The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

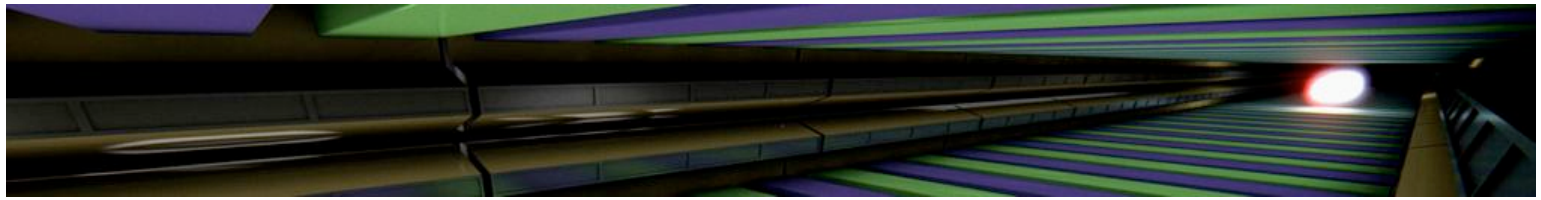
2139-2

School on Synchrotron and Free-Electron-Laser Sources and their Multidisciplinary Applications

26 April - 7 May, 2010

Scientific Use of Hard X-ray Free-Electron Lasers

Massimo Altarelli
European X-ray Free-Electron Laser Facility
Hamburg



Scientific Use of Hard X-ray Free-Electron Lasers

Massimo Altarelli

European X-ray Free-Electron Laser Facility
22607 Hamburg, Germany

www.xfel.eu for more information….

European XFEL

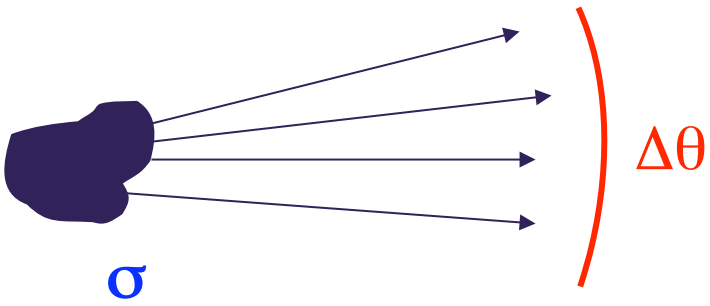
Third Generation Synchrotron Sources

Brilliance/Spectral Brightness

FLUX OF PHOTONS IN UNIT SPECTRAL RANGE

(SOURCE AREA) X (BEAM DIVERGENCE)

Units: photons/s/mm^2/mrad^2/0.1%BW



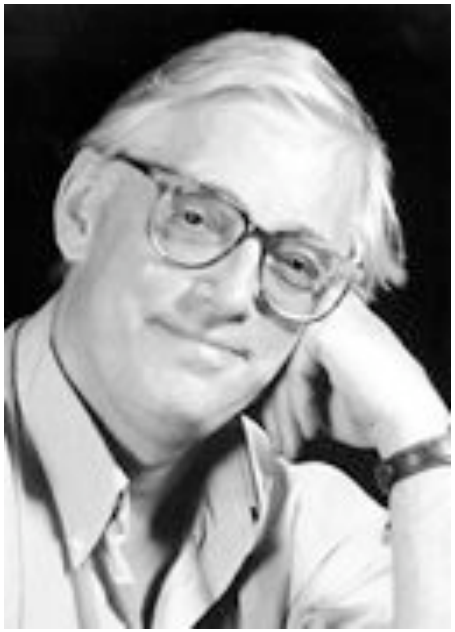
$$B = \frac{\Phi}{\sigma \, \Delta\theta_h \, \Delta\theta}$$

European XFEL

Nobel Prizes to Synchrotron Radiation Work

1997 John E. Walker

Structure of F1-ATPase



2003 Roderick McKinnon

Structure of Cellular Ion Channels

2006 Roger D. Kronberg

Structure of RNA polimerase

3 Win Nobel for Ribosome Research

Reuters

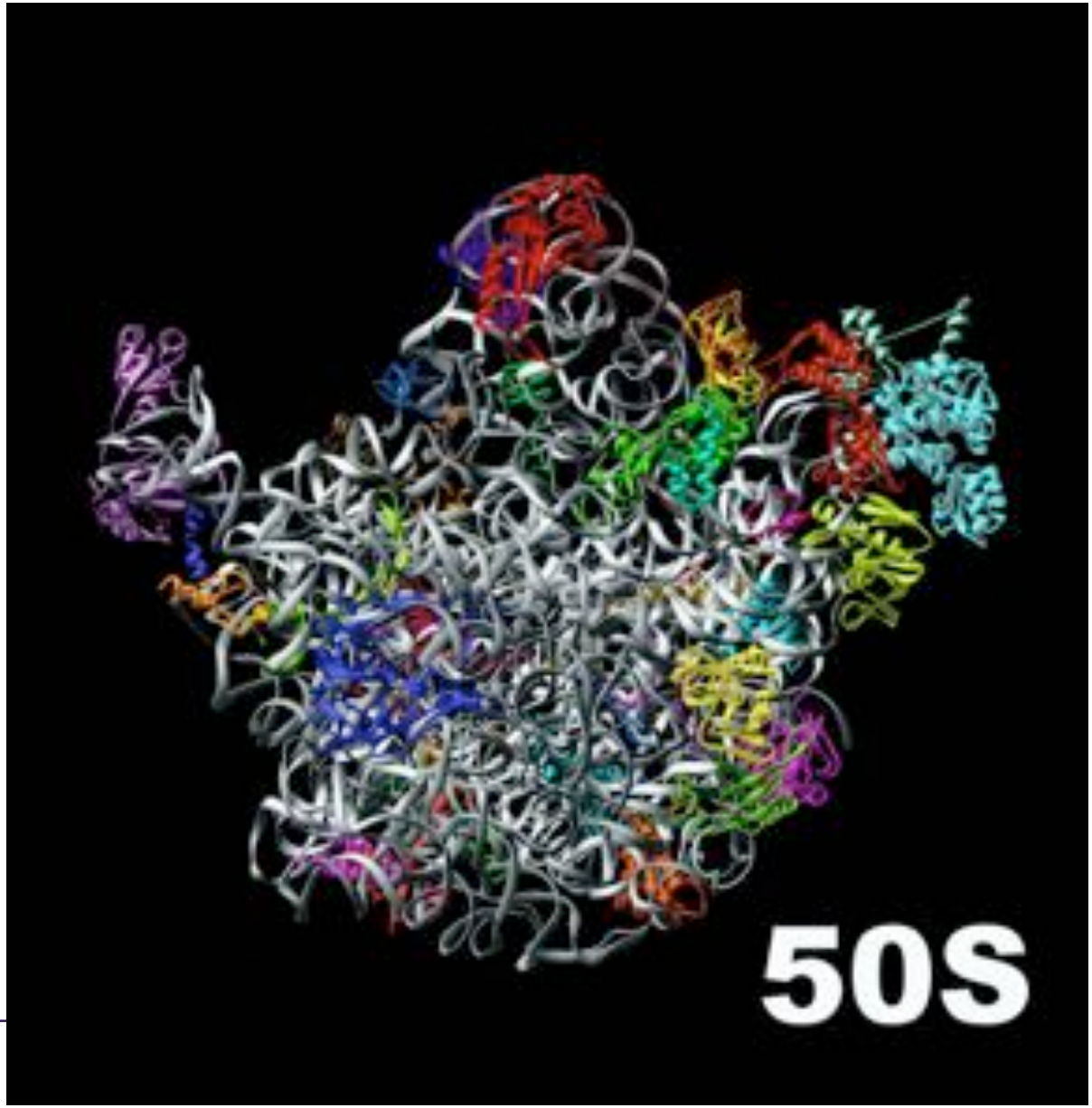
From left, Venkatraman Ramakrishnan of the MRC Laboratory of Molecular Biology in Cambridge, England; Thomas A. Steitz of Yale University; and Ada E. Yonath of the Weizmann Institute of Science in Rehovot, Israel, will share the 2009 Nobel Prize in Chemistry.

Working independently and using, among other things, the X-rays generated by powerful particle accelerators and prodigious computer calculations, the three winners and their colleagues succeeded in mapping the locations of the hundreds of thousands of atoms in the giant molecular complexes . . .

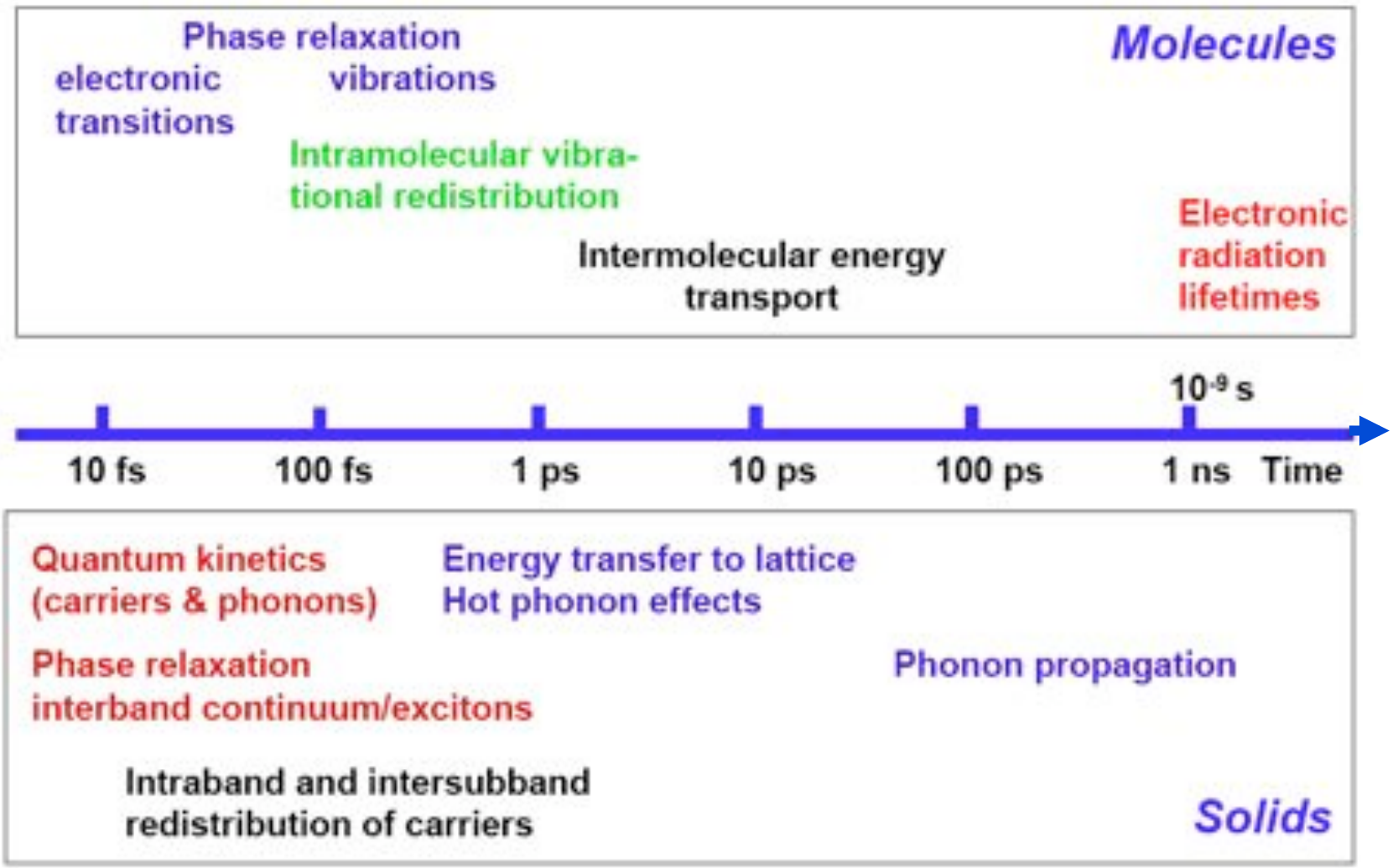
European XFEL

Ribosome: the Protein factory of the cell

From the home page of Ada Yonath



Time Scales for Dynamics

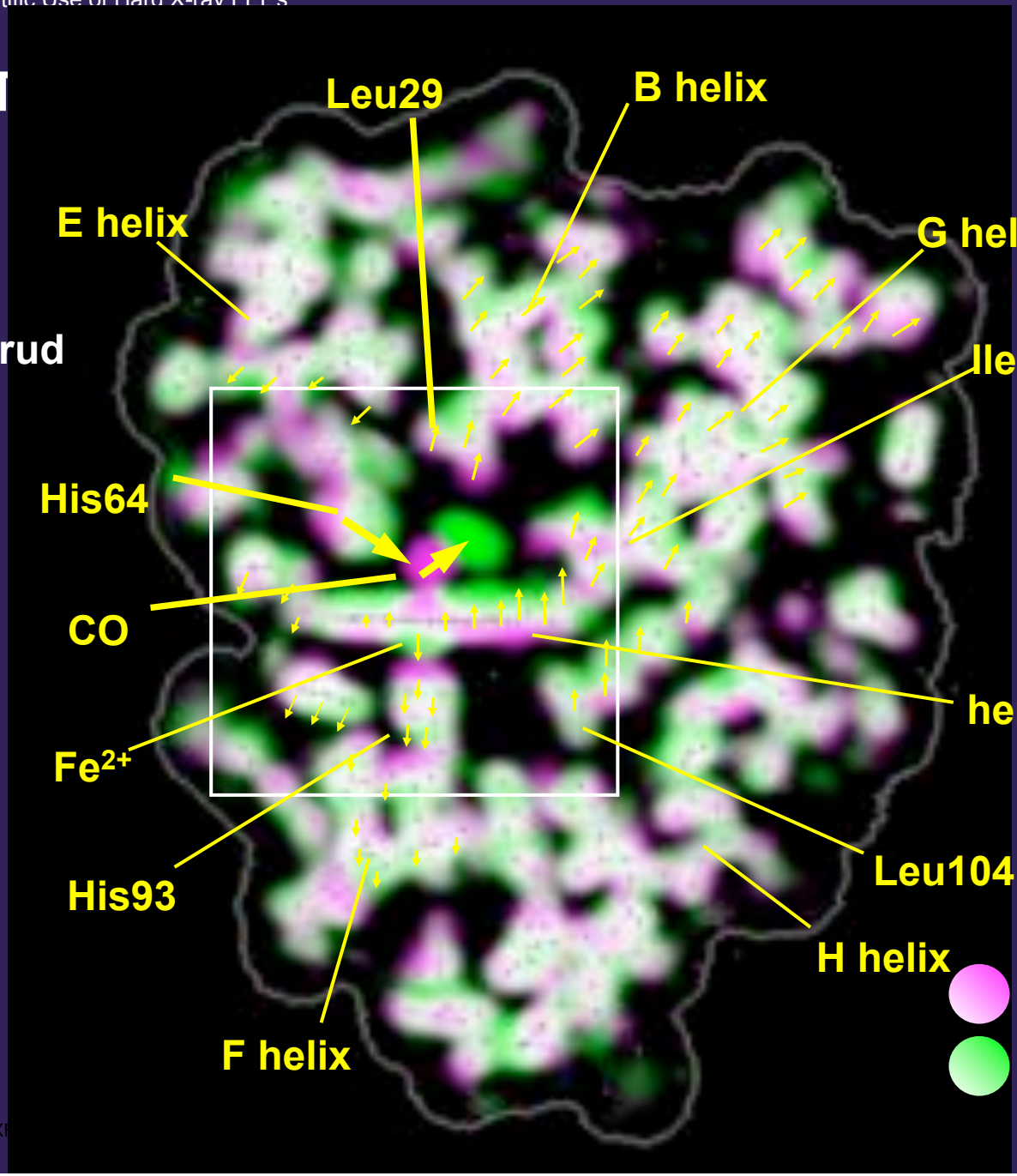


European XFEL

WT

After Ph. Afinrud

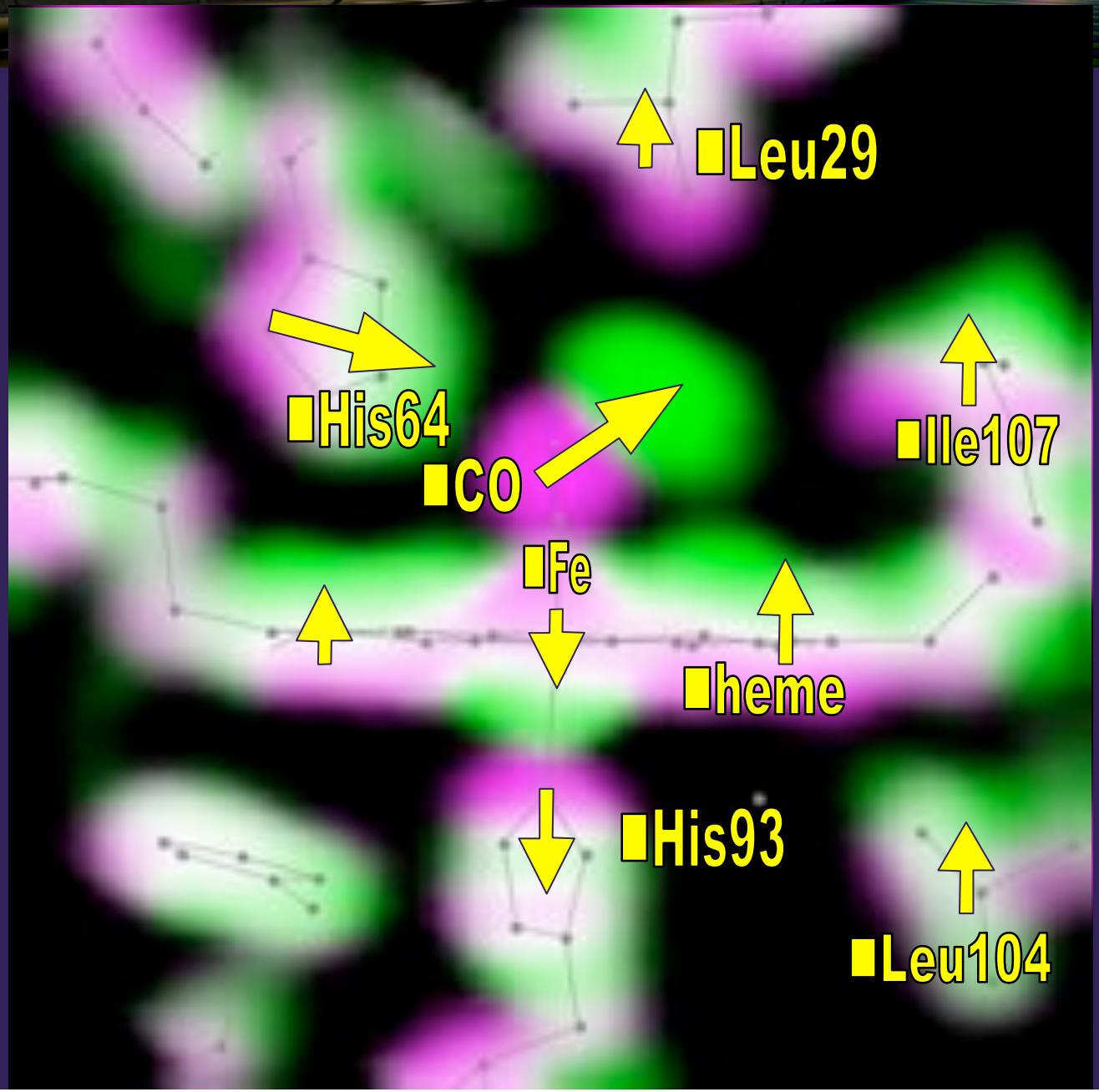
ESRF ID09



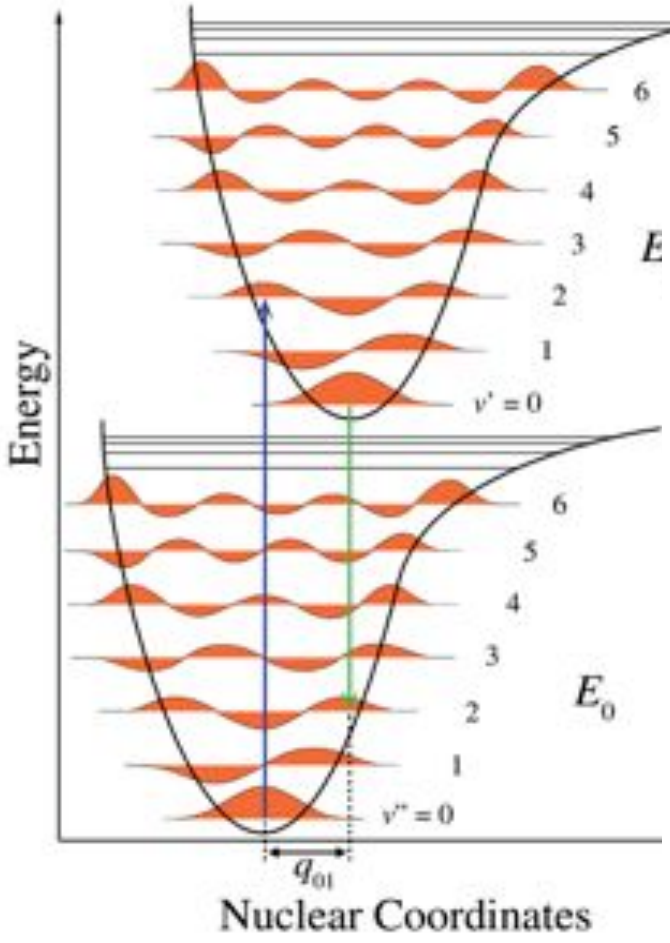
European XFEL

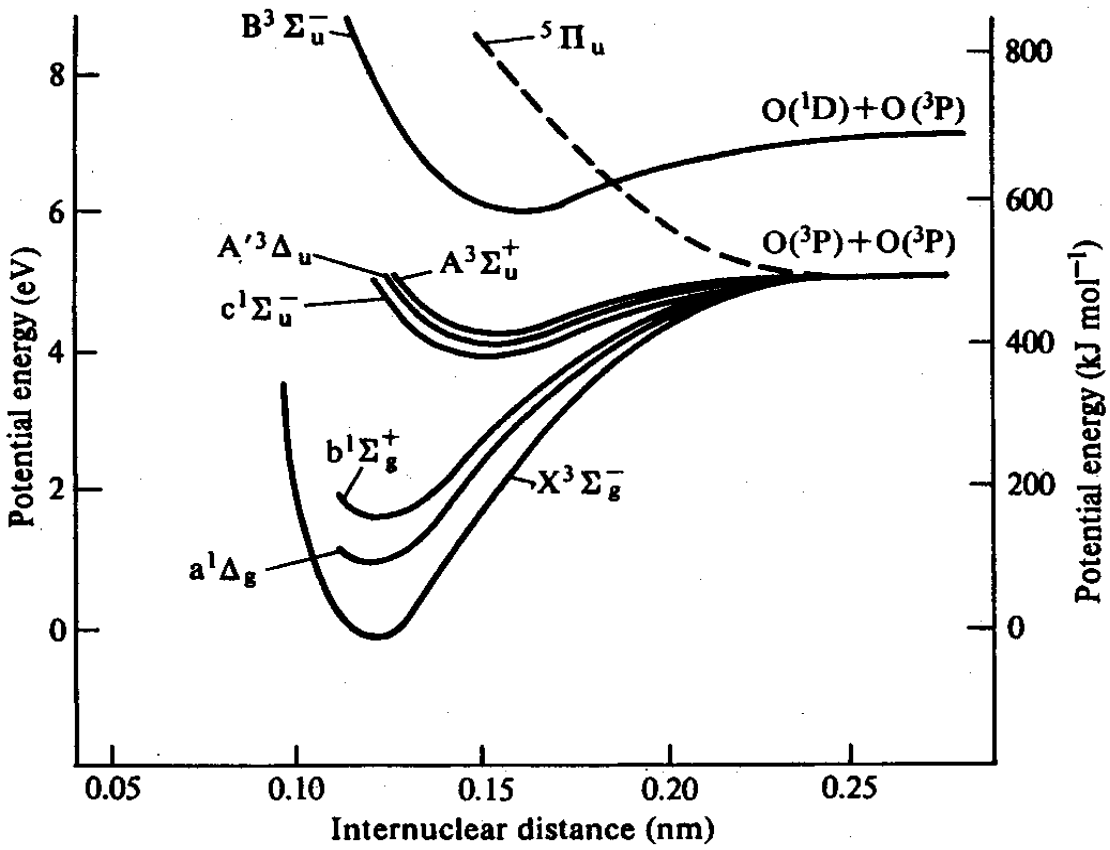
Photolyzed

Color-coded maps superimposed: MbCO at 100 ps



Exploring the Configuration Space Landscape

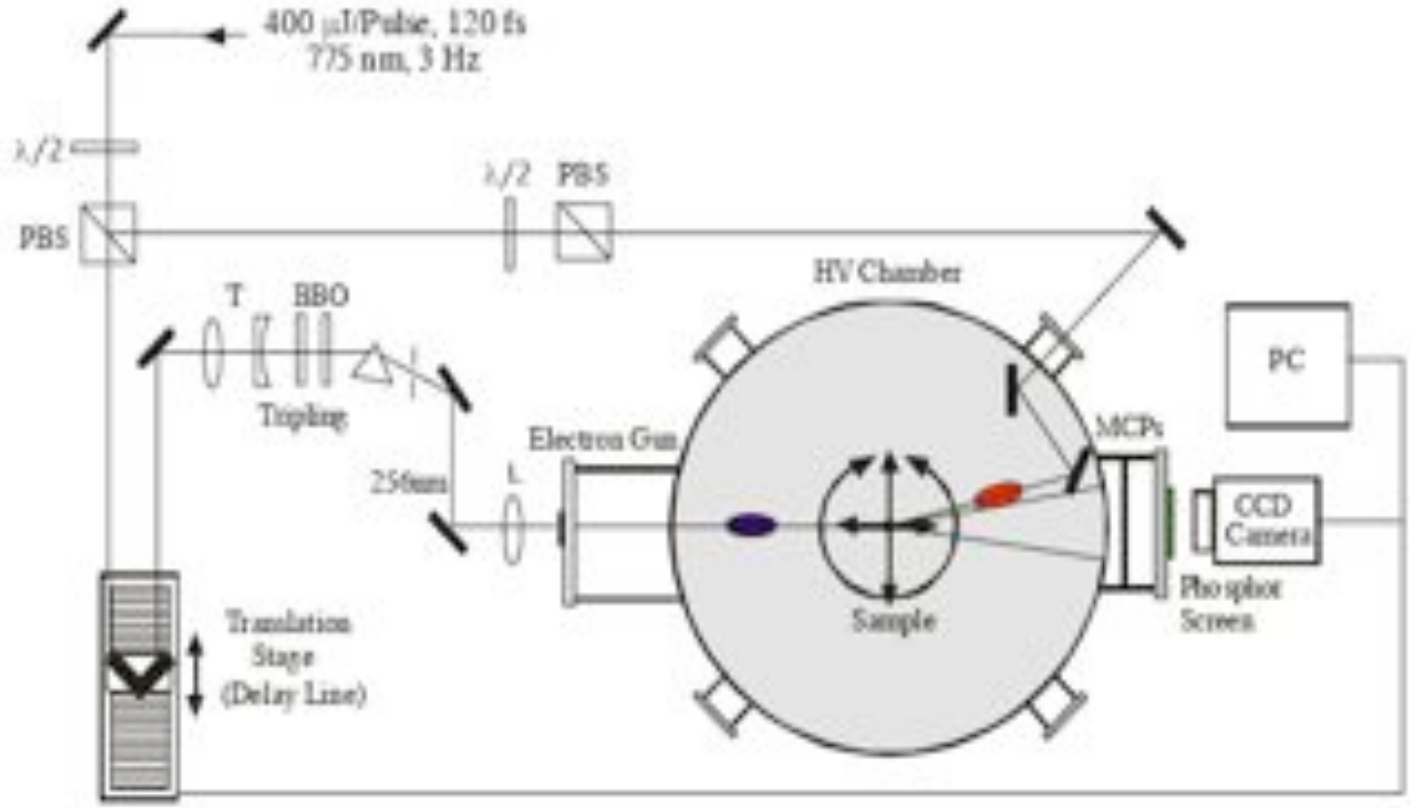




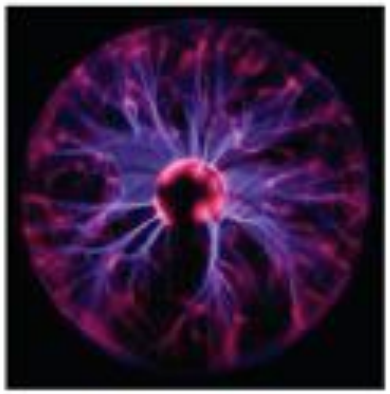
European XFEL

Tools for sub-ps structural dynamics

Ultrafast electron diffraction



Tools for ultrafast structural dynamics: x-rays

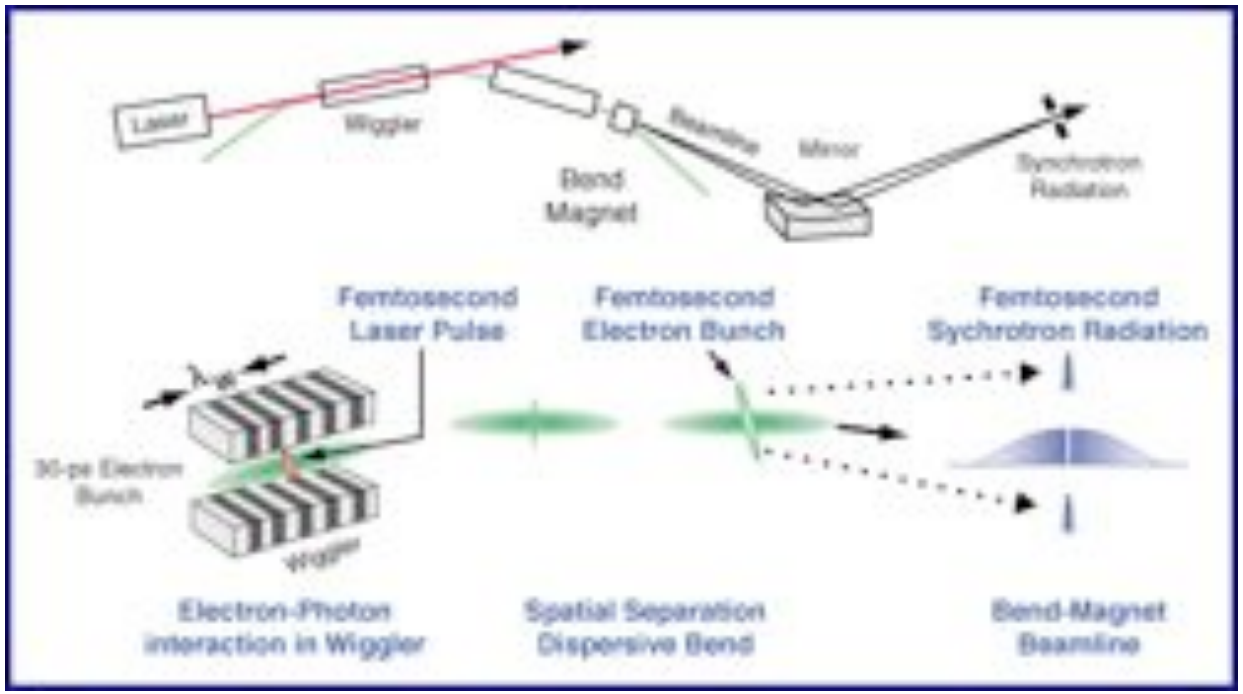


Laser-based: laser-plasma, plasma-wiggler, HHG,…

Accelerator-based:

Storage rings:

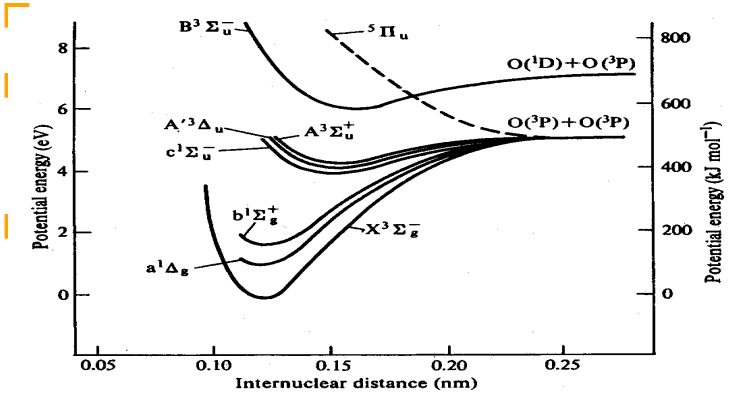
- **bunch-slicing,**
- **bunch-rotation**



European XFEL

Wanted…A more brilliant X-ray source, with:

wavelength down to ~ 0.1 nm ==> *atomic-scale resolution*

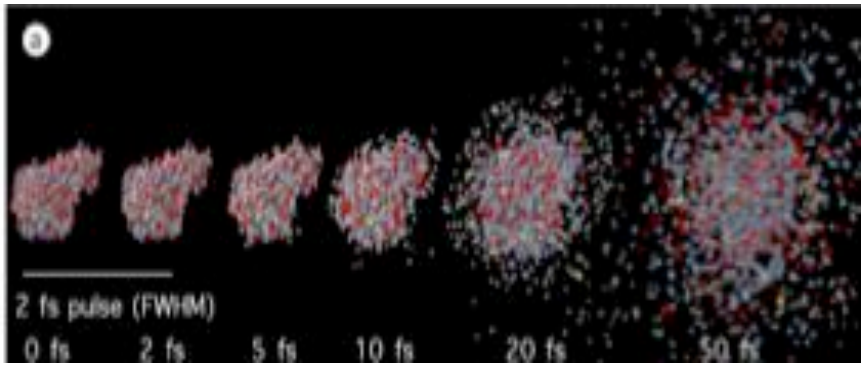


ultra-high peak brightness

==>investigation of matter under extreme conditions…

ultrashort (<1 ps) pulses

==> "molecular movies"



transverse spatial coherence

==> imaging of single nanoscale objects, possibly down to individual macromolecules (no crystals)

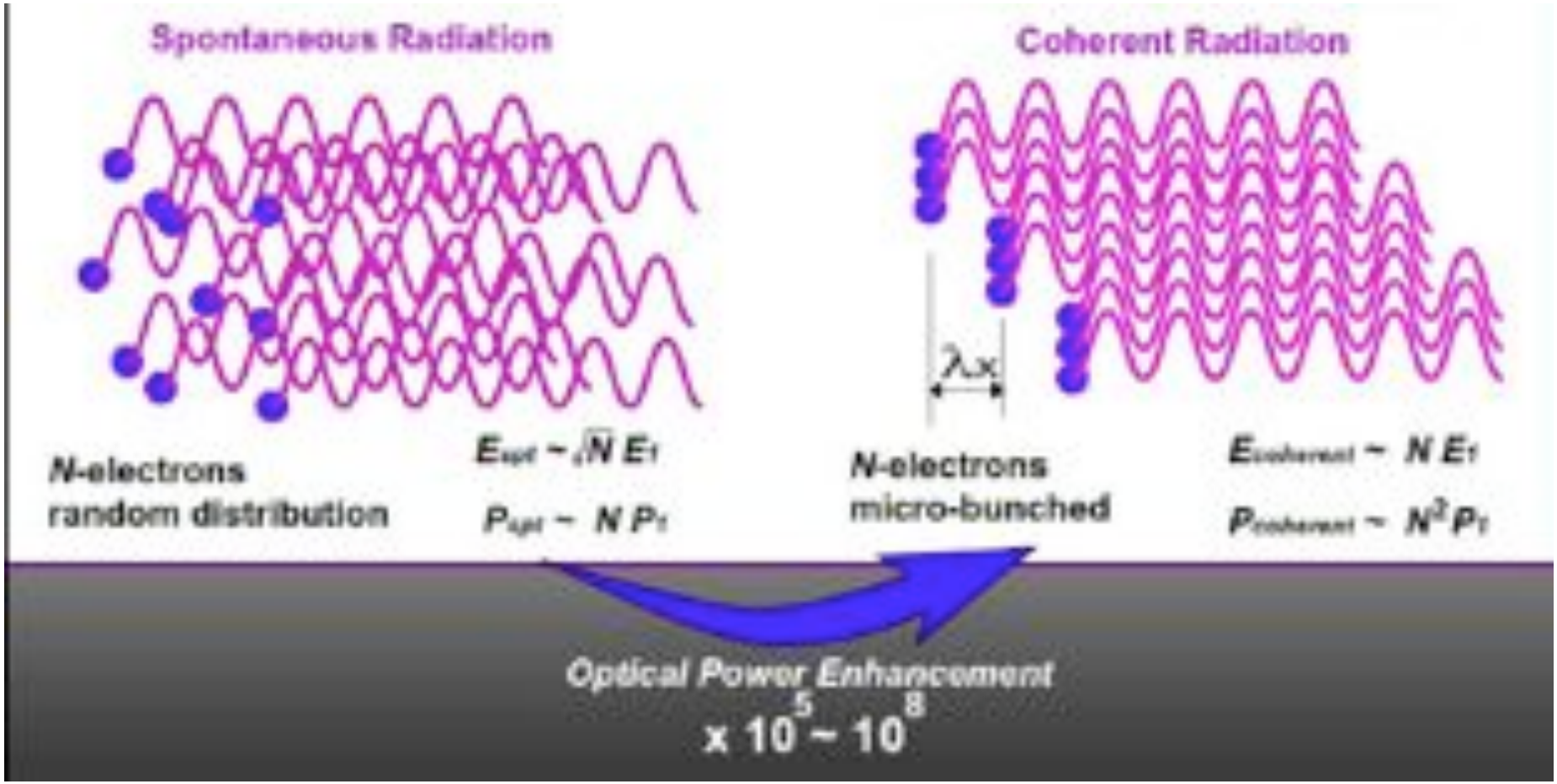
Fourth Generation: spatially coherent sources

Compression of electron bunches to ~100 fs preserving (or even increasing) the brilliance and number of photons per bunch is impossible in a storage ring configuration, where the same electrons run through the undulators 10^5 to 10^6 times per second.

This can however be achieved in a single-pass machine such as a linear accelerator, with suitable bunch compressors.

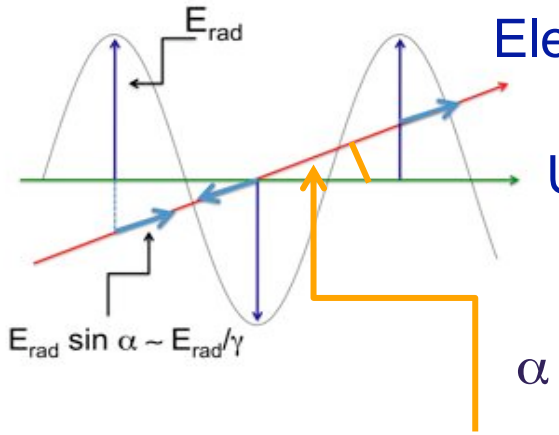
In addition, in a linac, emittance ε is NOT conserved, but $\varepsilon_n = \gamma\varepsilon \sim$ const., with $\gamma = E/mc^2$. It is then possible to reach the condition in which $\varepsilon \sim \lambda$.

Spontaneous vs. coherent rad. in Undulators



(after T. Shintake)

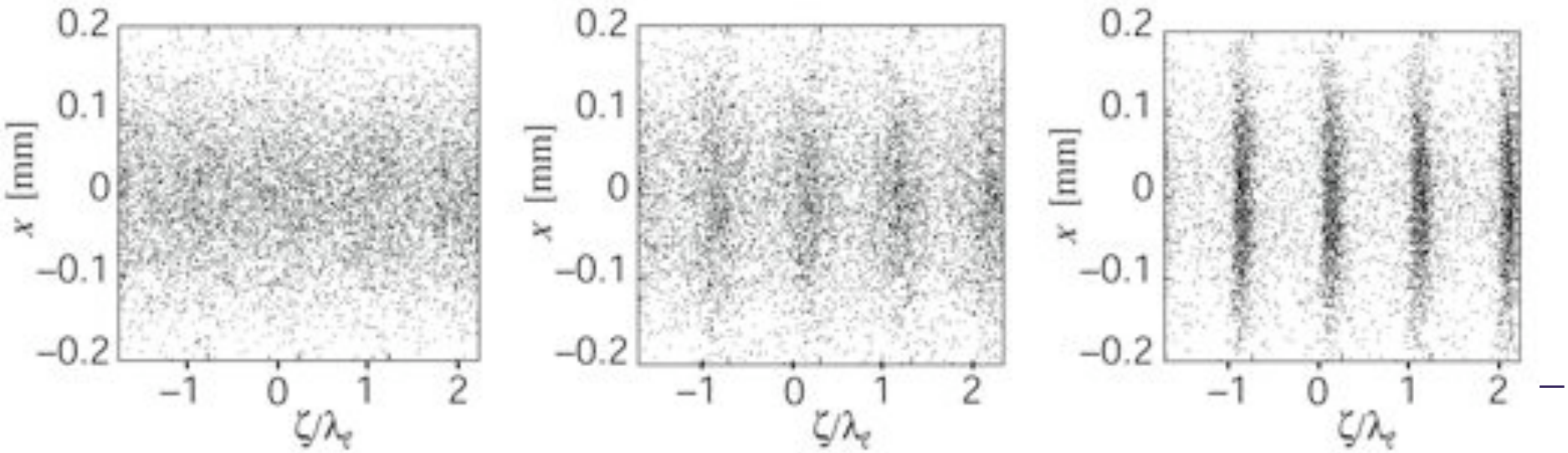
Origin of Microbunching



Electron trajectory

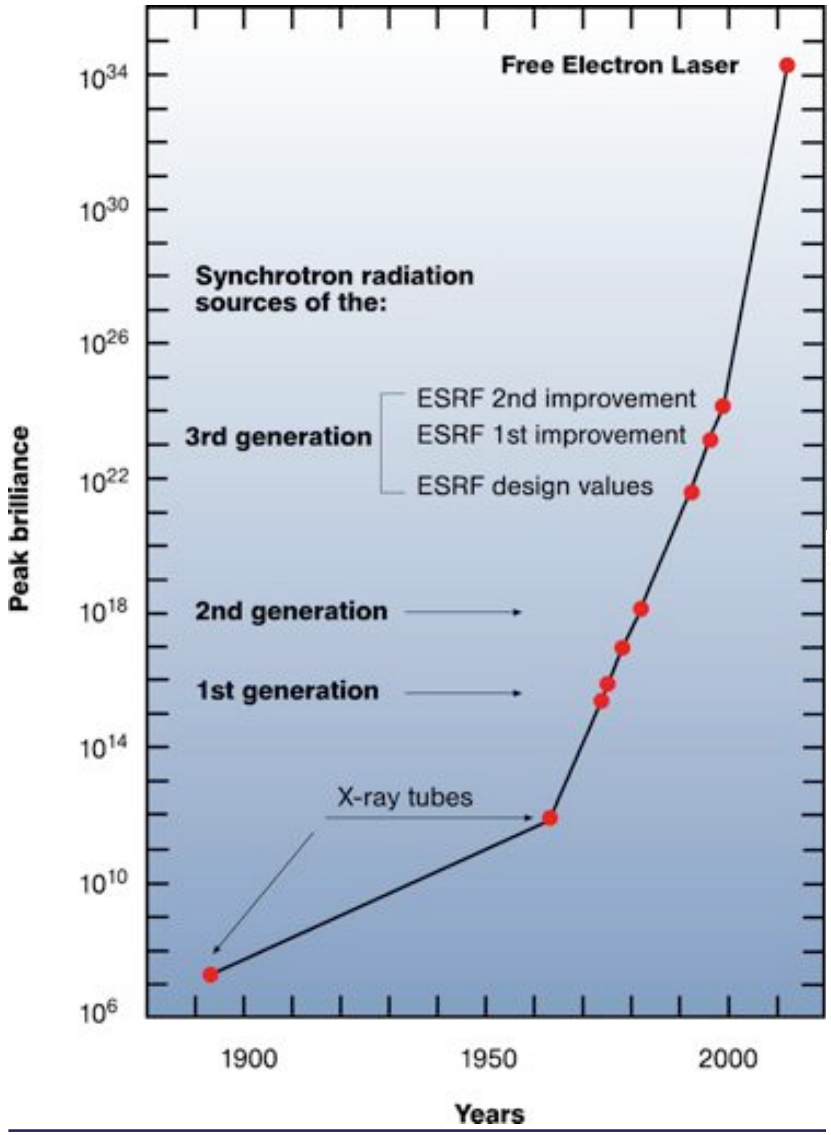
Undulator axis

Radiation electric field has a small component parallel to electron velocity, which can accelerate or decelerate electrons



European XFEL

Peak brilliance of X-ray Sources vs. time



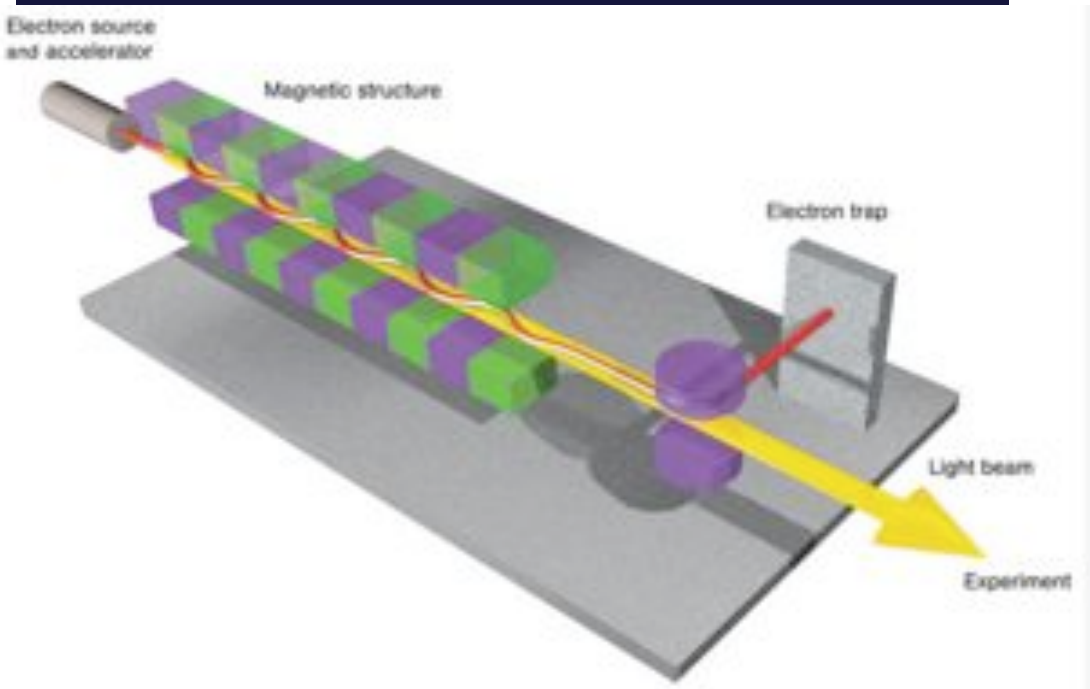
Free Electron Lasers:

- Based on Linear Accelerators

- Deliver ultrashort pulses

(100 fs = 0.1 ps= 10^{-13} s or less)

- (Transversely) Spatially coherent (laser-like) radiation



European XFEL

Today's state of the art

- **FLASH** – Ultraviolet and soft x-ray FEL user facility in Hamburg (down to $\lambda \sim 6.5$ nm) *10^{12} Ph/pulse*

- **SCSS Test Accelerator** – Ultraviolet and soft x-ray FEL user facility at Spring 8, Japan ($\lambda \sim 30 – 60$ nm)

- First beam from **LCLS** (Linac Coherent Light Source), the X-ray FEL using 13.6 GeV electrons from SLAC Linac, Stanford, CA, on April 10, 2009 *10^{12} Ph/pulse*

FLASH at DESY

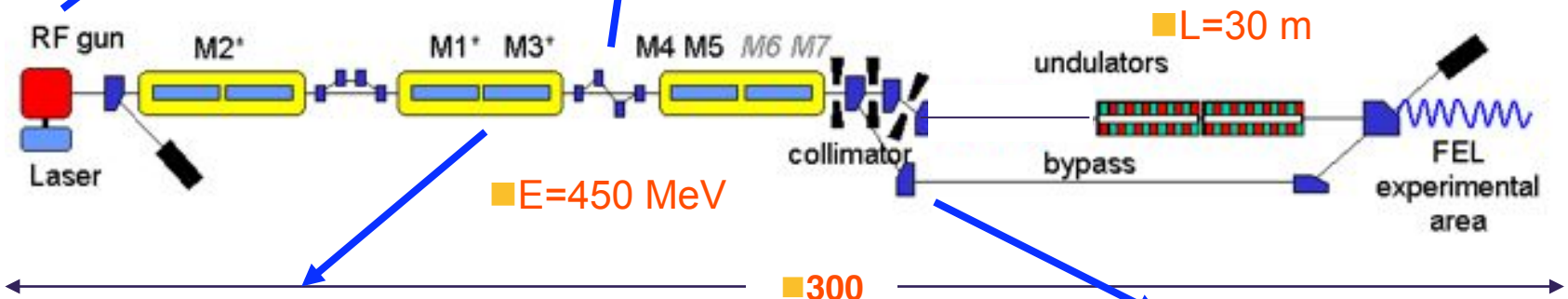
The first SASE FEL operating in the soft X-rays, down to 6.5 nm

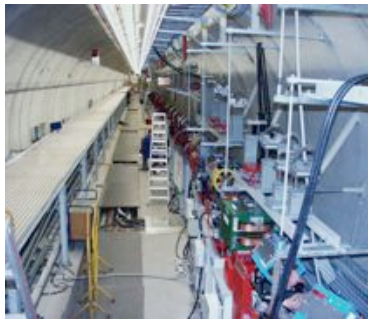
(+3rd, 5th harmonic!)

1 GeV Superconducting

Linear Accelerator



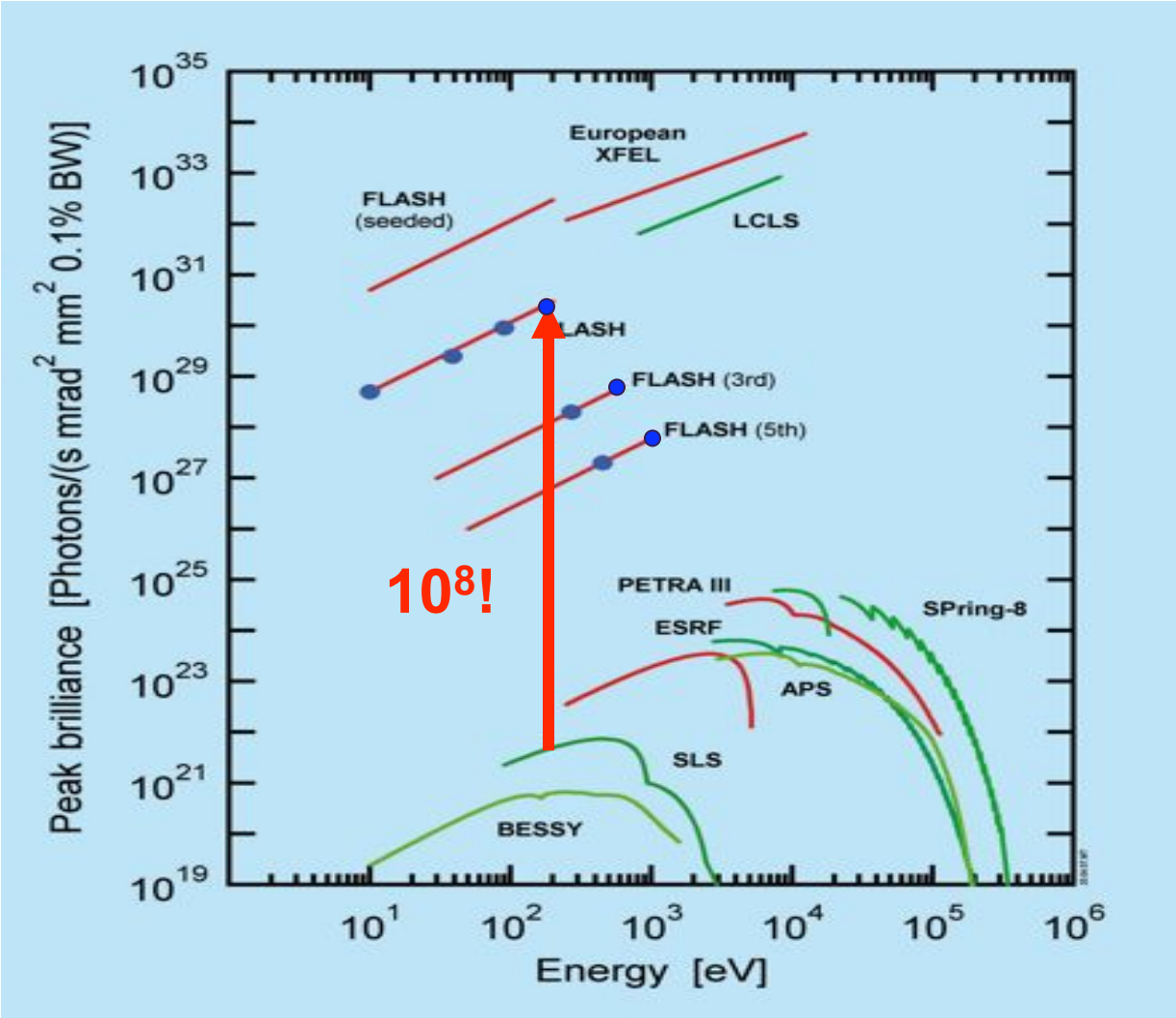



- Jan 2005: first lasing at 32 nm
- Aug 2005: first user exper.

European XFEL

Comparison of 3rd and 4th generation sources



FLASH at DESY

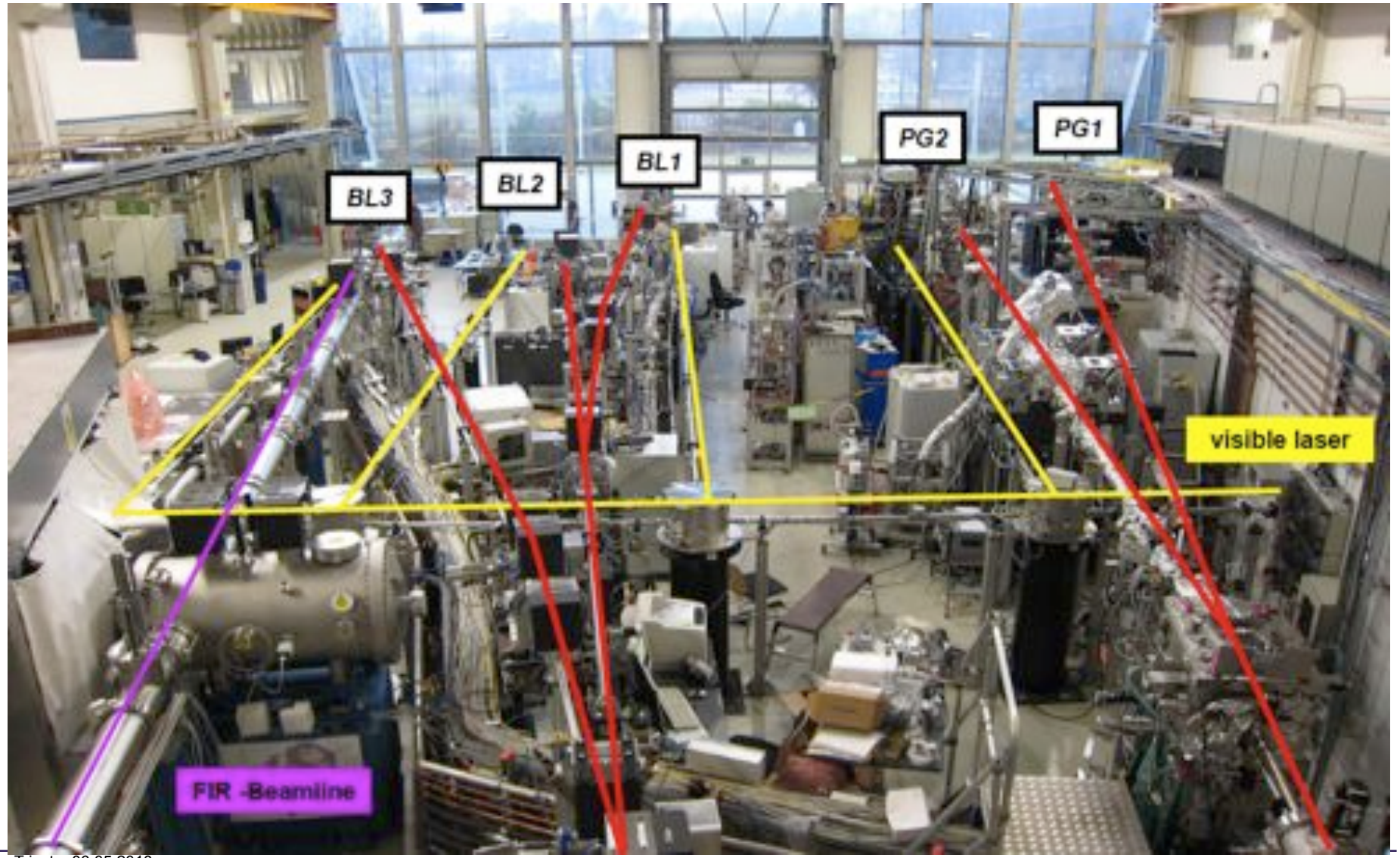
The first SASE FEL operating in the soft X-rays, down to 6.5 nm

(+3rd, 5th harmonic!)

1 GeV Superconducting

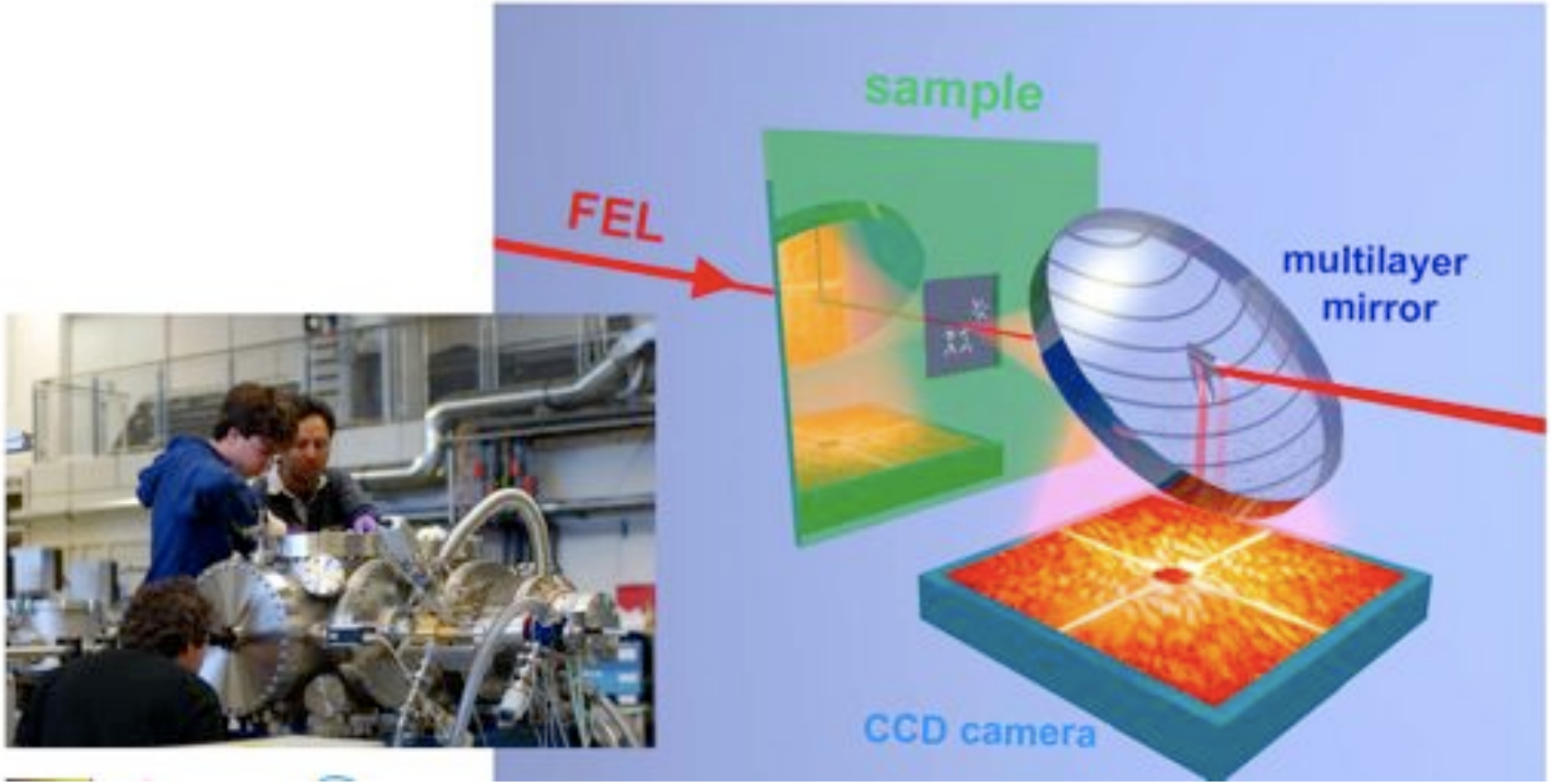
Linear Accelerator

FLASH Experimental Hall



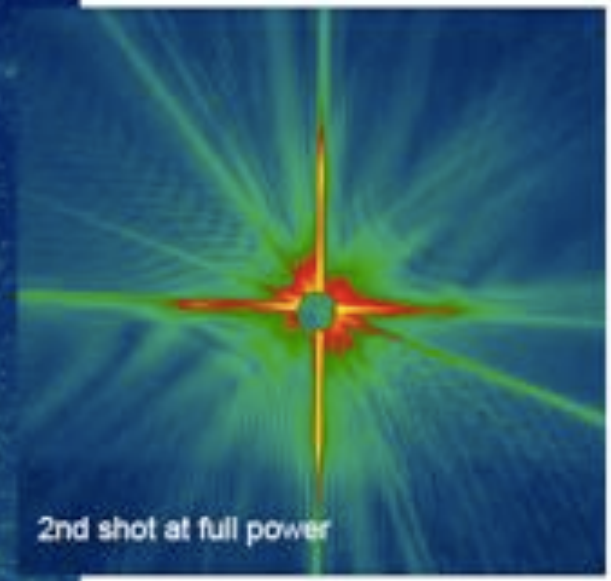
European XFEL

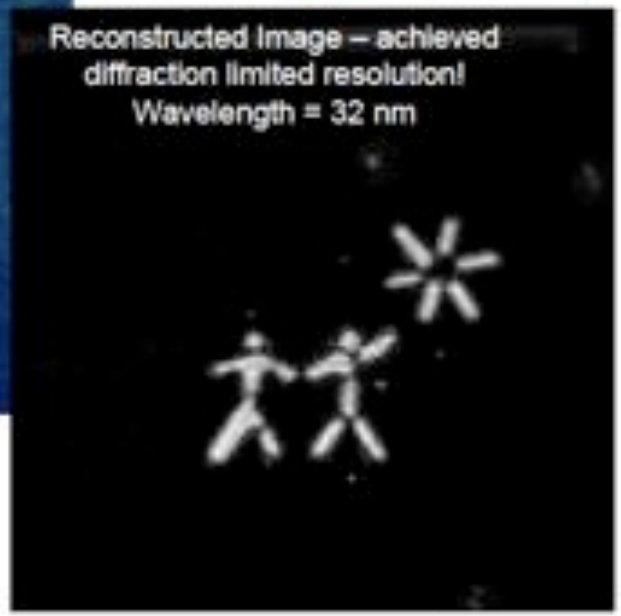
Single-shot (~25 fs, λ ~ 32 nm) imaging



H. Chapman, J. Hajdu et al., *Nature Physics* **2**, 839 - 843 (2006)

Reconstructed Image - 62 nm resolution

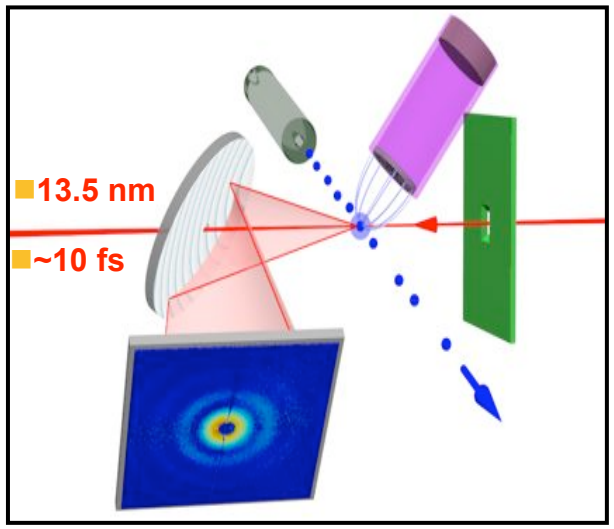


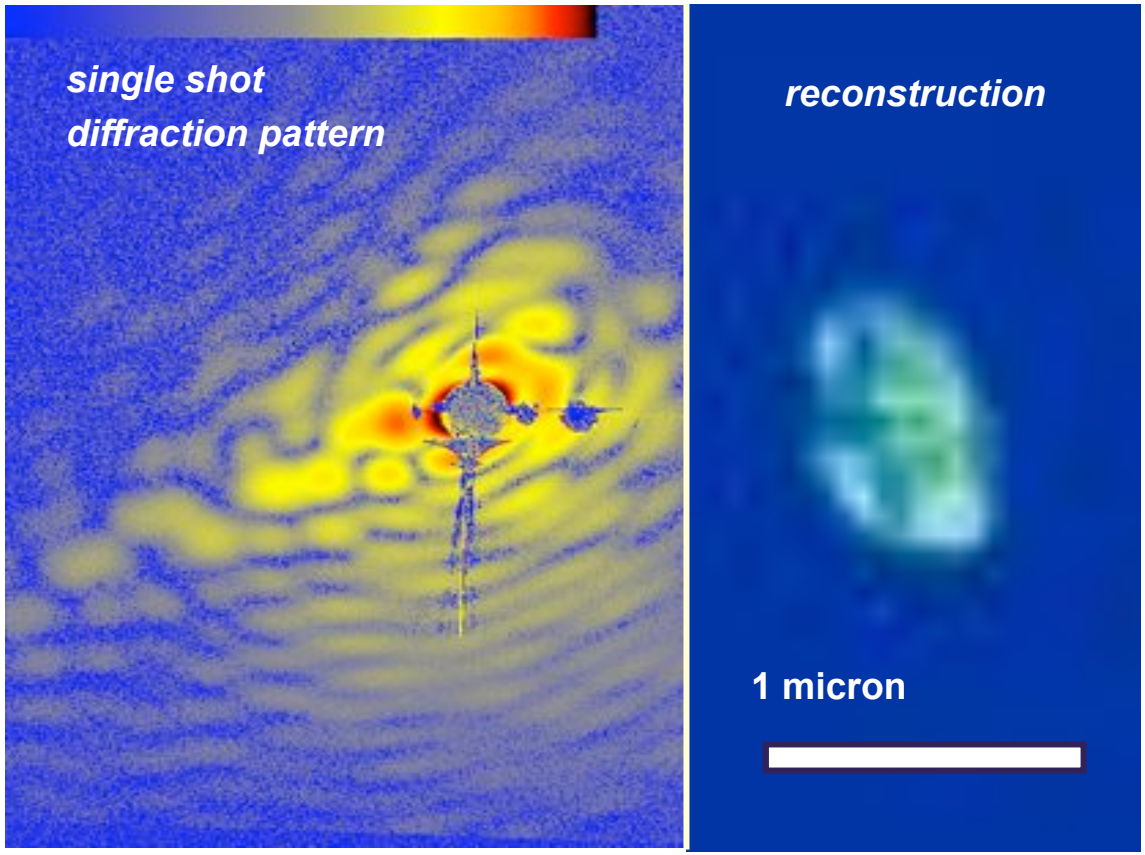


H.N.Chapman et al., Nature Physics 2, 839-843 (2006)

Imaging picoplankton *organism "on the fly"*

- **PICOPLANKTON** ***are the most abundant photosynthetic cells in the oceans (discovered in 1988)***





- ***This cell was injected into vacuum from solution, and shot through the beam at 200 m/s***

- J. Hajdu, I. Andersson, M. Svenda, M. Seibert (Uppsala)
- S. Boutet (SLAC)
- M. Bogan, H. Benner, U. Rohner, H. Chapman (LLNL)

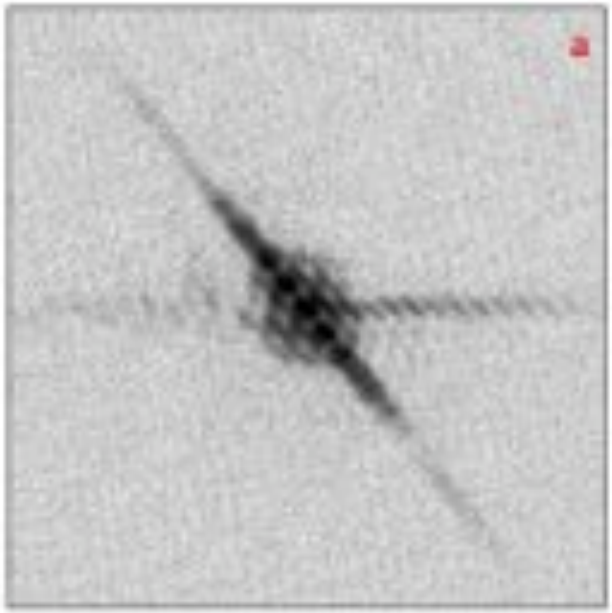
European XFEL

Laser generated harmonics at 32 nm catch up!!

PRL 103, 028104 (2009) PHYSICAL REVIEW LETTERS week ending 10 JULY 2009

Single-Shot Diffractive Imaging with a Table-Top Femtosecond Soft X-Ray Laser-Harmonics Source

A. Ravasio,[1] D. Gauthier,[1] F. R. N. C. Maia,[2] M. Billon,[1] J-P. Caumes,[1] D. Garzella,[1] M. Géléoc,[1] O. Gobert,[1] J-F. Hergott,[1] A-M. Pena,[1] H. Perez,[1] B. Carré,[1] E. Bourhis,[3] J. Gierak,[3] A. Madouri,[3] D. Mailly,[3] B. Schiedt,[3] M. Fajardo,[4] J. Gautier,[5] P. Zeitoun,[5] P. H. Bucksbaum,[6] J. Hajdu,[2,6] and H. Merdji[1,6,*]



HHG seeding demonstrated at SCSS test facility

LETTERS

Injection of harmonics generated in gas in a free-electron laser providing intense and coherent extreme-ultraviolet light

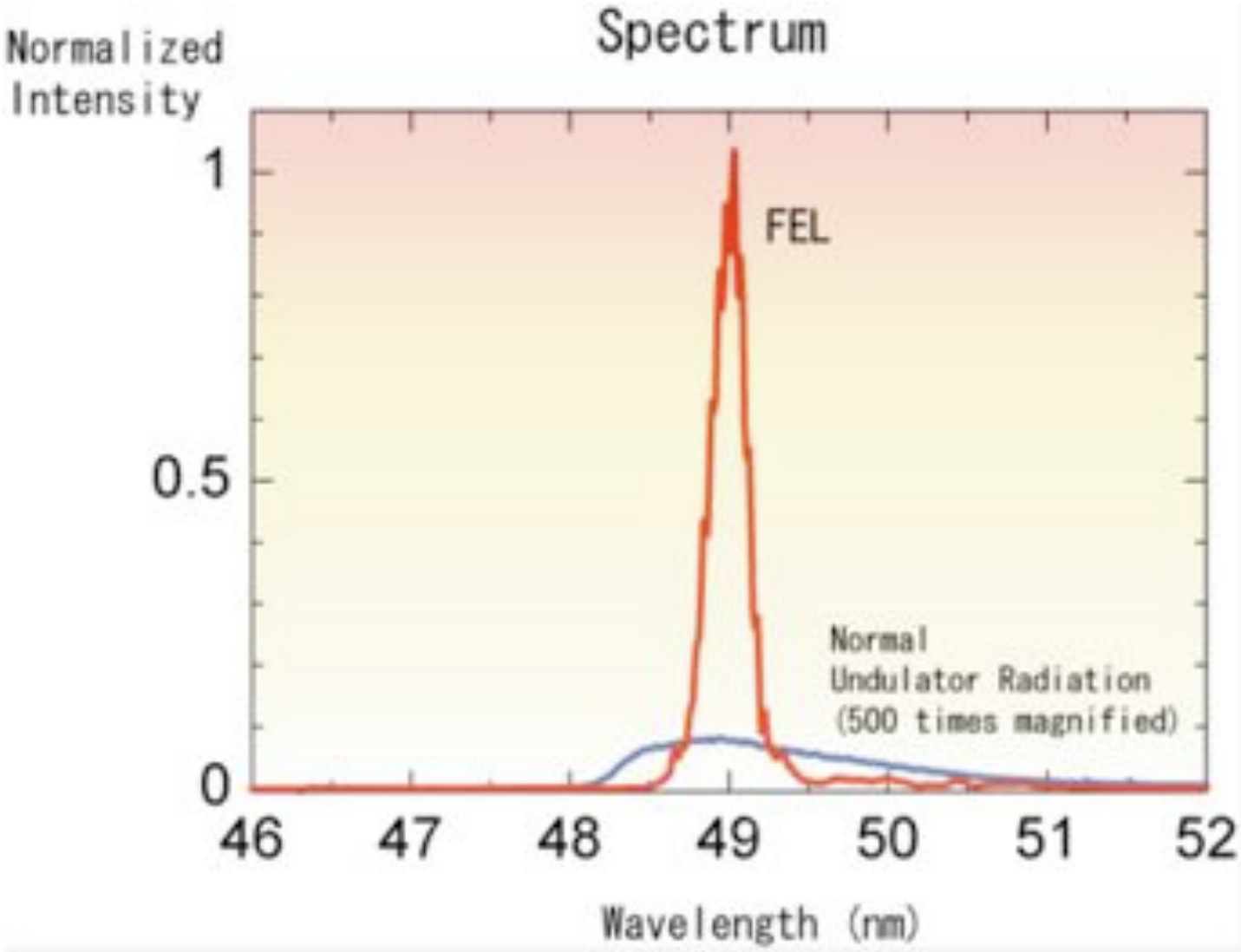
G. LAMBERT[1,2,3]*, T. HARA[2,4], D. GARZELLA[1], T. TANIKAWA[2], M. LABAT[1,3], B. CARRE[1], H. KITAMURA[2,4], T. SHINTAKE[2,4], M. BOUGEARD[1], S. INOUE[4], Y. TANAKA[2,4], P. SALIERES[1], H. MERDJI[1], O. CHUBAR[3], O. GOBERT[1], K. TAHARA[2] AND M.-E. COUPRIE[3]

[1]Service des Photons, Atomes et Molécules, DSM/DRECAM, CEA-Saclay, 91191 Gif-sur-Yvette, France
[2]RIKEN SPring-8 Centre, Harima Institute, 1-1-1, Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5148, Japan
[3]Groupe Magnétisme et Insertion, Synchrotron Soleil, L'Orme des Merisiers, Saint Aubin, 91192 Gif-sur-Yvette, France
[4]XFEL Project Head Office/RIKEN, 1-1-1, Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5148, Japan
*e-mail: guillaume.lambert@synchrotron-soleil.fr

Nature Physics **4**, 296 - 300 (01 Apr 2008)

Published online: 9 March 2008; doi:10.1038/nphys889

SASE at the SCSS test facility



150 MeV
Linac

Experimental Layout for HHG

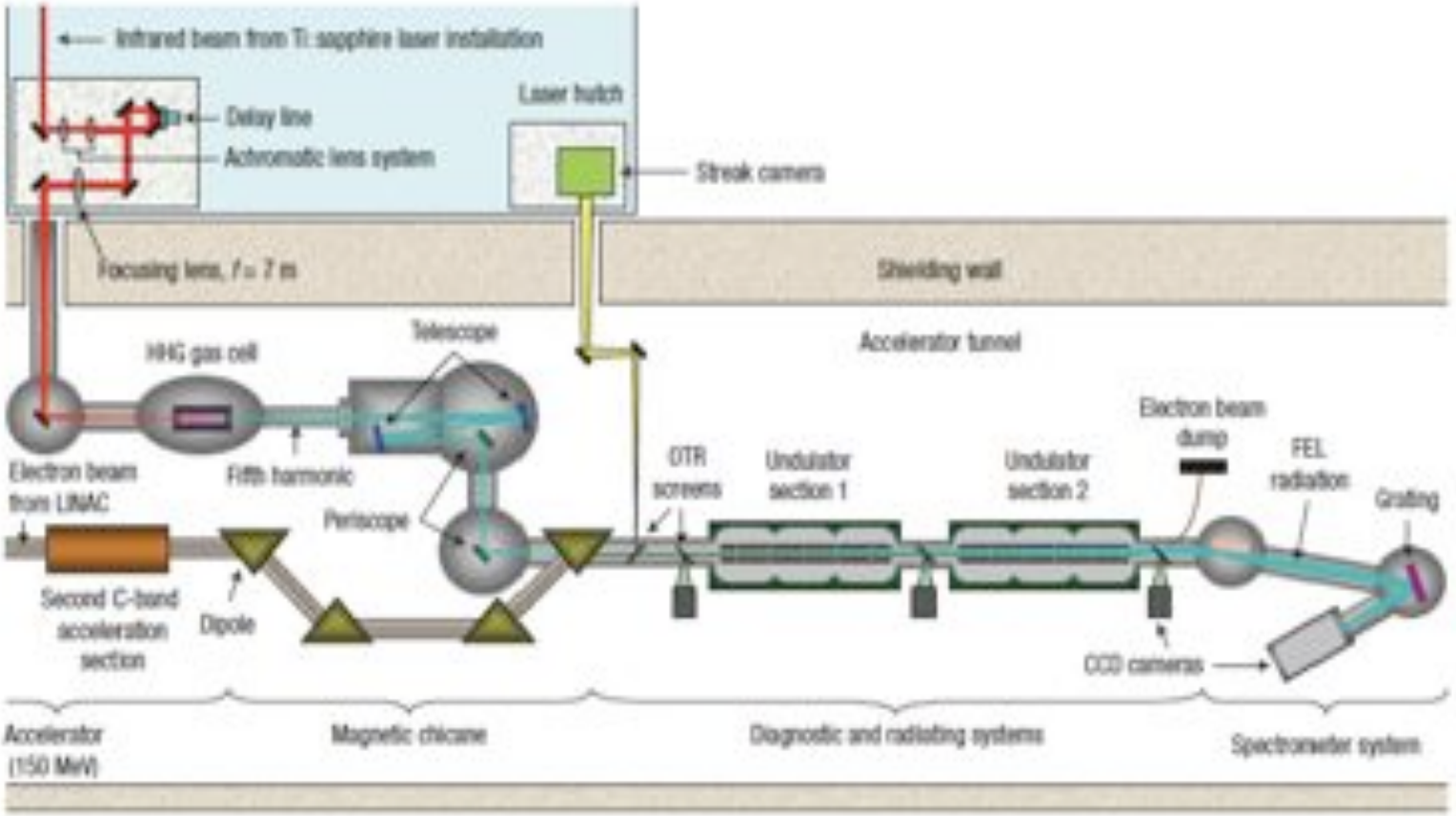


Figure 1 Layout of the experiment. A Ti:sapphire laser (800 nm, 20 mJ, 100 fs FWHM, 10 Hz) is loosely focused into a xenon gas cell (focal length $f = 7$ m), optimizing HHG output. Using the telescope and periscope optics (CaF_2 mirrors), the HHG seed beam is spectrally selected, refocused and spatially and temporally overlapped with the electron beam (150 MeV, 1 ps FWHM, 10 Hz—LINAC stands for linear accelerator) in the two consecutive undulator sections 1 and 2, which are both tuned to 160 nm, corresponding to the fifth harmonic of the laser. The beam position is monitored on optical transition radiation (OTR) screens.

Lambert et al.

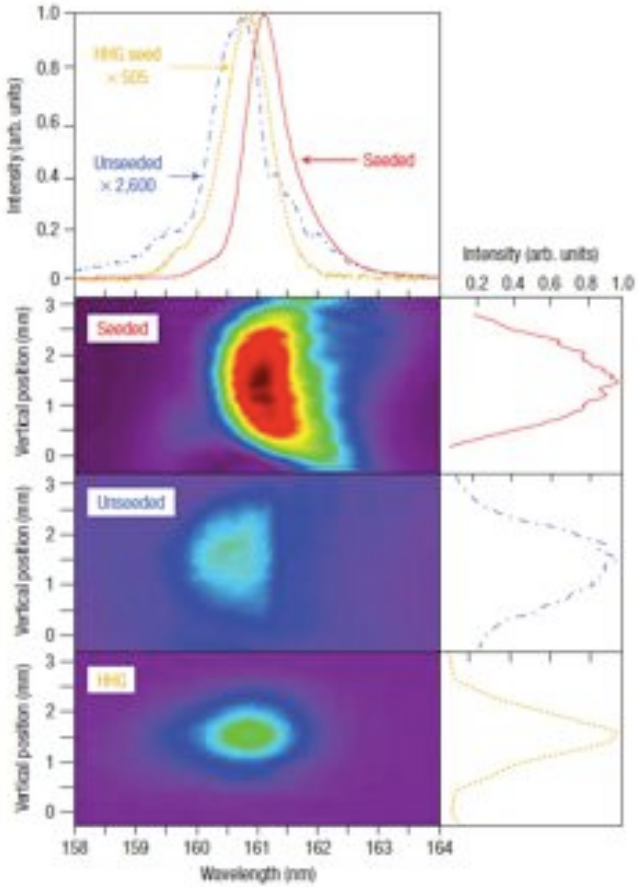


Figure 2 Comparison between the FEL seeded emission, the unseeded emission and the HHG seed at the fundamental wavelength (160 nm). The spatial (vertical) and spectral distributions are mapped on the CCD (charge-coupled device) camera of a spectrometer; spatial (right) and spectral (up) profiles are plotted at maximum intensity. The lines correspond to the seeded (single shot, line) and unseeded emission (averaged on 10 shots, dash–dot) and the HHG seed (single shot, dots). The seed pulse energy was 0.53 nJ and only the first undulator section was used for amplifying the HHG pulse.

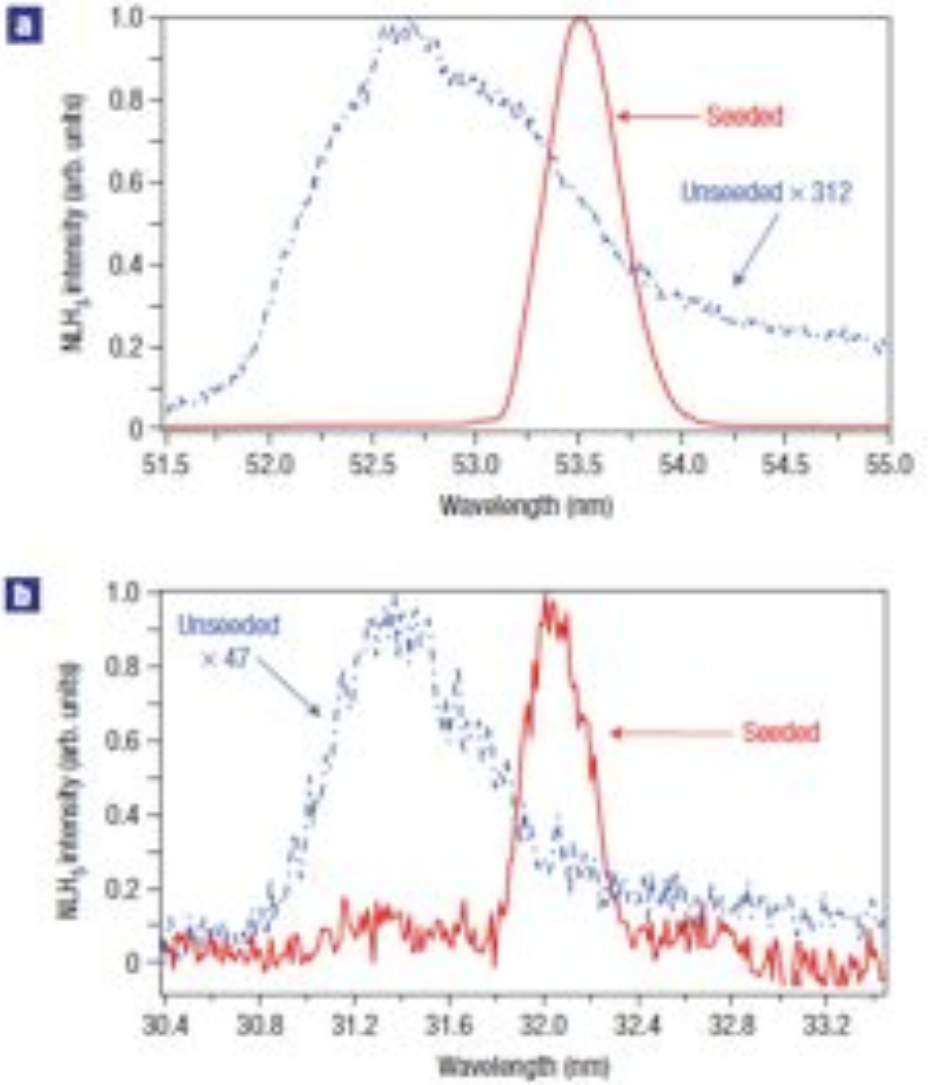


Figure 3 Spectra of the FEL seeded and unseeded emission at the wavelengths of the third and fifth NLHs. The spectra have been obtained by integrating the two-dimensional distributions of the CCD images (as for Fig. 2) over the vertical dimension. The seeded (single shot, line) and unseeded (averaged on 10 shots, dash–dot) FEL emissions are plotted for the third (a) and fifth (b) NLHs. The seed pulse energy was 0.53 nJ and only the first undulator section was used for radiating the NLHs.

European XFEL

April 10, 2009: the big news from LCLS!

1.5 Å Coherent X-rays!!

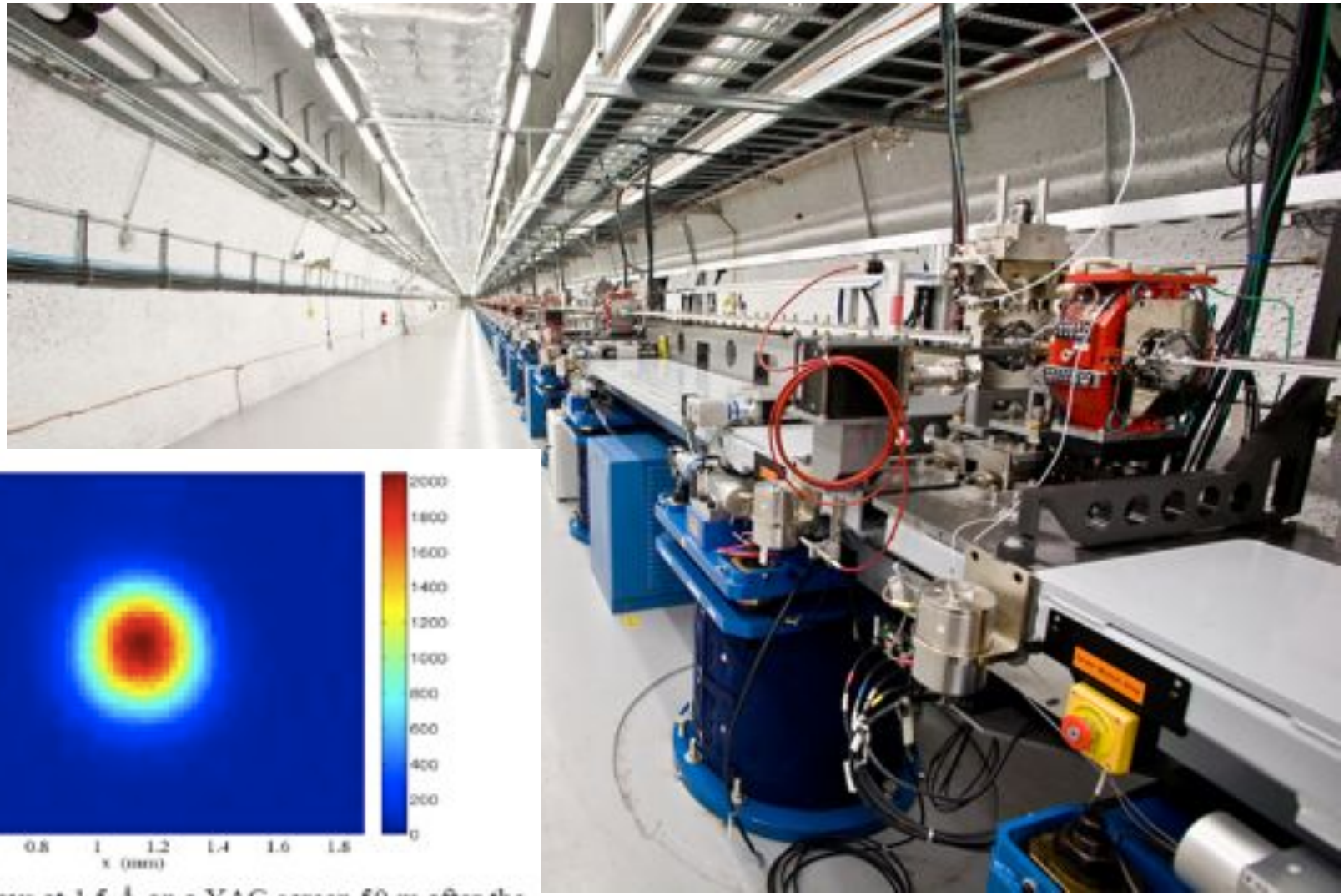


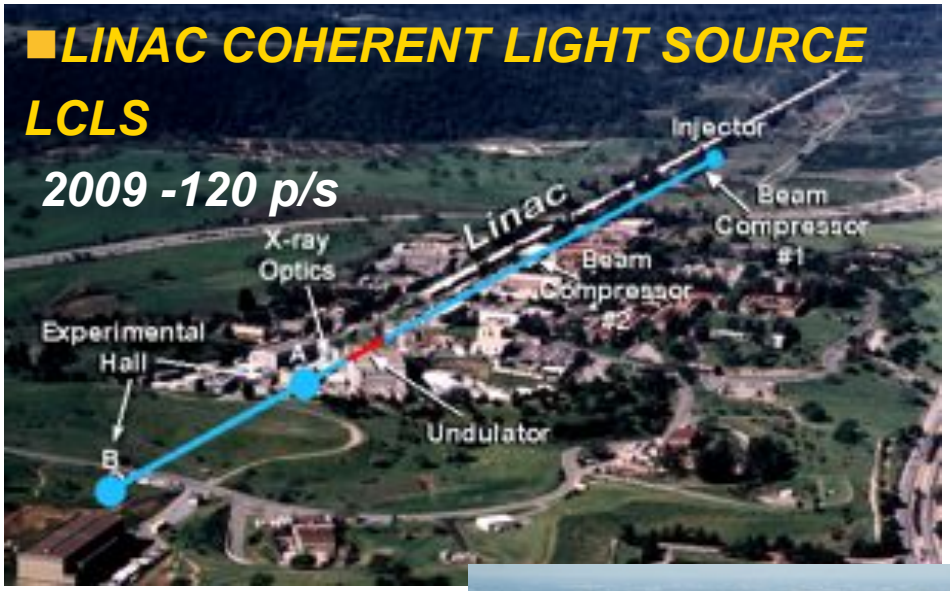
Figure 10: FEL x-rays at 1.5 Å on a YAG screen 50 m after the last inserted undulator (see Table 1 for measured parameters).

Hard x-ray FEL Projects

■ *LINAC COHERENT LIGHT SOURCE*

LCLS

2009 -120 p/s



2011-60 p/s

■ *SCSS*

SPring-8 Compact SASE Source

■ *European XFEL Facility*

2014 - 27 000 p/s

European XFEL

The European XFEL

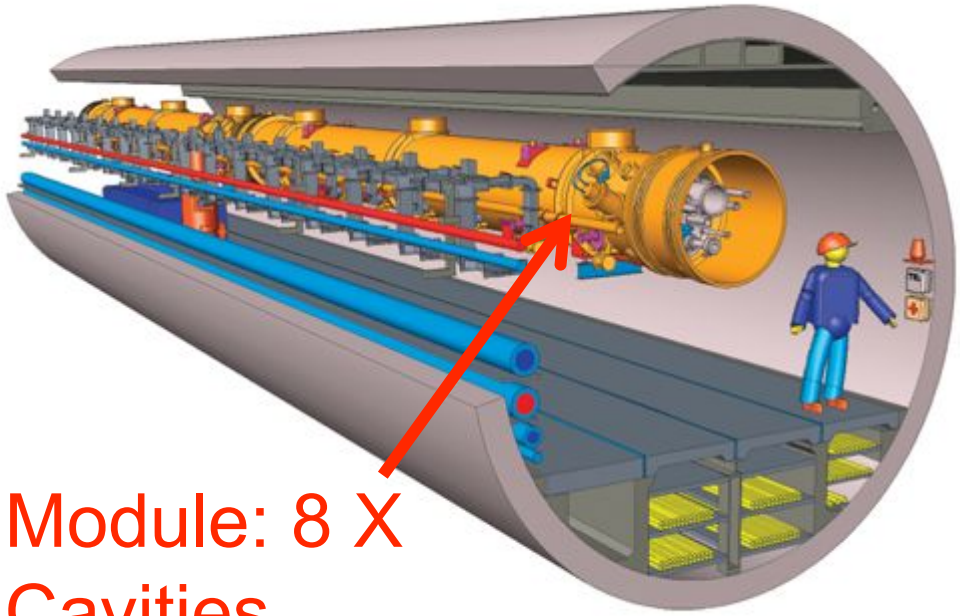

European XFEL
Enlightening Science
Licht der Zukunft
DESY
ARGE Tunnel XFEL


European XFEL
HOCHTIEF

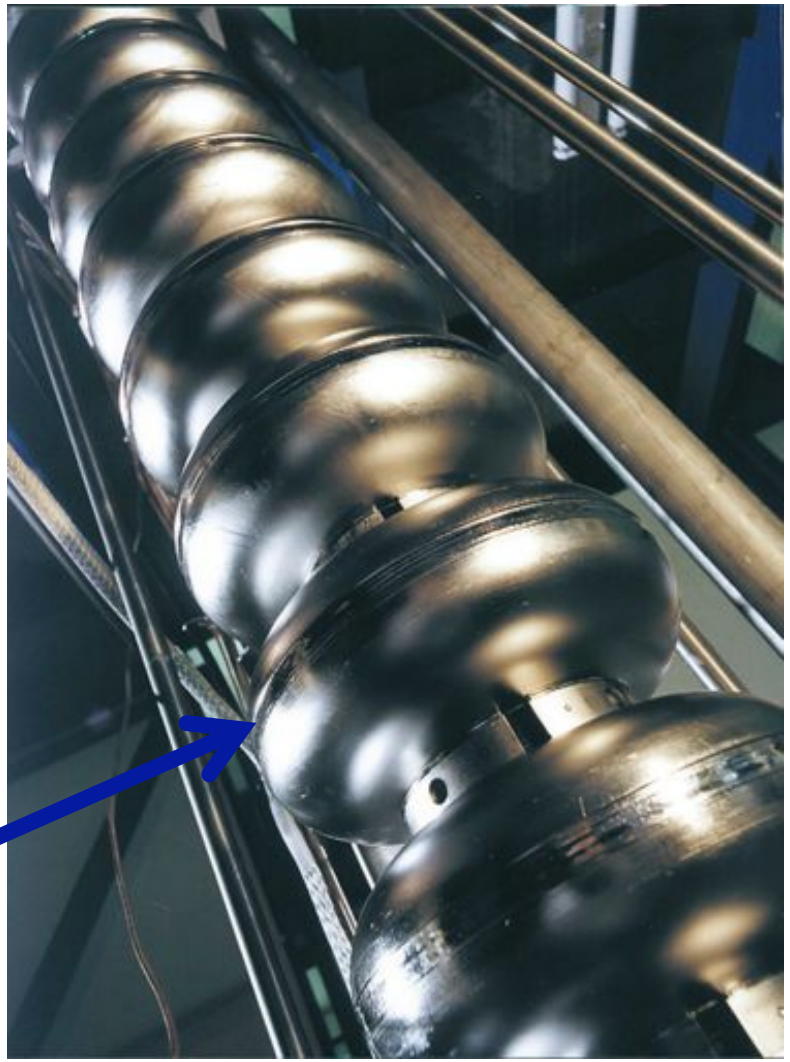
European XFEL

Superconducting "TESLA" Technology

100 8-Cavity modules, 1.4 km, 17.5 GeV Electron Energy



Module: 8 X Cavities



Niobium Cavities

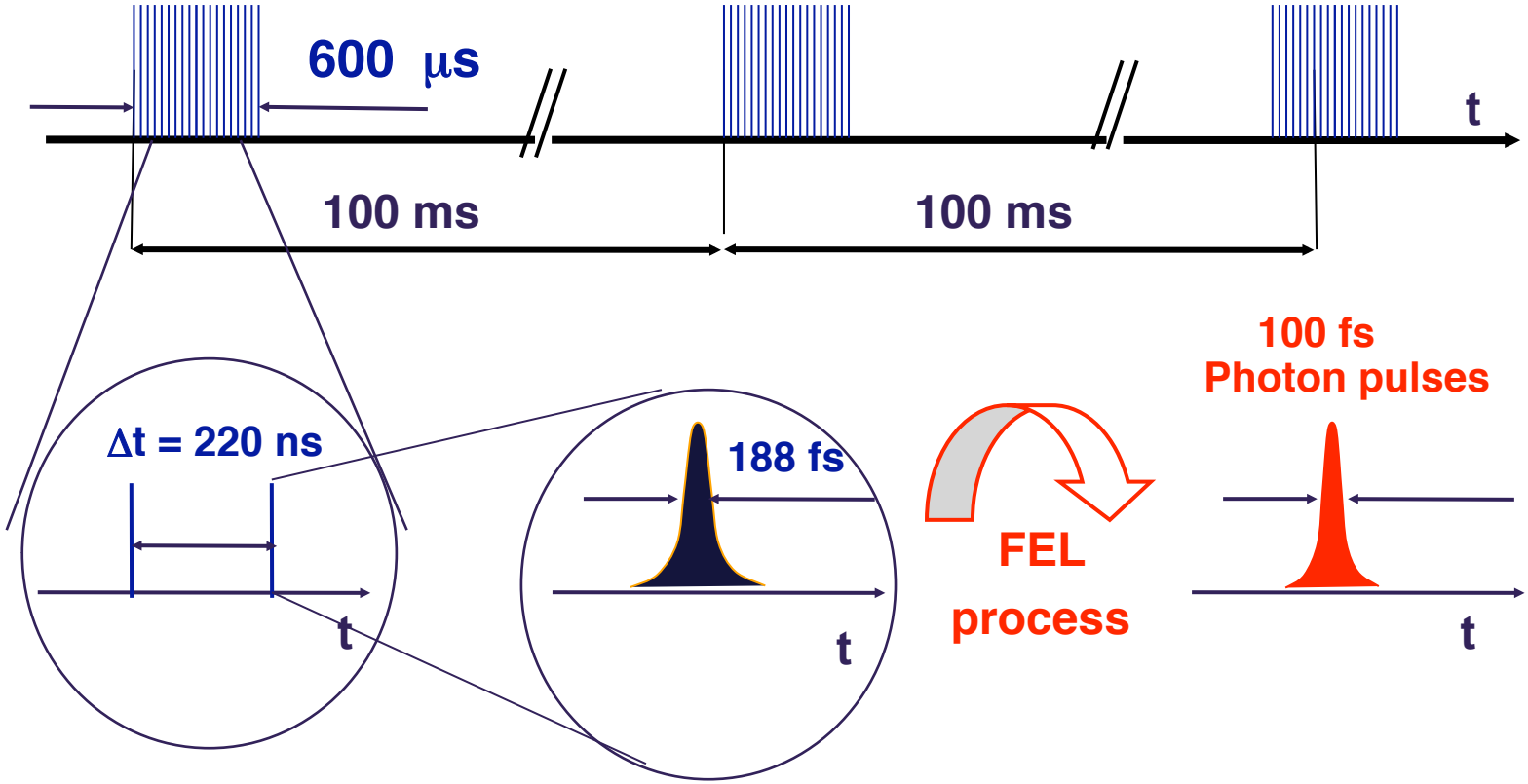
Module PXFEL1 on the test bench

China
France
Germany
Italy
Spain

Photo:
D. Kostin, DESY

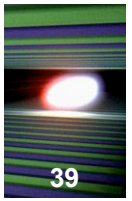
European XFEL Project - Time Structure

Electron bunch trains (with up to 2700 bunches à 1 nC)



Alternatively: 20 bunch trains / second, 300 µs long, with up to 1350 bunches each…

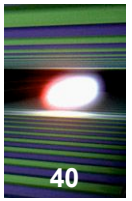
Comparison of the X-ray FEL Projects



	LCLS (USA)	SCSS (JAPAN)	EUROPEAN XFEL (SASE1)
Max. Electron Energy (GeV)	14.3	8.0	17.5
Minimum Wavelength(nm)	0.15	0.13	0.10
Peak Brilliance	1.5 10^33	1. 10^33	5. 10^33
Average Brilliance	4.5 10^22	1.5 10^23	1.6 10^25
Pulses/s	120	60	27 000
Photons/pulse	10^12	2 10^11	10^12
First Beam	2009	2011	2014

European XFEL

Scientific applications of X-ray FEL's

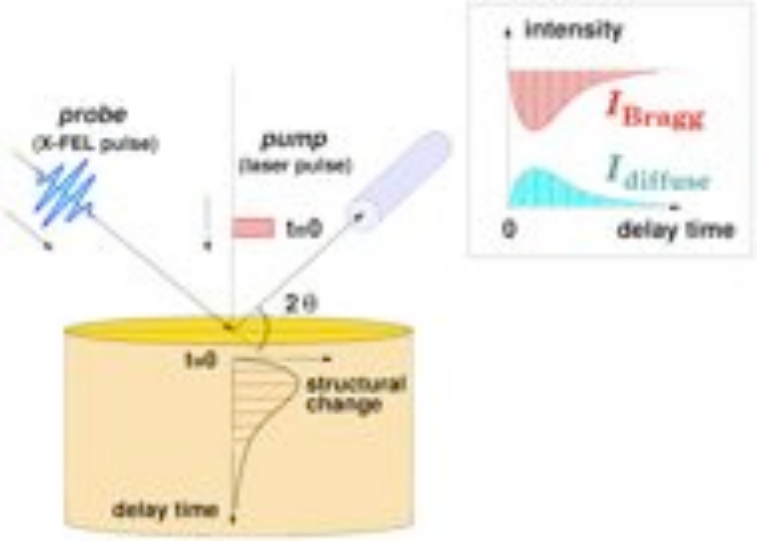


- Time-resolved, pump-and-probe experiments
- Coherent-diffraction imaging of nanoscale objects, down to *single macromolecules*
- Speckle Scattering and Photon-Correlation Spectroscopy
- High Energy-Density science

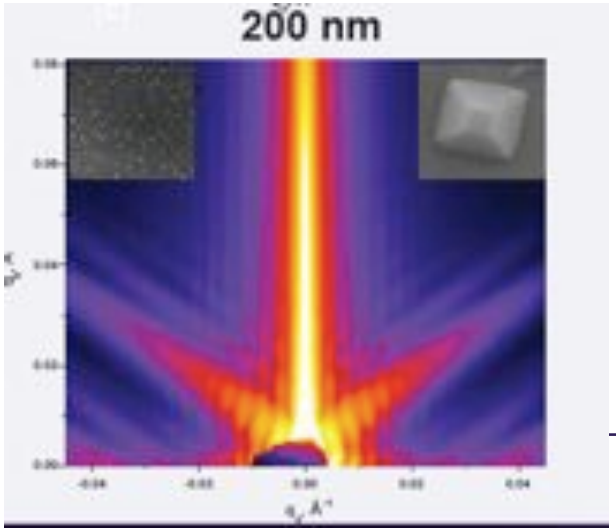
European XFEL

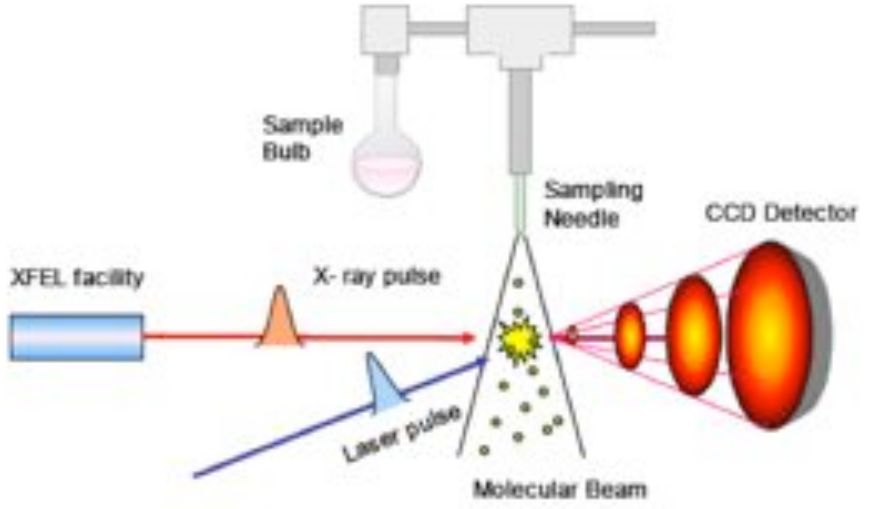
Scientific applications of hard X-ray FEL's

- Time-resolved, pump-and-probe experiments



- Coherent-diffraction imaging of nanoscale objects, down to *single macromolecules*

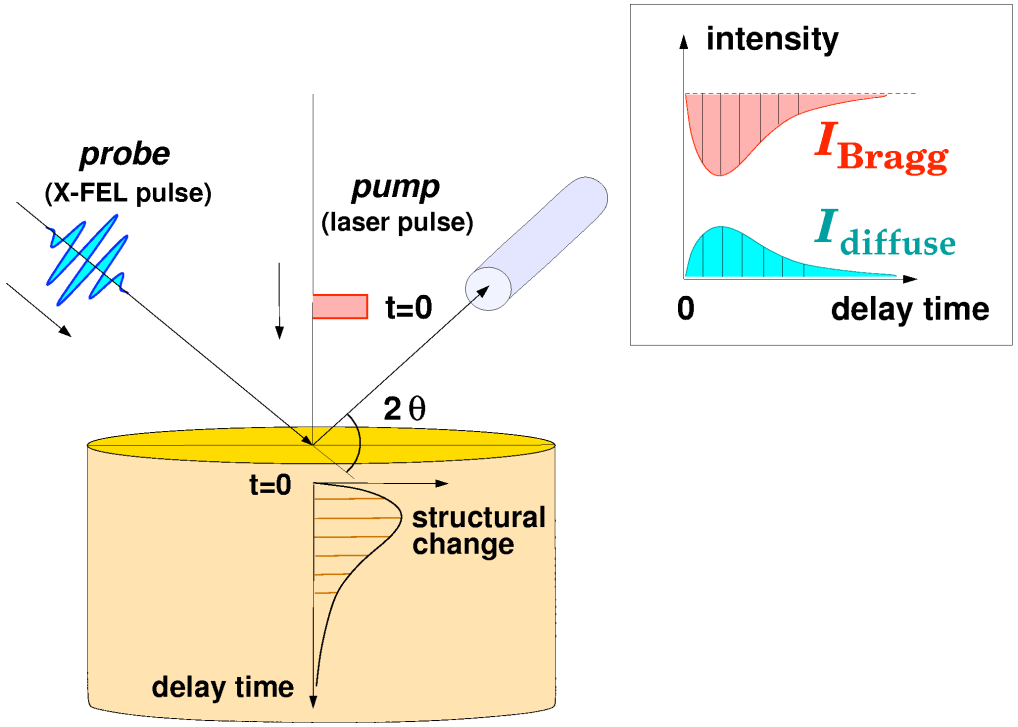




Pump and Probe Experiments

Today: study (structure) and dynamics on a ns to ps timescale

XFEL: study (structure) and dynamics on a ps to fs scale



European XFEL

InSb inertial dynamics at SPPS

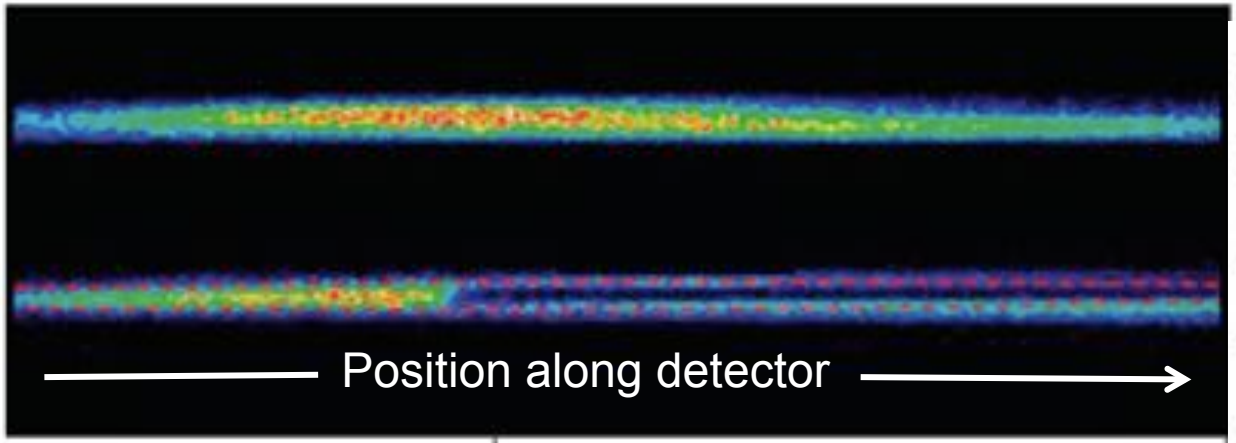
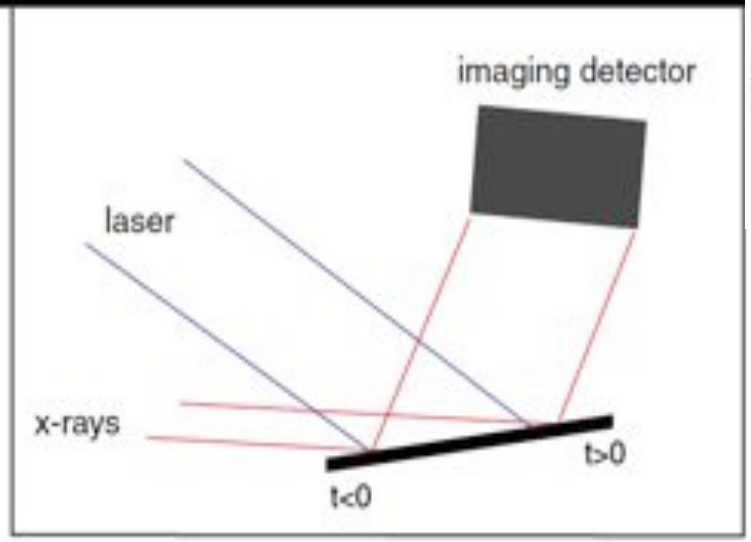
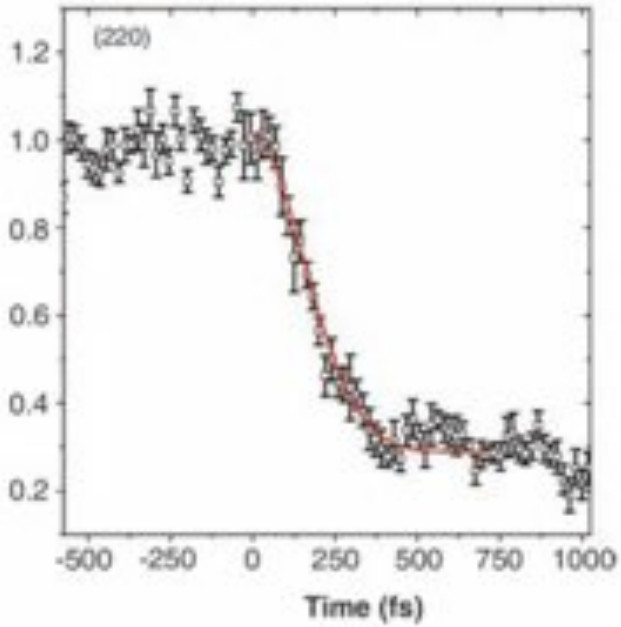


Fig. 1. (Top) A single-shot image of scattered x-rays from unperturbed sample above a single-shot image of perturbed sample. Dashed curves show region excited by laser pulse. (Bottom) Experimental setup showing cross-beam topography technique. By crossing the pump and probe beams on the sample and imaging the diffracted x-rays, we mapped temporal information into spatial information, enabling collection of the complete time history around time zero in a single shot. Time runs from left to right. The time window shown is ~8 ps.





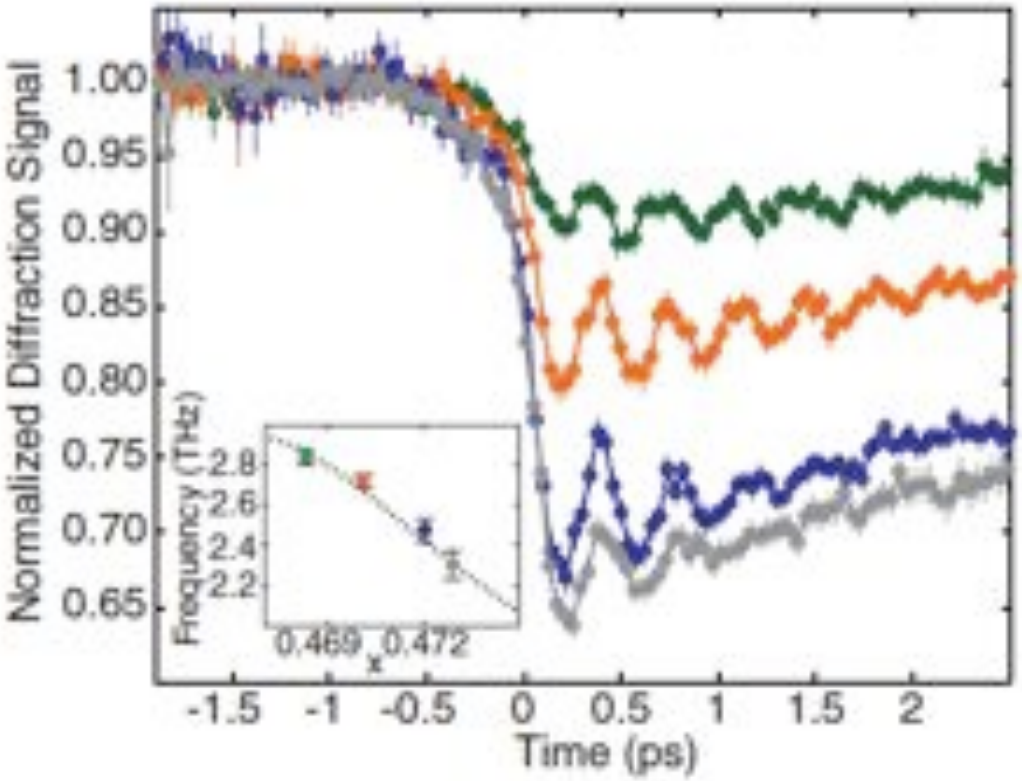
(220) Reflection intensity as a function of time

A.M. Lindenberg *et al.*, Science **308**, 392 (2005)

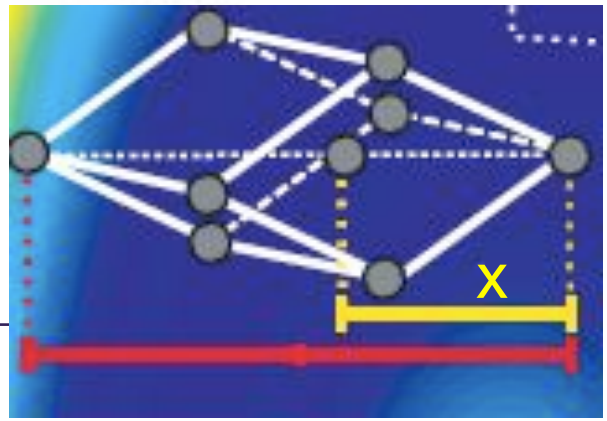
European XFEL

Ultrafast bond-softening in Bi (SPPS)

Fig. 1. Bismuth (111) x-ray diffraction efficiency as a function of time delay between the optical excitation pulse and x-ray probe for excitation fluences of 0.7 (green), 1.2 (red), 1.7 (blue), and 2.3 mJ/cm^2 (gray). The zero-delay point was set at the half maximum of the initial transient drop. The inset displays the optical phonon frequency as a function of the normalized atomic equilibrium position along the body diagonal of the unit cell x as measured by x-ray diffraction. The dotted curve represents the theoretical prediction obtained from DFT calculations of the excited-state potential-energy surface (*10*).



D.M. Fritz et al., Science, 315, 633 (2007)



European XFEL

What do protein crystallographers dream of ?

Nature **459**, 24 (7 May 2009)

STRUCTURES OF DESIRE

What do protein crystallographers dream of? The eukaryotic ribosome, the spliceosome, the nuclear-pore complex, the HIV trimer and almost any transmembrane protein, finds **Ananyo Bhattacharya**.

….Wayne Hendrickson of Columbia University in New York says there is also a lot of excitement about technologies that might be possible at facilities such as the European XFEL (X-Ray Free Electron Laser) under construction in Hamburg, Germany …The idea here is that an extremely short burst of X-rays could be scattered off a single protein molecule, blowing it apart but revealing something about its structure before the disintegration. "You are in principle able to capture the molecule in action," Hendrickson says....

European XFEL

(…After J. Hajdu)

Problems with conventional imaging in biology:

(1) Inability to obtain high resolution structures for non-reproducible objects of any type

(2) Problems with large reproducible objects

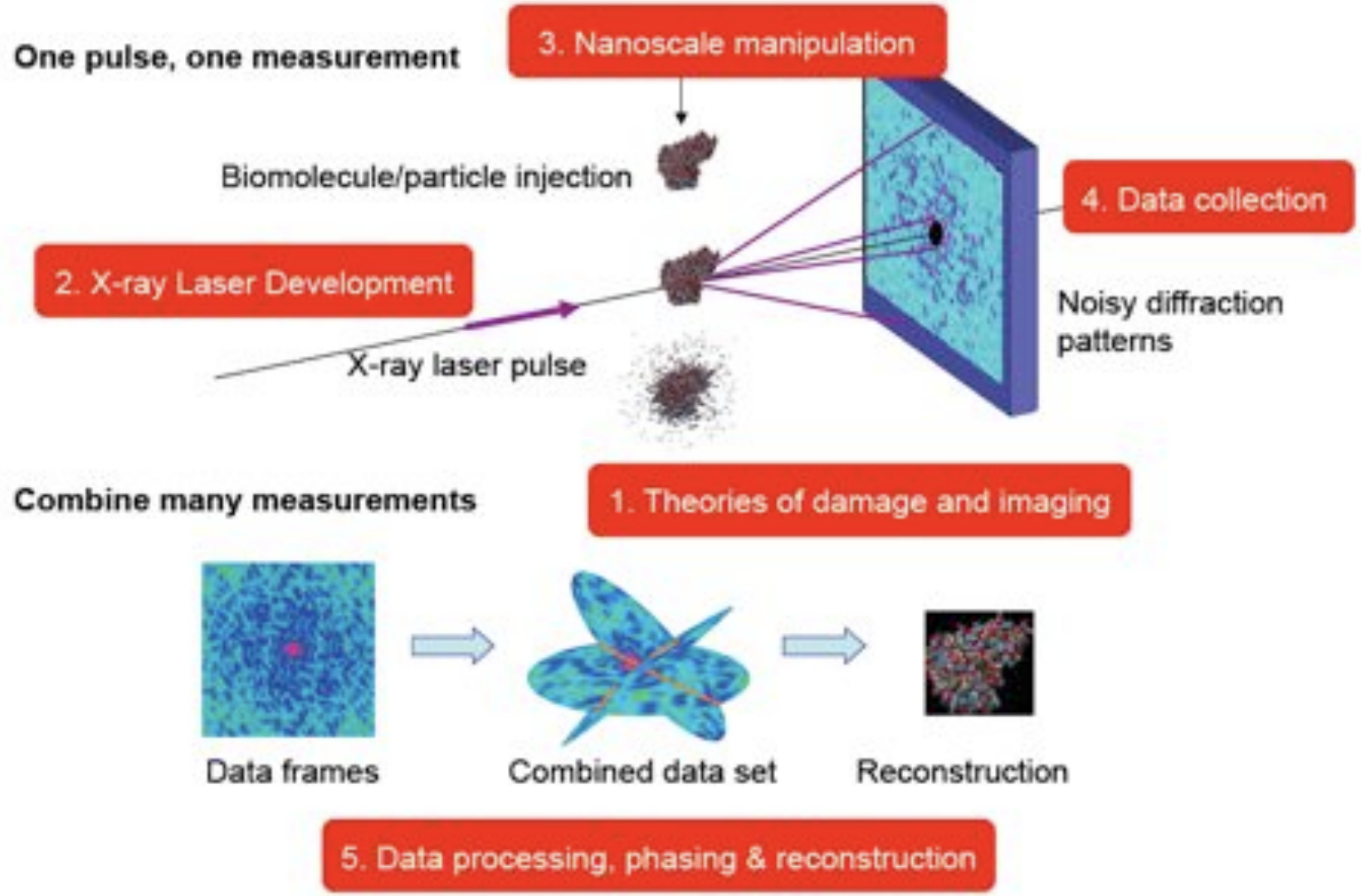
(3) Problems with crystallography
- Resolution depends on crystal quality (1D, 2D and 3D cryst.)
- Does it crystallise at all?

(4) Problems with the 4th dimension

Ultra-fast coherent scattering carries promise here

European XFEL

Single-Molecule X-ray Imaging



European XFEL

ARTICLES
PUBLISHED ONLINE: 9 NOVEMBER 2008 | DOI: 10.1038/NPHYS1129
nature physics

Structure from fleeting illumination of faint spinning objects in flight

Russell Fung, Valentin Shneerson, Dilano K. Saldin and Abbas Ourmazd*

Moves are afoot to illuminate particles in flight with powerful X-ray bursts, to determine the structure of single molecules, viruses and nanoparticles. … Using a new approach, we demonstrate the recovery of the structure of a weakly scattering macromolecule at the anticipated next-generation X-ray source intensities. Our work closes a critical gap in determining the structure of single molecules and nanoparticles by X-ray methods, and opens the way to reconstructing the structure of spinning, or randomly oriented objects at extremely low signal levels.

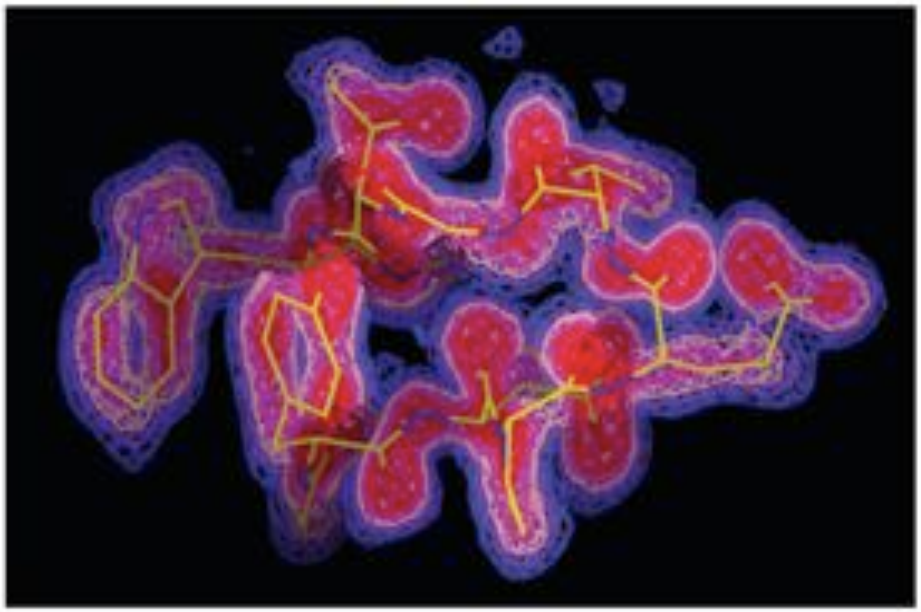
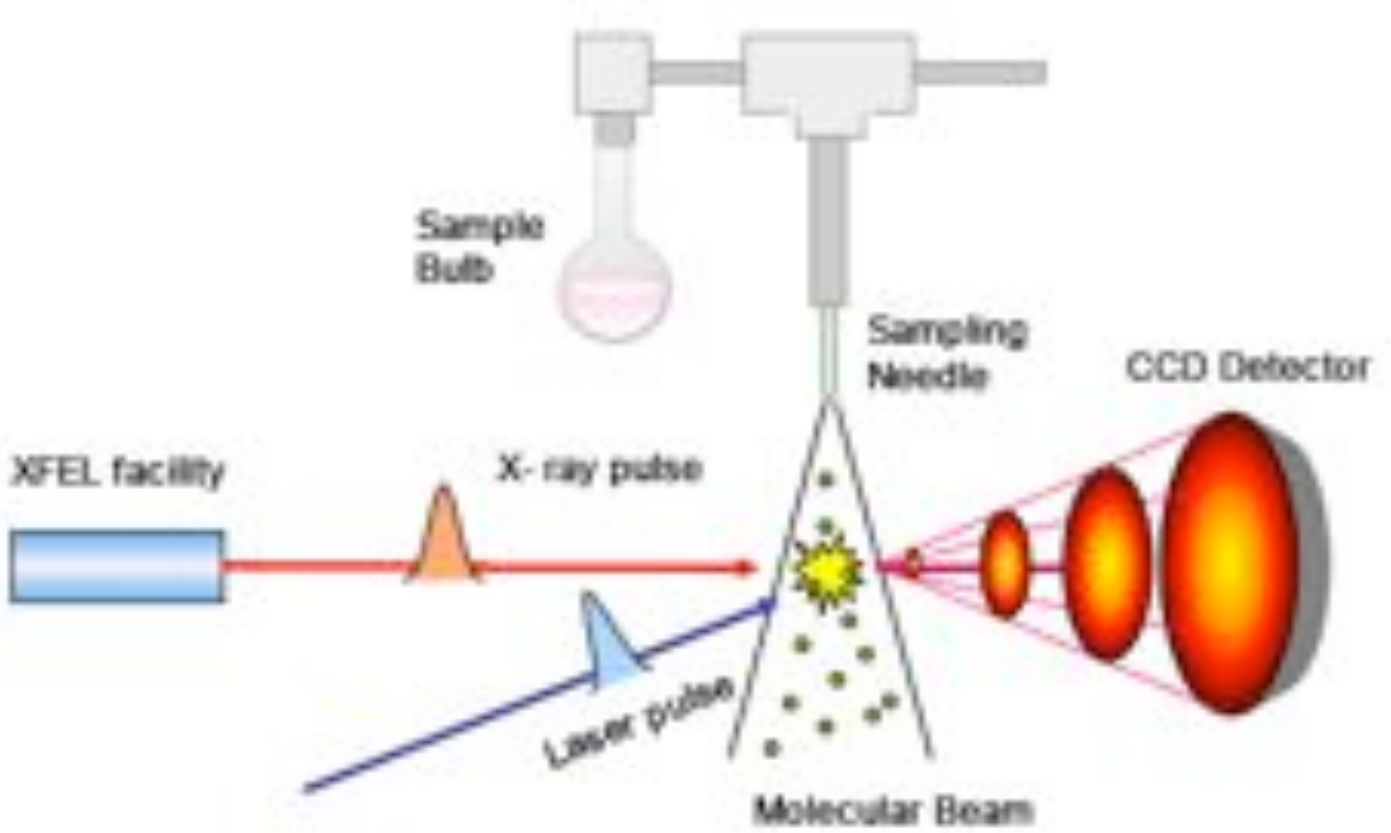


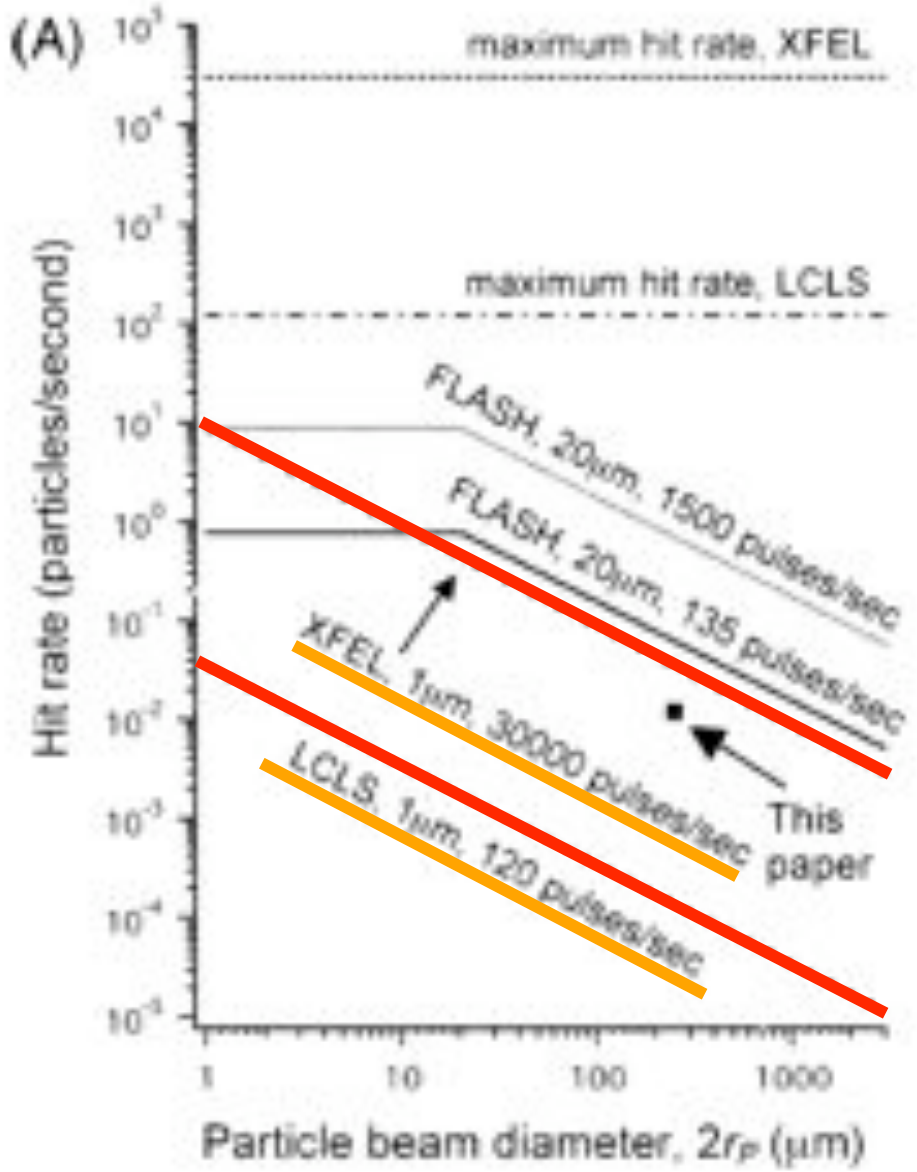
Figure 4 | Structure recovery. Isosurfaces of electron density of the protein chignolin, recovered from 72,000 diffraction patterns of unknown orientation at a MPC of 4×10^{-2} per pixel (see text). The molecular model is represented by the stick figure, with C bonds shown in yellow, N in blue and O in red. The 1, 2 and 3σ electron density contours are shown in blue, pink and red, respectively, with σ denoting the r.m.s. deviation from the mean electron density.

European XFEL

Average Brilliance: Single-Particle Imaging



M.J. Bogan et al., NanoLetters 8, 310 (2008)



How many molecules are hit per second?

aerosol concentration of 3 X10^4 particles/cm3

e.g.

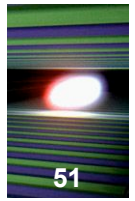
FEL beam diam. 1 μm

Particle beam ~200 μm

XFEL : ~ 0.1 hits per s

LCLS: < 10^{-3} hits per s

Exploitation of repetition rate



R&D projects of the European XFEL

- Detectors allowing acquisition of images at 5 MHz

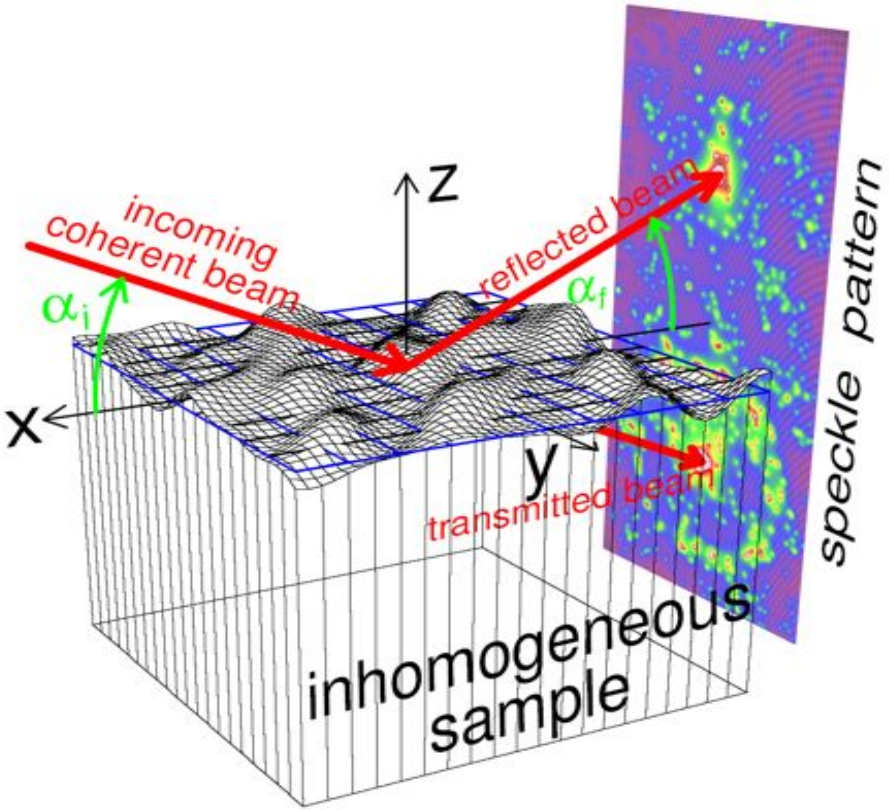
→ *3 Development projects under way for acquisition of up to 512 successive 1 M Pixel images at 5 MHz*

- Lasers allowing Pump and Probe at 5 MHz

→ *Plan launch of a development initiative in partnership with other institutes*

X-Ray Photon Correlation Spectroscopy

Coherent beam case: coherence length of light at sample >> correlation length of domains:

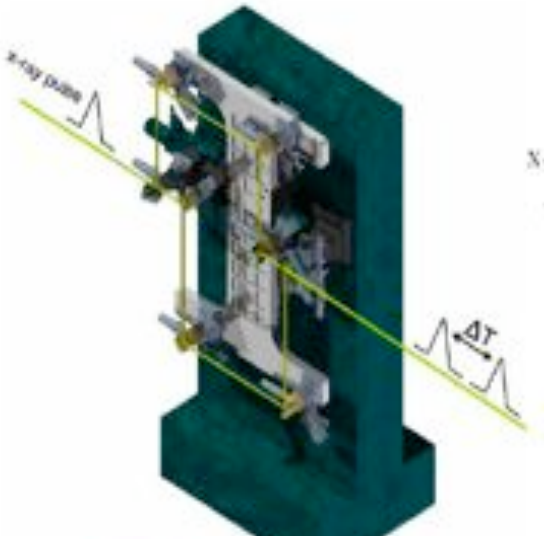


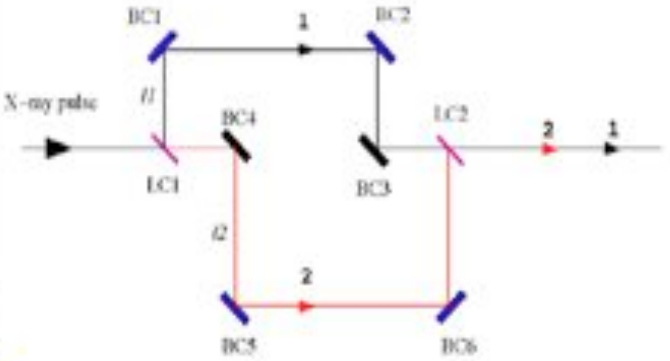
$$I(\mathbf{q}) = \left| \sum_{i=\,domains} e^{i\mathbf{q}\bullet\mathbf{R}_i} \; f_i \right|^2$$

Fluctuating Intensity :

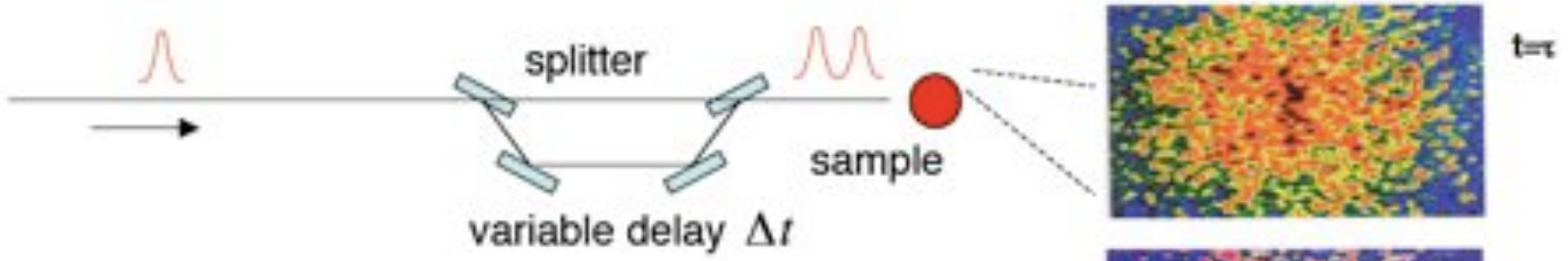
$$g_2(\tau) = \frac{\langle I(t+\tau)I(t)\rangle_t}{\langle I(t)\rangle_t^2}$$

Split-and-delay unit (Rosenker, Grübel *et al.*)





ps to ns delays

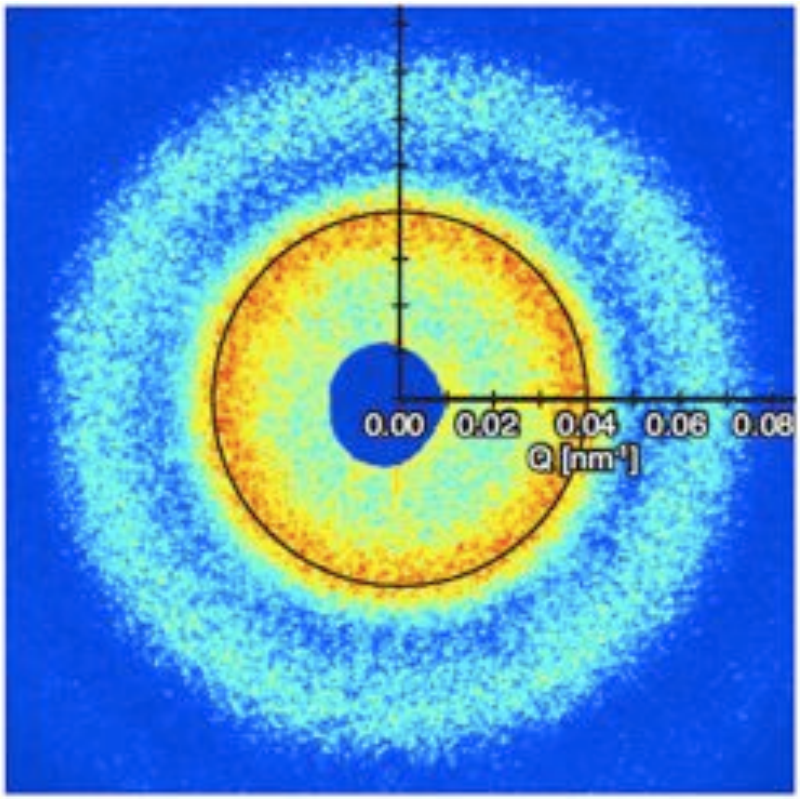


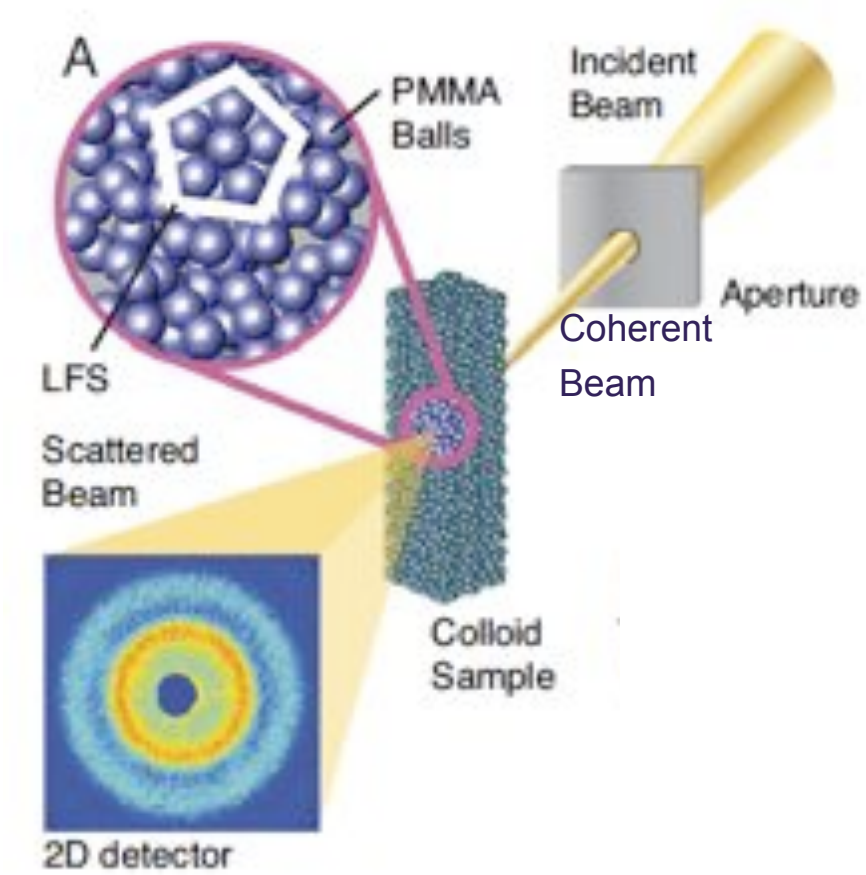
Analyze contrast as function of delay time
Observe time dependence of ordering in materials

European XFEL

Scientific applications of hard X-ray FEL's

- Speckle Scattering and Photon-Correlation Spectroscopy

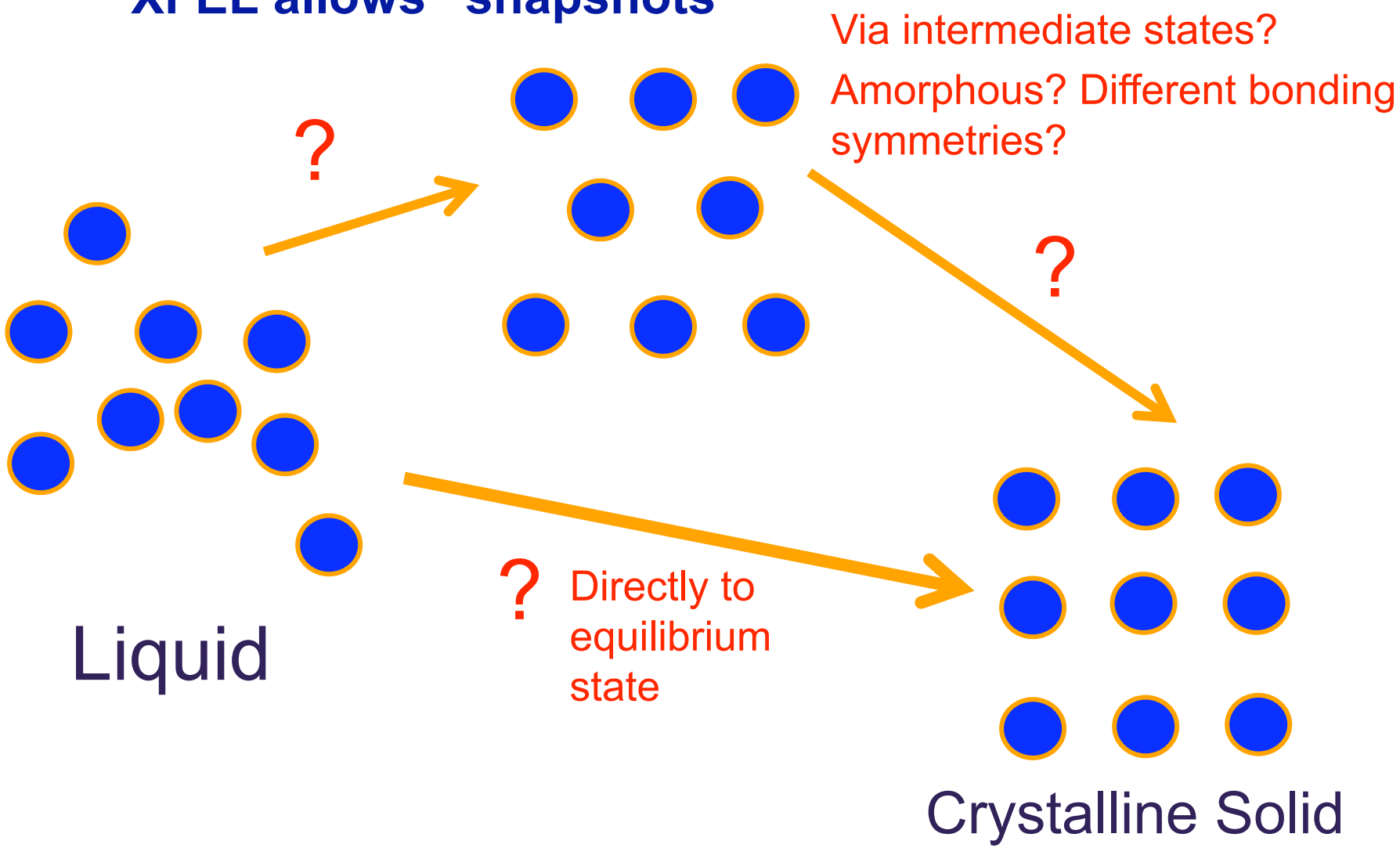




P. Wochner *et al.* PNAS (2009)

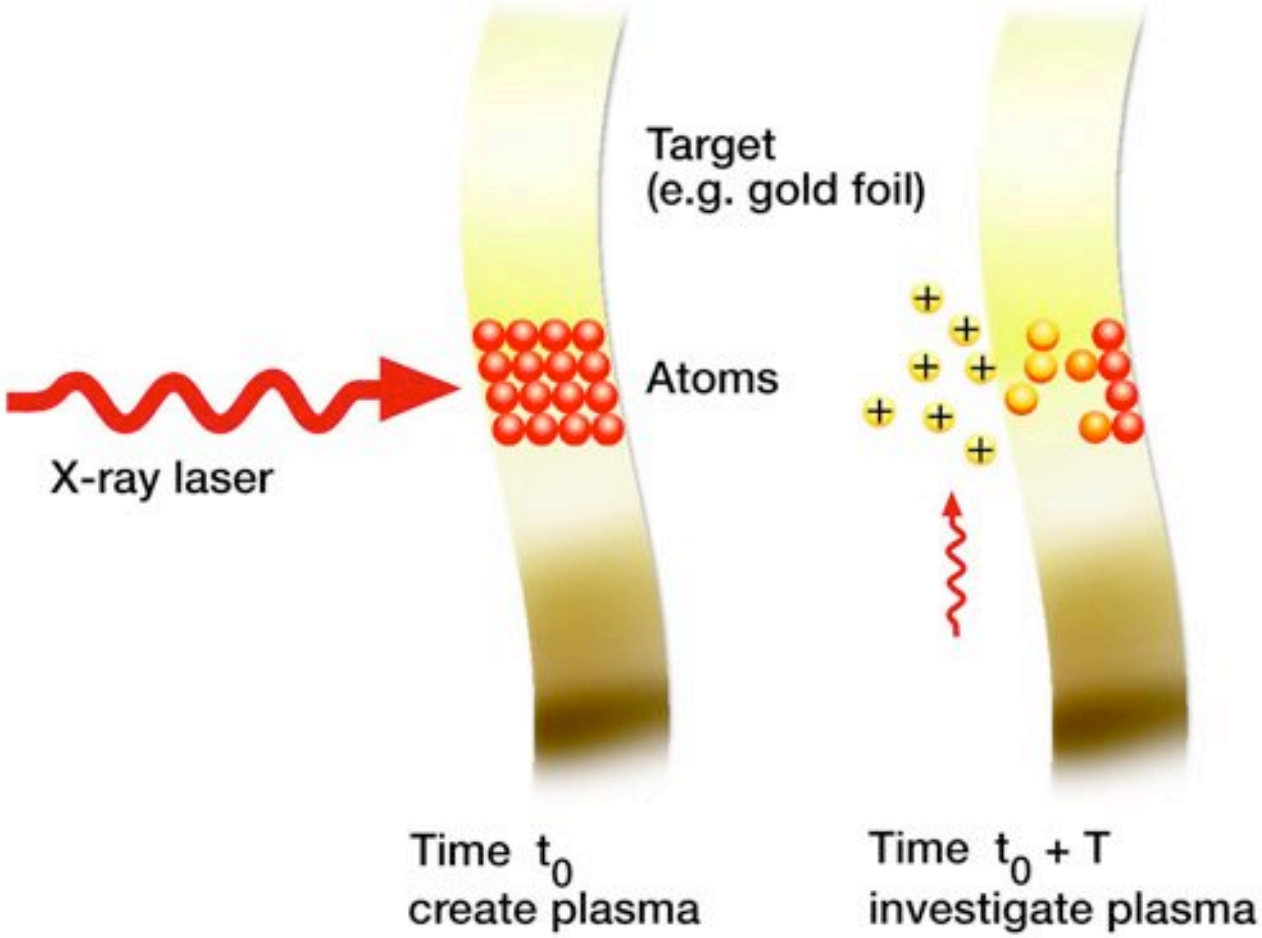
The formation of solid materials from liquids

XFEL allows "snapshots



European XFEL

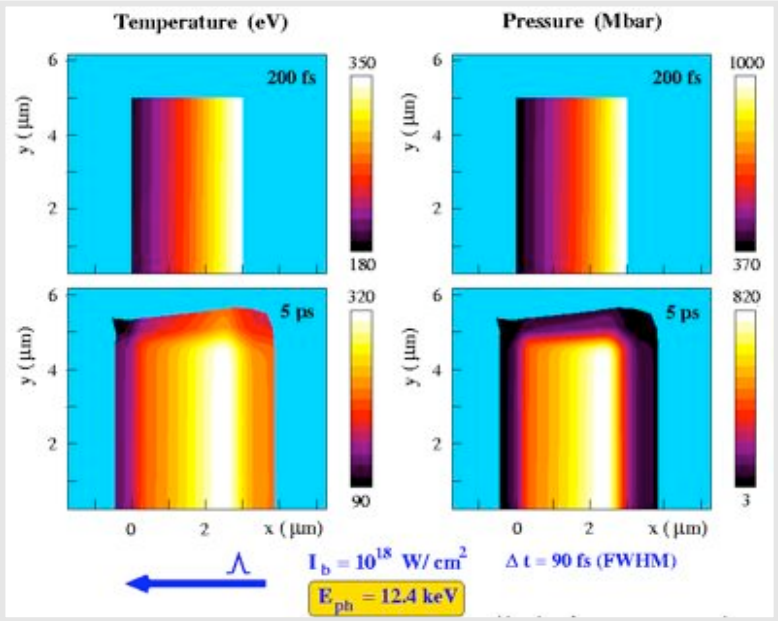
Plasma States by Pump-Probe Techniques



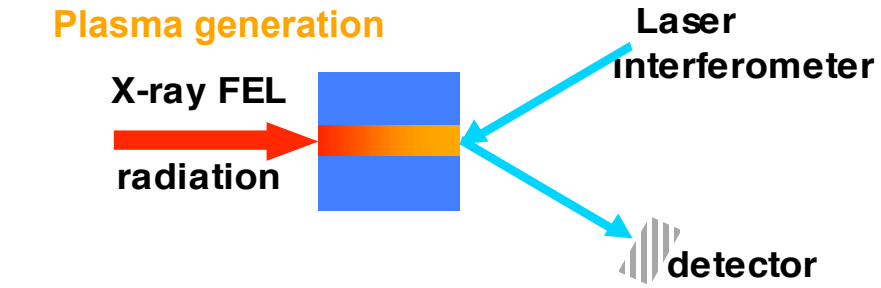
Warm Dense Matter

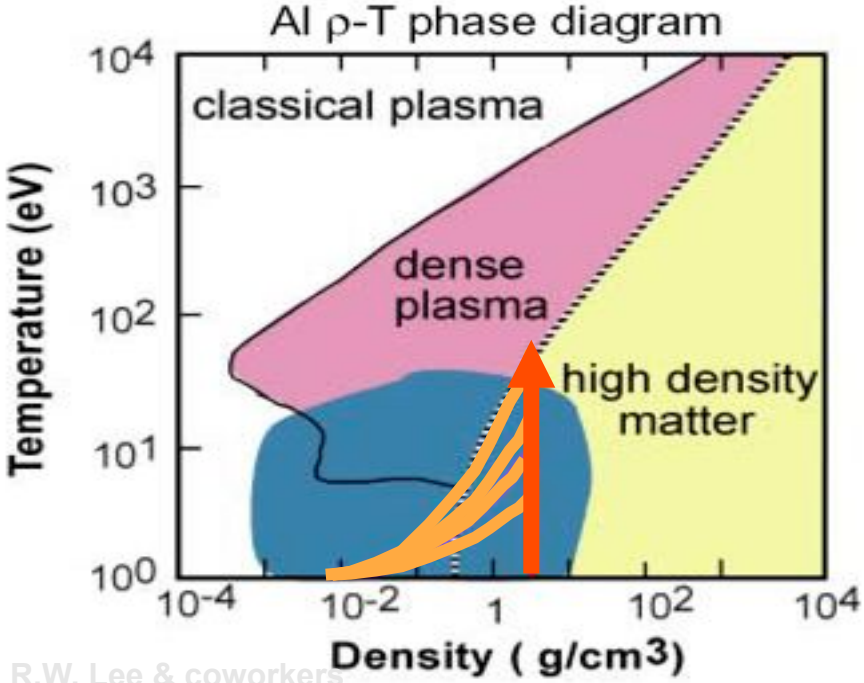
Isochoric heating of plasmas

- Solid density plasmas
- T_e up to few 100 eV
- Warm dense matter
- Pressure up to Gbar
- Plasma phase transitions



Schlegel et al., (2000)

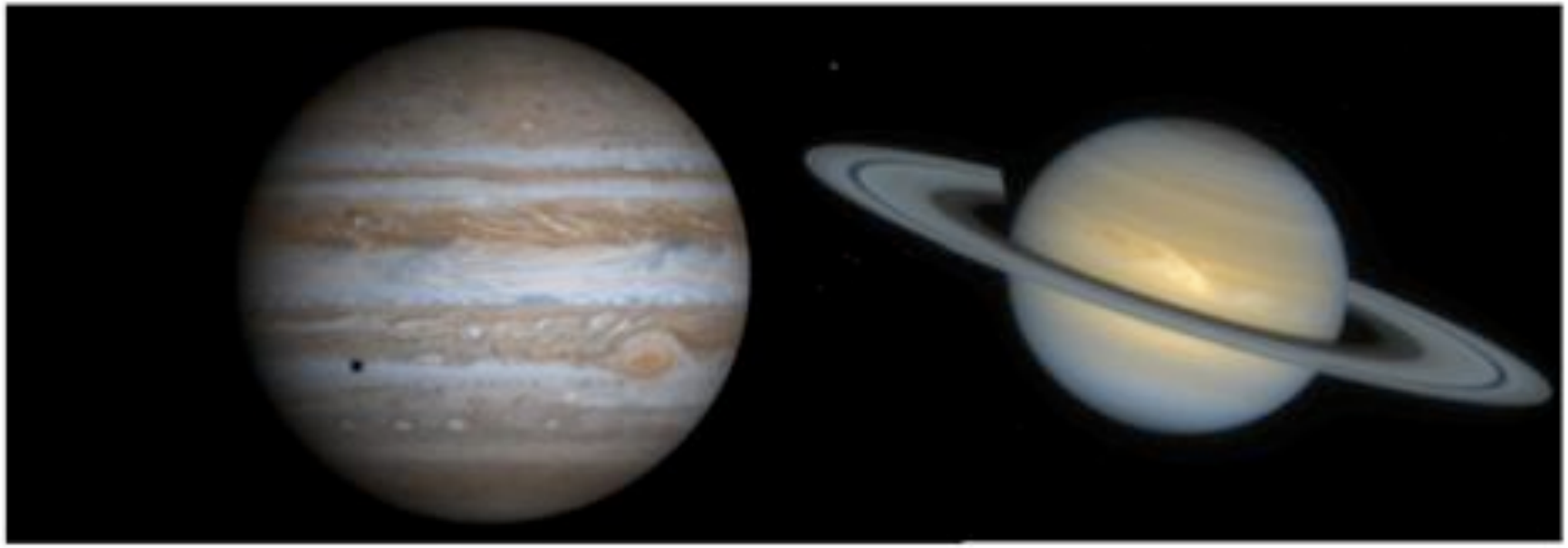




R.W. Lee & coworkers

Int. Workshop on the High Energy Density Science Endstation and Associated Instrumentation at the European XFEL, Oxford, March 30 – April 1, 2009

Thomson scattering, warm dense matter, and interior of giant planets



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INSTITUT FÜR PHYSIK

Trieste, 06.05.2010
Massimo Altarelli, European XFEL GmbH, Hamburg

Astrophysical objects

extreme states of matter

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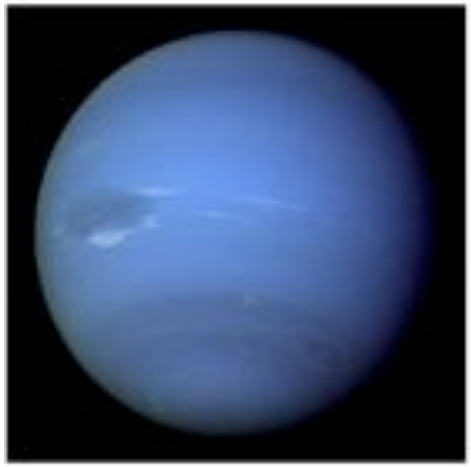
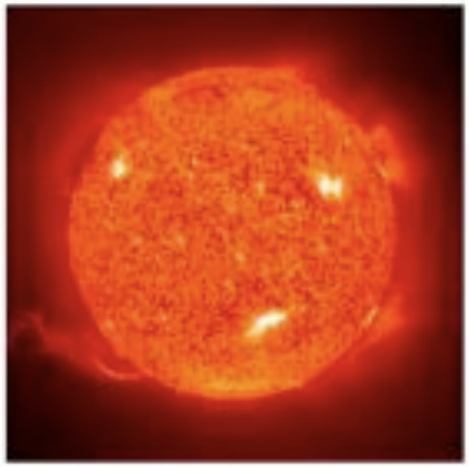
Giant Planets $M<13M_J$ | Brown Dwarfs $13M_J<M<75M_J$ | Stars $M>75M_J$





J, S, U, N and more than 300 exoplanets

… in the Orion Nebula seen in the IR spectrum

The Sun

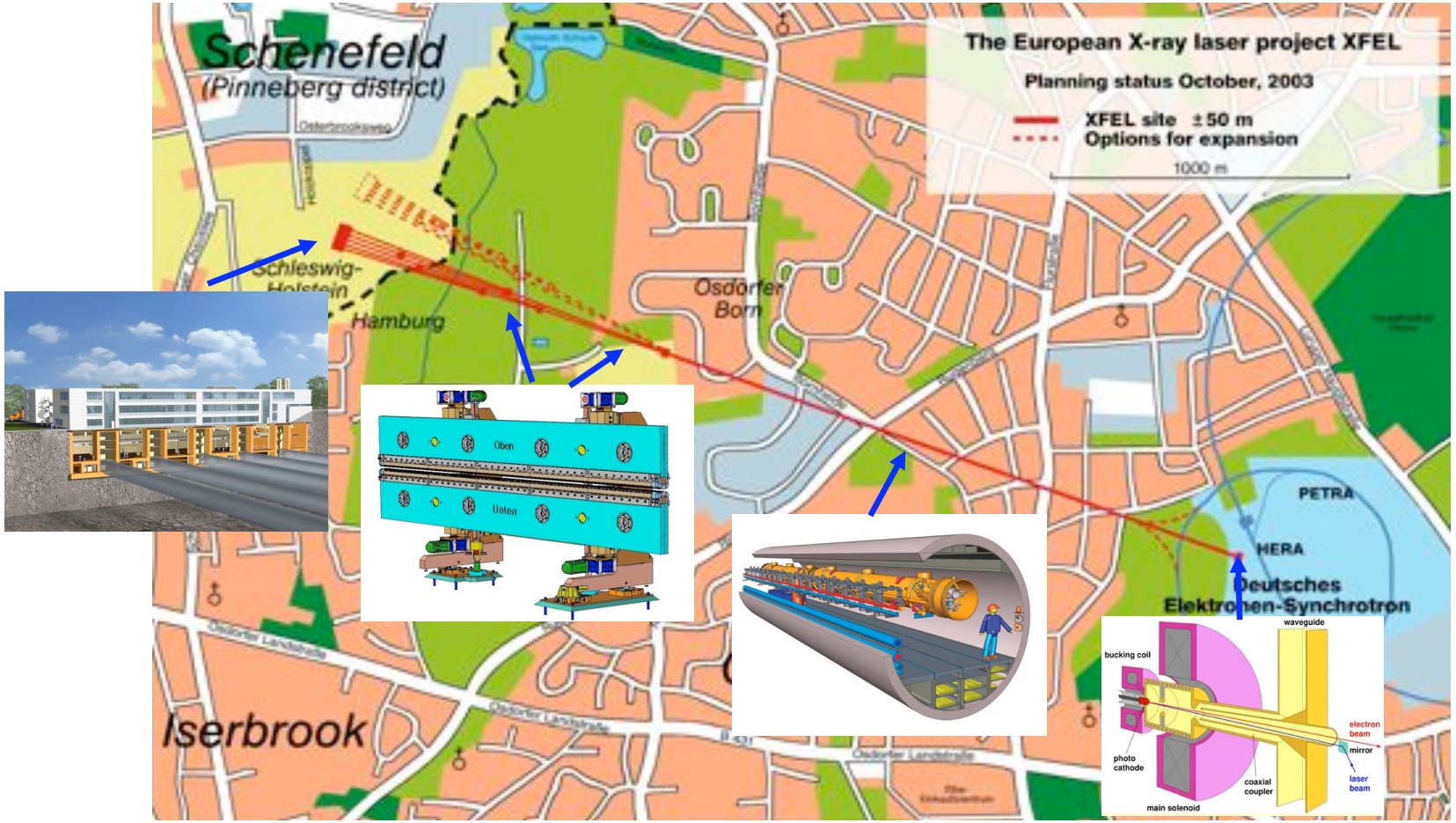
Cores of GPs:
≈ 10^4 K & 10 Mbar
warm dense matter

Cores of BDs:
≈ 10^6 K & Gbar

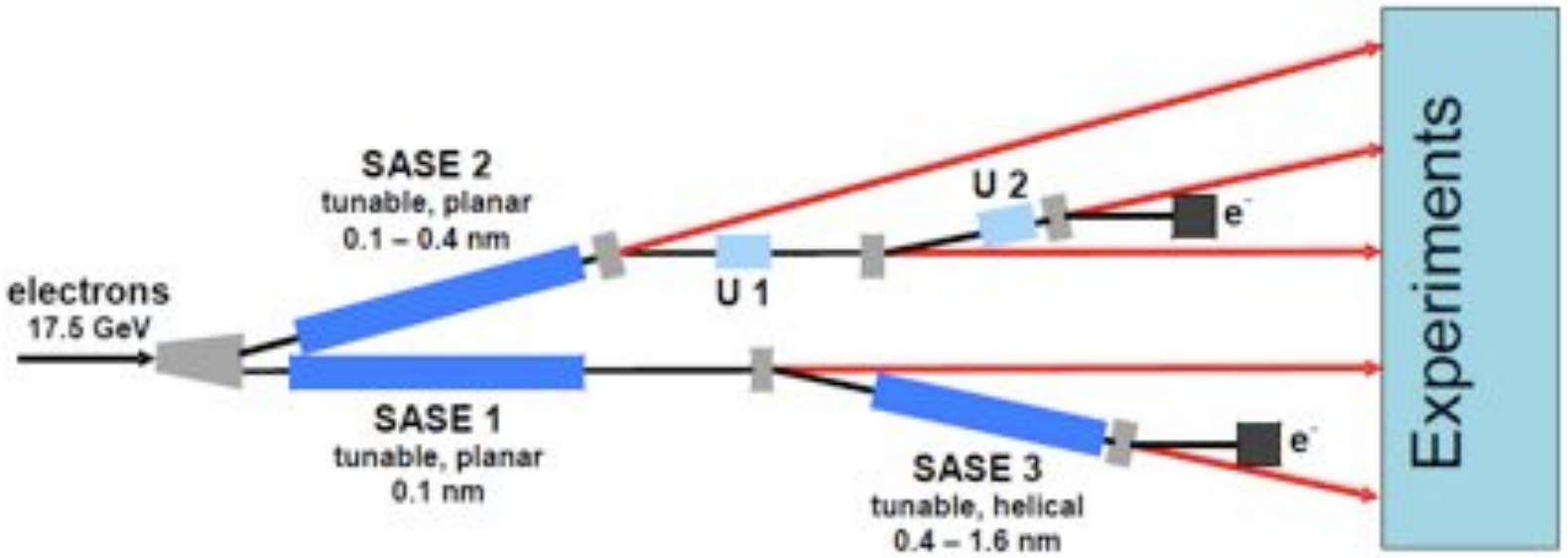
Core of the Sun:
≈ 10^7 K & 100 Gbar
hot dense matter

Overall layout of the European XFEL

3.4km

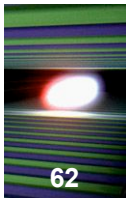


European XFEL Undulator Layout



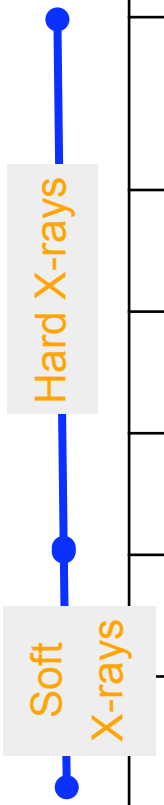
Initial configuration: SASE1, SASE2, SASE3 (planar) plus six instruments

Photon Beam Parameters



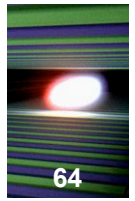
Parameter	Unit	SASE 1	SASE 2		SASE 3		
Electron energy	GeV	17.5	17.5	17.5	17.5	17.5	10.0**
Wavelength	nm	0.1	0.1	0.4	0.4	1.6	6.4
Photon energy	keV	12.4	12.4	3.1	3.1	0.8	0.2
Peak power	GW	20	20	80	80	130	135
Average power*	W	65	65	260	260	420	580
Photon beam size (FWHM)	μm	70	85	55	60	70	95
Photon beam divergence (FWHM)	μrad	1	0.84	3.4	3.4	11.4	27
Coherence time	fs	0.2	0.22	0.38	0.34	0.88	1.9
Spectral bandwidth	%	0.08	0.08	0.18	0.2	0.3	0.73
Pulse duration	fs	100	100	100	100	100	100
Photons per pulse	#	10^{12}	10^{12}	1.6×10^{13}	1.6×10^{13}	1.0×10^{14}	4.3×10^{14}
Average flux	#/s	3.3×10^{16}	3.3×10^{16}	5.2×10^{17}	5.2×10^{17}	3.4×10^{18}	1.4×10^{19}
Peak brilliance	B	5.0×10^{33}	5.0×10^{33}	2.2×10^{33}	2.0×10^{33}	5.0×10^{32}	0.6×10^{32}
Average brilliance*	B	1.6×10^{25}	1.6×10^{25}	7.1×10^{24}	6.4×10^{24}	1.6×10^{24}	2.0×10^{23}

Selection of first instruments



Instrument	Brief description of the instrument
SPB	Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules – **Structure determination of single particles: atomic clusters, bio-molecules, virus particles, cells.**
MID	Materials Imaging & Dynamics **–Structure determination of nano-devices and dynamics at the nanoscale.**
FDE	Femtosecond Diffraction Experiments – **Time-resolved investigations of the dynamics of solids, liquids, gases**
HED	High Energy Density Matter – **Investigation of matter under extreme conditions using hard x-rays, e.g. probing dense plasmas.**
SQS	Small Quantum Systems – **Investigation of atoms, ions, molecules and clusters in intense fields and non-linear phenomena.**
SCS	Soft x-ray Coherent Scattering **–Structure and dynamics of nano-systems and of non-reproducible biological objects using soft X-rays.**

Facing the competition



- Ensure exploitation of repetition rate at best
- Provide "simultaneous" beam time to different users' groups
- Ensure high reliability and stability, top level experimental facilities

Thank you for your attention!

And thanks to my colleagues:

Reinhard Brinkmann

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Andreas Schwarz

Mikhail Yurkov