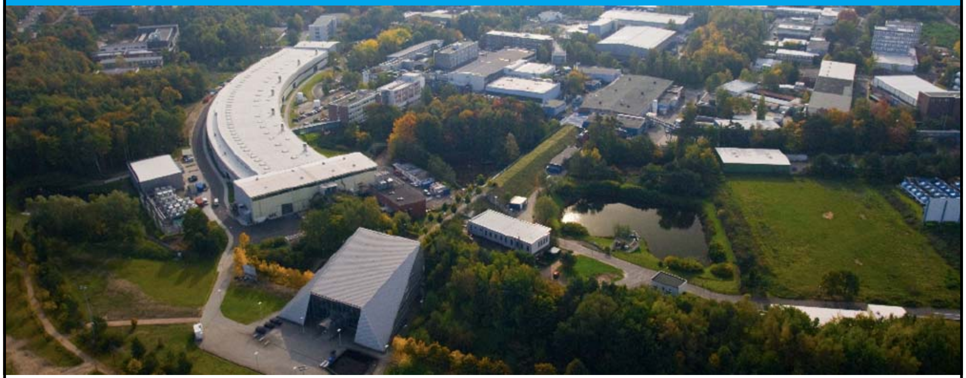
X-ray Free Electron Lasers: shedding light on nanoworld dynamics



Rolf Treusch
Summer Student Lectures,
DESY Zeuthen,
27. August 2009

HELMHOLTZ | GEMEINSCHAFT

Contents

X-ray sources in research

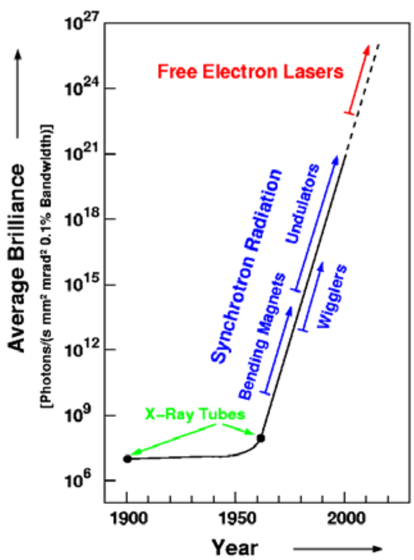
X-ray FELs

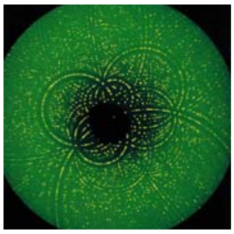
Synchrotron Radiation sources

X-ray tubes

From X-ray tubes to X-ray FELs

classical „X-ray“



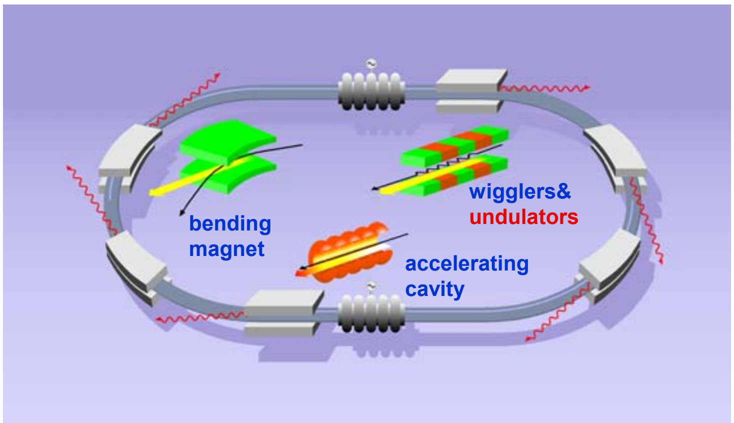


crystal structure analysis with atomic resolution

+

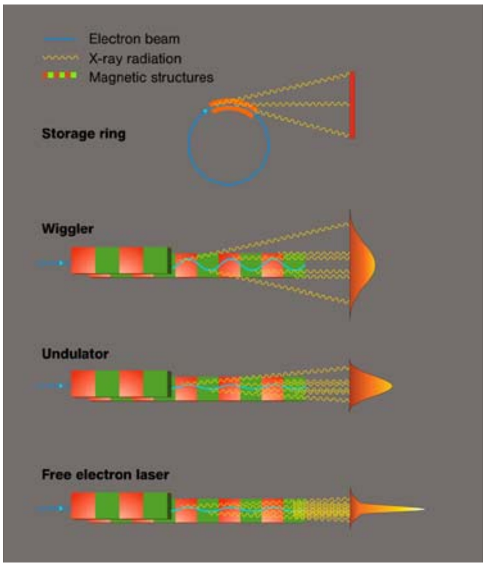
information about femtosecond dynamics

Synchrotron Radiation storage ring



Undulator = periodic magnetic field arrangement,
electrons emit light along sinusodial path,
photons can interfere constructively
➔ intensity enhancement $\propto N^2$ (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

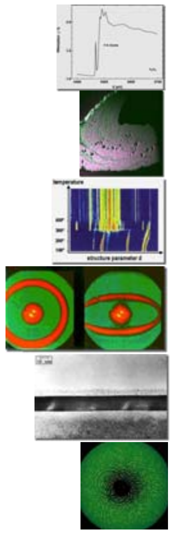
Fluorescence Analysis:
trace element analysis (e.g. Si-wafer impurities)

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 $\Rightarrow$ nonlinear effects,
plasma physics

Short Pulses:
Excitation $\leq$ timescale of molecular vibrations,
electronic relaxation, ...

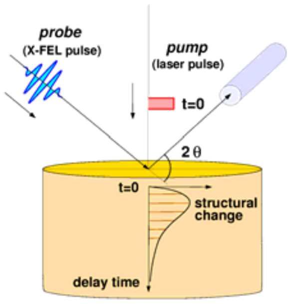
➔ Study of time dependent processes (*pump and probe* - experiments) or, e.g., X-ray microscopy on living cells

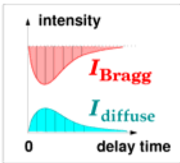
Contents

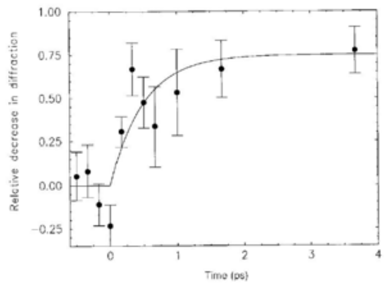
Examples of XFEL experiments

- **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?







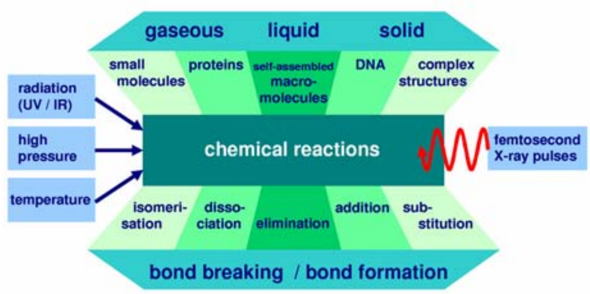
Rischel et al. (ESRF),

Nature 390, S. 490 ff.

Femtochemistry: Can we „film“ a chemical reaction?

Initial state

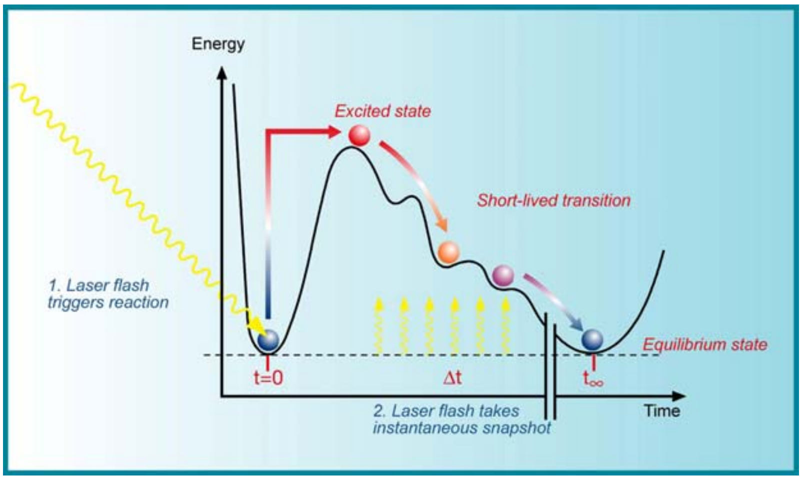
Excitation



Snapshot

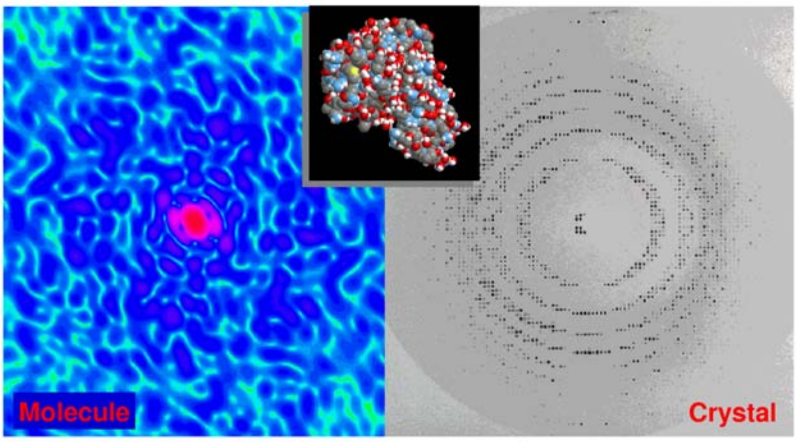
(time resolved)

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?

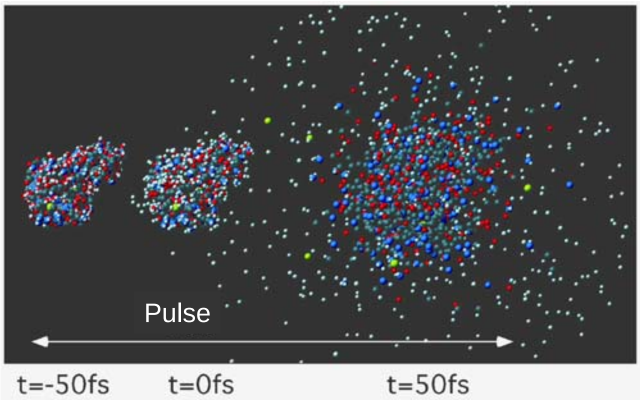


calculated diffraction image of a single Lysozyme molecule

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

J.Hajdu et al.

Obstacle: Coulomb-Explosion



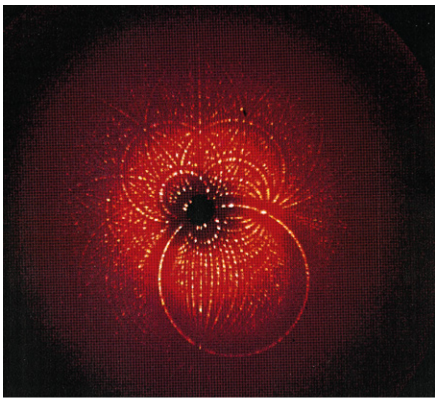
Example:
Lysozyme

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

R. Neutze et al.
Nature, August 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“

Contents

Free Electron Lasers: principles and properties

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

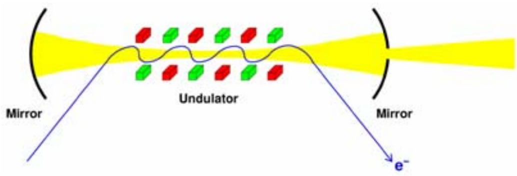
FEL vs. conventional Laser

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

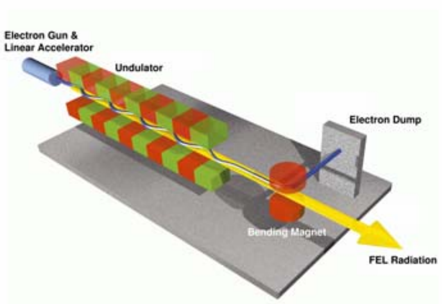
FEL was conceived by John Madey in his Ph.D. thesis, Stanford 1970:
J.M.J. Madey, J. Appl. Phys. 42, 1906 (1971)
First realization: D.A.G. Deacon, L.R. Elias, J.M.J. Madey, G.J. Ramian, H.A. Schwettman, T.I. Smith, Phys. Rev. Lett. 38, 892 (1977)

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

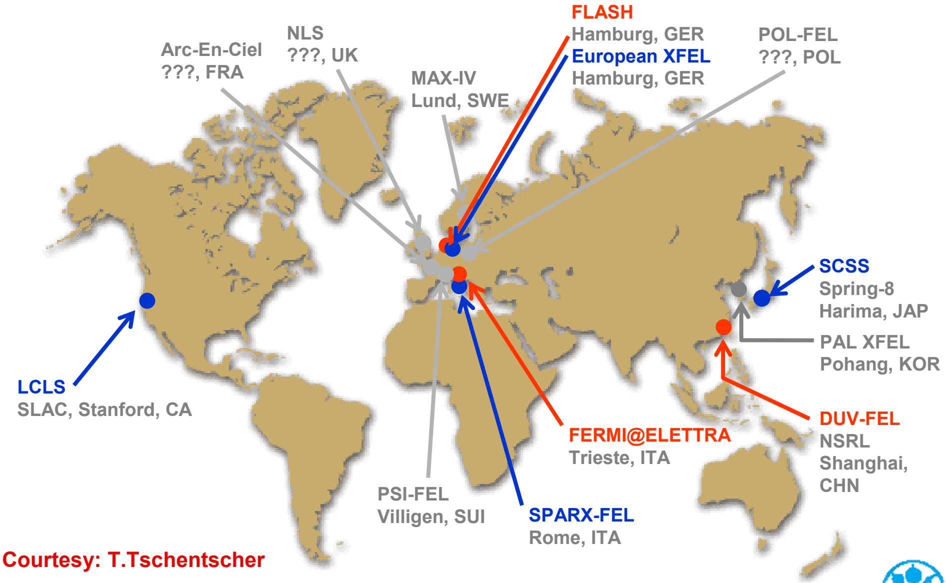


optical resonators are not usable for $\lambda < 150$ nm (low mirror reflectivities & possible damage)

below:
“single pass” SASE FELs



XUV & X-ray FEL Facilities and Projects



Courtesy: T.Tschentscher

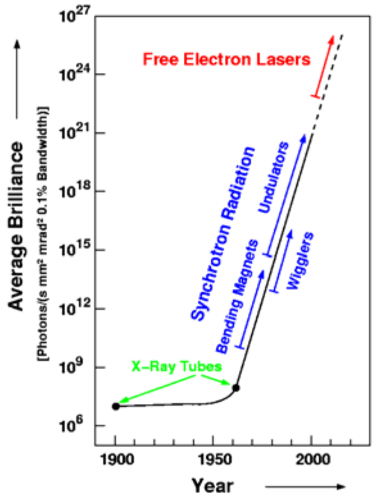
From synchrotron radiation towards SASE FELs

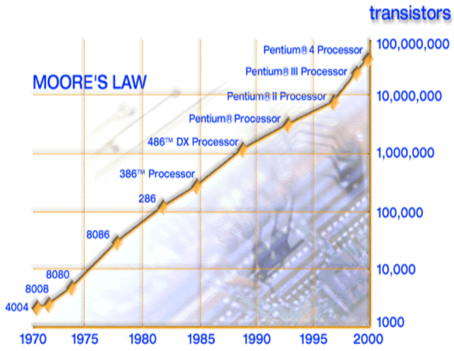
3rd generation synchrotron radiation source
(spontaneous undulator radiation)

+ 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

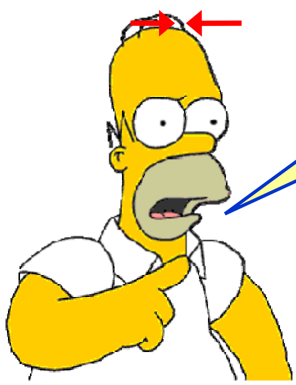




(http://www.intel.com/research/silicon/mooreslaw.htm)

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!!

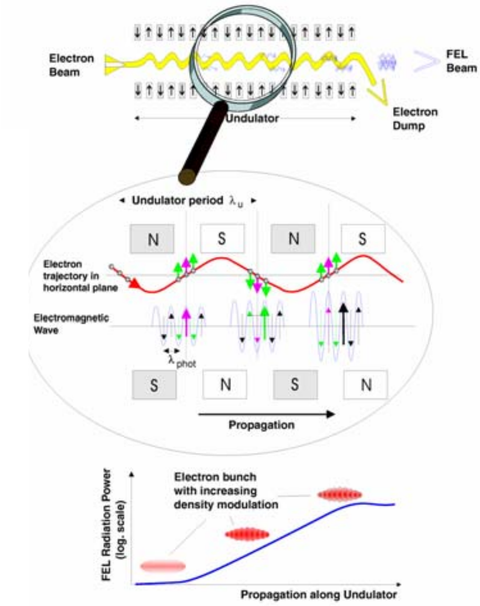
SASE (self-amplified spontaneous emission)

slippage between electrons and photons is λ_{phot} per undulator period

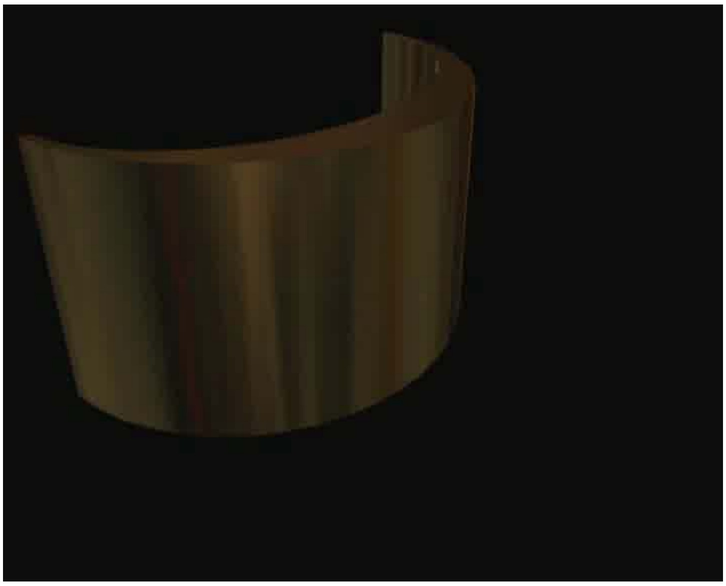
→ electrons in phase with e.m.-wave are retarded ("emit photons"), electrons with opposite phase gain energy ("absorb photons")

→ 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)



SASE movie



Requirements for SASE

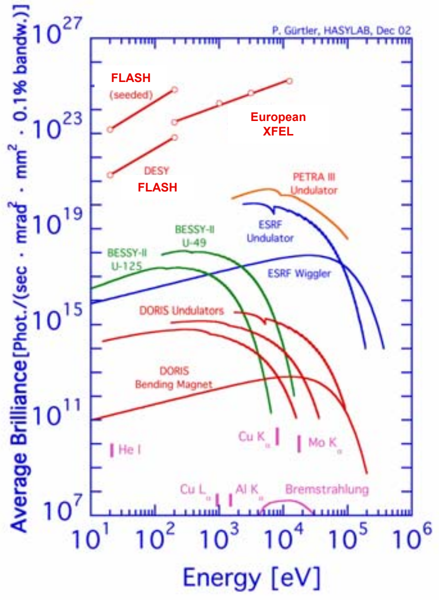
Good electron beam quality and sufficient overlap between e-beam and radiation pulse along the undulator, i.e.

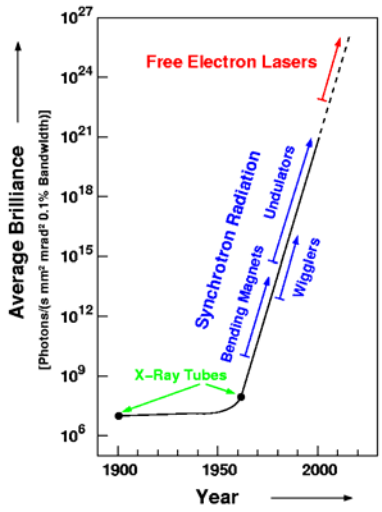
- low emittance, low energy spread electron beam
- extremely high charge density
  (kA peak currents)
- precise magnetic field of undulator
- accurate beam steering through undulator
  (few µm precision)

SASE FEL properties

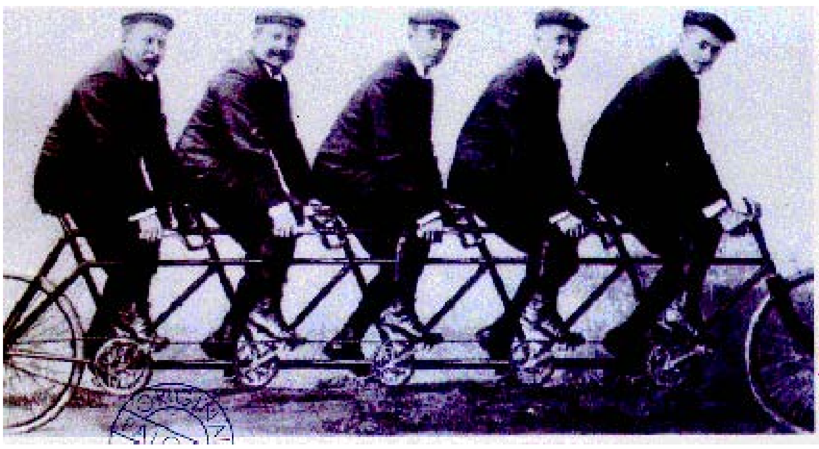
- high intensity (GW peak power)
- coherence
- femtosecond pulses
- narrow bandwidth
- wavelength tunability !
- down to X-rays !

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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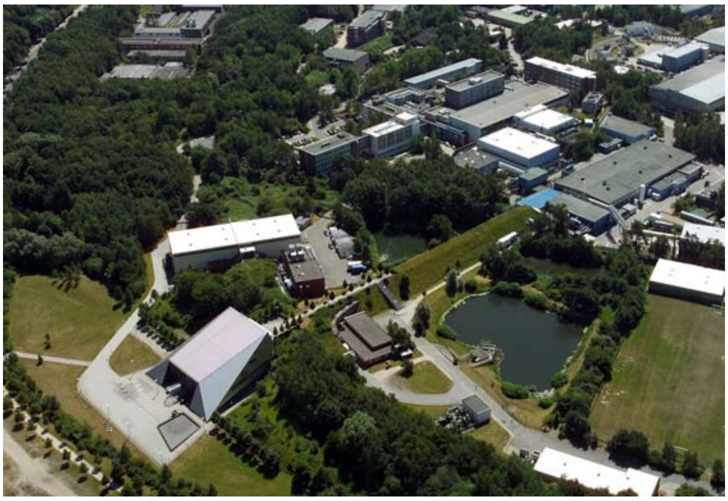
FLASH at DESY

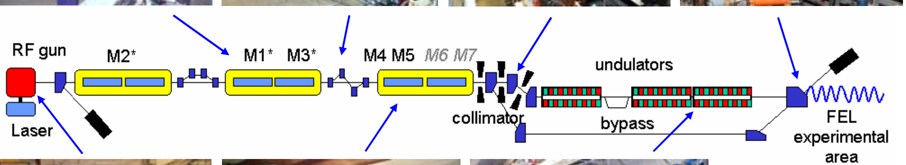


Installation of modules into the accelerator

Bunch compressor

Collimator area

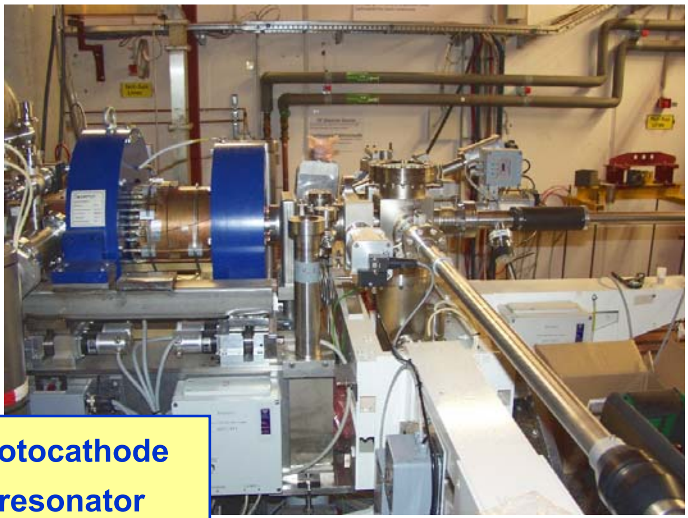
Deflection of electrons downwards into the dump



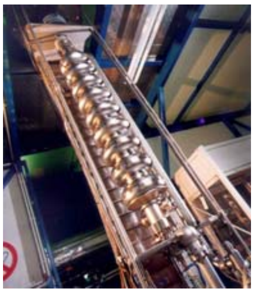
RF electron gun

Module #5

Undulator assembly



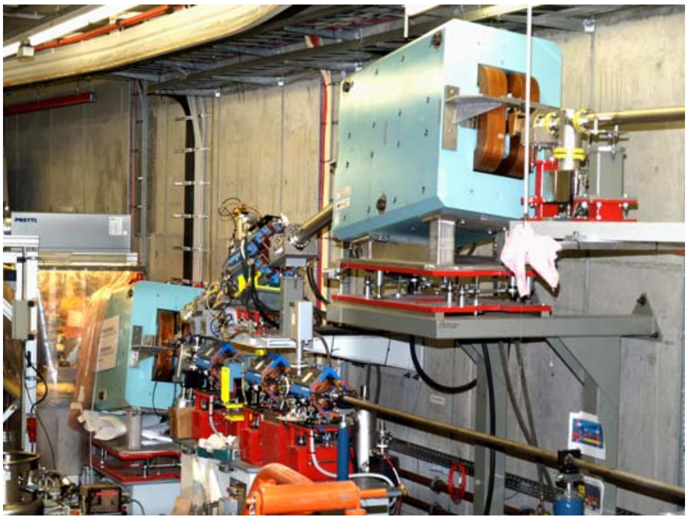
$CsTe_2$ photocathode
in 11/2 - cell resonator
1-3% quantum efficiency



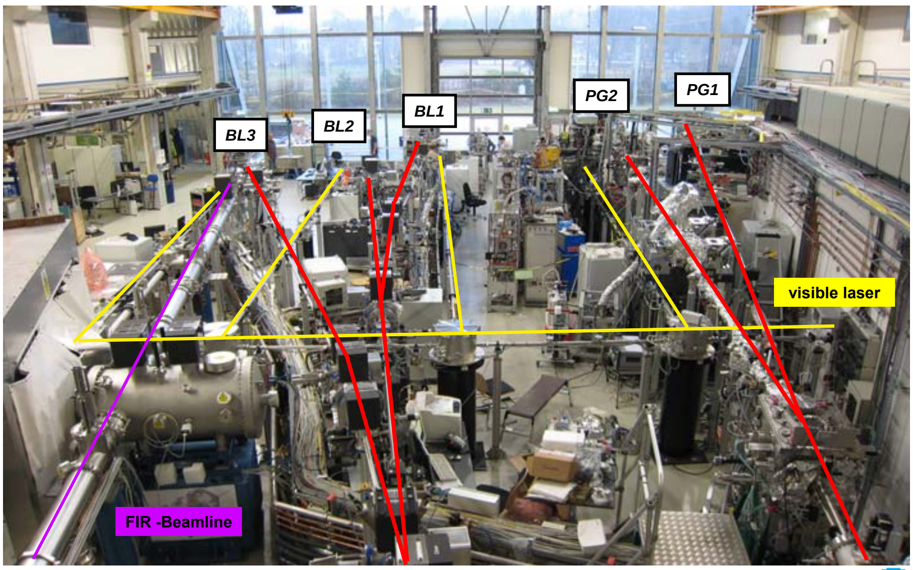
Accelerator module with
superconducting niobium cavities
25 MV/m routinely
Length: 12 m
Weight: about 10 tons!

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

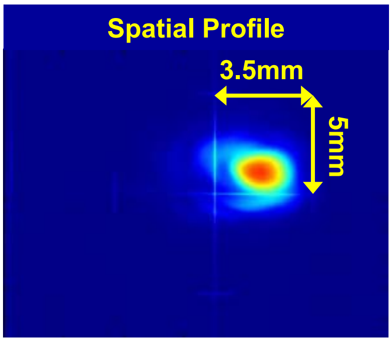
Fixed gap undulator, 30 m total length
with quadrupole doublets for focusing
the electron beam in intersections,
electron beam diagnostics
and steerer coils

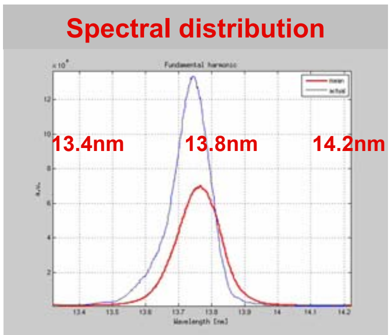


FLASH experimental hall



FLASH performance





Current parameters of FLASH

Wavelength range (fundamental):
6.5-48 nm

Spectral width (FWHM):
0.5-1 %

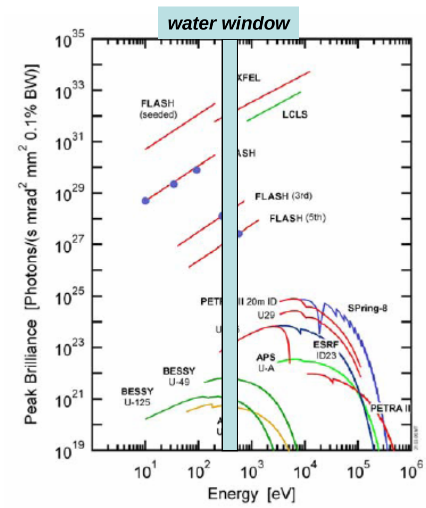
Pulse energy:
up to 100 µJ (average),
200 µJ (peak)

Pulse duration (FWHM):
5-50 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

Contents

Research Highlights from FLASH

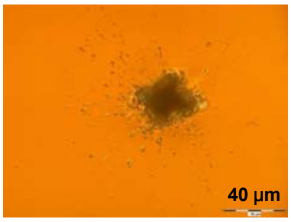
Research Areas

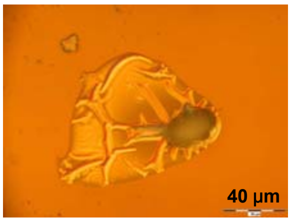
- Femtosecond time-resolved experiments
  - synchronisation FEL - optical laser
  - pump-probe experiments on atoms and molecules
  - sum-frequency generation
- Interaction of ultra-intense XUV pulses with matter
  - multiphoton excitation of atoms, molecules, clusters…
  - creation and characterisaton of dense plasmas
  - imaging of 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

- High energy density experiments (Lee et al.)
- Resonant ionization of highly charged ions (Crespo et al.)
- Pump-probe experiment on CO_2 alignment (M. Vrakkking et al.)
- Single shot diffraction imaging (Chapman, Hajdu et al.)

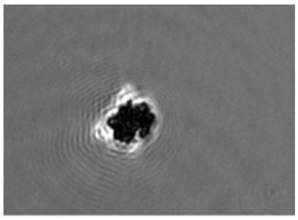
High energy density experiments
(R.W. Lee et al.)





Ablation of carbon coating on Si

R. Sobierajski et al.



Ablation of Si,
illuminated by optical laser pulse

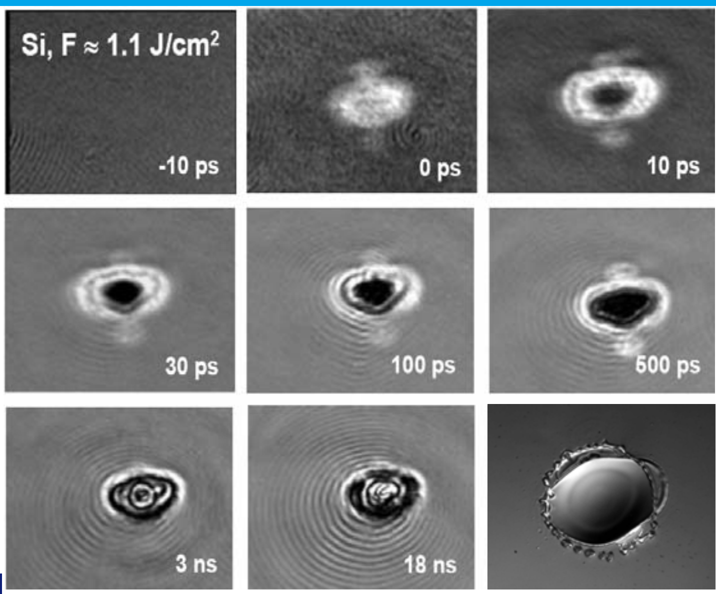
K. Sokolowski-Tinten et al.

… every flash a hit!

S.P. Hau-Riege et al., Appl. Phys. Lett. 90, 173128 (2007)

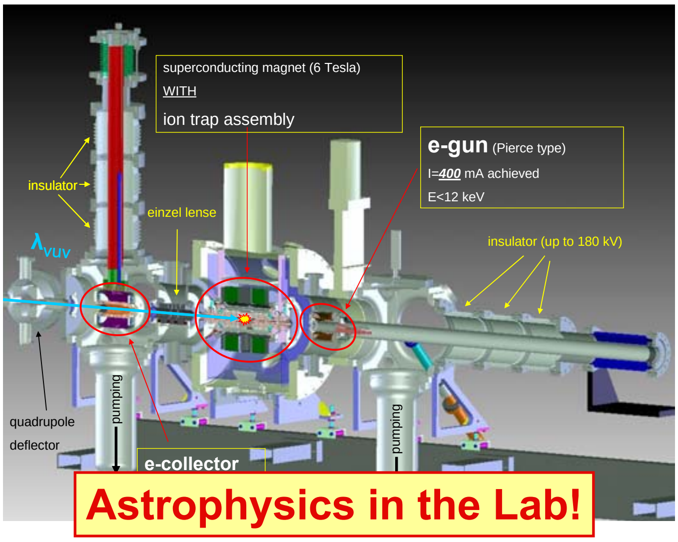
S.P. Hau-Riege et al., Phys. Rev. Lett. 98, 145502 (2007)

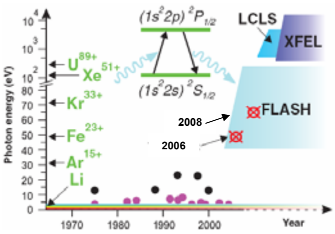
Results: Transient Reflectivity

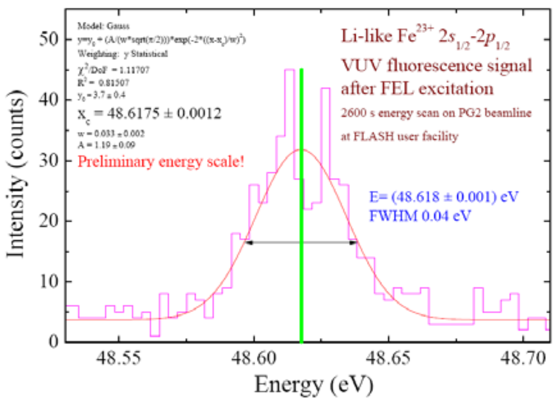


N. Stojanovic et al., Appl. Phys. Lett. 89, 241909 (2006)

Resonant ionization of highly charged ions
(J.Crespo et al.)





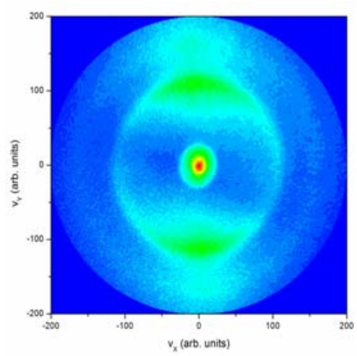


S.W.Epp et al.,
Phys. Rev. Lett. 98, 183001 (2007)

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

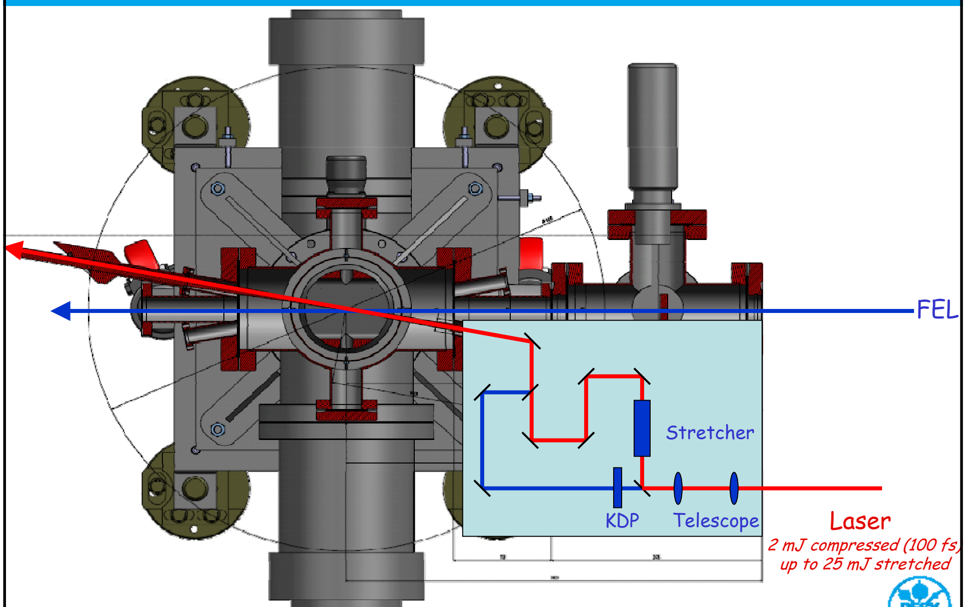
Time-dependent alignment of CO_2

- 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)



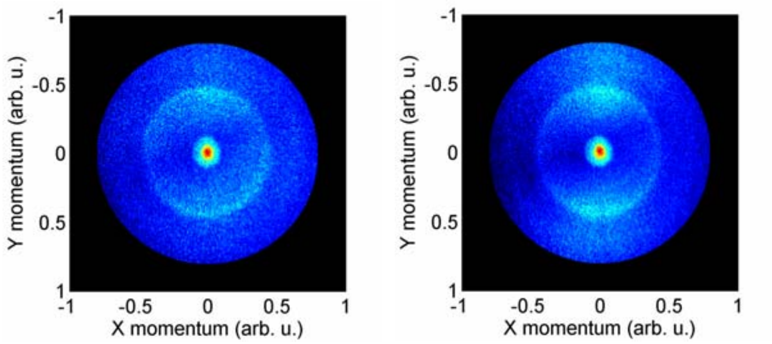
VMIS image
(*velocity map imaging spectrometer*)

AMOLF VMIS: Pump probe setup



M. Vrakking et al.

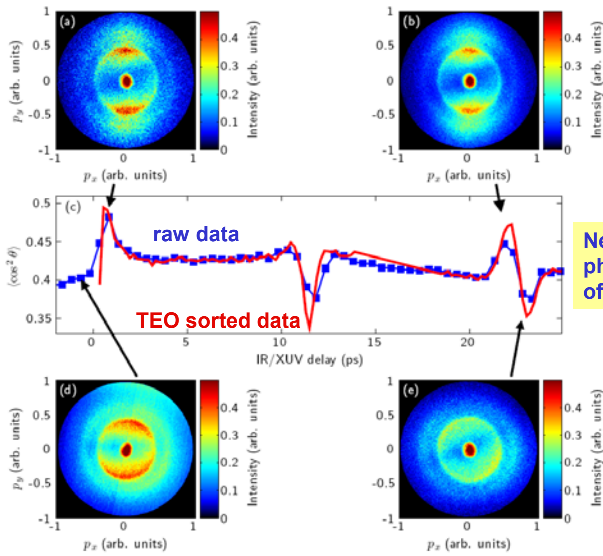
Dissociation of aligned CO2 molecules



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.



Next step: photodissociation of Br_2 (spring '09)

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

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

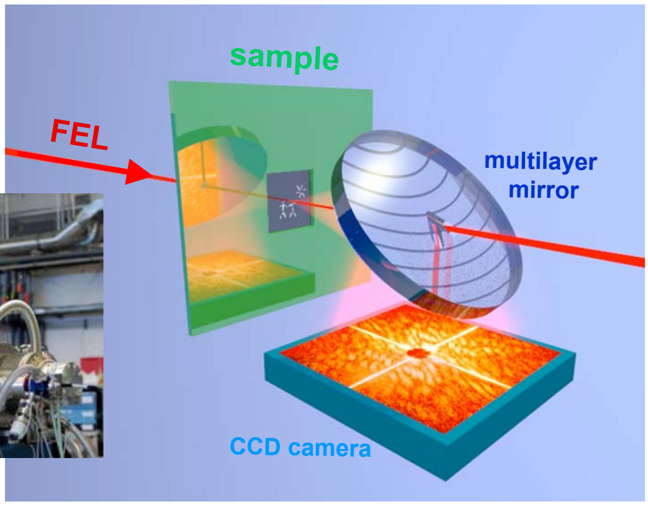
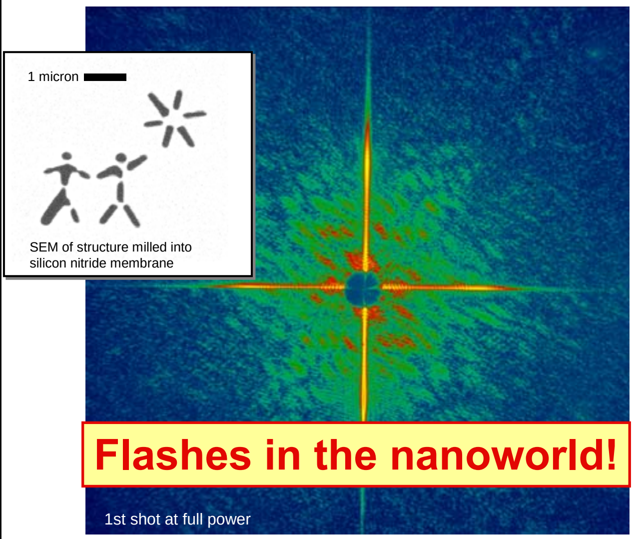
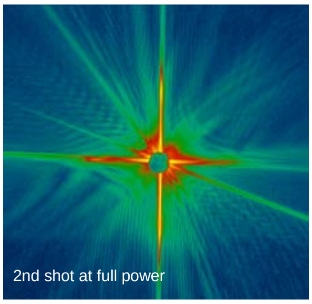
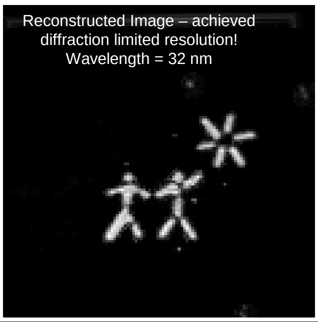


Image reconstructed from ultrafast diffraction pattern



Flashes in the nanoworld!





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

Dynamic X-ray diffraction imaging (pump-probe)

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

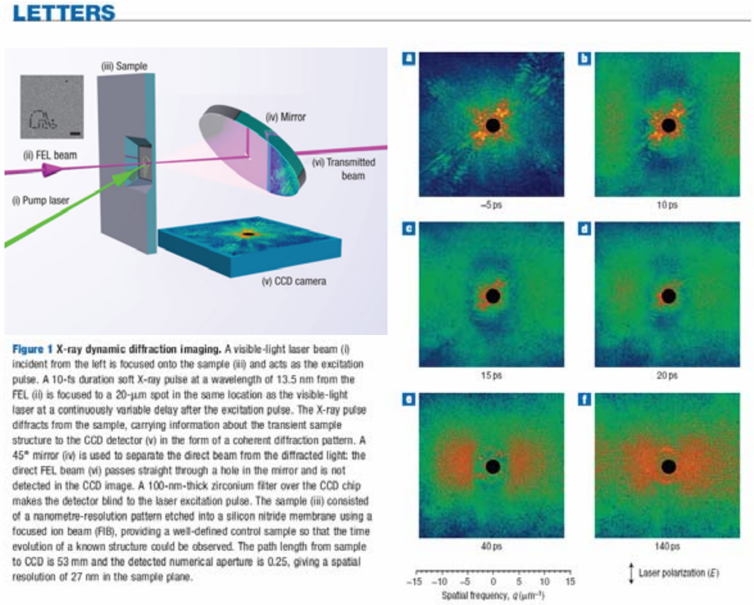
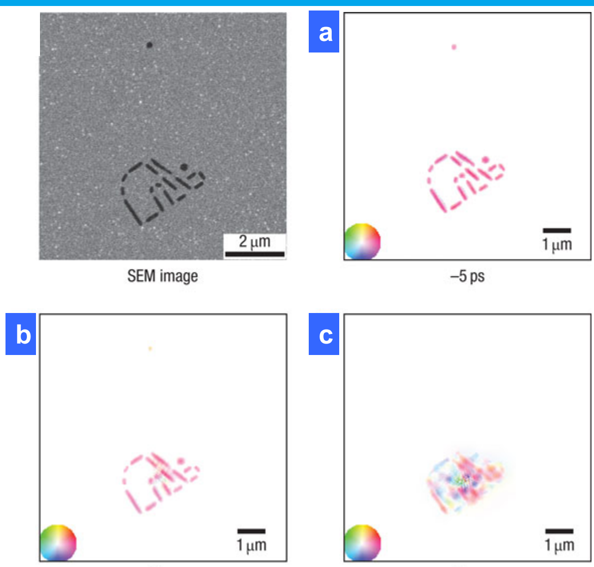


Figure 1 X-ray dynamic diffraction imaging. A visible-light laser beam (i) incident from the left is focused onto the sample (iii) and acts as the excitation pulse. A 10-fs duration soft X-ray pulse at a wavelength of 13.5 nm from the FEL (ii) is focused to a 20-μm spot in the same location as the visible-light 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.



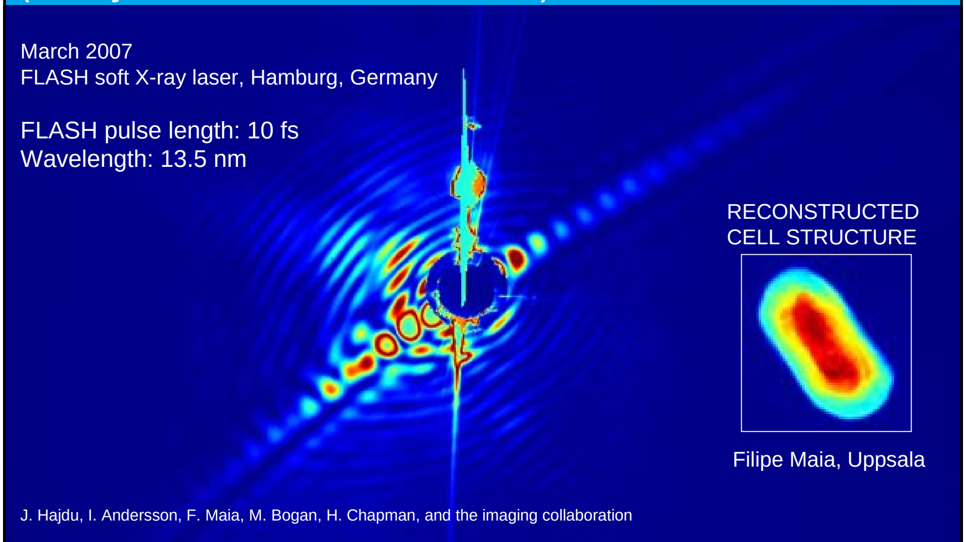
SEM image   –5 ps
10 ps   15 ps

True "high speed recording" of an explosion

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

March 2007
FLASH soft X-ray laser, Hamburg, Germany

FLASH pulse length: 10 fs
Wavelength: 13.5 nm



RECONSTRUCTED CELL STRUCTURE

Filipe Maia, Uppsala

J. Hajdu, I. Andersson, F. Maia, M. Bogan, H. Chapman, and the imaging collaboration

30 60 0 60 30

Resolution length on the detector (nm)

H.Chapman, J.Hajdu et al.

Publications

1. Bob Nagler, Ulf Zastrau, Roland R. Fäustlin, Sam M. Vinko, Thomas Whitcher, A.J. Nelson, Ryszard Sobierajski, Jacek Krzywinski, Jaromir Chalupsky, Elsa Abreu, Saša Bajt, Thomas Bornath, Tomas Burian, Henry Chapman, Jaroslav Cihelka, Tilo Döppner, Stefan Düsterer, Thomas Dzelzainis, Marta Fajardo, Eckhart Förster, Carsten Fortmann, Eric Galtier, Siegfried H. Glenzer, Sebastian Göde, Gianluca Gregori, Vera Hajkova, Phil Heimann, Libor Juha, Marek Jurek, Fida Y. Khattak, Ali Reza Khorsand, Dorota Klinger, Michaela Kozlova, Tim Laarmann, Hae Ja Lee, Richard W. Lee, Karl-Heinz Meiwes-Broer, Pascal Mercere, William J. Murphy, Andreas Przystawik, Ronald Redmer, Heidi Reinholz, David Riley, Gerd Röpke, Frank Rosmej, Karel Saksl, Romain Schott, Robert Thiele, Josef Tiggesbäumker, Sven Toleikis, Thomas Tschentscher, Ingo Uschmann, Hubert J. Vollmer and Justin S. Wark,
Turning solid aluminium transparent by intense soft X-ray photoionization,
Nature Physics, published online 26 July 2009; http://dx.doi.org/10.1038/NPHYS1341

2. H.B. Pedersen, S. Altevogt, B. Jordon-Thaden, O. Heber, L. Lammich, M.L. Rappaport, D. Schwalm, J. Ullrich, D. Zajfman, R. Treusch, N. Guerassimova, M. Martins and A. Wolf,
Neutral and charged photofragment coincidence imaging with soft x-rays on molecular ion beams: Breakup of H3O+ at 13.5 nm,
Phys. Rev. A 80, 012707 (2009); http://dx.doi.org/10.1103/PhysRevA.80.012707

3. M. Kurka, A. Rudenko, L. Foucar, K.U. Kühnel, Y.H. Jiang, Th. Ergler, T. Havermeier, M. Smolarski, S. Schössler, K. Cole, M. Schöffler, R. Dörner, M. Gensch, S. Düsterer, R. Treusch, S. Fritzsche, A.N. Grum-Grzhimajlo, E.V. Gryzlova, N.M. Kabachnik, C.D. Schröter, R. Moshammer, and J. Ullrich,
Two-photon double ionization of Ne by free-electron laser radiation: a kinematically complete experiment,
J. Phys. B: At. Mol. Opt. Phys. 42, 141002 (2009); http://dx.doi.org/10.1088/0953-4075/42/14/141002

4. C. Gutt, L.-M. Stadler, S. Streit-Nierobisch, A.P. Mancuso, A. Schropp, B. Pfau, C.M. Günther, R. Könnecke, J. Gulden, B. Reime, J. Feldhaus, E. Weckert, I.A. Vartaniants, O. Hellwig, F. Staier, R. Barth, M. Grunze, A. Rosenhahn, D. Stickler, H. Stillrich, R. Frömter, H.P. Oepen, M. Martins, T. Nisius, T. Wilhein, B. Faatz, N. Guerassimova, K. Honkavaara, V. Kocharyan, R. Treusch, E. Saldin, S. Schreiber, E.A. Schneidmiller, M.V. Yurkov, S. Eisebitt, and G. Grübel,
Resonant magnetic scattering with femtosecond soft X-ray pulses from a free electron laser operating at 1.59 nm,
Phys. Rev. B 79, 212406 (2009); http://dx.doi.org/10.1103/PhysRevB.79.212406

5. H. Thomas, C. Bostedt, M. Hoener, E. Eremina, H. Wabnitz, T. Laarmann, E. Plönjes, R. Treusch, A.R.B. de Castro and T.Möller,
Shell explosion and core expansion of xenon clusters irradiated with intense femtosecond soft x-ray pulses,
In Special Issue on attosecond and x-ray free electron laser physics:
J. Phys. B: At. Mol. Opt. Phys. 42, 134018 (2009); http://dx.doi.org/10.1088/0953-4075/42/13/134018

…

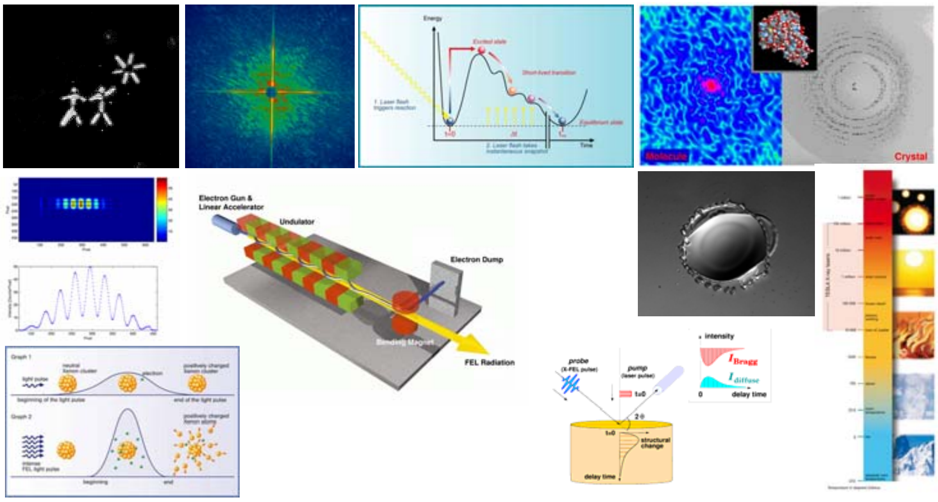
http://hasylab.desy.de/facilities/flash/publications/selected_publications/

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 48-6.5 nm in fundamental, and down to 1.6 nm in harmonics
  - GW peak power, 5-50 fs pulses
- Future: LCLS (autumn 2009), SCSS (~2011), XFEL (2014/15)

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



The end.