X-ray Free Electron Lasers: shedding light on nanoworld dynamics

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

HELMHOLTZ GEMEINSCHAFT

DESY

Contents

- **X-ray sources in research**
- **Examples of XFEL experiments**
- **Free Electron Lasers: principles and properties**
- **FLASH at DESY (setup and performance)**
- **Research Highlights from FLASH**
- **Conclusions / Outlook**

X-ray sources in research

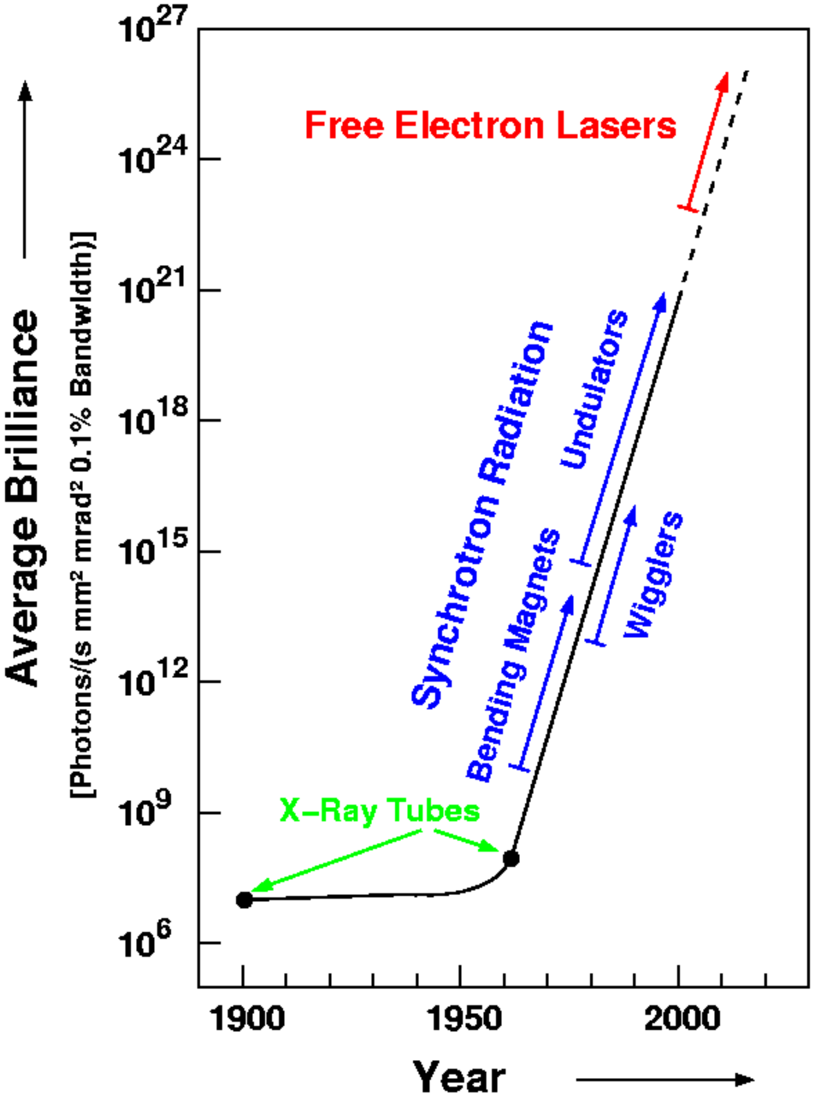
X-ray FELs

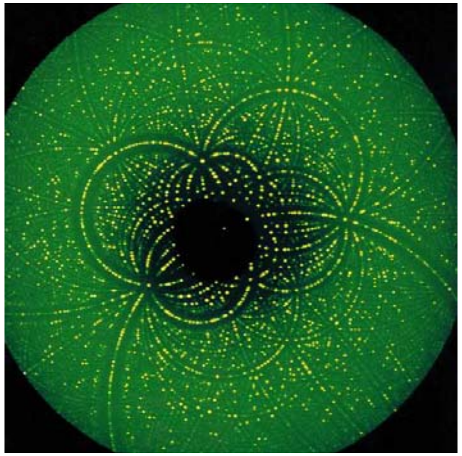
Synchrotron Radiation sources

X-ray tubes

From X-ray tubes to X-ray FELs

classical
„X-ray“



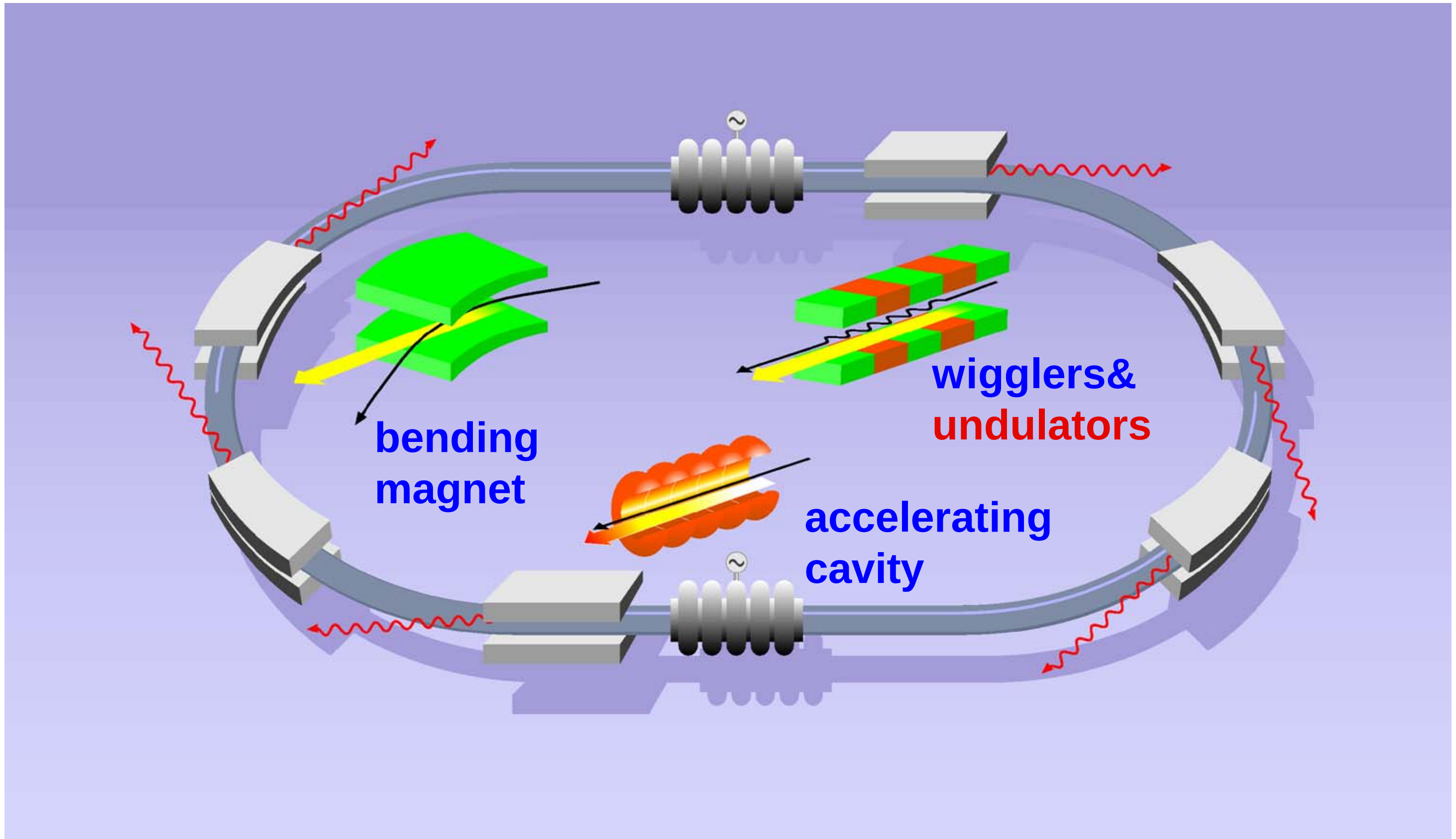


crystal structure analysis with atomic resolution

+

information about femtosecond dynamics

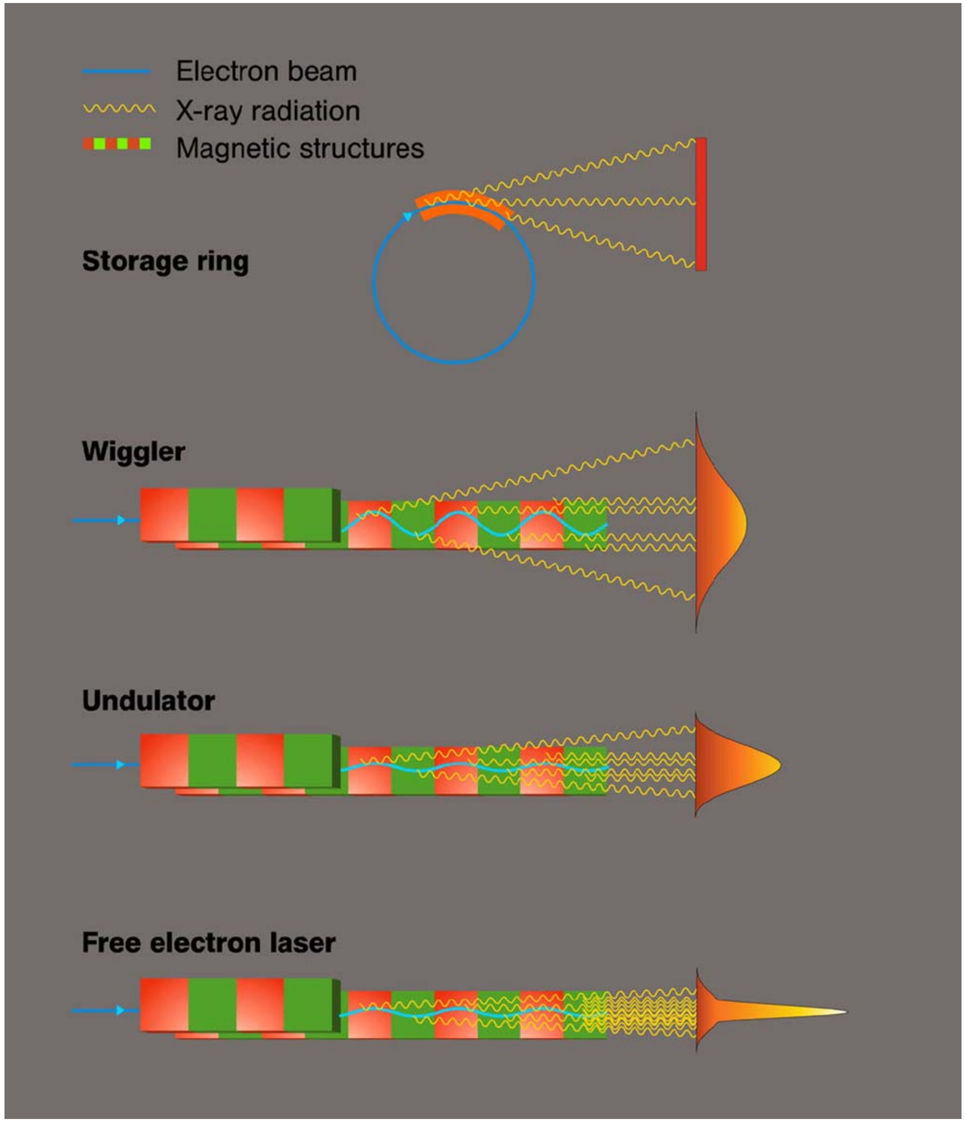
Synchrotron Radiation storage ring



Undulator = periodic magnetic field arrangement,
electrons emit light along sinusodial path,
photons can interfere constructively

➔ intensity enhancement ∝N^2 (N= # of undulator periods)

Synchrotron Radiation sources



bending magnet radiation

$\propto N_W$ x bending magnet

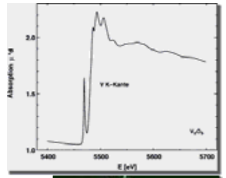
$\propto N_U^2$ x bending magnet

$\propto N_U^2$ x N_e x bending magnet

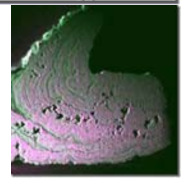
N_U , N_W = # of magnetic periods
N_e = # of electrons in a bunch

Applications of Synchrotron Radiation

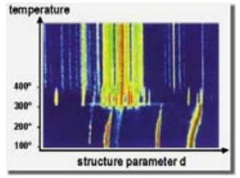
Absorption Spectroscopie (EXAFS / XANES):
local atomic surrounding, valence states, katalysis



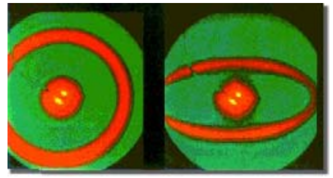
Fluorescence Analysis:
trace element analysis (e.g. Si-wafer impurities)



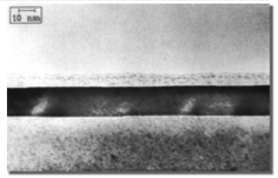
Diffraction:
structure analysis, stress, strain and textures in materials



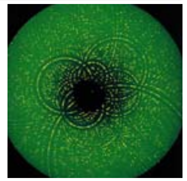
Small Angle Scattering:
soft and liquid materials (e.g. polymers)



Surfaces and Interfaces:
roughness, layer thicknesses, density of thin layers



Structure of Biomolecules (Protein Crystallography):
DNA, drug design, time-resolved dynamics of biological processes



„more light": What is it good for?

High Intensity:

diluted samples,
e.g spectroscopy on mass selected clusters in gas phase,
highly charged ions or
single molecule diffraction

Power Density:

focused to 1µm^2 > 10^{16} W/cm^2 ⇒ nonlinear effects,
plasma physics

Short Pulses:

Excitation ≤ timescale of molecular vibrations,
electronic relaxation, ...

➔ Study of time dependent processes (*pump and probe - experiments*) or, e.g., X-ray microscopy on living cells

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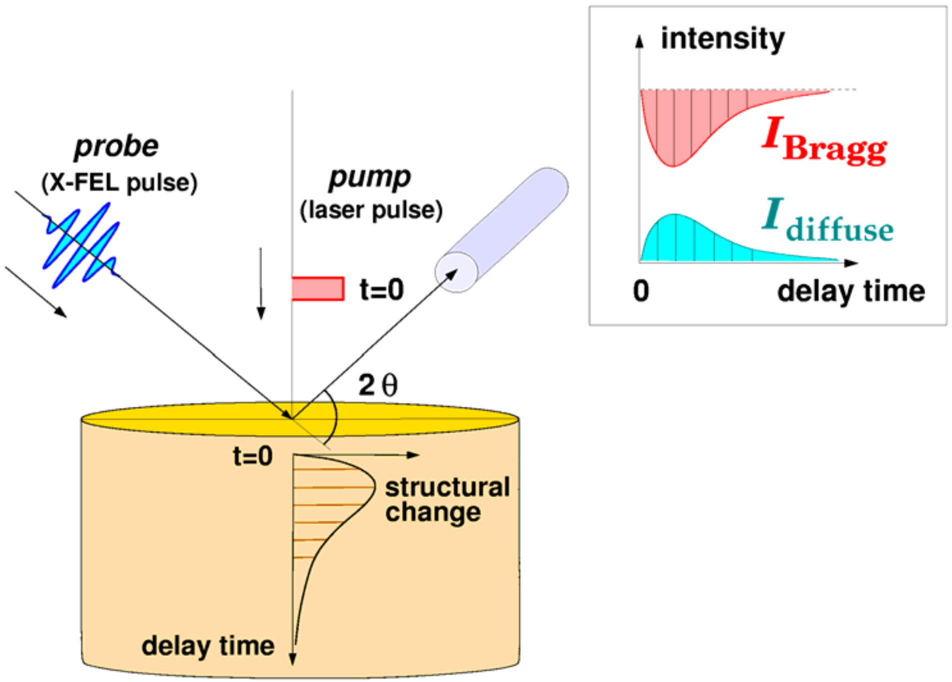
Examples of XFEL experiments

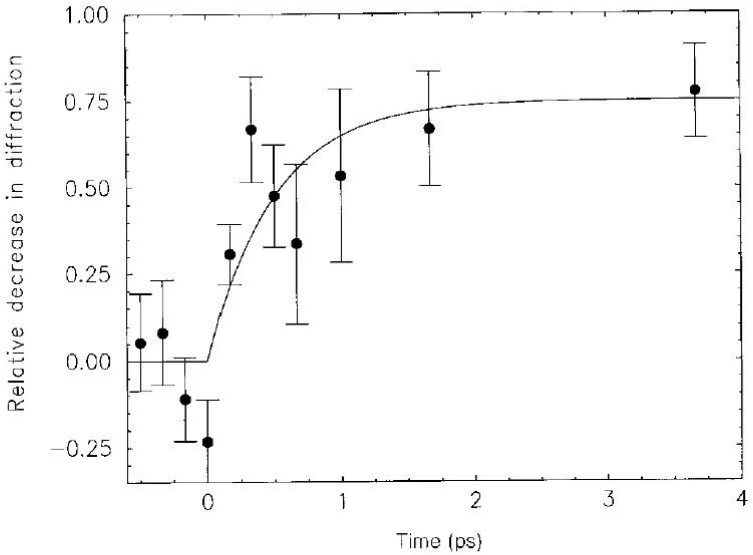
- **Condensed matter physics:**
  How does a surface melt?

- **Femtochemistry:**
  Can we „film“ a chemical reaction?

- **Biology:**
  Can we determine the structure of single protein molecules?
  Can ultrafast structural changes be detected?

Condensed matter Physics: How does a surface melt?



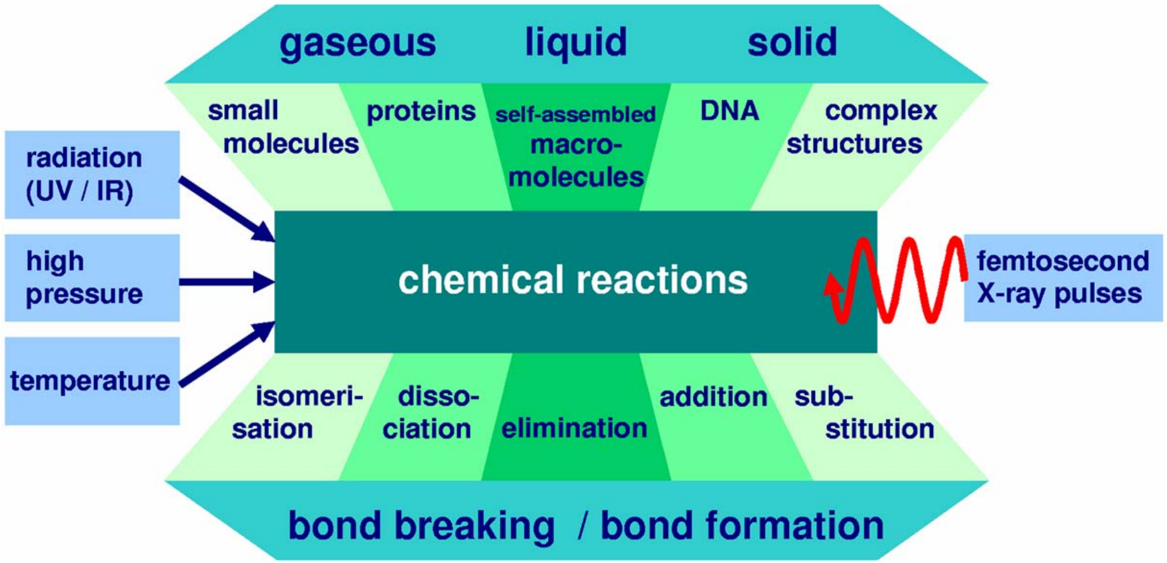


C. Rischel et al.,
Nature 390,
490-492 (1997)

Femtochemistry: Can we „film“ a chemical reaction?

Initial state

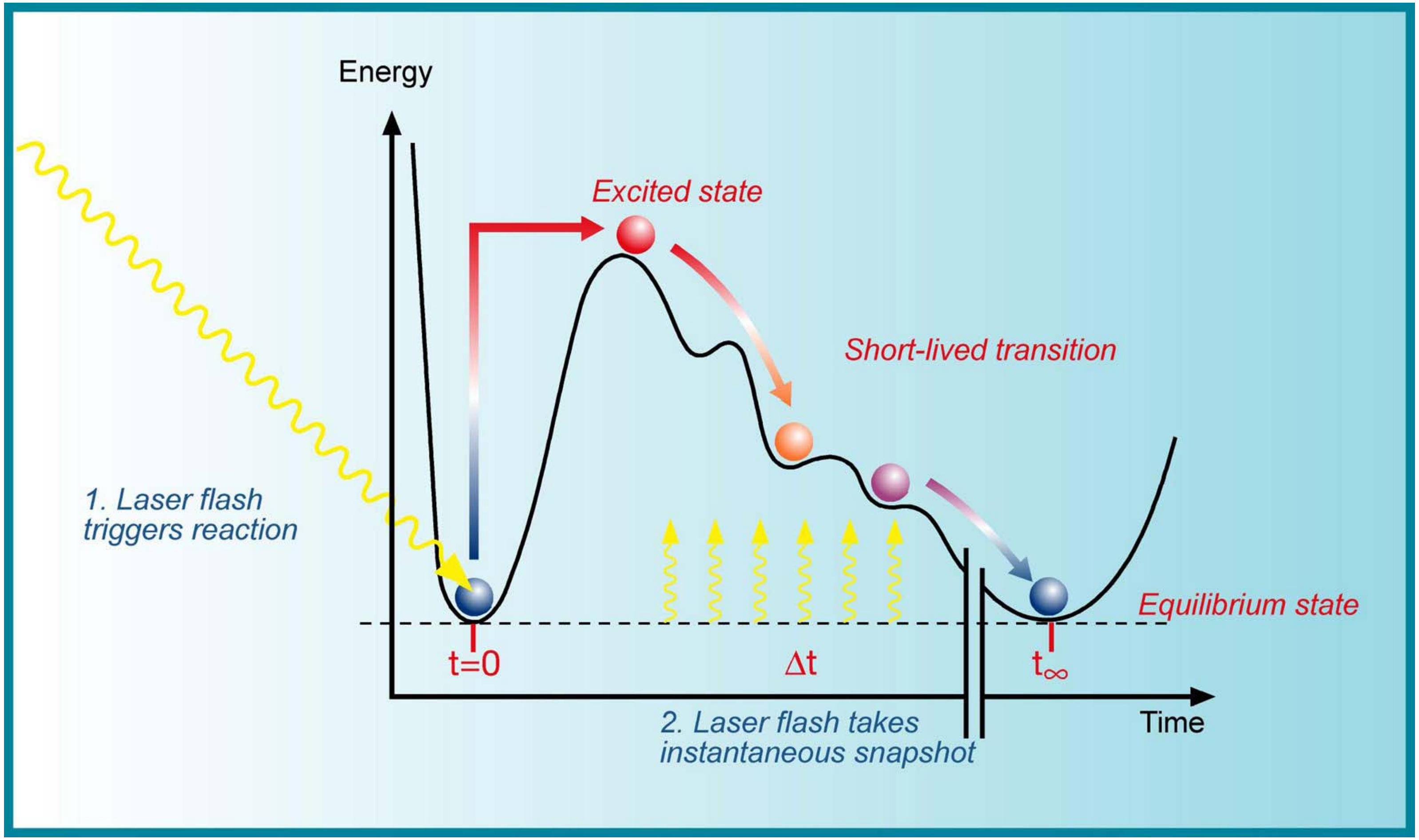
Excitation



Snapshot

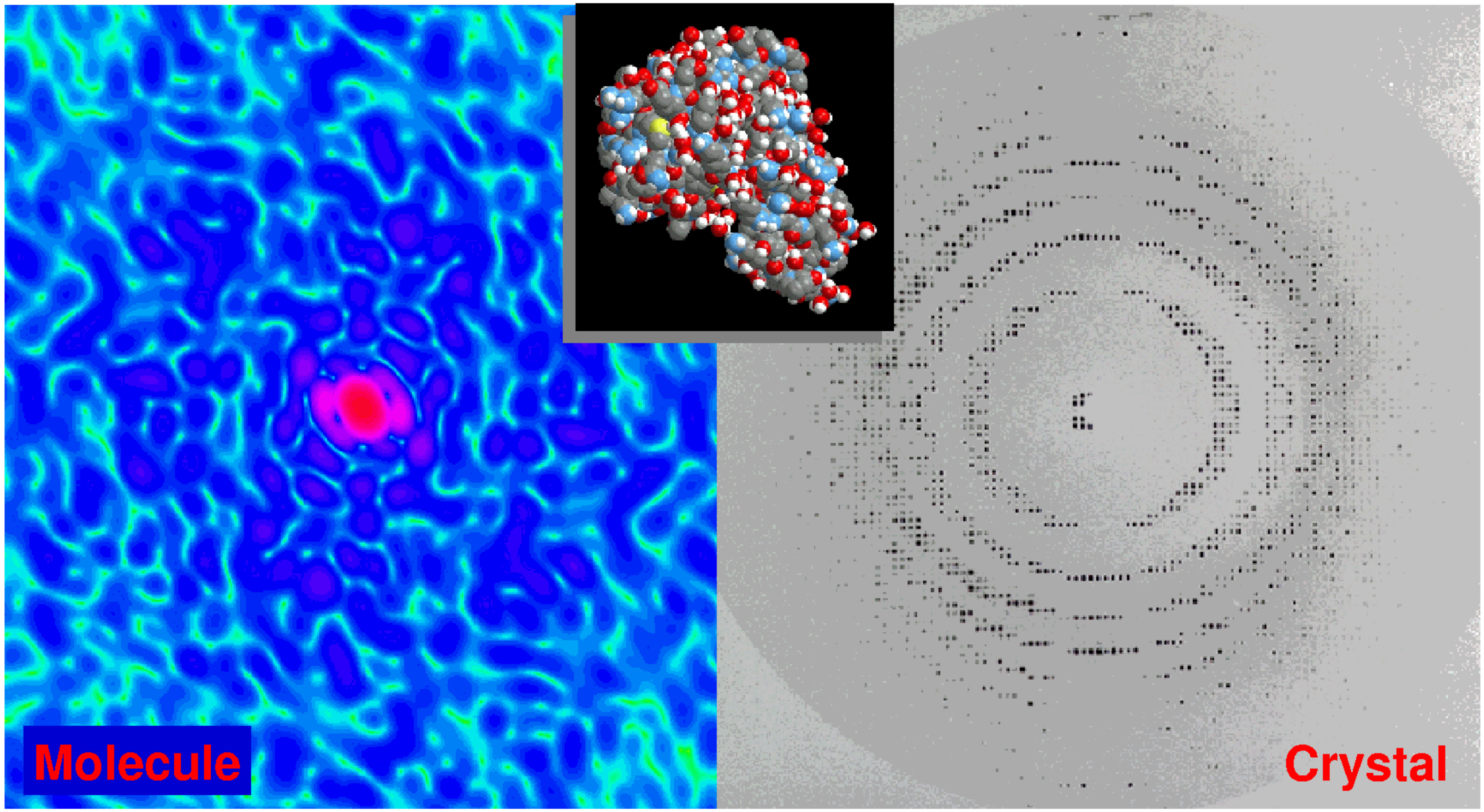
(time resolved)

Final state



Snapshots for different times after excitation
(“pump-probe experiment”) ➔ “film” of the reaction

Biology: Can we determine the structure of single protein molecules?

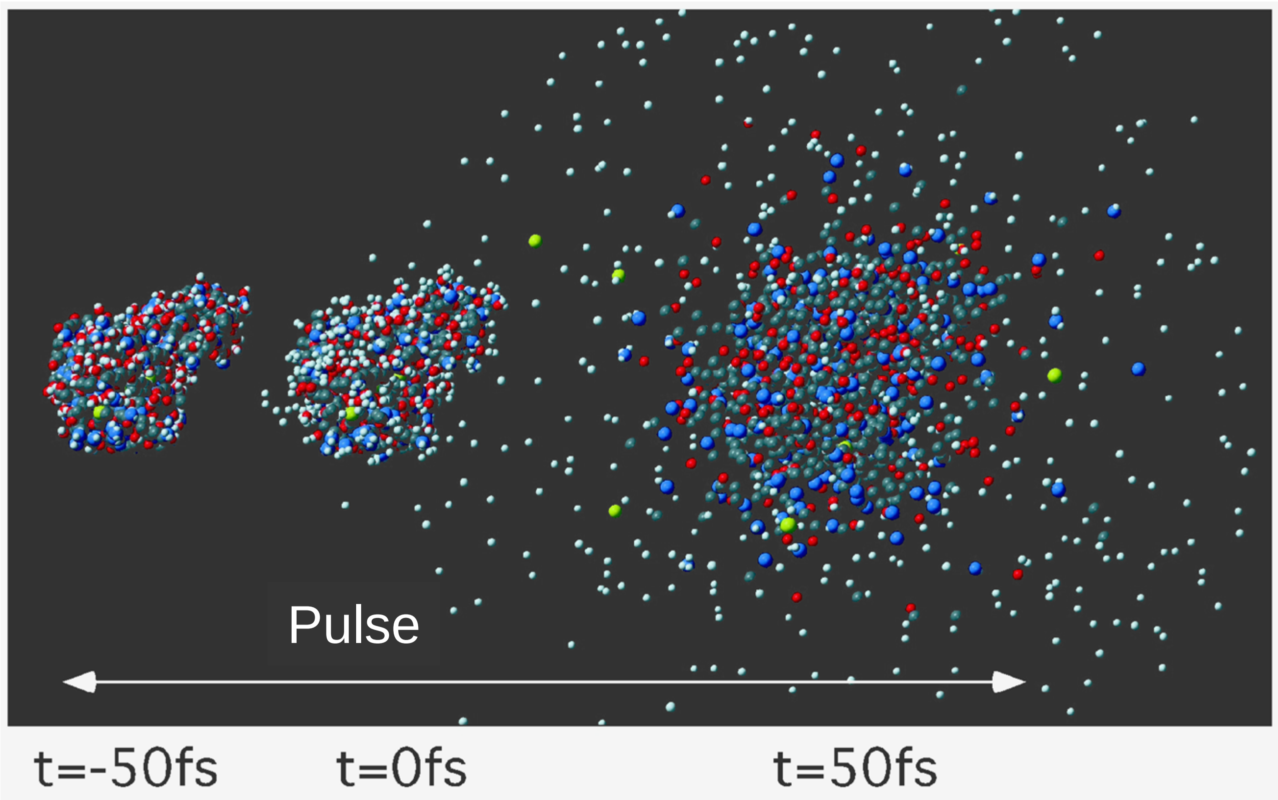


calculated diffraction image of a single Lysozyme molecule

measured diffraction pattern of a Lysozyme single crystal irradiated with Synchrotron Radiation

J.Hajdu et al.

Obstacle: Coulomb-Explosion



Example:

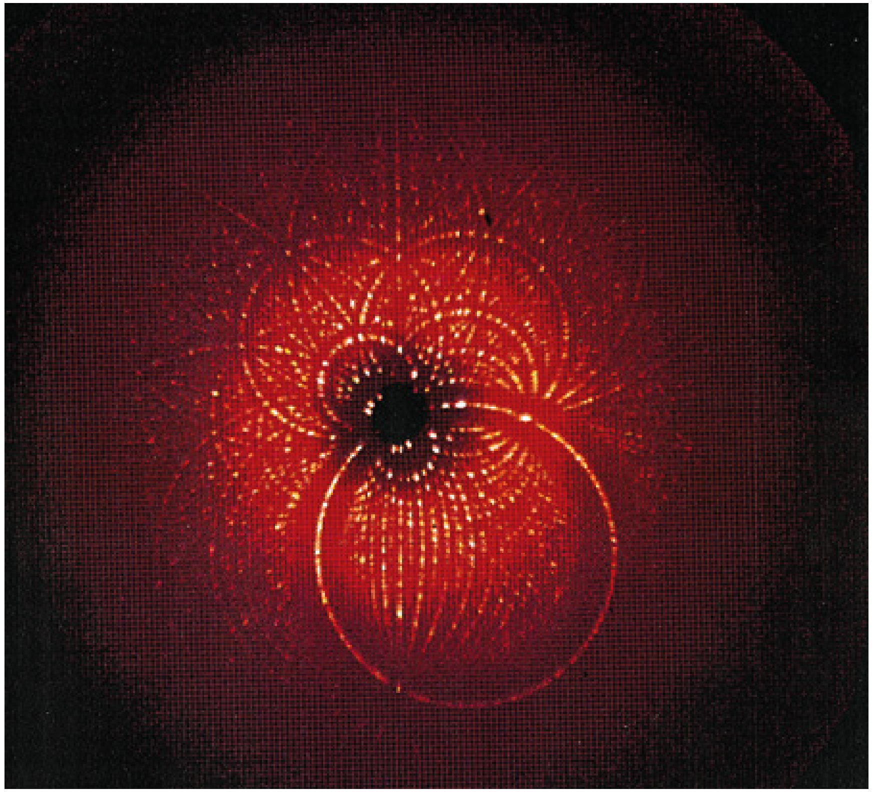
Lysozyme

white: Hydrogen,
grey: Carbon,
blue: Nitrogen,
red: Oxygen,
yellow: Sulfur

R. Neutze et al. Nature 406, 752-757 (2000)

Requirement: Pulse must be short enough and not to intense, to take picture before molecule disintegrates !

Can fast structural changes be measured?



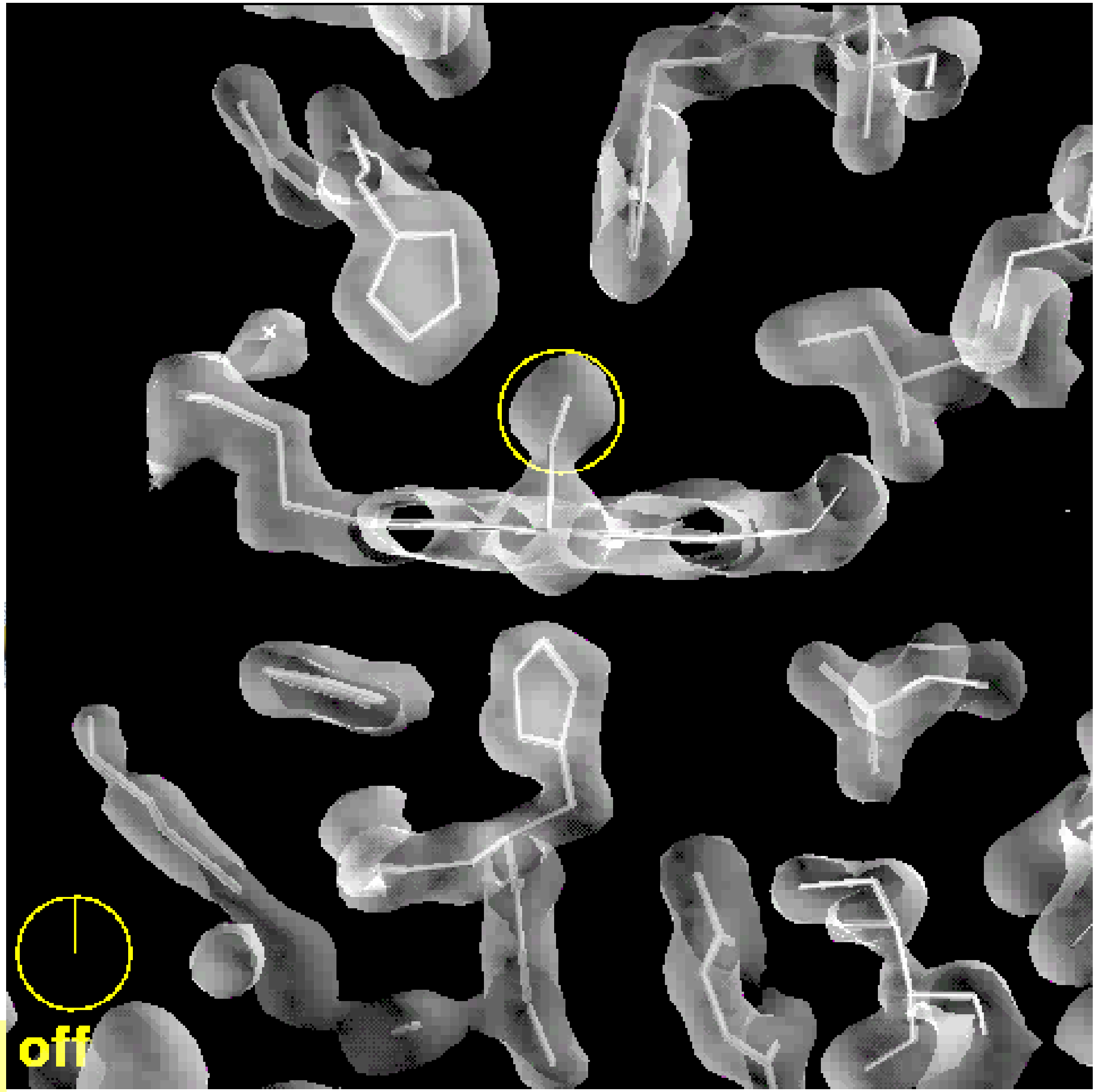
Laue-Diagram of a Myoglobine crystal with a carbon-monoxide ligand (MbCO), recorded with a single Synchrotron Radiation pulse of 150 picoseconds.

Image shows about 2000 reflections (the bright spots)
➔ crystal structure with a resolution of 0.18 nm (~ size of the CO molecule)

ESRF Highlights 1996/1997

➔ with X-ray FELs another 1000x shorter „exposure time“

Movie of CO detachment from Myoglobine



F. Schotte et al., Science 300, 1944 (2003)

Contents

Free Electron Lasers: principles and properties

- **FEL vs. conventional laser**
- **From synchrotron radiation towards FELs**
- **SASE (self amplified spontaneous emission)**

FEL vs. conventional Laser

Laser:

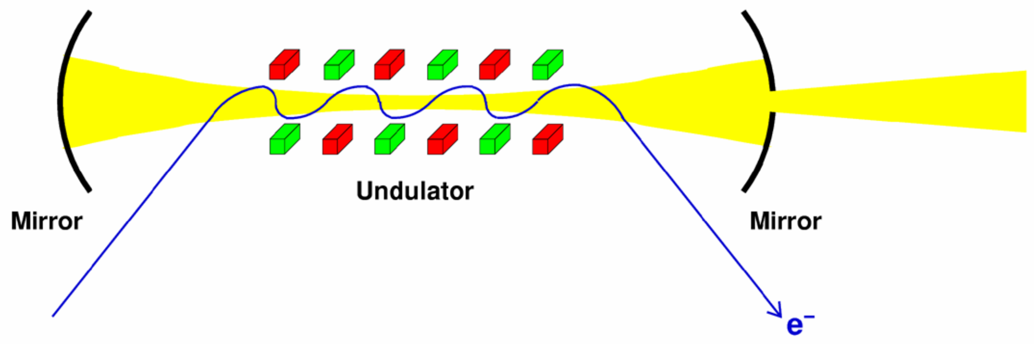
amplification due to stimulated emission of electrons bound to atoms (crystal, liquid dye, gas)

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

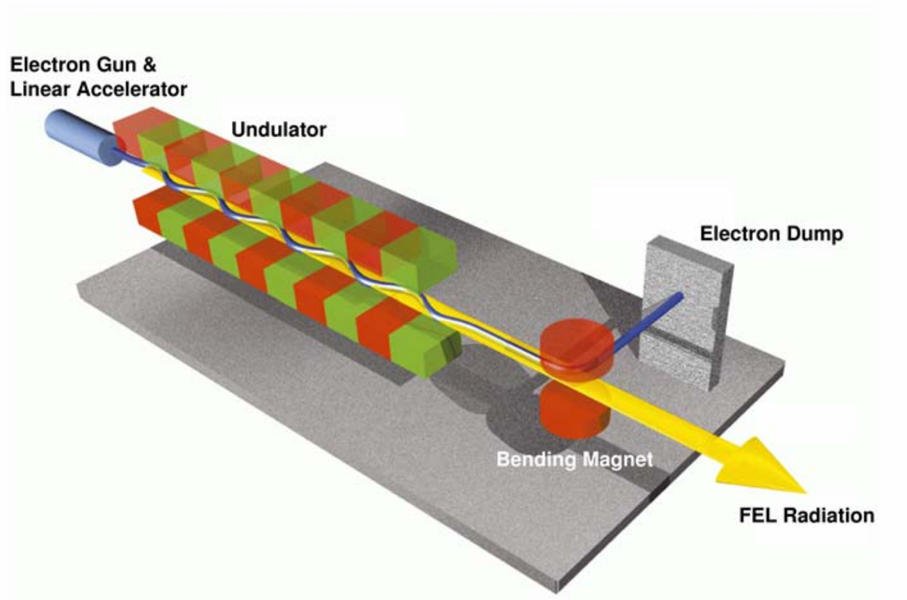
FEL was conceived by John Madey in his Ph.D. thesis, Stanford 1970:
J.M.J. Madey, J. Appl. Phys. 42, 1906 (1971)
First realization: D.A.G. Deacon, L.R. Elias, J.M.J. Madey, G.J. Ramian, H.A. Schwettman, T.I. Smith, Phys. Rev. Lett. 38, 892 (1977)

Most of todays FELs are operating in the mm and μm wavelength range using optical resonators

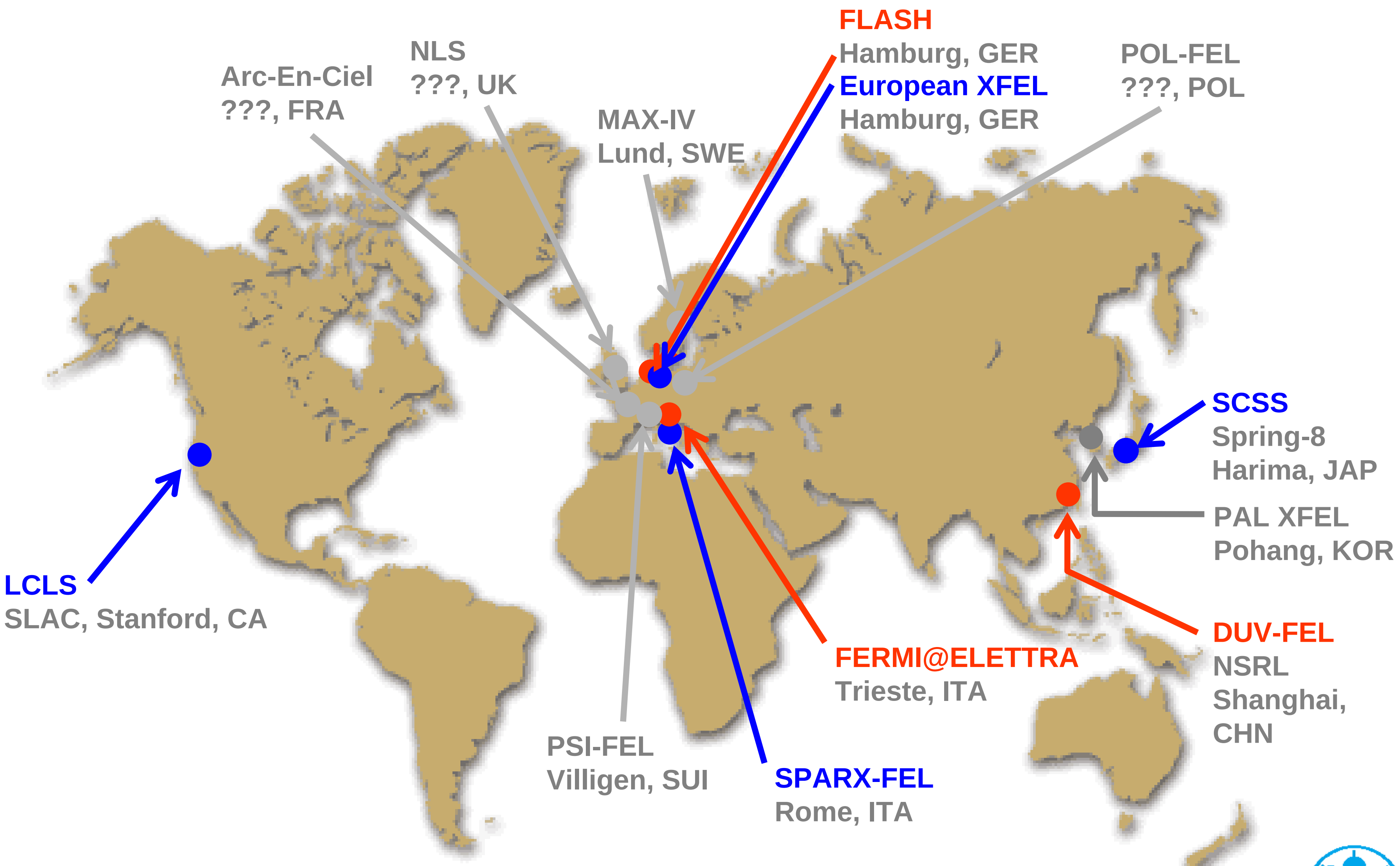


optical resonators are not usable for λ < 150 nm (low mirror reflectivities & possible damage)

below:
“single pass” SASE FELs



XUV & X-ray FEL Facilities and Projects



Courtesy: T.Tschentscher

From synchrotron radiation towards SASE FELs

3rd generation synchrotron radiation source

(spontaneous undulator radiation)

+ 10^8 x more peak brilliance

+ short pulses (≈100fs vs. 100ps)

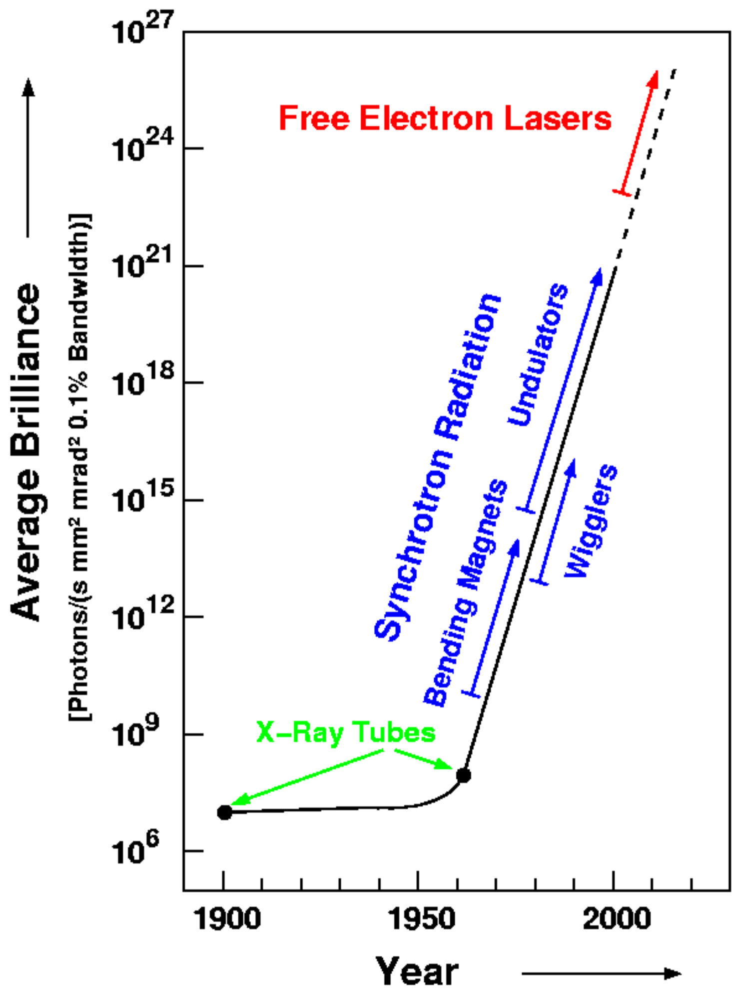
+ full transverse coherence

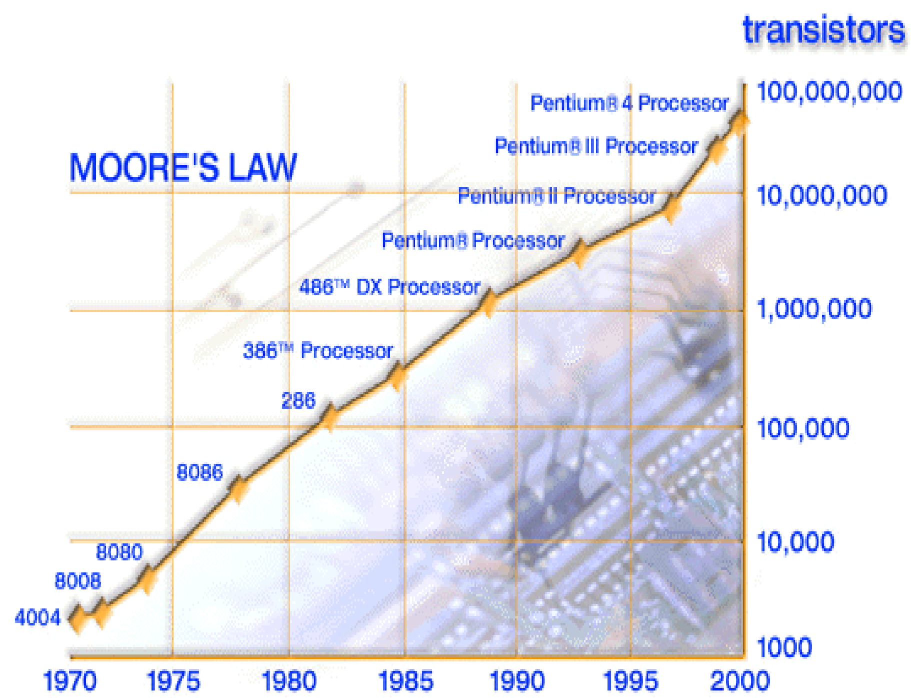
+ partial temporal coherence

(full temp. coherence with "seeding")

= Free Electron Laser (4th generation light source)

For comparison

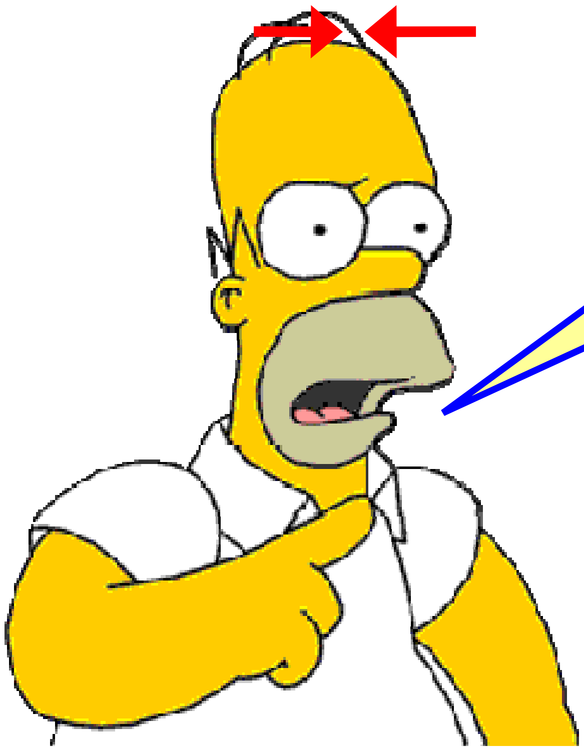




(http://www.intel.com/research/silicon/mooreslaw.htm)

10.000 x more "light" per decade since 1965

about 30 x more transistors per CPU per decade since 1970



100 fs (femtoseconds) correspond to a distance of 30 µm at the speed of light (≈ 300.000 km/s), i.e. the width of a hair!!

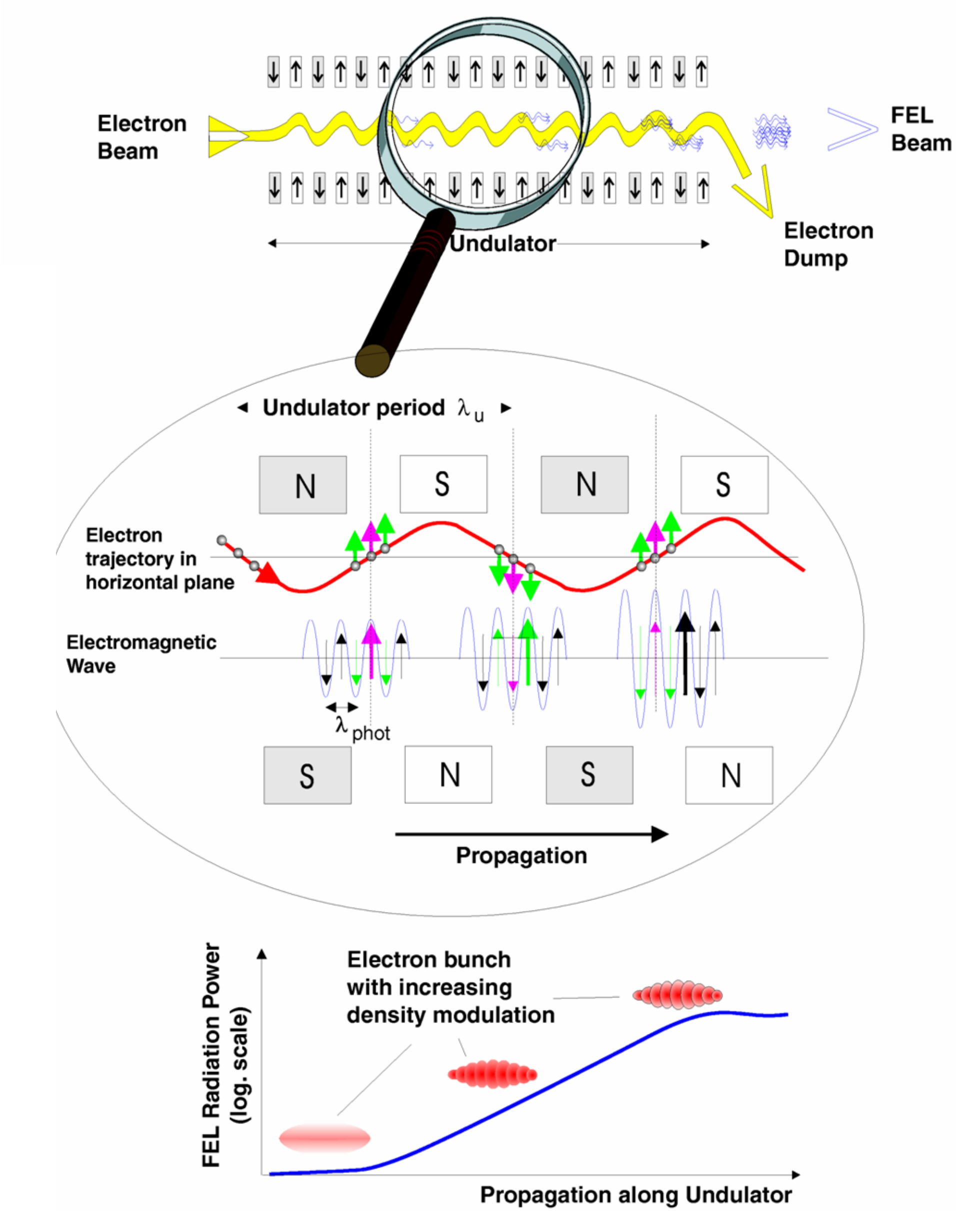
SASE (self-amplified spontaneous emission)

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")**

→ **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)**



(Just) some formulas …

$$\lambda_{\mathrm{phot}} = \frac{\lambda_{\mathrm{u}}}{2\gamma^2}\left(1 + \mathrm{K}_{\mathrm{rms}}^2\right)$$

Undulator resonance condition

(slippage between electrons and photons is λ_{phot} per undulator period for constructive interference)

$$\mathrm{K}_{\mathrm{rms}} = \frac{\mathrm{K}}{\sqrt{2}} = \frac{\mathrm{e}\,\mathrm{B}_{\mathrm{rms}}\,\lambda_{\mathrm{u}}}{2\,\pi\,\mathrm{m}_{\mathrm{e}}\mathrm{c}}$$

Undulator (K)-Parameter

(describes deflection of electrons in magnetic field with respect to opening angle of radiation cone)

Electron energy modulation

electrons travel on sinusoidal trajectory :

$$v_x(z) = K\frac{c}{\gamma}\cos(\frac{2\pi}{\lambda_u}z)$$

electromagnetic wave moving parallel with electron beam :

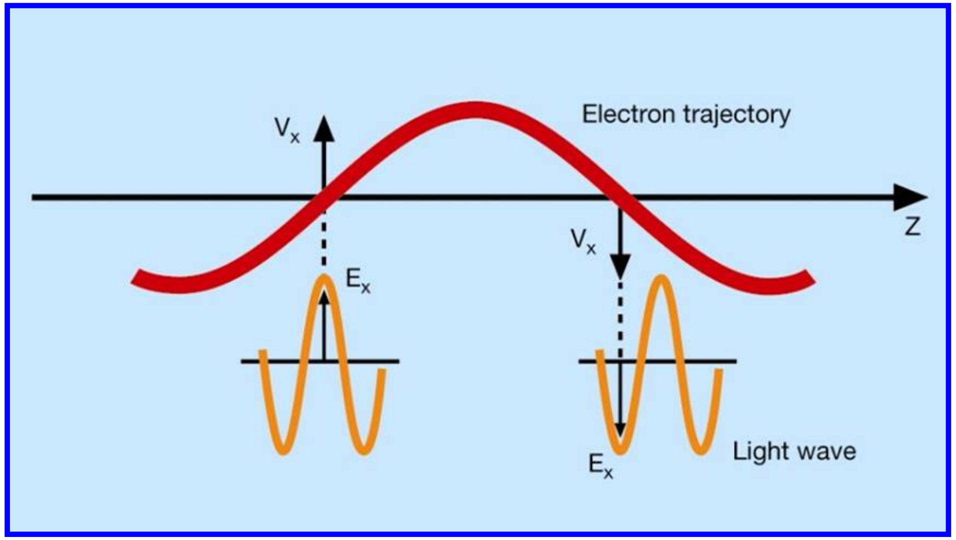
$$E_x(z,t) = E_0\cos(k_L z - \omega_L t)$$

change of electron energy due to electromagnetic field :

$$\frac{dW}{dz} = \frac{q}{v_z}\vec{v}\vec{E} = \frac{qE_0K}{\gamma\beta_z}\sin\Psi$$

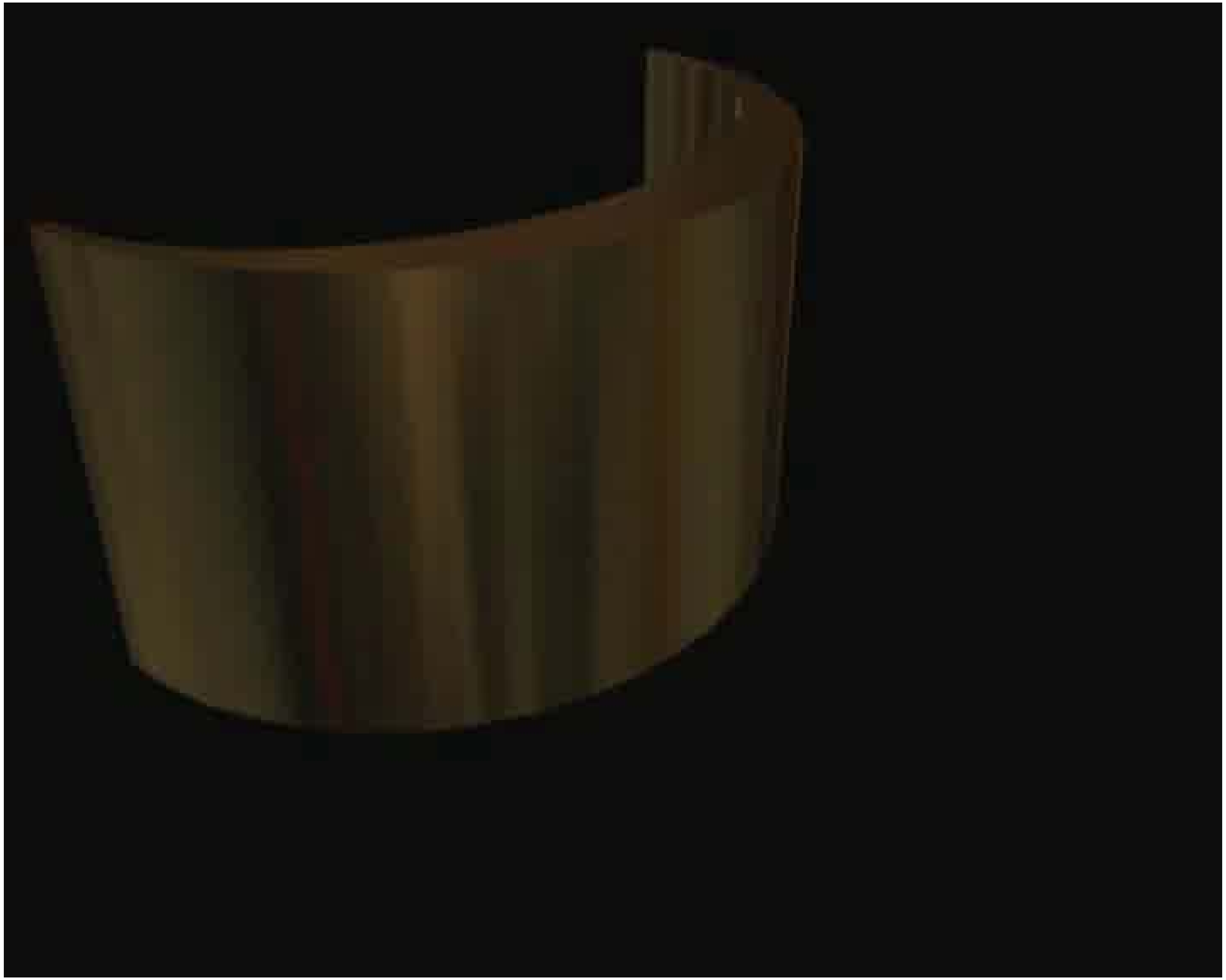
with the ponderomotive phase :

$$\Psi = (k_u + k_L)z - \omega_L t + \phi_0$$



for continuous energy transfer (constant phase Ψ)
➔ undulator resonance condition

SASE movie



Requirements for SASE

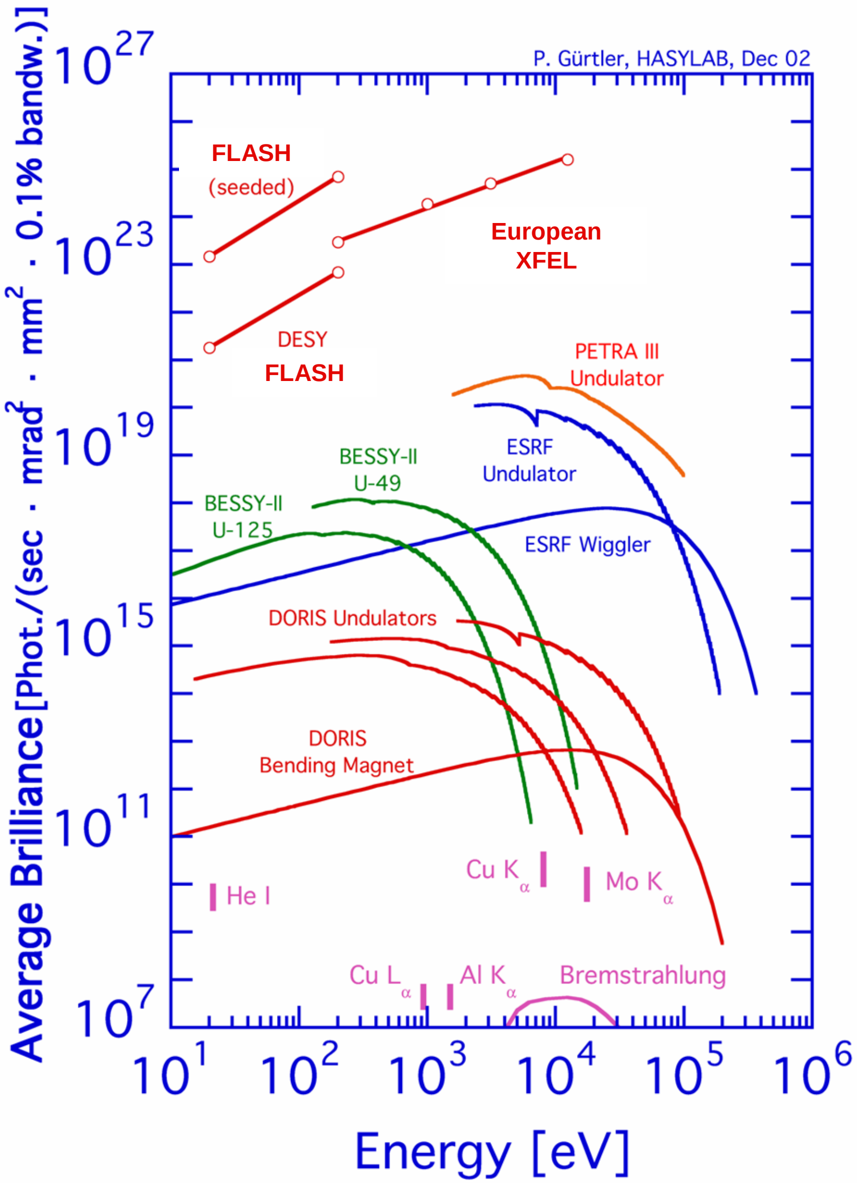
Good electron beam quality and sufficient overlap between e-beam and radiation pulse along the undulator, i.e.

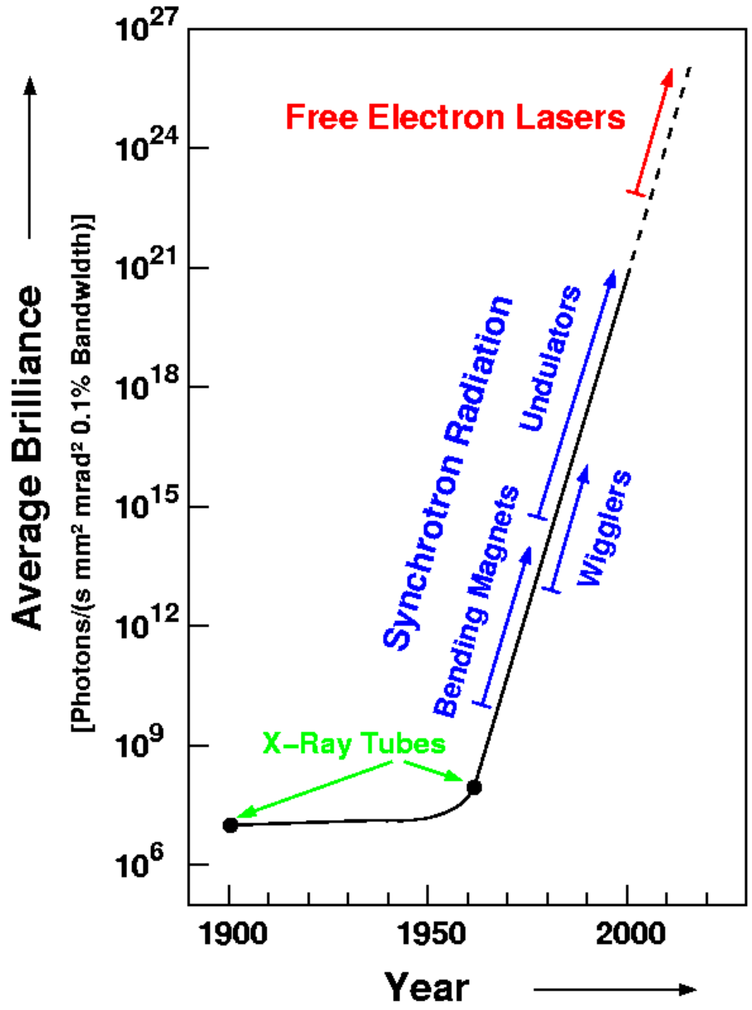
- **low emittance, low energy spread electron beam**
- **extremely high charge density (kA peak currents)**
- **precise magnetic field of undulator**
- **accurate beam steering through undulator (few µm precision)**

SASE FEL properties

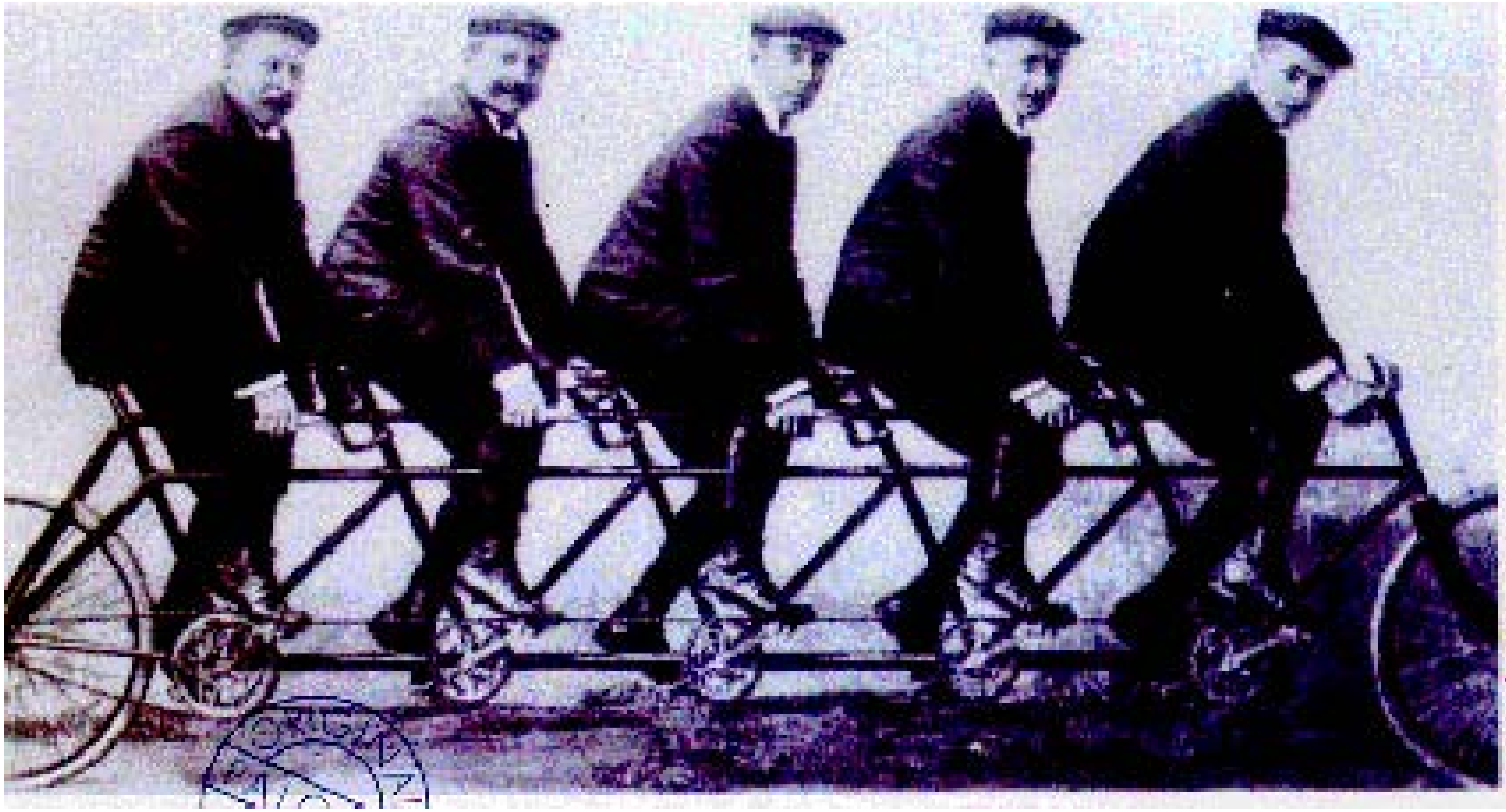
- **high intensity (GW peak power)**
- **coherence**
- **femtosecond pulses**
- **narrow bandwidth**
- **wavelength tunability !**
- **down to X-rays !**

Average brilliance of different sources





All you need is coherence !



Recommended reading on FELs

Basic papers ...	R.M. Philips, IRE Trans. Electron Devices **7**, 231 (1960)
	J.M.J. Madey, *Stimulated emission of bremsstrahlung in a periodic magnetic field*, J. Appl. Phys. **42**, 1906 (1971)
	D.A.G. Deacon, L.R. Elias, J.M.J. Madey, G.J. Ramian, H.A. Schwettman, T.I. Smith, *First Operation of a Free-Electron Laser*, Phys. Rev. Lett. **38**, 892 (1977)
	A.M. Kondratenko, E.L. Saldin, *Generation of coherent radiation by a relativistic electron beam in an ondulator*, Part. Acc. **10**, 207 (1980)
	R. Bonifacio, C. Pellegrini, L. Narducci, *Collective instabilities and high-gain regime in a free electron laser*, Opt. Commun. **50**, 373 (1984)
	S. Krinsky, L.H. Yu, *Output power in guided modes for amplified spontaneous emission in a single-pass free-electron laser*, Phys. Rev. A**35**, 3406 (1987)
	Kwang-Je Kim, *An analysis of self-amplified spontaneous emission*, Nucl. Instr. and Meth. A **250**, 396 (1986)
... and books :	T.C. Marshall, *Free Electron Lasers*, MacMillan, New York, NY (1985)
	A. Yariv, *Quantum Electronics* (3rd edition), J. Wiley&Sons, New York (1989)
	P. Luchini and H. Motz, *Undulators and Free-Electron Lasers*, Oxford Science publications, Oxford (1990)
	W.B. Colson, C. Pellegrini, A. Renieri (eds.), *Laser Handbook*, Vol. 6, North-Holland (1990)
	G. Dattoli, A. Renieri, A. Torre (eds.), *Lectures on the free electron laser theory and related topics*, World Scientific, London (1993)
	H.P. Freund and T.M. Antonsen Jr., *Principles of free-electron lasers*, Chapman and Hall, London, UK (1996)
	E.L. Saldin, E.A. Schneidmiller, M. Yurkov, *The Physics of Free Electron Lasers*, Springer, Berlin-Heidelberg (2000)

http://hasylab.desy.de/facilities/flash/publications/selected_publications/index_eng.html

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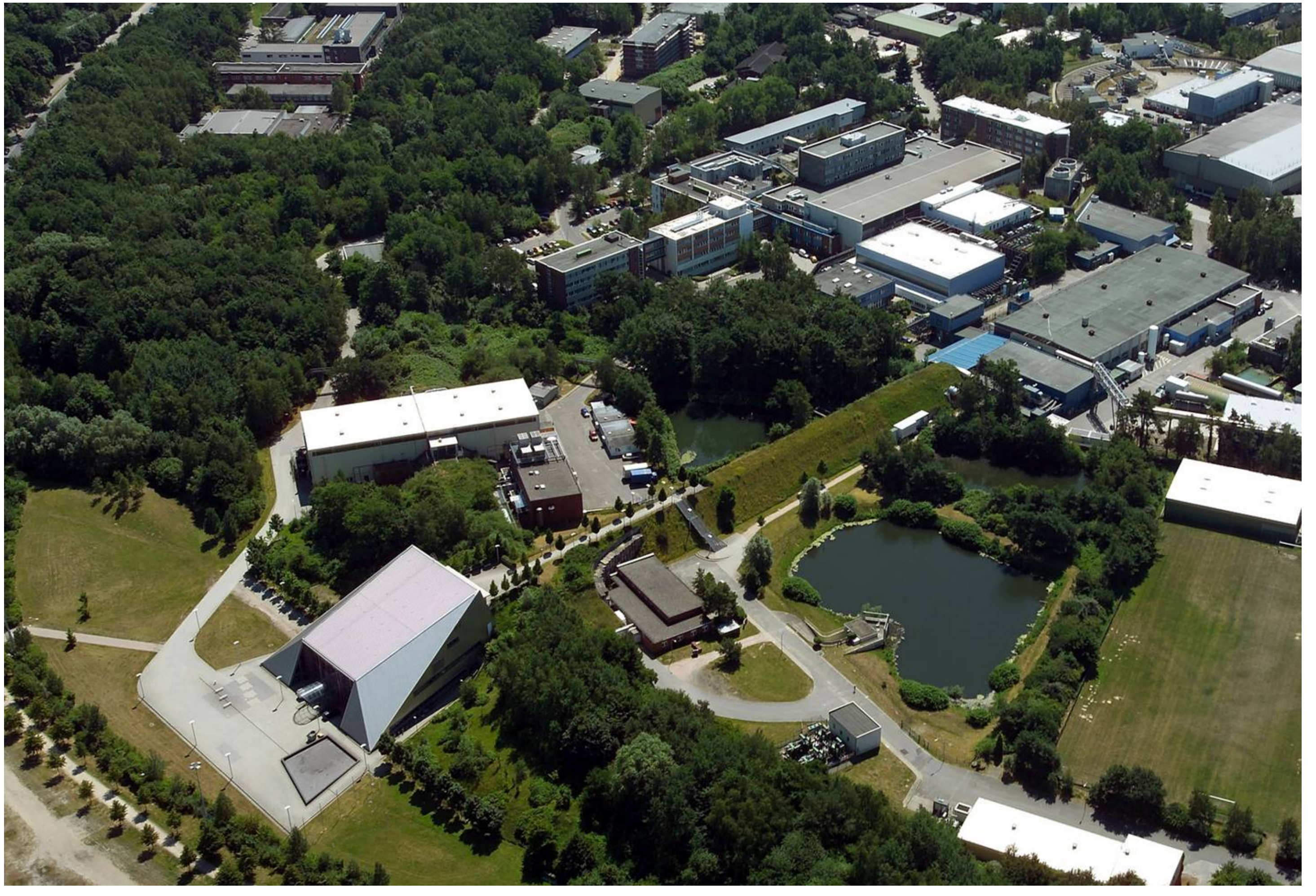
FLASH at DESY



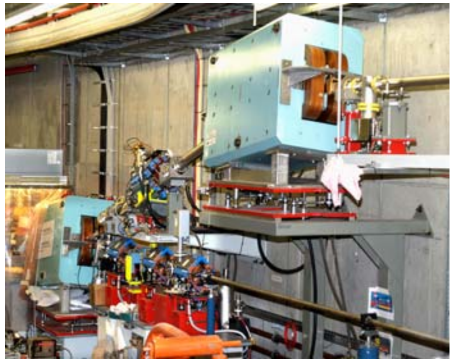
Setup before upgrade shutdown 2009/2010

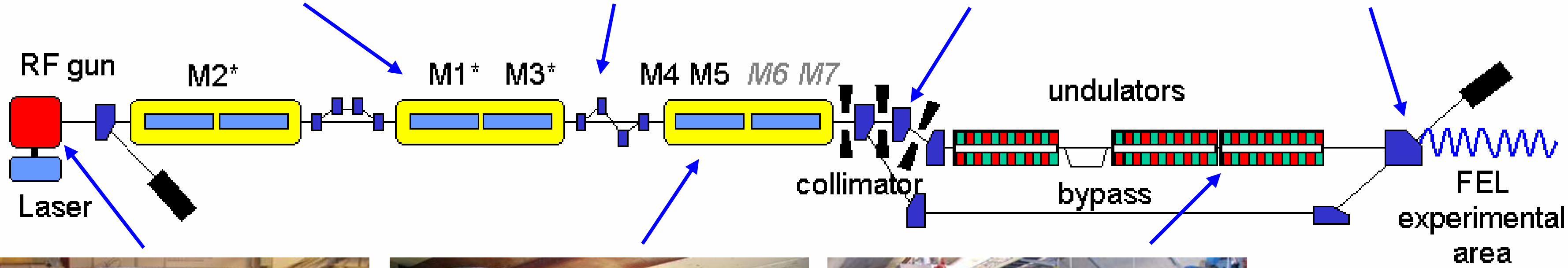
Installation of modules into the accelerator

Bunch compressor

Collimator area

Deflection of electrons downwards into the dump

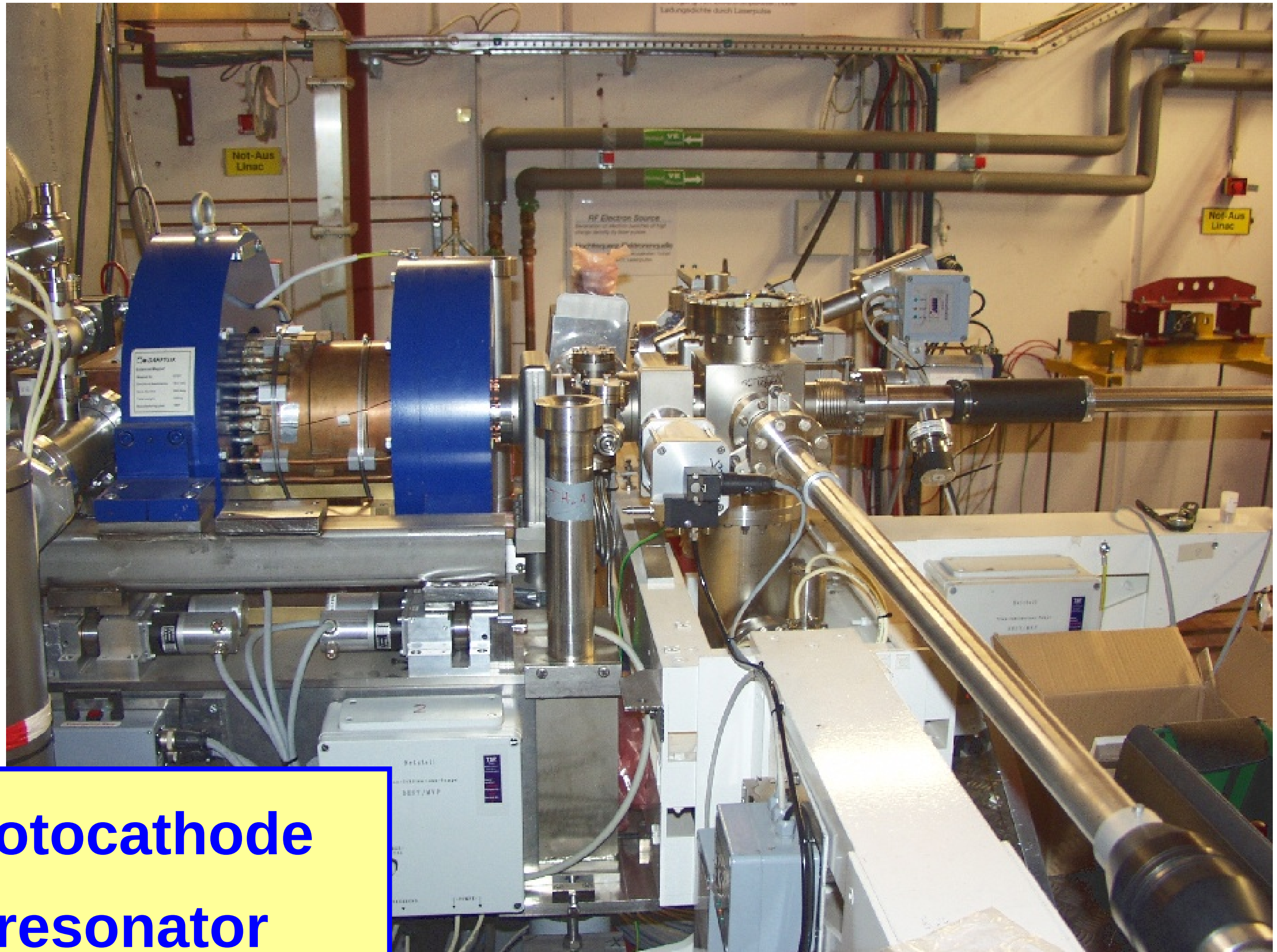




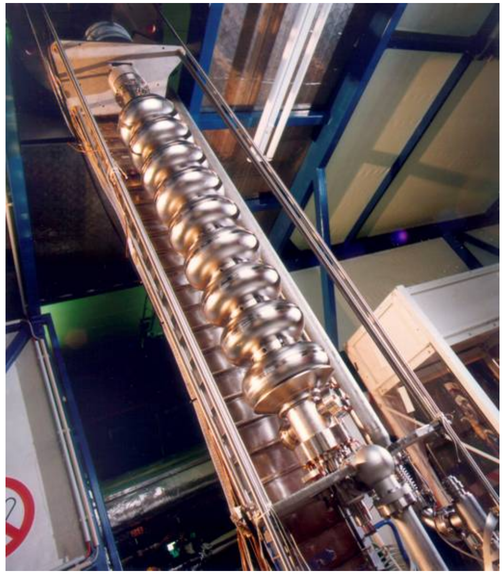
RF electron gun

Module #5

Undulator assembly



$CsTe_2$ photocathode
in 11/2 - cell resonator
1-3% quantum efficiency



Accelerator module with

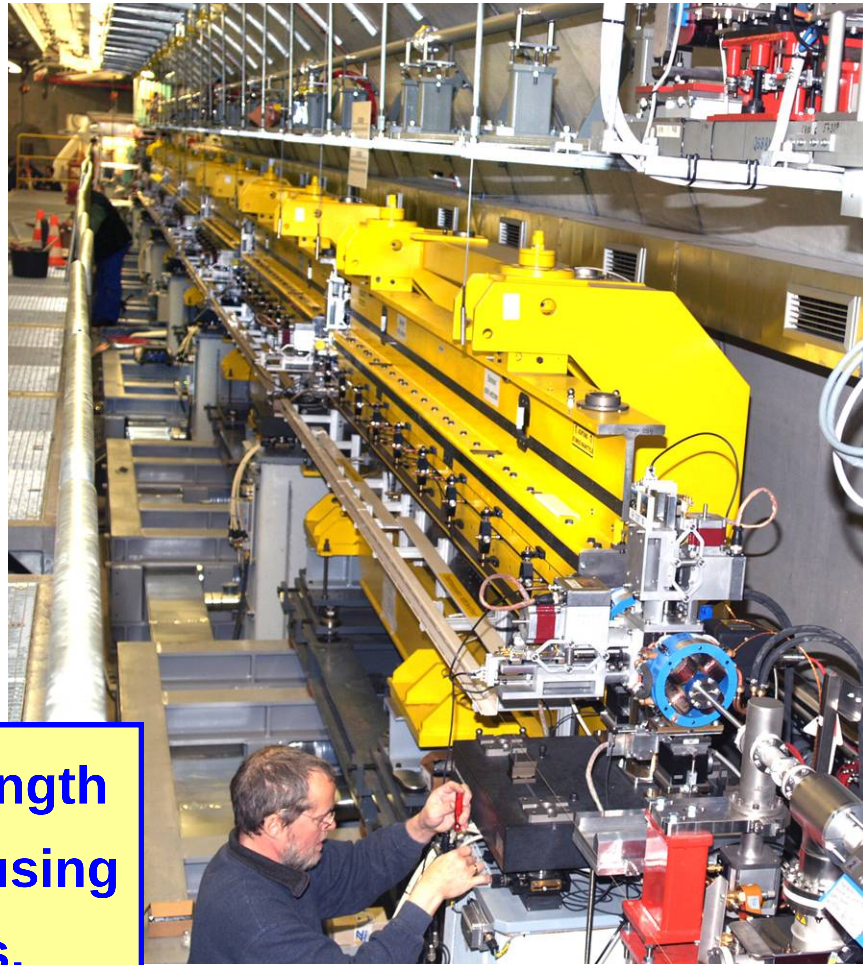
superconducting niobium cavities

25 MV/m routinely

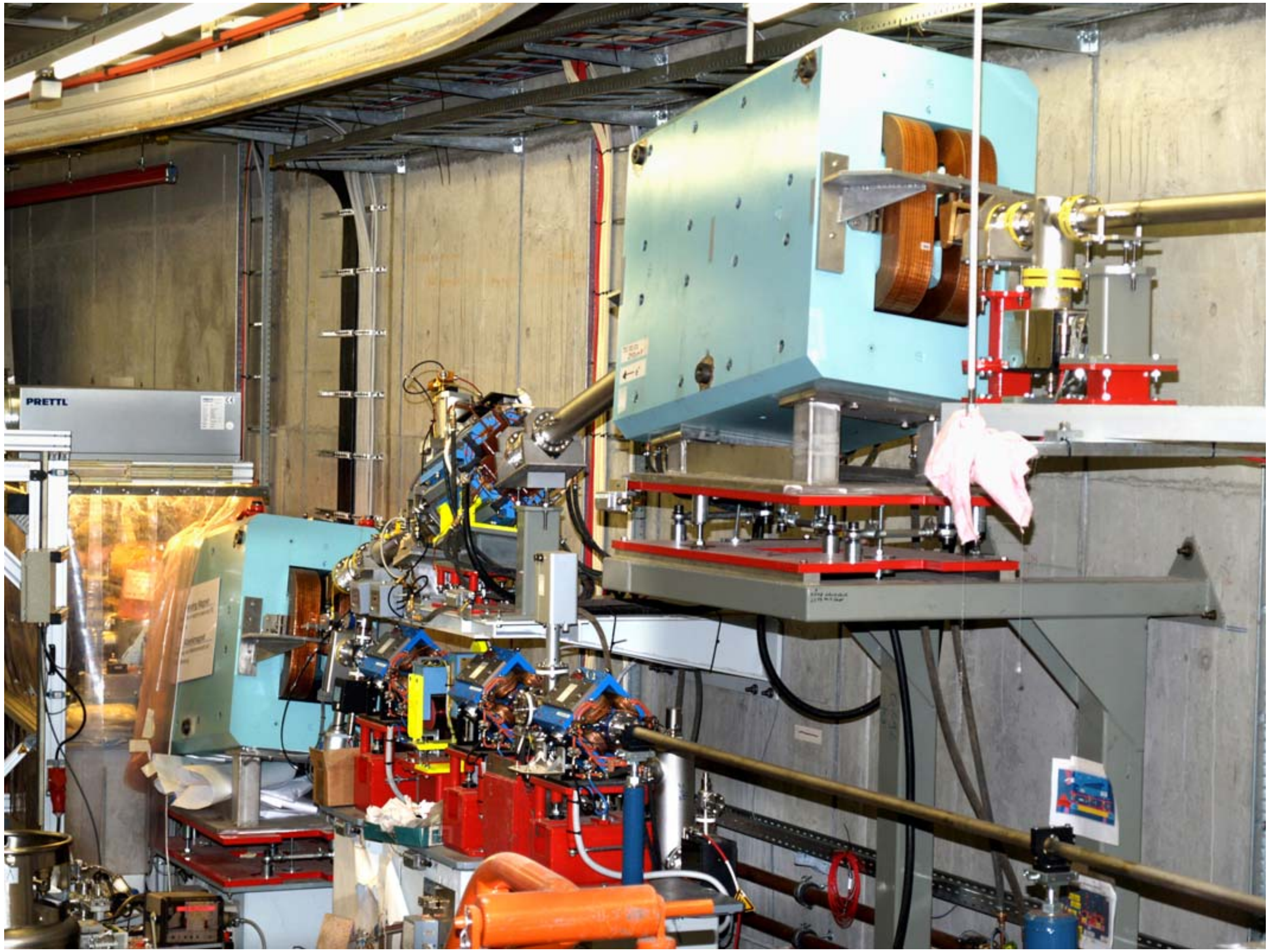
Length: 12 m

Weight: about 10 tons!

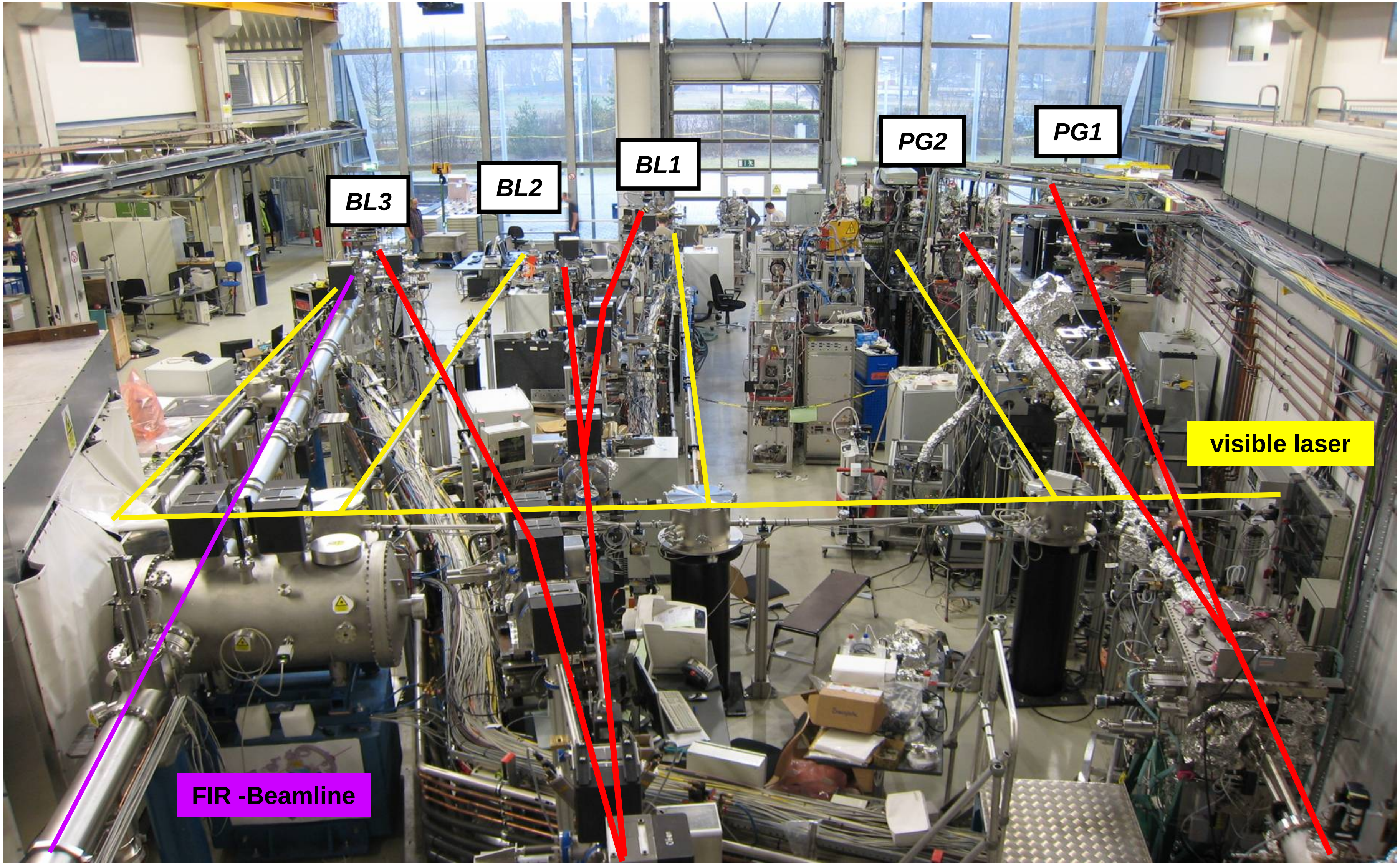
electromagnetic chicane
(4 dipole magnets) for
longitudinal compression
of electron bunches
(~1mm → 0.1mm)



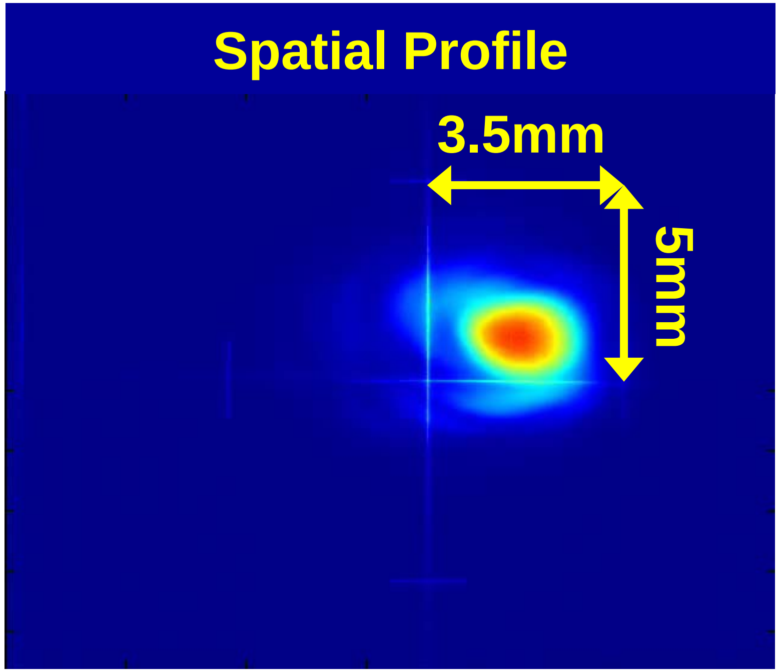
Fixed gap undulator, 30 m total length
with quadrupole doublets for focusing
the electron beam in intersections,
electron beam diagnostics
and steerer coils

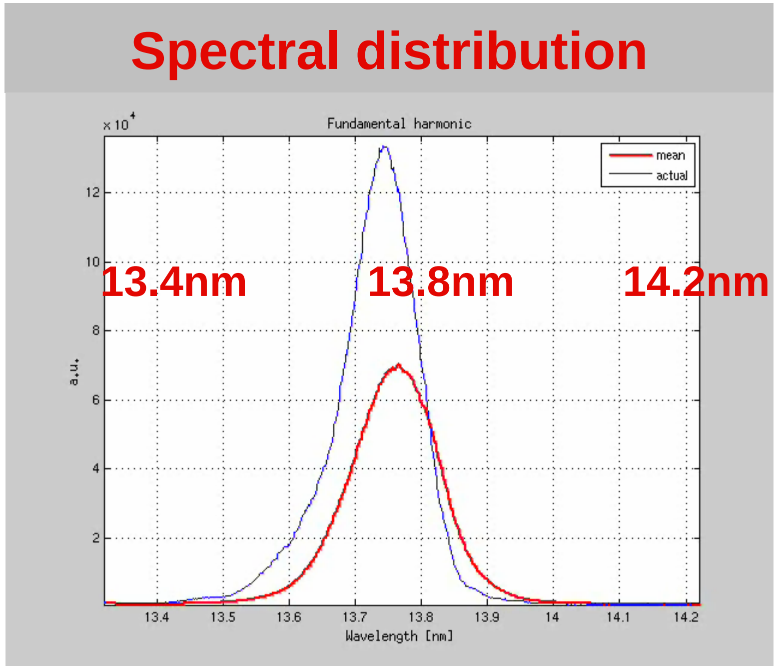

PRETTL

FLASH experimental hall



FLASH performance





Current parameters of FLASH

Wavelength range (fundamental):
6.8 - 47 nm

Spectral width (FWHM):
0.7 - 1 %

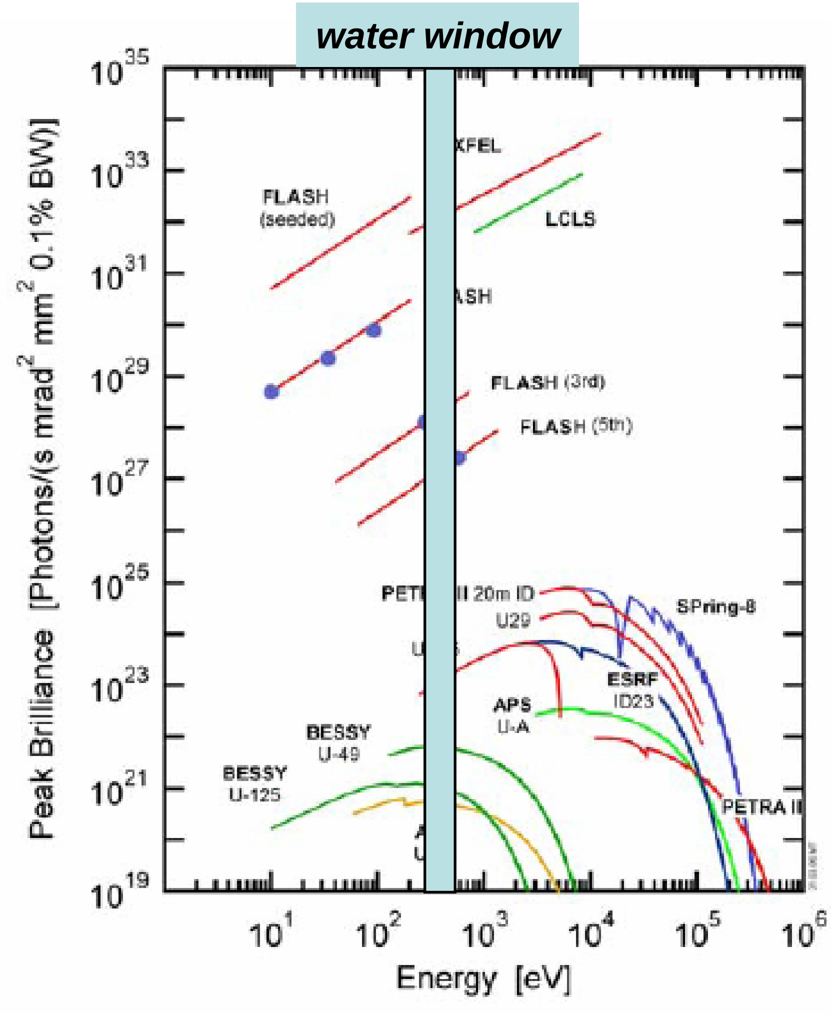
Pulse energy:
up to 100 µJ (average),
200 µJ (peak)

Pulse duration (FWHM):
10 - 70 fs

Peak power (fundamental):
1 - 5 GW

Average power (fundamental):
up to 0.1 W (up to 3000 pulses / sec)

Peak brilliance:
up to 5x10^{29}



peak brilliance

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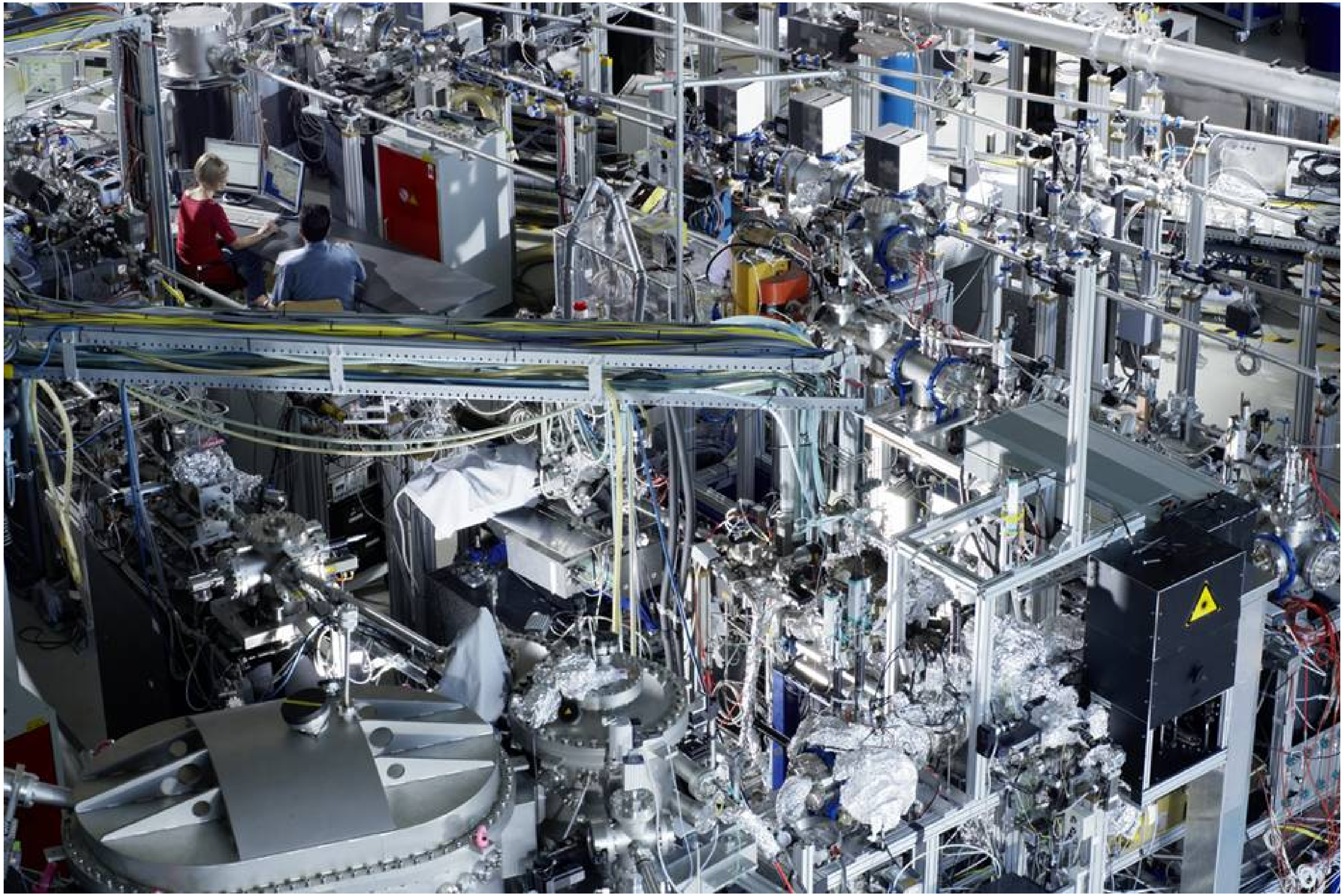
Research Highlights from FLASH



Research Areas

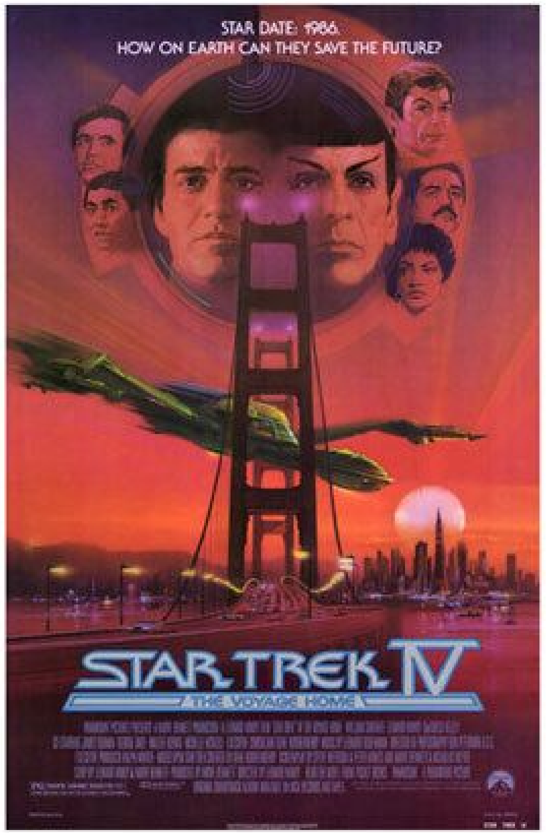
- **Femtosecond time-resolved experiments**
  - synchronization FEL - optical laser
  - pump-probe experiments on atoms and molecules
  - sum-frequency generation
- **Interaction of ultra-intense XUV pulses with matter**
  - multiphoton excitation of atoms, molecules, clusters…
  - creation and characterizaton of dense plasmas
  - imaging of nano-objects and biological samples
- **Investigation of extremely dilute samples**
  - photodissociation of molecular ions
  - highly charged ions
  - mass selected clusters
- **Investigation of surfaces and solids**
  - XUV laser desorption
  - surface dynamics
  - luminescence under FEL radiation
  - meV-resolution photon and photoelectron spectroscopy of surfaces and solids with nm resolution

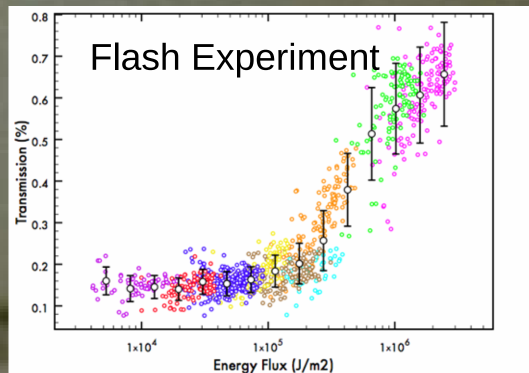
Science at FLASH : examples

- FLASH creates transparent aluminium (B. Nagler et al.)
- Pump-probe experiment on CO_2 alignment (M. Vrakkking et al.)
- Single shot diffraction imaging (H. Chapman, J. Hajdu et al.)

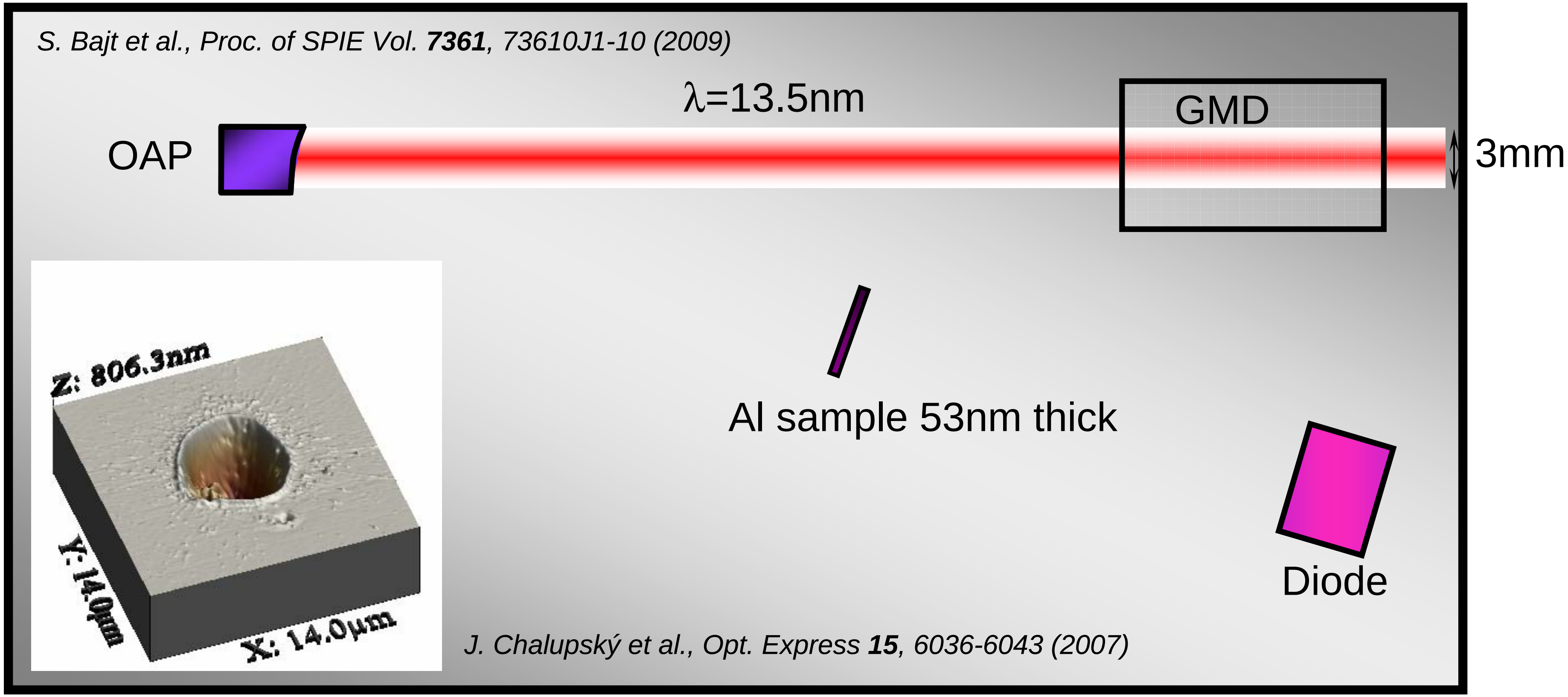
FLASH creates transparent Aluminium
(B.Nagler et al.)

Courtesy: S.Toleikis

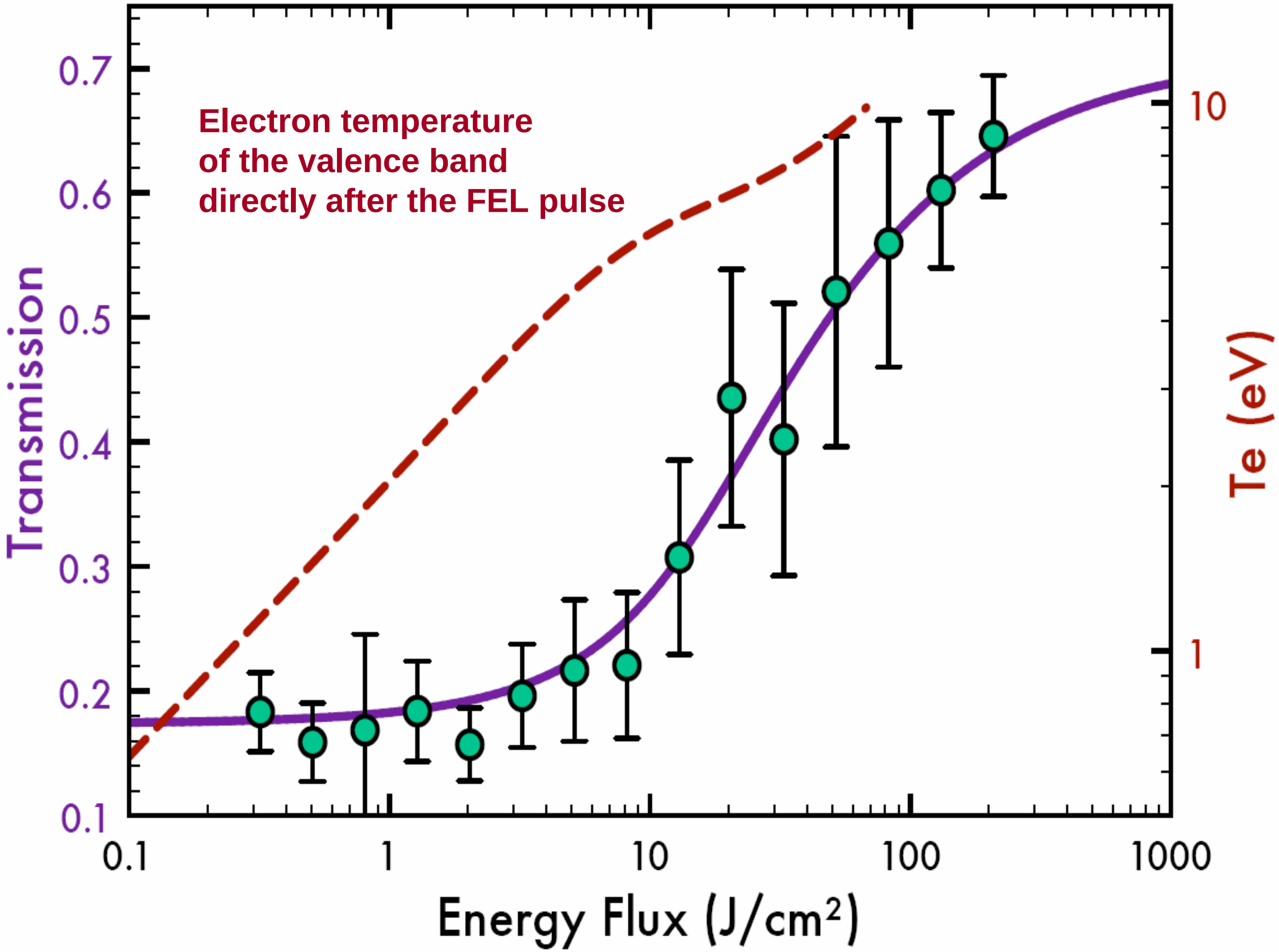




Microfocusing setup



Transmission dependent on power density



- Photoionization of L-shell electrons
- L-shell core hole state
- L-shell shift
- Recombination time: ~50 fs
- Quenching of bound-free absorption

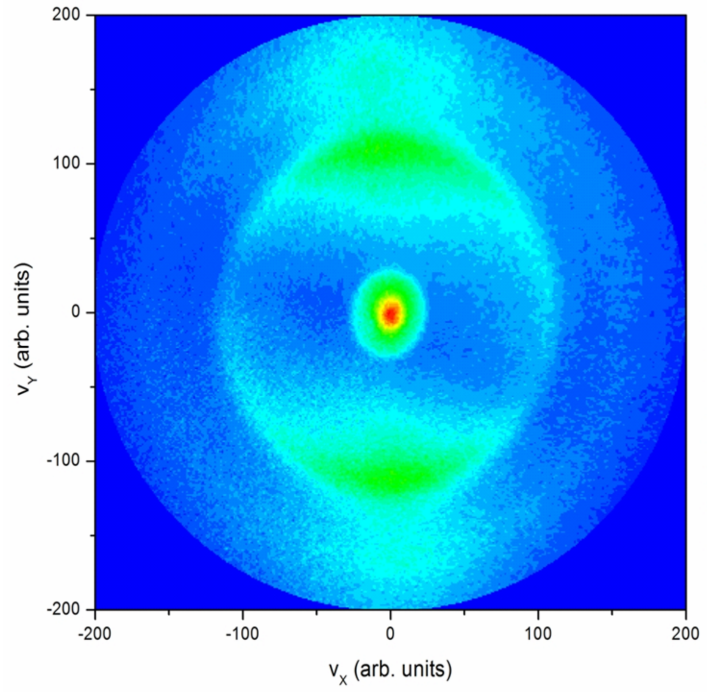
B. Nagler et al., Nature Physics 5, 693-696 (2009)

Drilling "holes" in femtoseconds!

Pump-probe experiment on CO_2 alignment
(M. Vrakkking, P. Johnsson et al.)

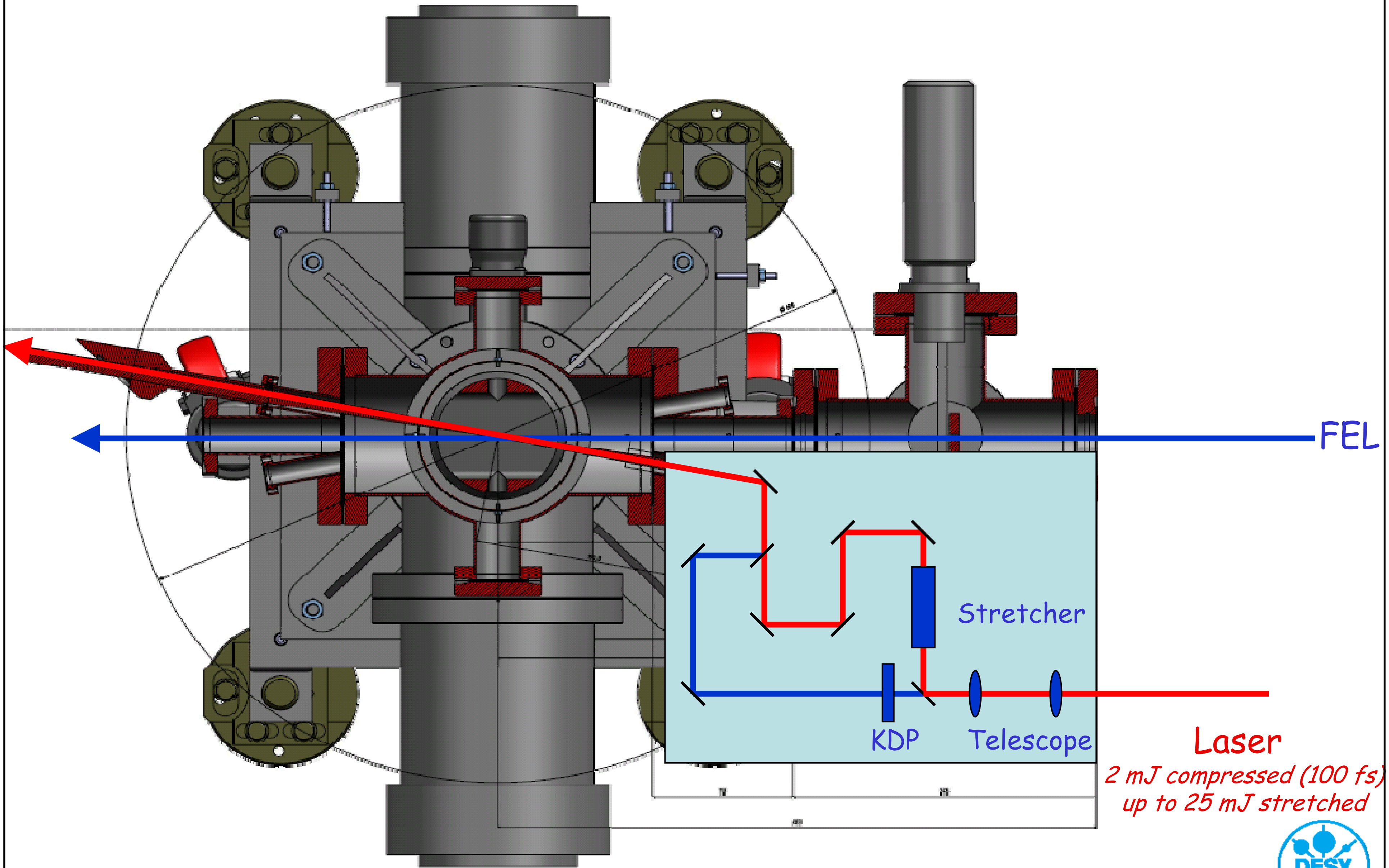
Time-dependent alignment of CO_2

- Use IR to align the molecule
- Use FLASH FEL to dissociatively ionize
- Velocity and angle-resolved detection of O^+
- Step towards molecular frame dynamics (fragmentation, imaging)

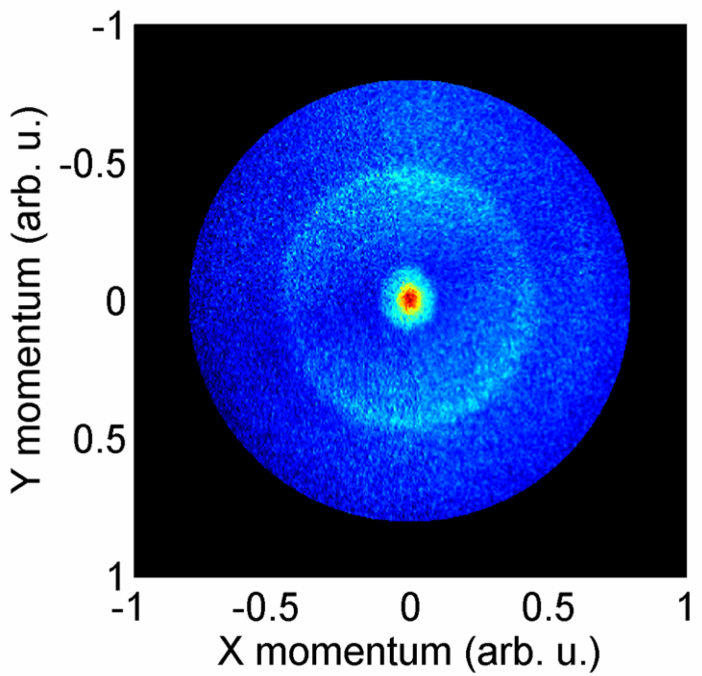


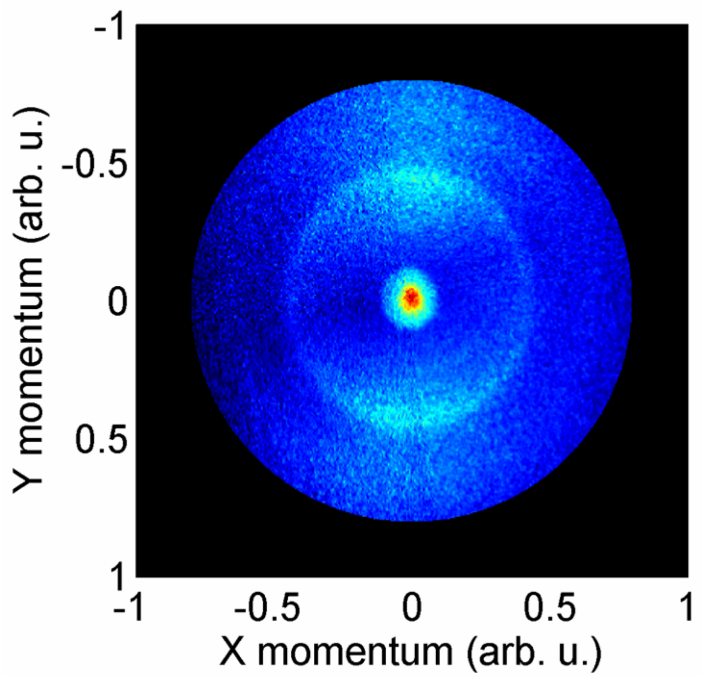
VMIS image
(velocity map imaging spectrometer)

AMOLF VMIS: Pump probe setup



Dissociation of aligned CO2 molecules

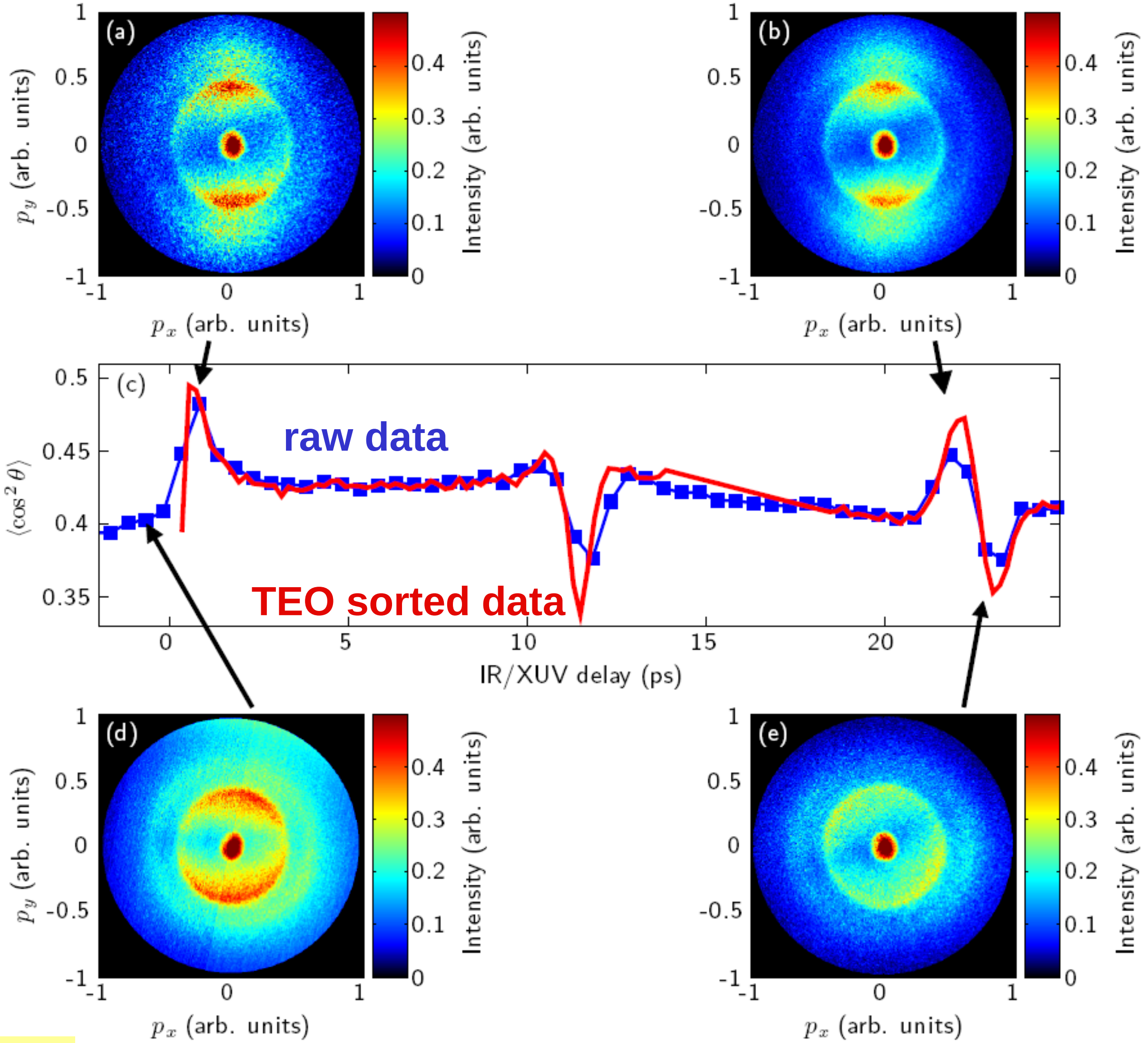




Velocity map image of O^+ ions from dissociating CO_2 molecules, taken before (left) and during (right) alignment of the molecules

(courtesy P. Johnsson, AMOLF, Amsterdam)

Goal:
Studies of ultra-fast dissociation dynamics by observing photoelectron diffraction in the molecular frame.



P. Johnsson et al., J. Phys. B 42, 134017 (2009)

Line up and split up!

Coherent single-shot X-ray diffraction imaging
(H. Chapman, J. Hajdu)

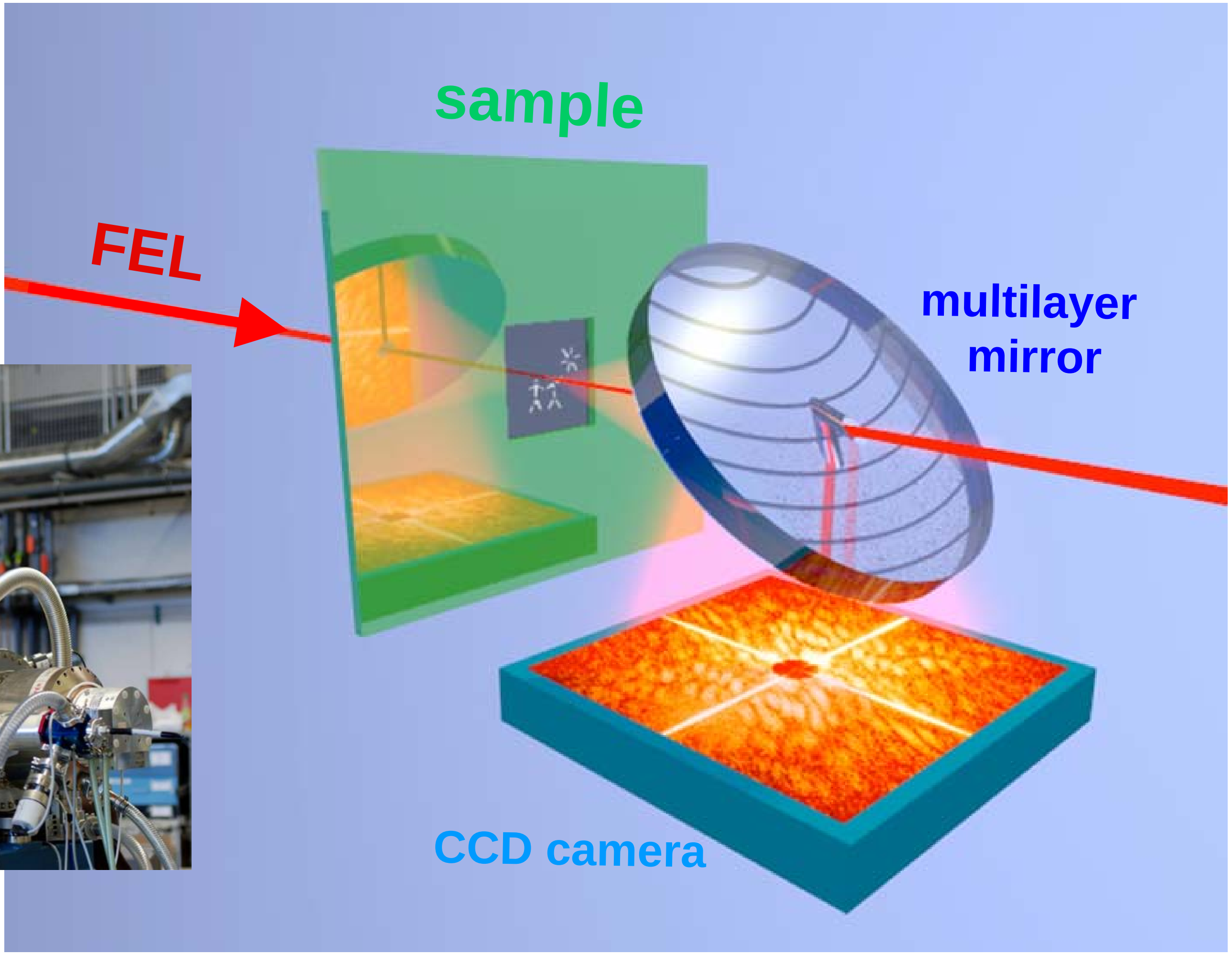
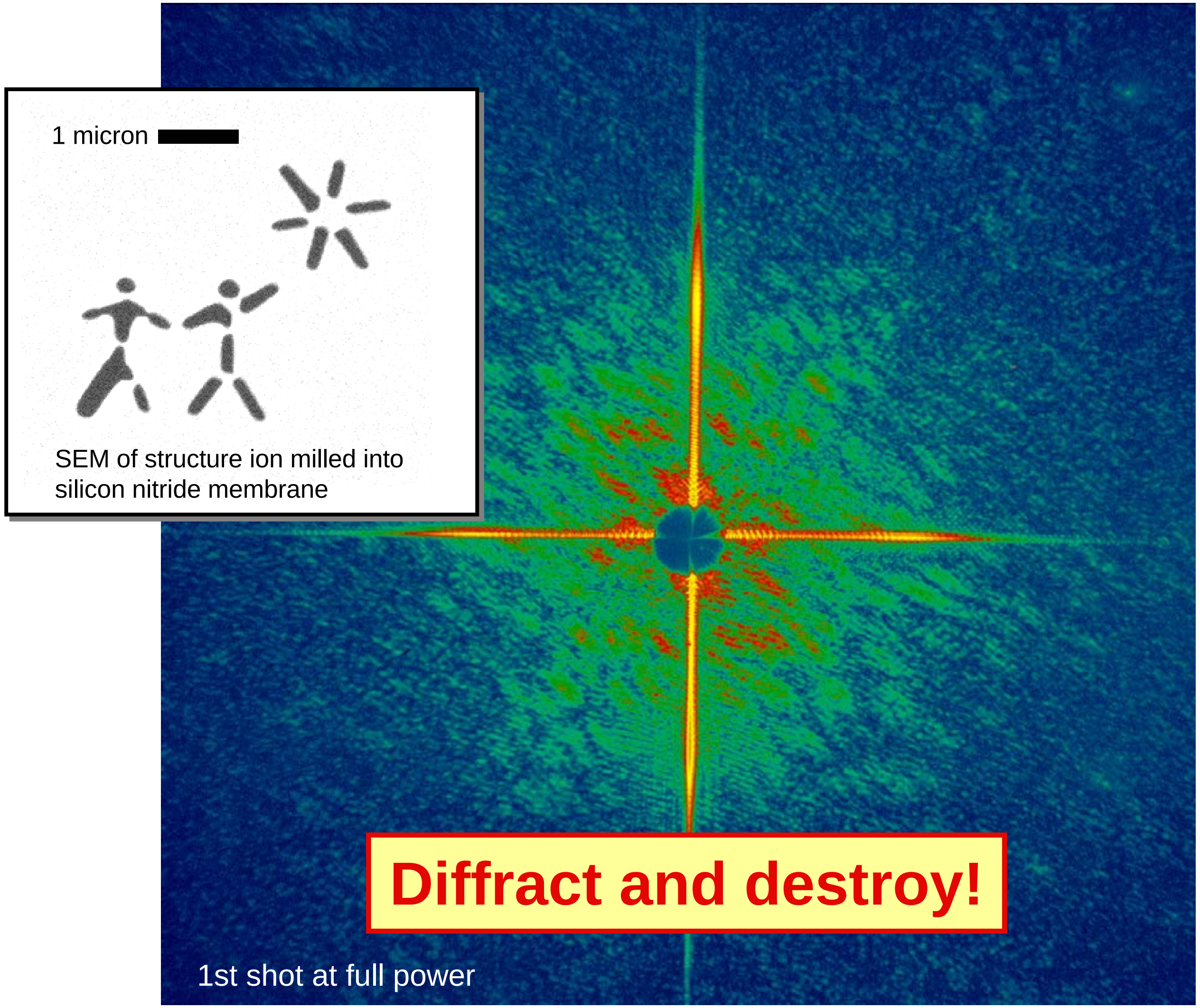
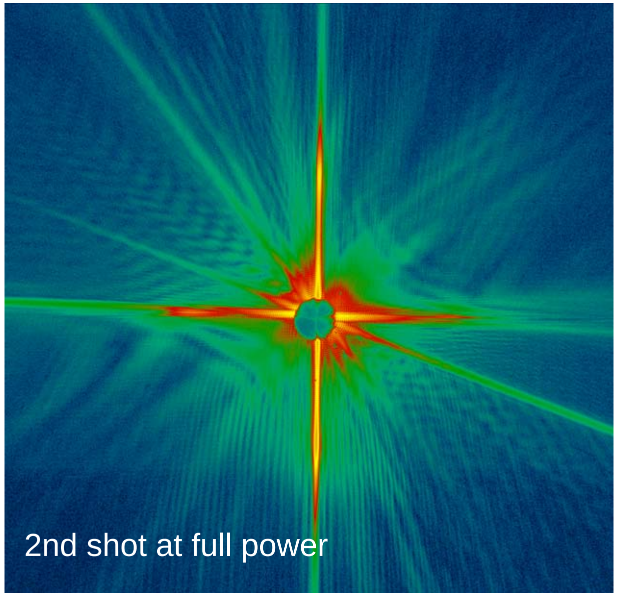
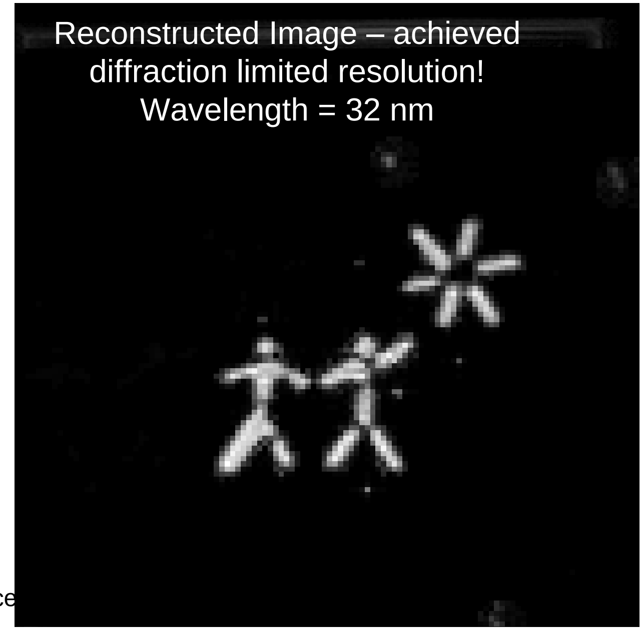


Image reconstruction from ultrafast diffraction pattern







H.N.Chapman et al., Nature Physics 2, 839-843 (2006)

Dynamic X-ray diffraction imaging (pump-probe)

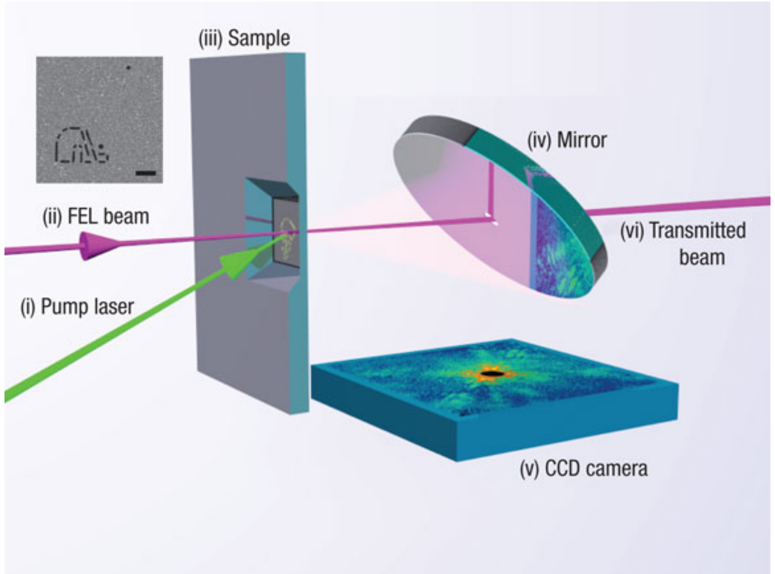
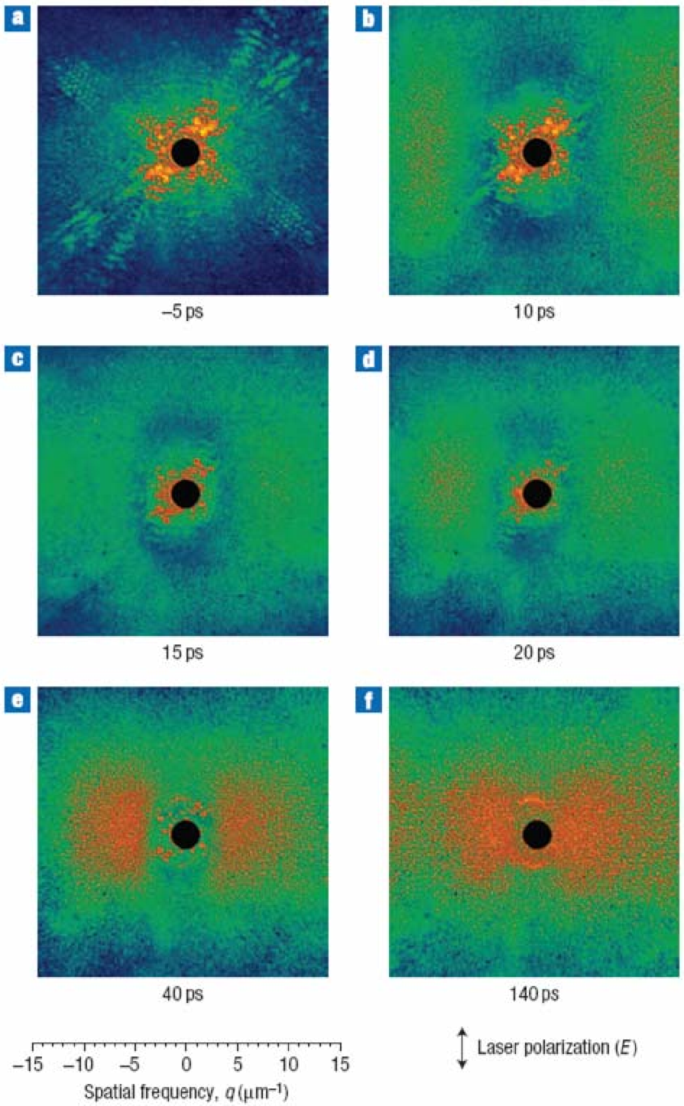
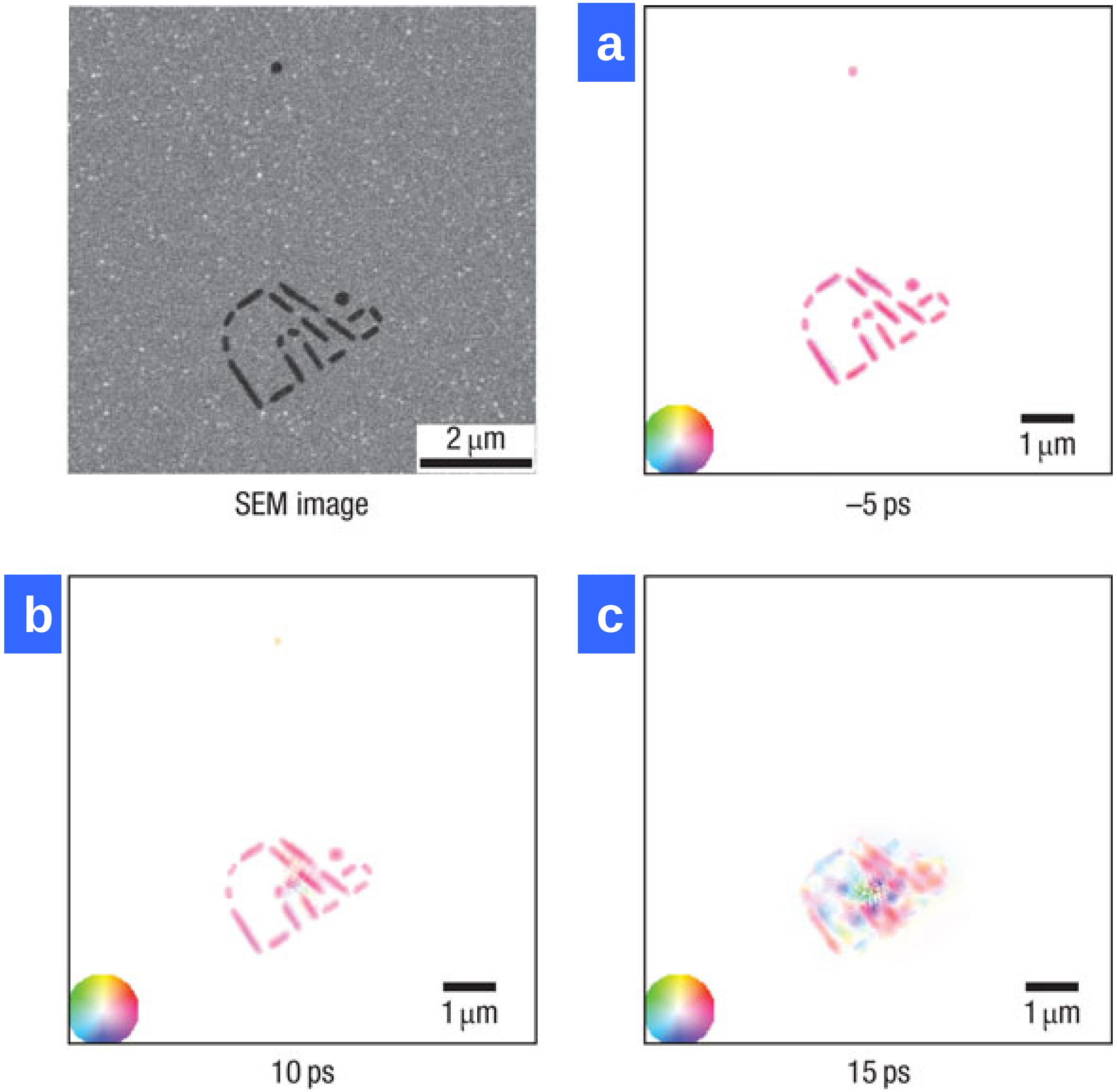


Figure 1 X-ray dynamic diffraction imaging. A visible-light laser beam (i) incident from the left is focused onto the sample (iii) and acts as the excitation pulse. A 10-fs duration soft X-ray pulse at a wavelength of 13.5 nm from the FEL (ii) is focused to a 20-µm spot in the same location as the visible-light laser at a continuously variable delay after the excitation pulse. The X-ray pulse diffracts from the sample, carrying information about the transient sample structure to the CCD detector (v) in the form of a coherent diffraction pattern. A 45° mirror (iv) is used to separate the direct beam from the diffracted light: the direct FEL beam (vi) passes straight through a hole in the mirror and is not detected in the CCD image. A 100-nm-thick zirconium filter over the CCD chip makes the detector blind to the laser excitation pulse. The sample (iii) consisted of a nanometre-resolution pattern etched into a silicon nitride membrane using a focused ion beam (FIB), providing a well-defined control sample so that the time evolution of a known structure could be observed. The path length from sample to CCD is 53 mm and the detected numerical aperture is 0.25, giving a spatial resolution of 27 nm in the sample plane.



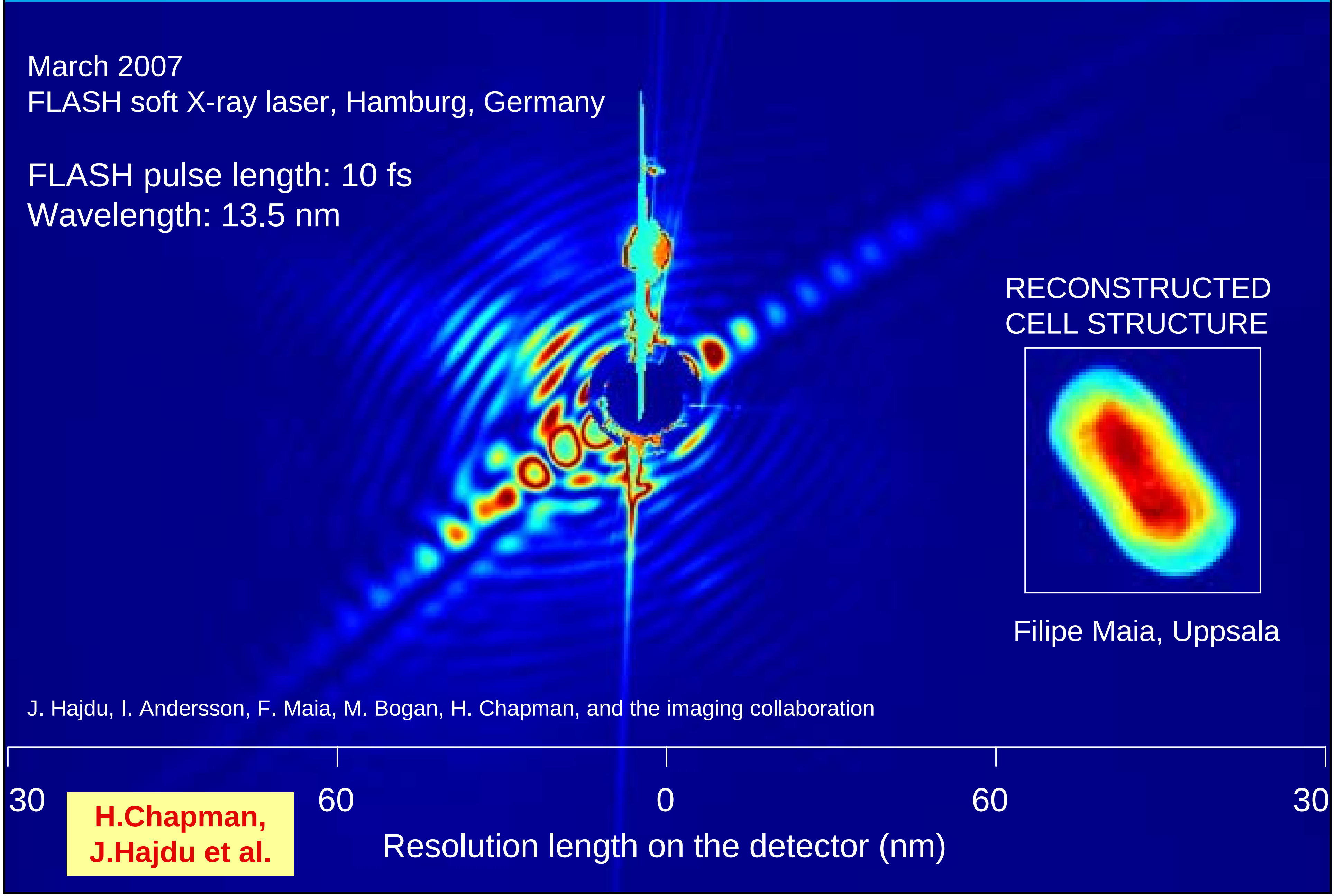
A.Barty et al., Nature Photonics 2, 415-419 (2008)

DESY



True "high speed recording" of an explosion

FIRST FLASH DIFFRACTION IMAGE OF A LIVE PICOPLANKTON (cell injected into the beam at 200m/s)



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2. T.W.J. Dzelzainis, J. Chalupsky, M. Fajardo, R. Fäustlin, P.A. Heimann, V. Hajkova, L. Juha, M. Jurek, F.Y. Khattak, M. Kozlova, J. Krzywinski, R.W. Lee, B. Nagler, A.J. Nelson, F.B. Rosmej, R. Sobierajski, S. Toleikis, T. Tschentscher, S.M. Vinko, J.S. Wark, T. Whitcher, D. Riley, *Plasma emission spectroscopy of solids irradiated by intense XUV pulses from a free electron laser*, High Energy Density Phys. 6, 109-112 (2010); http://dx.doi.org/10.1016/j.hedp.2009.05.017

3. A.J. Nelson, S. Toleikis, H. Chapman, S. Bajt, J. Krzywinski, J. Chalupsky, L. Juha, J. Cihelka, V. Hajkova, L. Vysin, T. Burian, M. Kozlova, R.R. Fäustlin, B. Nagler, S.M. Vinko, T. Whitcher, T. Dzelzainis, O. Renner, K. Saksl, A.R. Khorsand, P.A. Heimann, R. Sobierajski, D. Klinger, M. Jurek, J. Pelka, B. Iwan, J. Andreasson, N. Timneanu, M. Fajardo, J.S. Wark, D. Riley, T. Tschentscher, J. Hajdu, and R.W. Lee, *Soft x-ray free electron laser microfocus for exploring matter under extreme conditions*, Opt. Express 17, 18271-18278 (2009); http://dx.doi.org/10.1364/OE.17.018271

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5. S.P. Hau-Riege, R.A. London, R.M. Bionta, D. Ryutov, R. Soufli, S. Bajt, M.A. McKernan, S.L. Baker, J. Krzywinski, R. Sobierajski, R. Nietubyc, D. Klinger, J.B. Pelka, M. Jurek, L. Juha, J. Chalupský, J. Cihelka, V. Hájková, A. Velyhan, J. Krása, K. Tiedtke, S. Toleikis, H. Wabnitz, M. Bergh, C. Caleman, and N. Timneanu, *Wavelength dependence of the damage threshold of inorganic materials under extreme-ultraviolet free-electron-laser irradiation*, Appl. Phys. Lett. 95, 111104 (2009); http://dx.doi.org/10.1063/1.3216845

…

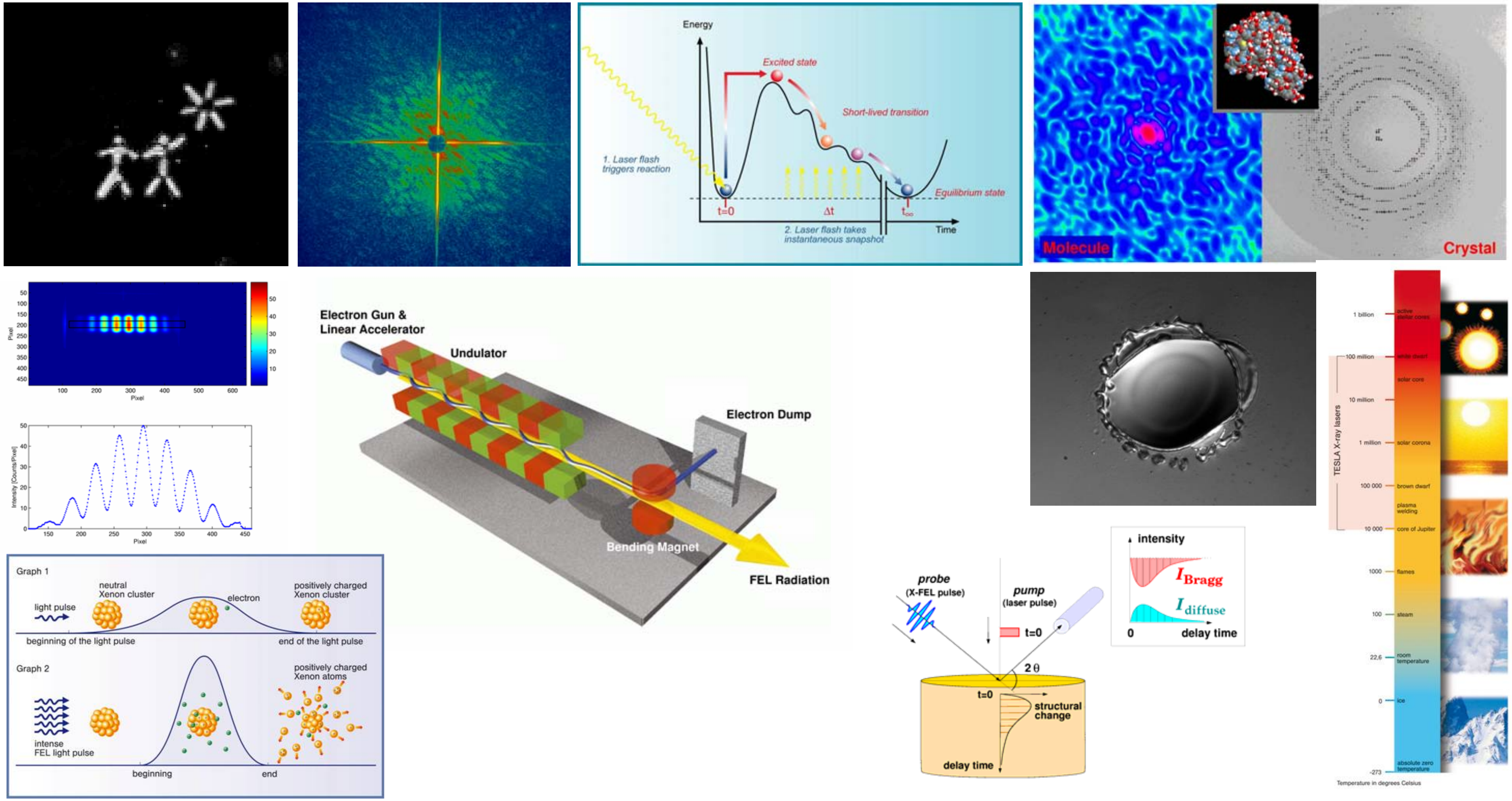
http://hasylab.desy.de/facilities/flash/publications/selected_publications/

Contents

Conclusions / Outlook

- **FELs are presently unrivaled radiation sources in a spectral range hardly accessible with "conventional" lasers:**
  - **extremely intense**
  - **coherent**
  - **short pulses**
  - **tunable wavelength**
- **Successful user operation of FLASH:**
  - **SASE from 47-6.8 nm in fundamental, and down to 1.6 nm in harmonics**
  - **GW peak power, 10-70 fs pulses**
- **Future: LCLS, USA (user operation since end 2009), SCSS, Japan (~end 2011), European XFEL (2014/15)**

X-ray Free Electron Lasers:
shedding light on nanoworld dynamics



The end.