

Photons at DESY: A coherent and bright perspective

Jochen R. Schneider





X-rays

X-rays have a wavelength of the same order of magnitude as the distance of atoms in matter

X-rays interact with the electrons

X-rays penetrate matter

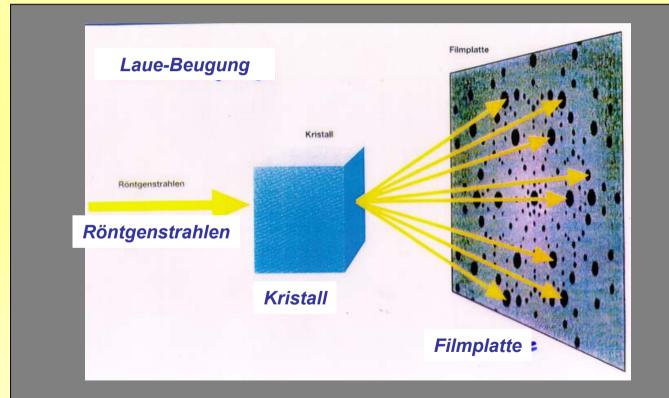
X-rays are used to study the electronic and geometrical structure of matter

X-rays are applied in basic research and engineering science as well as in medicine

Wilhelm Conrad Röntgen



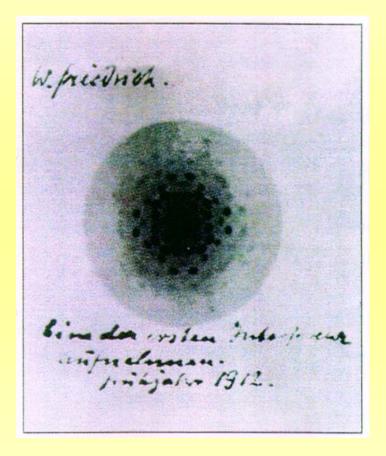
Röntgen-Strukturbestimmung

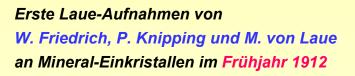


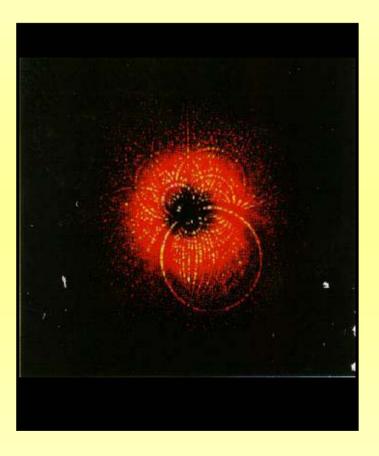
Bestimmung der Atomlagen aus den Intensitäten der Bragg-Reflexe



Laue Beugungsdiagramme



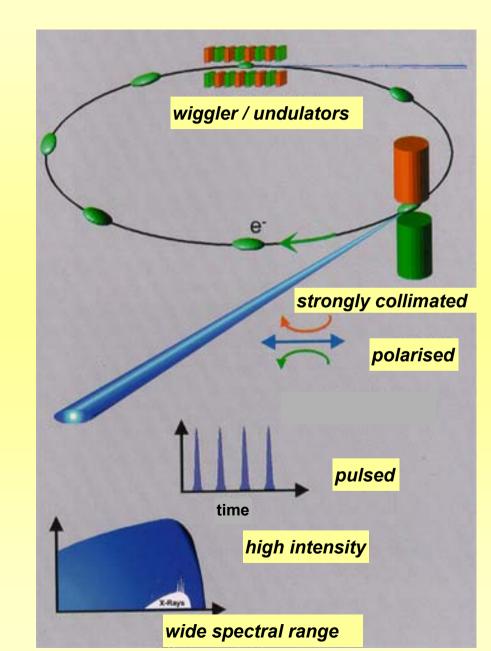




Laue-Aufnahme an Kohlen-Monoxyd-Myoglobin in 150 psec (M. Wulff et al., ESRF-Grenoble)



So far, the pace of progress in X-ray sciences has been closely tied to the development of synchrotron radiation sources, where 3 orders of magnitude in brilliance were gained every 10 years since 1960.





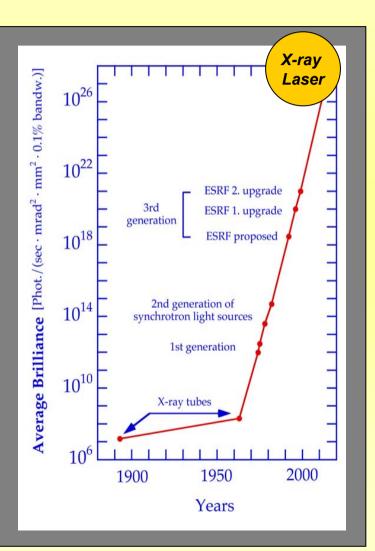
European Synchrotron Radiation Facility



European flagship for hard X-ray sciences



Development of the brilliance of X-ray sources



Since the discovery of X-rays in 1895 the brilliance increased by more than 3 orders of magnitude every 10 years

New generations of X-ray sources

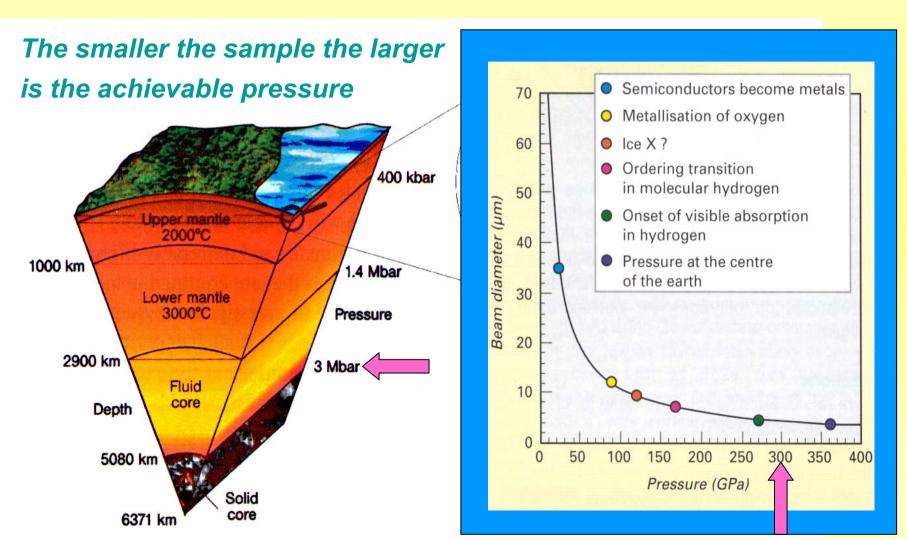
Open new opportunities for sciences without making the established work on older facilities less valuable

As a result: steady increase of synchrotron radiation users





Diffraction under extreme pressure

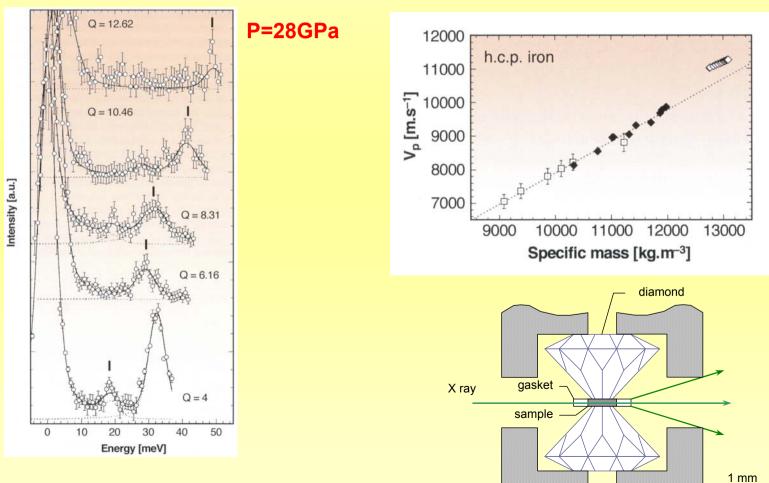




Inelastic scattering under high pressure



Speed of sound of Fe under pressure (ESRF: 2 ph/min)



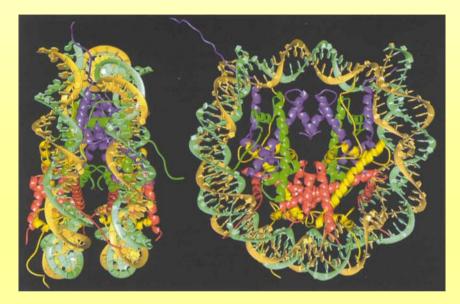
G. Fiquet et al., Science (accepted)



Microfocus application (diffraction)



Multiple views of the nucleosome core particle crystal structure at 2.0 Å resolution. Over 800 water molecules (cyan) and divalent ions (magenta) have been added to the more than 12,000 C,N,O atoms of the proteins and DNA that make up this fundamental repeating unit found in chromosomes (see article on page 9).



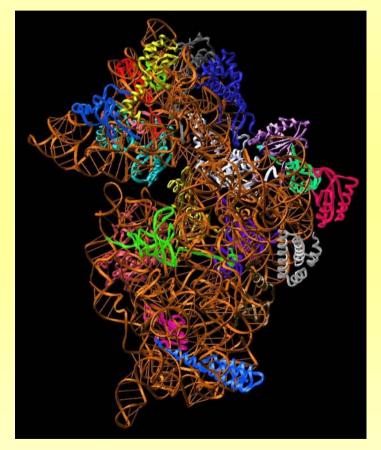
nucleosome core particle

K. Luger, A.W. Mäder, R.K. Richmond, D.F. Sargent and T.J. Richmond, Nature, 389, 251-260 (1997).



Life sciences/Structural Biology

30S ribosomal subunit:



F. Schlünzen, R. Zarivach, J. Harms, A. Bashan, A. Tocilj, R. Albrecht, A. Yonath, Nature <u>413</u> (2001) 814-821

Small crystals:

Micro focus and still small divergence

Large complexes:

• Extremely intense and parallel radiation

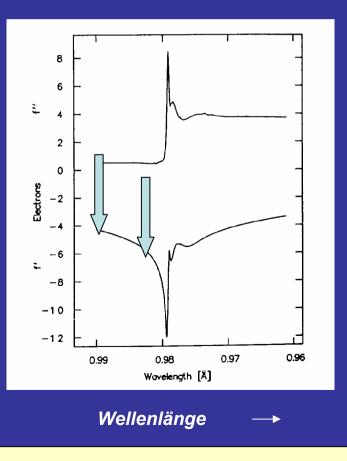
Optimum anomalous signal:

High energy resolution and stability



Beugungsexperimente mit Synchrotronstrahlung

Resonante Streuung am Se Atom



Mittlere Leuchtstärke ~10²¹ *Photonen/sec/#*

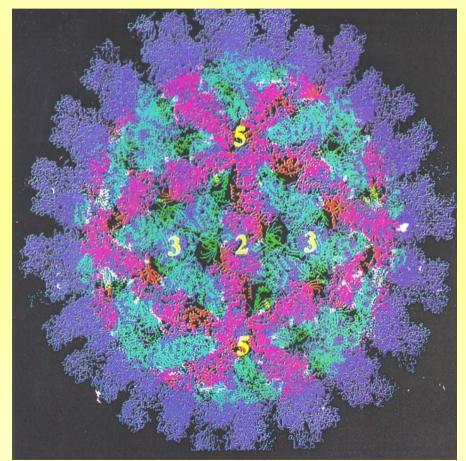
Energieauflösung ∆E/E im 0,001 Bereich

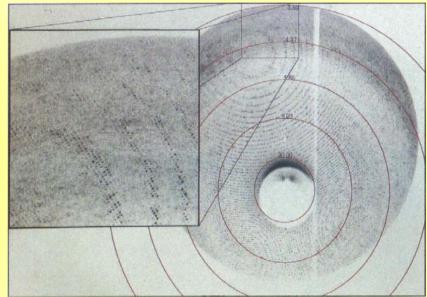
~10¹³ Photonen/sec auf Probe



Structure of a Virus







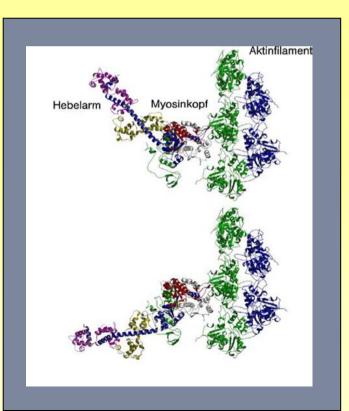
core particle of the blue-tongue virus David Stuart et al., ESRF data



Synchrotron-Strahlung in der Biologie

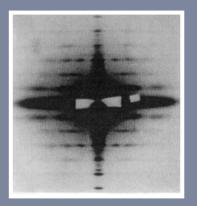
Muskeln bewegen alles,

aber wie bewegt sich ein Muskel?



es begann bei DESY:

G. Rosenbaum, K.C. Holmes & J. Witz Nature <u>230</u> (1971) 434-437



Zeit aufgelöste Klein-Winkel-Streuung



History

- **1964** 1st SR Laboratory at DESY Synchrotron
- **1973** 1st EMBL Laboratory at DESY
- 1974 SR Laboratory at DORIS storage ring
- **1981 HASYLAB experimental hall**
- 1986 HARWI experimental hall
- 1987 MPG unit for structural molecular biology
- 1991 Start of operation of DORIS III
- **1992 HASYLAB wiggler laboratory**
- **1993 DORIS III becomes dedicated SR source**
- 1995 SR from an undulator at PETRA II
- 2000 Demonstration of SASE at TESLA Test Facility
- 2001 1st experiment at TTF SASE FEL
- 2003 Decision of German Government to support PETRA III and the European XFEL Laboratory in Hamburg



Some early scientific highlights

- First precise determination of absorption coefficients
- X-ray small angle scattering from muscles
- Photo-electron yield spectroscopy
- X-ray interferometry
- X-ray microscopy with zone plates
- Mößbauer spectroscopy with synchrotron radiation
- Scattering from liquid surfaces
- Studies of surfaces and interfaces with standing waves
- Inelastic scattering at eV and meV resolution
- Spin dependent absorption spectroscopy
- Coronary angiography



Careers starting at DESY-HASYLAB

- Wolfgang Eberhardt (Director BESSY)
- Wolfgang Gudat (Director BESSY)
- Ruprecht Haensel (Director General ESRF)
- Ernst E. Koch (Director BESSY)
- Helmut Krech (Admistrative Director BESSY, DESY, ESRF)
- Christof Kunz (Research Director ESRF)
- Gerhard Materlik (CEO Diamond)
- Gottfried Mühlhaupt (Machine Director BESSY, ESRF, SLS)
- Volker Saile (Director CAMD)
- Alwin Wrulich (Machine Director Elettra, SLS)

Professors at Universities:

R. Frahm (Wuppertal), T. Brückel (FZJ-Aachen), J. Falta (U. Bremen),



Research with Photons at DESY

Storage ring based facilities

DORIS III: Experiments needing high photon flux

PETRA II: high brilliance test beamline

PETRA III: Project Optimized for high brilliance LINAC based facilities

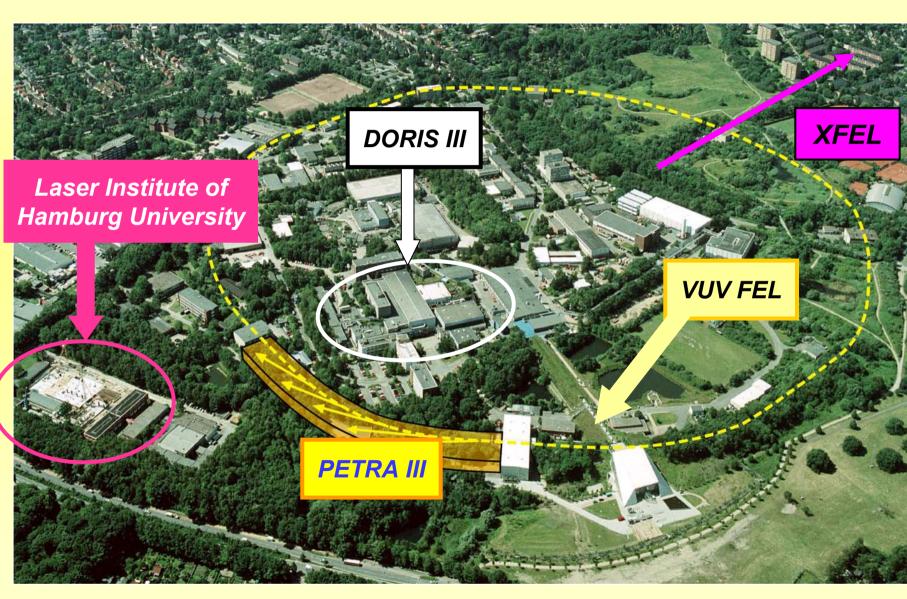
VUV FEL:

wavelengths from ~6 to 100 nm

European X-FEL Laboratory: Project wavelengths from ~0.085 to 6 nm

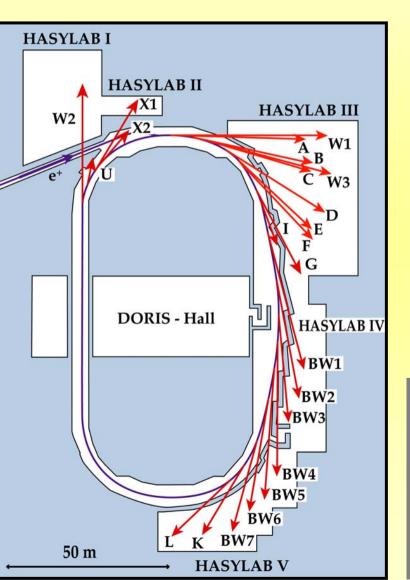


Research with photons at DESY





HASYLAB operation



DORIS III:

40 beamlines 76 experimental stations

7 stations operated by EMBL Outstation

1 station operated by MPG

10 stations operated with support from external institutions (Verbundforschung)

<u>PETRA II:</u>

1 test beamline 2 experimental stations

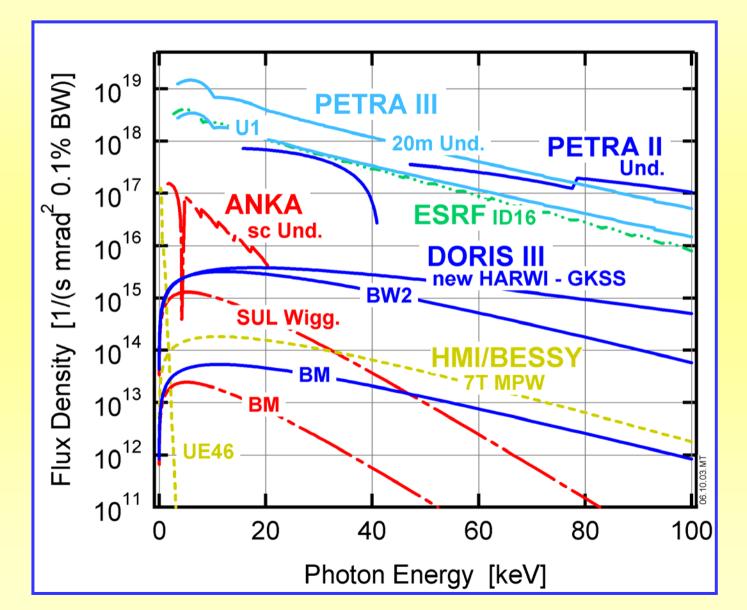
HASYLAB staff in 2003

27 (17) scientists 31 (6) engineers and technicians 6 management, administration, secretariat

+ DESY infrastructure, machine operation and general administration

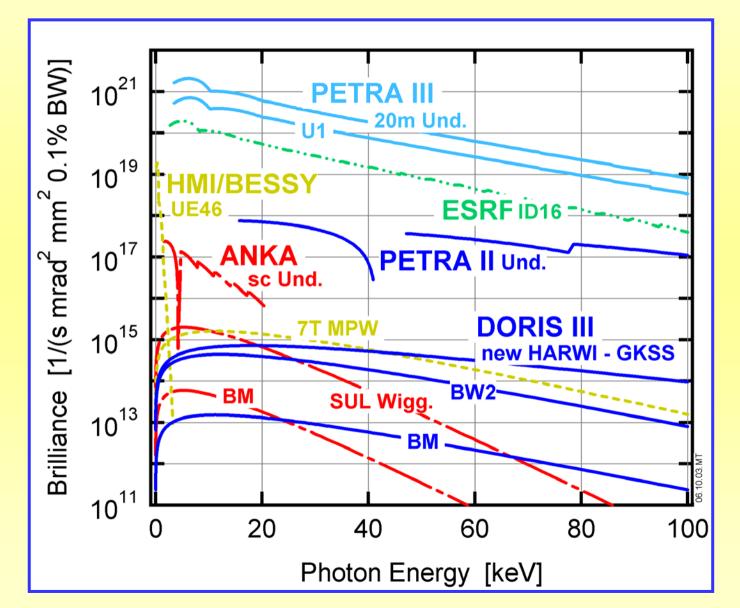


Flux density at storage ring facilities





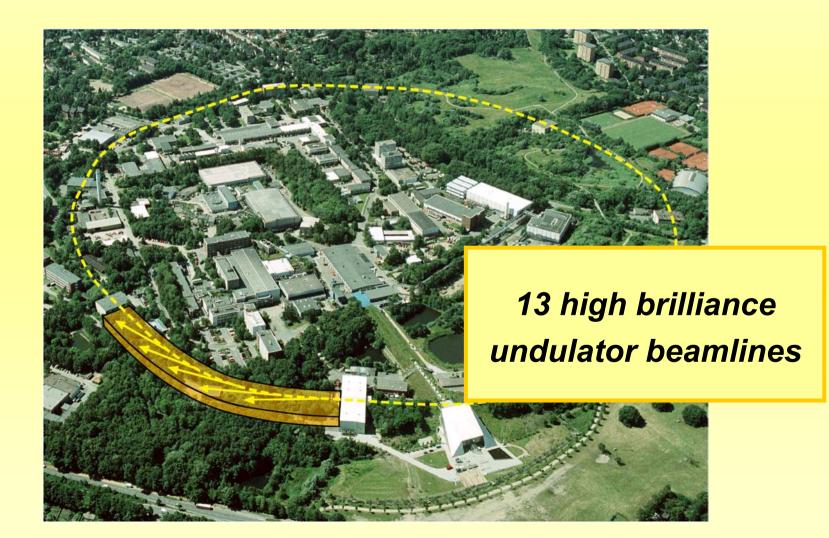
Brilliance at storage ring facilities





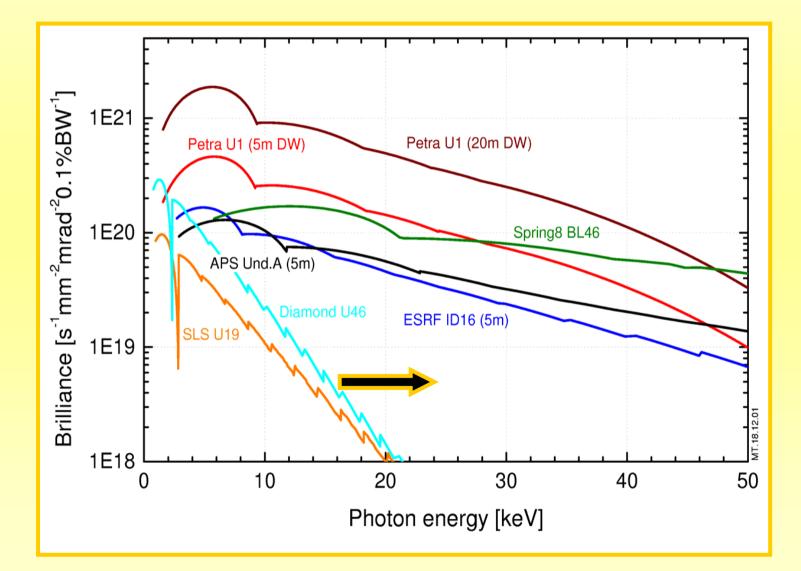
Project

PETRA III synchrotron radiation facility





PETRA III: brilliance comparison





Time Resolved Studies



Probing matter with atomic resolution

Present day X-ray and neutron experiments probe in most cases equilibrium states of matter.

The next goal is to probe the dynamic state of matter with atomic resolution in space and time in order to allow for studies of non-equilibrium states, and very fast transitions between the different states of matter.



Watching a Protein as it Functions with 150-ps Time-Resolved X-ray Crystallography

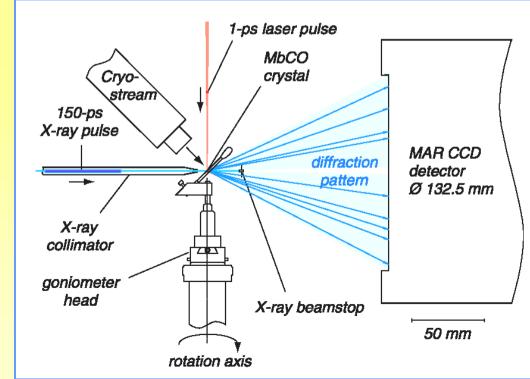
Friedrich Schotte,¹ Manho Lim,² Timothy A. Jackson,³ Aleksandr V. Smirnov,¹ Jayashree Soman,⁴ John S. Olson,⁴ George N. Phillips Jr.,⁵ Michael Wulff, ⁶ Philip A. Anfinrud¹



ID 09 E

X-ray pulses (~150 psec, ~1010 photons, 0.1mm²) from ESRF ID09B in "single bunch" mode.

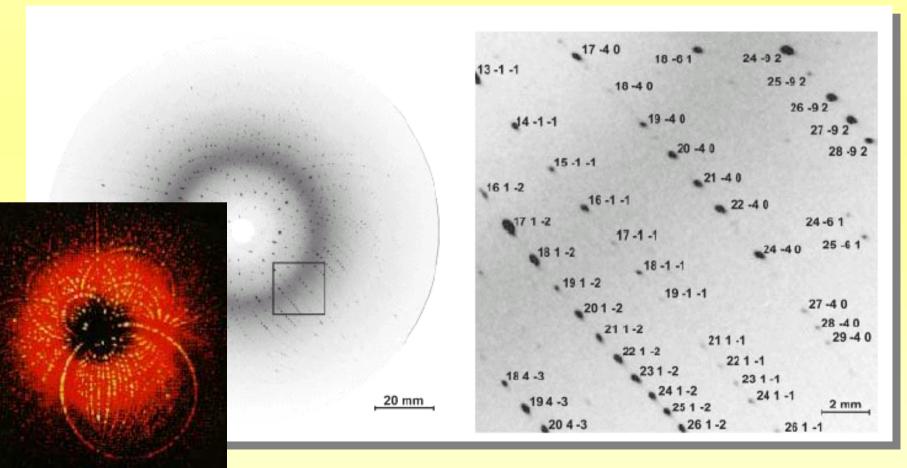
Laser pump pulses (570 nm, 1 psec, 23 µJ) induced photodissociation, better than 50 psec time jitter.





MbCO photodissociation dynamics

Myoglobin Laue data (3.5% bw, 15.6 keV) recorded on CCD



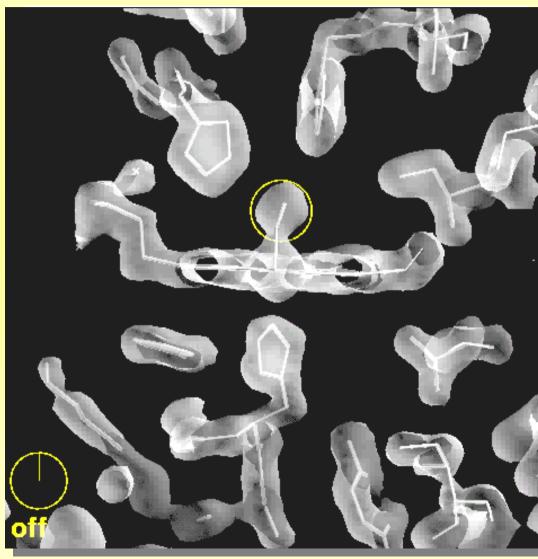


MbCO photodissociation dynamics

Myoglobin

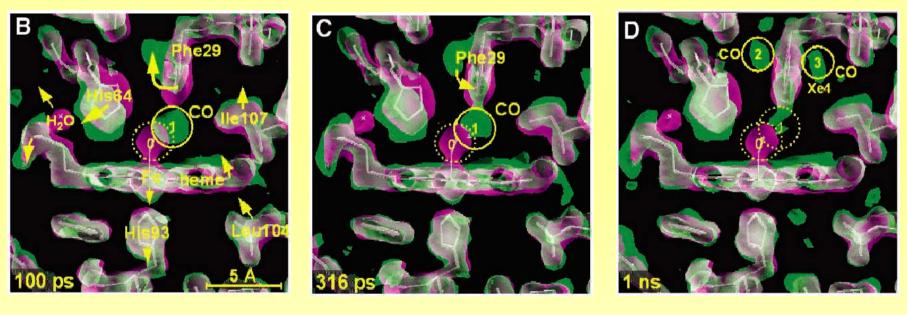
Correlated motions of heme, protein backbone and side chains already evident at 100 psec

Early displacements of side chains much more dramatic than static differences between Mb and MbCO





Watching a protein as it functions



100 psec

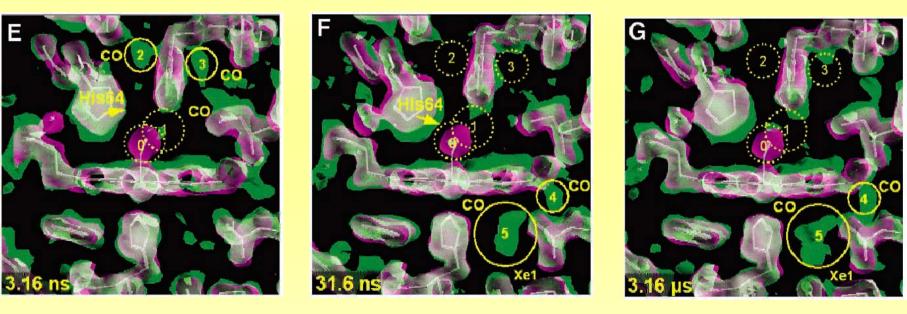
316 psec

1000 psec 1 nsec

MbCO photodissociation dynamics



Watching a protein as it functions



3.6 nsec

31.6 nsec

<mark>3160 nsec</mark> 3,16 μsec

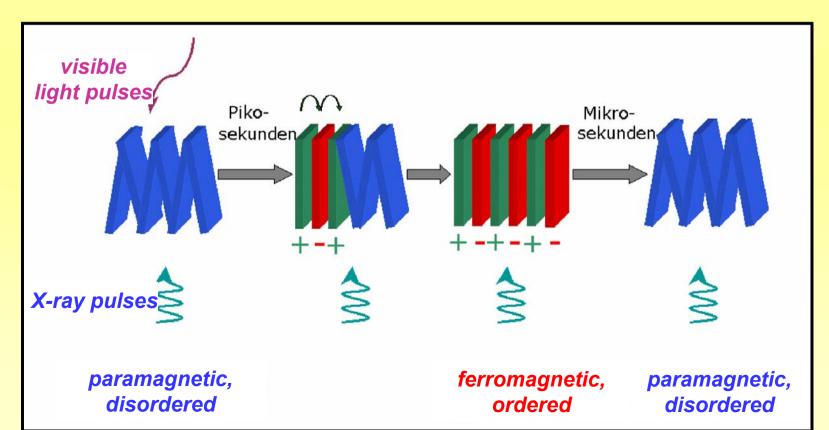
MbCO photodissociation dynamics



Laser-induced ferroelectric structural order in an organic charge-transfer crystal tetrathiafulvalene-p-chloranil

E. Collet, M.-H. Lemée-Cailleau, M. Buron-Le Cointe, H. Cailleau, S. Techert, M. Wulff, T. Luty, S.-Y. Koshihara, M. Meyer, L. Toupet, P. Rabiller

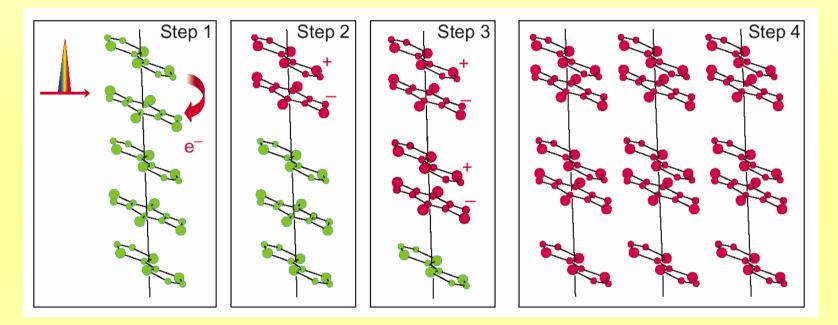
Science, Vol. 300, 25 April 2003, 612





Laser-induced ferroelectric structural order in an organic charge-transfer crystal

Collet et al, Science, Vol. 300, 25 April 2003, 612

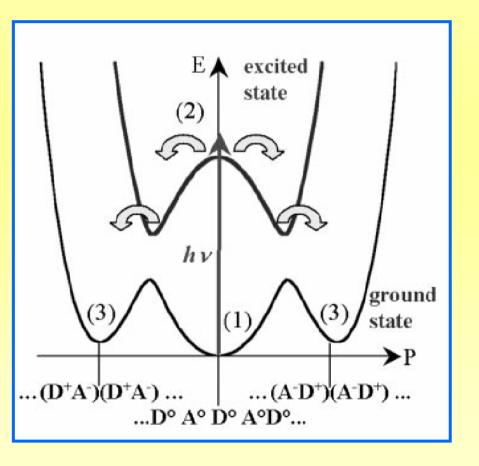


- 1. an optical pulse excites a molecule
- 2. an intermolecular charge transfer occurs accompanied by a lattice relaxation, i.e. a dimerization process trapping the excitation
- 3. cooperative phenomena take place with the self-multiplication of the excited molecule in the stack
- 4. interstack interactions lead to the 3D ordering of the dimers, with a photon efficiency so high that one photon transforms a few hundred molecules



Photoinduced neutral-to-ionic transformation path along the polar order parameter P

Collet et al, Science, Vol. 300, 25 April 2003, 612

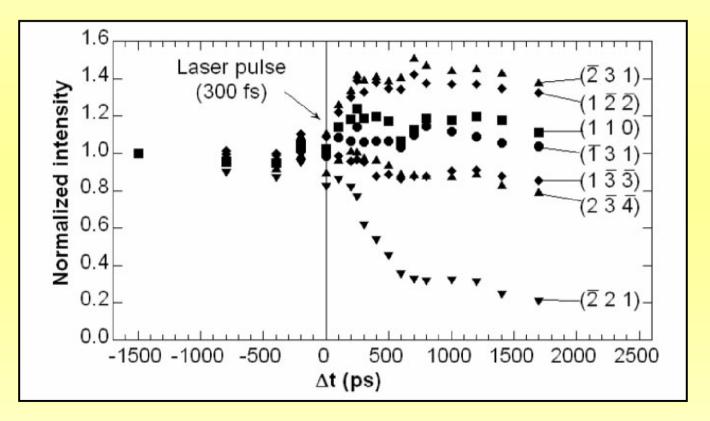


- 1. The stable neutral state is made of homogeneous, nonpolar neutral chains where electron donar (D) and acceptor (A) molecules are regularly stacked.
- 2. Photons excite DA pairs into an ionic state inducing a lattice relaxation.
- 3. The coupling between the relaxed species makes the system switch to a metastable macroscopic state.



Laser-induced ferroelectric structural order in an organic charge-transfer crystal

Collet et al, Science, Vol. 300, 25 April 2003, 612

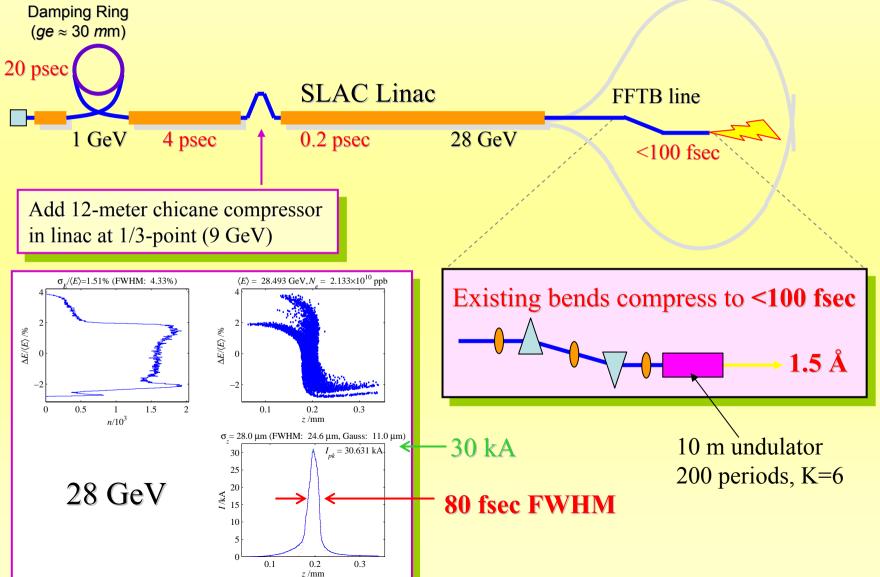


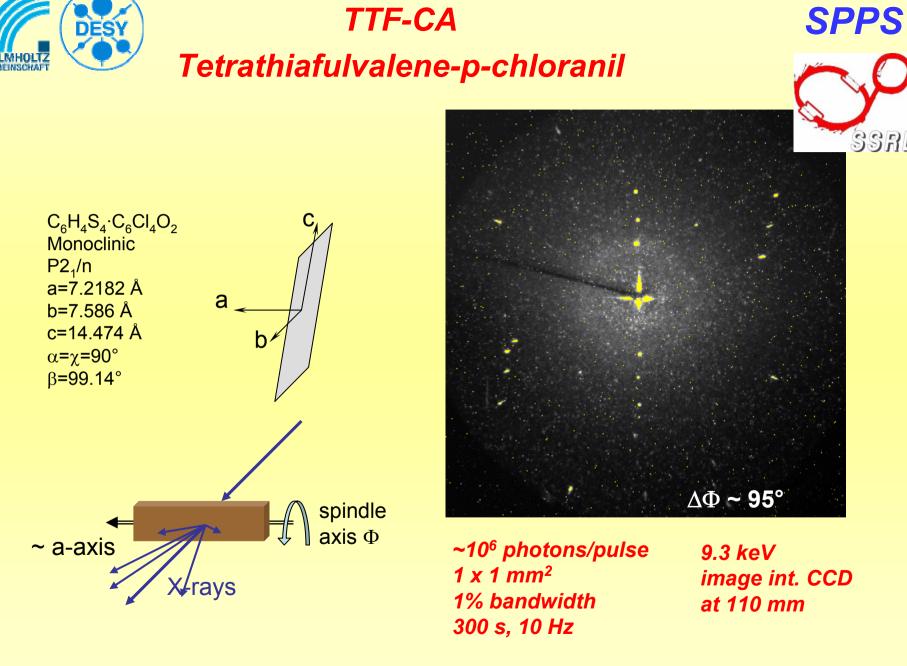
ESRF

Relative intensity of some single crystal Bragg peaks versus the delay time between the laser pump and the X-ray probe. After about 500 ps the light-driven metastable state is established.

Sub-Picosecond Pulse Source (SPPS) R&D Program (a Component of the LCLS R&D Effort)







T Tschentscher H Schulte-Schrenning S Techert SPPS-Team (1 Hastings)



Diffraction from Salol

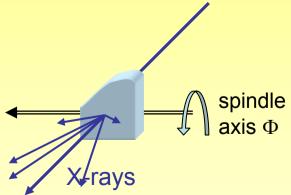
SPPS

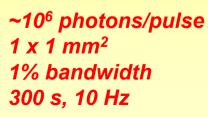
SR.

Phenylsalicylate

 $\begin{array}{l} C_{13}H_{10}O_{3} \\ \text{Orthorombic} \\ \text{Pbca} \\ a=7.961 \text{ Å} \\ b=11.258 \text{ Å} \\ c=23.402 \text{ Å} \\ \alpha=\beta=\gamma=90^{\circ} \\ \Delta\theta \ (0 \ 16 \ 0)=0.3 \ \text{mdeg} \end{array}$







9.365 keV image intensif. CCD at 120 mm

T Tschentscher H Schulte-Schrenning F Weckert SPPS-Team (1 Hastings)



LINAC driven



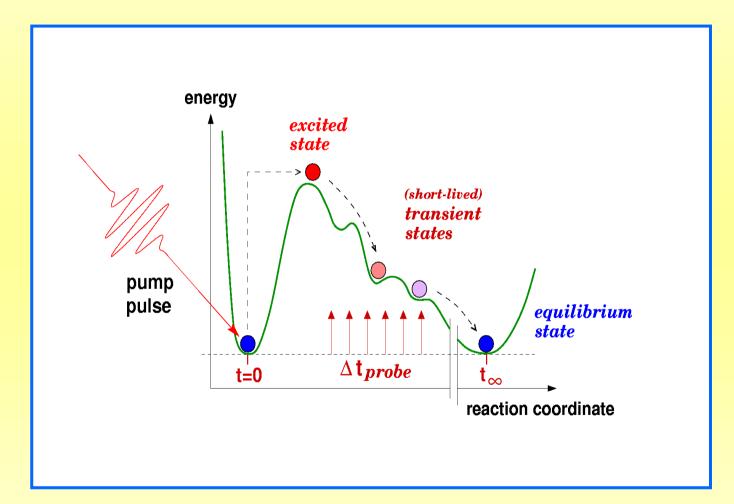
Probing matter with atomic resolution

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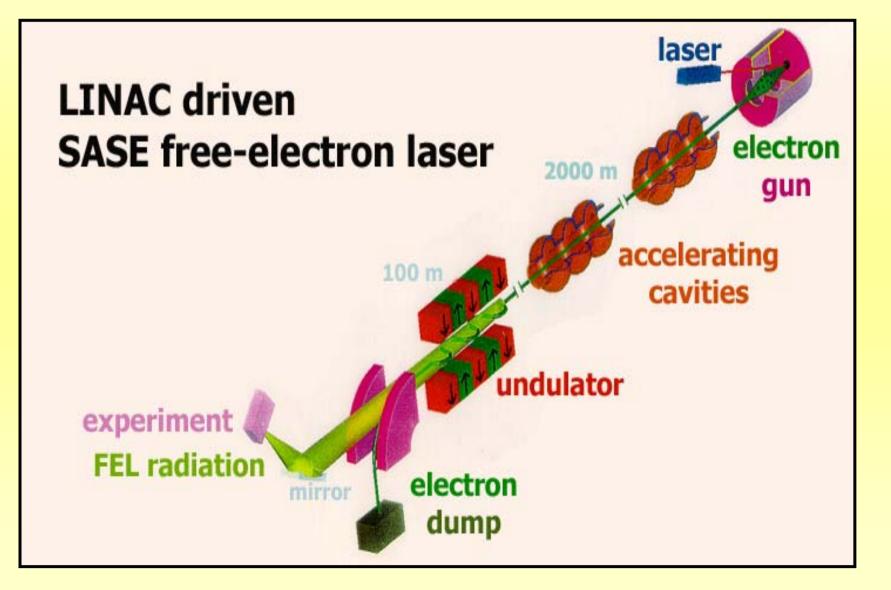


Take a movie of chemical reactions



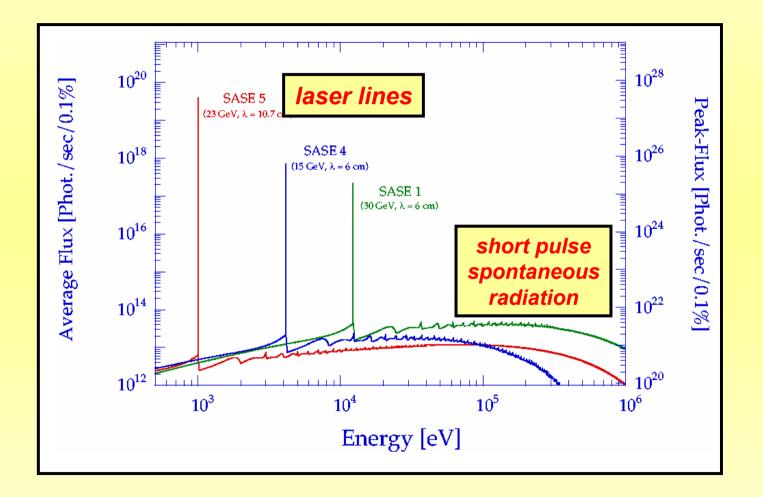
Schematic presentation of transition states in a chemical reaction







SASE X-FEL: Spectral flux



Spectral distribution of angle integrated SASE FEL radiation



European X-FEL Laboratory

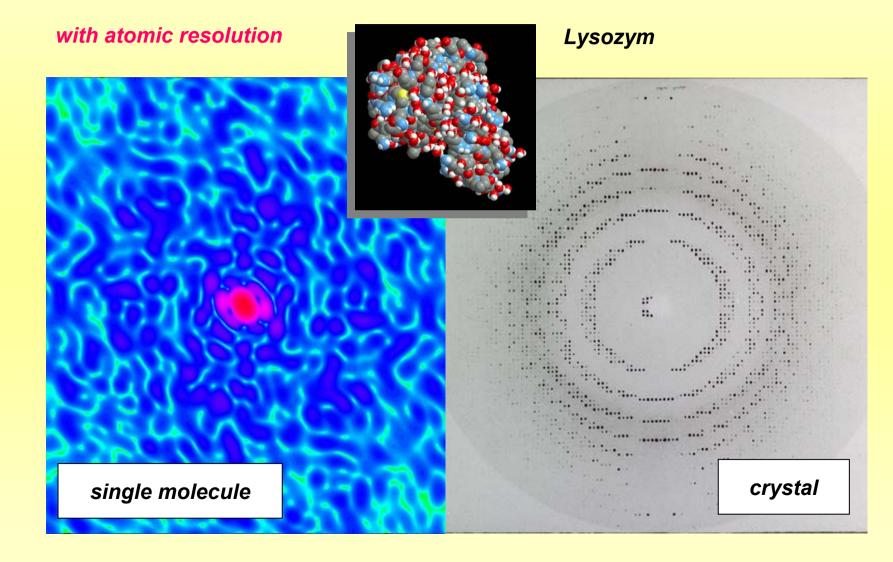
Compared to 3rd generation storage ring based synchrotron radiation facilities, the gain factors are:

- peak brilliance: 10⁹ at the FEL line
 - **10⁴ for spontaneous radiation**
- average brilliance: 10⁴ at FEL line
- coherence: 10⁹ at FEL line (numbers of photons per mode)

With gain factors of **10⁴** ... **10⁹** the scientific case is based on extrapolation from today's needs and/or on wild dreams



Imaging of a single bio-molecule



Oversampling: J. Miao, K.O. Hodgson and D. Sayre, PNAS <u>98</u> (2001) 6641-6645

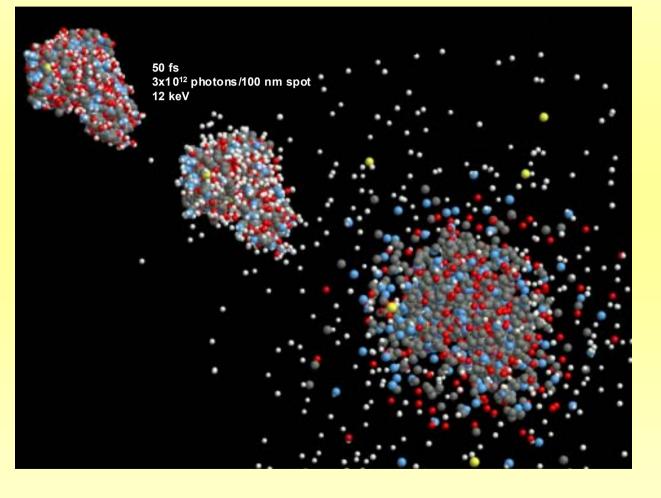


Coulomb Explosion von Lyzosym



t=50 fsec

t=100 fsec



R. Neutze, R. Wouts, D. van der Spoerl, E. Weckert, J. Hajdu: Nature 406 (2000) 752-757



European XFEL Laboratory

Main fields of application

- atomic, molecular and cluster phenomena, plasma physics
- non-linear processes and quantum optics
- condensed matter physics and materials science
- ultra-fast chemistry and life-sciences

The scientific case has been discussed in recent reports from SLAC/SSRL, DESY/HASYLAB, BESSY, ELETTRA, SRS Daresbury, MIT Bates Lab



Strategy for the realization of hard X-ray FEL facilities at DESY

Step wise approach because of the challenges involved

FEL at TTF I (1999 - 2002): Proof-of-Principle for SASE in 2001 at 80 – 120 nm, first experiments in 2001/2

integrated system tests are needed

VUV FEL user facility (2005): Soft X-rays in the 100 - 6 nm wavelength range

European XFEL Laboratory:

hard X-rays: 6 - 0.1 nm, funding under way, beam for users expected in 2012

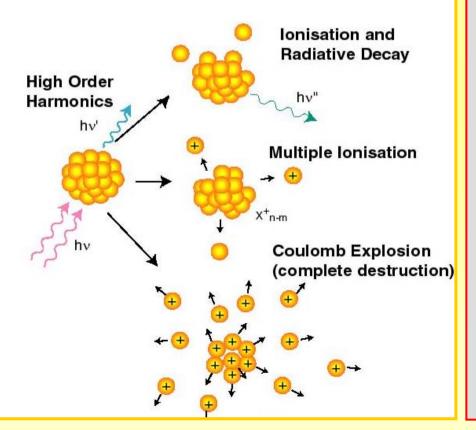


VUV FEL

in TESLA Technology



Goals of a cluster experiment

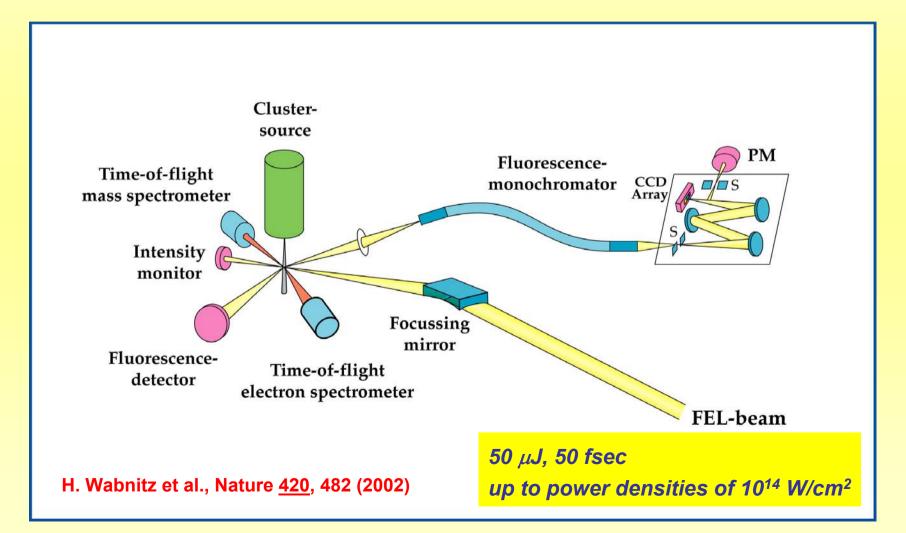


Questions asked:

- which multi-photon processes are observed
- cross sections (surface, bulk)
- which ions are prepared (charge state, electronically excited states)
- life time of intermediate states
- high-order harmonic generation

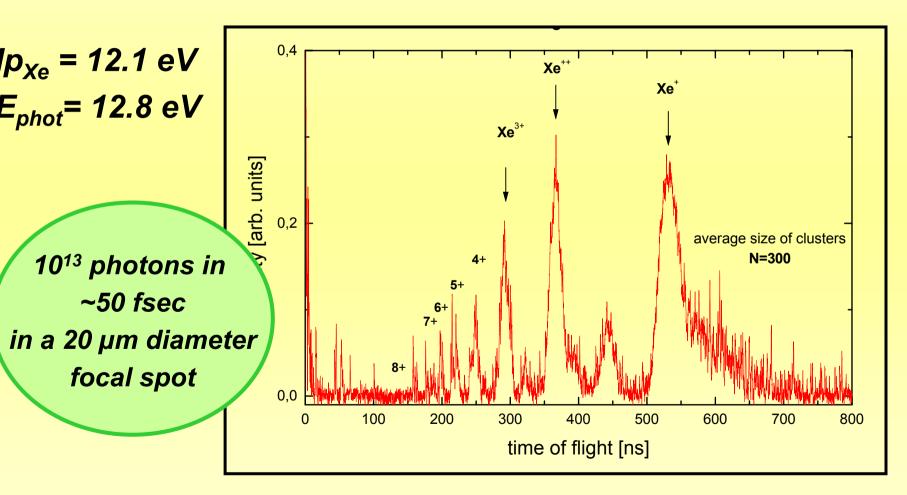


FEL Cluster Experiment at 100 nm





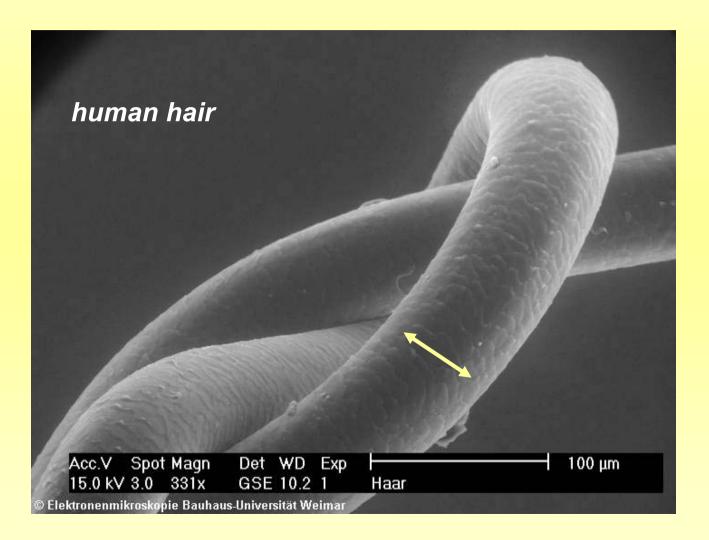
Single shot time-of-flight spectrum



Coulomb explosion of Xenon clusters with ~ 300 atoms

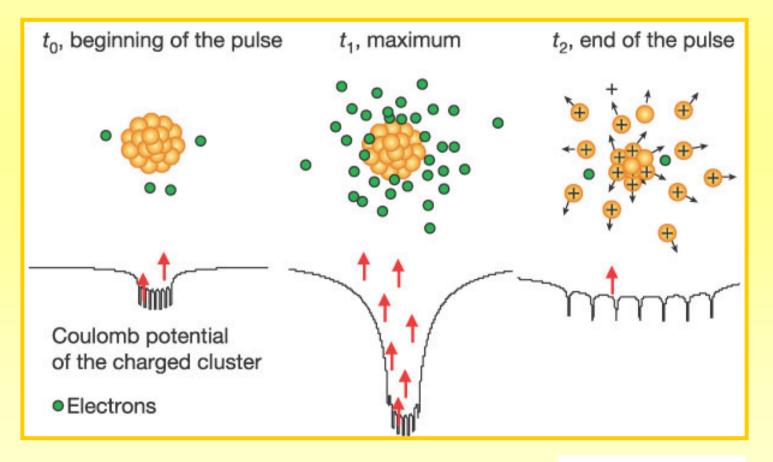


100 femtoseconds ↔ 30 µm



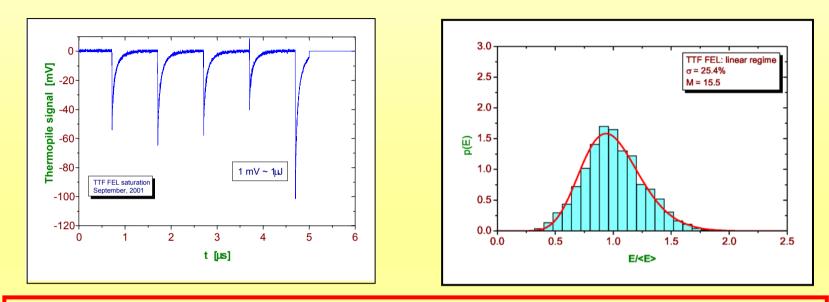


Coulomb explosion of clusters induced by multi-photon absorption



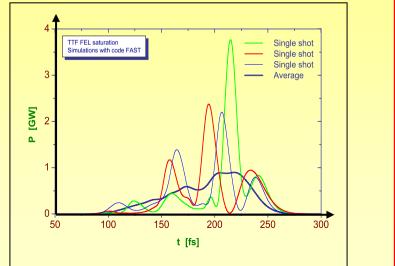
Th. Moeller et al.

Fluctuation properties of SASE radiation at TTF



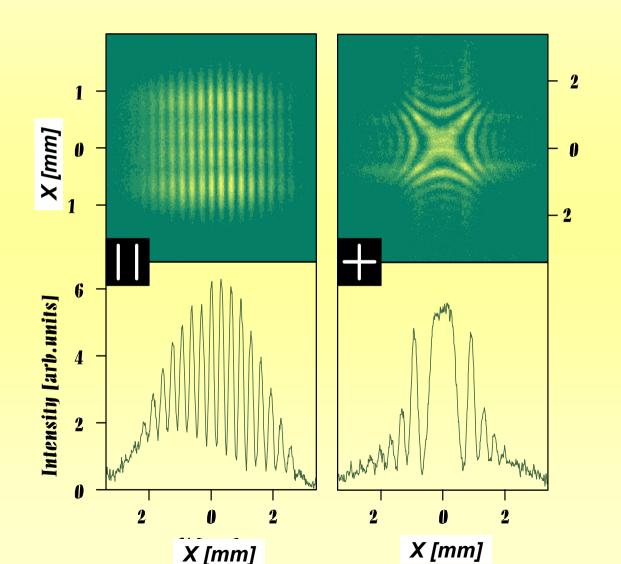
Simulated spike structure in SASE saturation based on measured fluctuations of the pulse energy

EUSCHAE



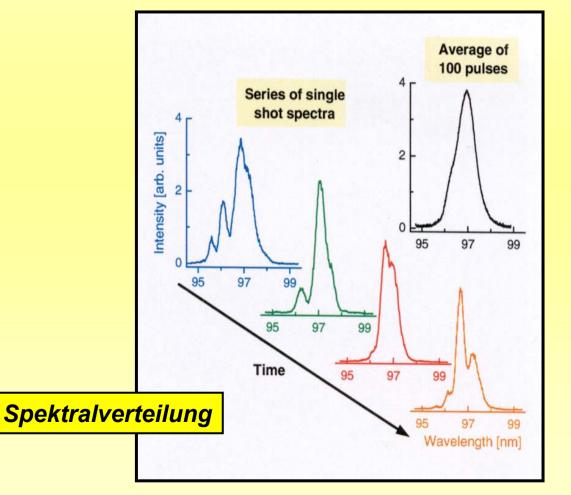


Transversale Kohärenz





SASE FEL: Start aus dem Rauschen

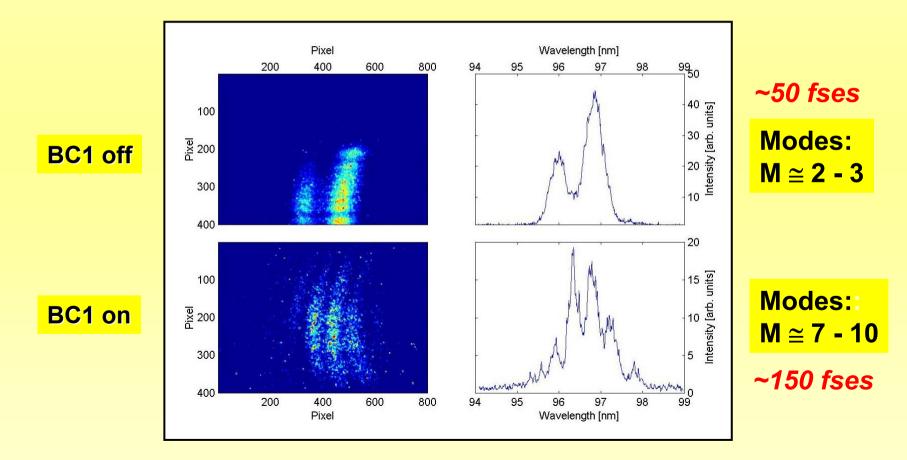


Pulsdauer zwischen 50 und 100 fsec



TTF Phase I

Pulse length variation via bunch compressor (BC1)





Performance of

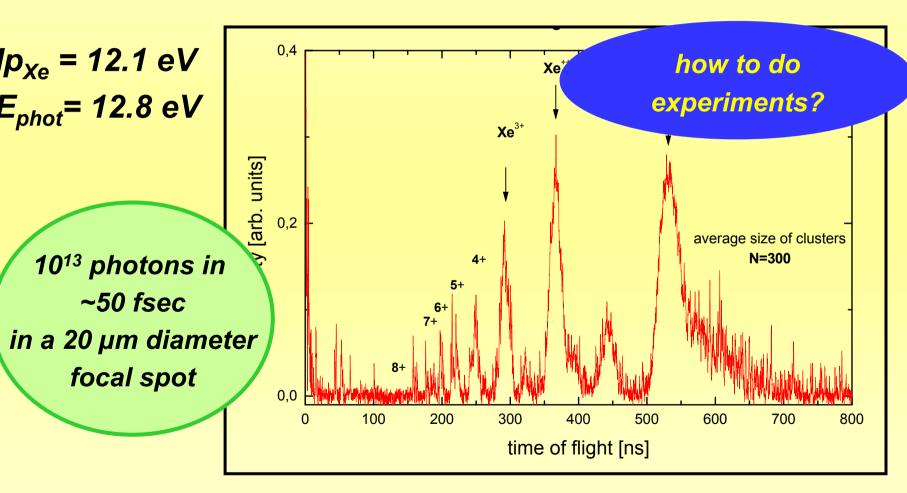
TESLA Test Facility VUV FEL (80-100 nm)

- saturation
- photon statistics
- single pulse spectral distribution
- lateral coherence
- second harmonic
- pulse length variation 50 150 fsec

all measured quantities agree very well with SASE FEL theory



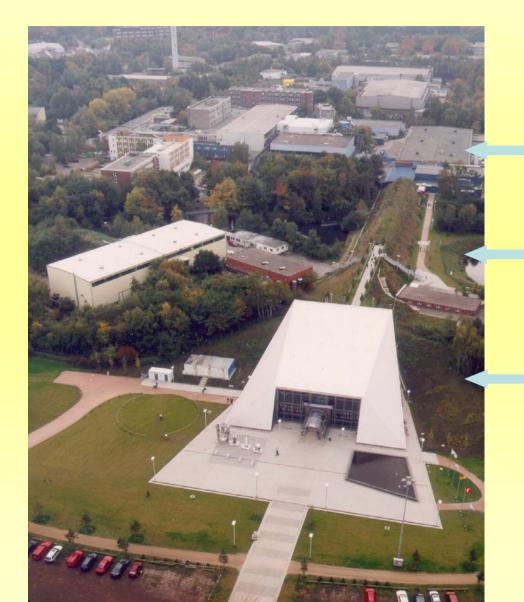
Single shot time-of-flight spectrum



Coulomb explosion of Xenon clusters with ~ 300 atoms



VUV FEL User Facility at DESY



TTF 1

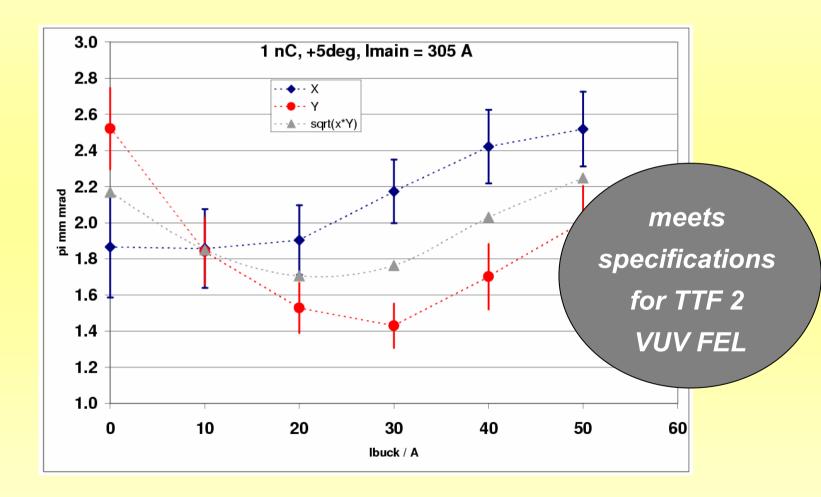
TTF 2

experimental hall

start of operation in 2004



Latest results from PITZ



current in the solenoid compensating the magnetic field at the cathode



VUV FEL at TTF

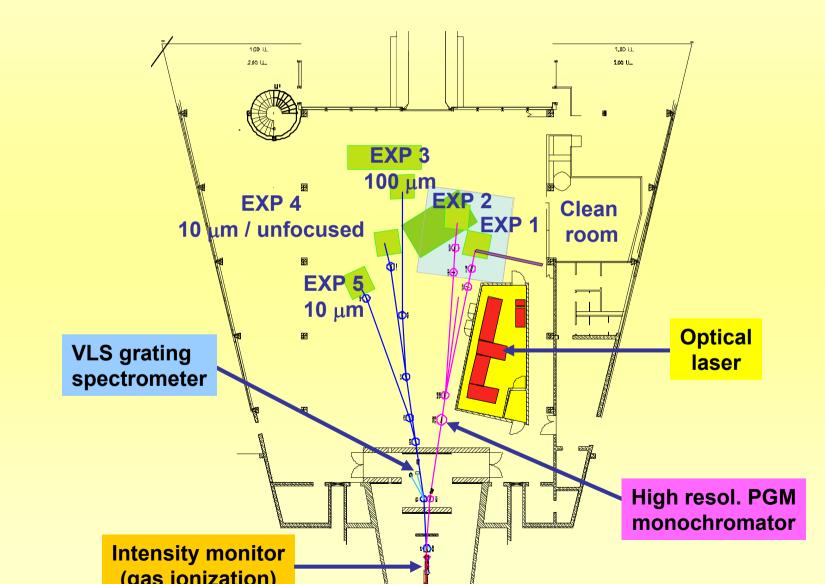


undulators



Layout of VUV FEL user facility

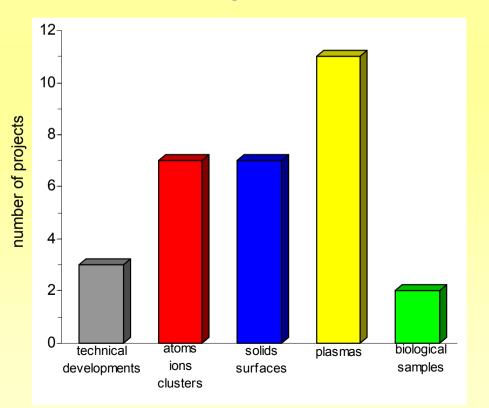
5 experimental stations





Review of VUV FEL Proposals Sep. 25-27, 2002

Areas of Proposed Research



- 30 proposals submitted
- about 200 scientists from
 60 institutes in 11 countries involved

optical lasers community: 18

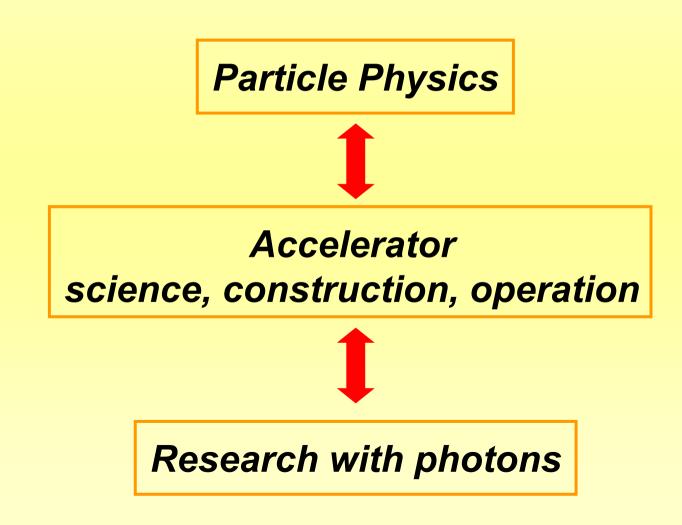
synchrotron community: 12



European XFEL Laboratory

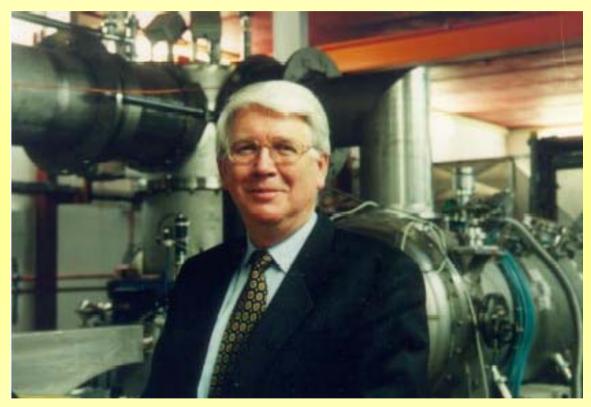


DESY's formula for success:





1992: The vision for DESY's future



Björn H. Wiik

TESLA: A linear e⁺-e⁻ collider with incorporated X-ray laser based on a super conducting linear accelerator



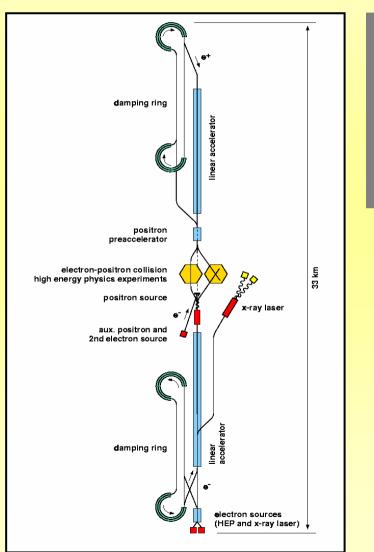
TESLA project





TESLA:

Linear Collider with integrated X-ray laser laboratory



500 GeV linear collider3136 Mio EuroDetector for particle physics210 Mio EuroAccelerator components for X-FEL241 Mio EuroX-ray laser laboratory290 Mio Euro

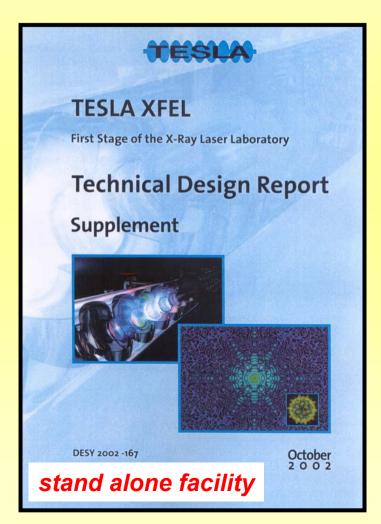
7000 person years





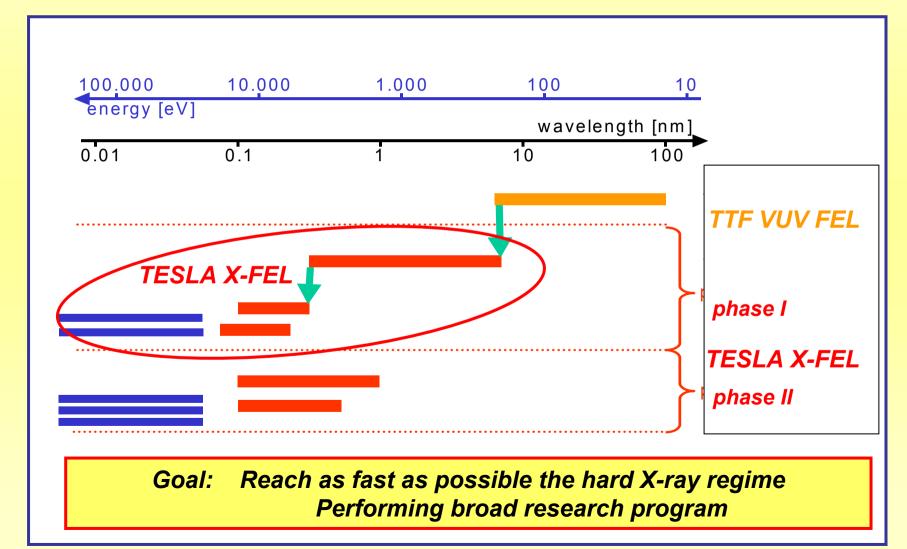
German Science Council Statements concerning the X-FEL

DESY and the **TESLA** collaboration are asked to present as soon as possible a technical proposal which is optimised for the X-FEL, based on the existing **Technical Design Report for** the integrated solution. This proposal should include a cost evaluation.

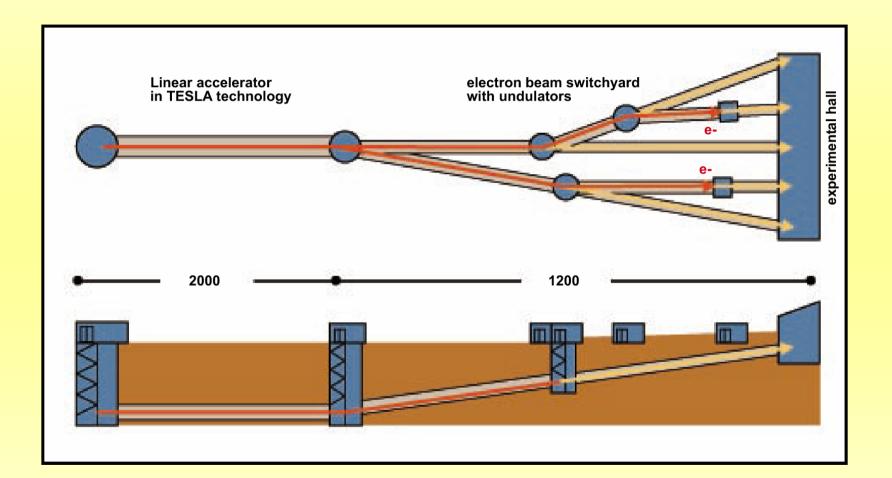




Spectral distribution at XFELs in Hamburg



European XFEL Laboratory (Oct. 2002)



3 FEL and 2 beamlines for spontaneous synchrotron radiation with 10 independent experimental stations



European XFEL Laboratory

Cost estimate at year 2000 prices

Linear accelerator including 110 million EUR for personnel 446 million EUR

XFEL Laboratory with beamlines and 10 experimental stations including 30 million EUR for personnel

238 million EUR

Project preparation

25 million EUR



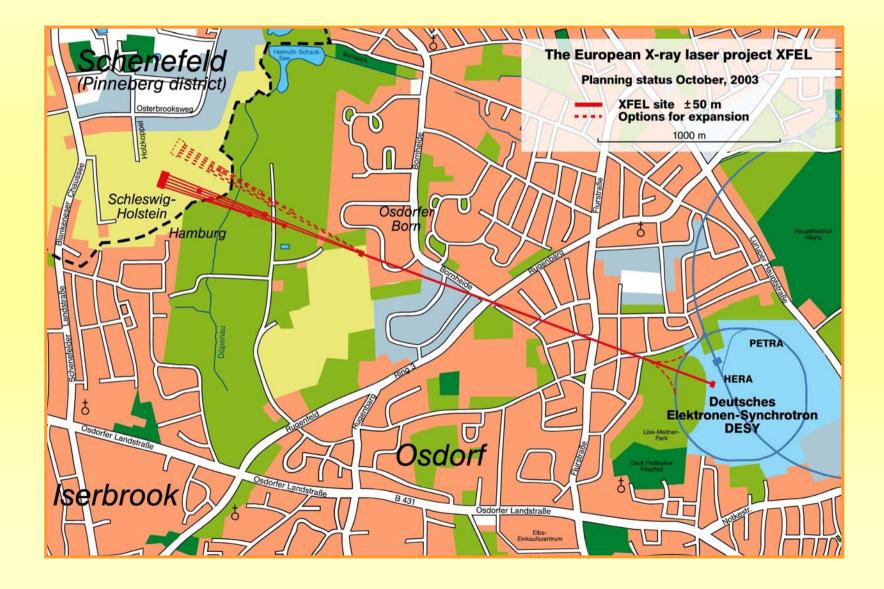
Decisions by German Government on Large Scale Facilities for Research

announced 5 February 2003

- 50 % of the investment costs of 673 MEuro for a European XFEL Laboratory
- 120 MEuro for upgrade of PETRA storage ring
- No comment on possible sites for TESLA Linear Collider, DESY encouraged to continue strong program in particle physics



European XFEL Laboratory – Site Proposal





Discussions in Europe





EUROPEAN STRATEGY FORUM on RESEARCH INFRASTRUCTURES

Sixth meeting

Brussels, Friday July 4, 2003 (09:30-17:00)

- 5. X-ray FEL at DESY
 - a issues encountered by delegations considering the question
 "whether or not to join?" (science case, technical case, business case)
 - **b** exchange of views and experiences
 - c conclusions with respect to continuation of negotiations
- 6. Working groups on Free Electron Lasers
 - a final version of joint report (I, UK): discussion
 - b conclusions and follow-up

Suggestion: Workshop on the

Technical Challenges at the Proposed European XFEL Laboratory



Conclusions of ESFRI workshop

- A lot more needs to be done, but technical solutions are in reach to meet the parameters of the proposed European XFEL Laboratory in due time
 - photo-cathodes, injectors
 - optimization of Linac, however, it is already clear today that the TESLA technology is flexible enough to be able to profit from progress expected in the coming years for different sub-systems
 - fast switching within a bunch train preserving the beam quality
 - electron and photon beam diagnostics
 - synchronization
 - X-ray optics, instrumentation, detectors



Discussion at ESFRI - Trieste 20. Nov. 2003

- Ministers have on the table a German proposal for a European hard X-ray FEL facility in Hamburg. Declarations of interest by various Member States justify continuing along the following lines:
 - setting up of a European working group for engineering design
 - update of the science case, with the view of starting construction in about two years

- For the VUV/soft X-ray regime there are several initiatives from various countries, exploiting different technologies and leading to complementary applications:
 - Trieste FEL (IT), VUV FEL at TTF-2 (DE), 4GLS (UK), Max4 Laboratory (SE), BESSY-FEL (DE), Arc-en-Ciel (FR)



Discussion at ESFRI - Trieste 20 Nov. 2003

 Most initiatives are at various stages of maturity, but the majority of projects can start within 2-3 years: for example the TTF-2 soft X-ray facility will start as a user facility in Hamburg in 2005. R&D has already taken place on practically all proposed facilities.

 A joint project for advanced R&D on key technological issues, covering both the hard X-ray and the VUV/soft X-ray regimes, is intended to start within months.

"EC Call for Design Studies"



EUROPEAN INITIATIVE FOR GROWTH QUICKSTART PROGRAMME

This Quick-start programme identifies key areas for investment in network and knowledge.

The projects, where work and investment can be under way within three years, accelerate progress towards achieving existing EU goals.

The total volume of investment that this Initiative mobilises will be around €60 billion between now and 2010 and, in some cases, beyond.

The specific projects foreseen cover:

- nanoelectronics
- next generation lasers (VUVs and XFEL in Hamburg)
- use of hydrogen as a source of energy and electricity



Photons at DESY:

A coherent and bright perspective

With the VUV FEL, PETRA III and XFEL project DESY will provide a unique spectrum of outstanding facilities for research with X-rays to the national and international science communities.

DESY's accelerator department will focus more and more on the development, construction and operation of accelerator based light sources.

Together with its international partners, especially in the TESLA collaboration, DESY has an extraordinary potential to promote progress in accelerator based light sources and photon sciences as a whole.