

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture 1	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2017 G. Grübel, A. Philippi-Kobs, O. Seeck, T. Schneider, L. Frenzel, M. Martins, W. Wurth		
Location	Lecture hall AP, Physics, Jungiusstraße		
Date	Tuesday	12:30 - 14:00	(starting 4.4.)
	Thursday	8:30 - 10:00	(until 13.7.)



Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture:	4 SWS	Tuesday and Thursday
Tutorial/Übungen:	2 SWS	Tuesday (if agreed on)

Proseminar: *For Bachelor students*
8 creditpoints For Master students

Fixed dates:	Tuesday	12:30 - 14:00
	Thursday	8:30 - 10:00

First meeting "Tutorial":	Tuesday, April 11	14:30 - 16:00
Location:	Seminar room 4	



Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecturers: Gerhard Grübel (GG), Thomas Schneider (TS),
Oliver Seek (OS), Andre Philippi-Kobs (AK),

- Part I:** **Basics of X-ray Physics** (GG)
- Part II:** **Magnetism - Thin Films** (AK)
- Part III:** **Surfaces and Interfaces** (OS)
- Part IV:** **Macromolecular Crystallography** (TS)
Site Visit



Methoden moderner Röntgenphysik II: Streuung und Abbildung

Part I:

Basics of X-ray Physics

by Gerhard Grübel (GG)

- [4.4.] Organisation and Introduction
- [6.4.] Introduction
- [11.4.] X-ray Scattering Primer
- [13.4.] Sources of X-rays, Synchrotron Radiation
- [18.4.] Refraction and Reflection
- [20.4.] Kinematical Scattering Theory (I)
- [25.4.] Kinematical Scattering Theory (II), Applications
- [27.4.] Small Angle Scattering and Soft Matter
- [2.5.] Anomalous Scattering
- [9.5.] Introduction: Coherence I
- [11.5.] Coherence II; Applications of Coherent X-ray Beams

Literature

Basic concepts:

Elements of Modern X-Ray Physics

J. A. Nielsen and D. McMorrow, J. Wiley&Sons (2001)

X-Ray Diffraction

B.E. Warren, DOVER Publications Inc., New York

Principles of Optics

M. Born and E. Wolf, Cambridge University Press, 7th ed.

Soft X-rays and Extreme Ultraviolet Radiation

D. Attwood, Cambridge University Press (2000)

<http://www.coe.berkeley.edu/AST/sxreuv/>

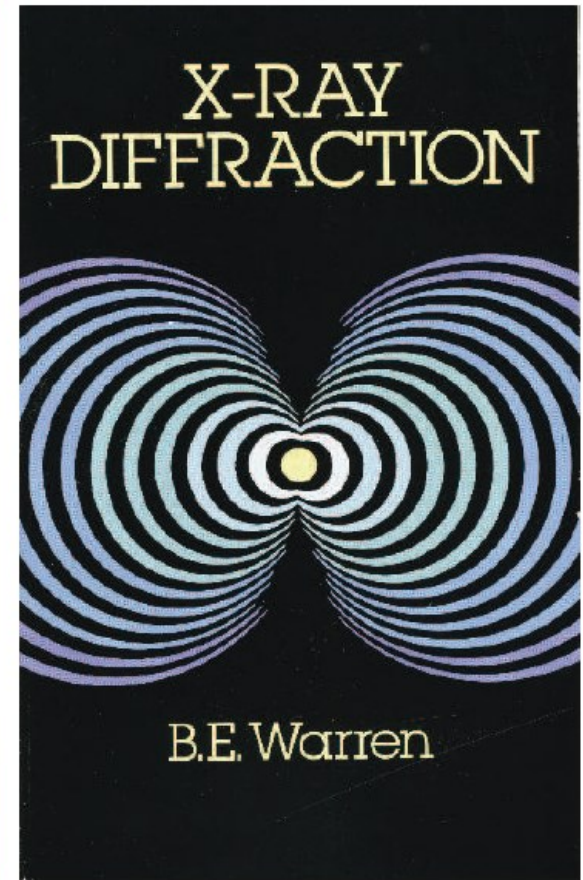
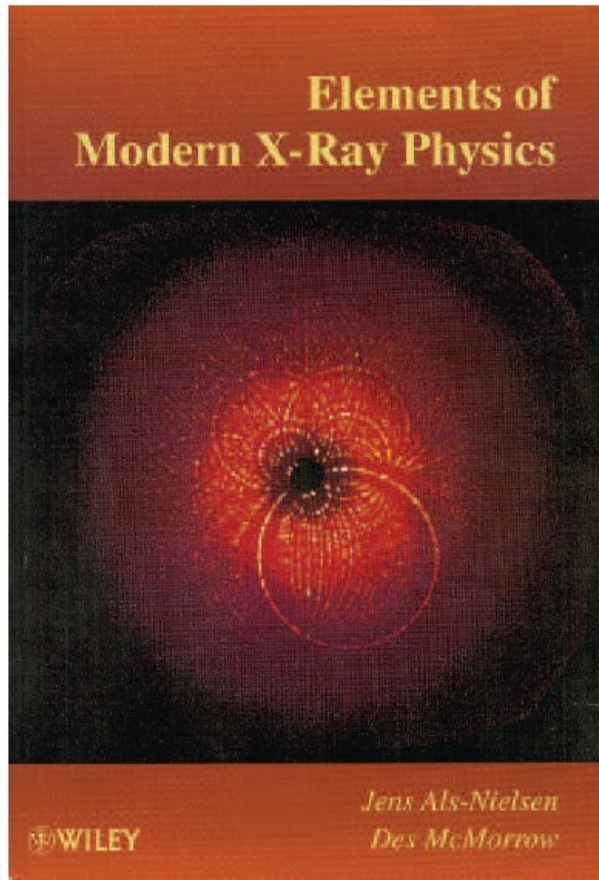
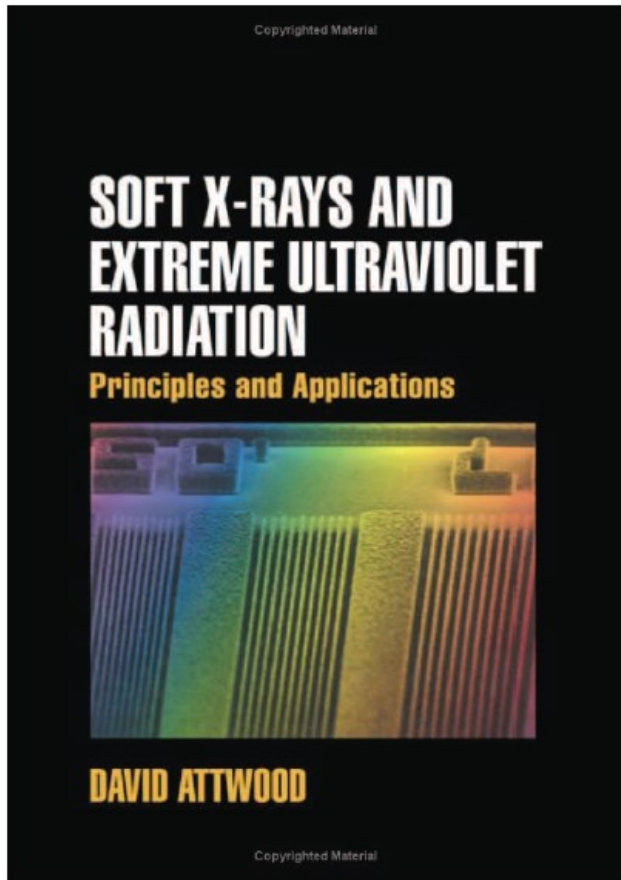
Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen

K. Wille, Teubner Studienbücher 1996

Lecture Notes

http://photon-science.desy.de/research/studentsteaching/lectures_seminars/ss17





* some of the slides are courtesy of M. Tolan, C. Gutt and A. Hermmerich

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Part I:

Basics of X-ray Physics

by Gerhard Grübel (GG)

Introduction

Overview, Introduction to X-ray Scattering



X-ray Scattering Primer

Elements of X-ray Scattering

Sources of X-rays, Synchrotron Radiation

Laboratory Sources, Accelerator Bases Sources

Reflection and Refraction from Interfaces

Snell's Law, Fresnel Equations

Kinematical Diffraction (I)

Diffraction from an Atom, a Molecule, from Liquids, Glasses, ...

Kinematical Diffraction (II)

Diffraction from a Crystal, Reciprocal Lattice, Structure Factor, ...

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Small Angle Scattering, and Soft Matter

Introduction, Form Factor, Structure Factor, Applications, ...

Anomalous Diffraction

Introduction into Anomalous Scattering, ...

Introduction into Coherence

Concept, First Order Coherence, ...

Coherent Scattering

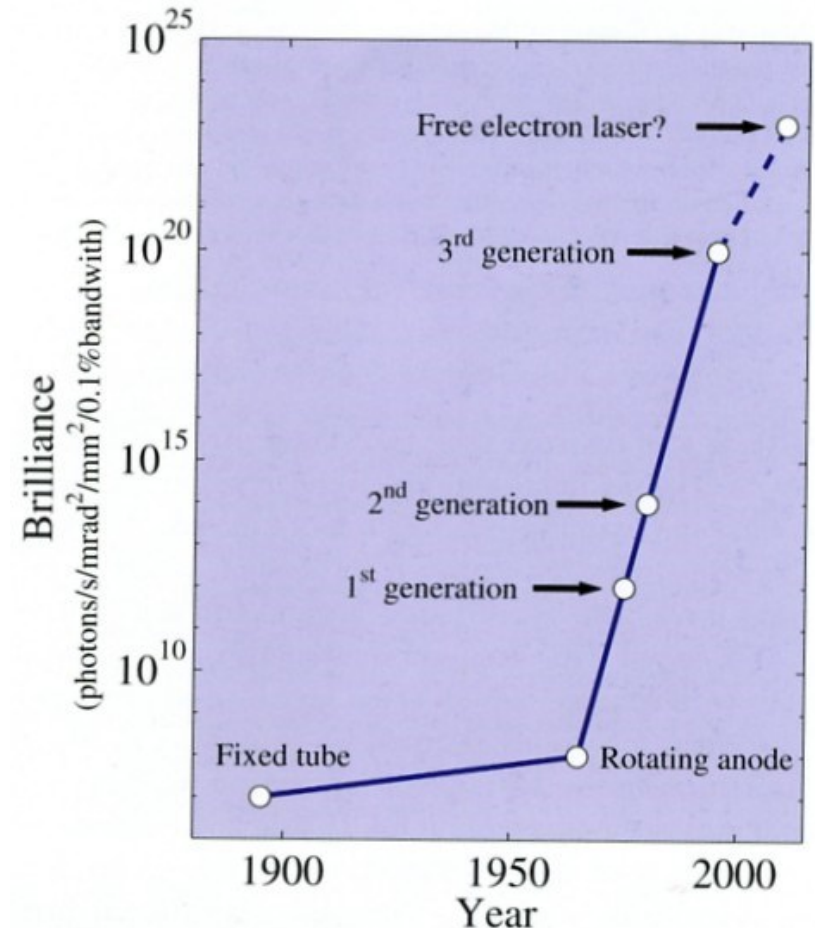
Spatial Coherence, Second Order Coherence, ...

Applications of Coherent Scattering

Imaging and Correlation Spectroscopy, ...

Introduction by Gerhard Grübel

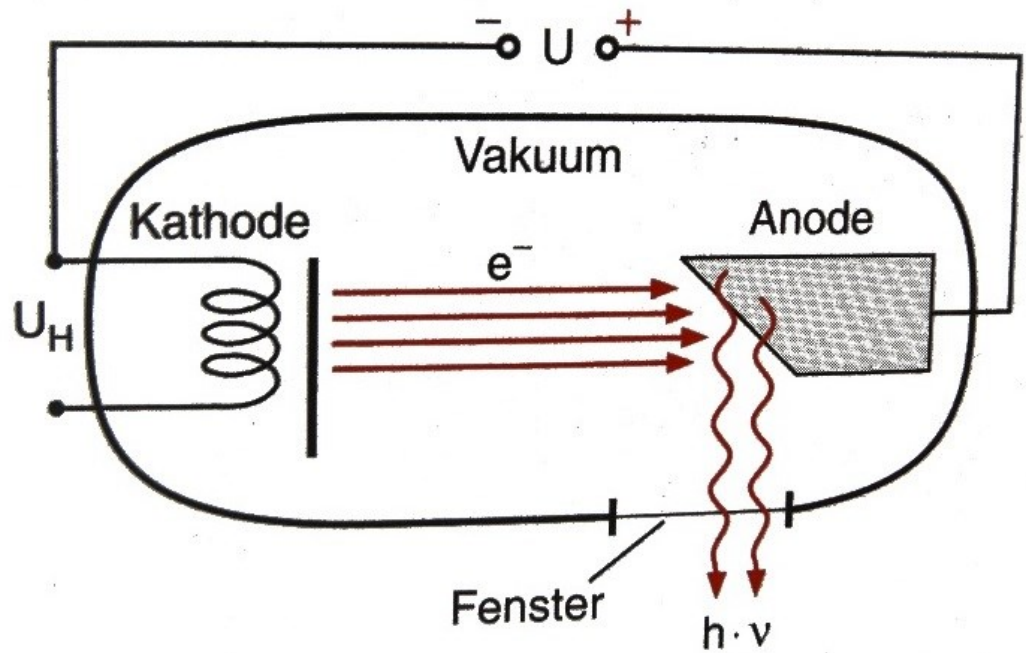
- 1895 X-ray discovered by W.C. Röntgen
- 1901 Nobel Prize; since then, unprecedented success in unraveling the structure of materials
- 1970 Synchrotron radiation revolutionizes the field
- 2005 Start operation FLASH (first SASE based FEL)
- 2009 Free Electron Lasers (XFEL)



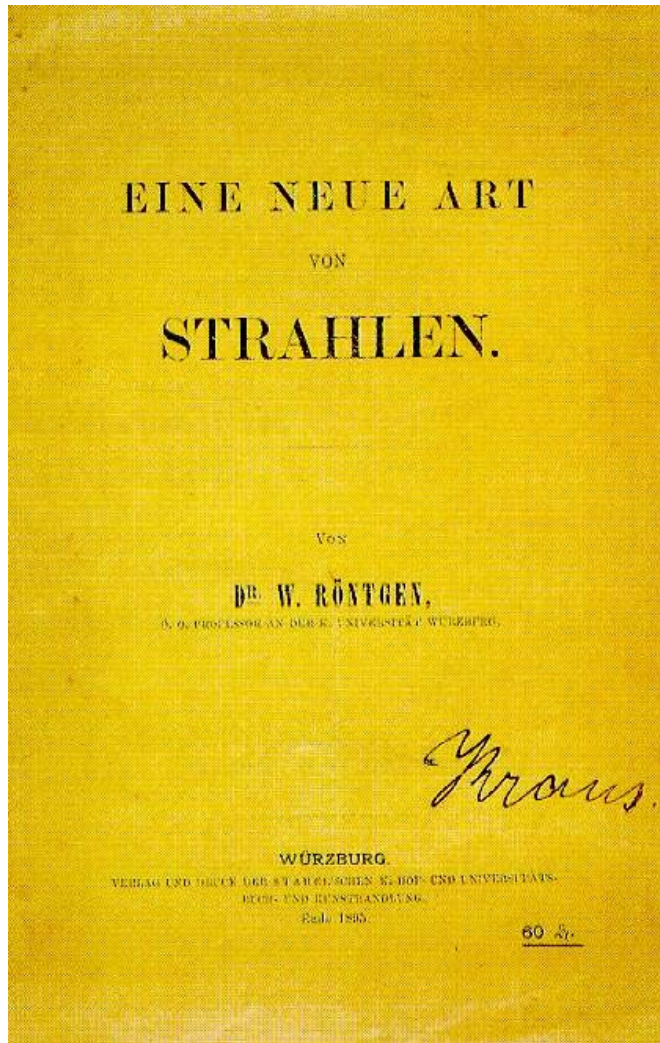
Würzburg, 8. November 1895



Wilhelm C. Röntgen (1845 - 1923)



Klassische Röntgenröhre



X-rays

≡

Electromagnetic Radiation

≡

Wavelength

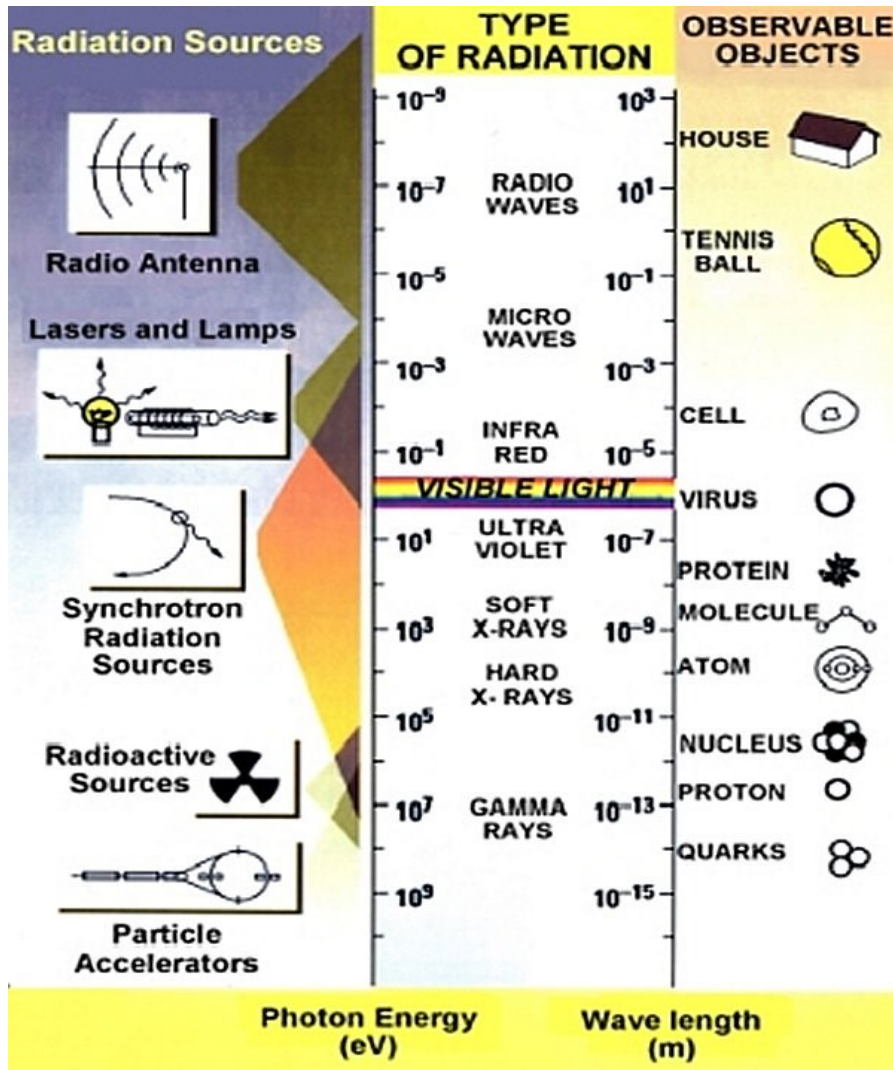
$$(\lambda[\text{\AA}] = \frac{12.398}{E [\text{keV}]})$$

≡

Object Size

≡

Angstroms
 for Condensed
 Matter Research



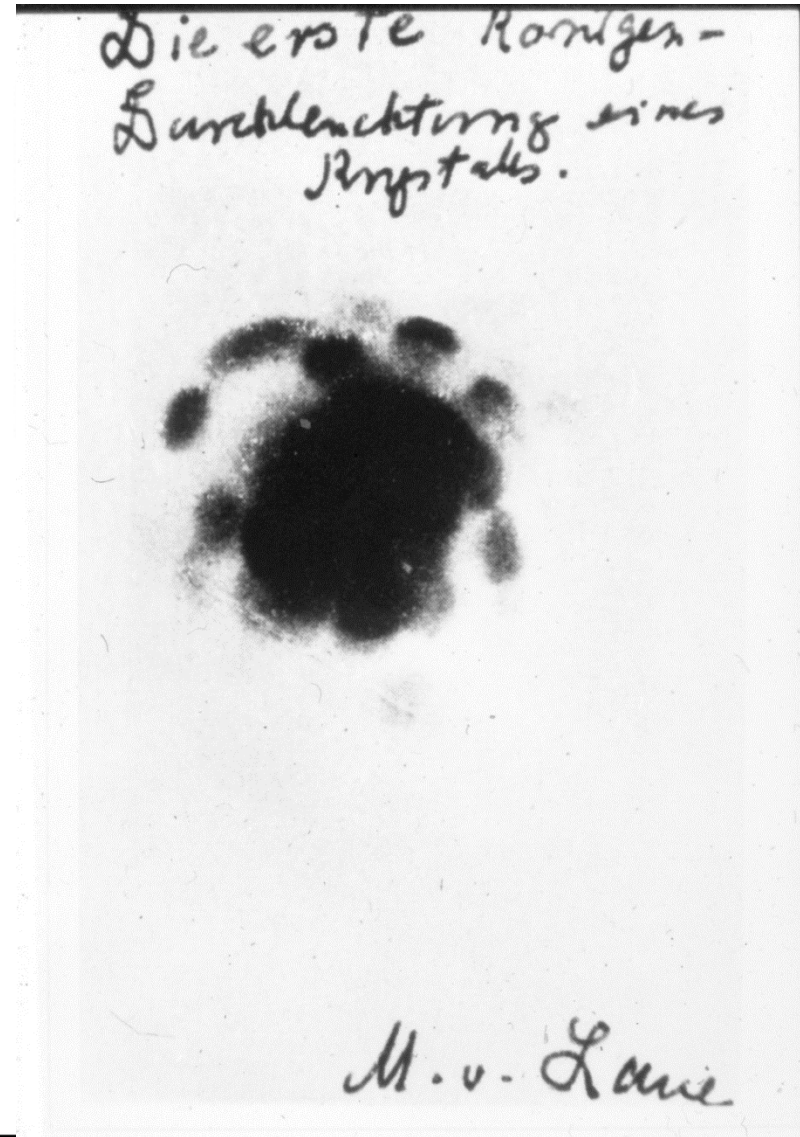
Nobel Prices

- 1901 W.C. Röntgen in **Physik** für die **Entdeckung der Röntgenstrahlen**
- 1914 M. von Laue in **Physik** für **Röntgenbeugung an Kristallen**
- 1915 W.H. Bragg und W.L. Bragg in **Physik** für Bestimmung der **Kristallstruktur mit Röntgenbeugung**
- 1917 C.G. Barkla in **Physik** für die **charakteristische Strahlung der Elemente**
- 1924 K.M.G. Siegbahn in **Physik** für **Röntgenspektroskopie**
- 1927 A.H. Compton in **Physik** für **Streuung von Röntgenstrahlen durch Elektronen**
- 1936 P. Debye in **Chemie** für **Beugung von Röntgenstrahlen und Elektronen in Gasen**
- 1946 H.J. Muller in **Medizin** für die Entdeckung von **Mutationen durch Röntgenstrahlung**
- 1954 L. Pauling in **Chemie** für Entwicklungen in der **Strukturchemie**
- 1956 A.F. Cournand, W. Forssmann und D.W. Richards in **Medizin** für die **Entwicklung des Herzkatheters unter Röntgenkontrolle**
- 1962 J. Watson, M. Wilkins und F. Crick in **Medizin** für die **Strukturaufklärung des DNA-Moleküls**
- 1962 M. Perutz und J. Kendrew in **Chemie** für die **Strukturaufklärung von Hämoglobin**
- 1964 D.C. Hodgkin in **Chemie** für die **Röntgenstrukturanalyse von Penicillin** und wichtigen biochemischen Substanzen
- 1976 W.N. Lipscomb in **Chemie** für **Röntgenstrukturuntersuchungen an Boranen**
- 1979 A.M. Cormack und G.N. Hounsfield in **Medizin** für **Computertomographie**
- 1981 K.M. Siegbahn in **Physik** für **hochaufgelöste Elektronenspektroskopie**
- 1985 H.A. Hauptman und J. Karle in **Chemie** für die Entwicklung direkter Methoden zur **Bestimmung von Röntgenstrukturen**
- 1988 J. Deisenhofer, R. Huber und H. Michel in **Chemie** für die **Bestimmung der dreidimensionalen Struktur von Proteinen für die Photosynthese**
- 1997 P.D. Boyer, J.E. Walker und J.C. Skou in **Chemie** für **Aufklärung der Funktion des Enzyms ATP**
- 2002 R. Giacconi in **Physik** für die **Entwicklung der Röntgenastronomie**
- 2003 R. MacKinnon in **Chemie** für **Röntgenstrukturbestimmung von Ionenkanälen in Zellmembranen**
- 2009 V. Ramakrishnan, T. A. Steitz, A. E. Yonath in **Chemie** für **Studies of the Structure and Function of the Ribosome**

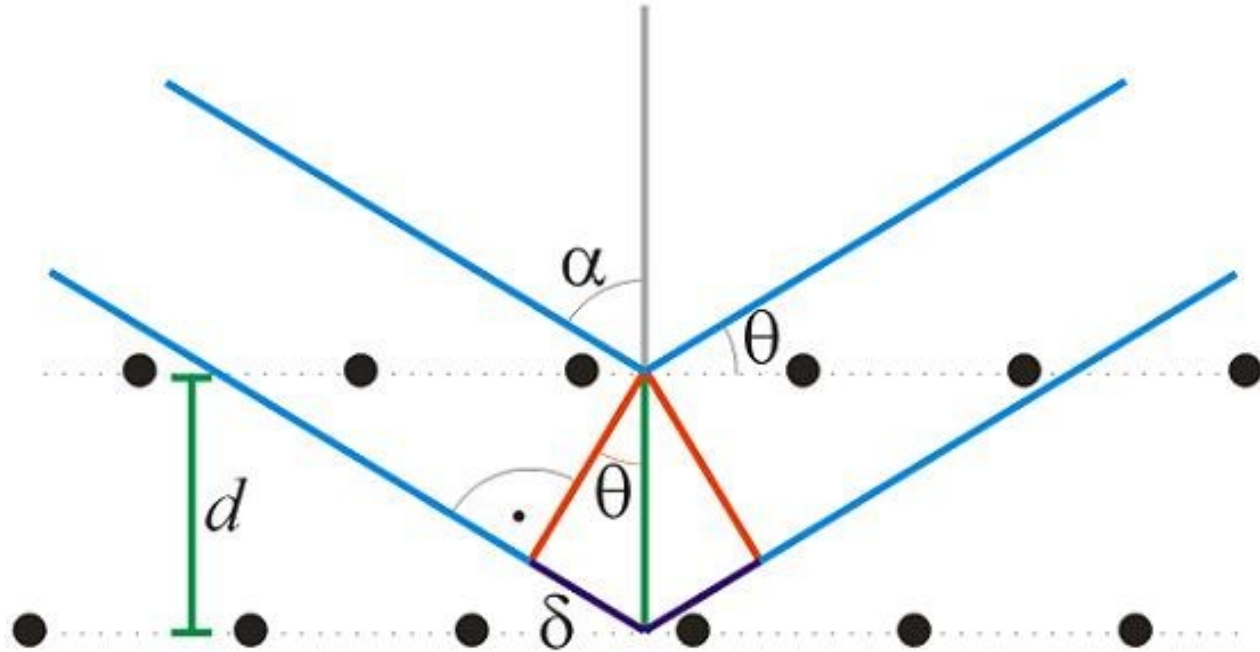
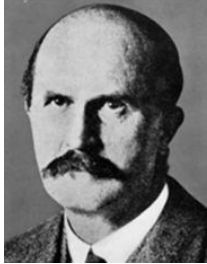
v. Laue et. al.

Interferenzen am Kristallgitter

Laue, Friedrich und Knipping 1912

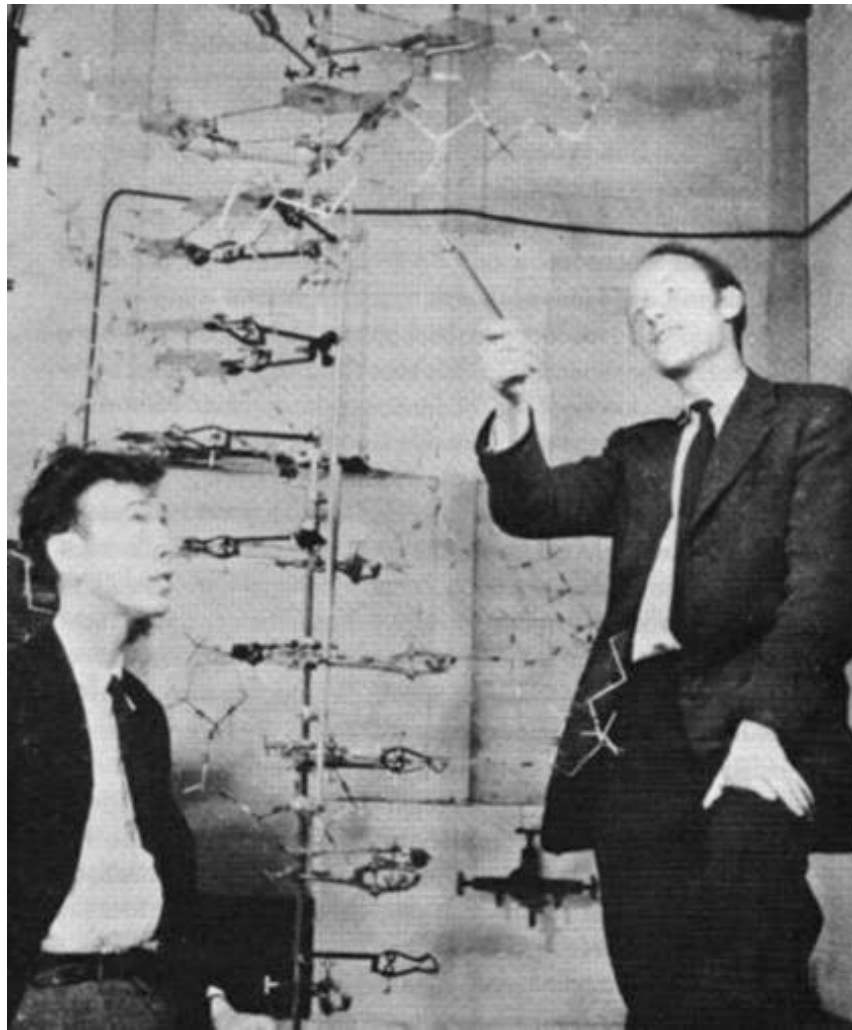


Bragg's Law



Scattering intensity only if: $n\lambda = 2d \sin(\Theta)$

Watson & Crick 1953



A Structure for DNA

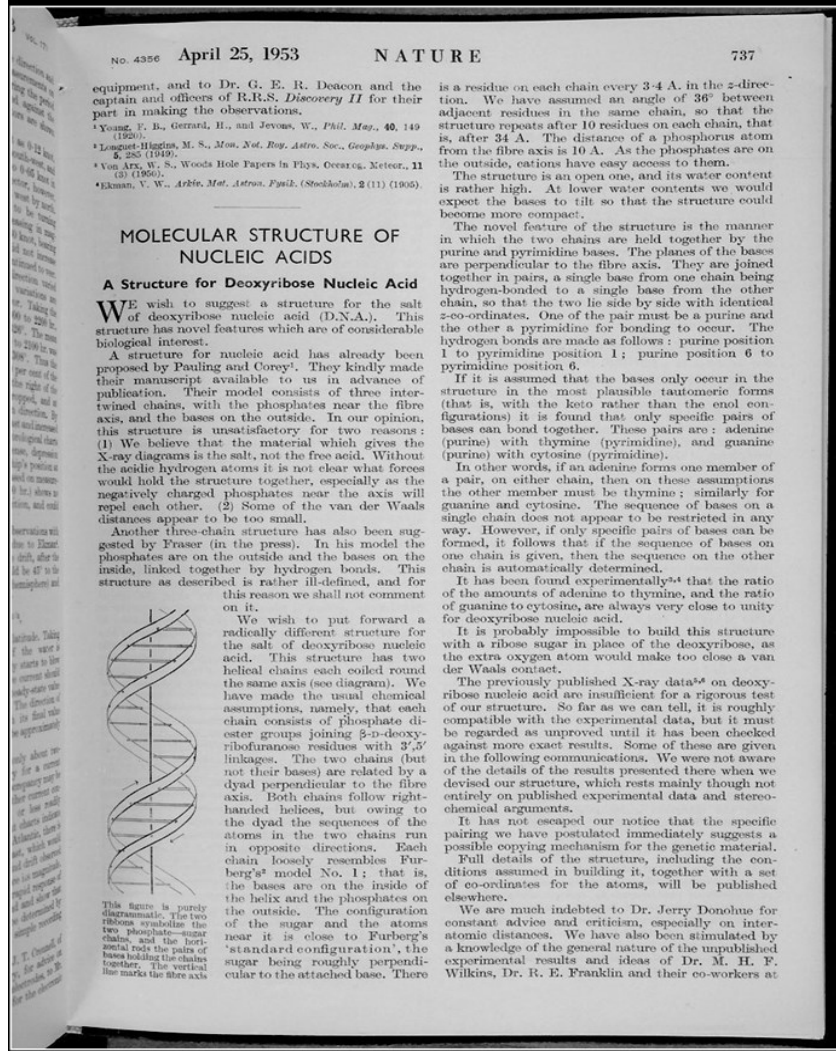
James D. Watson and Francis H.C. Crick (1953)

It has not escaped our notice that the specific pairing we have postulated immediately suggests a possible copying mechanism for the genetic material.

Full details of the structure, including the conditions assumed in building it, together with a set of co-ordinates for the atoms, will be published elsewhere.

We are much indebted to Dr. Jerry Donohue for constant advice and criticism, especially on interatomic distances. We have also been stimulated by a knowledge of the general nature of the unpublished experimental results and ideas of Dr. M. H. F. Wilkins, Dr. R. E. Franklin and their co-workers at

James D. Watson and Francis H. C. Crick
"Molecular Structure of Nucleic Acids: A Structure for Deoxyribose Nucleic Acid" (1953)

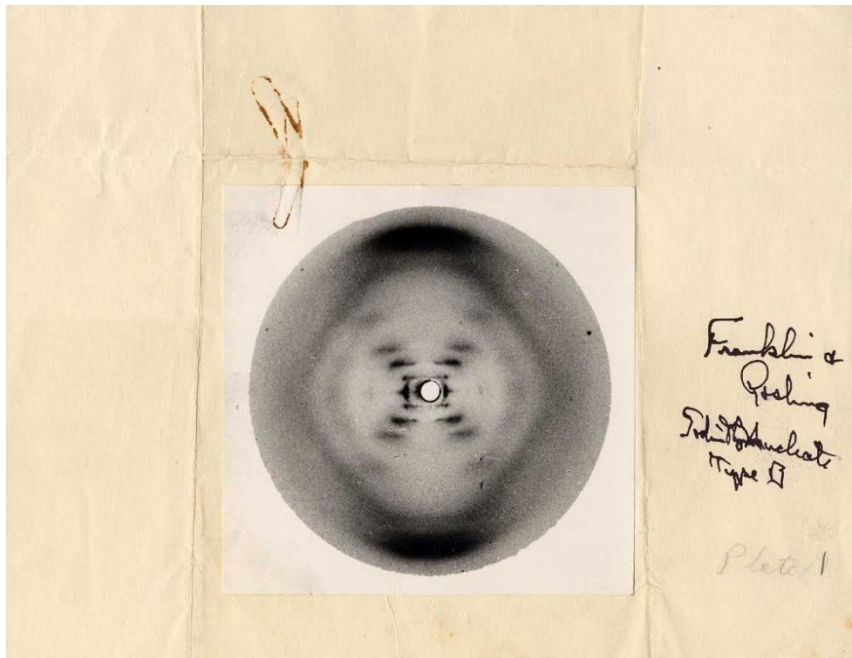
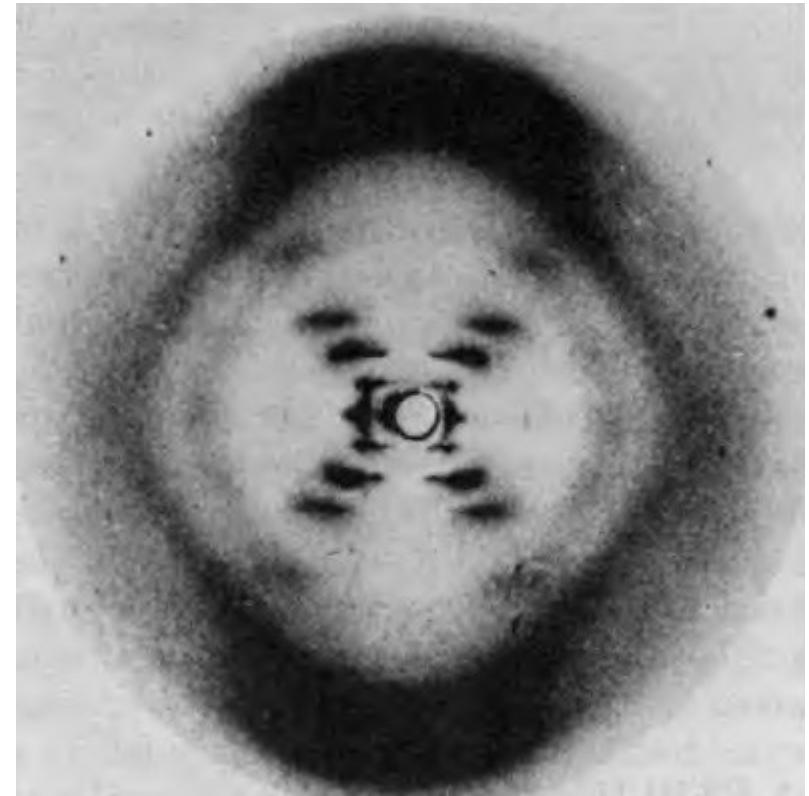


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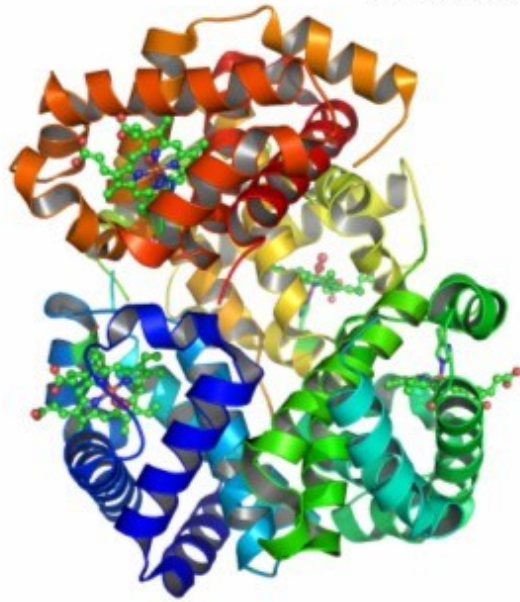
Illustration reprinted with permission from *Nature* (171: 736-37). Copyright 1953, Macmillan Magazines Ltd; and with the permissions of James Watson and Francis Crick.



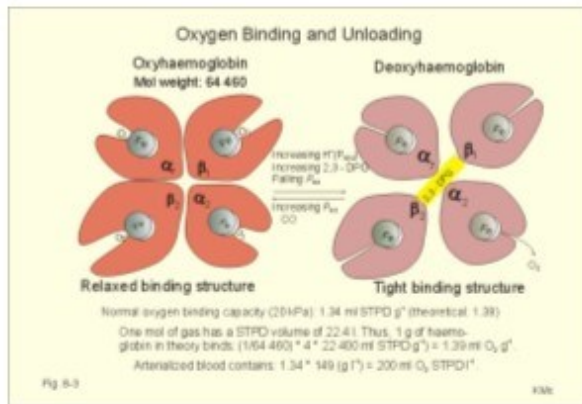
Rosalind Franklin's Famous X-ray that provided enough evidence to establish that DNA was a helix.



Hämoglobin und Myoglobin Struktur mit Röntgenstrahlen



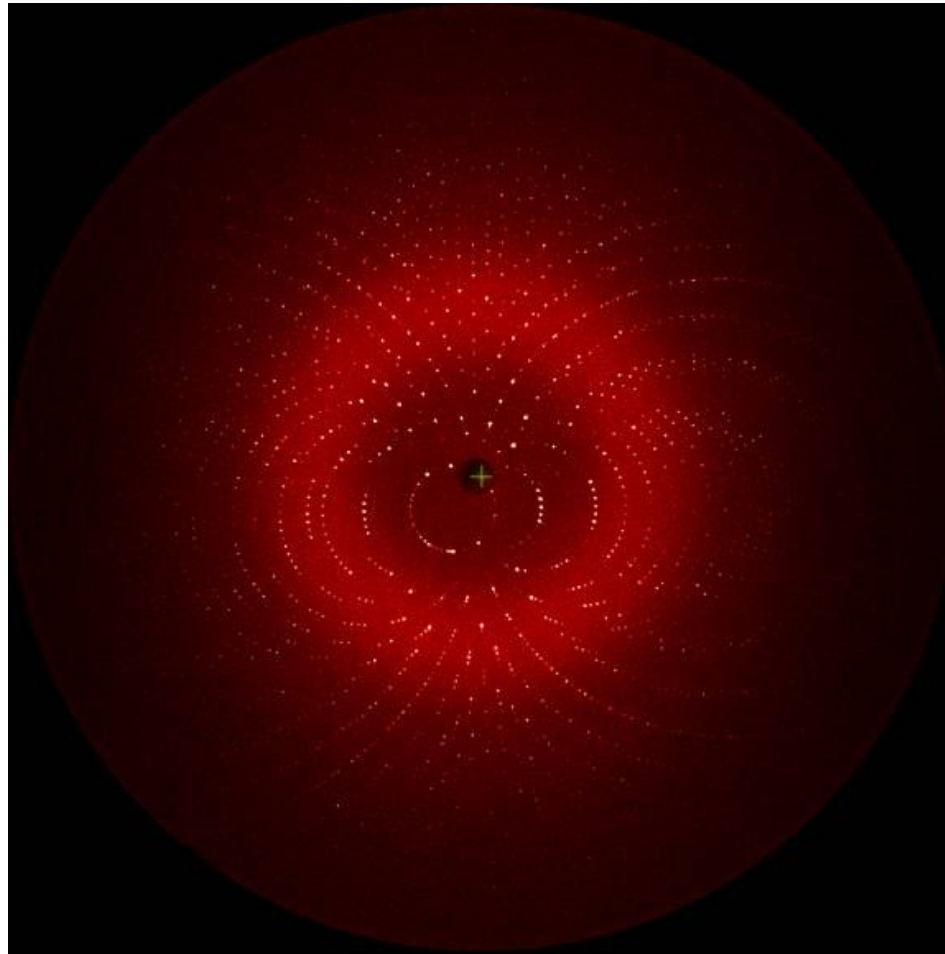
John Cowdery Kendrew
 Max Perutz
 Nobelpreis 1962



X-ray Scattering Research Today



Modern Protein Crystallography



BioCARS 14-ID-B station of APS using an undulator with a gap of 25 mm from a crystal of the M37V mutant of CO-bound dimeric clam hemoglobin.

Dynamics of Biomolecules

Example:

Myoglobin protein found in muscle, stores oxygen for conversion into energy. Structure solved in 1960 (Kendrew).

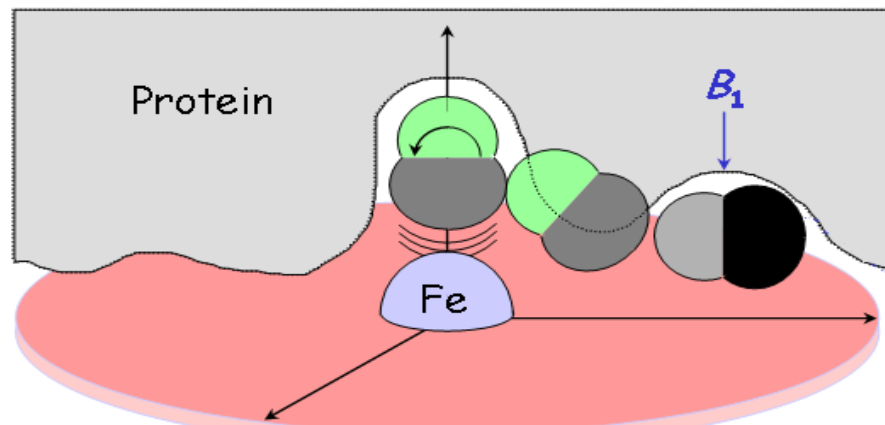
Puzzle:

How does the oxygen get into and out of the myoglobin molecule?

The protein is not static but dynamic with channels opening and closing?

→ Time resolved Laue Diffraction

Use CO instead of O₂. Use 10 ns optical pulse to CO from the Fe docking site. Probe dynamics with a 100 ps x-ray pulse.

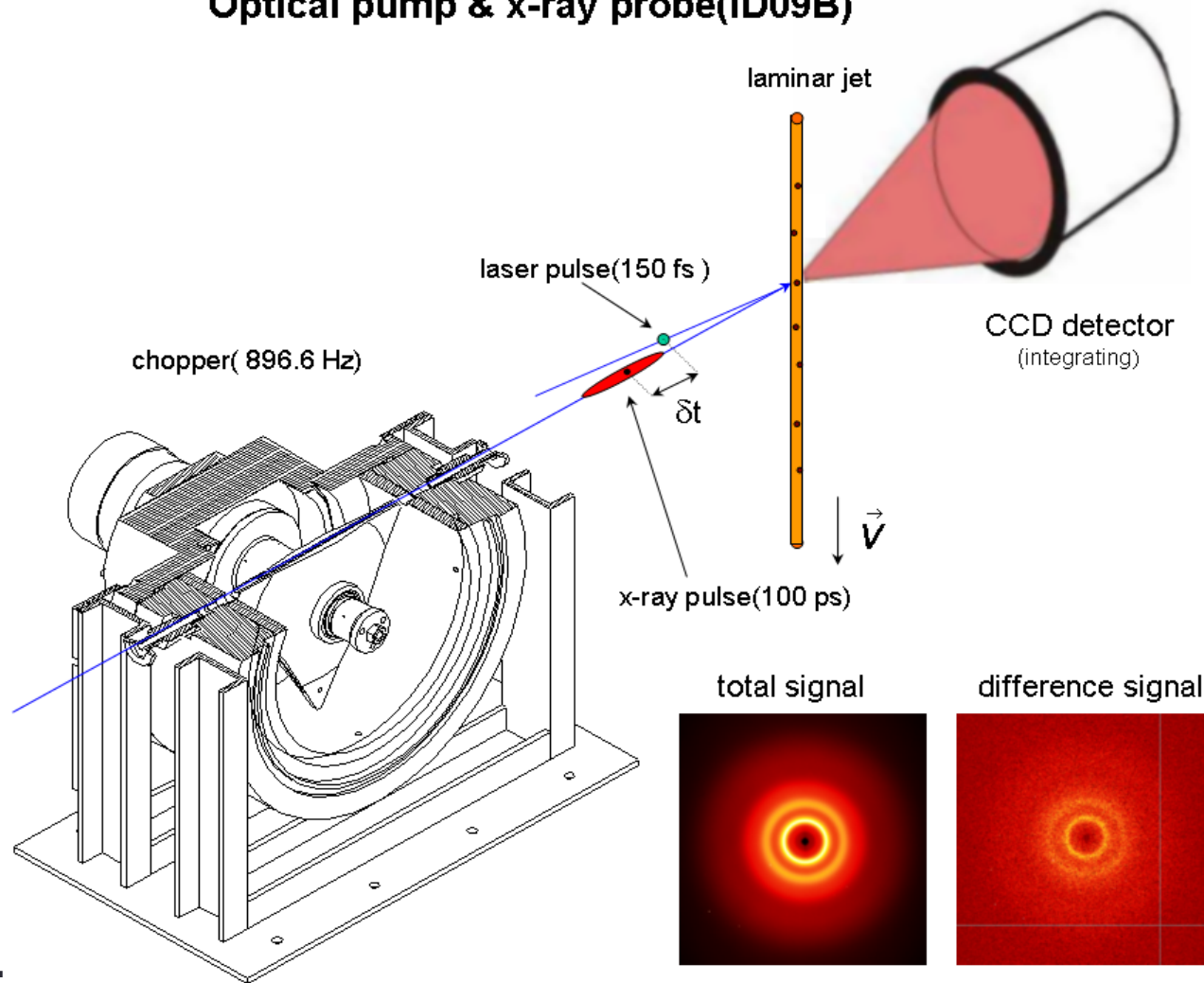


Courtesy M. Wulff



Time Resolved Protein Dynamics

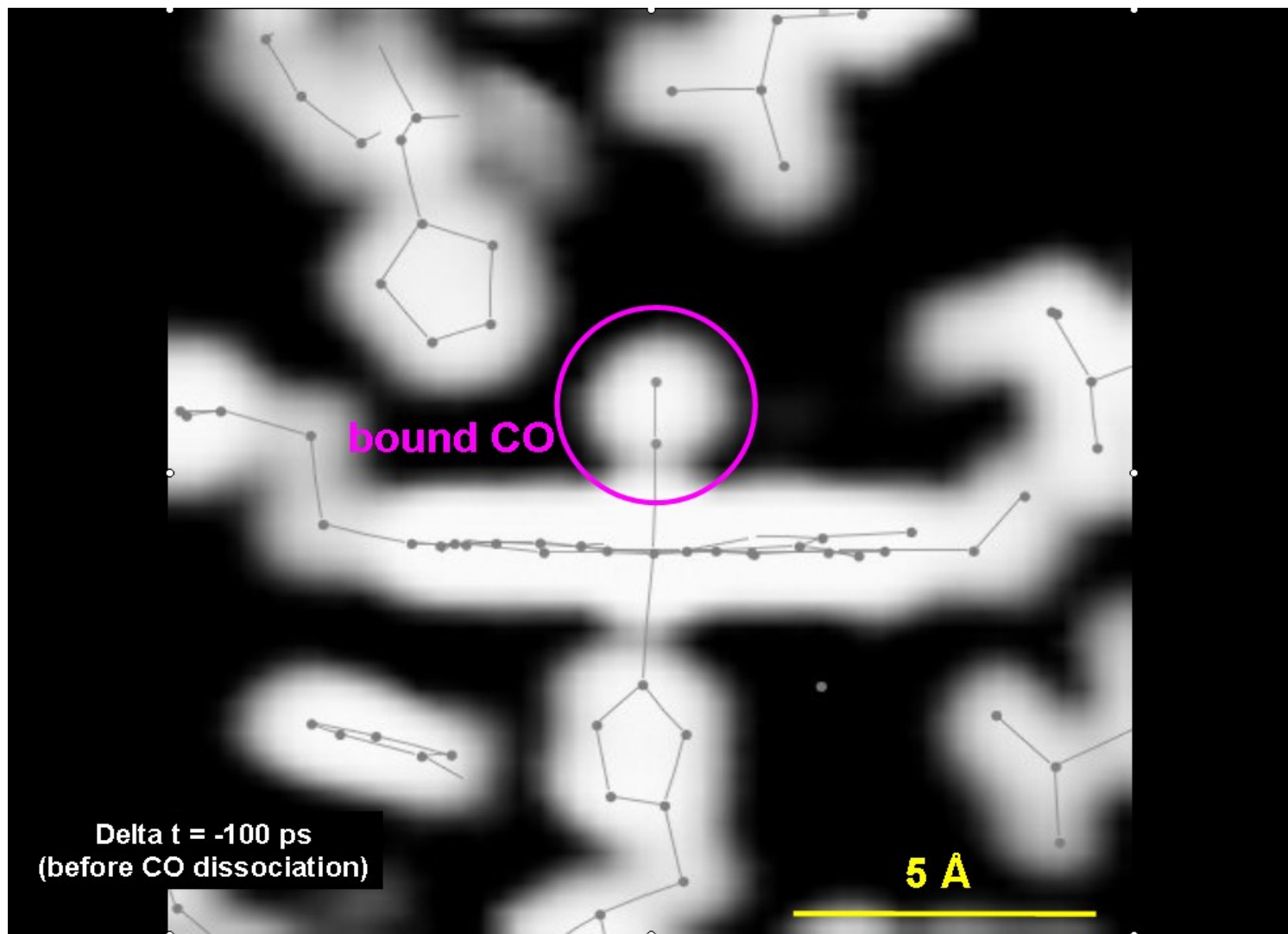
Optical pump & x-ray probe (ID09B)



Courtesy M. Wulff

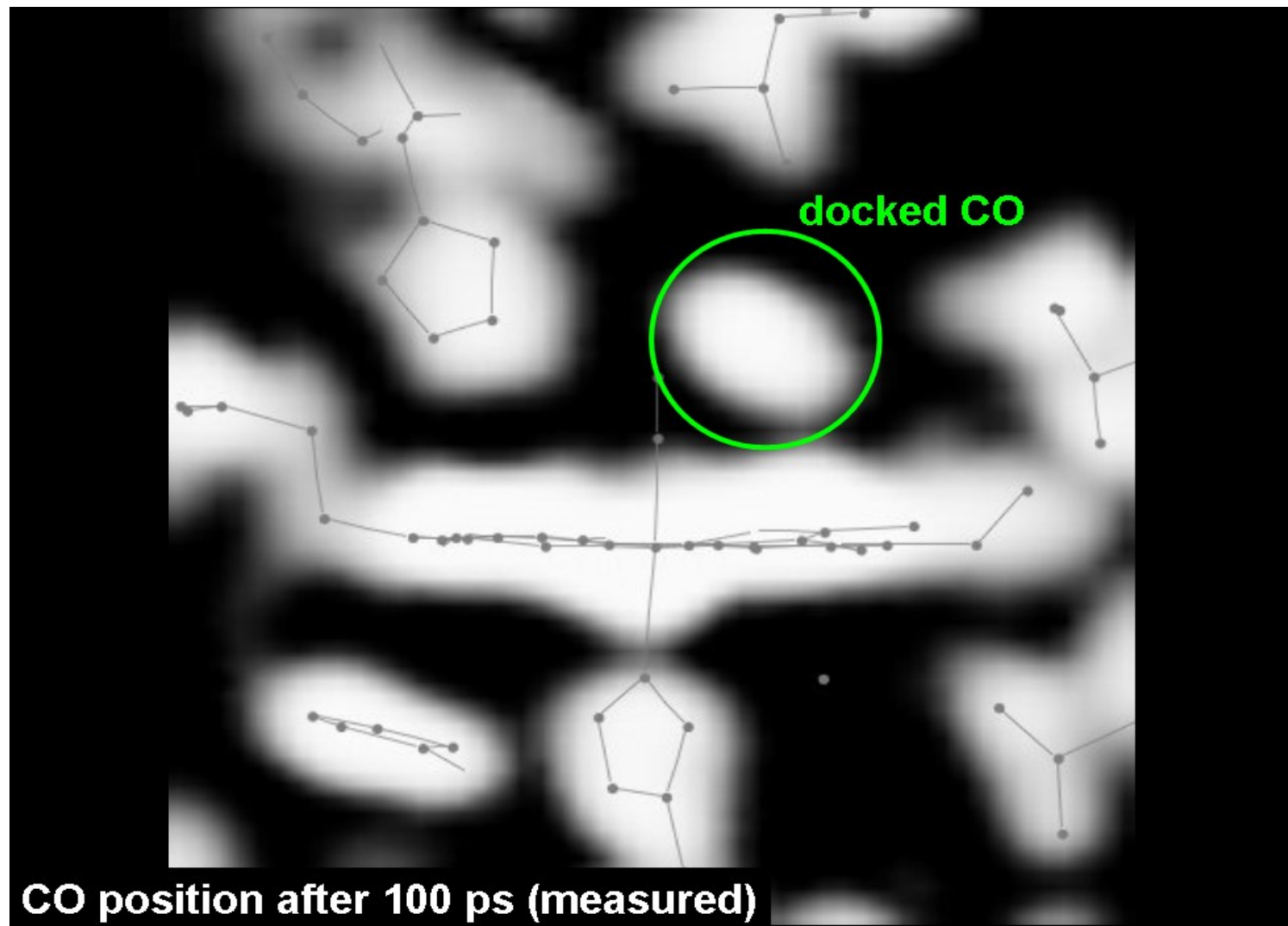
Time Resolved Protein Dynamics

Courtesy
M. Wulff



Time Resolved Protein Dynamics

Courtesy
M. Wulff

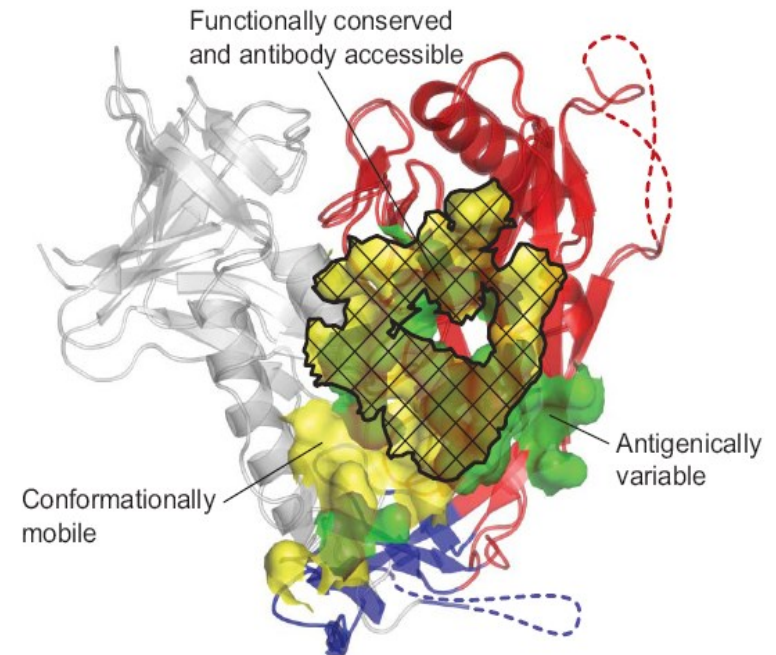


ARTICLES

Structural definition of a conserved neutralization epitope on HIV-1 gp120

Tongqing Zhou¹, Ling Xu¹, Barna Dey¹, Ann J. Hessel³, Donald Van Ryk², Shi-Hua Xiang⁴, Xinzhen Yang⁴, Mei-Yun Zhang⁵, Michael B. Zwick³, James Arthos², Dennis R. Burton³, Dimiter S. Dimitrov⁵, Joseph Sodroski⁴, Richard Wyatt¹, Gary J. Nabel¹ & Peter D. Kwong¹

The remarkable diversity, glycosylation and conformational flexibility of the human immunodeficiency virus type 1 (HIV-1) envelope (Env), including substantial rearrangement of the gp120 glycoprotein upon binding the CD4 receptor, allow it to evade antibody-mediated neutralization. Despite this complexity, the HIV-1 Env must retain conserved determinants that mediate CD4 binding. To evaluate how these determinants might provide opportunities for antibody recognition, we created variants of gp120 stabilized in the CD4-bound state, assessed binding of CD4 and of receptor-binding-site antibodies, and determined the structure at 2.3 Å resolution of the broadly neutralizing antibody b12 in complex with gp120. b12 binds to a conformationally invariant surface that overlaps a distinct subset of the CD4-binding site. This surface is involved in the metastable attachment of CD4, before the gp120 rearrangement required for stable engagement. A site of vulnerability, related to a functional requirement for efficient association with CD4, can therefore be targeted by antibody to neutralize HIV-1.





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Deutsches Elektronen-Synchrotron
Ein Forschungszentrum der Helmholtz-Gemeinschaft



FORSCHERWELT.

Wir machen Erkenntnis möglich



Home

INFORMATIONEN FÜR

- » Journalisten
- » Wirtschaftspartner
- » Schüler und Lehrer

DESY beglückwünscht Ada Yonath zum Chemie-Nobelpreis



Die israelische Forscherin Prof. Ada E. Yonath hat zusammen mit zwei Amerikanern den Nobelpreis für Chemie verliehen bekommen. Ihre Forschungen zur Struktur und Funktion der Ribosomen, denjenigen Molekülkomplexen, die aus der DNA-Erbinformation die für das Leben notwendigen Eiweißmoleküle herstellen, führte sie hauptsächlich an DESYs DORIS-Beschleuniger durch.

» mehr

50 Jahre DESY

» Alle Infos zum Jubiläumsjahr



Veranstaltungen

» VERANSTALTUNGSKALENDER FÜR
DESY IN HAMBURG UND ZEUTHEN



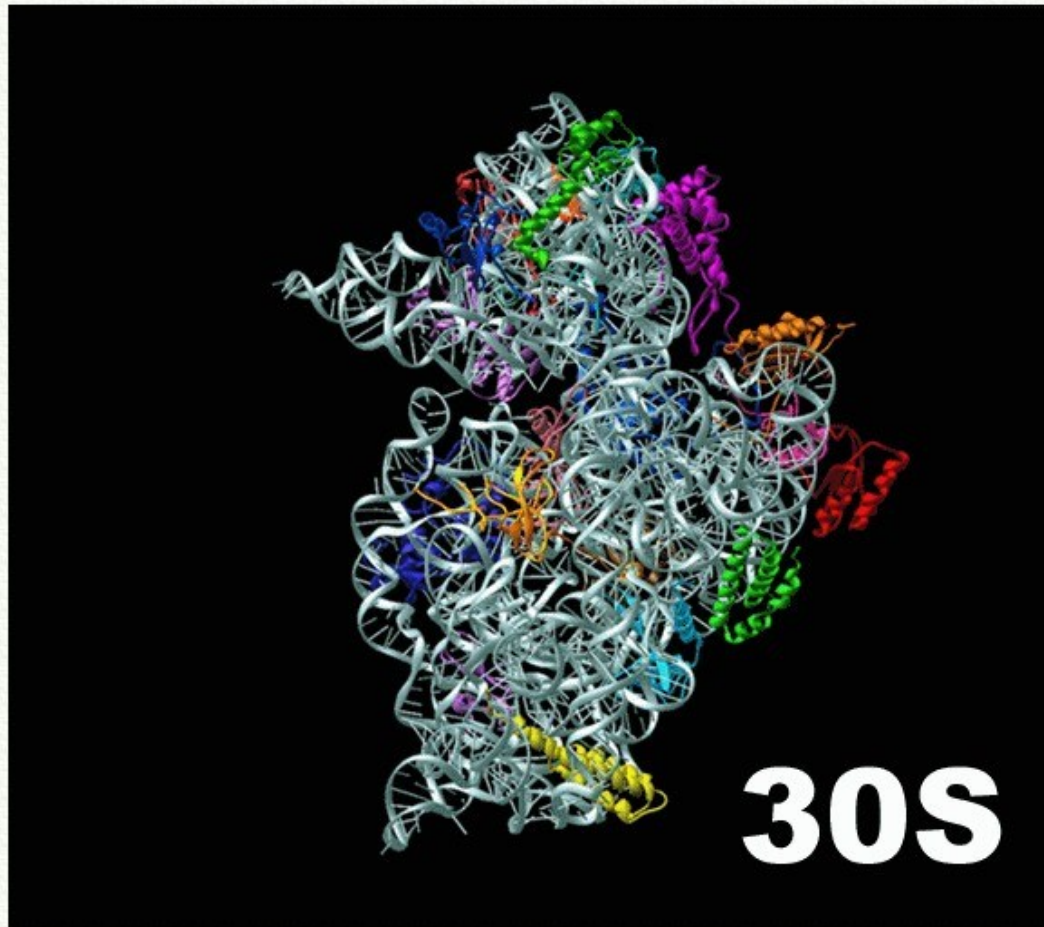


Figure A:

The Small Ribosomal Subunit

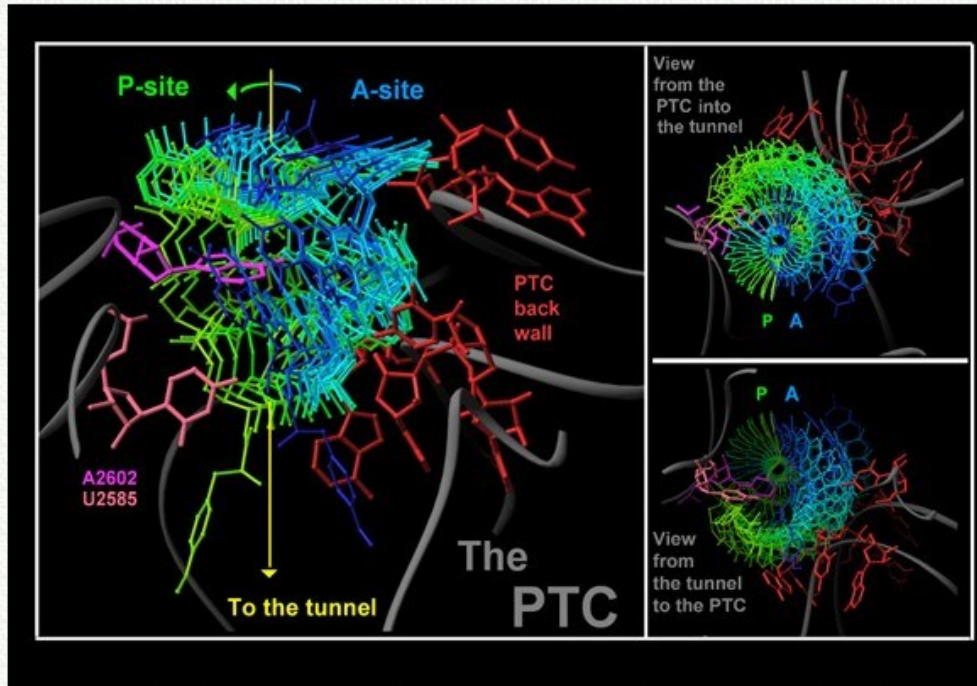
Schlutzen et al., Cell, 102, 615-23 (2000)



Figure B:

The Large Ribosomal Subunit

[Harms et al., Cell, 107, 679-88 \(2001\)](#)



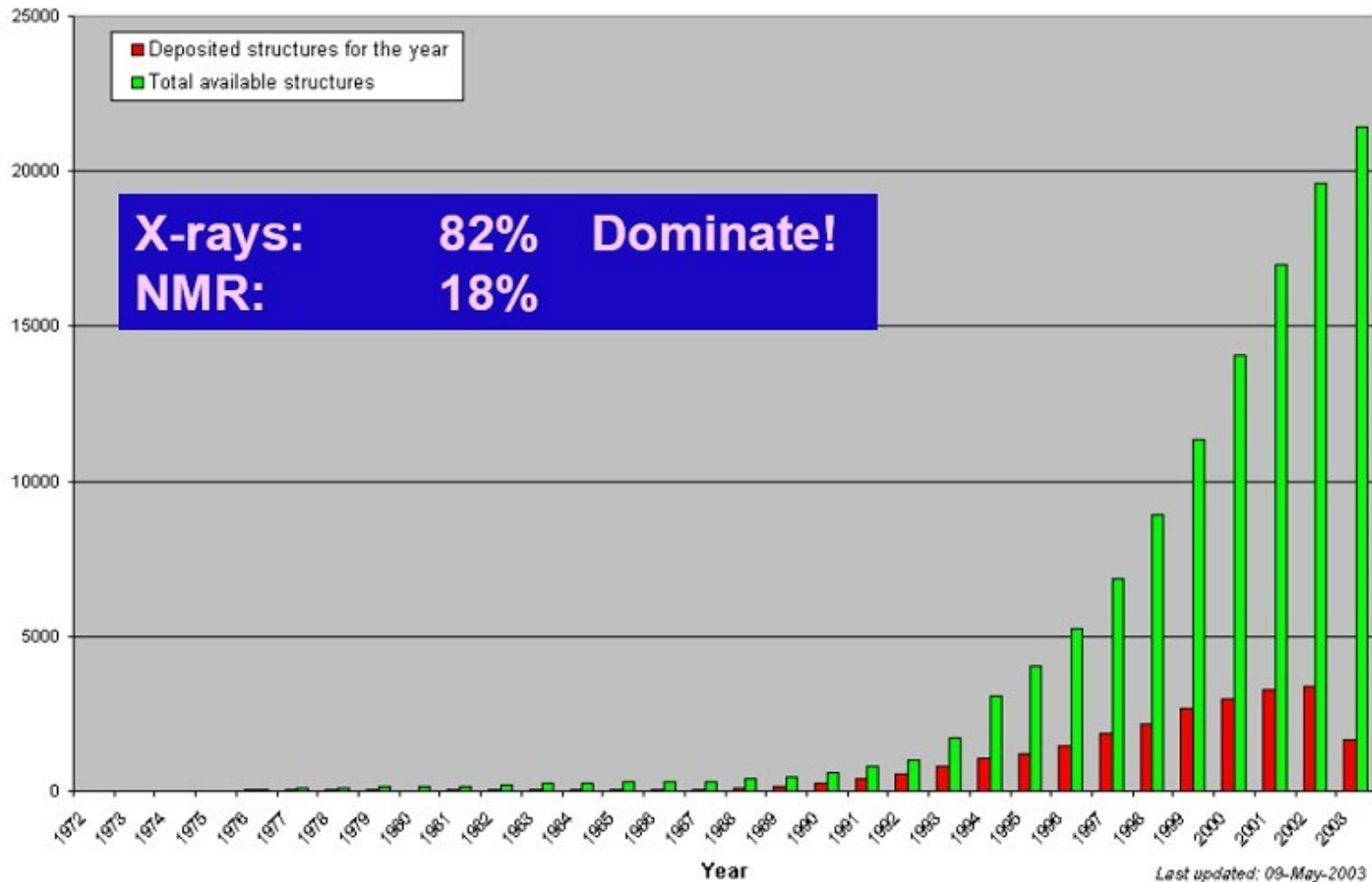
***Figure C:**

tRNA A-site \rightarrow P site

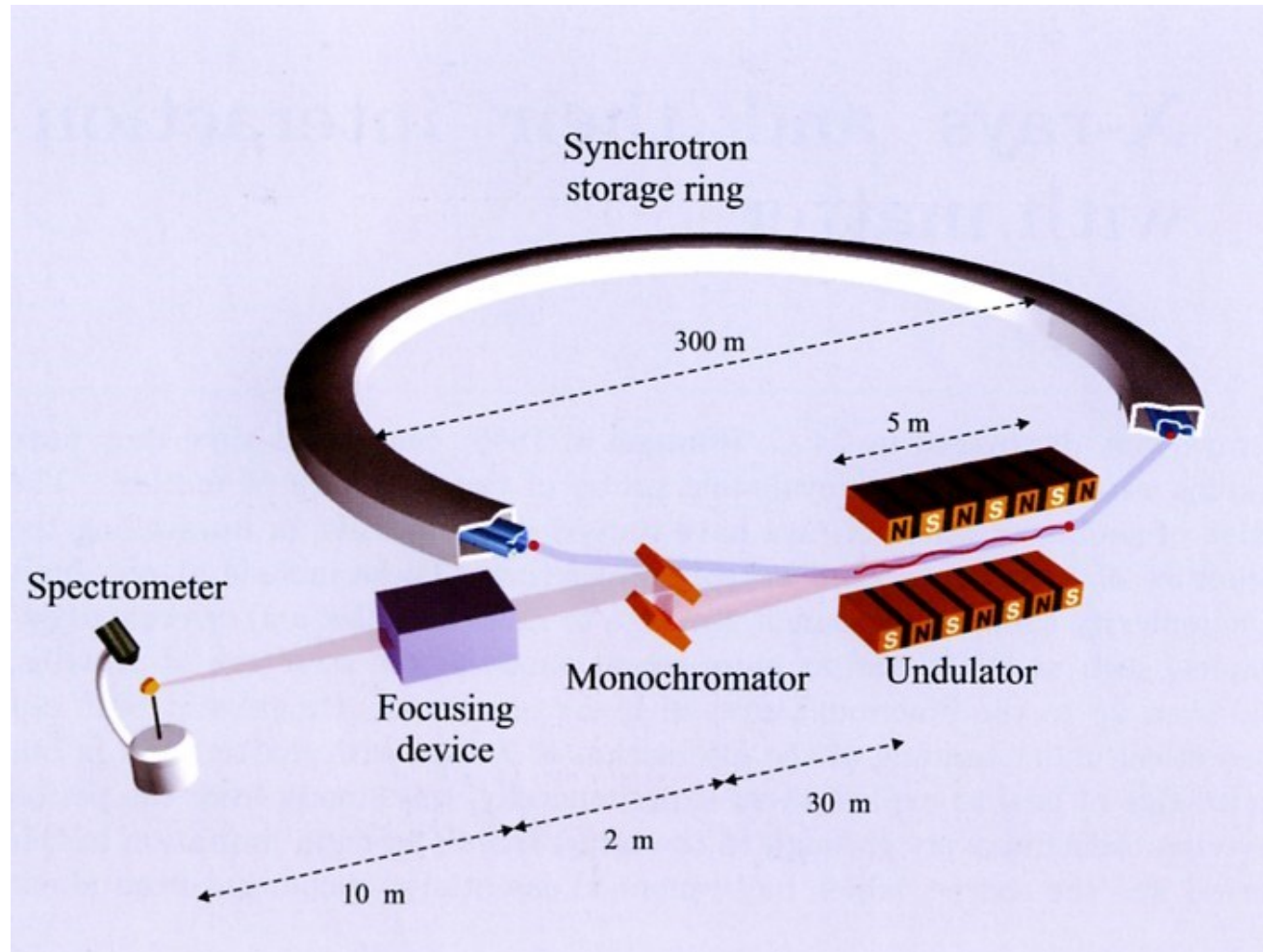
Agmon et al., 2003; Bashan et al., 2003

*For details go to "Scientific Activities" (Figure 5)

Spectacular growth of structural biology



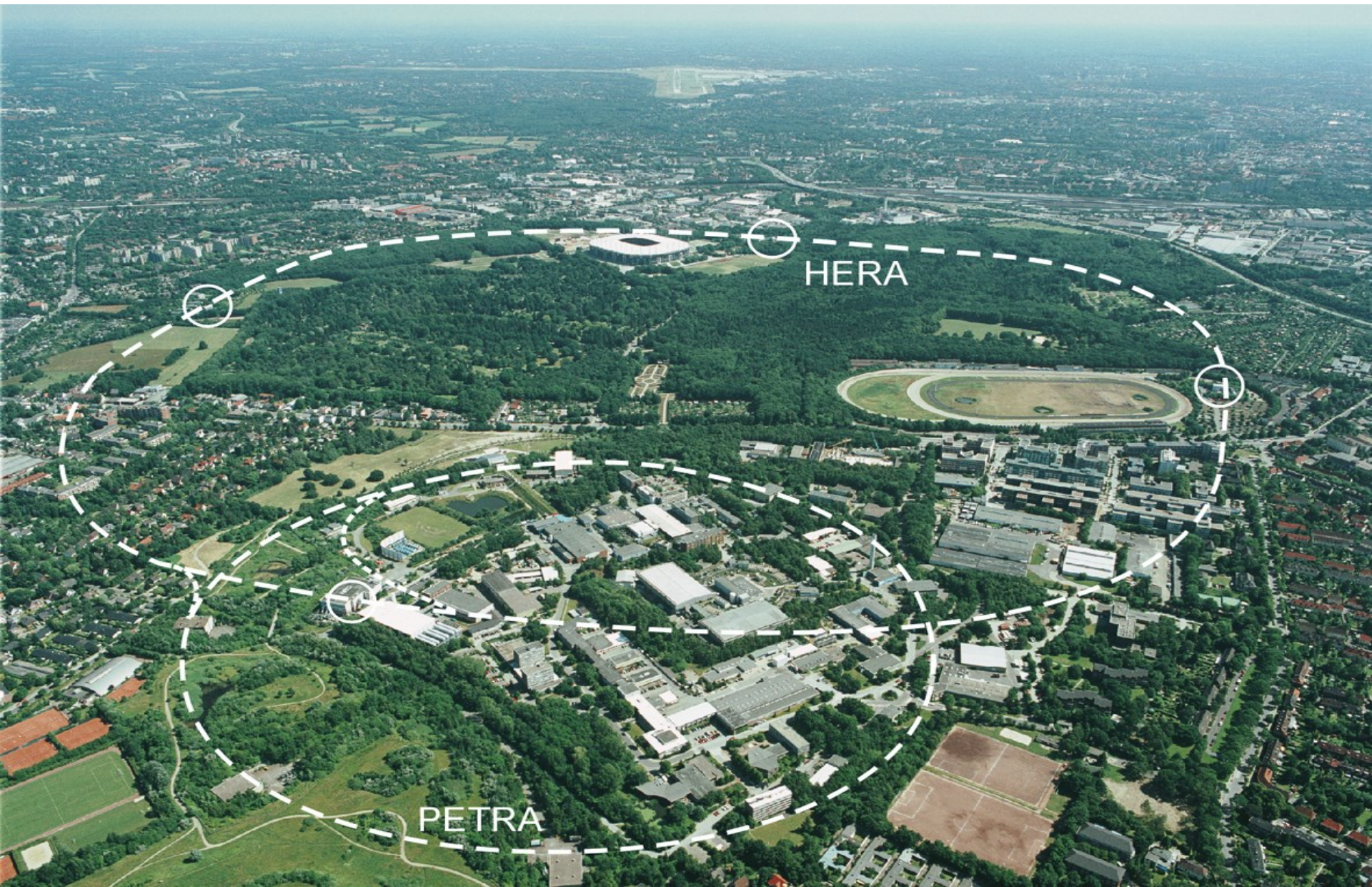
Made Possible by Storage-Rings



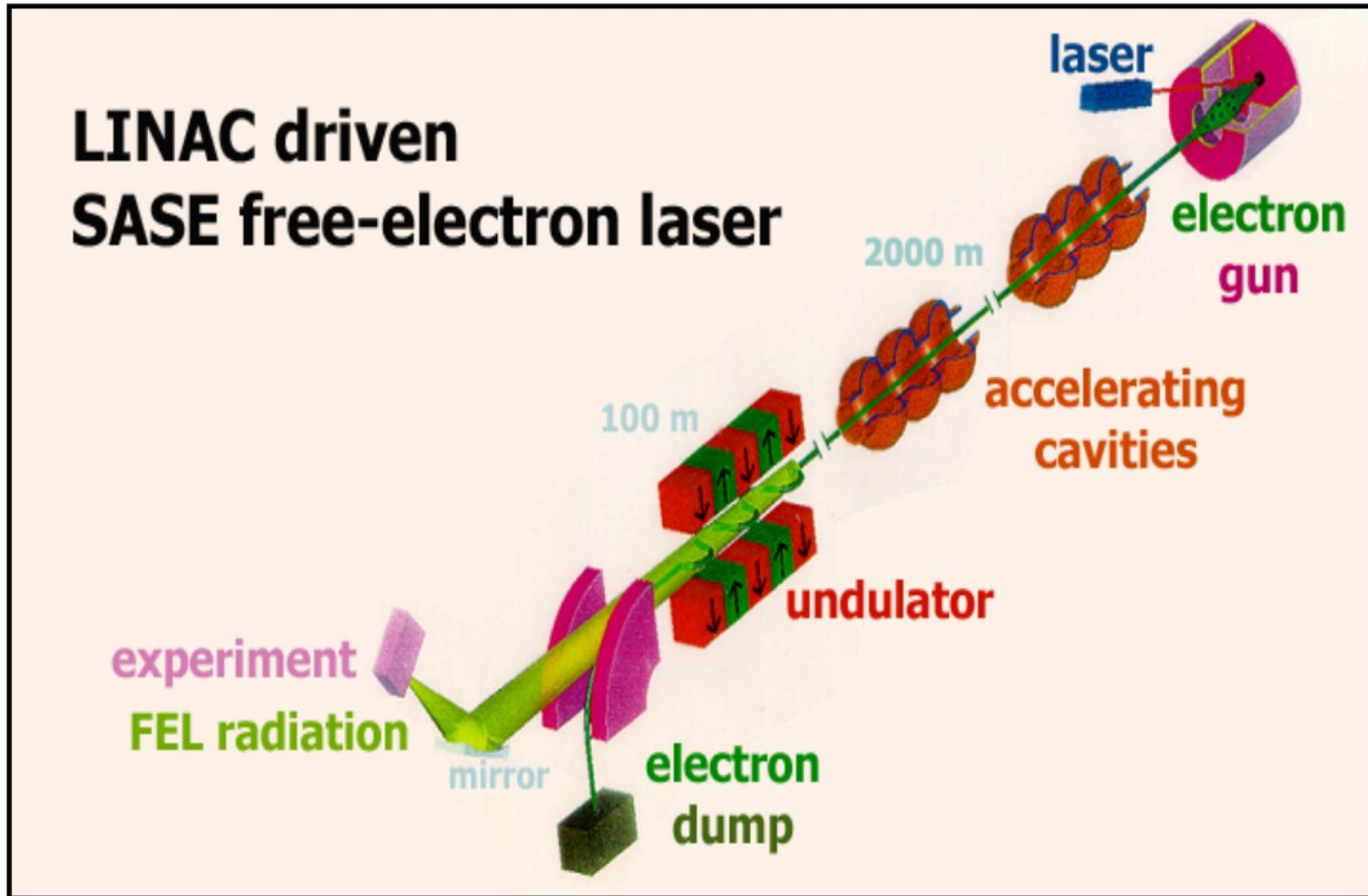
European Synchrotron Radiation Facility (ESRF)



Deutsches Elektronen Synchrotron (DESY)



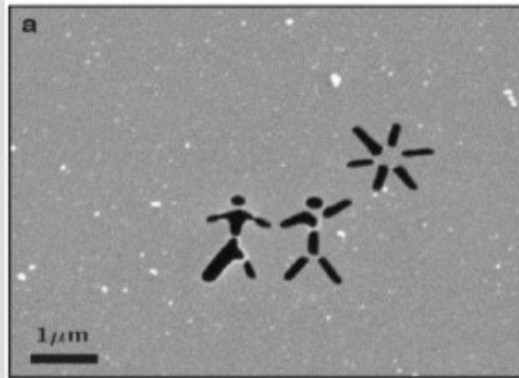
Free Electron Lasers (FELs)



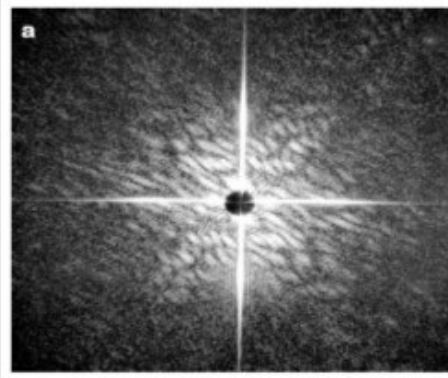
The FLASH Facility in Hamburg



The Femtosecond World



Model structure in 20 nm SiN membrane



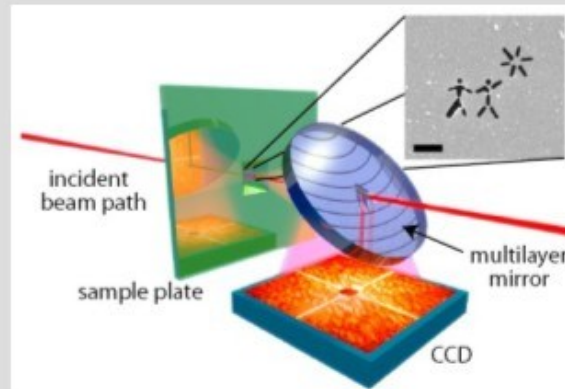
Speckle pattern recorded with a single (25 fs) pulse



Reconstructed image

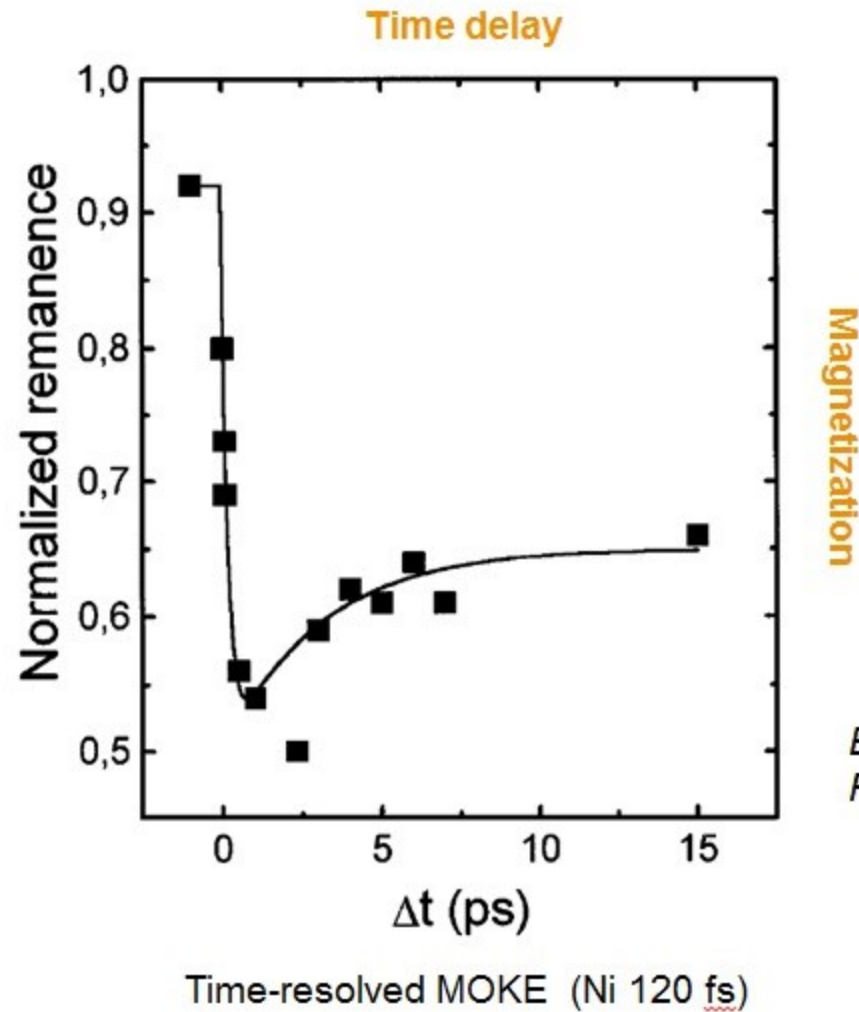
*

Incident FEL pulse:
25 fs, 32 nm,
 $4 \times 10^{14} \text{ W cm}^{-2}$
(10^{12} ph/pulse)



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

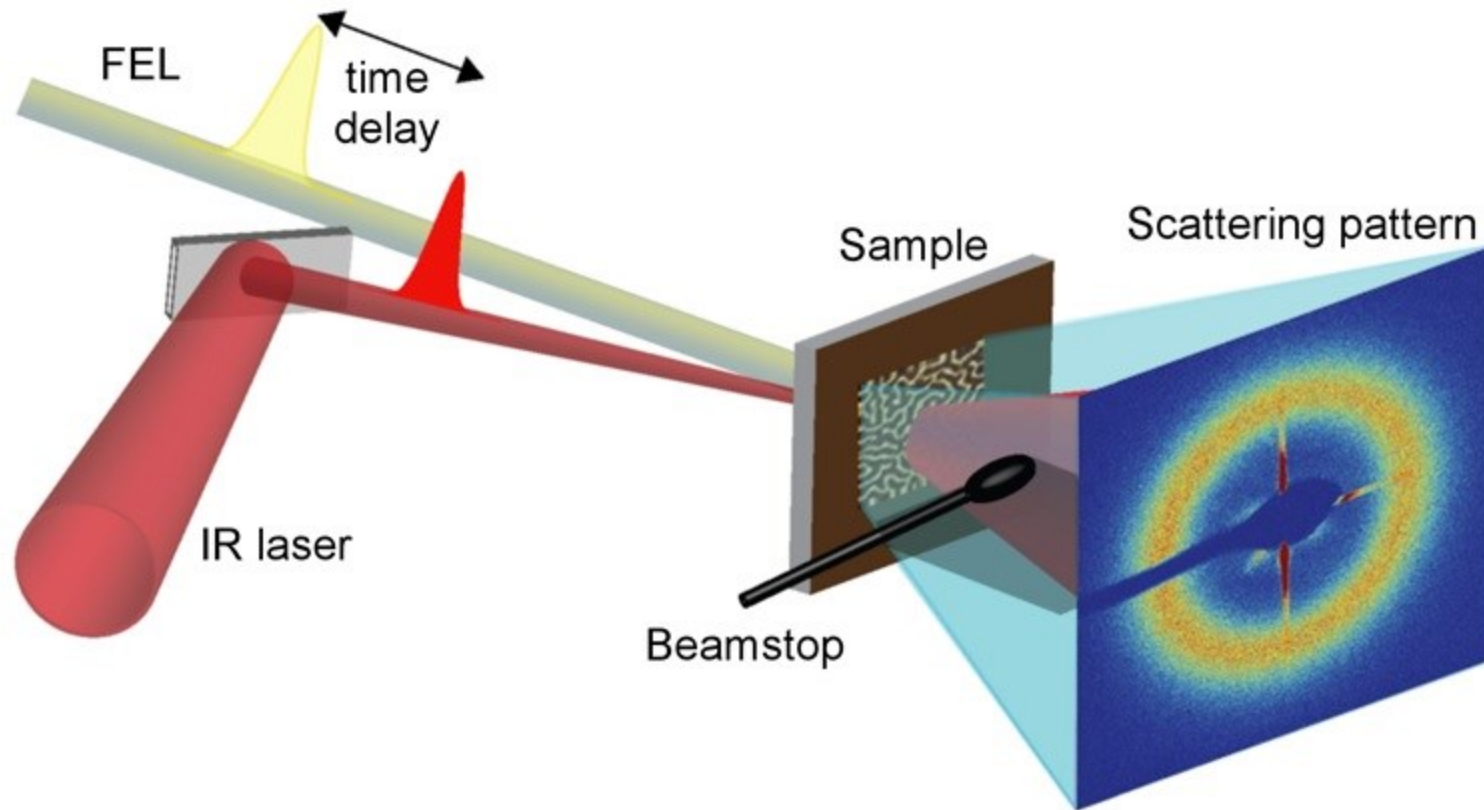
Femtomagnetism



*E. Beaurepaire et al.,
PRL 76 (1996) 4250*

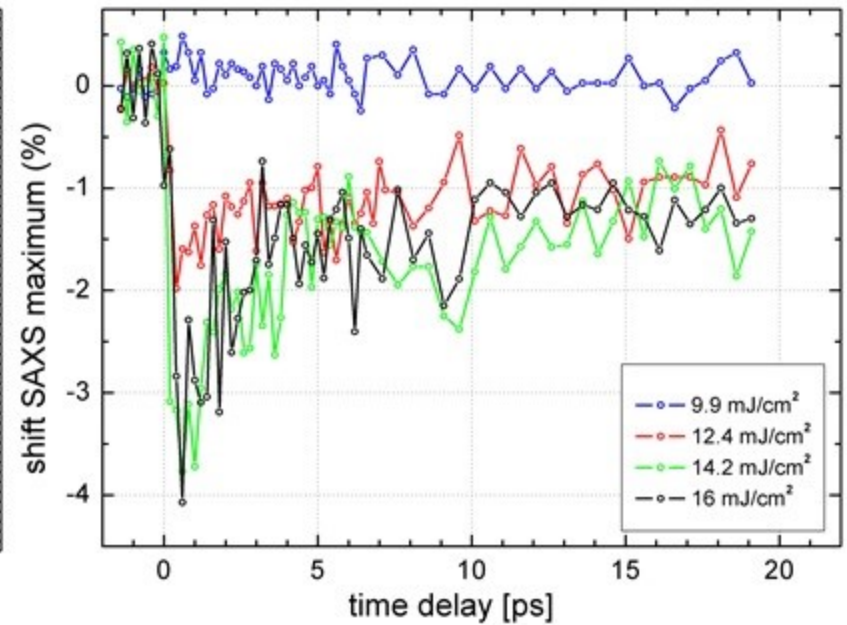
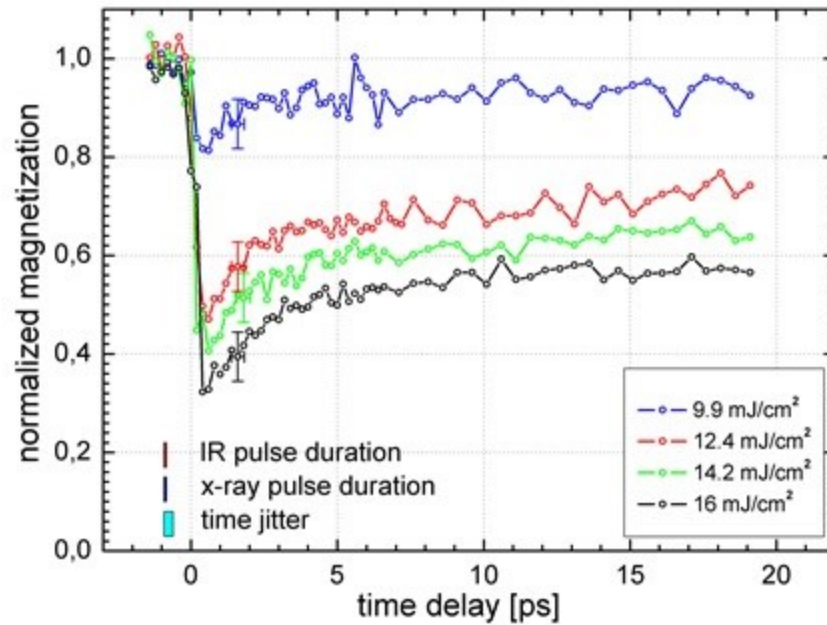
*Gd (100 \pm 80 ps) via
time resolved
photoemission
A. Vaterlaus et al.,
PRL 67, 3315 (1991)*

Femtomagnetism



B. Pfau et al., Nature Communications, Vol. 3, 11; DOI:doi:10.1038/ncomms2108 (2012)
L.Müller et al., Rev. Sci. Instrum. 84, 013906 (2013)

Femtomagnetism



Ultrafast demagnetization

Ultrafast magnetic domain structure changes?

Femtomagnetism

PRL 105, 027203 (2010)

PHYSICAL REVIEW LETTERS

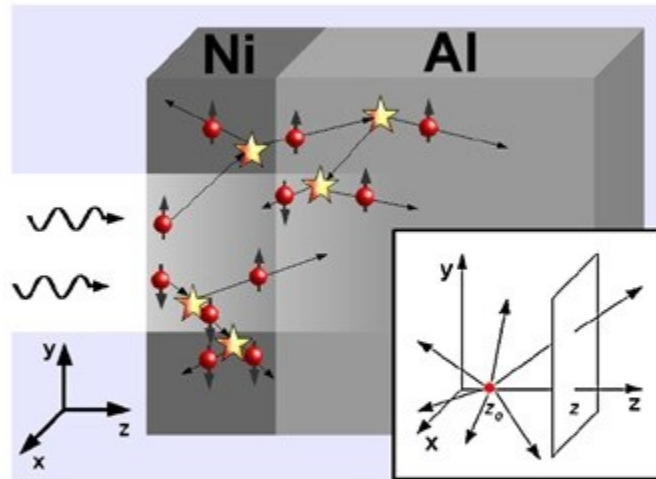
week ending
9 JULY 2010

Superdiffusive Spin Transport as a Mechanism of Ultrafast Demagnetization

M. Battiato,* K. Carva,† and P. M. Oppeneer

Department of Physics and Astronomy, Uppsala University, Box 516, SE-75120 Uppsala, Sweden

(Received 31 March 2010; published 9 July 2010)



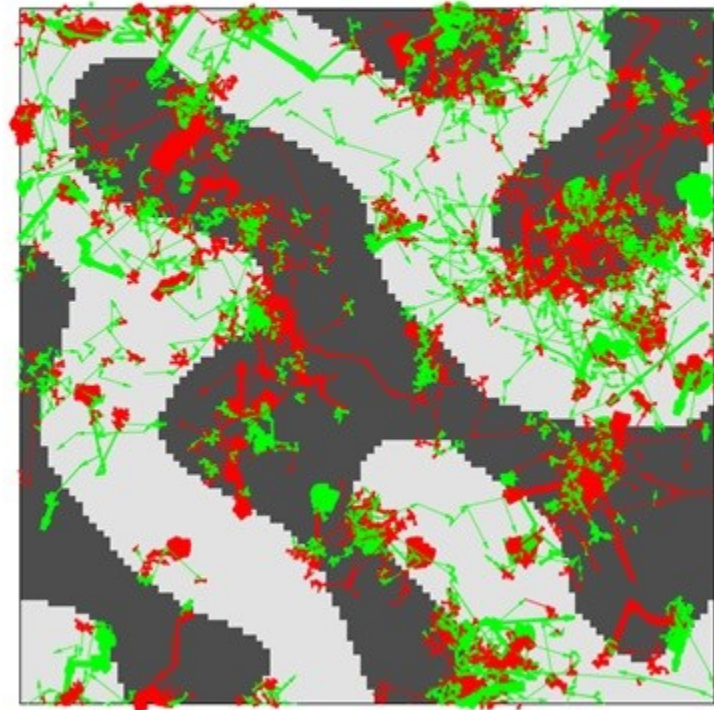
sp-band



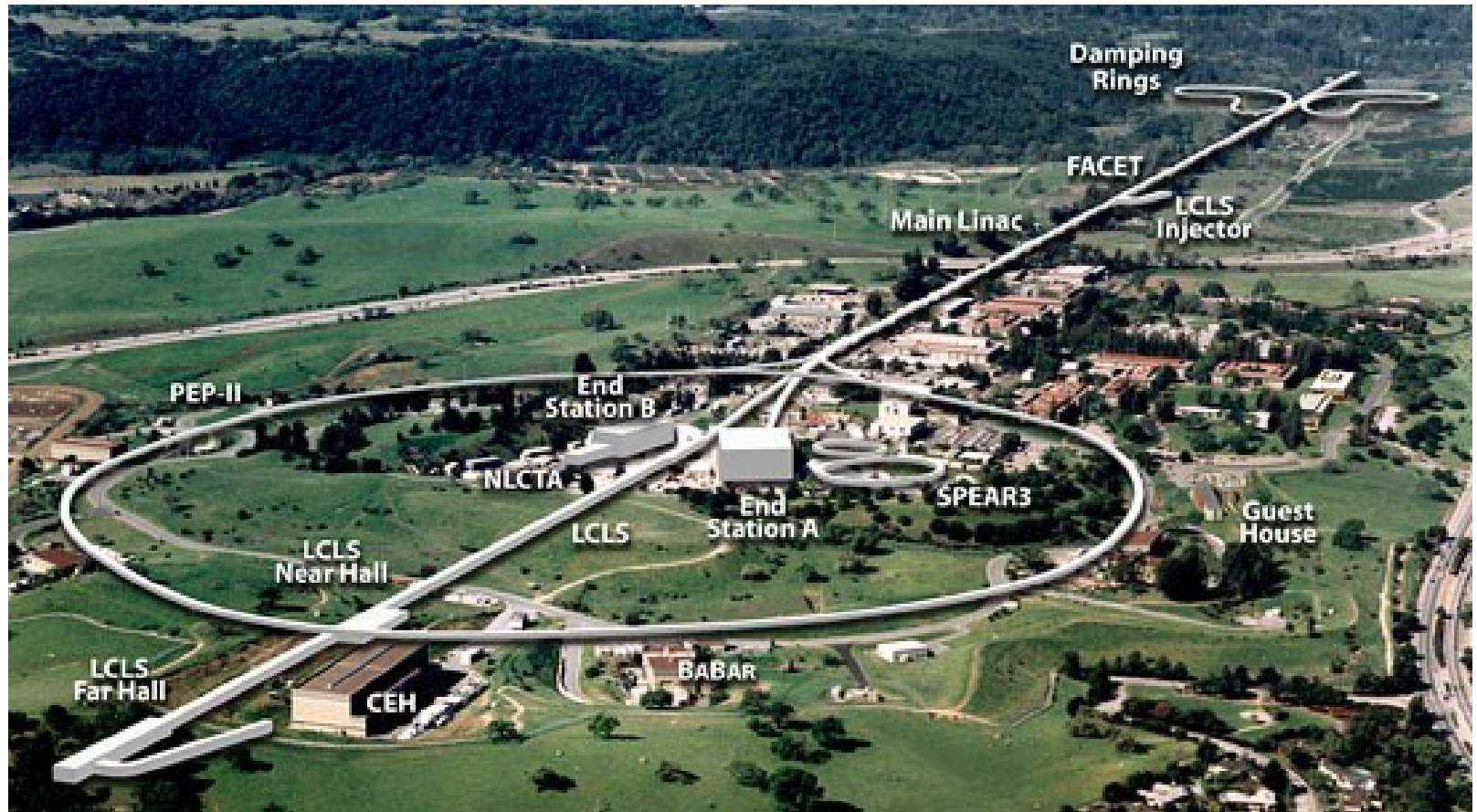
d-band

sp-electrons are fast (1nm/fs)
spin majority and spin minority
electrons have different lifetime

→ depletion of majority spin
 carriers at an interface/domain wall
 → **increasing domain wall width**



LCLS – Linac Coherent Light Source - SLAC



Serial Femtosecond Crystallography

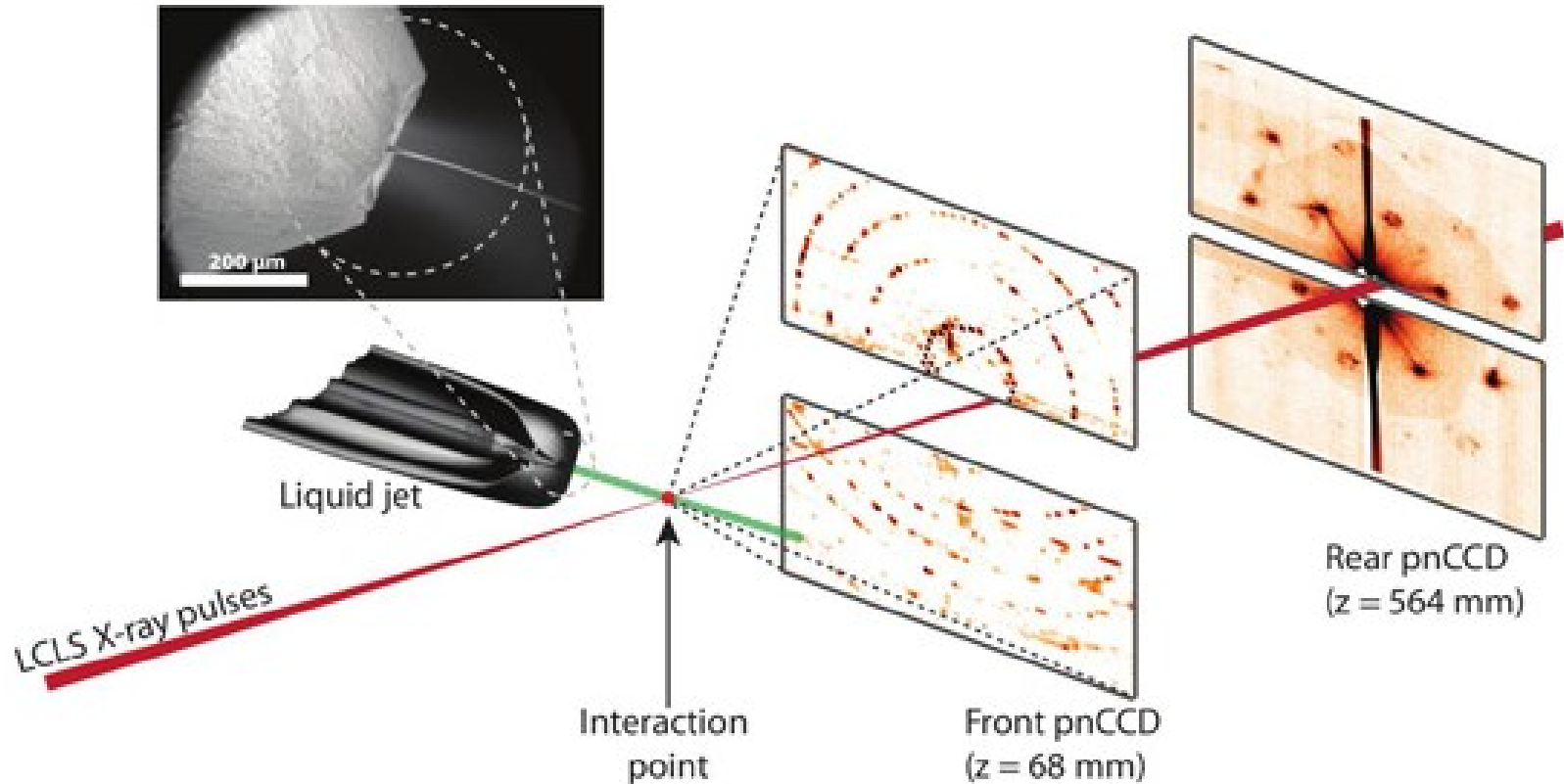
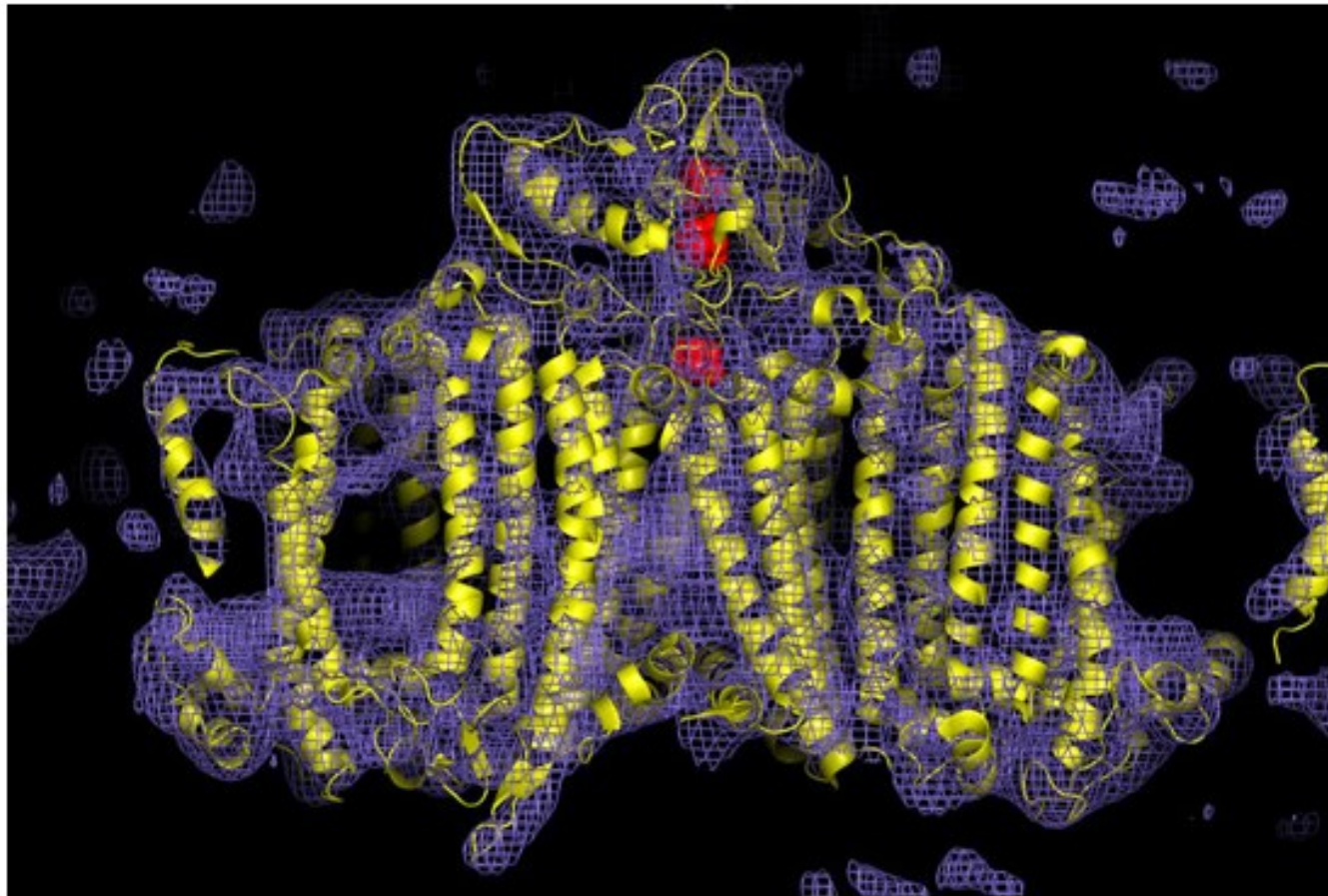


Figure 1

Experimental set-up for serial femtosecond crystallography. First published in Nature 470, 73 – 78 (2011).

Henry N. Chapman et al., NATURE 470, 73 (2011)

Serial Femtosecond Crystallography



Extracted from 3 million diffraction patterns from photosystem I nanocrystals (200nm to 2 micron size)
LCLS:30 Hz at 1.8 keV

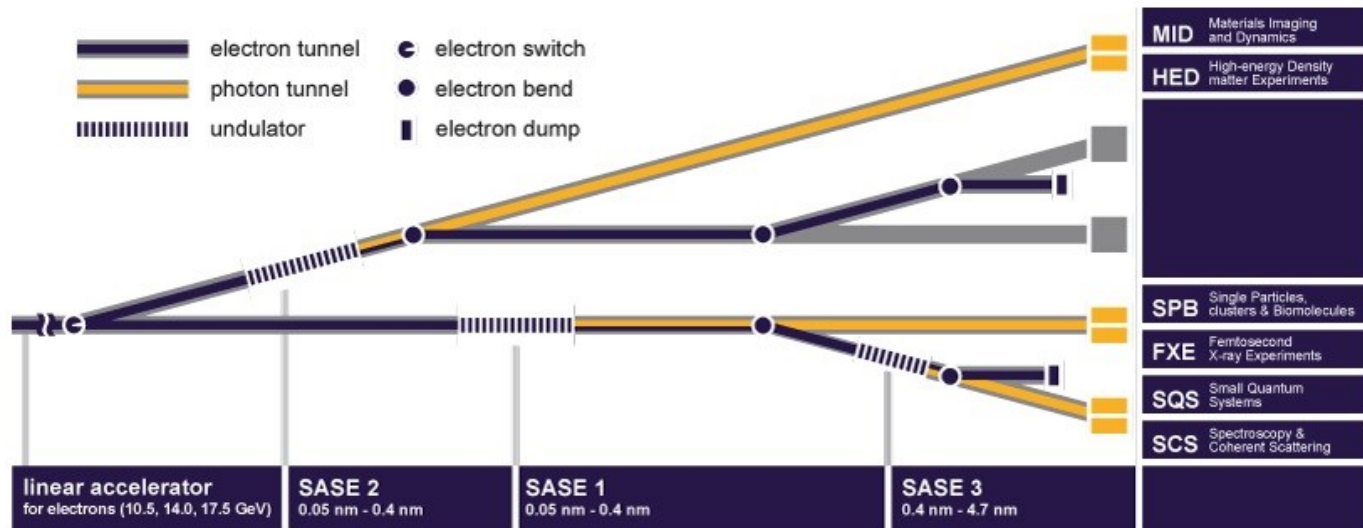
Figure 3
Electron density map of the photosystem I protein complex obtained from the LCLS diffraction data. First published in Nature 470, 73 – 78 (2011). Nanocrystals were grown by Petra Fromme of Arizona State University.

European XFEL

BEAMLINES

The European XFEL will provide light sources (beamlines) for X-ray flashes with different properties.

When electron bunches are induced to follow a slalom course in the magnet arrangements—the so-called undulators—of the European XFEL, they emit flashes of X-ray radiation. The European XFEL will comprise different undulators, i.e. different light sources providing X-ray flashes with different properties.



LCLS

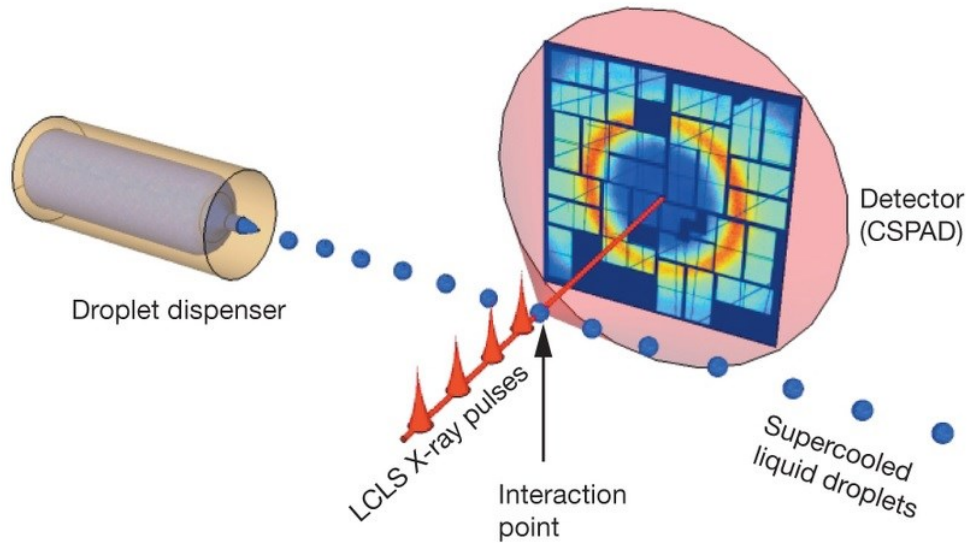
Ultrafast X-ray probing of water structure below the homogeneous ice nucleation temperature

J. A. Sellberg, C. Huang, T. A. McQueen, N. D. Loh, H. Laksmono, D. Schlesinger, R. G. Sierra, D. Nordlund, C. Y. Hampton, D. Starodub, D. P. DePonte, M. Beye, C. Chen, A. V. Martin, A. Barty, K. T. Wikfeldt, T. M. Weiss, C. Caronna, J. Feldkamp, L. B. Skinner, M. M. Seibert, M. Messerschmidt, G. J. Williams, S. Boutet, L. G. M. Pettersson *et al.*

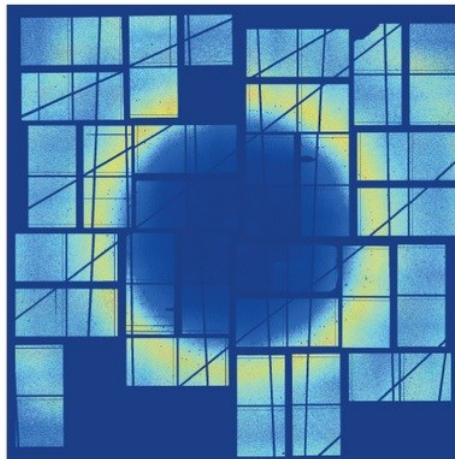
Affiliations | Contributions | Corresponding authors

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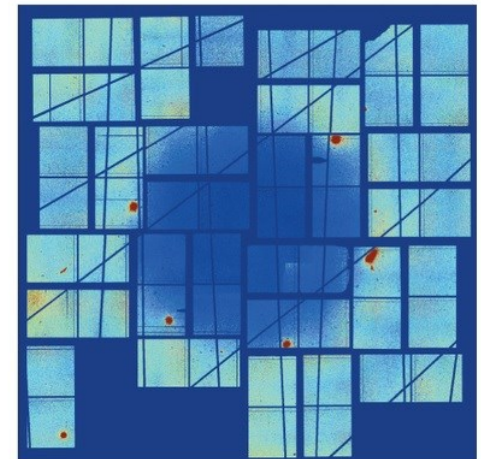
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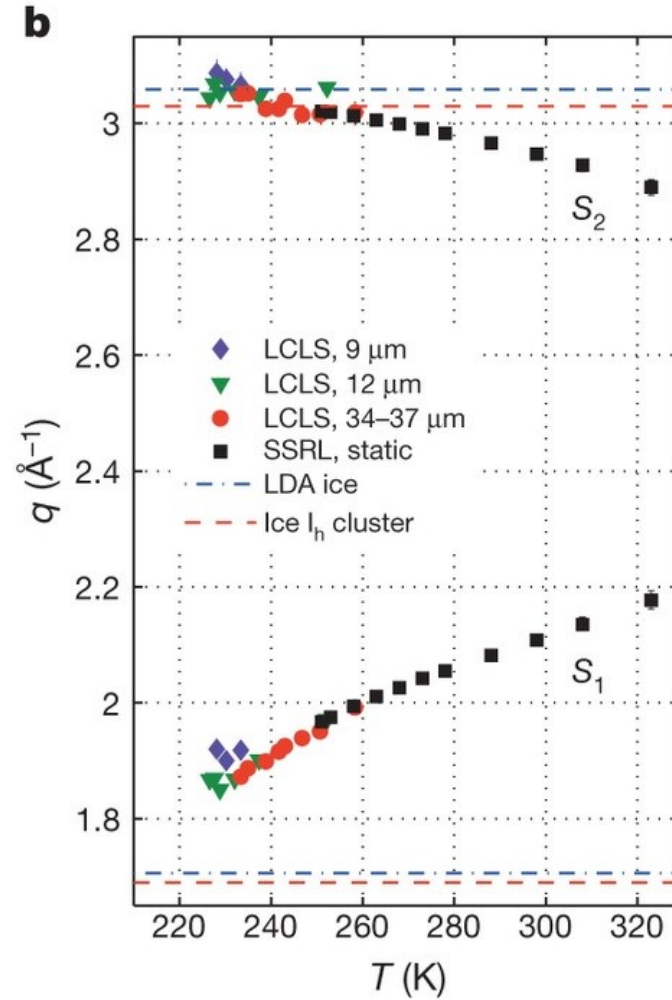
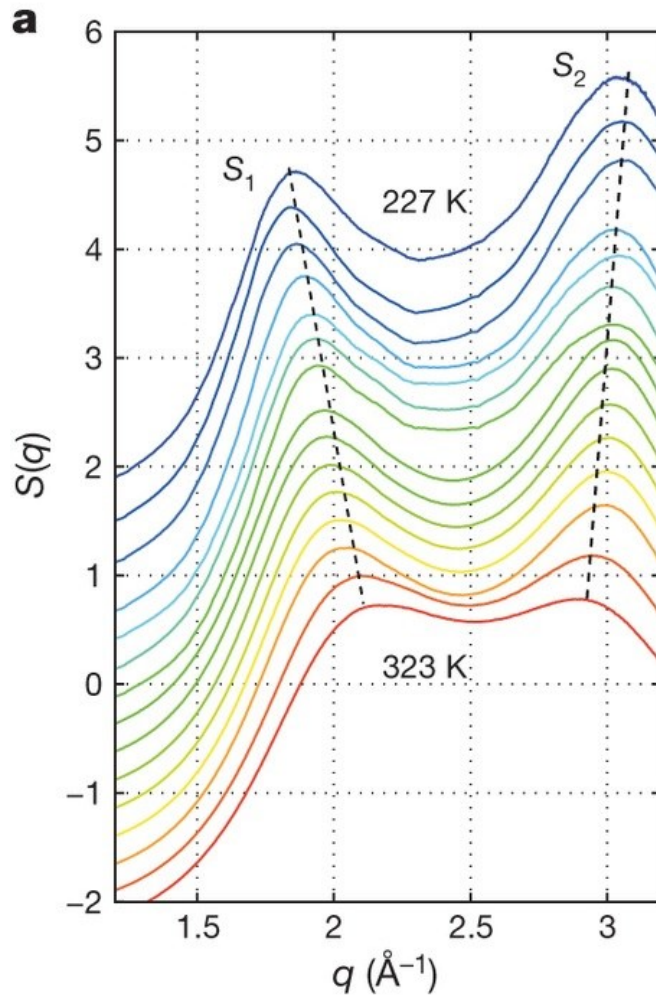
b



c



Supercooled Water



SACLA



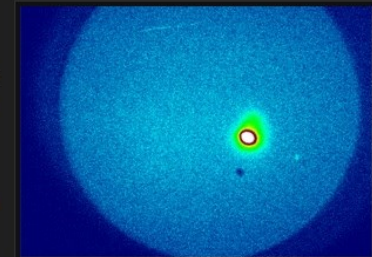
Lasing Achieved at SACLA, Japan's X-ray Free Electron Laser (XFEL) facility

We are pleased to announce that the SPring-8 Angstrom Compact free electron Laser (SACLA) came on line at the RIKEN Harima Institute. SACLA is the second laser of its type in operation, following LCLS at the U.S. Department of Energy's SLAC National Accelerator Laboratory. Producing the world's highest energy X-ray laser light, SACLA offers scientists a new tool for studying and understanding the arrangement of atoms moving extremely rapidly in various materials.



SACLA was built jointly by RIKEN and JASRI as one of the five Key Technologies of National Importance designated in 2006. Electron beam commissioning began in February 2011. By March 23, the beam reached the designed electron energy of 8 GeV and successfully generated 0.08 nm X-rays. This demonstrated the basic performance of the accelerator components so that we could start tuning the system for lasing. After only three months, lasing at the highest energy was achieved on June 7.

Finer tuning will continue in the months ahead. We expect to open the facility to both domestic and international public users by the end of the 2011 fiscal year.

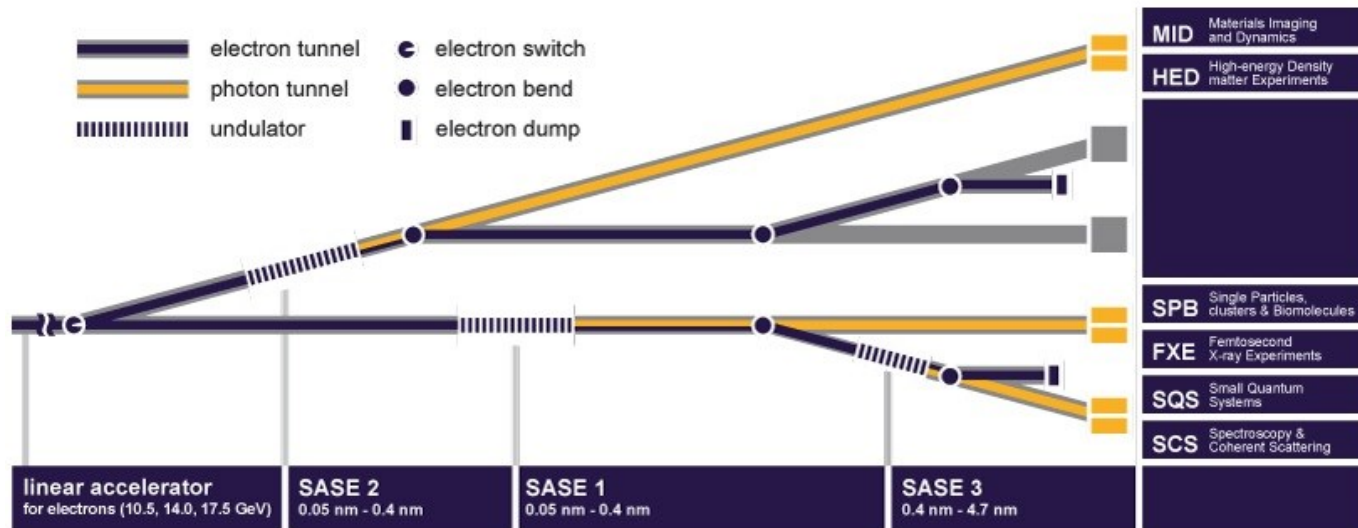


European XFEL

BEAMLINES

The European XFEL will provide light sources (beamlines) for X-ray flashes with different properties.

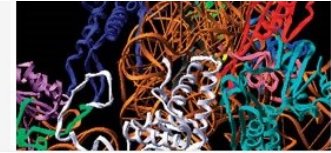
When electron bunches are induced to follow a slalom course in the magnet arrangements—the so-called undulators—of the European XFEL, they emit flashes of X-ray radiation. The European XFEL will comprise different undulators, i.e. different light sources providing X-ray flashes with different properties.



European XFEL

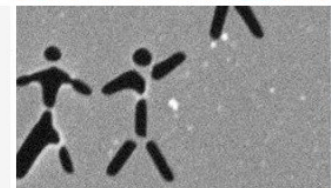
Deciphering the structure of biomolecules

Using the X-ray flashes of the European XFEL, scientists can decipher the 3D structure of biomolecules, cell constituents and whole viruses. This will provide the basis for the medicines of the future.



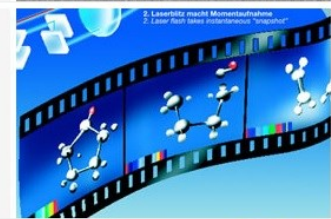
Exploring the nanoworld in 3D

The X-ray flashes of the European XFEL will enable completely novel, three-dimensional insights into the nanoworld and thus shed light on future technological applications.



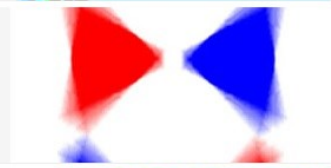
Filming chemical reactions

With the X-ray flashes of the European XFEL, scientists can film how molecules form and separate again or how they fulfil important functions in biological cells. This may contribute to improvements in energy generation or the production of chemical substances and lead to progress in medicine.



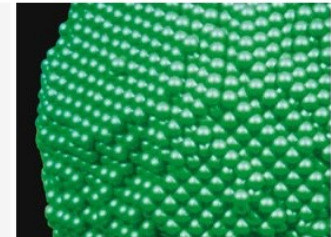
Unravelling magnetization

The X-ray flashes of the European XFEL will enable scientists to study exciting aspects of magnetization – with direct applications in data storage.



Observing small objects in strong fields

The European XFEL will create unique conditions for the investigation of atoms, molecules, atomic clusters or nanoparticles in extremely high X-ray radiation fields. These insights can lead not only to progress in basic research, but also to new products – such as novel catalysts or electronic devices controlled by X-ray radiation.



Investigating extreme states of matter

The focused X-ray flashes of the European XFEL can create states of matter under extremely high pressures and temperatures. This will help to both develop new astrophysical models for planets and push ahead with fusion research for future energy generation here on Earth.

