XFEL radiation sources and properties

Ryszard Sobierajski
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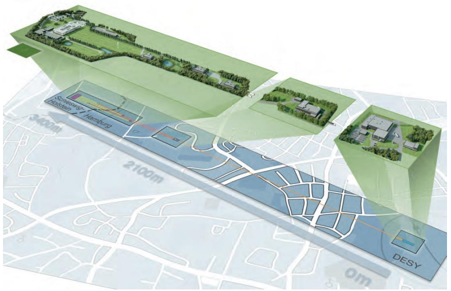
What will it be about…

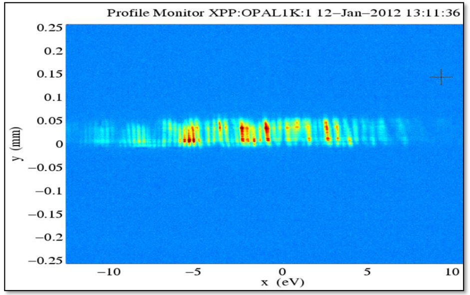
Interdisciplinary research with the use of X-ray free electron lasers in the fields of physics, materials sciences, chemistry and biology.

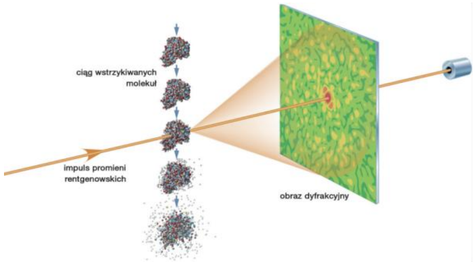
- **principles of operation and radiation properties of XFEL sources,**
- X-ray interaction with matter
- basic x-ray research techniques
- examples of XFELs applications in:
  - protein crystallography,
  - photochemistry,
  - dynamics of atomic and electronic structure of materials,
  - magnetism
  - matter under extreme pressure and temperature conditions,
  - non-linear x-ray optics etc.
- the instrumentation used in XFEL facilities

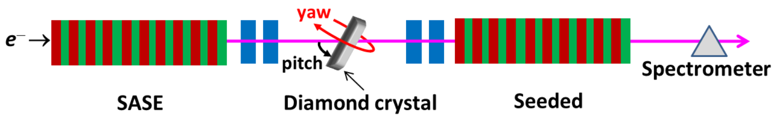
Outline

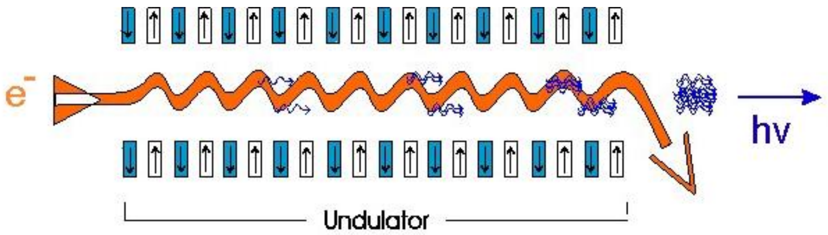
1. What are XFELs?
2. How XFEL radiation is generated?
3. Main properties of the XFEL radiation
4. XFELs in the world - comparison
5. Typical XFEL applications
6. New XFEL technologies











XFELs – general layout

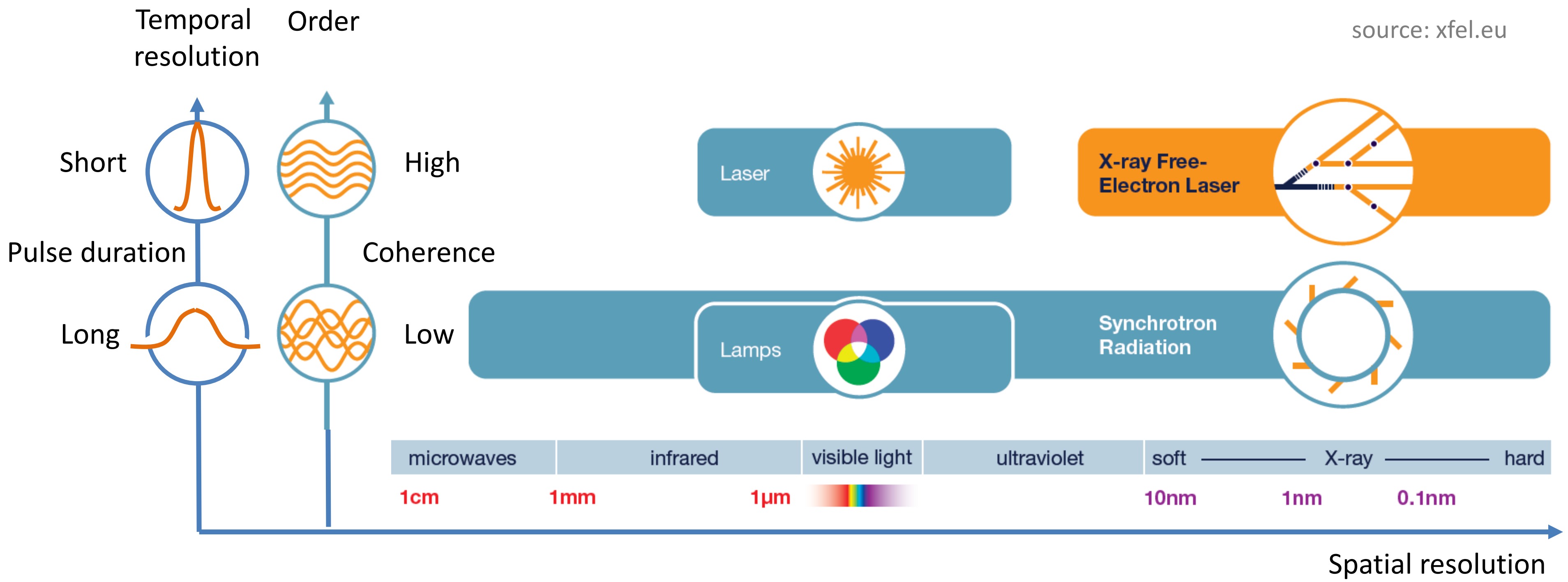
source: xfel.eu

XFELs of the World

source: xfel.eu

XFELs vs lasers and synchrotrons

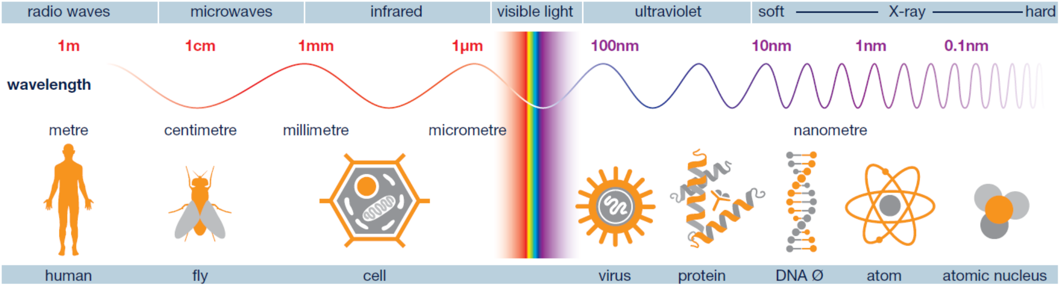
source: xfel.eu



XFELs vs lasers and synchrotrons

XFEL HUB-POLAND

Wavelength / Photon energy



Electrons in molecules / Valence and conduction electrons

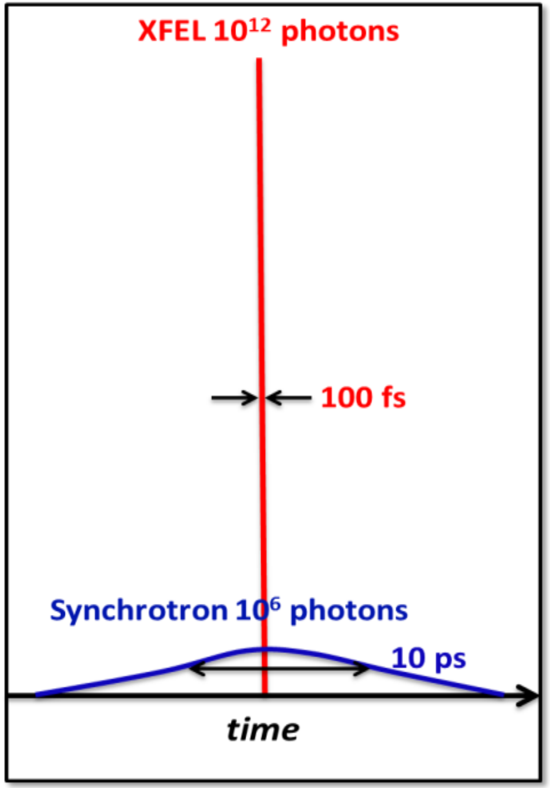
Core-shell electrons ionisation

10 meV – 10 eV

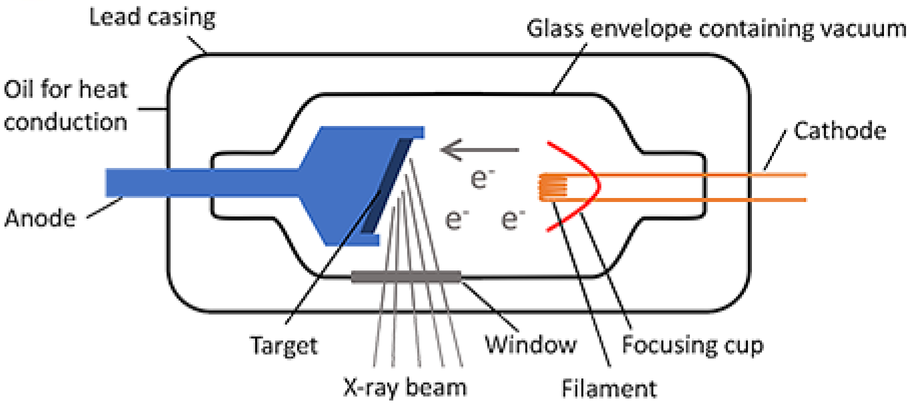
0.1 – 10 keV

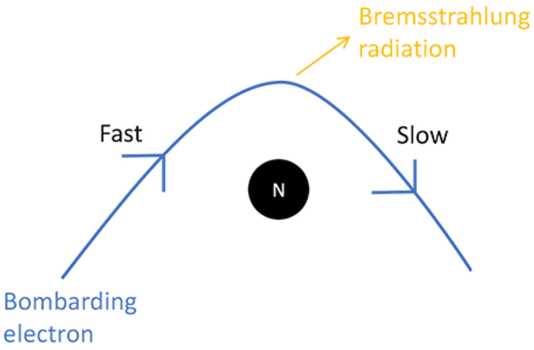
source: xfel.eu

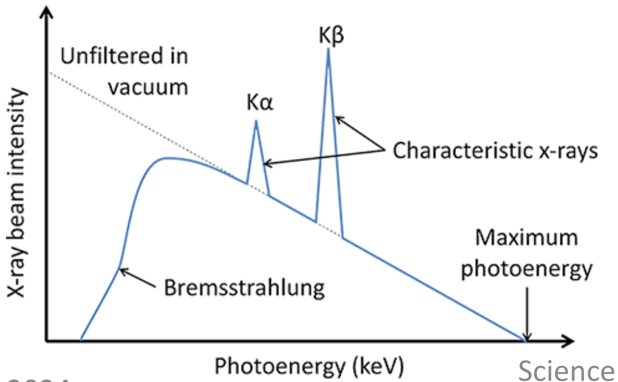
Pulse duration

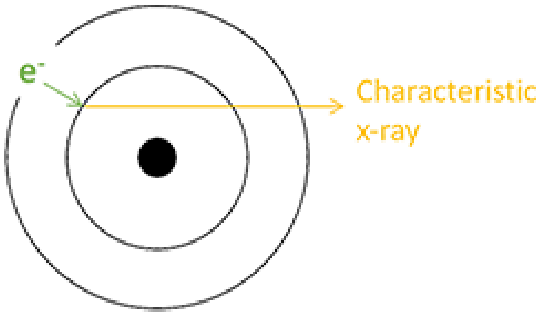


X-ray sources: X-ray tubes



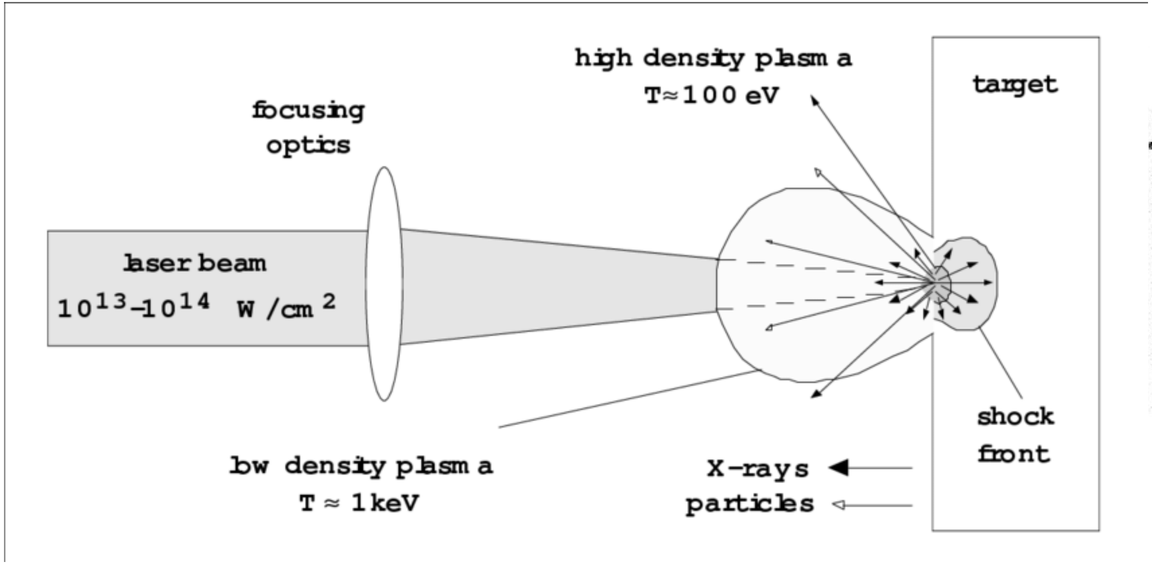


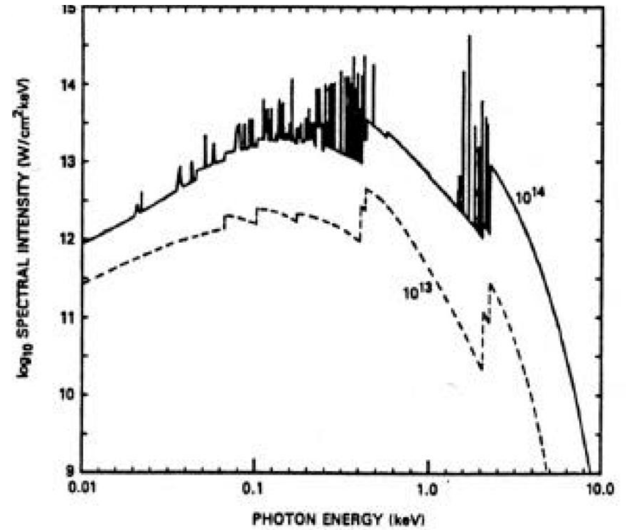




source: www.radiologycafe.com

X-ray sources: Laser-produced plasma

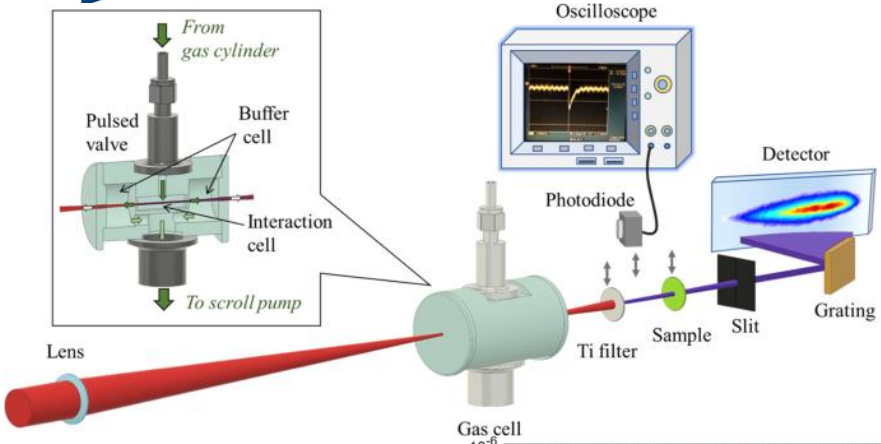


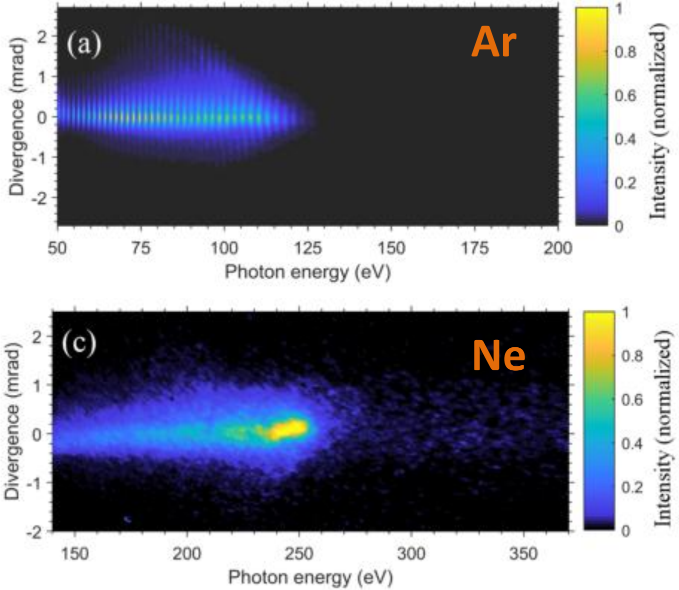


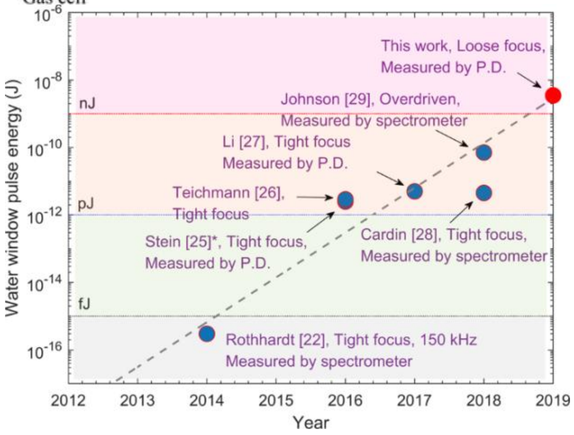
Calculated X-ray spectrum from laser heated Al target irradiated at intensities of 10^{13} and 10^{14} W/cm^2 [67].

DOI: 10.1007/BF02874624

X-ray sources: HHG







DOI: 10.1038/s42005-020-0355-x

Synchrotron radiation discovery

PHYSICAL REVIEW VOLUME 65, NUMBERS 11 AND 12 JUNE 1 AND 15, 1944

Letter to the Editor

PROMPT publication of brief reports of important discoveries in physics may be secured by addressing them to this department. The closing date for this department is the third of the month. Because of the late closing date for the section no proof can be shown to authors. The Board of Editors does not hold itself responsible for the opinions expressed by the correspondents. Communications should not in general exceed 600 words in length.

On the Maximal Energy Attainable in a Betatron

D. IWANENKO AND I. POMERANCHUK
Physical Institute of the Moscow State University, Moscow, and Physico-Technical Institute of the Academy of Sciences of the U. S. S. R., Leningrad, U. S. S. R.
May 18, 1944

BY means of a recently constructed induction accelerator-betatron, Kerst succeeded in obtaining electrons up to 20 Mev.[1] The principle of operation of the betatron is the acceleration of electrons by a tangential electric field produced by a changing magnetic flux, which is connected with the magnetic field keeping electrons on the orbit by a simple relation. In contrast to a cyclotron, whose applicability is essentially limited to the non-relativistic region on the ground of defocusing of orbits due to the change of mass at high energies, there is no such limitation for the betatron.

We may point out, however, that quite another circumstance would lead as well to the existence of a limitation for maximal energy attainable in a betatron. This is the radiation of electrons in the magnetic field. Indeed, electrons moving in a magnetic field will be accelerated and must radiate in accordance with the classical electrodynamics. One can easily see that quantum effects do not play here any important role as the dimension of the orbit is very great. As was shown by one of us[2] an electron moving in a magnetic field **H** radiates per unit of path the energy

$$-(dE/dX)=2/3(e^2/mc^2)^2(E/mc^2)^2[(\mathbf{V}/c)\mathbf{H}]^2 \qquad (1)$$

where e is the charge, m the mass, **V** the velocity, and E the energy of the electron; E is assumed much greater than mc^2.

In the betatron **V** is normal to H and practically for the whole path equal to c. Then we have

$$-(dE/dX)=2/3(e^2/mc^2)^2(EH/mc^2)^2. \qquad (2)$$

The limiting value of energy E_0 is to be determined from the condition that the radiated energy (2) will be equal to energy gained by the electron in the electric field produced by magnetic flux per unit of path:[3]

$$\frac{2}{3}r_0^2\left(\frac{E_0H}{mc^2}\right)^2=\frac{e|d\phi/dt|}{2\pi R_0c}=\frac{e}{c}R_0|\dot{H}| \qquad (3)$$

$$\dot{H}=dH/dt \qquad r_0=e^2/mc^2.$$

Here R_0 is the radius of the orbit, ϕ is the induction flux.[1]

Hence:

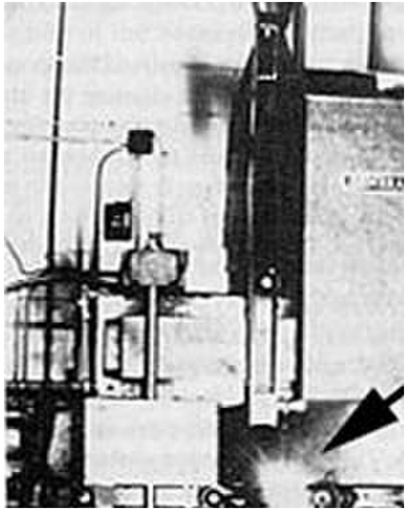
$$\frac{E_0}{mc^2}=\left(\frac{3eR_0}{2r_0^2c}\frac{\dot{H}}{H^2}\right)^{\frac{1}{2}}. \qquad (4)$$

Taking for H and E the values now being in use we get $E_0\approx5\times10^8$ ev, which is only five times as great as the energy which one expects to obtain in the betatron now under construction. From (4) one sees that E_0 is inversely proportional to the magnetic field applied and proportional to the square root of energy gained in the rotation electric field per unit of path. All this requires the using of smaller H or of higher frequencies with the purpose of getting higher limiting values of E_0.

The radiative dissipation of energy of electrons moving in a magnetic field must be also of importance for the discussion of the focusing of the electronic beam, as the energy of particles being accelerated will grow more slowly with the growth of H if the radiation is taken into account. This latter question may deserve a separate discussion.

[1] D. W. Kerst, Phys. Rev. **61**, 93 (1942).
[2] I. Pomeranchuk, J. Phys. **2**, 65 (1940).
[3] D. W. Kerst and R. Serber, Phys. Rev. **60**, 53 (1941).

Synchrotron radiation discovery



27.04.1947 General Electric Research Laboratory- first observation of synchrotron radiation

THE
PHYSICAL REVIEW
A journal of experimental and theoretical physics established by E. L. Nichols in 1893
SECOND SERIES, VOL. 102, No. 6 JUNE 15, 1956

Spectral and Angular Distribution of Ultraviolet Radiation from the 300-Mev Cornell Synchrotron*

D. H. TOMBOULIAN AND P. L. HARTMAN
Department of Physics, Cornell University, Ithaca, New York
(Received November 22, 1955)

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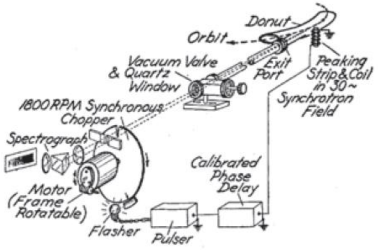


FIG. 11. Diagram showing the arrangement to be used for recording the radiation from essentially monoenergetic electrons. For work in the vacuum ultraviolet the rotating disk is enclosed, the drive shaft coming through a vacuum seal. So far the disk has not been used in the investigation of the far-ultraviolet spectrum. However, the plate of Fig. 12 was obtained with this arrangement and the quartz optical system indicated here.

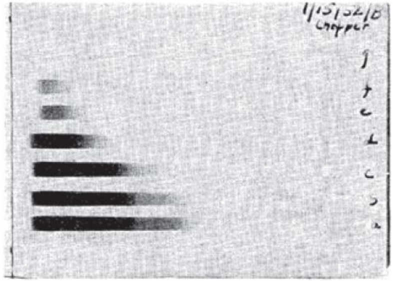
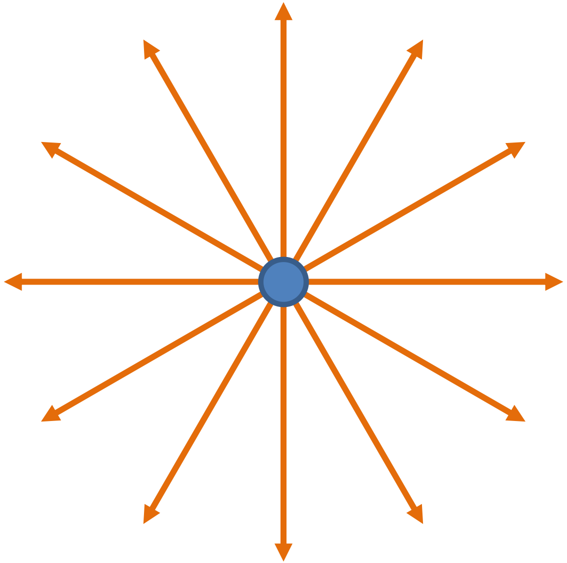


FIG. 12. Reproduction of a plate obtained with the arrangement of Fig. 11, showing spectra of the continuous radiation emitted by essentially monoenergetic electrons. The various exposures correspond to electron energies ranging from 60 Mev at the top to 110 Mev at the bottom. An exposure at 50 Mev is not visible in the reproduction. The exposures were adjusted so that, in each case, approximately the same total number of radiating electrons was involved.

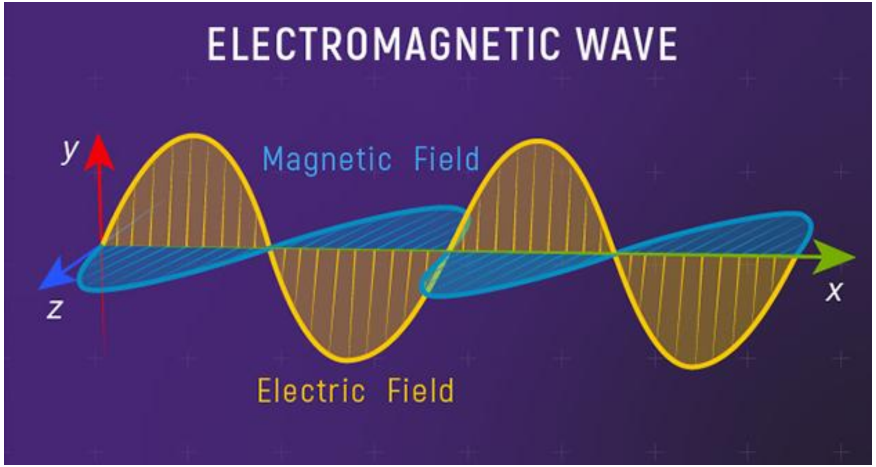
DOI: 10.1103/PhysRev.71.829.5

Electric field of a static charge vs. electromagnetic wave

Static electric field

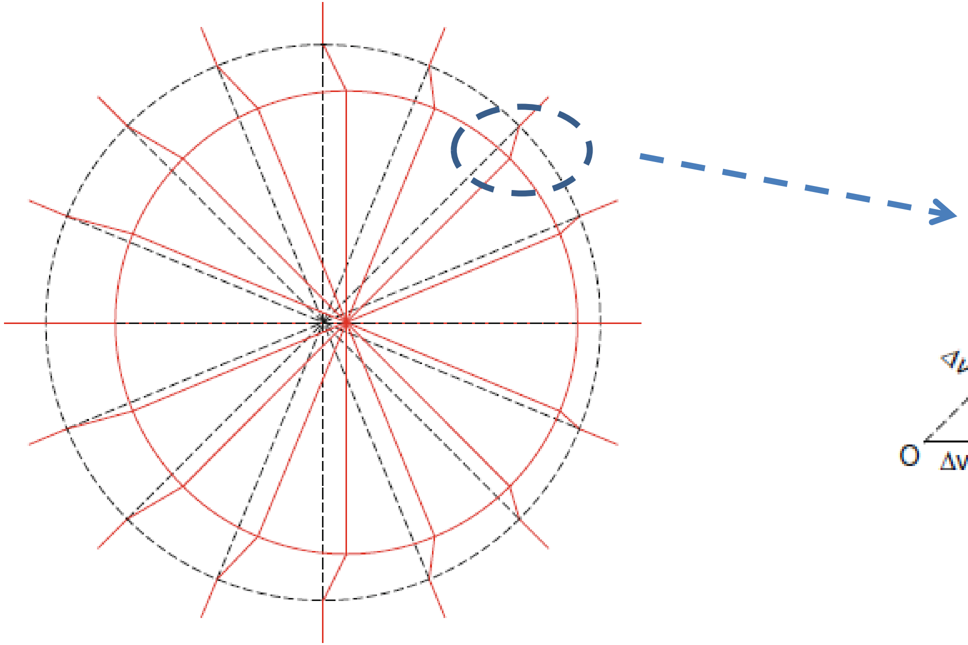


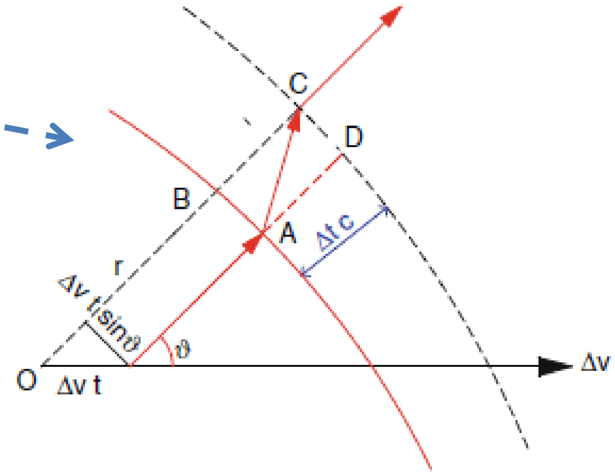
Electromagnetic wave



webbtelescope.org

Radiation of an accelerating charged particle – Purcell method



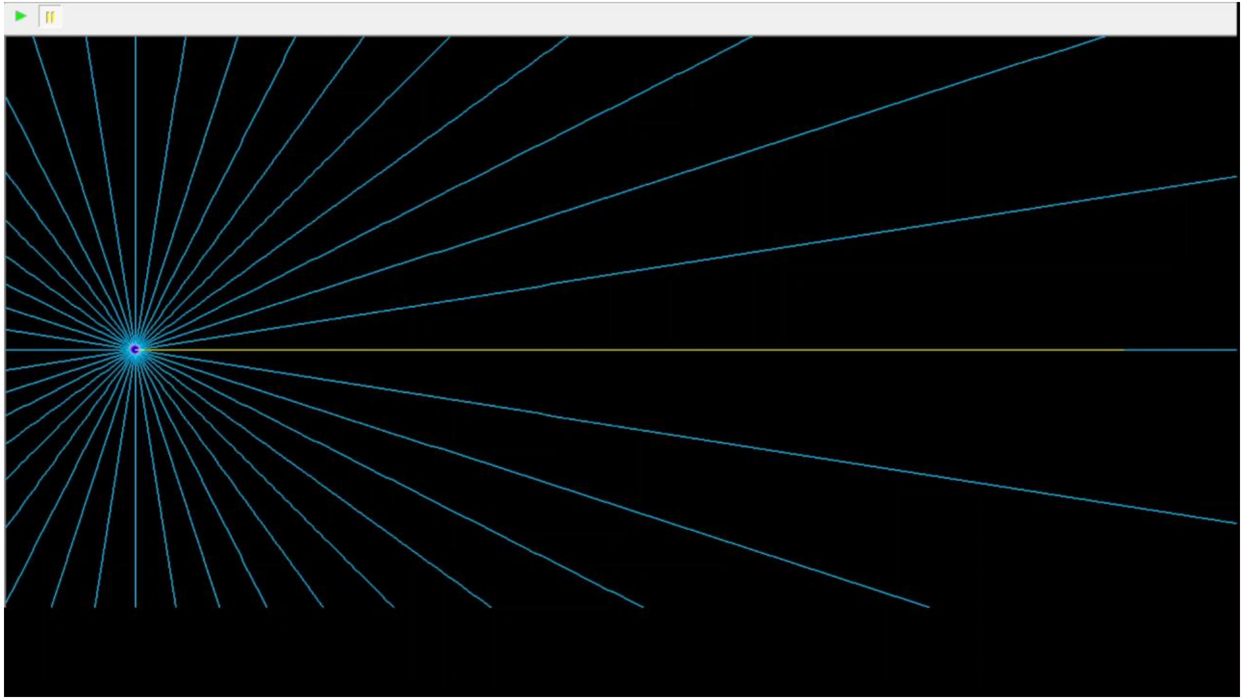


High Energy astrophysics. An Introduction.
T. J.-L. Courvoisier (2013) Springet

physics.weber.edu/schroeder/mrr/MRRtalk.html

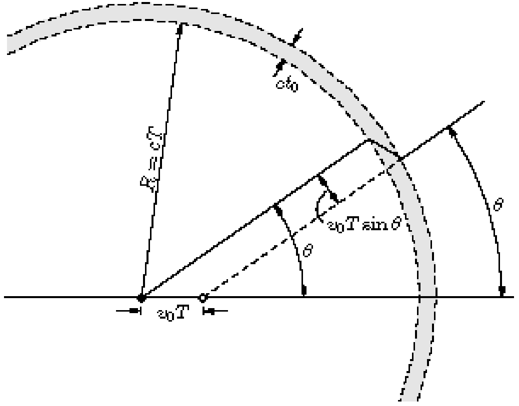
Electric field – charge at const. velocity

https://uspas.fnal.gov/resources/tutorials/physics-demos.shtml



Radiation of an accelerating charged particle – Purcell method

Consider the case of a point charge q initially moving at speed $v_0 \ll c$ which then stops, decelerating uniformly for a duration of t_0. At a time $T \gg t_0$ after this happens, the pulse of radiation has reached a radius of $R = cT$, as shown below.



For an arbitrary field line at an angle θ, the geometry of the "kink" requires that the ratio of the transverse field to the radial field be

$$\frac{E_t}{E_r} = \frac{v_0 T \sin\theta}{c t_0} = \frac{a R \sin\theta}{c^2} \tag{4}$$

where a is the magnitude of the particle's acceleration. But the radial field is given by Coulomb's law, so the transverse field is

$$E_t = \left(\frac{a R \sin\theta}{c^2}\right)\left(\frac{q}{4\pi\epsilon_0 R^2}\right) = \frac{q}{4\pi\epsilon_0 c^2}\frac{a\sin\theta}{R}. \tag{5}$$

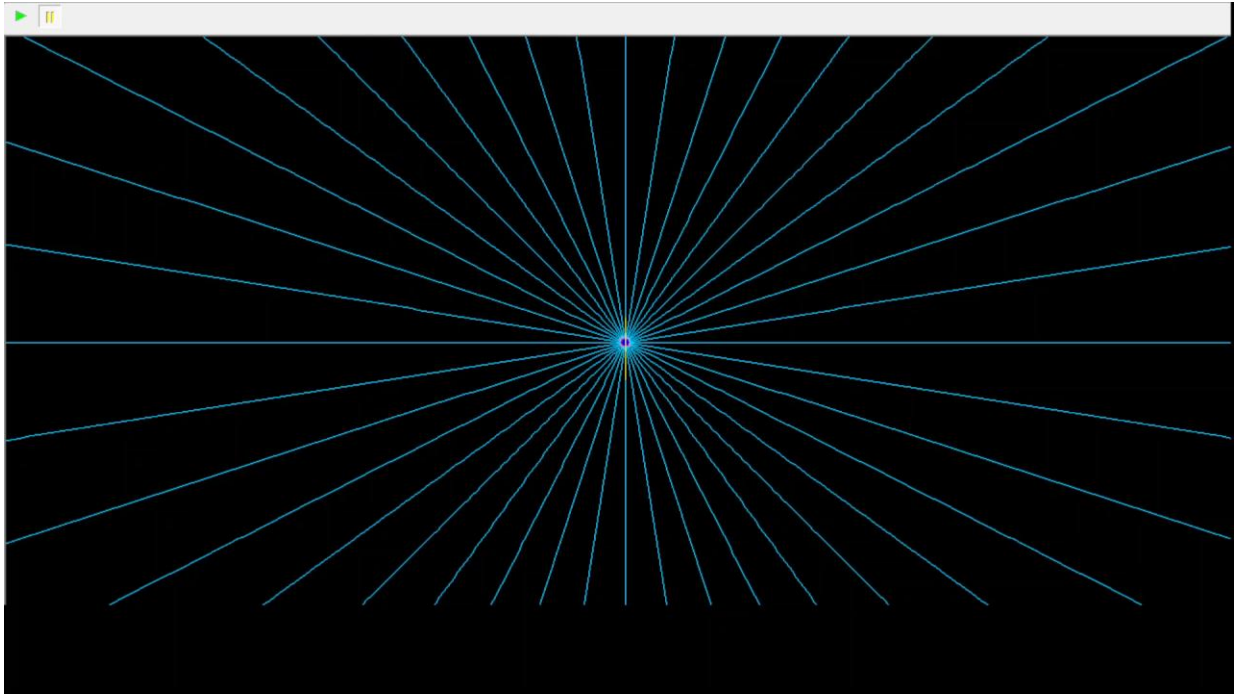
Notice that this falls off with distance as $1/R$, not $1/R^2$. The energy per unit volume stored in this field, proportional to $|\vec{E}|^2$, therefore falls of as $1/R^2$, so the total energy contained in the shell is unchanged as the shell expands. To calculate the power radiated you have to average over angles (which gives a factor of 2/3) and also multiply by 2 to include the equal energy stored in the magnetic field. The result is the Larmor formula,

$$\text{Power radiated} = \frac{q^2 a^2}{6\pi\epsilon_0 c^3}. \tag{6}$$

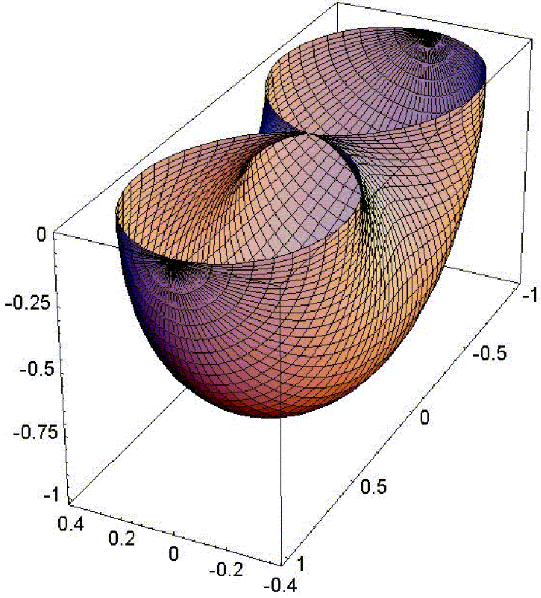
Edward M. Purcell „Electricity and Magnetism”

Electric field – dipol radiation

https://uspas.fnal.gov/resources/tutorials/physics-demos.shtml

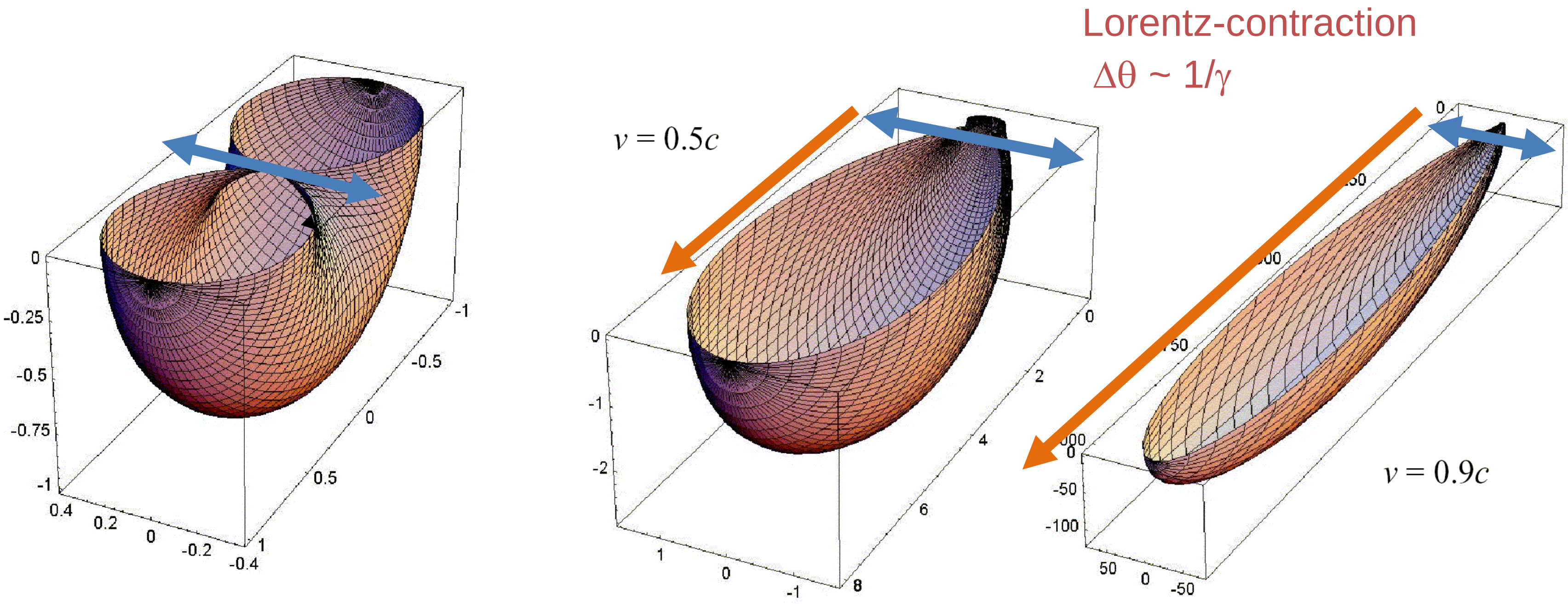


$$I_t \sim (E_t)^2 \sim \sin^2\theta$$



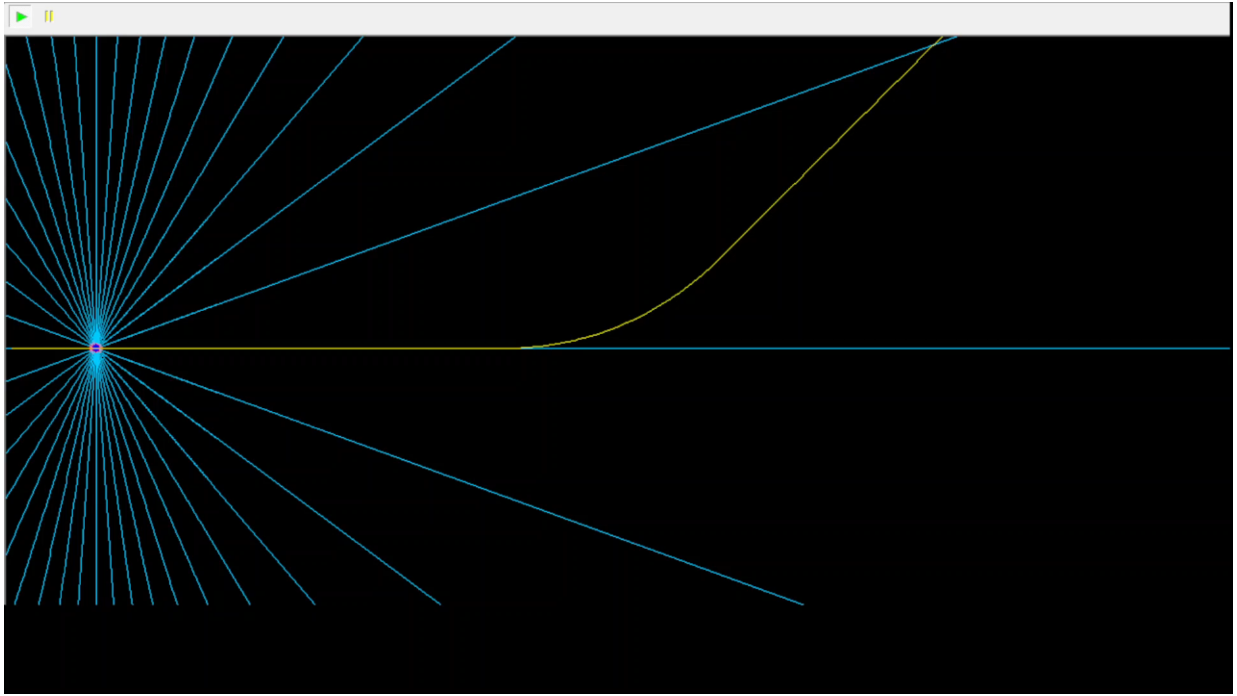
K. Wille, Univ. Dortmund

Radiation of a dipole under relativistic conditions



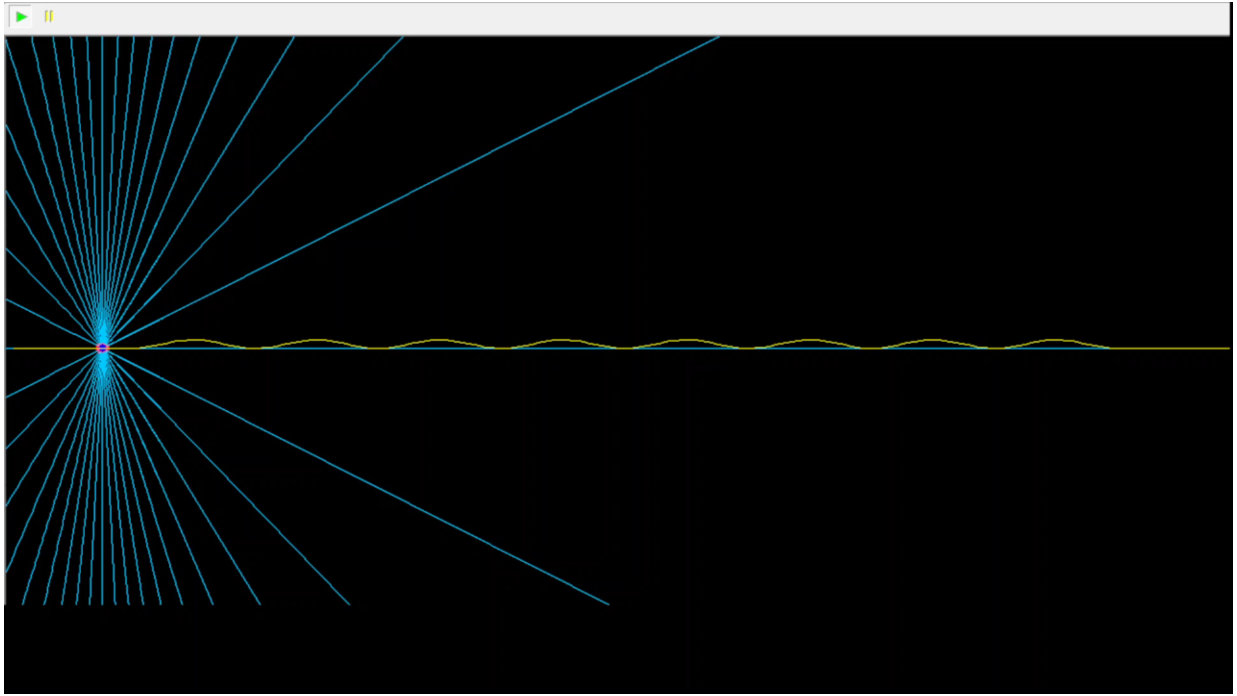
Electric field – charge in bending magnet

https://uspas.fnal.gov/resources/tutorials/physics-demos.shtml



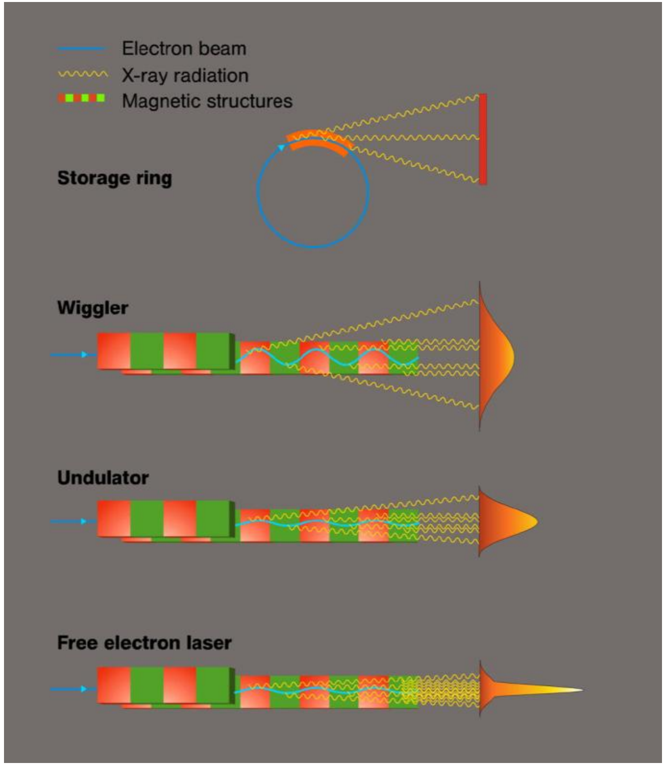
Electric field – charge in undulator

https://uspas.fnal.gov/resources/tutorials/physics-demos.shtml



Intensity vs. Electric field

source: xfel.eu



N_U , N_W = # of magnetic periods
N_e = # of electrons in a bunch
(1 nC ~ 10^9 – 10^{10} electrons)

$\propto N_e$

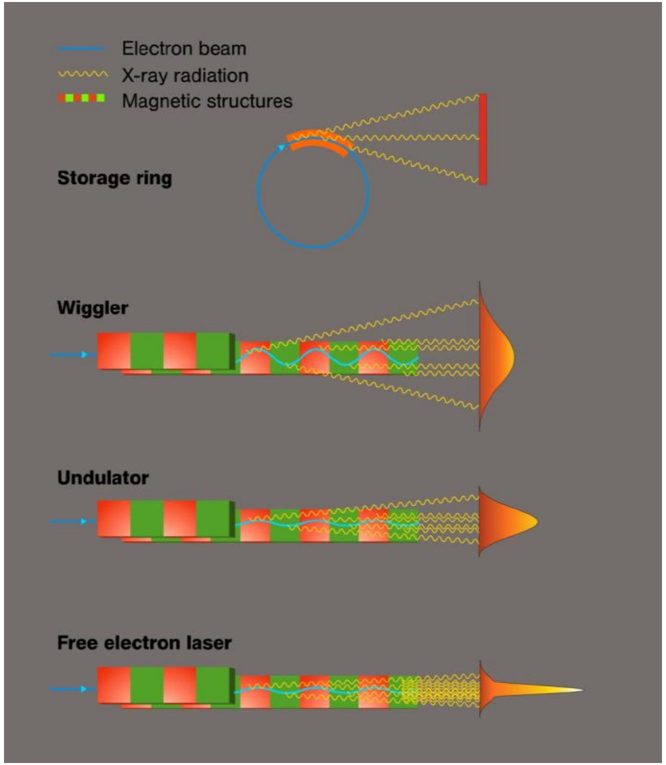
$\propto N_W \times N_e$

$\propto N_U^2 \times N_e$

$\propto N_U^2 \times N_e^2$

Synchrotron radiation sources

source: xfel.eu



N_U, N_W = # of magnetic periods
N_e = # of electrons in a bunch
(1 nC ~ 10^9 – 10^{10} electrons)

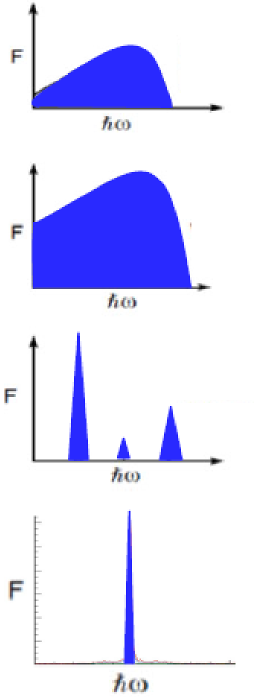
Spectrum $\hbar\omega$

$\propto N_e$

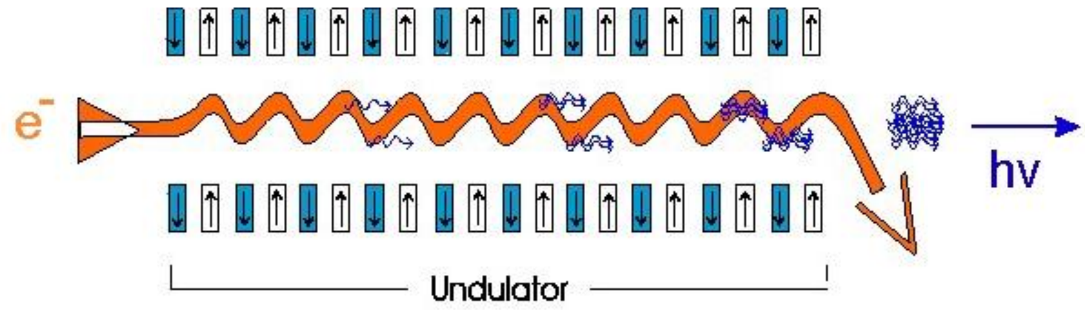
$\propto N_W \times N_e$

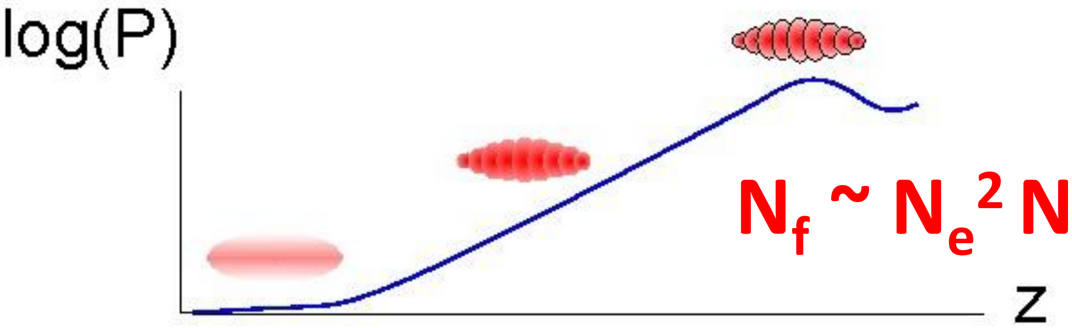
$\propto N_U^2 \times N_e$

$\propto N_U^2 \times N_e^2$



SASE - Self Amplified Spontaneous Emission



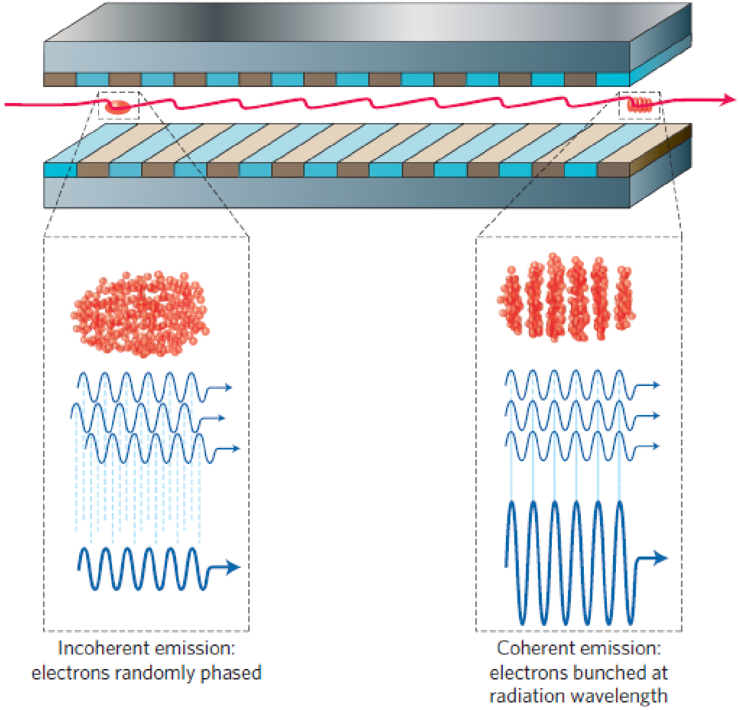


$$N_f \sim N_e^2 N_m^2$$

source: xfel.eu

SASE - Self Amplified Spontaneous Emission

10.1038/nphoton.2010.239



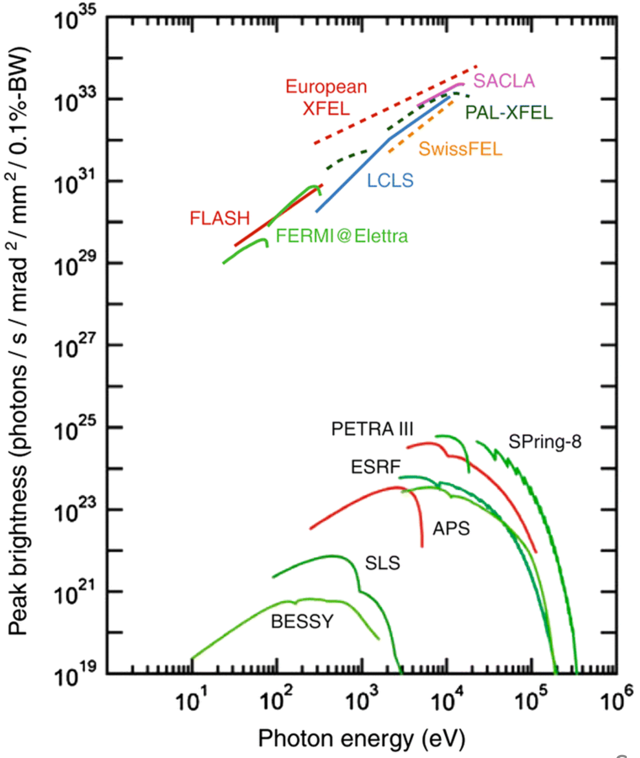
Incoherent

$$E = \sum_{k=0}^{N} \mathrm{E}\exp(i\varphi_k) = \sqrt{N}E \quad I \sim E^2 = NE^2$$

Coherent

$$E = \sum_{k=0}^{N} \mathrm{E}\exp(i\varphi) = NE \quad I \sim E^2 = N^2E^2$$

Peak brightness of SR sources

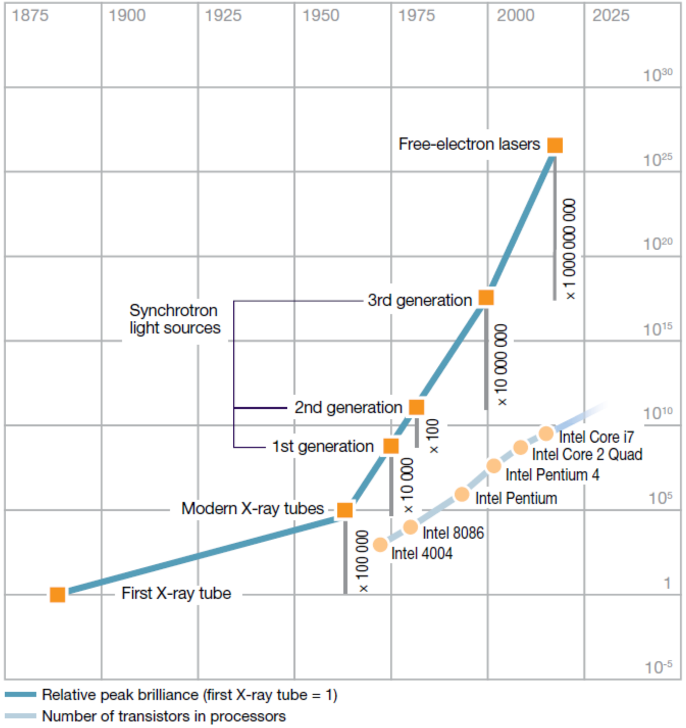


$$\frac{\text{Photons per second}}{\text{Source Area * Source Divergence * bandwidth}}$$

Photons / s / mm^2 / mrad^2 / 0.1%BW

DOI: 10.1039/9781782624097-00001

For comparison



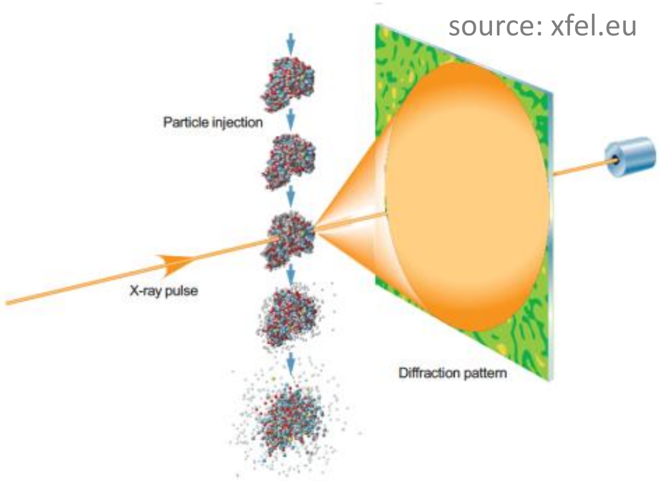
Comparison in rates of development between X-ray light sources and computer processors. The rate of increase of relative brightness of X-ray sources since the 1890s surpasses the increase in the number of transistors on a silicon processor chip since the 1960s (the latter described as "Moore's Law").

source: xfel.eu

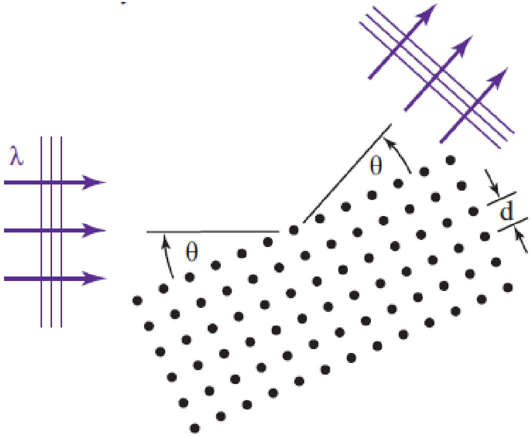
XFEL radiation properties

Wavelength – 50 ÷ 0.5 Å

Atomic spatial resolution



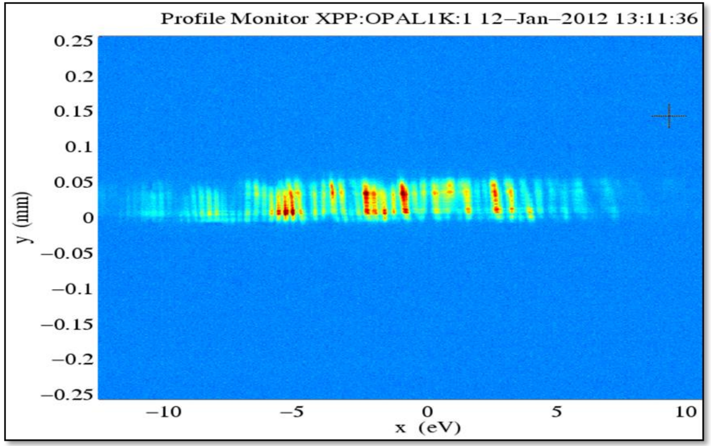
source: xfel.eu



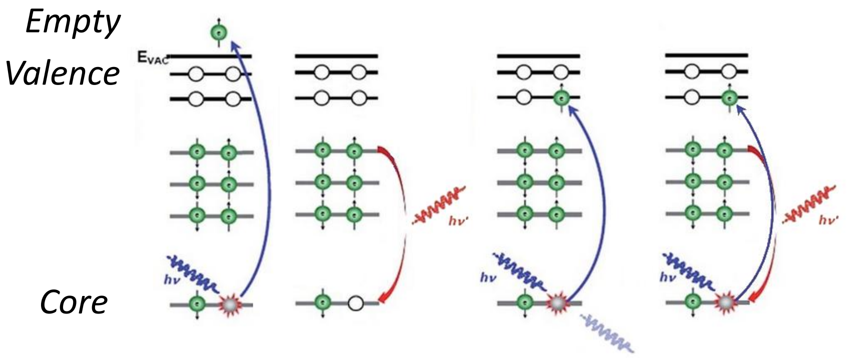
$$m\lambda = 2d_{hkl}\sin\theta$$

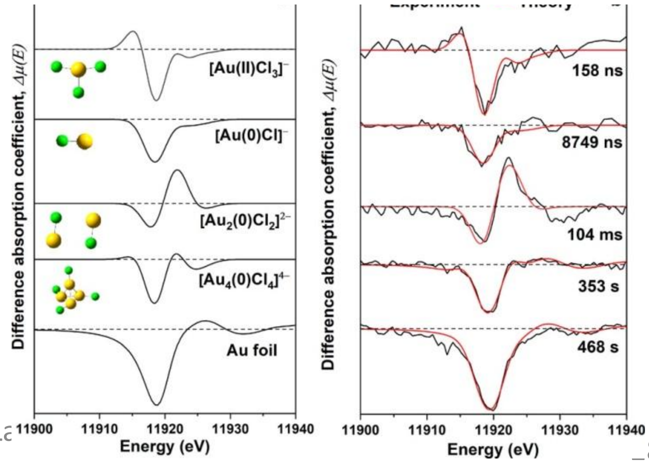
XFEL radiation properties

Wavelength – 50 ÷ 0.5 Å
Photon energy – 0.25 ÷ 25 keV
Spectral bandwidth - 0.1%



Courtesy: J.Krzywinski, SLAC

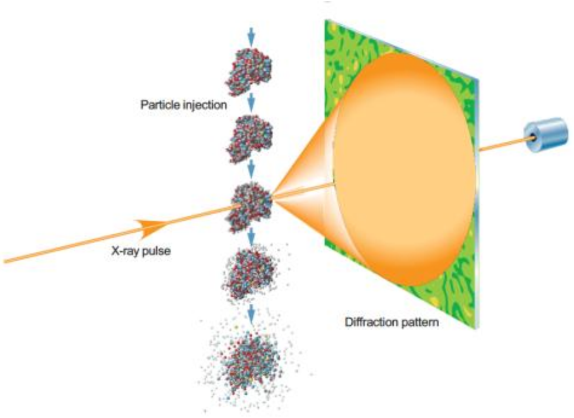




Photon energy adjusted to abosrption edges of various elements/species

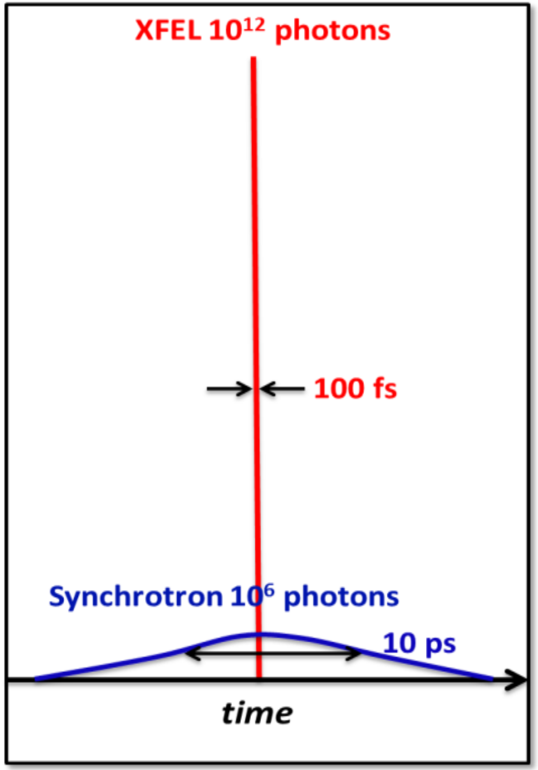
XFEL radiation properties

Wavelength – 50 ÷ 0.5 Å
Photon energy – 0.25 ÷ 25 keV
Spectral bandwidth - 0.1%
Pulse energy – 1 mJ or $10^{11\text{-}12}$ photons
Pulse duration – 1- 200 fs



„Probe before destroy”

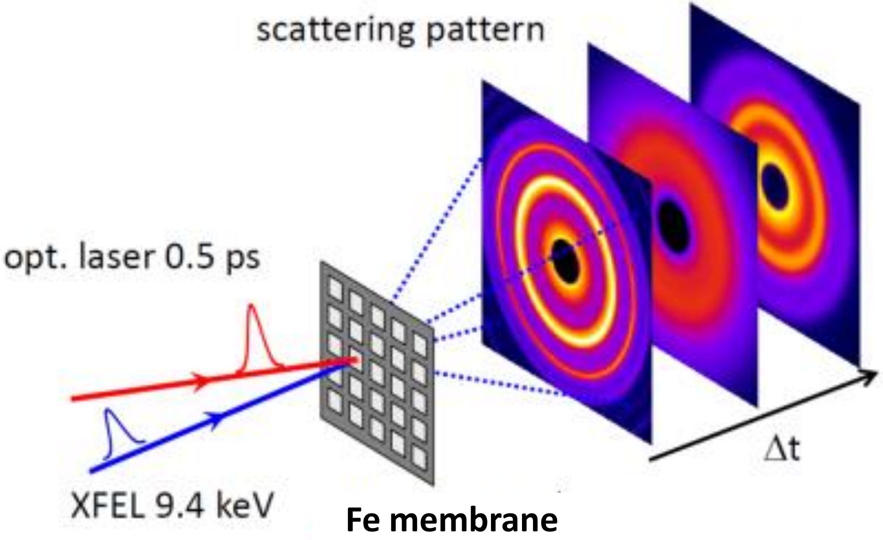
All information
in one pulse



XFEL radiation properties

Wavelength – 50 ÷ 0.5 Å
Photon energy – 0.25 ÷ 25 keV
Spectral bandwidth - 0.1%
Pulse energy – 1 mJ or $10^{11\text{-}12}$ photon
Pulse duration – 1- 200 fs

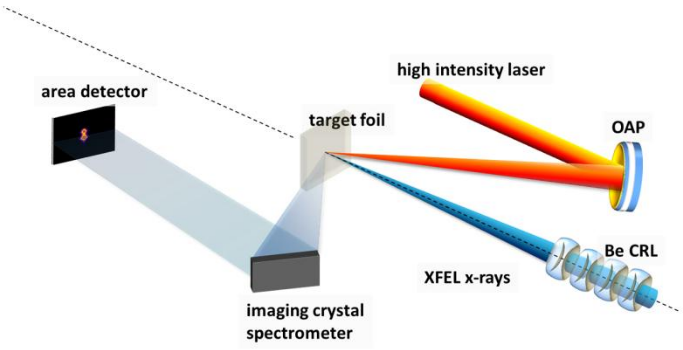
Time-resolved studies
(pump-probe)



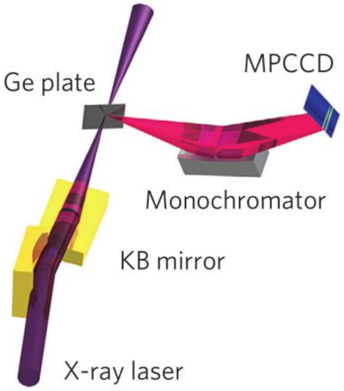
XFEL radiation properties

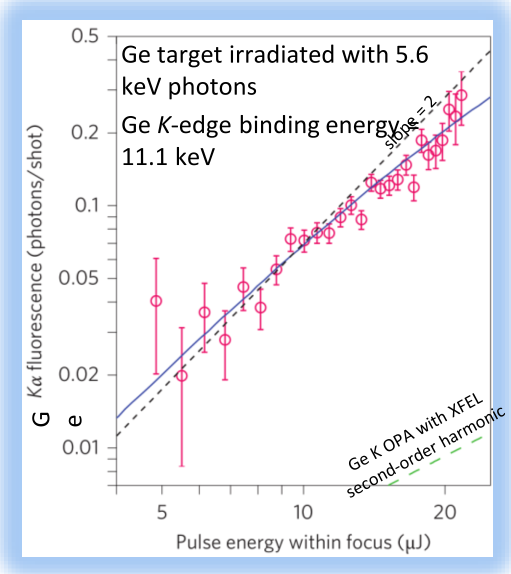
Wavelength – 50 ÷ 0.5 Å
Photon energy – 0.25 ÷ 25 keV
Spectral bandwidth - 0.1%
Pulse energy – 1 mJ or $10^{11\text{-}12}$ photons
Pulse duration – 1- 200 fs
Peak Power ~ sub Terawatt

„Warm Dense Matter”



X-ray non-linear optics



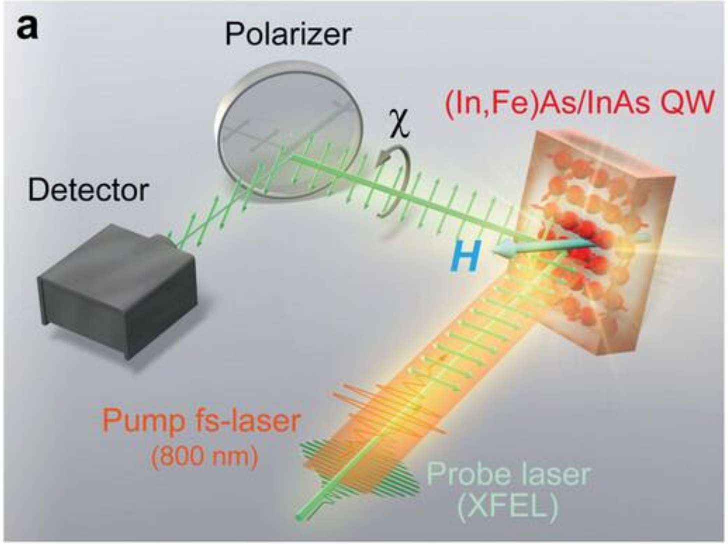


DOI: 10.1038/nphoton.2014.10

XFEL radiation properties

Wavelength – 50 ÷ 0.5 Å
Photon energy – 0.25 ÷ 25 keV
Spectral bandwidth - 0.1%
Pulse energy – 1 mJ or 10^{11-12} photons
Pulse duration – 1- 200 fs
Peak Power ~ sub Terawatt
Polarisation – linear or circular

Magnetic measurements (e.g. Kerr effect)

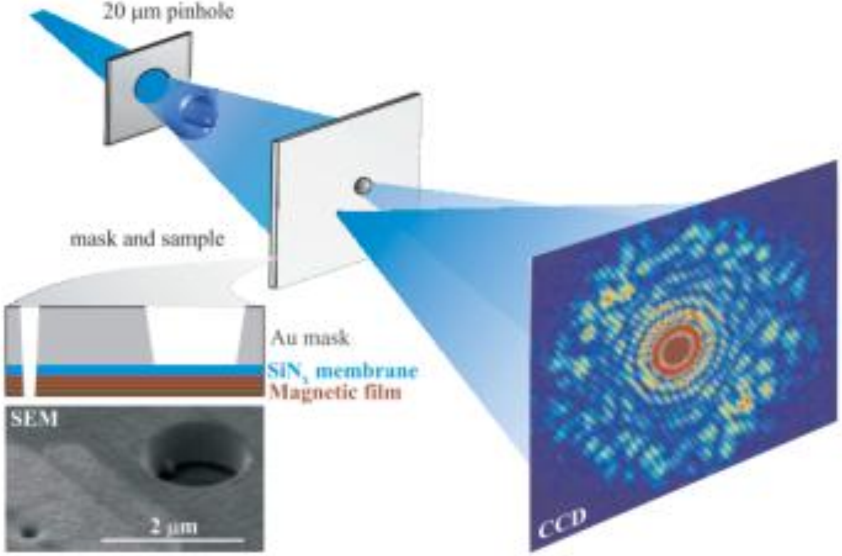


DOI: 10.1002/adma.202301347

XFEL radiation properties

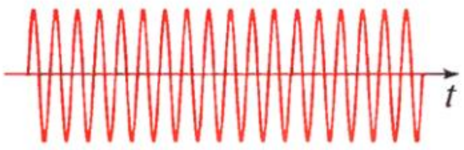
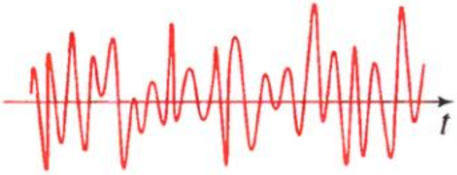
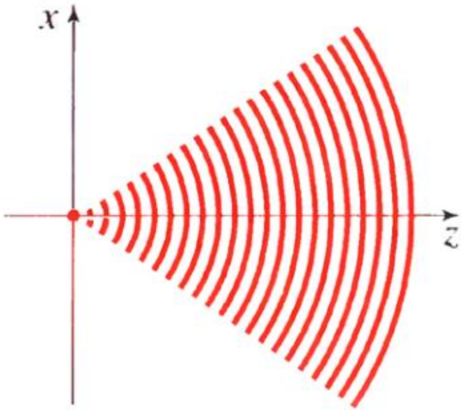
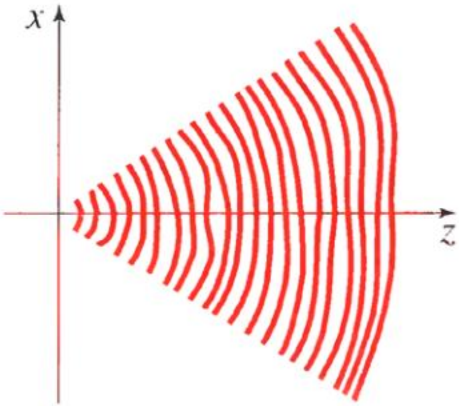
Wavelength – 50 ÷ 0.5 Å
Photon energy – 0.25 ÷ 25 keV
Spectral bandwidth - 0.1%
Pulse energy – 1 mJ or $10^{11\text{-}12}$ photons
Pulse duration – 1- 200 fs
Peak Power ~ sub Terawatt
Polarisation – linear or circular
Spatial coherence

X-ray holography
Correlation spectroscopy



J.A.Nielsen, D. McMorrow, Elements of Modern X-ray Physics, Wiley (2011)

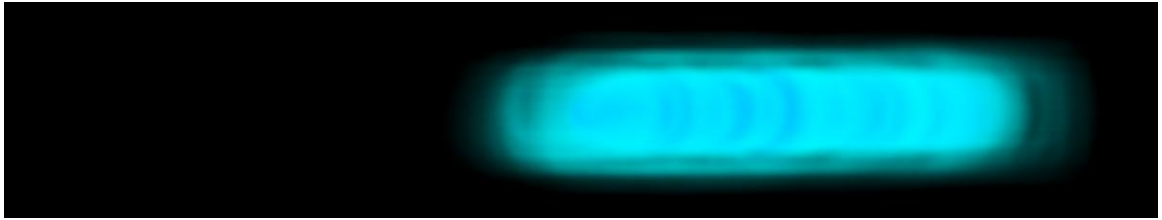
Coherence

	Coherent	In-coherent
Time (longitudinal)		
Space (transversal)		

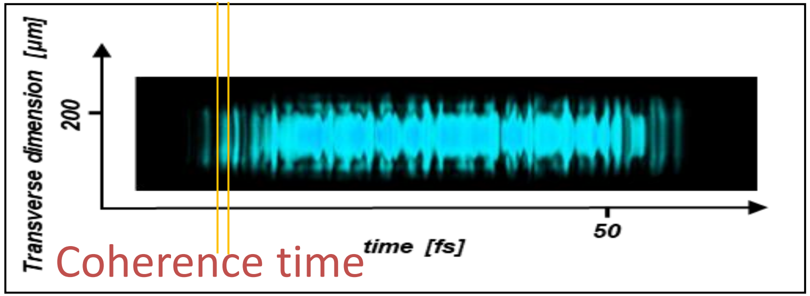
Saleh, Teich, Fundamentals of Photonics , Wiley 2007

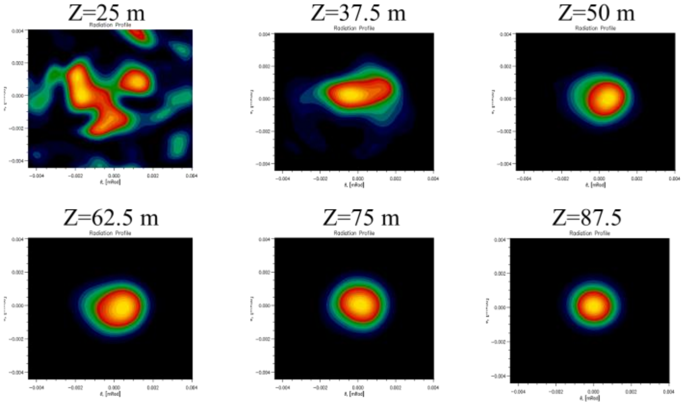
Coherent properties of SASE photon bunch

3D representation of the photon pulse exiting the undulator line



Temporal coherence





Courtesy: J.Krzywinski, SLAC

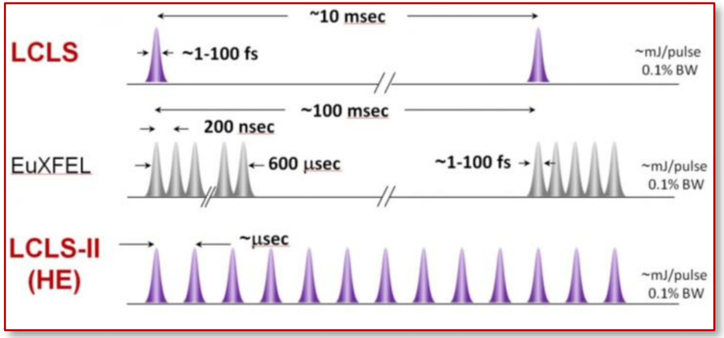
Spatial coherence

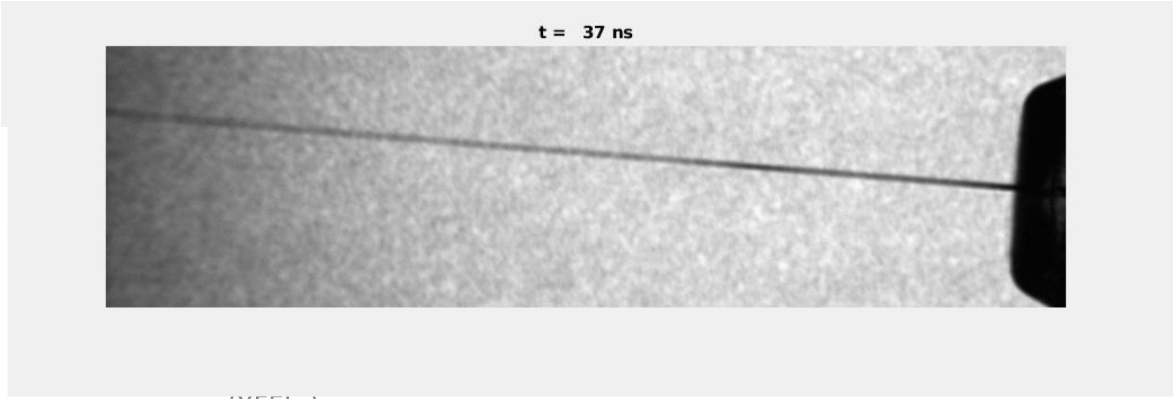
XFEL radiation properties

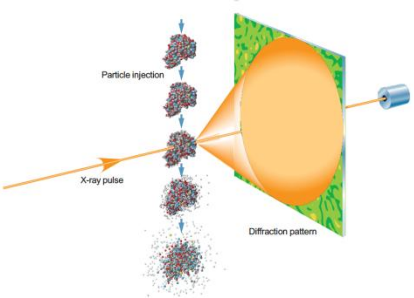
Time resolution in micro-/milisecond domain

HUB-POLAND

Wavelength – 50 ÷ 0.5 Å
Photon energy – 0.25 ÷ 25 keV
Spectral bandwidth - 0.1%
Pulse energy – 1 mJ or 10^{11-12} photons
Pulse duration – 1- 200 fs
Peak Power ~ sub Terawatt
Polarisation – linear or circular
Spatial coherence
Pulse structure



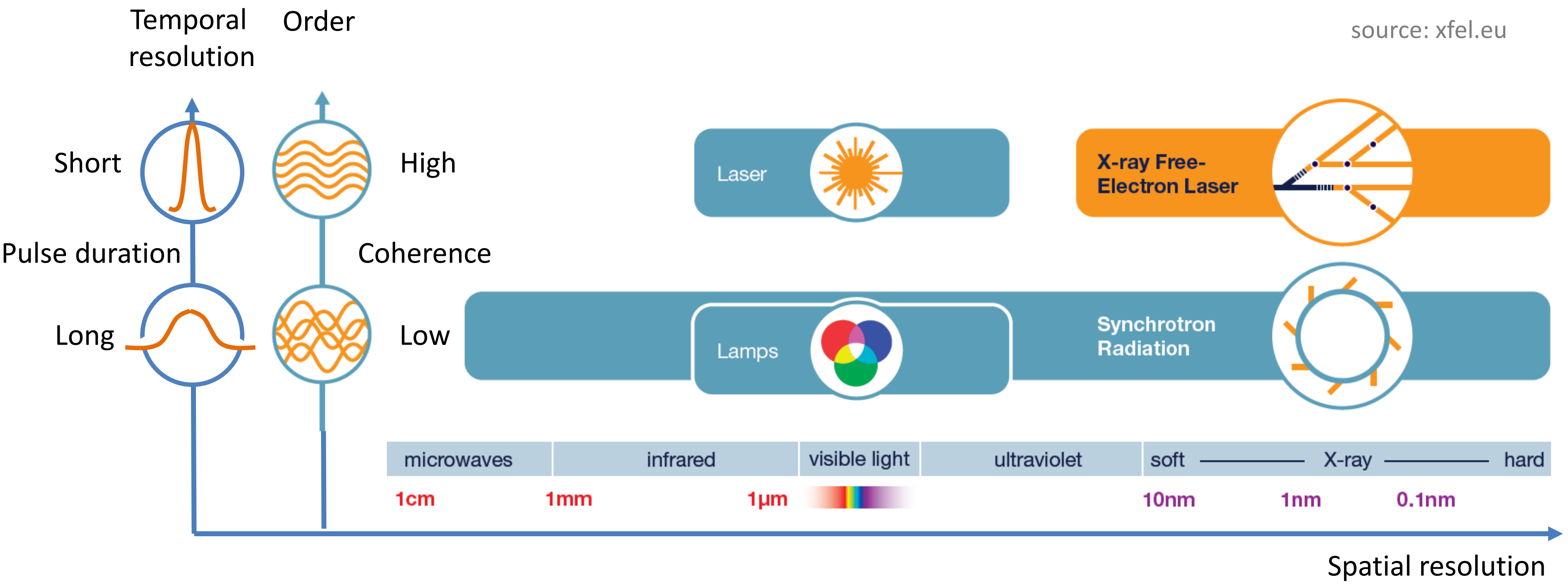




(XFELs)

XFELs vs lasers and synchrotrons

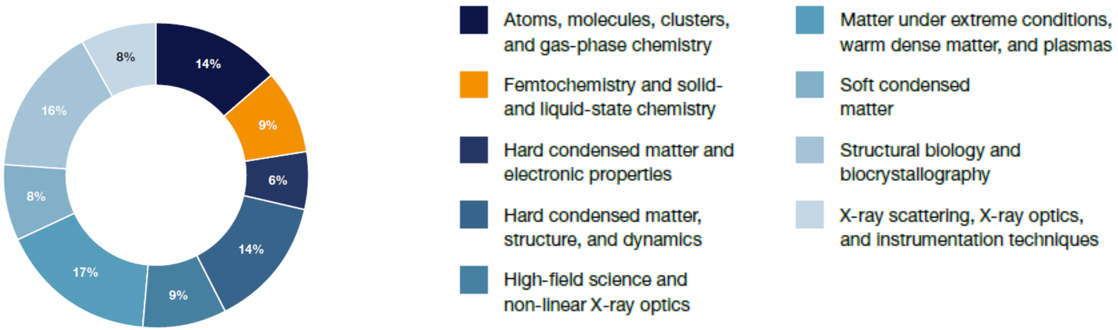
source: xfel.eu

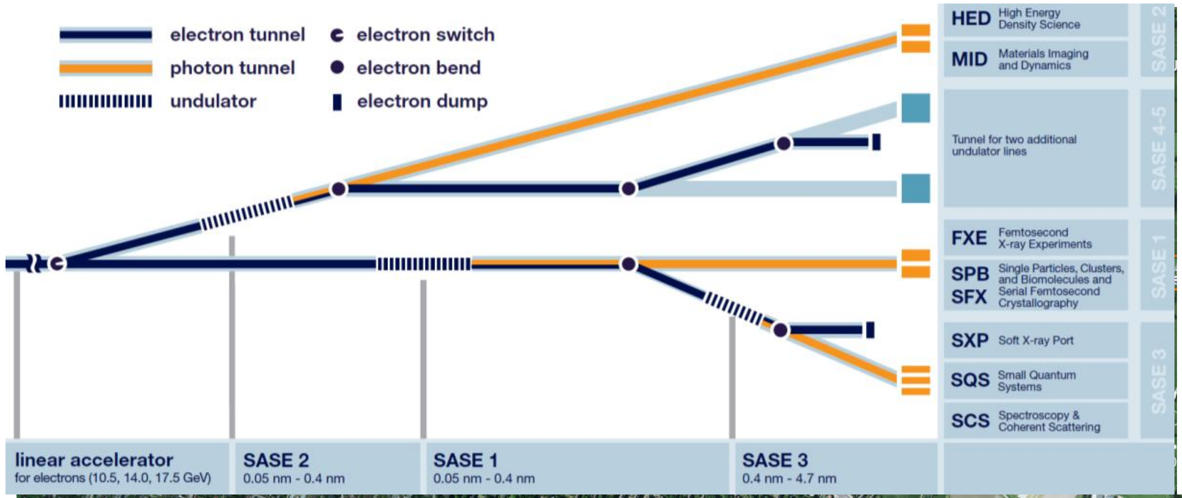


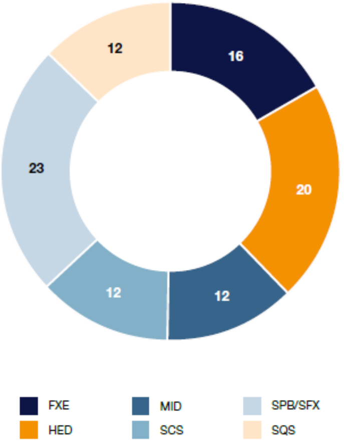
XFELs of the World

source: xfel.eu

European XFEL



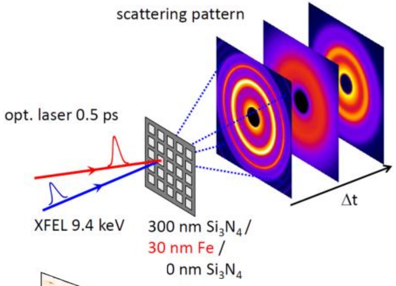


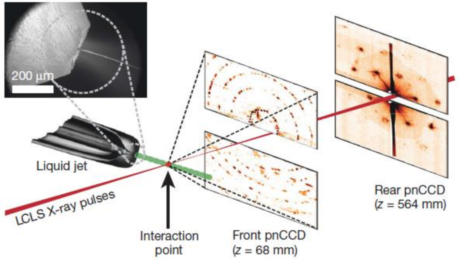


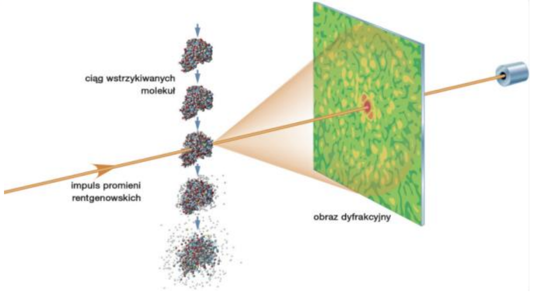
source: xfel.eu

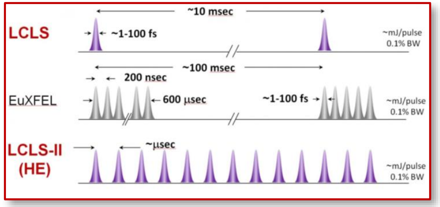
EuXFEL radiation properties

Wavelength – 50 ÷ 0.5 Å & 2-color
Photon energy – 0.25 ÷ 25 keV
Spectral bandwidth - 0.1% & seeding
Pulse energy – 1 mJ or $10^{11\text{-}12}$ photons
Pulse duration – 1- 200 fs & as
Polarisation – linear or circular
Spatial coherence
Pulse structure









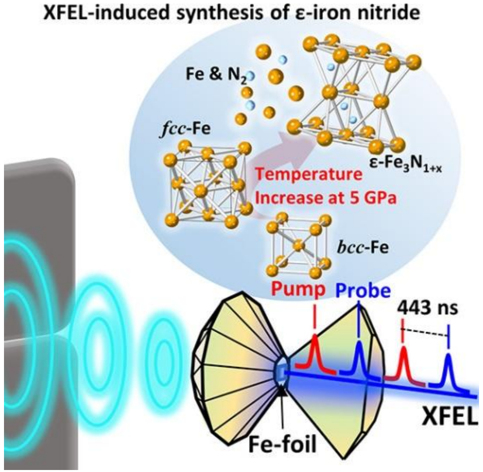
EuXFEL radiation properties

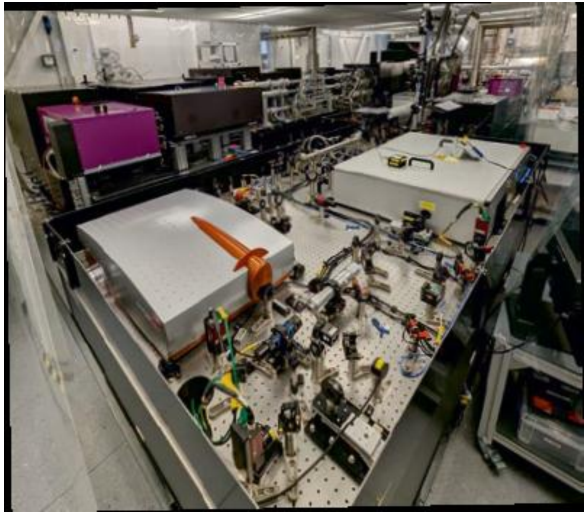
HUB-POLAND

Wavelength – 50 ÷ 0.5 Å & 2-color
Photon energy – 0.25 ÷ 25 keV
Spectral bandwidth - 0.1% & seeding
Pulse energy – 1 mJ or 10^{11-12} photons
Pulse duration – 1- 200 fs & as
Polarisation – linear or circular
Spatial coherence
Pulse structure

+

High energy/intensity lasers
Diamond Anvil Cell (DAC)

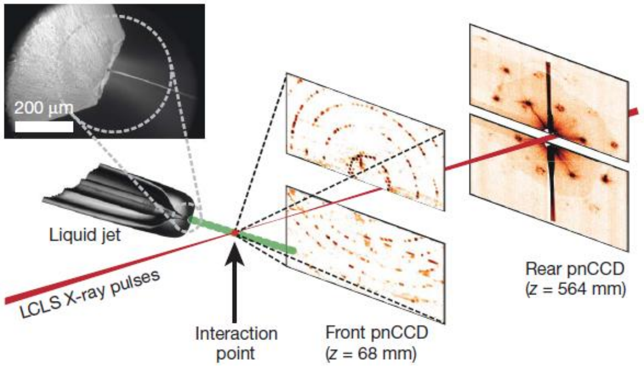




Biology – structure determination with atomic resolution

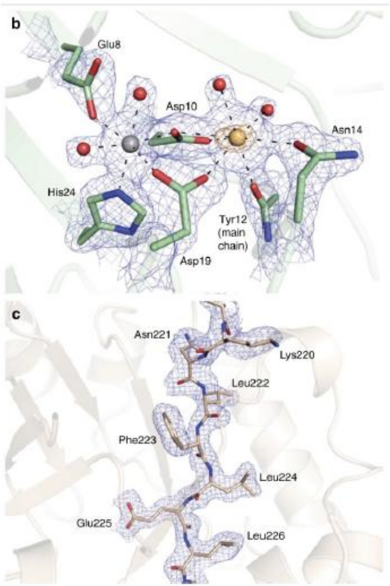
Serial femtosecond crystallography (SFX)

μm-size crystals



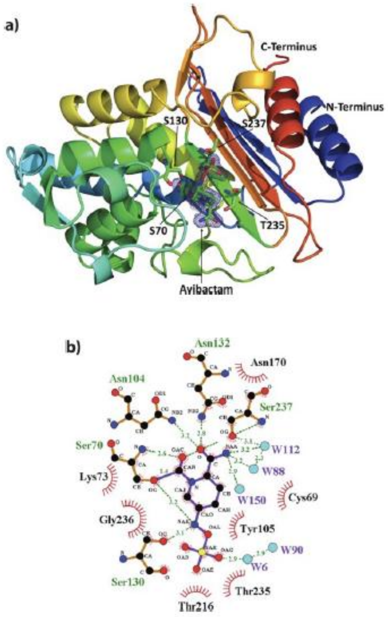
H.N. Chapman et al., Nature 470, 73 (2011)

Jack bean protein



Grünbein et al, *Nat. Commun.* 9, 3487 (2018)

CTX-M-14 β-lactamase

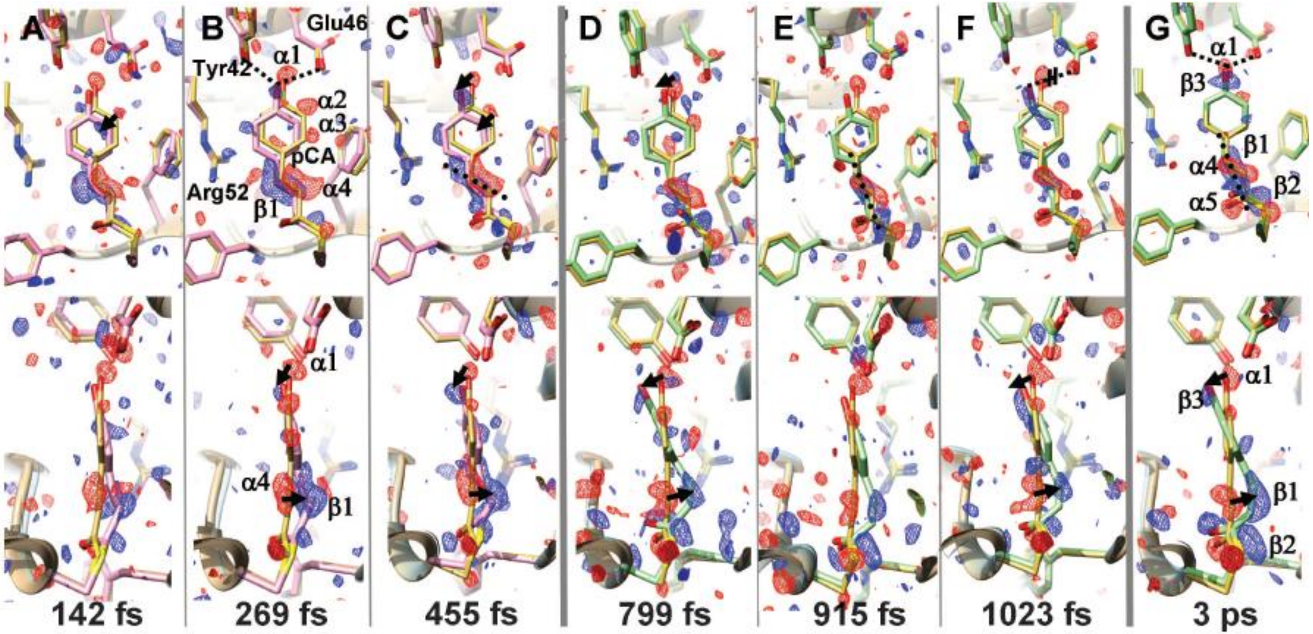


Wiedorn et al, *Nat. Commun.* 9, 4025 (2018)

Courtesy: W.Gawełda, UAM

Molecular movies

Photo-active Yellow Protein (100 fs to 3 ps):



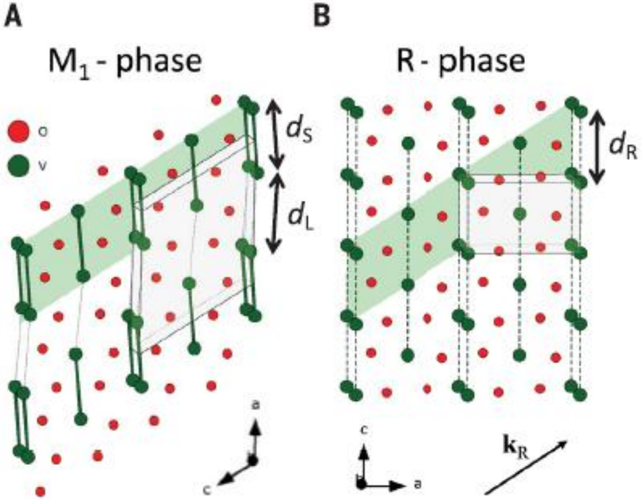
Courtesy: W.Gawełda, UAM

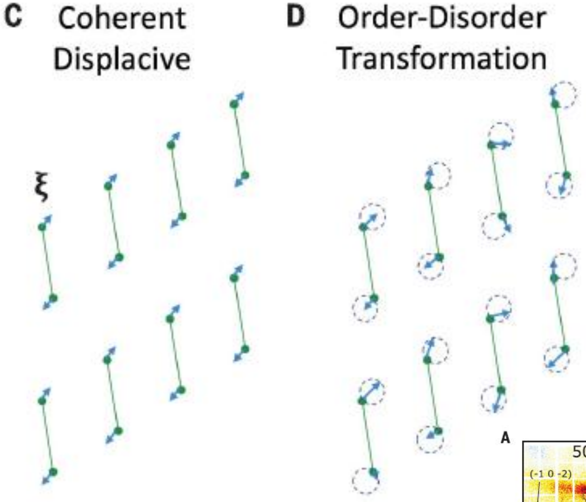
K. Pande et al., Science 352, 725 (2016)

Ultrafast disorder

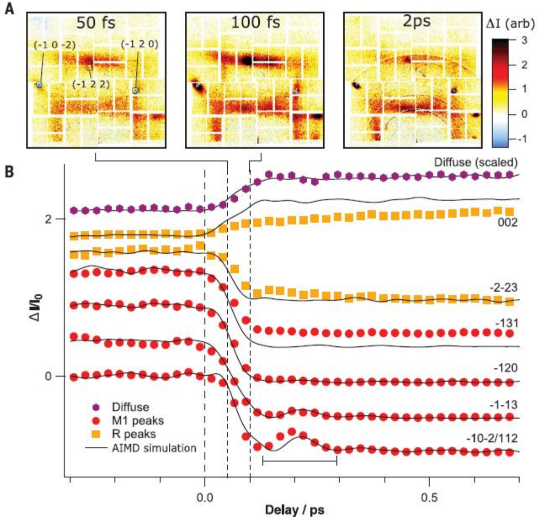
Ultrafast disordering of vanadium dimers in photoexcited VO_2

Simon Wall[1]*†, Shan Yang[2]†, Luciana Vidas[1], Matthieu Chollet[3], James M. Glownia[3], Michael Kozina[4], Tetsuo Katayama[5], Thomas Henighan[4], Mason Jiang[4], Timothy A. Miller[1], David A. Reis[4,6,7], Lynn A. Boatner[8], Olivier Delaire[2,9]*, Mariano Trigo[4,6]*





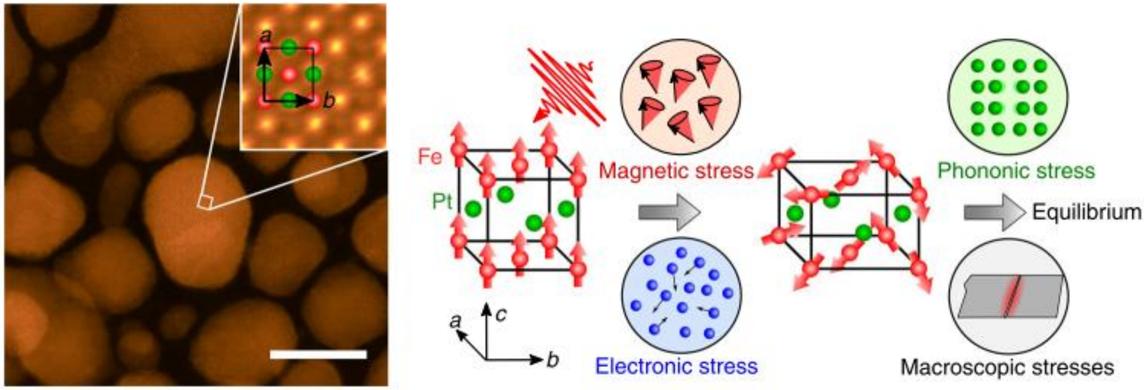
Science 362, 572–576 (2018)



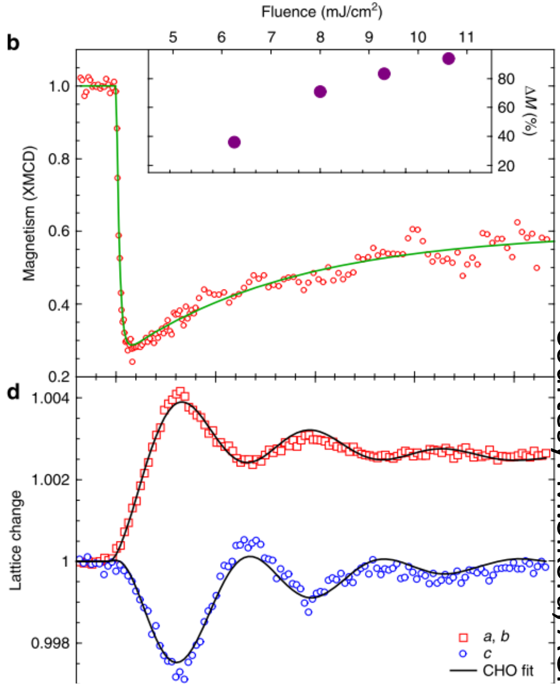
Ultrafast demagnetization

A.H. Reid, et al., Nature Commun. (2018)

X-ray magnetic diffraction



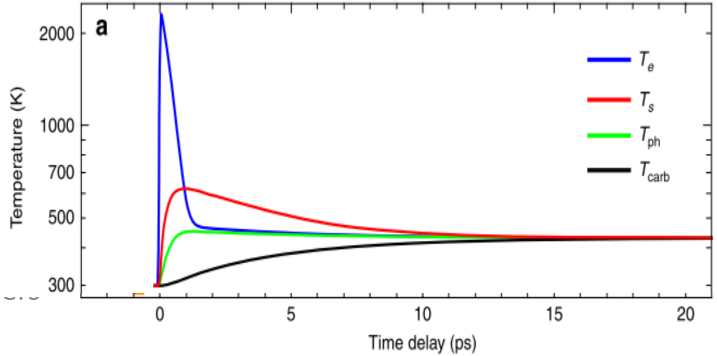
Unstrained samples: CoPt nanoparticles



Courtesy: M.Sikora, AGH

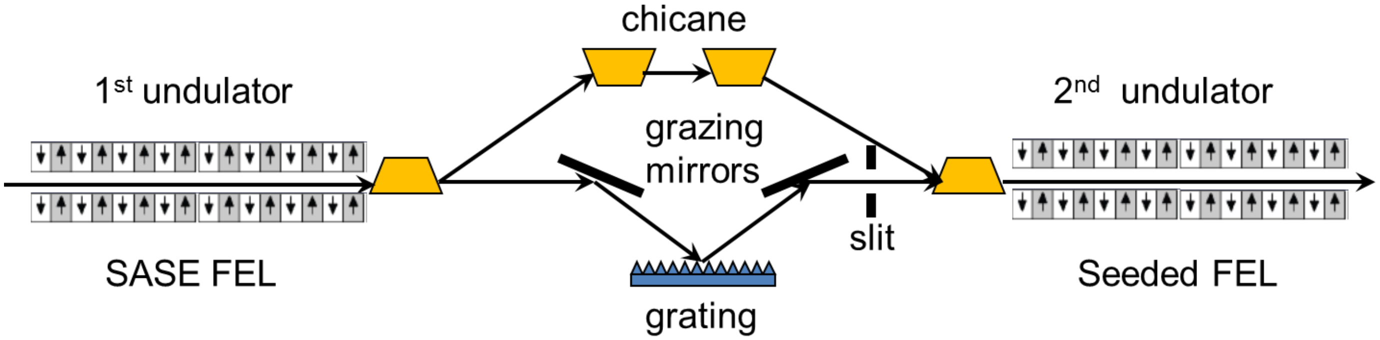
Magnetoelastic stress builds up on the sub-ps timescale, characteristic of ultrafast demagnetization

Stress from transiently populated phonons takes over on the ps timescale → reduced magn. anisotropy



Self-Seeding - How to improve the coherence time ?

- First undulator generates SASE
- X-ray monochromator filters SASE and generates seed
- Chicane delays electrons and washes out SASE microbunching
- Second undulator amplifies seed to saturation



1. J. Feldhaus et al., NIMA, 1997.

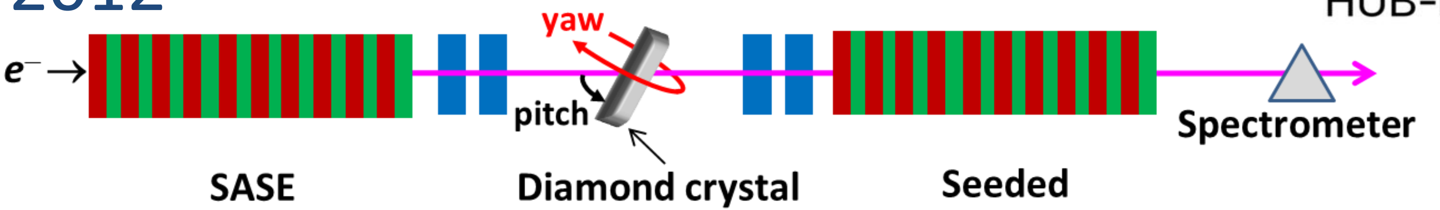
2. E. Saldin et al., NIMA, 2001.

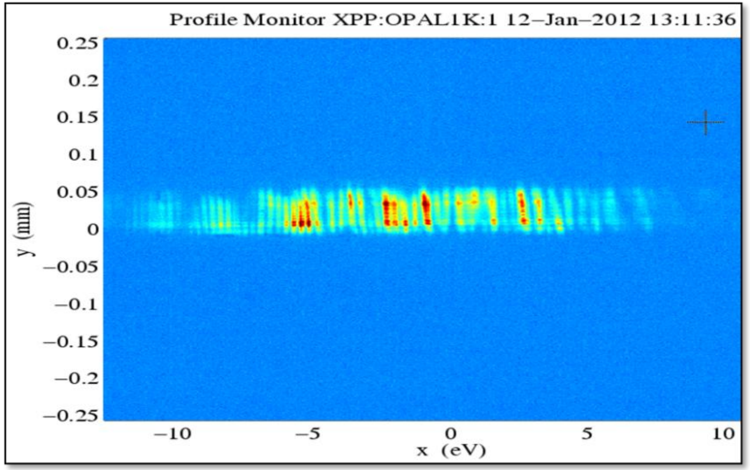
3. Y. Ding, Z. Huang, R. Ruth, PRSTAB, 2010.

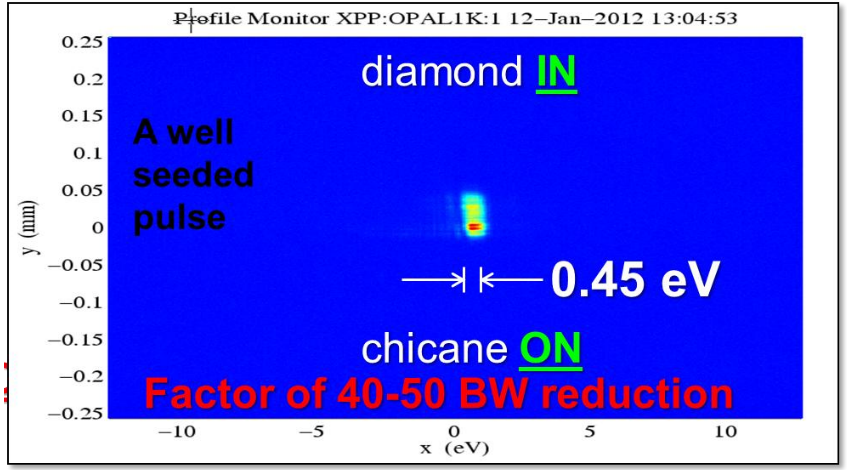
4. G. Geloni, G. Kocharyan, E. Saldin, DESY 10-133, 2010.

Courtesy: J.Krzywinski, SLAC

Hard X-ray self seeding at SLAC 2012







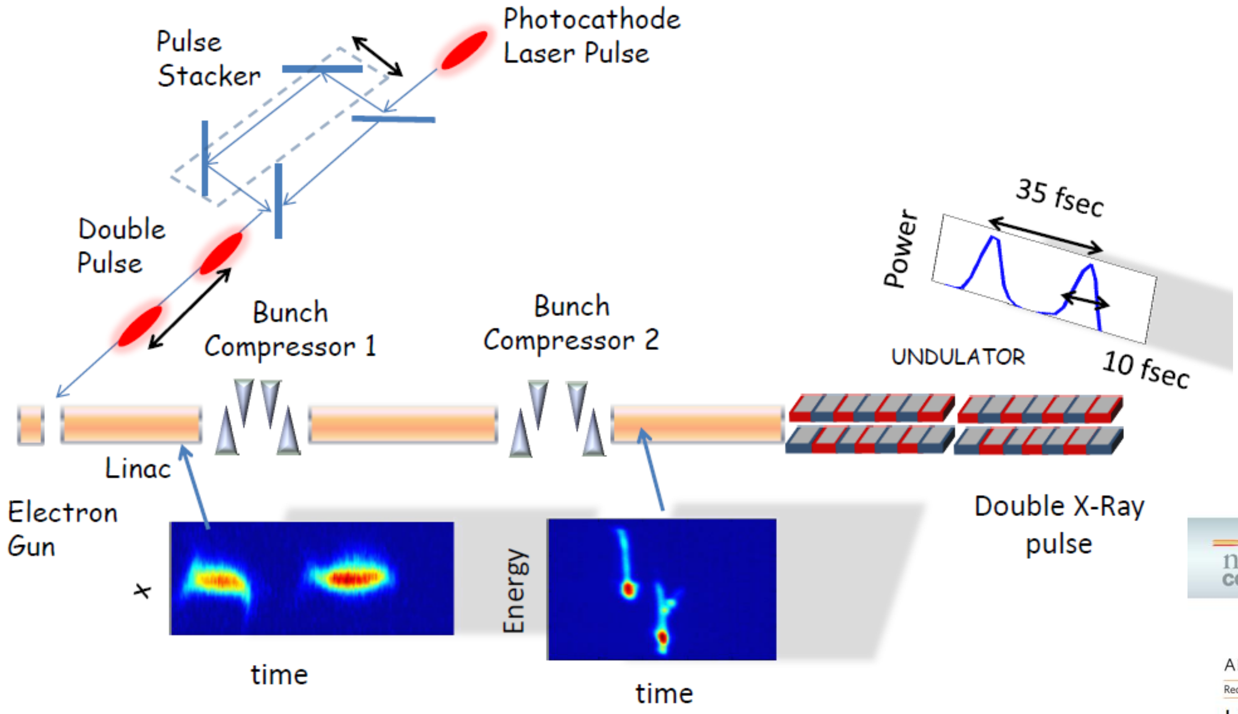
Demonstration of self-seeding in a hard-X-ray free-electron laser

Nature Photonics **6**, 693–698 (2012) | doi:10.1038/nphoton.2012.180

J. Amann, W. Berg, V. Blank, F.-J. Decker, Y. Ding, P. Emma, Y. Feng, J. Frisch, D. Fritz, J. Hastings, Z. Huang, J. Krzywinski, R. Lindberg, H. Loos, A. Lutman, H.-D. Nuhn, D. Ratner, J. Rzepiela, D. Shu, Yu. Shvyd'ko, S. Spampinati, S. Stoupin, S. Terentyev, E. Trakhtenberg, D. Walz *et al.*

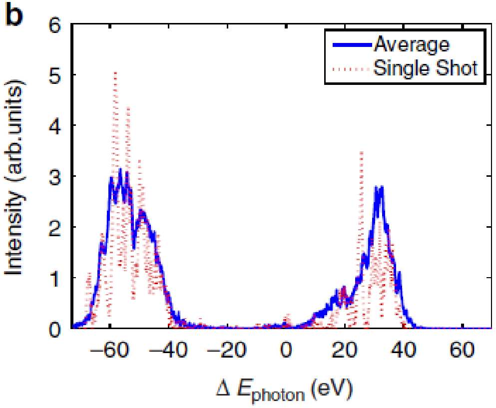
Courtesy: J.Krzywinski, SLAC

2 color XFEL



psec delay

femtosec delay
~1% energy separation



nature COMMUNICATIONS

ARTICLE

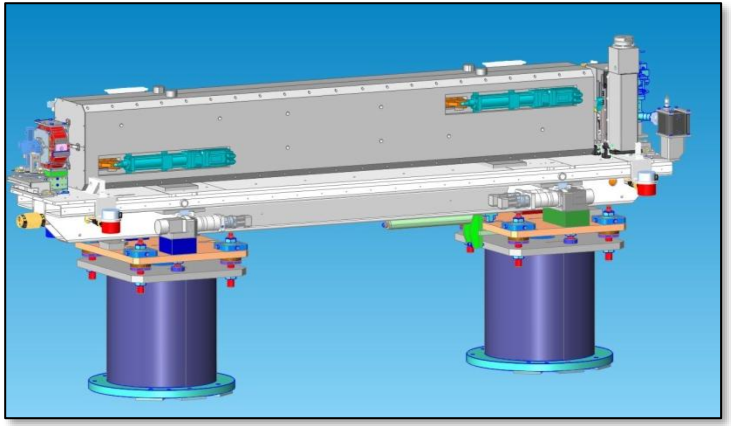
Received 16 Oct 2014 | Accepted 22 Jan 2015 | Published 6 Mar 2015
DOI: 10.1038/ncomms7369 OPEN

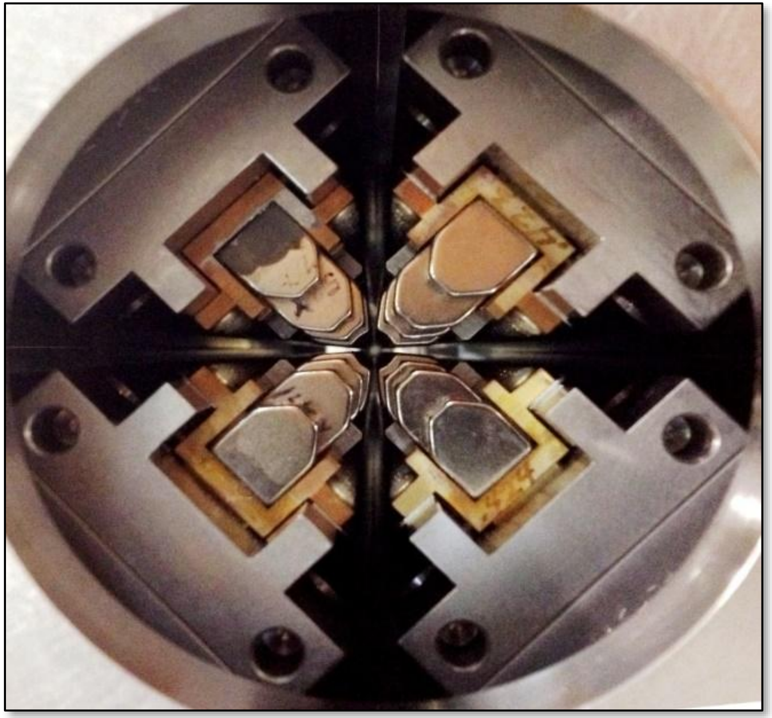
High-intensity double-pulse X-ray free-electron laser

A. Marinelli[1], D. Ratner[1], A.A. Lutman[1], J. Turner[1], J. Welch[1], F.-J. Decker[1], H. Loos[1], C. Behrens[1,2], S. Gilevich[1], A.A. Miahnahri[1], S. Vetter[1], T.J. Maxwell[1], Y. Ding[1], R. Coffee[1], S. Wakatsuki[1,3] & Z. Huang[1]

Courtesy: J.Krzywinski, SLAC

Polarization control

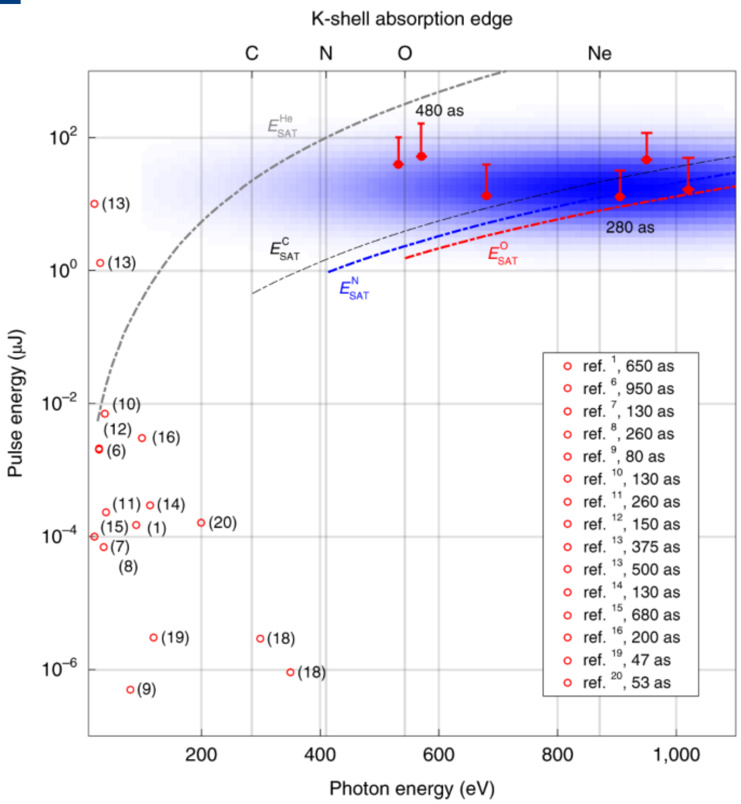


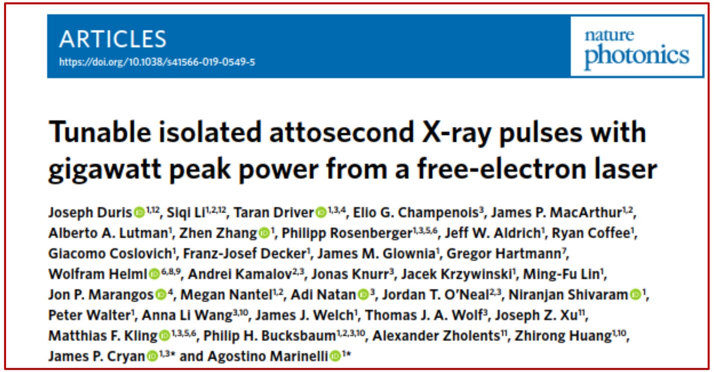


Four independent rows of permanent magnets move longitudinally at fixed gap

Courtesy: J.Krzywinski, SLAC

Attosecond pulses





ARTICLES

nature photonics

https://doi.org/10.1038/s41566-019-0549-5

Tunable isolated attosecond X-ray pulses with gigawatt peak power from a free-electron laser

Joseph Duris[1,12], Siqi Li[1,2,12], Taran Driver[1,3,4], Elio G. Champenois[3], James P. MacArthur[1,2], Alberto A. Lutman[1], Zhen Zhang[1], Philipp Rosenberger[1,3,5,6], Jeff W. Aldrich[1], Ryan Coffee[1], Giacomo Coslovich[1], Franz-Josef Decker[1], James M. Glownia[1], Gregor Hartmann[7], Wolfram Helml[6,8,9], Andrei Kamalov[2,3], Jonas Knurr[3], Jacek Krzywinski[1], Ming-Fu Lin[1], Jon P. Marangos[4], Megan Nantel[1,2], Adi Natan[3], Jordan T. O'Neal[2,3], Niranjan Shivaram[1], Peter Walter[1], Anna Li Wang[3,10], James J. Welch[1], Thomas J. A. Wolf[3], Joseph Z. Xu[11], Matthias F. Kling[1,3,5,6], Philip H. Bucksbaum[1,2,3,10], Alexander Zholents[11], Zhirong Huang[1,10], James P. Cryan[1,3]* and Agostino Marinelli[1]*

Further reading

- **D. Attwood and A. Sakdinwat**, X-rays and Extreme Ultraviolet Radiation (Cambridge, UK 2017), Chapter 6,

  YouTube lectures:

  AST C210 EE C213 Spring 2021 Lecture 13 –YouTube

  https://www.youtube.com/watch?v=v8_I4dbYyR8

  AST C210 EE C213 Spring 2021 Lecture 14 –YouTube

  https://www.youtube.com/watch?v=peyI6aVXua4

- **Philip Willmott**, SLS, PSI, „An Introduction to Synchrotron Radiation"
- **K.-J. Kim, Z. Huang and R. Lindberg**, Synchrotron Radiation and Free Electron Lasers: Principles of Coherent X-ray Generation (Cambridge, UK, 2017).
- **P. Schmüser, M. Dohlus**, J. Rossbachand C. Behrens, Free-Electron Lasers in the Ultraviolet and X-ray Regime(Springer, Heidelberg, 2014).

Thank you for your attention

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