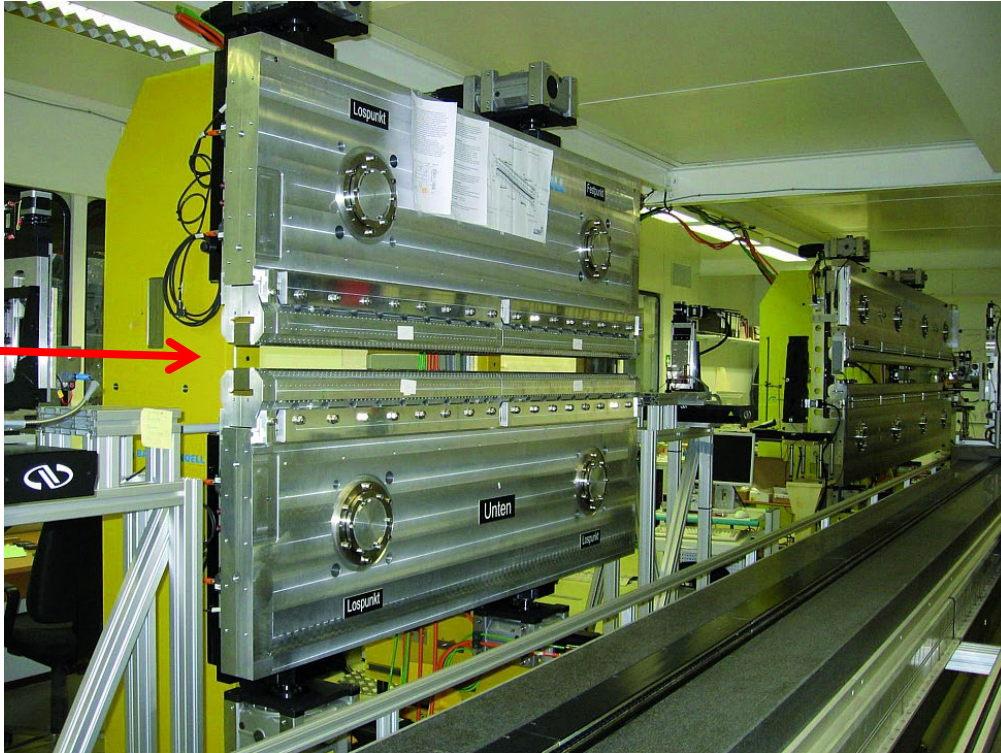
$$\text{brilliance} = \frac{\text{Photon flux}}{\sigma_x \sigma_y \sigma'_x \sigma'_y \text{ BW}}$$

- Photon flux = photons/s
- σ_x, σ_y = transverse area from which SR is emitted
- σ'_x, σ'_y = solid angle into which the SR is emitted
- BW = bandwidth of the monochromator



PETRA III @ DESY

Characteristic parameters



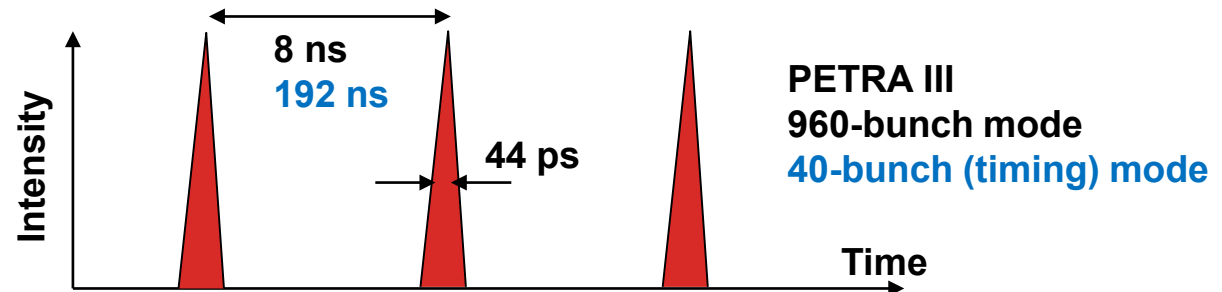
Vertical aperture of vacuum chamber: 7 mm

PETRA III machine parameters

Electron energy: **6 GeV**
Circumference: 2304 m
Revolution time: 7.685 μ s
Number of bunches: 960, 480, 40
Bunch separation: 8, 16, 192 ns
Bunch length: 13.2 mm, **44 ps**
Total beam current: **100 mA (top-up mode)**

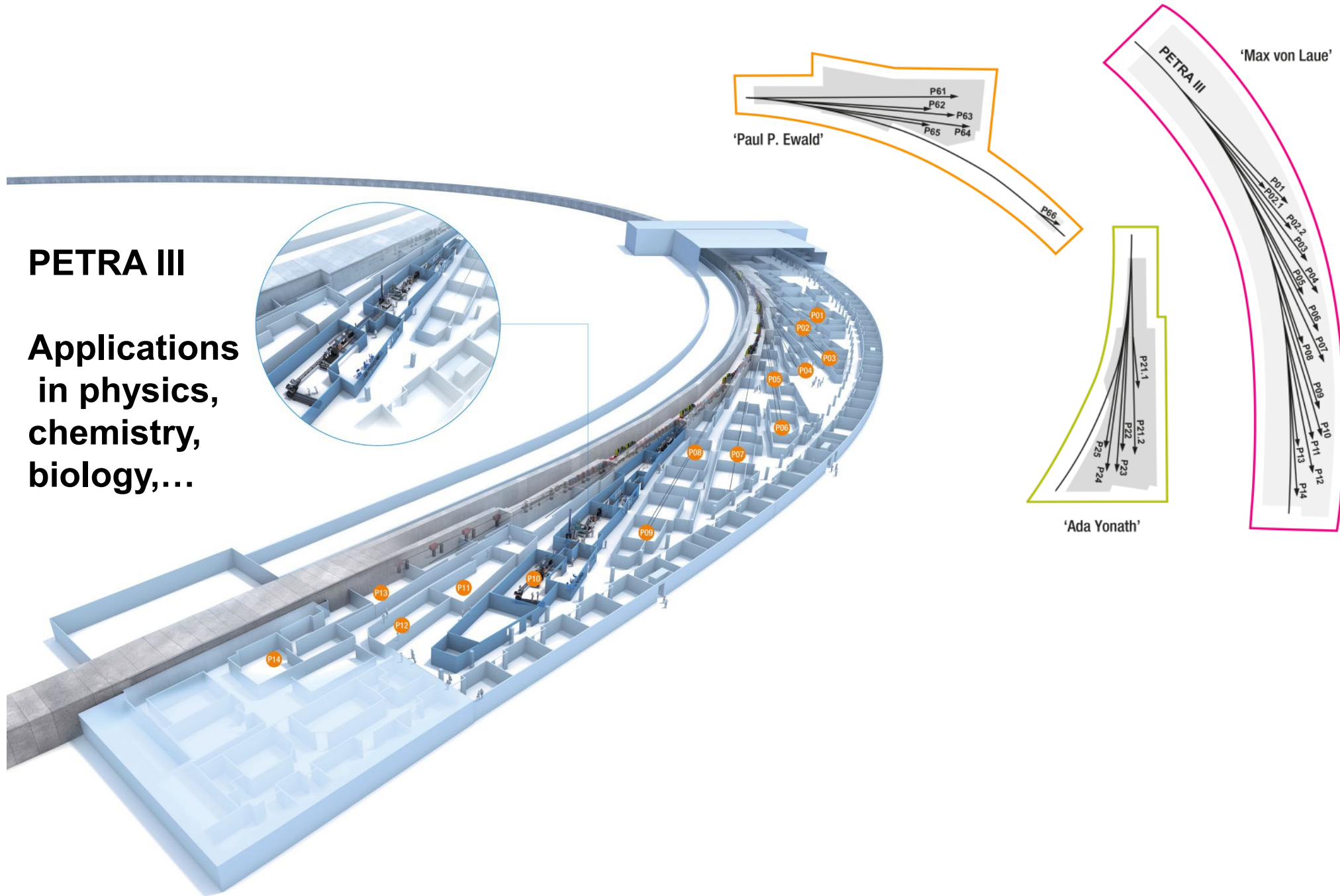
Horizontal emittance: **1.2 nm rad**
Vertical emittance: **0.012 nm rad**

Bending magnet field: 0.873 T
Bending magnet radius: 22.92 m
Critical photon energy: **20.9 keV**



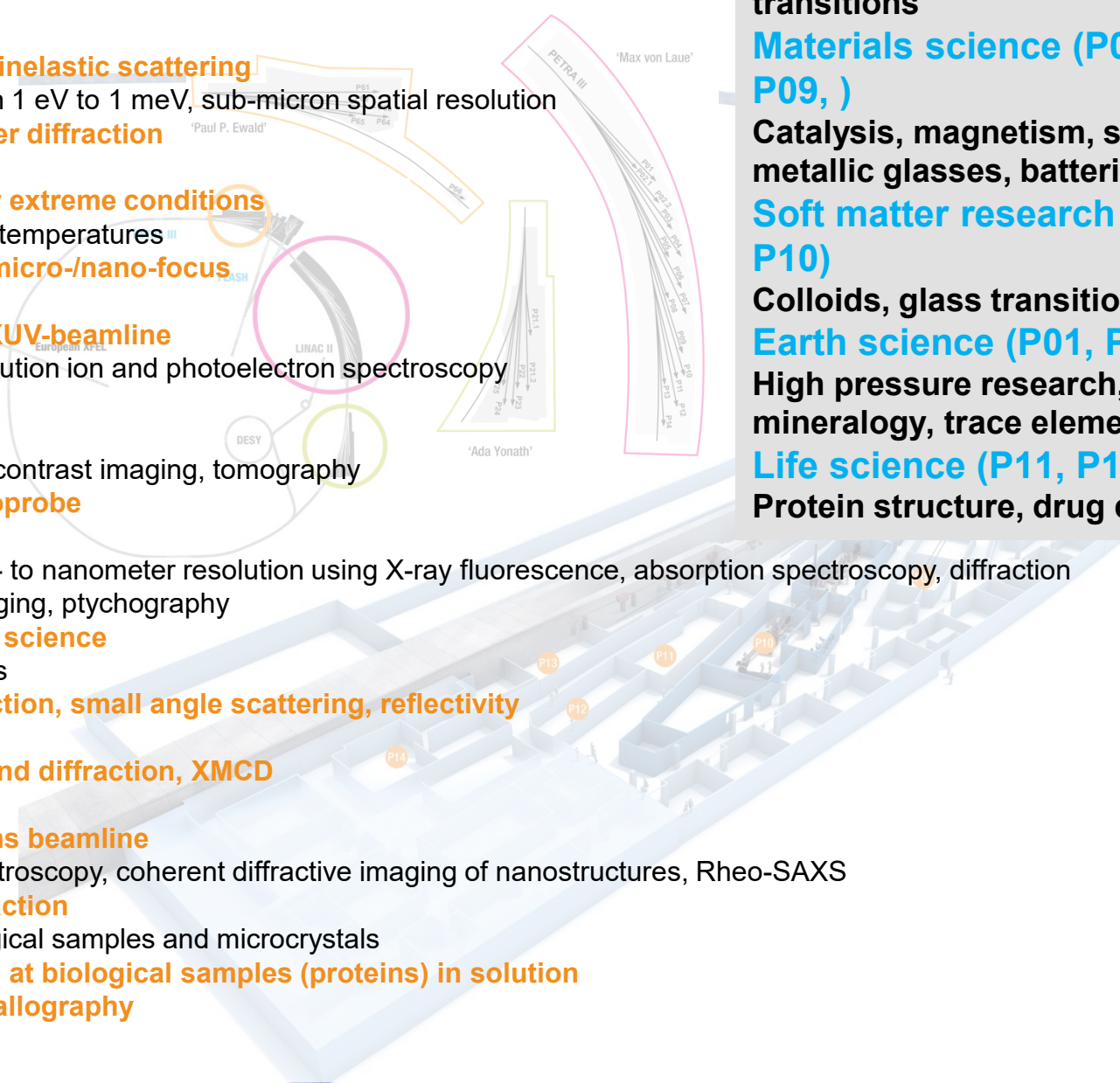
PETRA III

Applications
in physics,
chemistry,
biology,...



PETRA III Facilities

- P01: Nuclear resonant and inelastic scattering**
 2.5 - 80 keV, Resolution 1 eV to 1 meV, sub-micron spatial resolution
- P02.1: High-resolution powder diffraction**
 60 keV, Resolution
- P02.2: Microdiffraction under extreme conditions**
 25 - 60 keV, high pressure, high/low temperatures
- P03: X-ray scattering with micro-/nano-focus**
 9 - 23 keV
- P04: Variable polarization XUV-beamline**
 250 - 3000 eV High-resolution ion and photoelectron spectroscopy
- P05: Imaging beamline**
 5- 50 keV
 Phase- and absorption contrast imaging, tomography
- P06: Hard X-ray micro/nanoprobe**
 5 - 21 keV
 Visualization with micro- to nanometer resolution using X-ray fluorescence, absorption spectroscopy, diffraction
 coherent diffraction imaging, ptychography
- P07: High energy materials science**
 30 - 200 keV, Microfocus
- P08: High resolution diffraction, small angle scattering, reflectivity**
 5 - 29 keV, Microfocus
- P09: Resonant scattering and diffraction, XMCD**
 2.7 - 50 keV
- P10: Coherence applications beamline**
 5 - 25 keV Photon correlation spectroscopy, coherent diffractive imaging of nanostructures, Rheo-SAXS
- P11: Bio-Imaging and diffraction**
 5 - 30 keV, Micro/nanobeam, biological samples and microcrystals
- P12: Small angle scattering at biological samples (proteins) in solution**
- P13/P14: Macromolecular crystallography**

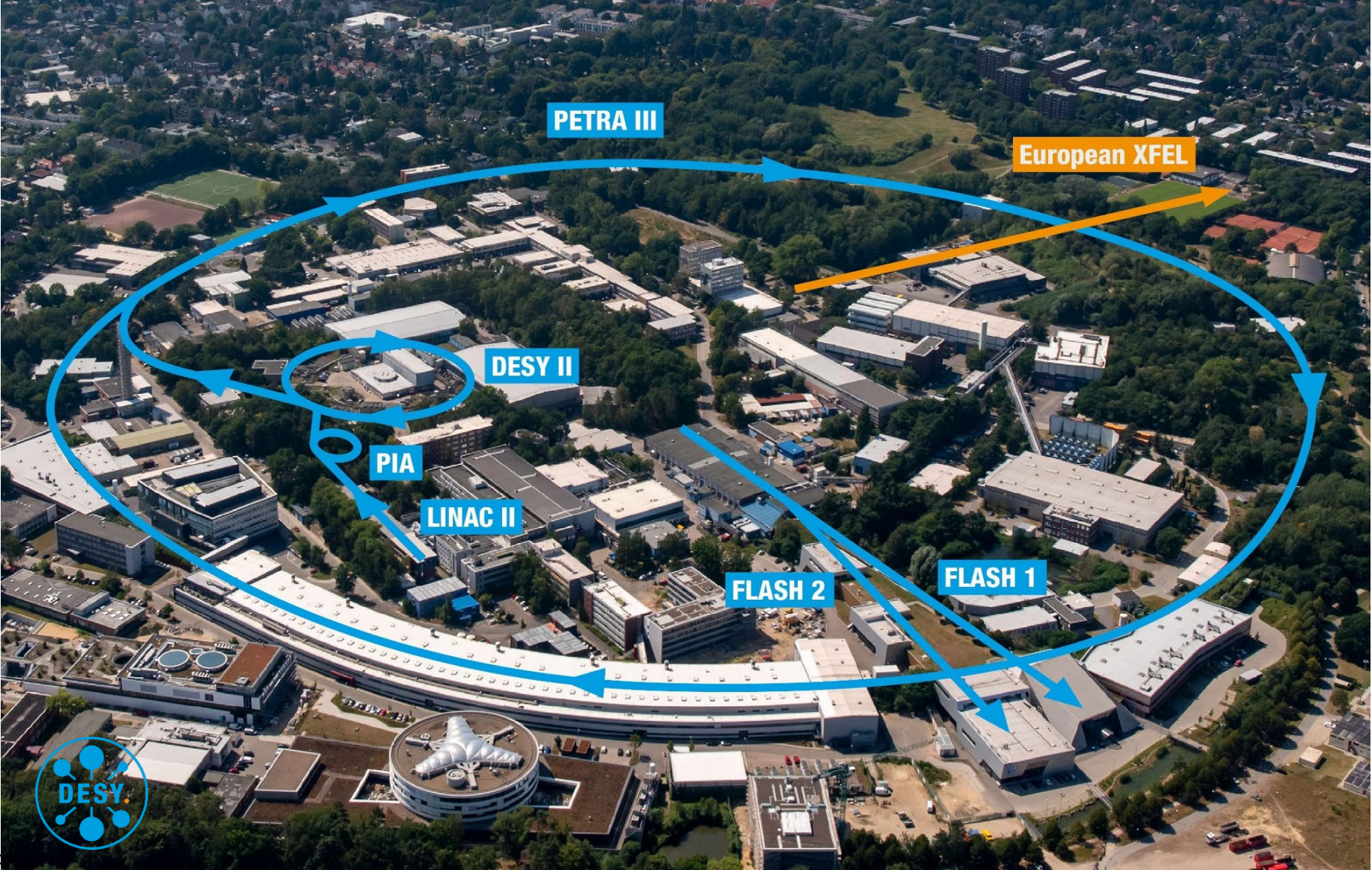


- Atomic and molecular science (P04)
- Surface science (P01, P03, P08, P10)
- Thin films, wetting phenomena, phase transitions
- Materials science (P01, P02, P04, P07, P09,)
- Catalysis, magnetism, superconductivity, metallic glasses, batteries
- Soft matter research (P01, P03, P08, P09, P10)
- Colloids, glass transitions
- Earth science (P01, P02, P08, P09)
- High pressure research, geophysics, mineralogy, trace element analysis
- Life science (P11, P12, P13, P14)
- Protein structure, drug development

Principle of Free-Electron Lasers (FELs)

FELs at DESY

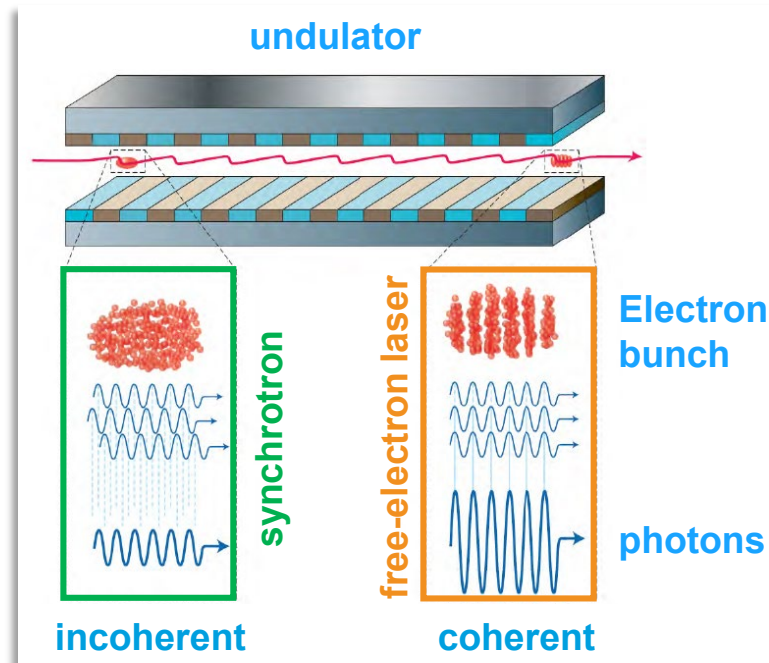
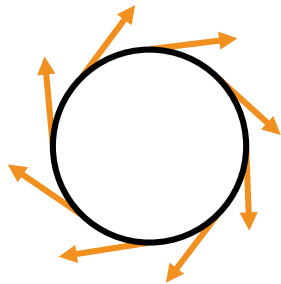
FLASH and European XFEL



Synchrotrons vs. free-electron lasers

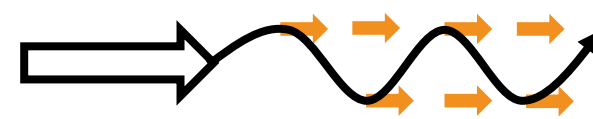
Synchrotrons

- Electrons traveling in a wide circular path, emitting light as they change directions
- Light is UV or X-ray, but not (fully) coherent
- Multiple users

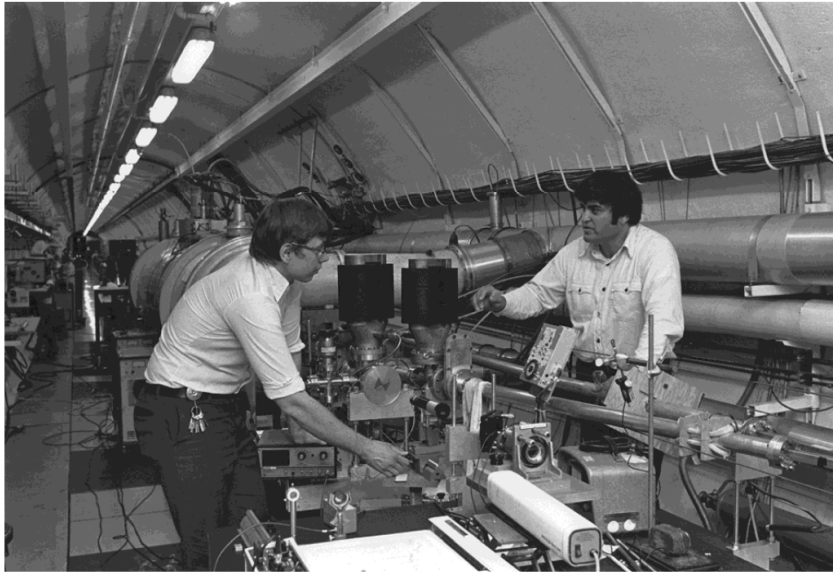


Free-electron lasers

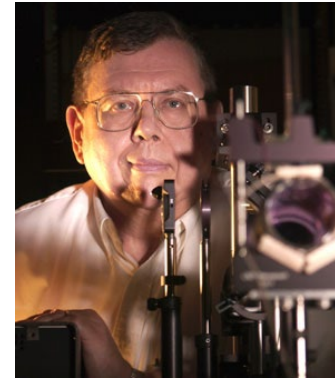
- Electrons accelerated in a straight line and manipulated to generate light
- **Light is coherent and intensely bright in very short pulses**
- Single user



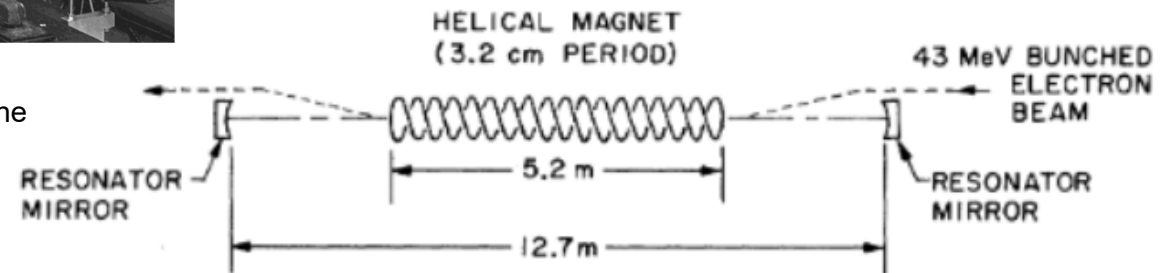
Invention of free-electron laser



John Madey and Luis Elias working inside the Superconducting Acceleration (SCA) tunnel with the FEL equipment, Stanford University, 1995



John Madey, The University of Hawai'i



FEL was theorized by John Madey in his Ph.D. thesis, Stanford 1970:

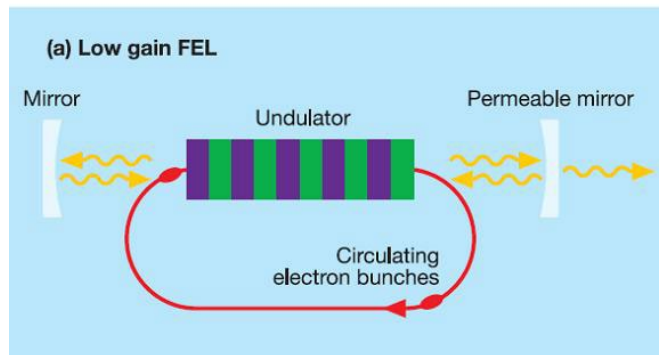
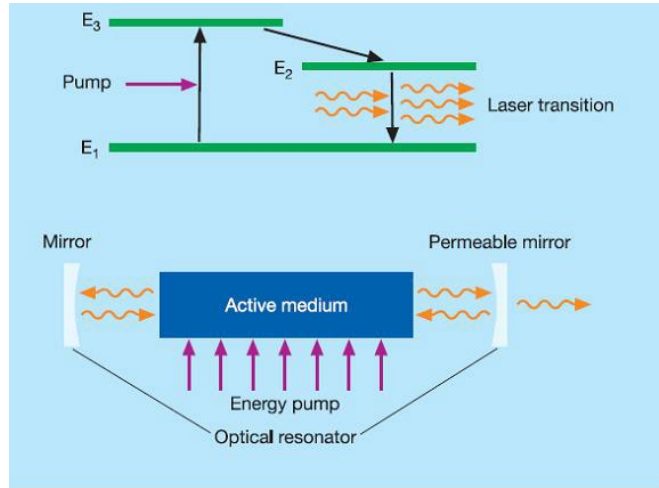
J.M.J. Madey, J. Appl. Phys. 42, 1906 (1971)

First realization: Stanford, Electron energy: 43.5 MeV, FEL radiation: 3.4 μm
D.A.G. Deacon, L.R. Elias, J.M.J. Madey, G.J. Ramian, H.A. Schwettman, T.I. Smith; Phys. Rev. Lett. 38, 892 (1977)

Free-electron laser (FEL) vs. conventional laser

- **Laser:**
amplification due to stimulated emission of electrons bound to atoms (crystal, liquid dye, gas)
- **FEL:**
amplification / gain medium = „free“ (unbound) electrons, stripped from atoms in an electron gun, accelerated to relativistic velocities and travelling through an undulator (= periodic magnetic multipole structure) to produce intense radiation

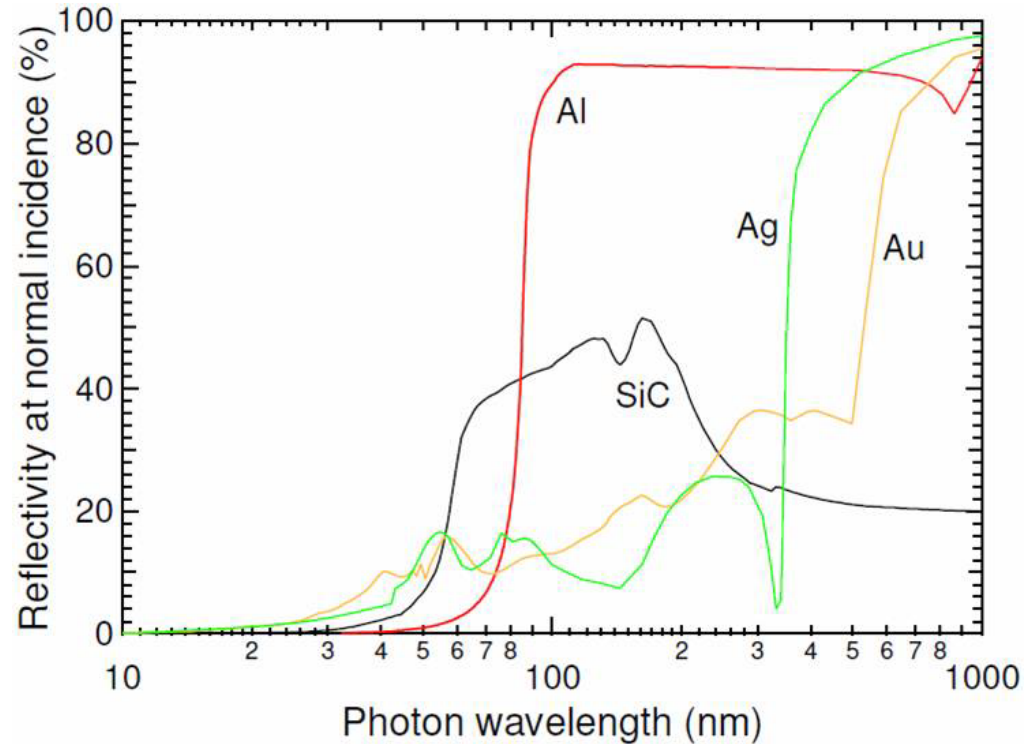
Free-electron laser (FEL) vs. conventional laser



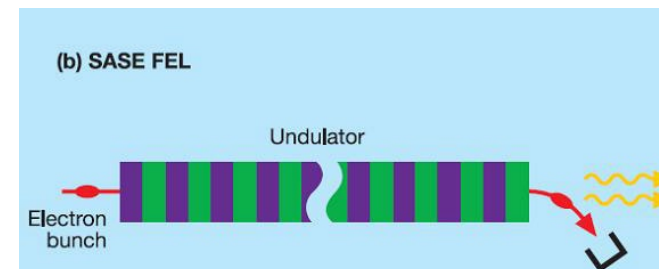
- Quantized energy levels
 - Pump energy initiates population inversion
 - Stimulated emission
 - Optical resonator (cavity)
-
- Electron energy is not quantized
 - "Pump energy" is the kinetic energy of the electrons
 - Stimulated emission
 - Optical cavity or single pass SASE

Free-electron laser at short wavelength

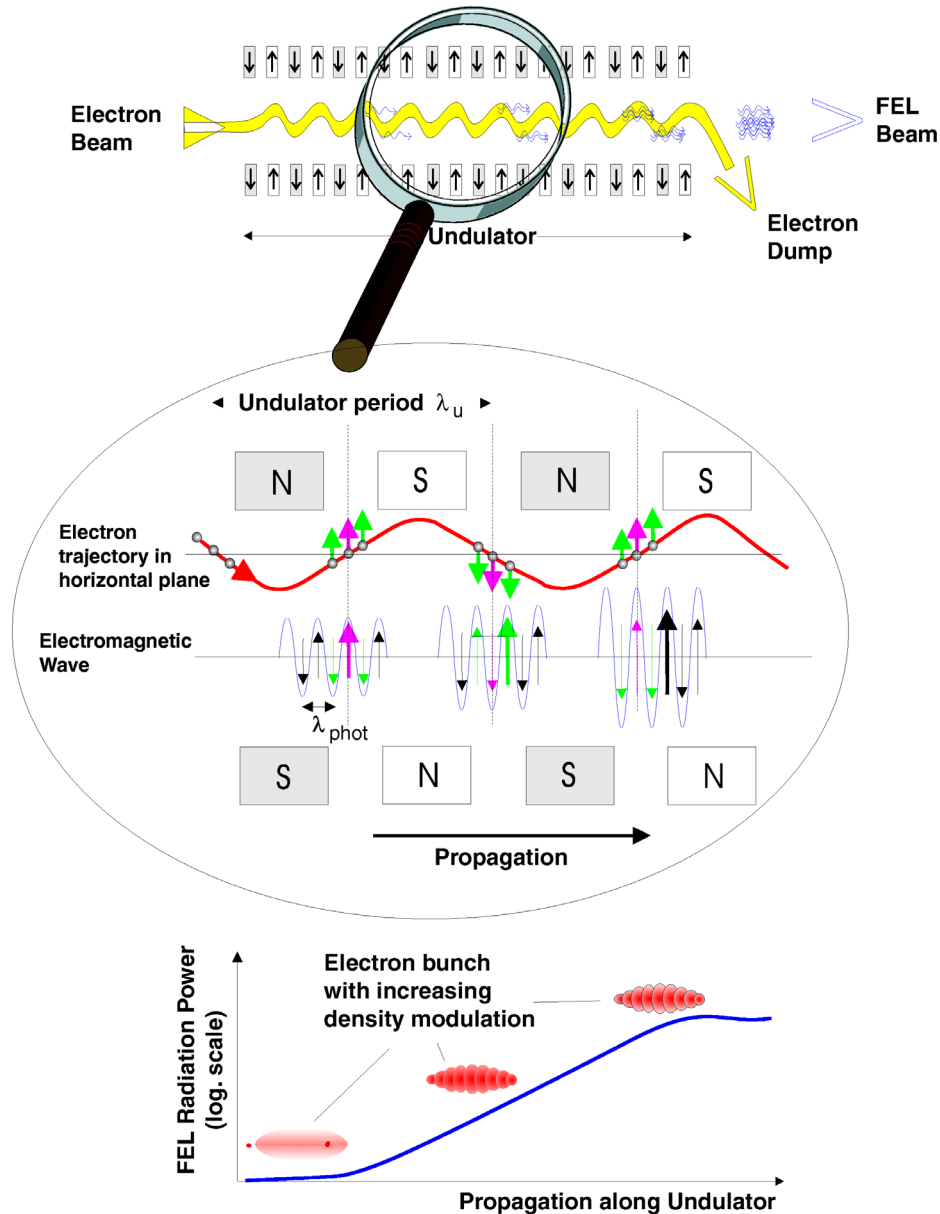
- Optical cavity does not work for wavelength $\lambda < 100\text{nm}$ (low reflectivity, radiation damage)



- single pass SASE FEL



Self-amplified spontaneous emission – SASE FEL



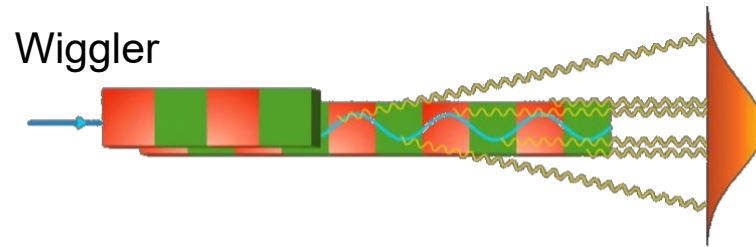
- Slippage between electrons and photons is λ_{phot} per undulator period
- Electrons in phase with e.m.-wave are retarded (“emit photons”), electrons with opposite phase gain energy (“absorb photons”)
- Different trajectories in the undulator (see Lorentz force)
- > Longitudinal charge density modulation (“micro-bunching”) with periodicity equal to λ_{phot}
- > Self-amplification of spontaneous emission due to increasingly coherent emission from micro-bunches (like point charge)
- $I \sim N_e^2 N_p^2$

Insertion devices: Wigglers and Undulators

Intensity of the emitted radiation

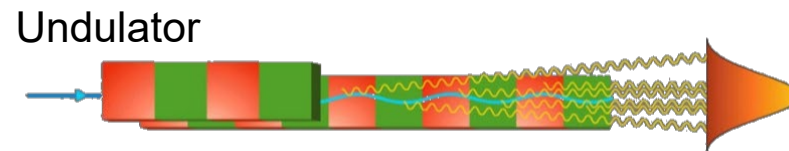
N_p = Number of magnet poles

N_e = Number of electrons/bunch



Incoherent superposition

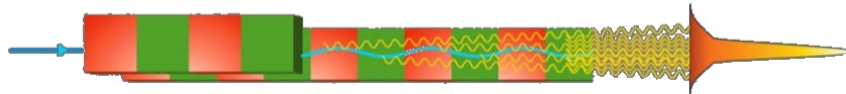
$$I \sim N_e N_p$$



Partially coherent superposition

$$I \sim N_e N_p^2$$

Free-Electron Laser



Fully coherent superposition

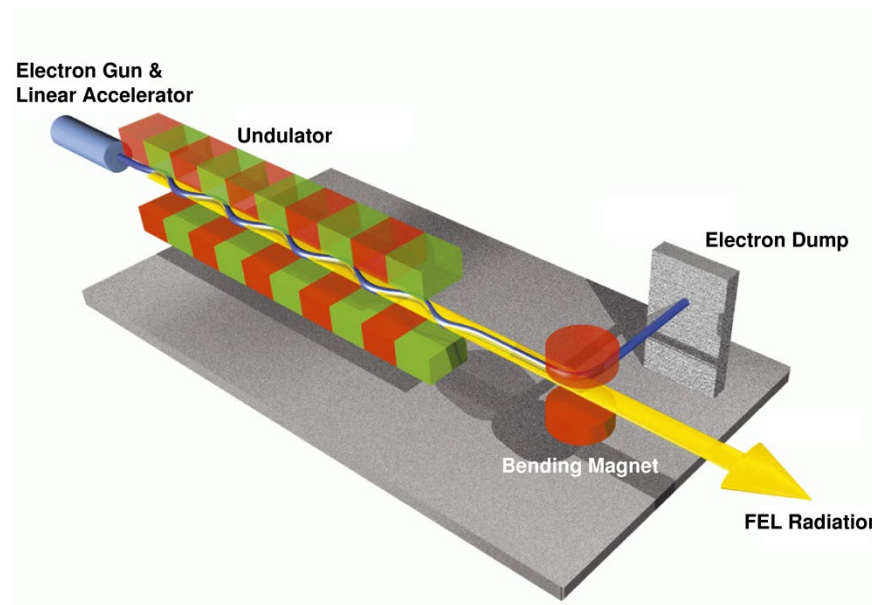
$$I \sim N_e^2 N_p^2$$

Self-Amplified Spontaneous Emission (SASE)

Self-amplified spontaneous emission – SASE

Requirement for SASE

- Good electron beam quality and sufficient overlap between electron-beam and radiation pulse along the undulator:
 - low emittance, low energy spread of electron beam
 - extremely high charge density (kA peak currents)
 - precise magnetic field of undulator
- accurate beam steering through undulator (few μm precision)



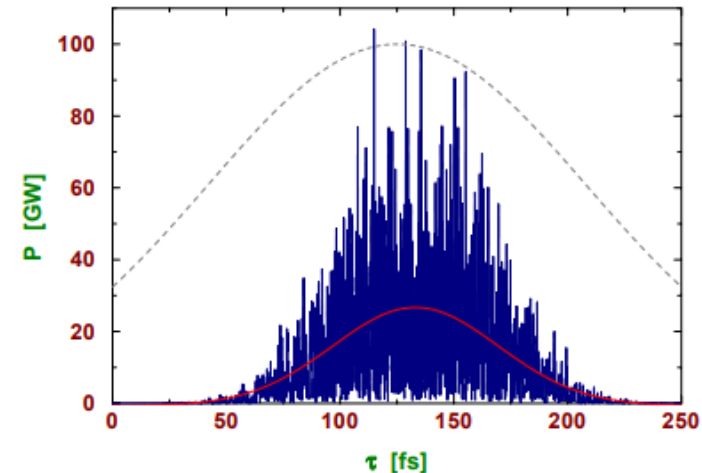
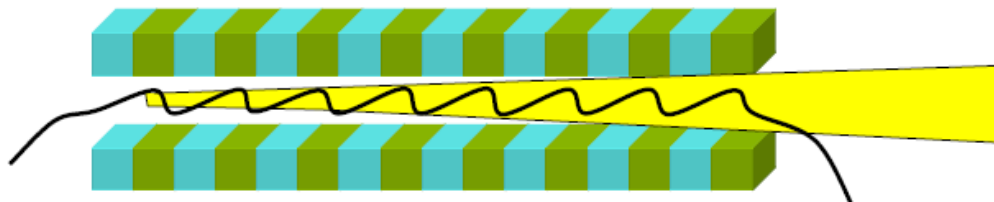
Self-amplified spontaneous emission – SASE

Emitted light, temporal distribution

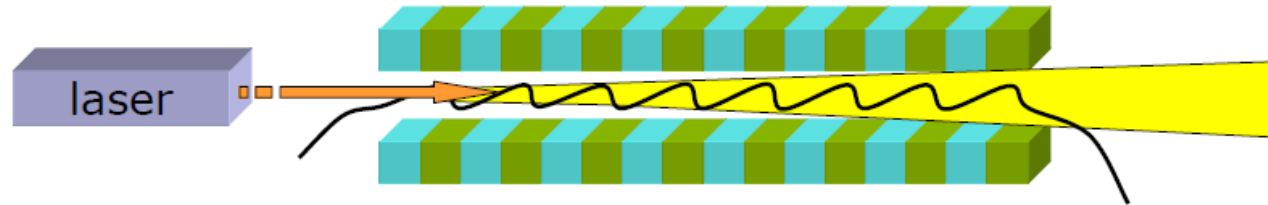
- For a given wavelength there is only one resonant electron energy (continuous energy transfer)

$$\lambda_l = \frac{\lambda_u}{2\gamma^2} \left(1 + \frac{K^2}{2} \right)$$

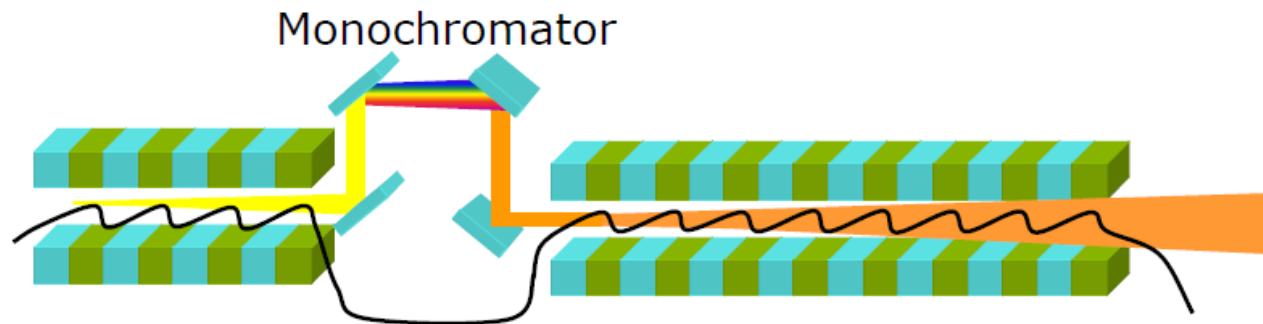
- Wavelength change by changing the electron energy or magnetic field strength
- FEL process starts from noise: randomly distributed electron bunch and spontaneous undulator radiation
- Radiation pulse is “spiky” in time (and frequency) domain



Seeded – FEL



- External laser seeding



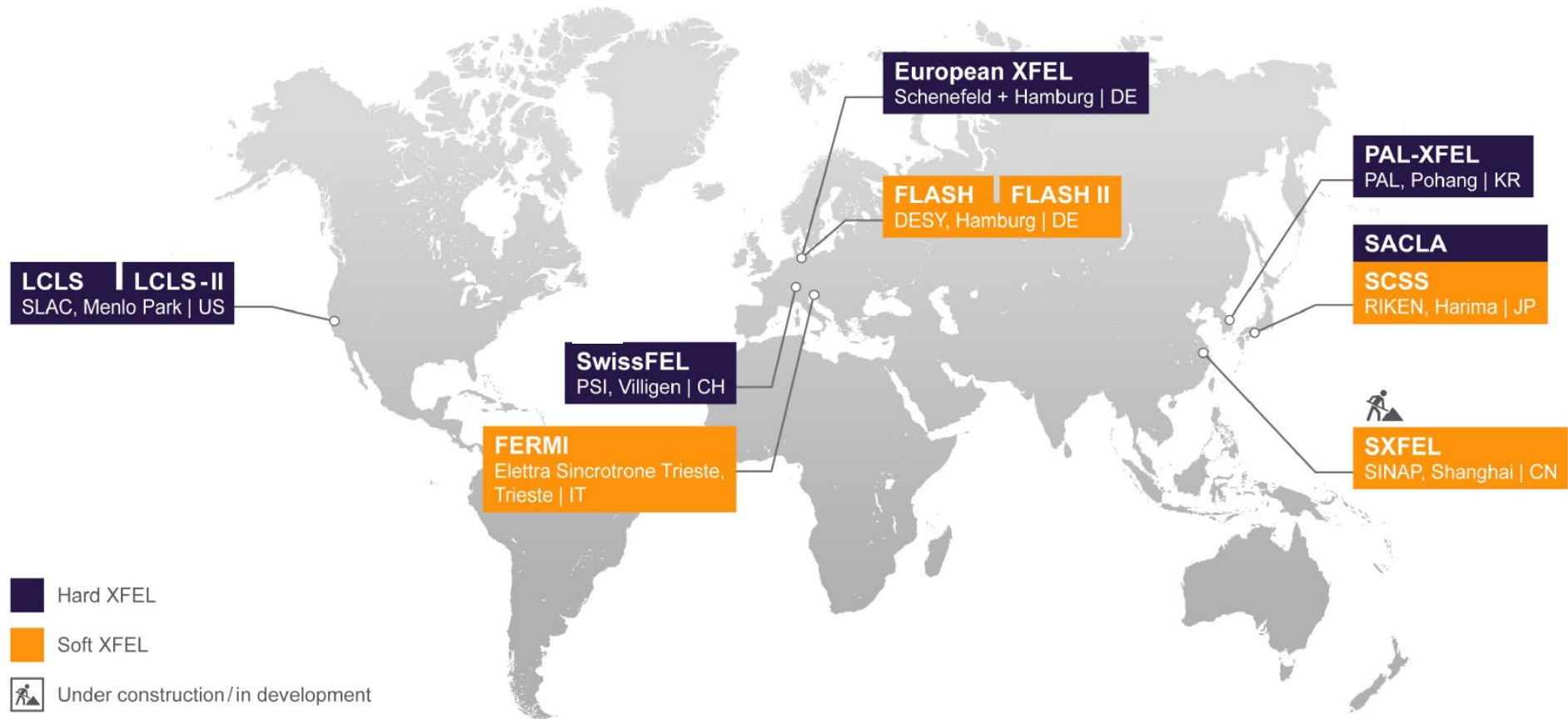
- Self-seeding

SASE FEL properties

- > high intensity (GW peak power)**
- > coherence (laser-like radiation)**
- > femtosecond pulses!**
- > narrow bandwidth!**
- > full wavelength tunability!**
- > down to X-rays!**

- > but: shot-to-shot fluctuations (w/o seeding)**
 - > very good photon diagnostics are mandatory!**

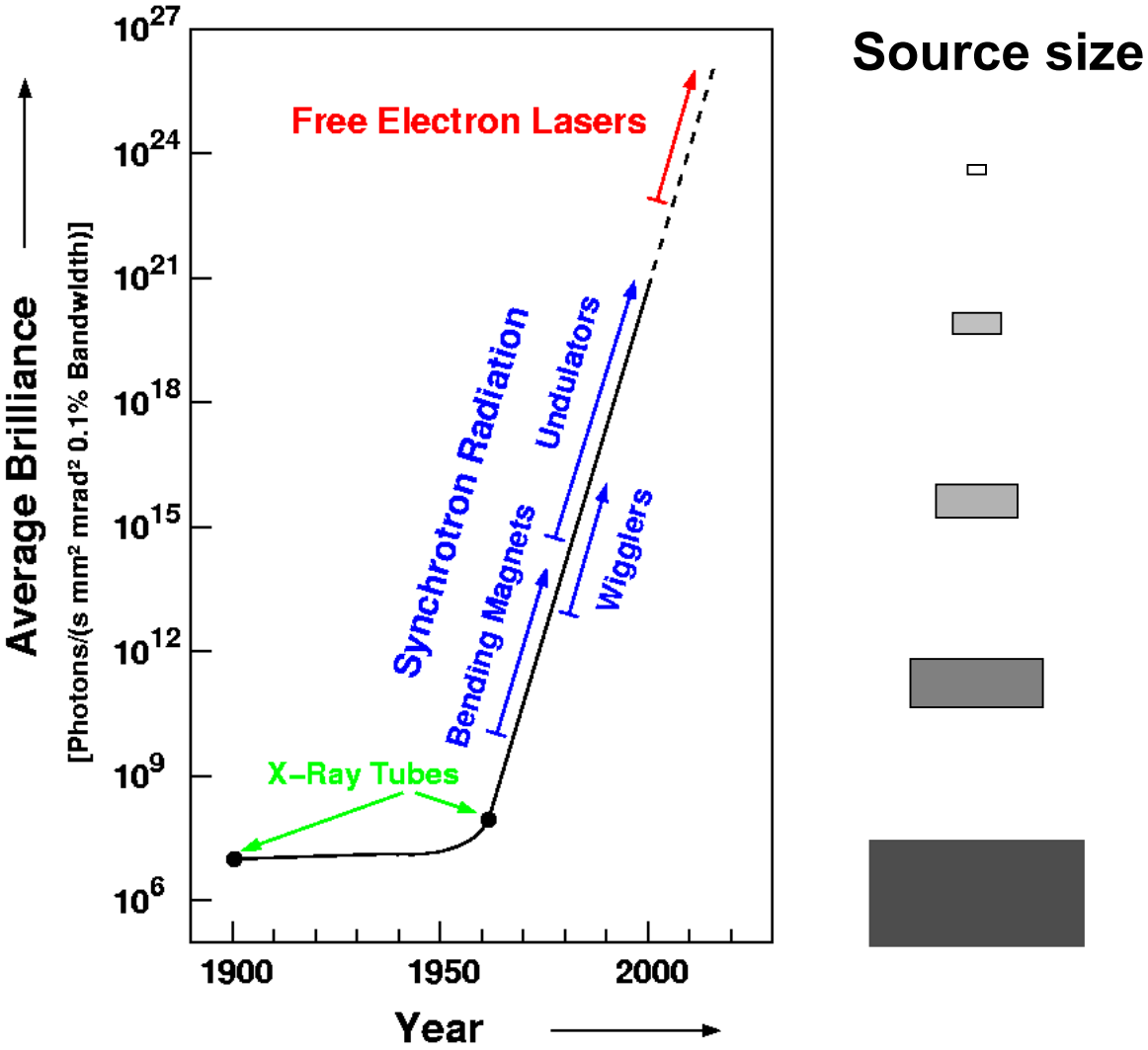
X-ray free-electron lasers worldwide



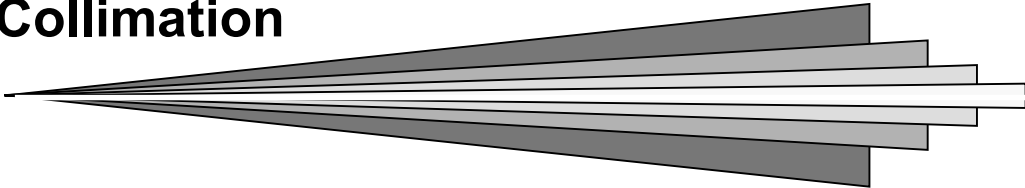
Free-electron lasers



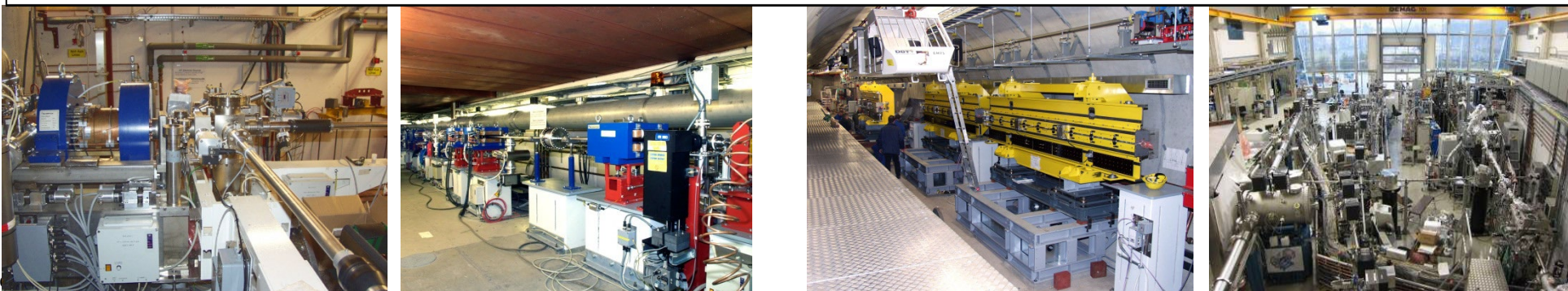
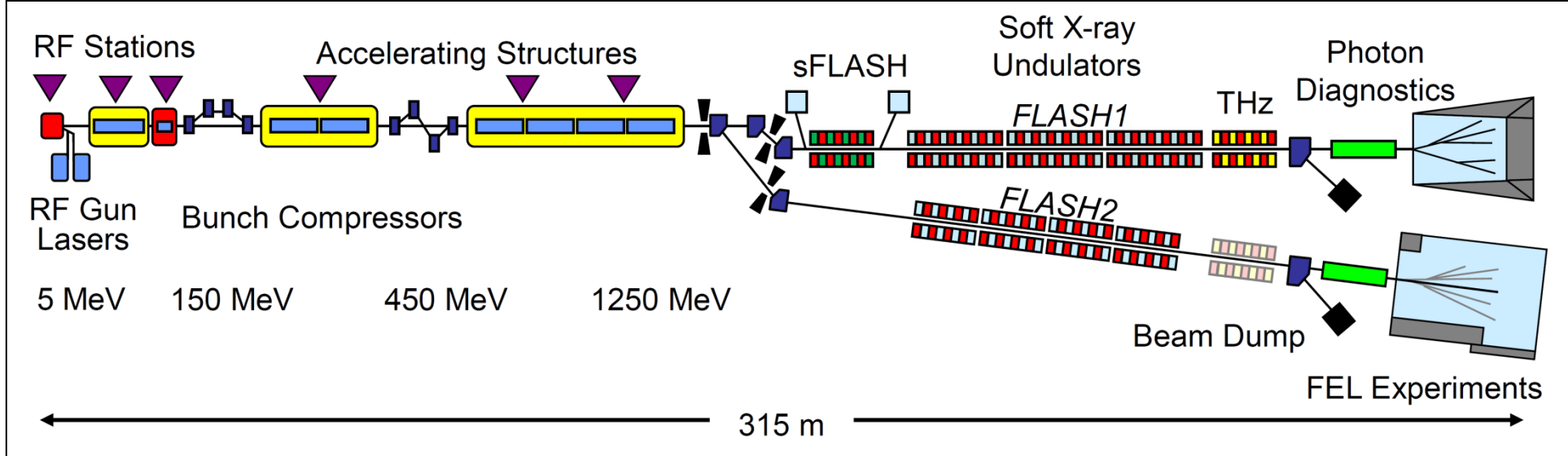
FLASH



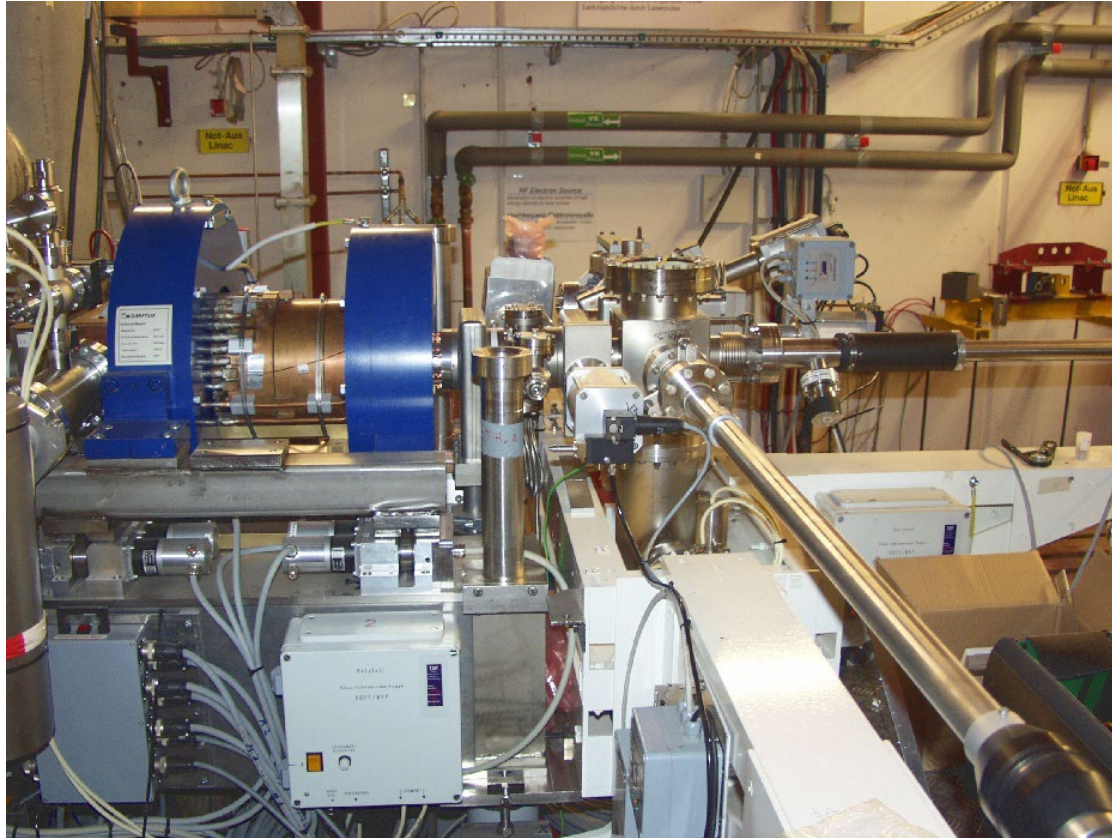
Collimation



The FLASH facility

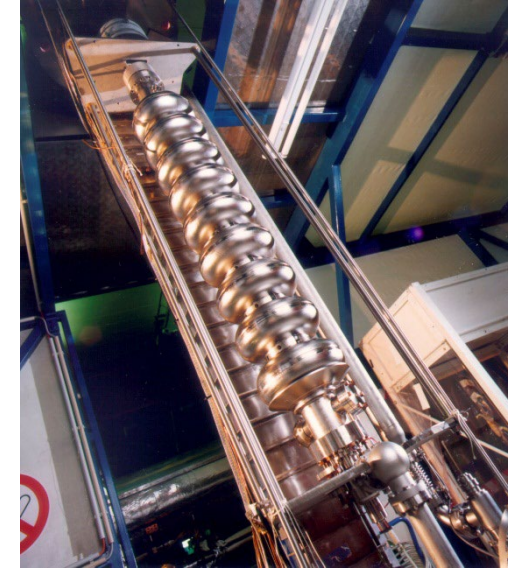


Injector: creating bunches of electrons



- > Optical laser strikes Cs_2Te photocathode, releasing a cloud of electrons (1-3% quantum efficiency)
- > Electrons move into a magnetic field, $11/2$ -cell resonator, shaping into a bunch
- > Small accelerator module “fires” bunch into the main electron accelerator

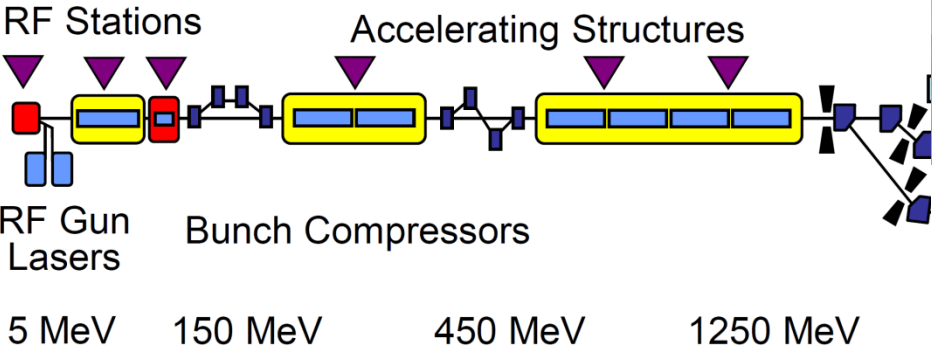
Superconducting accelerator module



- Accelerator module with superconducting niobium cavities
- 25 MV/m routinely
- Length: 12 m
- Weight: about 10 tons!

Bunch compressors

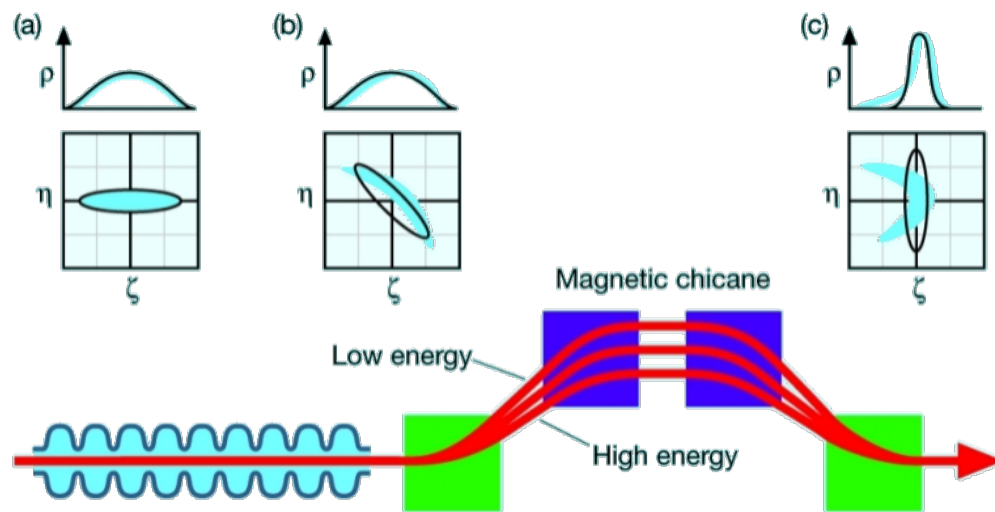
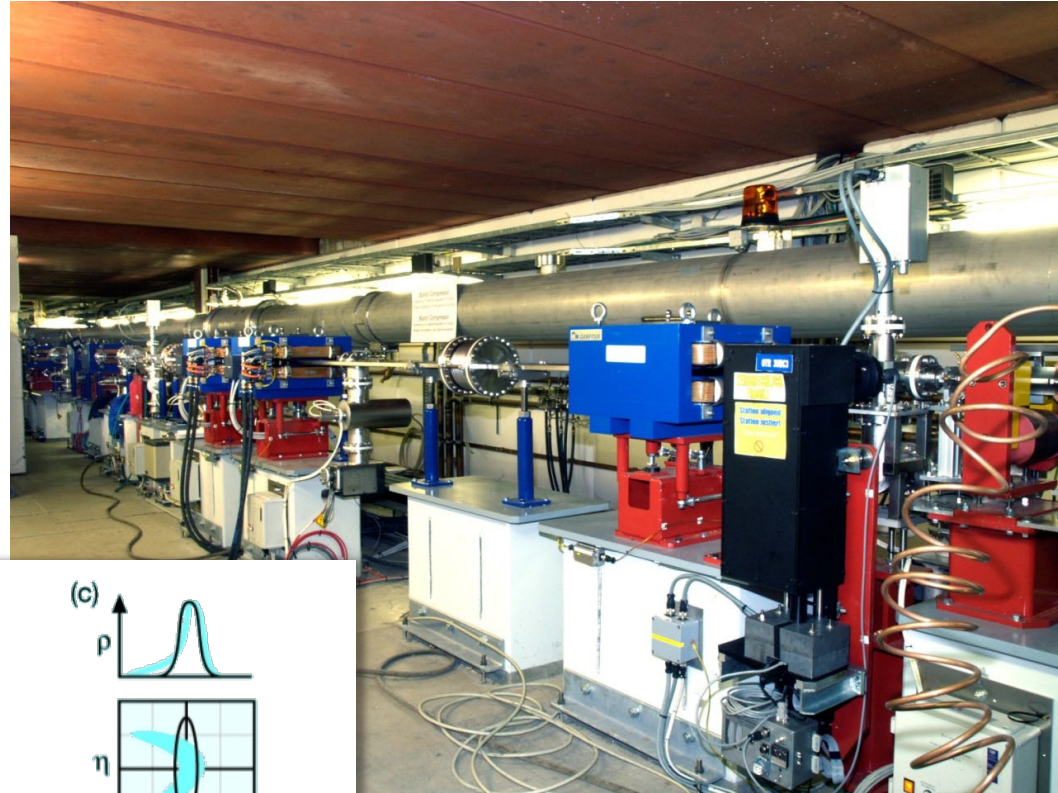
- > electromagnetic chicane (4 dipole magnets)
- > longitudinal compression of electron bunches
- > $\sim 1 \text{ mm} \rightarrow 0.1 \text{ mm}$



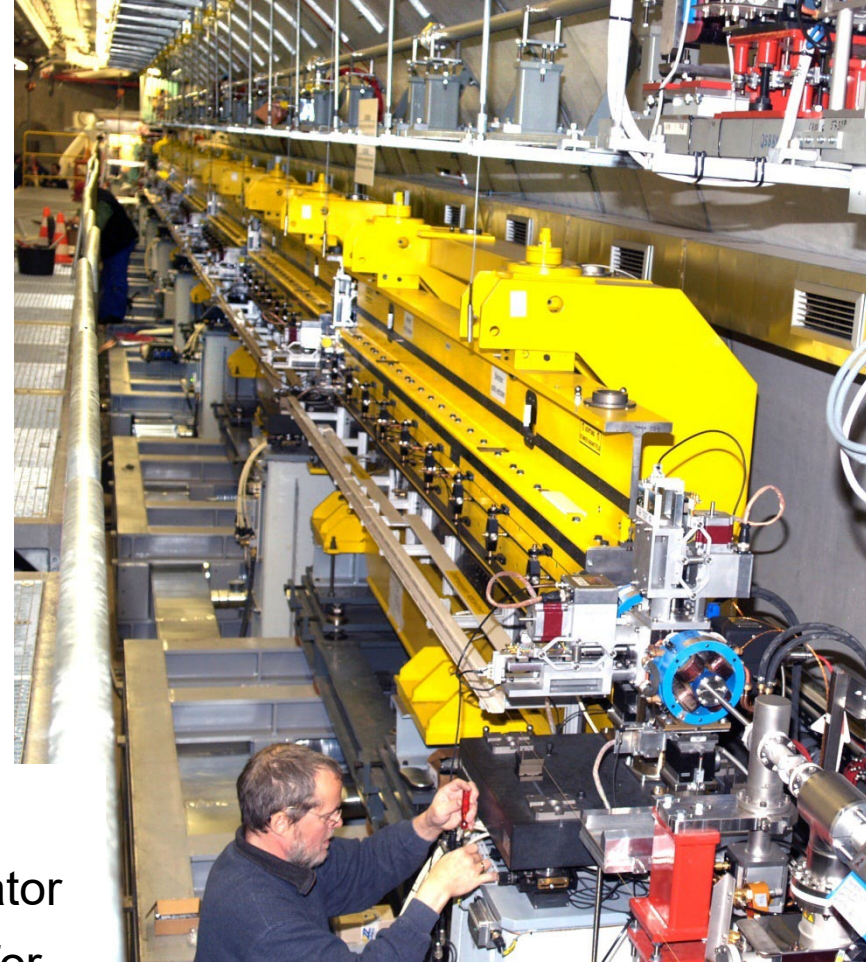
Electron bunch compression

Increase of electron peak current

- > electromagnetic chicane (4 dipole magnets)
- > longitudinal compression of electron bunches
- > $\sim 1\text{-}2\text{ mm} \rightarrow 0.1\text{ mm}$
70 A to $>1\text{ kA}$ peak current

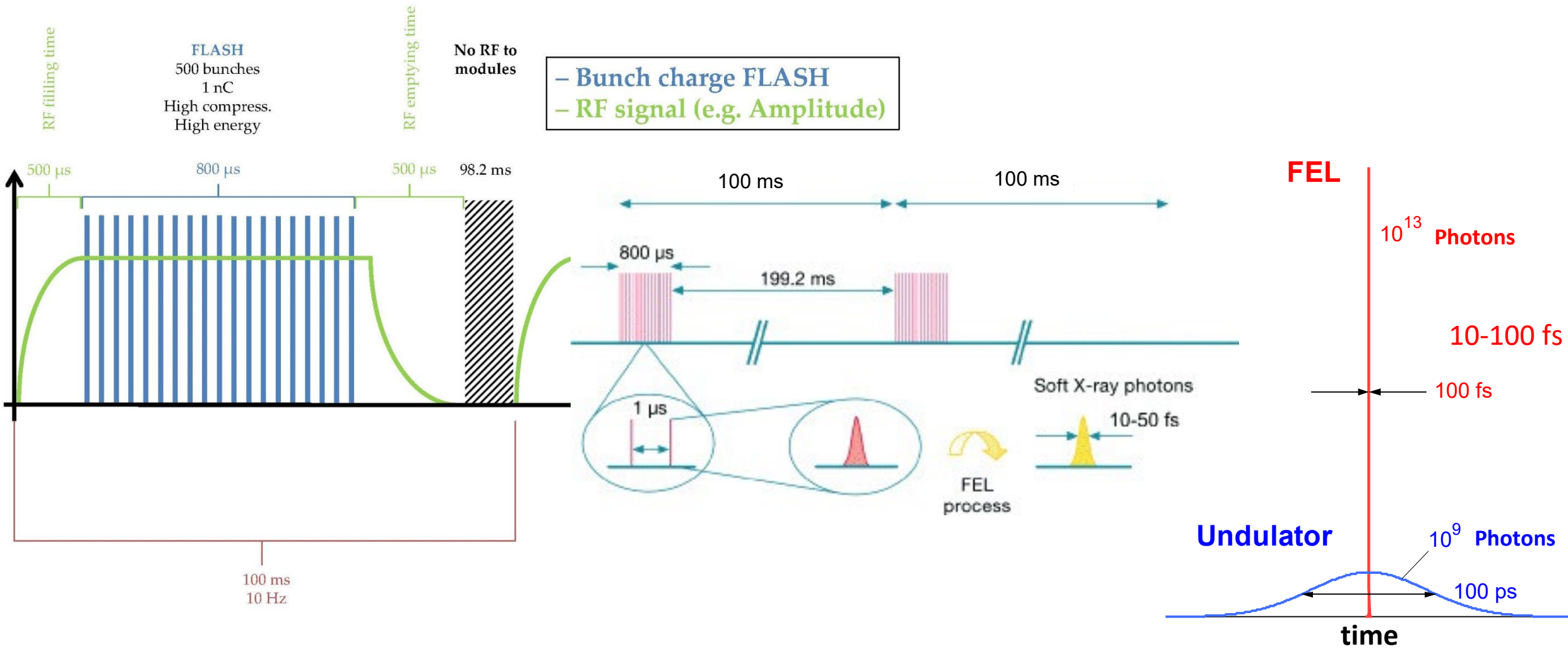


Undulators

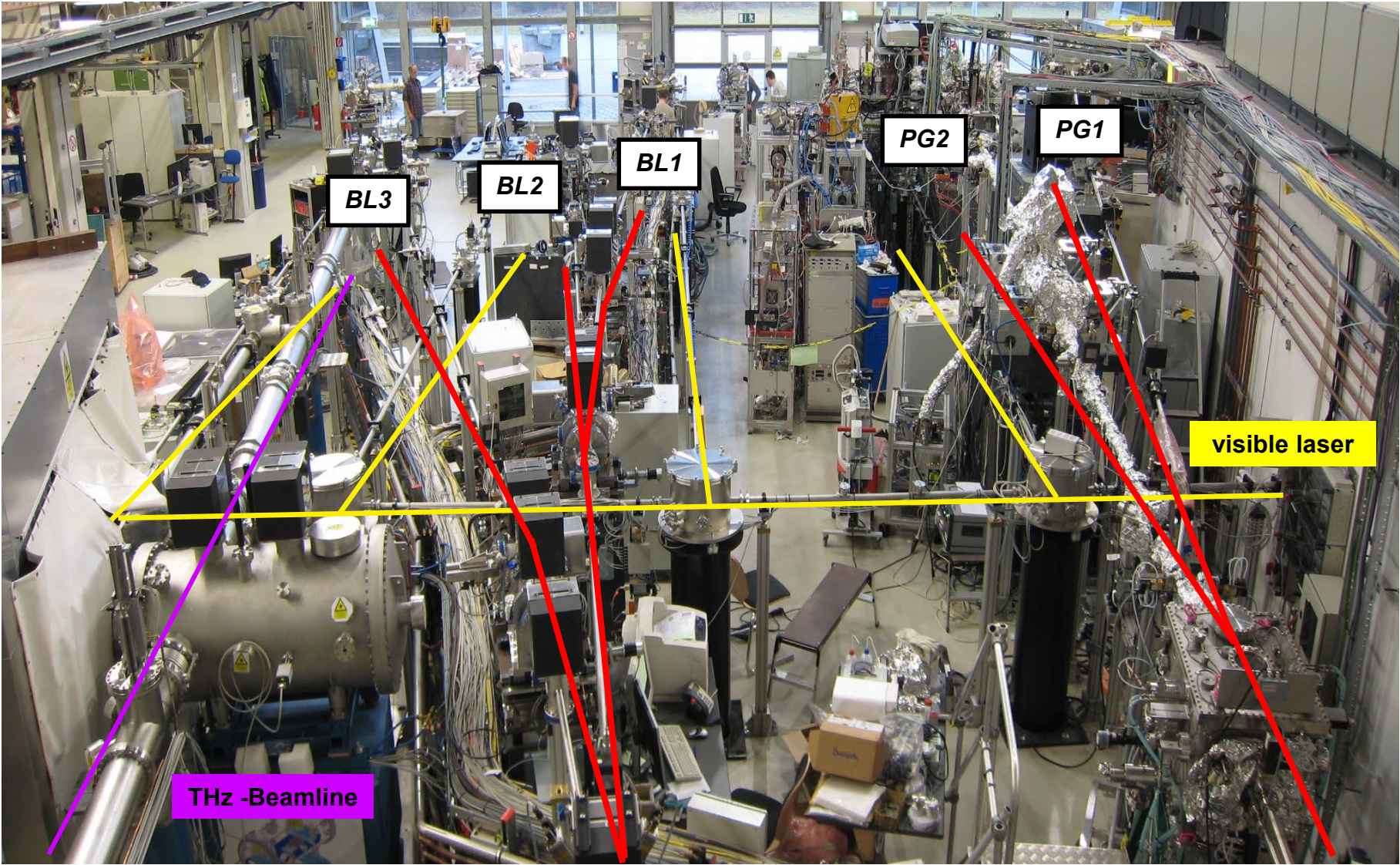


- 27 m undulator
- 12 mm fixed gap → tuning with accelerator
- Intersections with quadrupole doublets for focusing electron beam, electron beam diagnostics and steerer coils

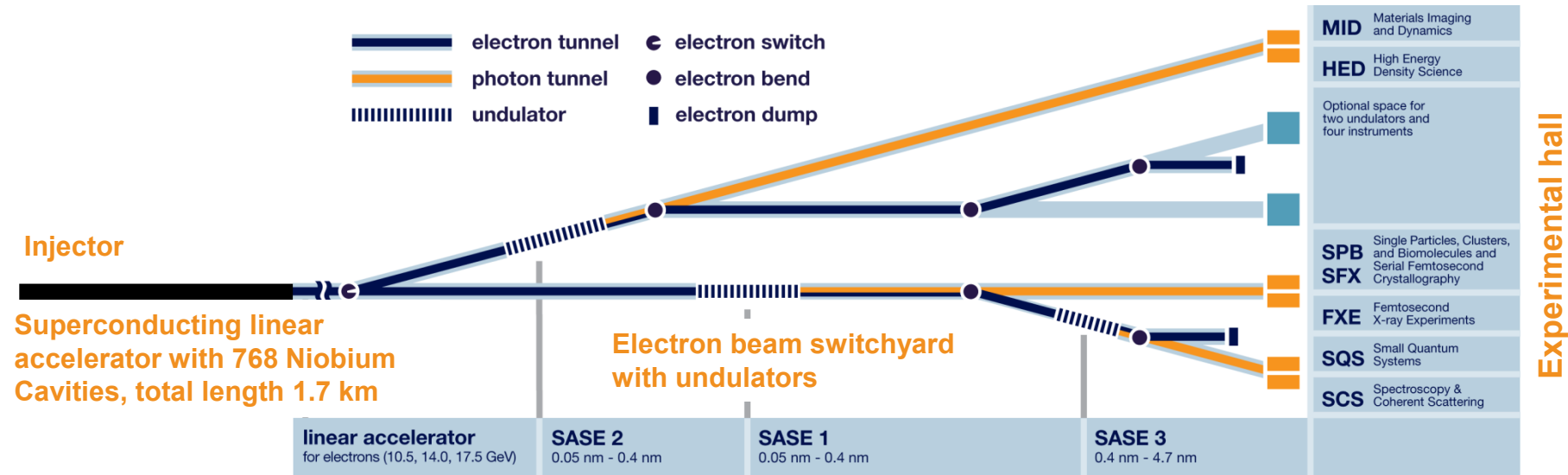
Superconducting modules: bunch structure



FLASH1 experimental hall – Albert-Einstein hall



European XFEL: schematic layout



Supercond. Linac: up to 17.5 GeV

Undulators:

SASE1/2: 34 modules, 212 m total length

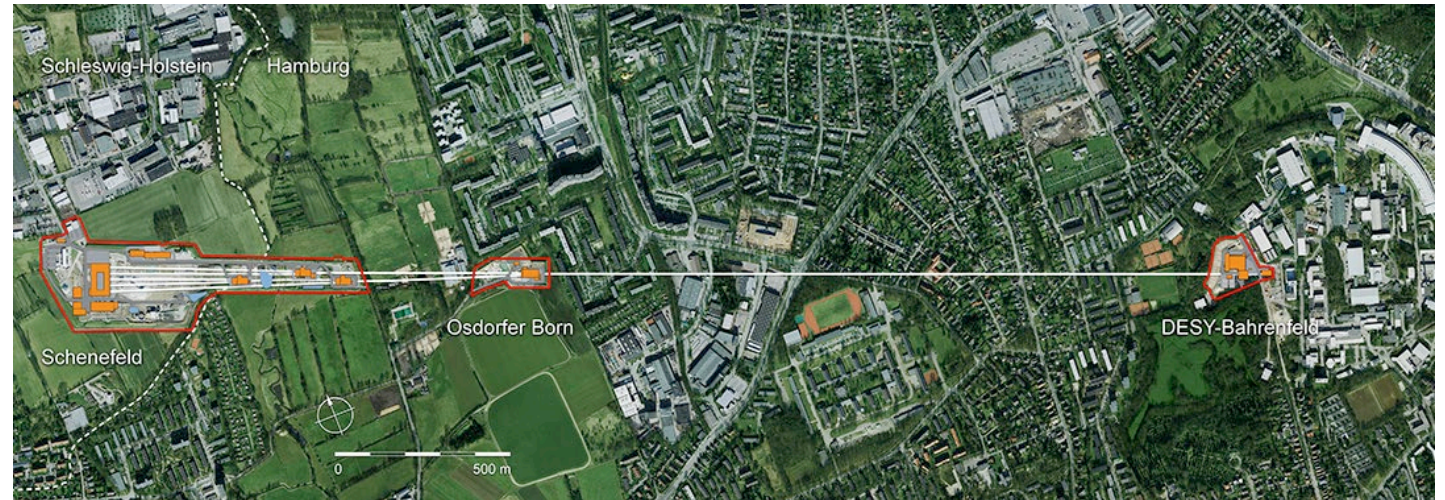
SASE 3 : 20 modules, 125 m total length

Photon energies: 0.2 – 3 – 26 keV

Average brilliance: $\sim 10^{25}$ 1/(s·mm²·mrad²·0.1%BW)

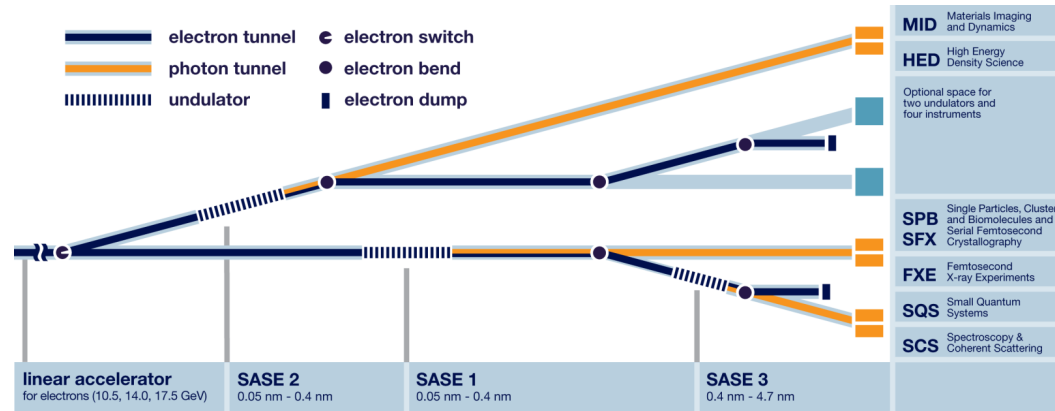
Peak brilliance: $\sim 10^{33}$

Pulse length: <100 fs



European XFEL

Science at the beamlines



Endstation	Science
3100-24800 eV	MID Materials imaging & dynamics: structure determination of nanodevices and dynamics at the nanoscale
	HED High energy density science: investigation of matter under extreme conditions using hard X-ray FEL radiation, e.g. probing dense plasmas
	SPB/SFX Ultrafast coherent diffraction imaging of single particles, clusters and biomolecules: structure determination of single particles (atomic clusters, biomolecules, virus particles, cells), serial femtosecond crystallography
260-3100 eV	FXE Femtosecond X-ray experiments: time-resolved investigations of the dynamics of solids, liquids, gases
	SQS Small quantum systems: investigation of atoms, ions, molecules and clusters in intense fields and non-linear phenomena
	SCS Spectroscopy & coherent scattering: Electronic and atomic structure and dynamics of nanosystems and of non-reproducible biological objects using soft X-rays

Summary

- Basics of synchrotron radiation
 - Wiggler/undulator
 - Synchrotrons/FELs
 - Self-amplified spontaneous emission – SASE
-
- Properties: high brilliance, wide tunable energy range, small source size
(for FELs: short pulses, full coherence)

Questions for tomorrow:

- What properties of the light must be considered in experiments?
- What are they important for, for example?
- What is so useful in using synchrotrons or FELs? Why X-rays?