

# Methoden moderner Röntgenphysik: Streuung und Abbildung

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Lecture 1	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2021 G. Grübel, O. Seeck, V. Markmann, F. Lehmkuhler, Andre Philippi-Kobs, M. Martins		
Location	online		
Date	Tuesdays	12:30 - 14:00	(starting 6.4.)
	Thursdays	8:30 - 10:00	(until 8.7.)



# Methoden moderner Röntgenphysik: 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 13	14:15 - 15:45
Location:	online	



# Methoden moderner Röntgenphysik: Online Info

Tuesday Zoom-Meeting

<https://desy.zoom.us/j/92674682486>

Meeting ID: 926 7468 2486

Passcode: 144456

Thursday Zoom-Meeting

<https://desy.zoom.us/j/99738625981>

Meeting ID: 997 3862 5981

Passcode: 841881

Tutorial Zoom-Meeting

<https://desy.zoom.us/j/95288979489>

Meeting ID: 952 8897 9489

Passcode: 832350



# Methoden moderner Röntgenphysik: Streuung und Abbildung

**Lecturers:** Gerhard Grübel (GG), Felix Lehmkuhler (FL),  
Oliver Seek (OS), Andre Philippi-Kobs (AK)

<b>Part I:</b>	<b>Basics of X-ray Physics</b>	(GG)
<b>Part II:</b>	<b>Surfaces and Interfaces</b>	(OS)
<b>Part III:</b>	<b>Soft Matter Studies</b>	(FL)
<b>Part IV:</b>	<b>Magnetism - Thin Films</b>	(AK)

# Methoden moderner Röntgenphysik: Streuung und Abbildung

## Part I:

### Basics of X-ray Physics

by Gerhard Grübel (GG)

- [ 6.4.] Organisation and Introduction
- [ 8.4.] X-ray Scattering Primer, Sources of X-rays, Synchrotron Radiation
- [13.4.] Refraction and Reflection
- [15.4.] Kinematical Scattering Theory (I)
- [20.4.] Kinematical Scattering Theory (II)
- [22.4.] Small Angle Scattering and Soft Matter/ Anomalous Scattering
- [27.4.] Introduction: Coherence I
- [29.4.] Coherence II
- [ 4.5.] Applications of Coherent X-ray Beams

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## Part II:

### Surfaces and Interfaces

by Oliver Seeck (OS)

- [ 6.5.] Crystal Truncation Rods
- [11.5.] X-ray Reflectivity
- [18.5.] Grating incidence diffraction
- [29.5.] Surface diffuse scattering
- [25.5.] Outlook

# Methoden moderner Röntgenphysik: Streuung und Abbildung

## Part III:

### Soft Matter Studies

by Felix Lehmkuhler (FL)

- [27.5.] Soft Matter studies I: Methods & experiments
- [ 1.6.] Soft Matter studies II: Structure
- [ 3.6.] Soft Matter studies III: Dynamics
- [ 8.6.] Case study I: Glass transition
- [10.6.] Case Study II: Water and Ice
- [15.6.] Outlook I
- [17.6.] Outlook II

# Methoden moderner Röntgenphysik: Streuung und Abbildung

## Part IV:

### Studies on Magnetic Nanostructures

by Andre Philippi-Kobs (AK)

[22.6.] Ferromagnetism in a Nutshell

[24.6.] Interaction of Polarized Photons with Ferromagnetic Materials

[29.6.] X-ray Magnetic Circular Dichroism (XMCD) and Resonant Magnetic  
Small Angle X-ray Scattering (mSAXS)

[ 1.7.] Femtomagnetism / Imaging of Magnetic Domains

[ 6.7.] Outlook



# 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, 7<sup>th</sup> ed.

### Soft X-rays and Extreme Ultraviolet Radiation

D. Attwood, Cambridge University Press (2000)

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

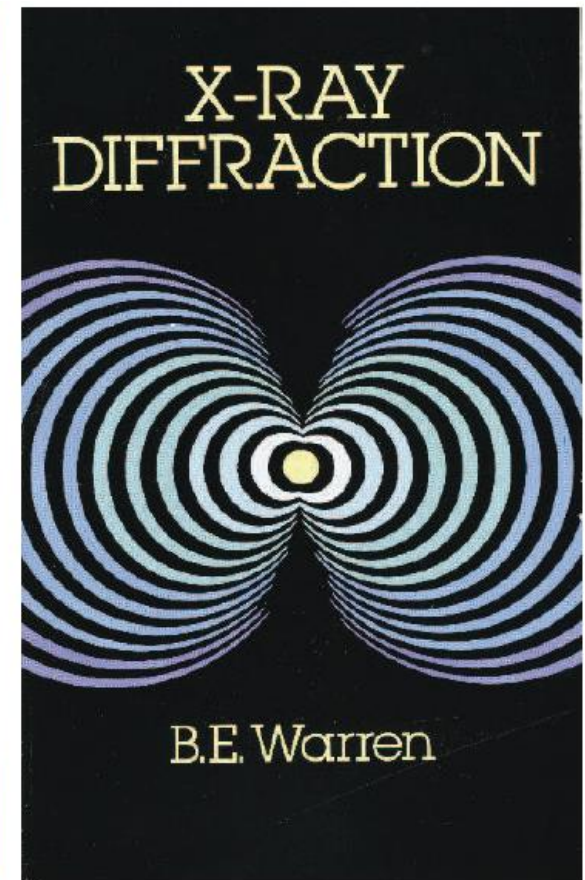
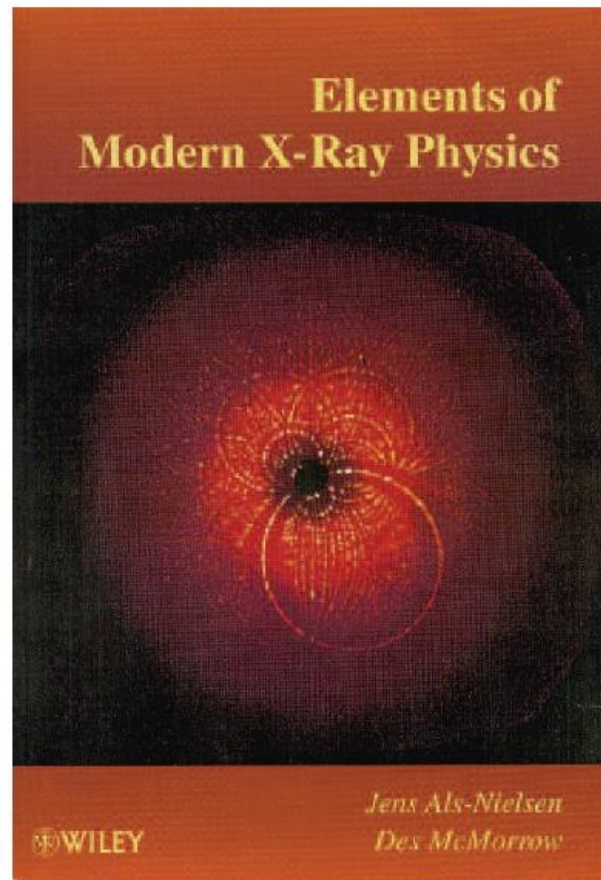
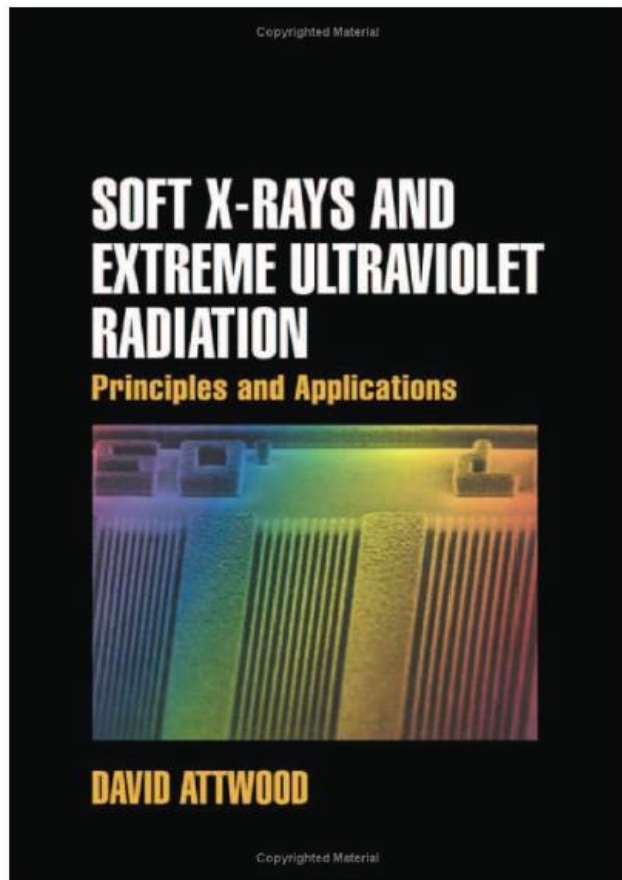
### Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen

K. Wille, Teubner Studienbücher 1996

# Lecture Notes

[https://photon-science.desy.de/research/research\\_teams/coherent\\_x\\_ray\\_scattering/teaching/index\\_eng.html](https://photon-science.desy.de/research/research_teams/coherent_x_ray_scattering/teaching/index_eng.html)





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

# Methoden moderner Röntgenphysik: 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 & Sources of X-rays +Synchrotron Radiation

Elements of X-ray Scattering, 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: 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, Spatial Coherence, Second Order Coherence, ...

## Coherent Scattering

Imaging and Correlation Spectroscopy, ...

# Methoden moderner Röntgenphysik: Streuung und Abbildung

## Part II/1:

### Surfaces and Interfaces

by Oliver Seeck (OS)

#### Crystal Truncation Rods

Concept of surfaces scattering as convolution of the surface structure factor with the bulk structure factor, Scattering from single crystal surfaces and epitactic films, Example: 2x1 surface reconstruction of Si 004 surfaces

#### X-ray Reflectivity

Concept of surface scattering as deduced from the kinematic approximation (Born Approximation), X-ray reflectivity of multilayers in Born Approximation and following dynamic scattering using Parratt, Refractive index, Example: Low density interfaces in Polymers

# Methoden moderner Röntgenphysik: Streuung und Abbildung

## Part II/2:

### Surfaces and Interfaces

by Oliver Seeck (OS)

#### Grazing incidence diffraction

Concept of evanescent waves, Penetration depth of X-rays, Example: Surface Phase Transition of Ising type  $\text{NH}_4\text{Cl}$  crystals

#### Surface diffuse scattering

Concept of scattering from disordered surfaces, Auto-correlation function and spectral power density, diffuse scattering in Born Approximation, Example: Capillary wave roughness on liquid ethanol



# Methoden moderner Röntgenphysik: Streuung und Abbildung

## Part III:

### Soft Matter Studies

by Felix Lehmkuhler (FL)

Soft Matter studies I: Methods & experiments

Soft Matter studies II: Structure

Soft Matter studies III: Dynamics

Case study I: Glass transition

Case study II: Water and Ice

Outlook I + II



# Methoden moderner Röntgenphysik: Streuung und Abbildung

## Part IV:

### Studies on Magnetic Nanostructures

by Andre Philippi-Kobs (AK)

#### Ferromagnetism in a Nutshell

Introduction to magnetic materials, magnetic phenomena, Magnetic Free Energy, Perpendicular Magnetic Anisotropy, Magnetic Domains and Domain Walls

#### Interaction of Polarized Photons with Ferromagnetic Materials

Charge and Spin X-ray Scattering by a Single Electron, Absorption and Resonant Scattering of Ferromagnets (Semi-Classical and Quantum-Mechanical Concepts)

#### X-ray Magnetic Circular Dichroism (XMCD) and Resonant Magnetic Small Angle X-ray Scattering (mSAXS)

XMCD Effect, Role of Spin-Orbit Coupling and Exchange Splitting, Sum Rules, XMLD and Natural Dichroisms, mSAXS of Magnetic Domain Patterns\

#### Femtomagnetism / Imaging of Magnetic Domains

Introduction to Ultrafast Magnetization Dynamics Induced by Femtosecond Infrared Pulses, Pump-Probe Experiments of Nano-Scale Magnetic Domain Patterns, All-Optical Switching, Manipulating Magnetism by XUV and THz Pulses

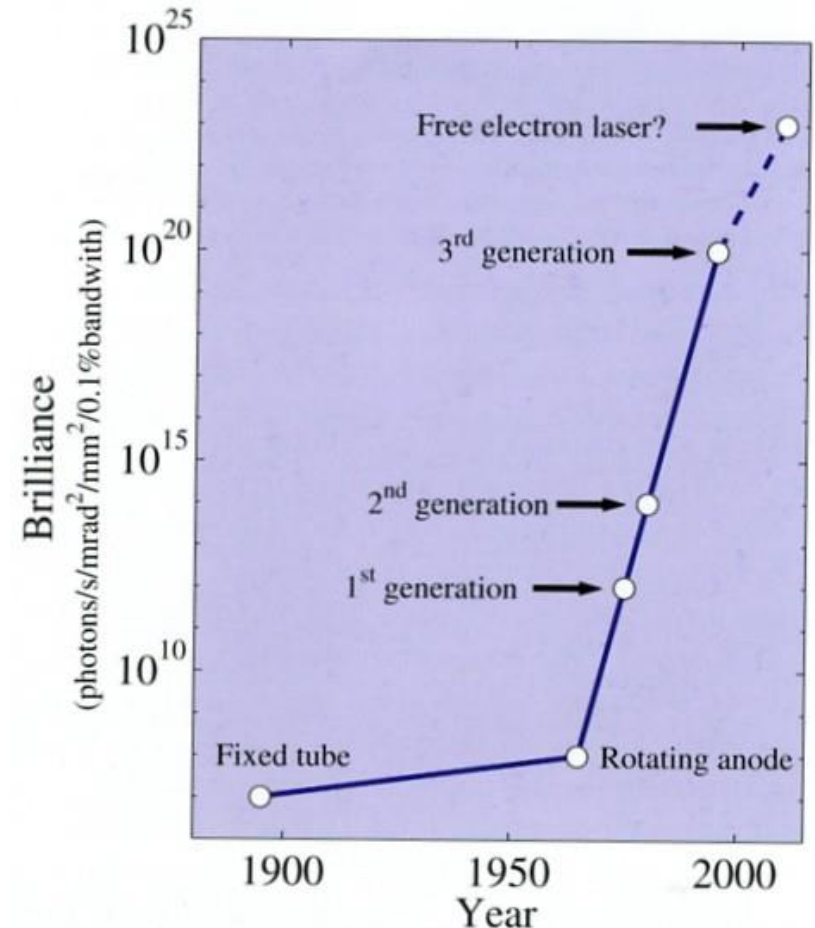
Fourier Transform Holography (FTH), Scanning Transmission X-ray Microscopy (STXM), Coherent Diffraction Imaging (CDI)

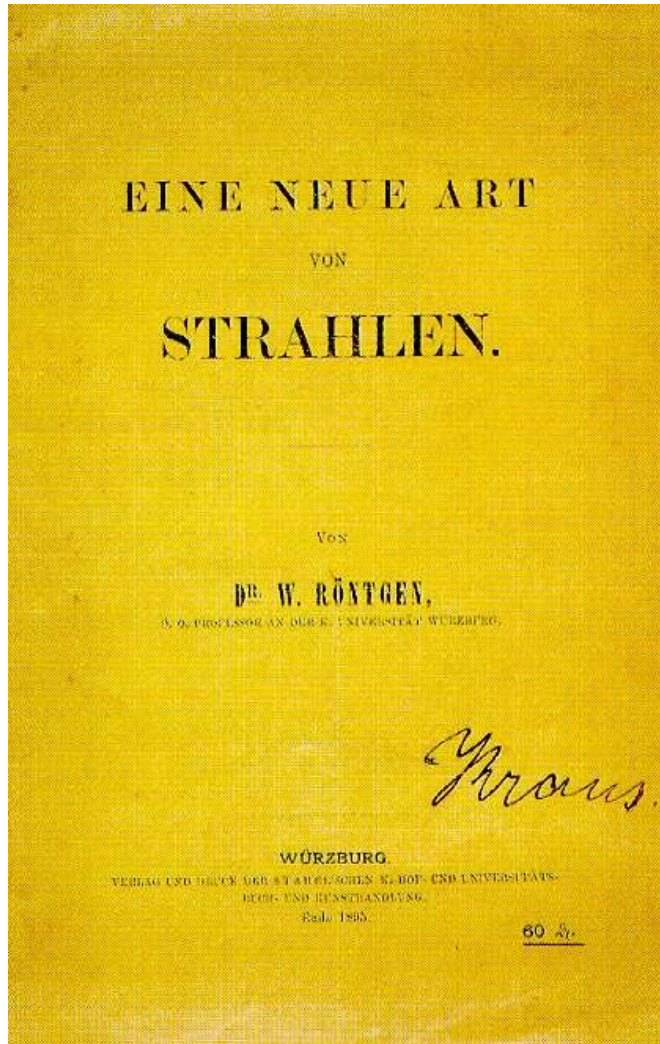




# Introduction by Gerhard Grübel

- 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)





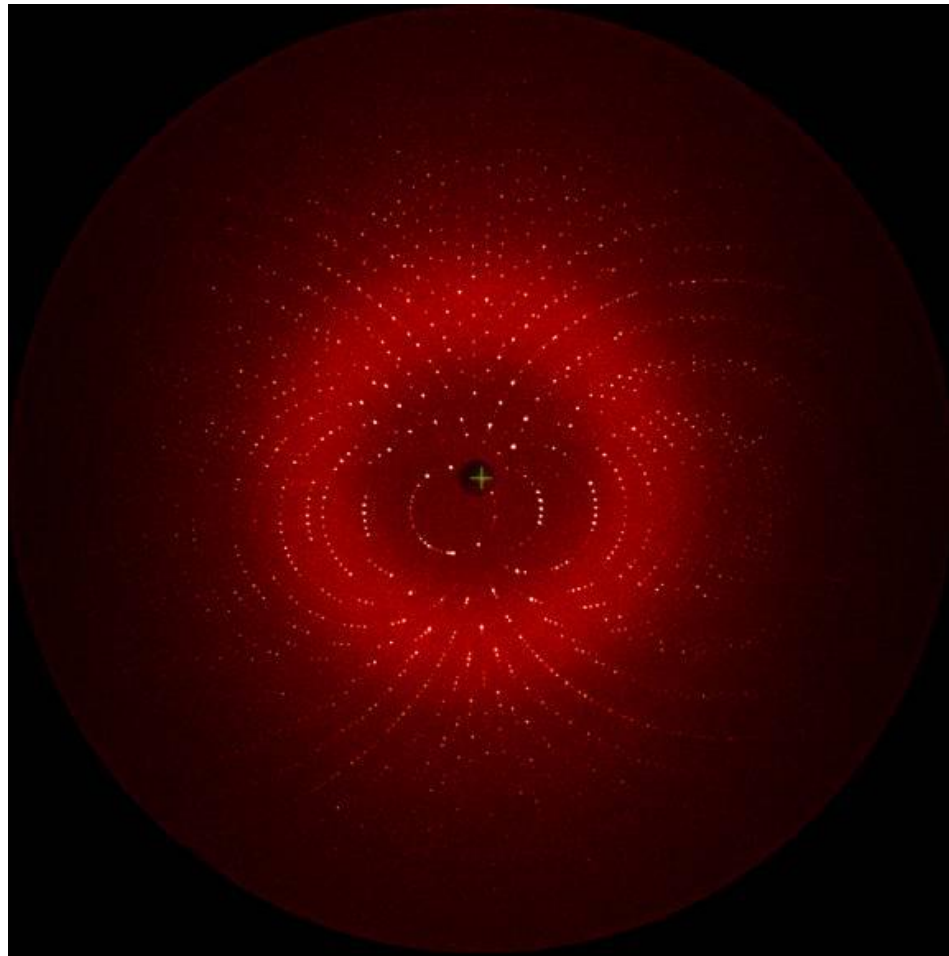
# Nobel Prices

- 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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Deutsches Elektronen-Synchrotron  
Ein Forschungszentrum der Helmholtz-Gemeinschaft



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## INFORMATIONEN FÜR

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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

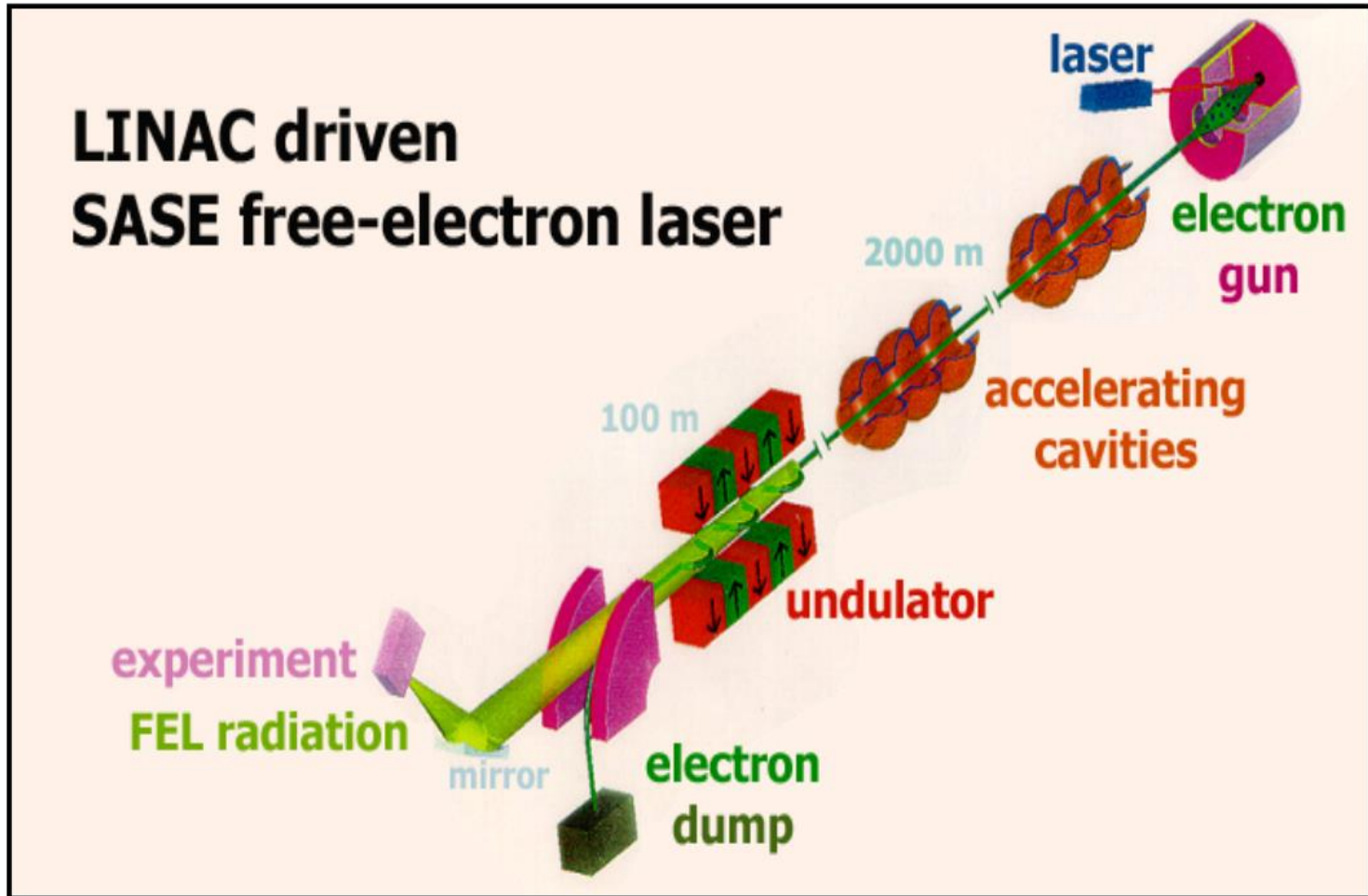
» [VERANSTALTUNGSKALENDER FÜR DESY IN HAMBURG UND ZEUTHEN](#)



# European Synchrotron Radiation Facility (ESRF)

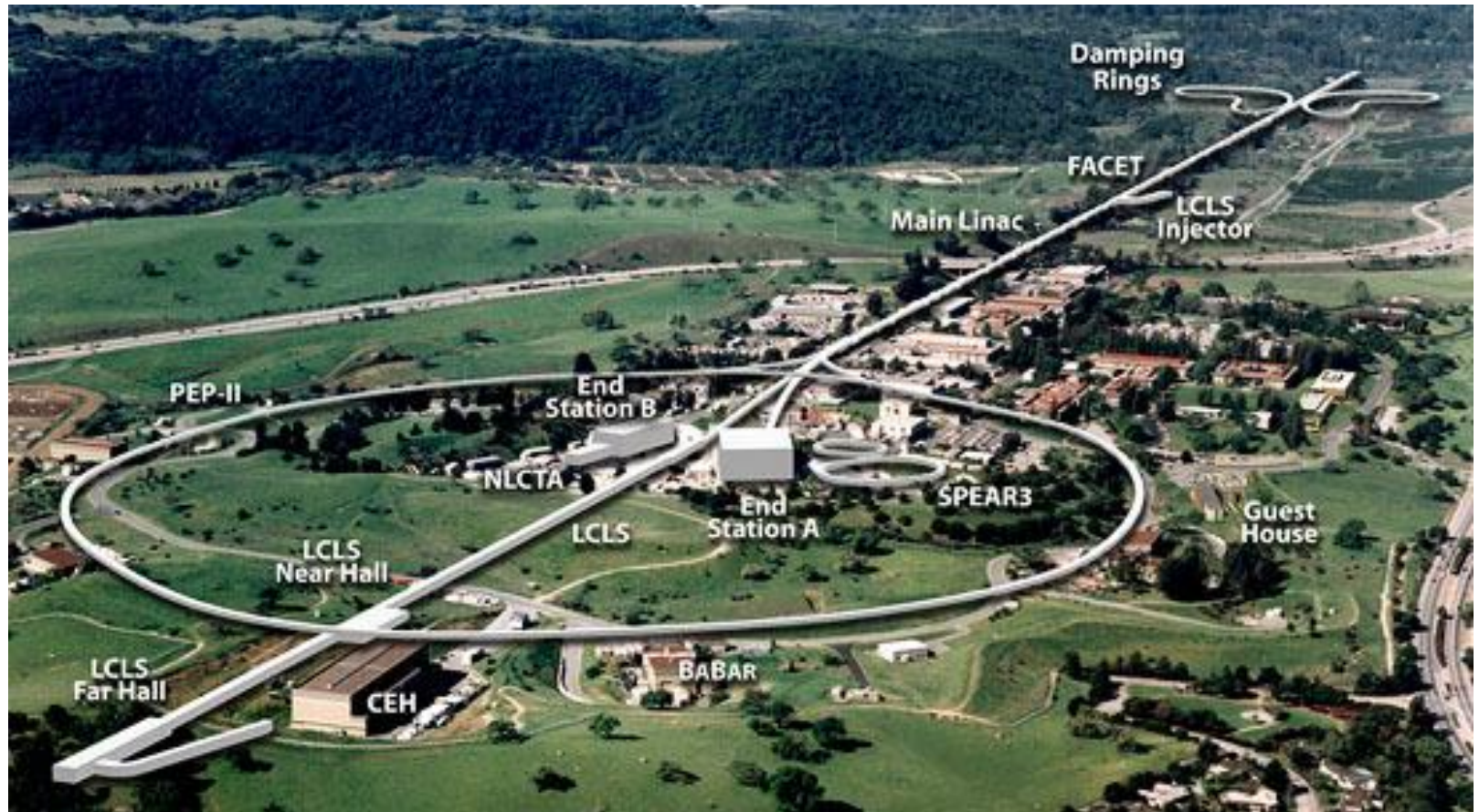


# Free Electron Lasers (FELs)

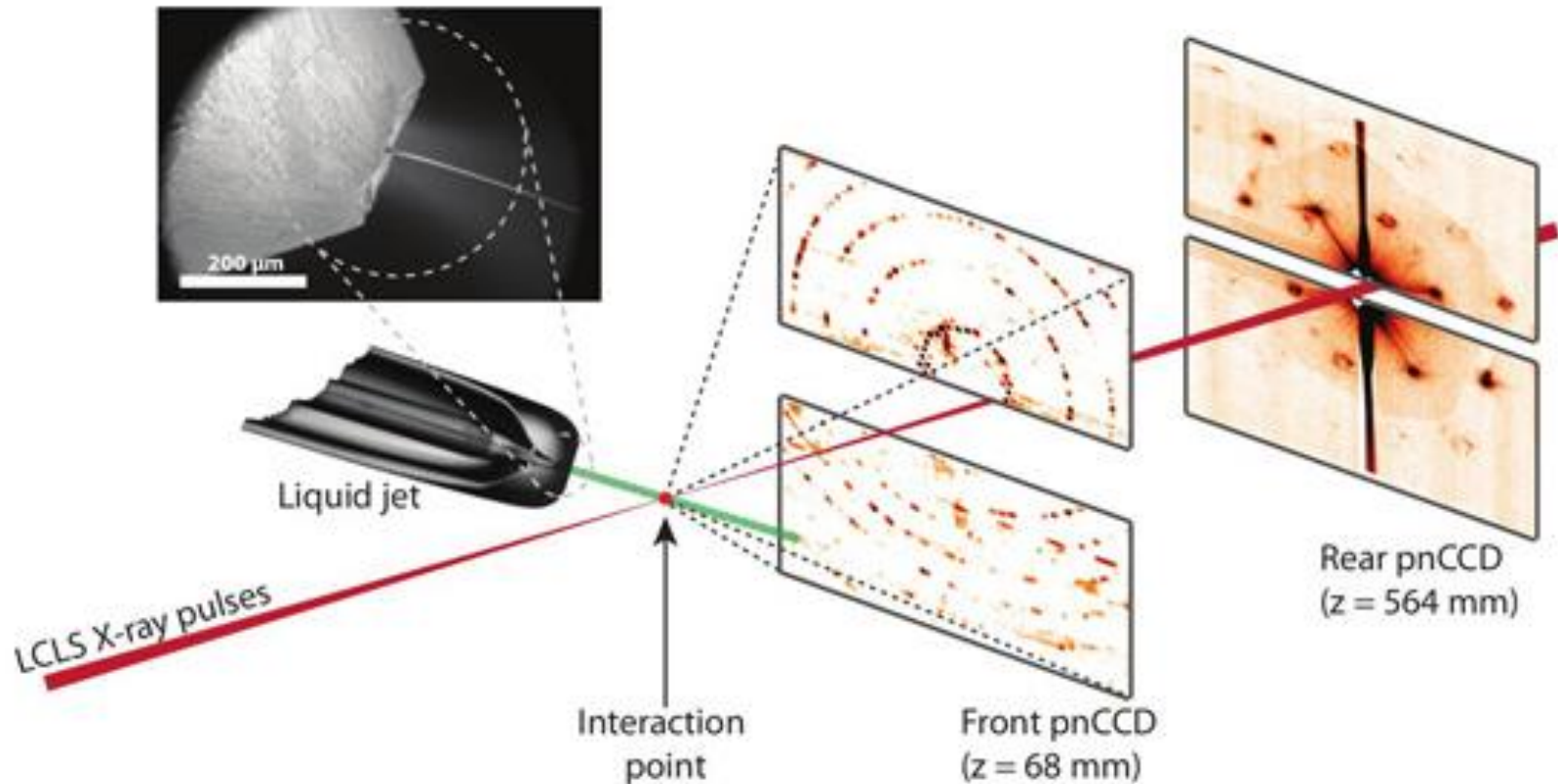




# LCLS – Linac Coherent Light Source - SLAC



# Serial Femtosecond Crystallography



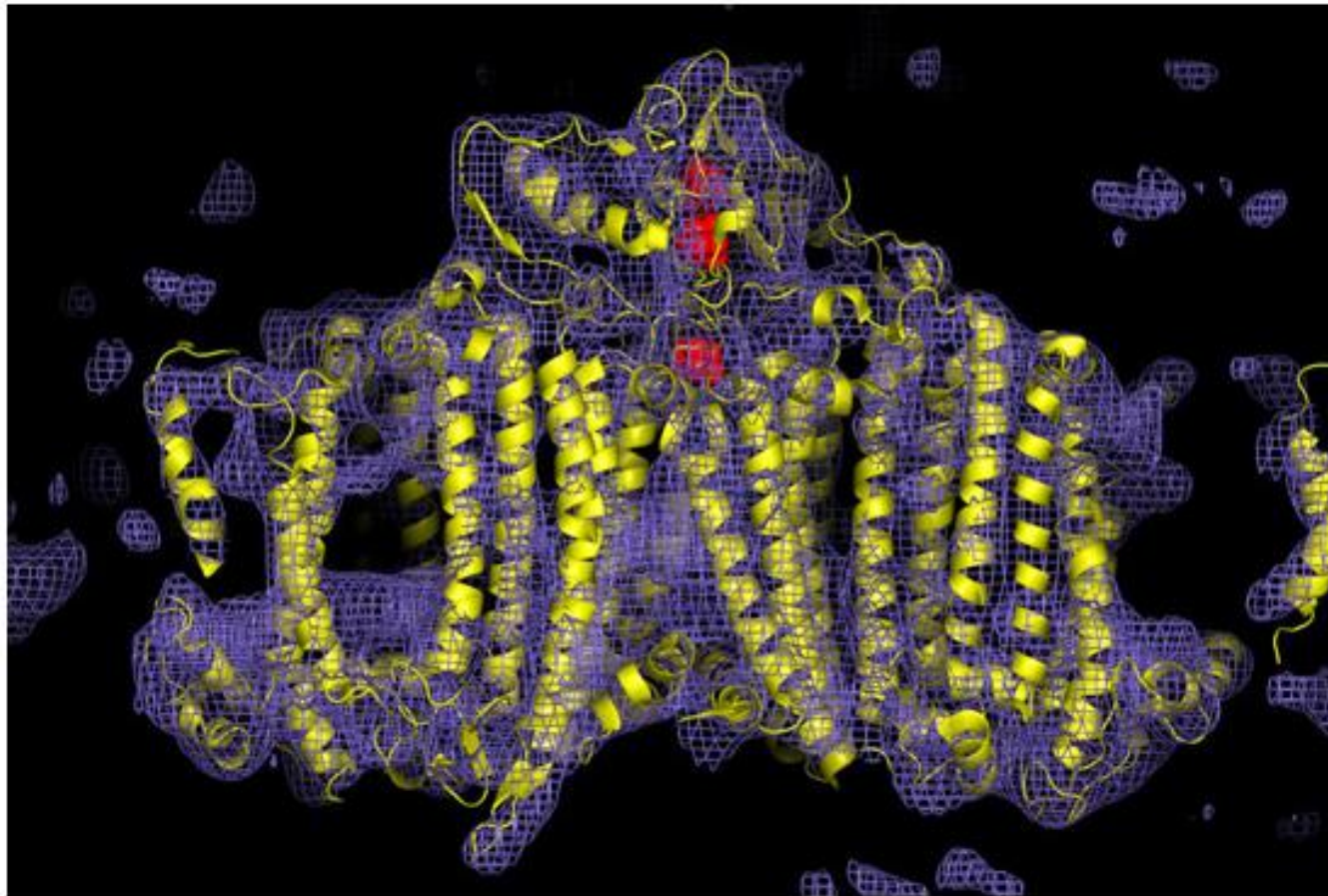
**Figure 1**

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.

