Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture 0	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.)

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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	

DESY

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

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Part II:

Magnetism – Magnetic Thin Films

by André Philippi-Kobs (AP)

[23.5.] Magnetic small angle scattering of magnetic domain patterns
[30.5.] Imaging of magnetic domains
[1.6.] Femtomagnetism
[13.6.] Related aspects

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Part III:

Surfaces and Interfaces

by Oliver Seek (OS)

[15.6.] Introduction & Crystal Truncation Rods
[20.6.] X-ray Reflectivity I (Born-Approximation)
[22.6.] X-ray Reflectivity II (Dynamical Theory and Experiments)
[27.6.] Grazing Incidence Diffraction & Surface Diffuse Scattering

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Part IV:

Macromolecular Crystallography

by Thomas Schneider (TS)

[29.6.] Site Visit
[4.7.] Structural Biology & MX
[6.7.] Collection and processing of Diffraction Data
[11.7.] Phasing an Model refinement
[13.7.] Site Visit

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

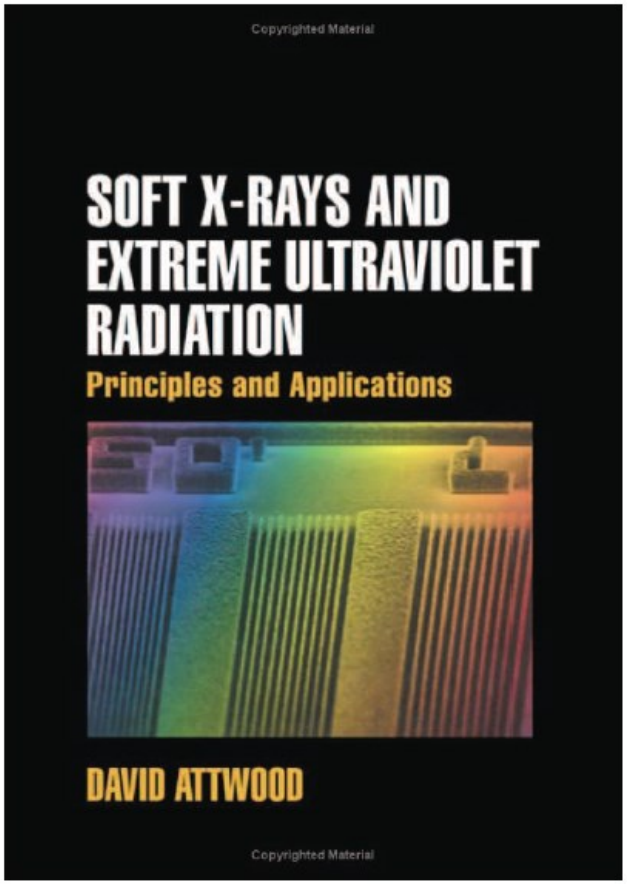
Principles of Optics
M. Born and E. Wolf, Cambridge University Press, 7th ed.

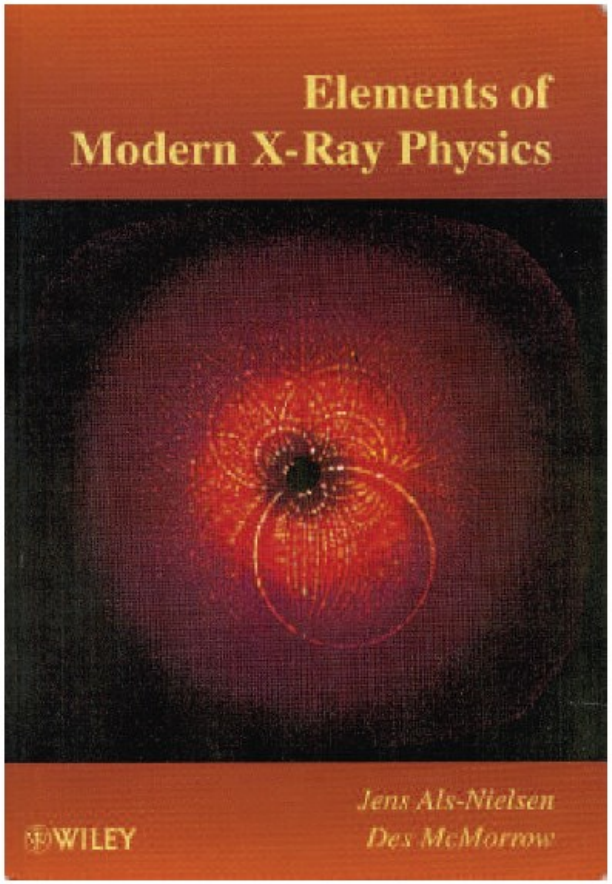
Soft X-rays and Extreme Ultraviolet Radiation
D. Attwood, Cambridge University Press (2000)
http://www.coe.berkeley.edu/AST/sxreuv/

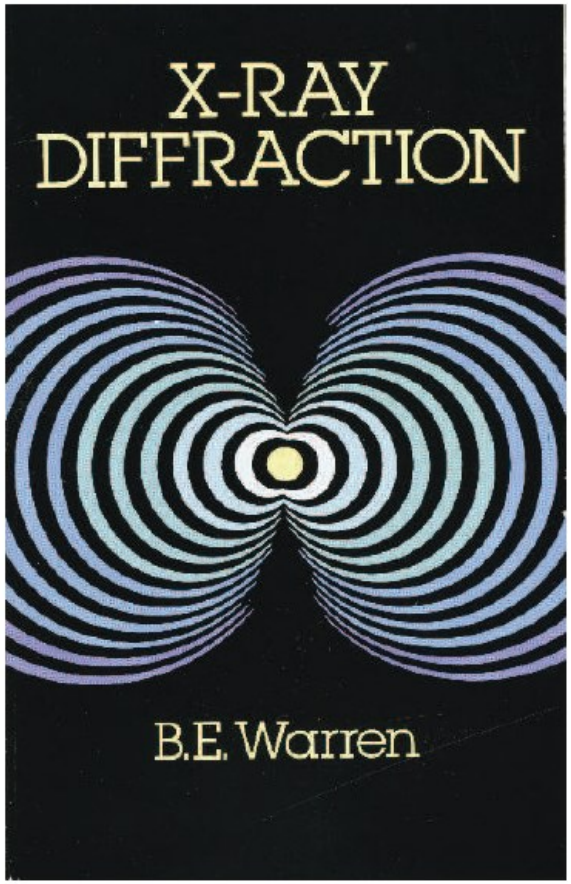
Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen
K. Wille, Teubner Studienbücher 1996

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, …

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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, ...

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Part II:

Magnetism – Magnetic Thin Films

by André Philippi-Kobs (AP)

[23.5.] Magnetic small angle scattering of magnetic domain patterns
- Introduction of magnetism in thin films
- Resonant scattering & X-ray magnetic circular dichroism (XMCD), XMLinearD

[30.5.] Imaging of magnetic domains
- Fourier transform holography (FTH)
- Scanning transmission X-ray microscopy (STXM)
- Coherent diffraction imaging (CDI), Ptychography

[1.6.] Femtomagnetism
- Introduction of ultrafast magnetization dynamics
- Pump-probe experiments of nano-scale magnetic domain patterns

[13.6.] Related aspects
- Determination of coherence via magnetic domain patterns
- Magnetic XRD of antiferromagnets and chiral systems
- Further electronic inhomogeneities probed by X-rays (charge density wave; Abrikosov vortices in superconductors)

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Part III:
Surfaces and Interfaces
by Oliver Seek (OS)

[15.6.] Introduction &Crystal Truncation Rods

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[22.6.] X-Ray Reflectivity II (Dynamical Theory and Experiments)

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Part IV:
Macromolecular Crystallography
by Thomas Schneider (TS)

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Macromolecular Crystallography
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MX – The Method
Bragg's law
Structure Factors, Argand Diagrams
Real and Reciprocal Space
Phase Problem *What is the 'Phase Problem'
Symmetry in Real and Reciprocal Space
Anomalous Diffraction
Overview of Phasing Methods

MX – Collection and Processing of Diffraction Data
Crystals and Their Properties/Problems
Synchrotron Radiation Beams for MX
Diffractometry for MX
Detectors for MX
2D Diffraction Images. Ewald Construction?
Data Processing
- Integration
- Scaling
- Anomalous Data
- Data Quality Indicators
- Resolution
- Radiation Damage

Part IV:
Macromolecular Crystallography
by Thomas Schneider (TS)

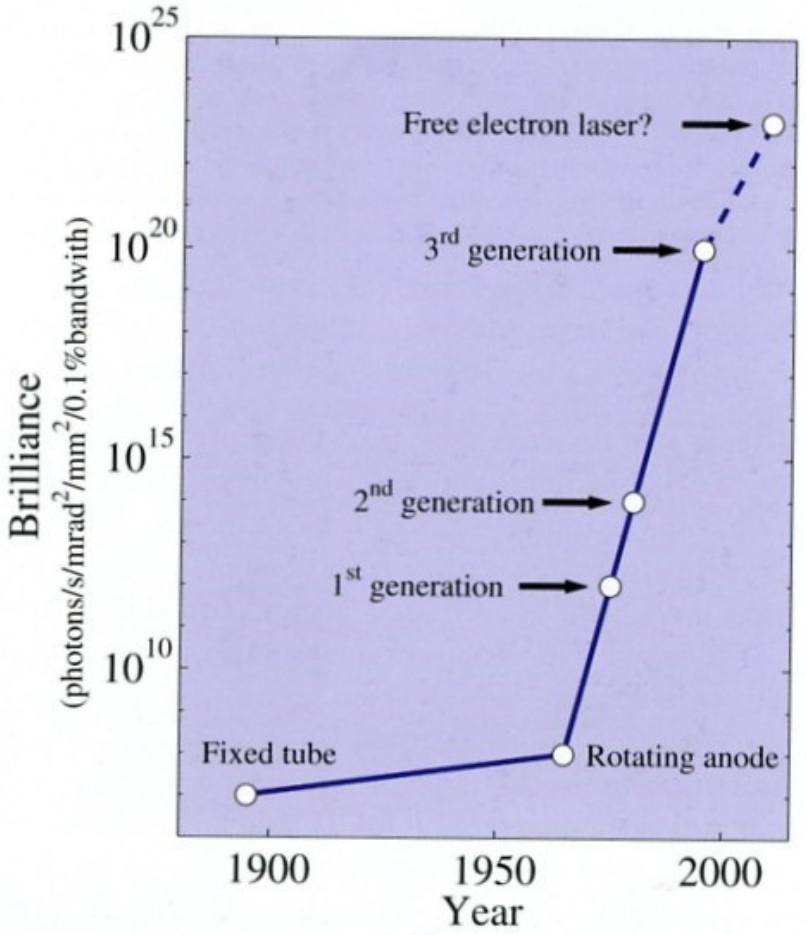
MX – Building Models & Future
Experimental Phasing: MAD
Experimental Phasing: Derivatives
Knowledge-based Phasing: Molecular Replacement
Model bias
Model Building
Refinement
X-FEL crystallography

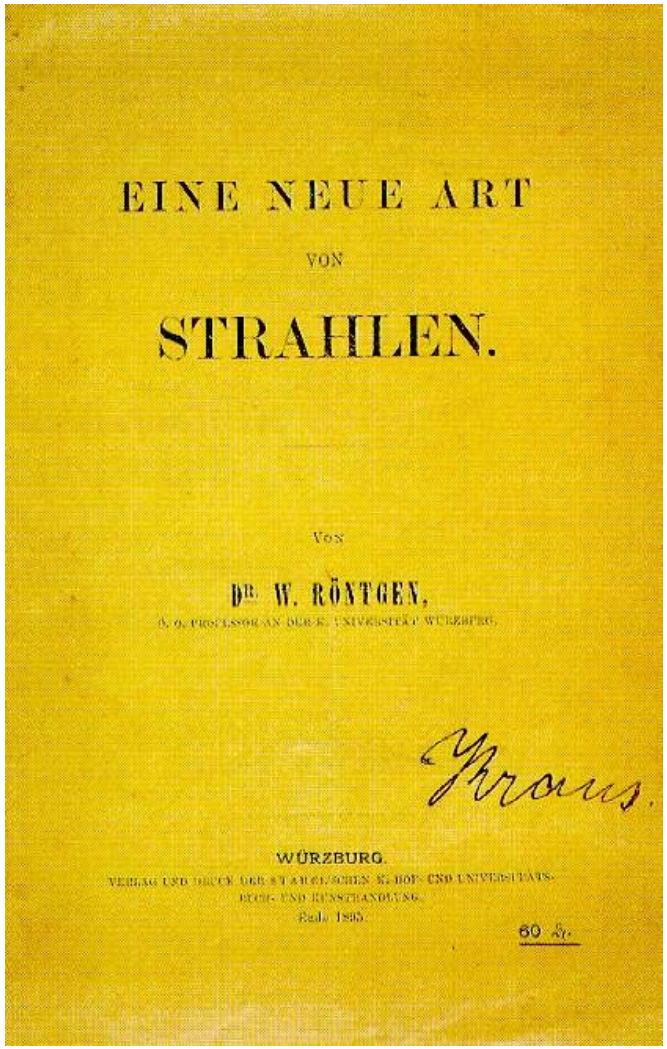
DEMO 1: Crystallographic Data Processing
DEMO 2: Crystallographic Structure Determination

Literature:
Als-Nielsen
D. Blow: Outline of Crystallography for Biologists. Oxford University press. ISBN: 978-0198510512. € 39.00 (amazon)
G. Rodes: Crystallography made crystal clear. Academic press. ISBN: 978-0-12-587073-3. € 40.95 (amazon)
http://www-structmed.cimr.cam.ac.uk/course.html
G. Taylor (2003): 'The phase problem', Acta Cryst. D59:1881.

Introduction by Gerhard Grübel

1895	X-ray discovered by W.C. Röntgen
1901	Nobel Price; 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)





EINE NEUE ART

VON

STRAHLEN.

Von

Dr. W. RÖNTGEN,

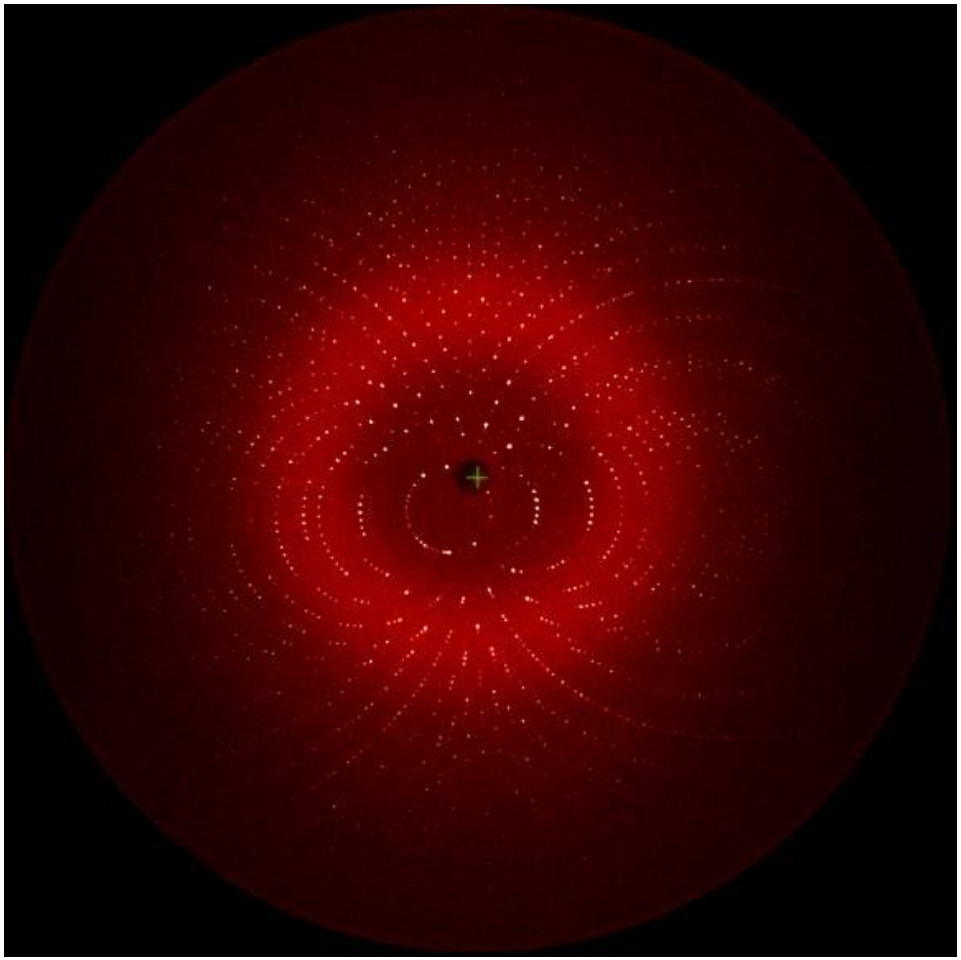
WÜRZBURG.

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**

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.

BESCHLEUNIGER | FORSCHUNG MIT PHOTONEN | TEILCHENPHYSIK
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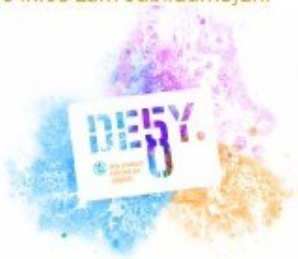
DESY beglückwünscht Ada Yonath zum Chemie-Nobelpreis

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

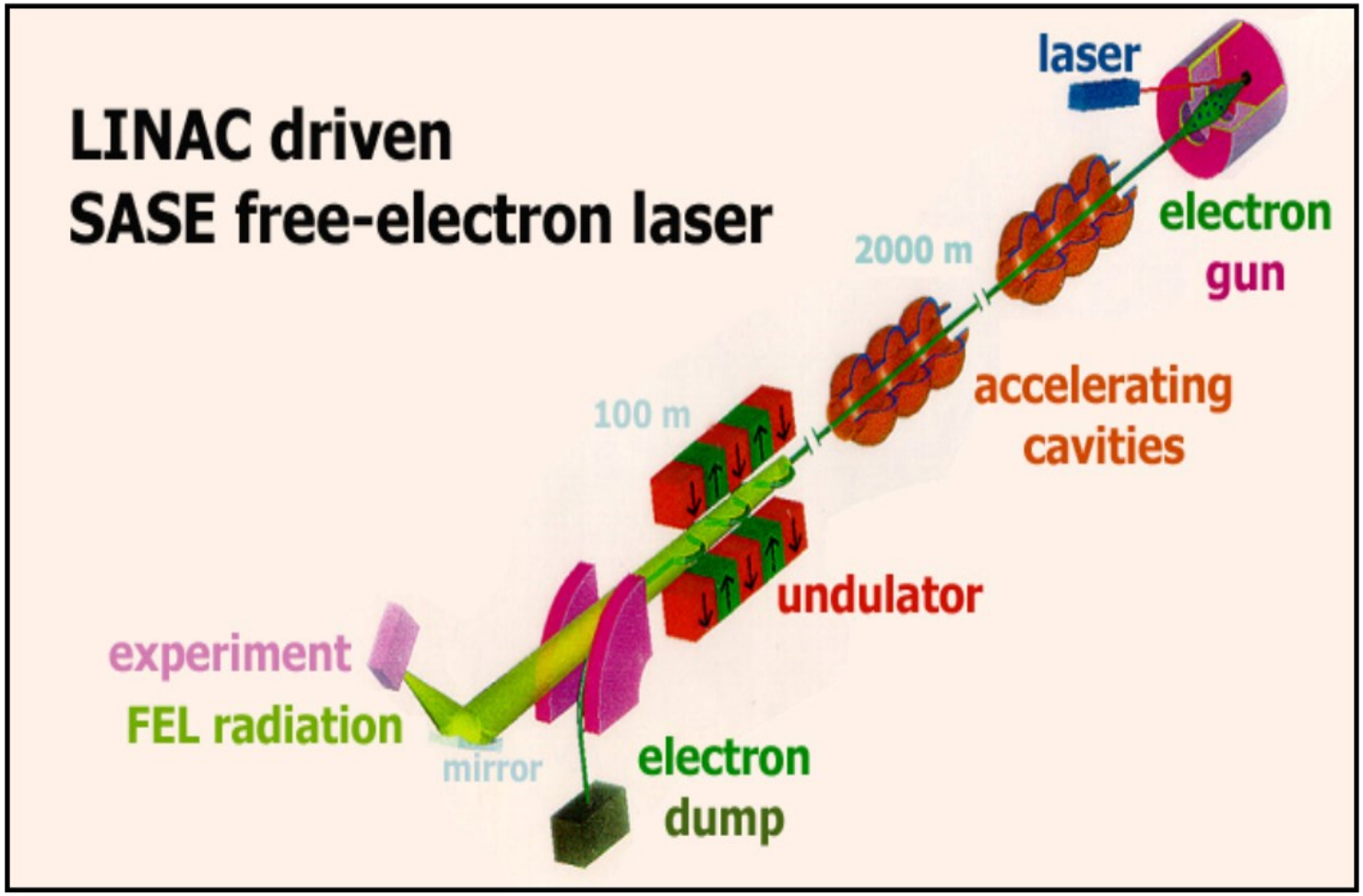


Veranstaltungen

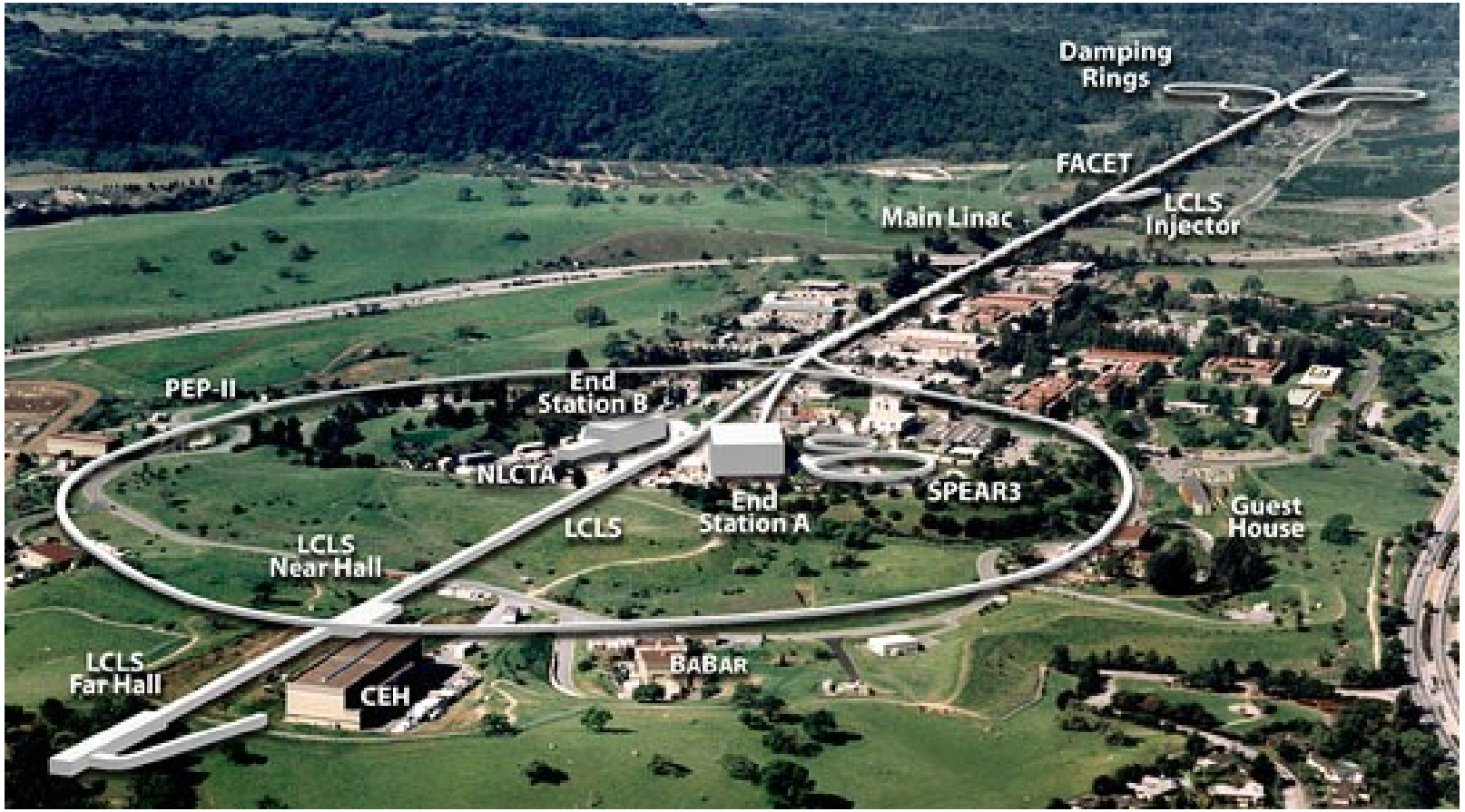
» VERANSTALTUNGSKALENDER FÜR DESY IN HAMBURG UND ZEUTHEN

European Synchrotron Radiation Facility (ESRF)

Free Electron Lasers (FELs)



LCLS – Linac Coherent Light Source - SLAC



Serial Femtosceond Crystallography

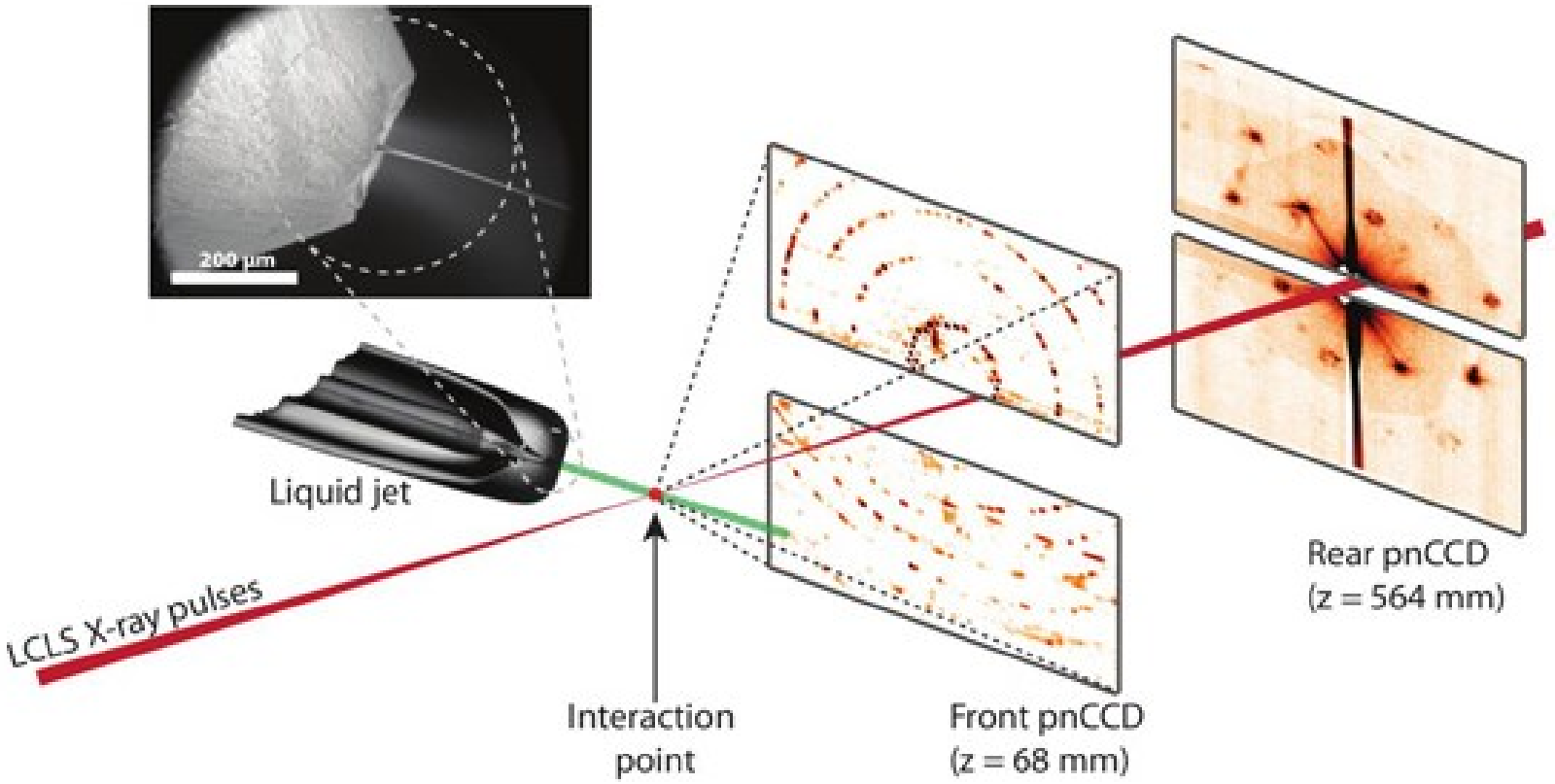


Figure 1
Experimental set-up for serial femtosecond crystallography. First published in Nature 470, 73 – 78 (2011).

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

Serial Femtosceond Crystallography

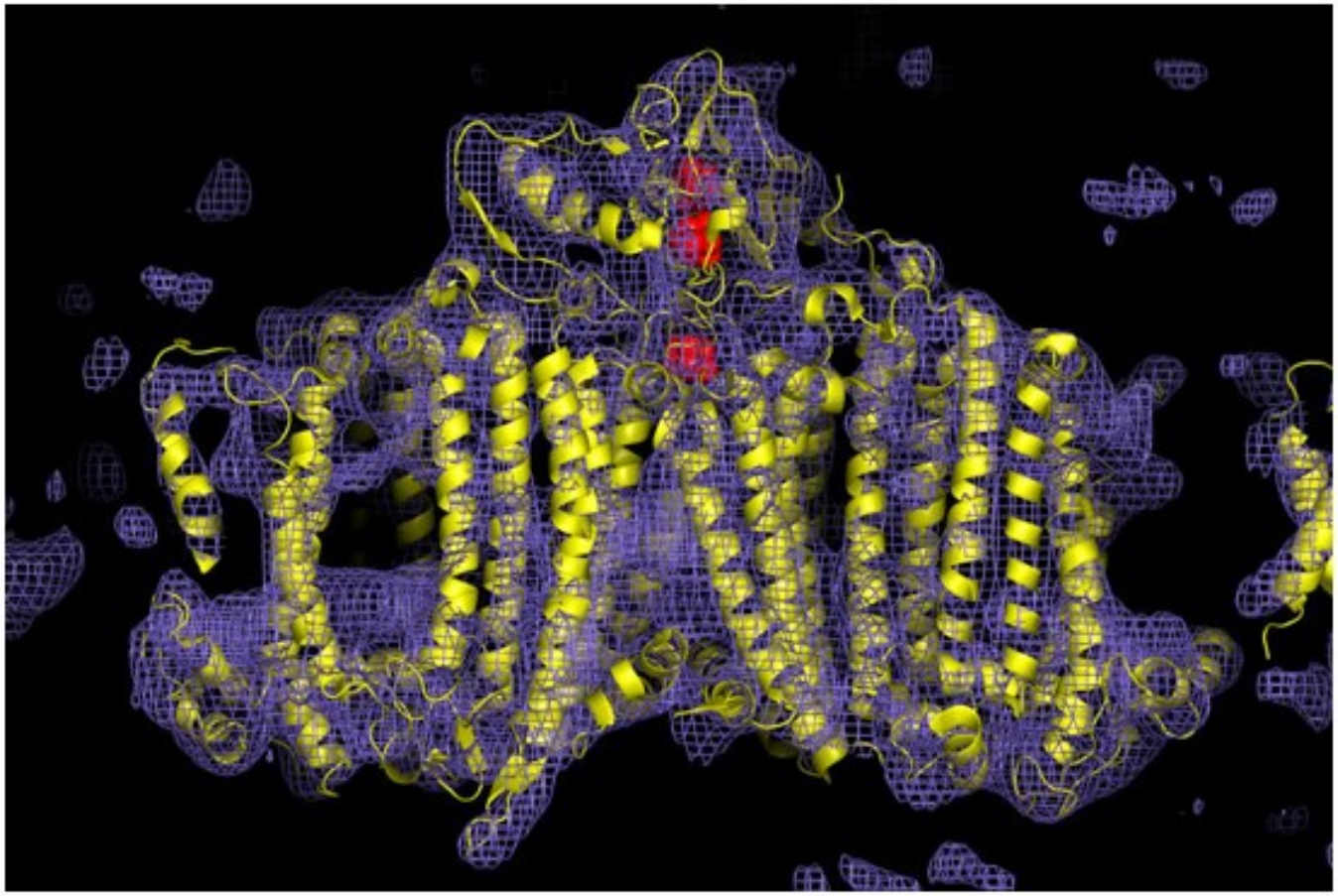


Figure 3
Electron density map of the photosystem I protein complex obtained from the LCLS diffraction data. First published in Nature 470, 73 – 78 (2011). Nanocrystals were grown by Petra Fromme of Arizona State University.

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

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.