

# Methoden moderner Röntgenphysik II: Streuung und Abbildung

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Lecture 1	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2016 G. Grübel, M. Martins, S. Roth, O. Seeck, T. Schneider	
Location	Lecture hall AP, Physics, Jungiusstraße	
Date	Tuesday	12:45 - 14:15
	Thursday	8:30 - 10:00



# 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	12:45 - 14:15
	Thursday	8:30 - 10:00

First meeting "Tutorial":	Tuesday, April 19	14:30 - 16:00
Location:	Seminar room 4	



# Methoden moderner Röntgenphysik II: Streuung und Abbildung

**Proseminar:** For Bachelor students

Regularly date: Tuesdays at 16:30 - 18:00

Preliminary discussion: April 5, 2016  
Seminar room 4

Starting date: To be discussed

Location: To be discussed



# Methoden moderner Röntgenphysik II: Streuung und Abbildung

## A. Grundlagen und Methodik

- 1 Quellen für hochbrillante Röntgenstrahlung
- 2 Fokussierung von Röntgenstrahlung: Auf dem Weg zur 1 nm Auflösung
- 3 Winkelaufgelöste Photoelektronenspektroskopie
- 4 Röntgenabsorption
- 5 Fluoreszenzspektroskopie
- 6 Magnetische Röntgenspektroskopie und Streuung
- 7 Diffraction Imaging und Röntgenholographie
- 8 Correlation Spectroscopy
- 9 Reaktionsmikroskop

# Methoden moderner Röntgenphysik II: Streuung und Abbildung

## B. Anwendungen und Nutzung von Röntgenstrahlung

### 1 Ultraschnelle dynamische Prozesse

Streuung an Oberflächen und Grenzflächen

### 2 Untersuchung von dünnen Schichten mittels Streuung

### 3 Metallische Oberflächen – Vom Atom zum Kontakt

### 4 Reflektivität und Streuung von Grenzflächen

Spezielle Anwendungen

### 5 Kolloidale Suspensionen

### 6 Metallische Gläser

### 7 Röntgenspektroskopie an freien Ionen

# Methoden moderner Röntgenphysik II: Streuung und Abbildung

**Lecturers:** Gerhard Grübel (GG), Thomas Schneider (TS),  
Oliver Seek (OS), Stephan Roth (SR),

**Part I:** **Basics of X-ray Physics** (GG)  
**Part II:** **Soft Matter** (SR)  
**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)

- [ 5.4.] Organisation and Introduction
- [ 7.4.] Introduction
- [12.4.] X-ray Scattering Primer
- [14.4.] Sources of X-rays, Synchrotron Radiation
- [19.4.] Refraction and Reflection
- [21.4.] Kinematical Scattering Theory (I)
- [26.4.] Kinematical Scattering Theory (II), Applications
- [28.4.] Small Angle Scattering and Soft Matter
- [ 3.5.] Anomalous Scattering
- [10.5.] Introduction: Coherence I
- [12.5.] Coherence II; Applications of Coherent X-ray Beams



# Methoden moderner Röntgenphysik II: Streuung und Abbildung

## Part II:

### Soft Matter

by Stephan Roth (SR)

- [24.5.] What is Soft Matter
- [26.5.] Soft Matter and Biological Multilayer Membranes
- [31.5.] Soft Matter and Biological Multilayer Membranes
- [ 2.6.] Structures Surfaces/Gratings and Molecular In-plane Ordering,  
Off-specular Diffraction
- [ 7.6.] Capillary Waves, Diffuse X-ray Scattering



# Methoden moderner Röntgenphysik II: Streuung und Abbildung

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

- [ 9.6.] Introduction
  - Concepts of surfaces
  - Scattering (Born approximation)
  
- [14.6.] Crystal Truncation Rods
  - The basic idea
  - How to calculate
  - Examples
  
- [16.6.] Reflectivity
  - In Born approximation
  - Exact formalism (Fresnel)
  - Examples
  
- [21.6.] Grazing Incidence Diffraction
  - The basic idea
  - Penetration depth
  - Example
  
- [23.6.] Diffuse Scattering
  - Concepts of rough surfaces
  - Correlation functions
  - Scattering Born-approximation
  - DWBA
  - Examples

# Methoden moderner Röntgenphysik II: Streuung und Abbildung

## Part III: **Macromolecular Crystallography**

by Thomas Schneider (TS)

- [28.6.] **Site Visit**
- [30.6.] **Structural Biology & MX**
- Proteins
  - Protein crystals
  - Recombinant production of proteins
  - Radiation damage and cryogenic cooling
  - Bragg's law
- [ 5.7.] **Collection and processing of Diffraction Data**
- Real and reciprocal space
  - The crystallographic phase problem
  - Symmetry in real and reciprocal space  
(+ Demonstration Practical)
- [ 7.7.] **Phasing an Model refinement**
- Phasing methods
  - Ab initio
  - Molecular Replacement – 25%. Model bias
  - Multiple Isomorphous Replacement
  - Multiple Anomalous Diffraction
  - Refinement
- [ 12.7.] **Reserve**

# 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/>

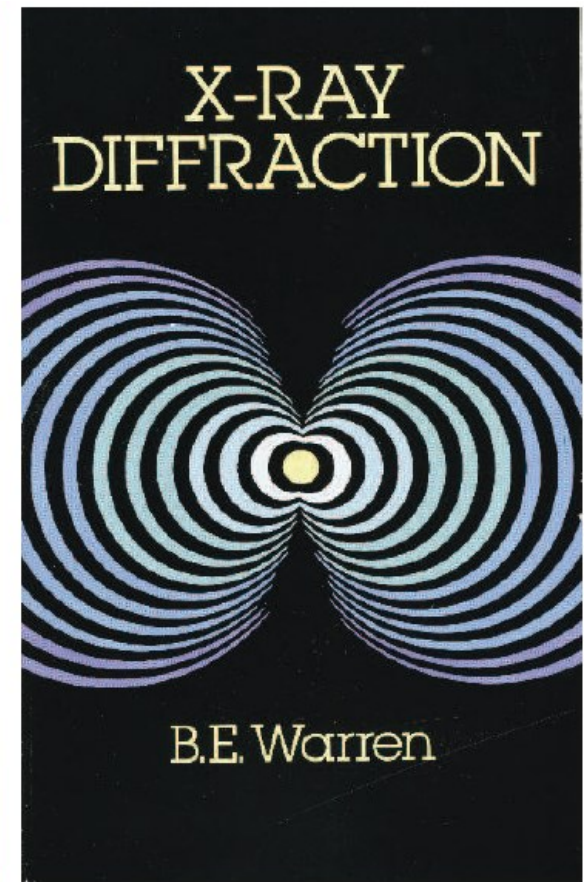
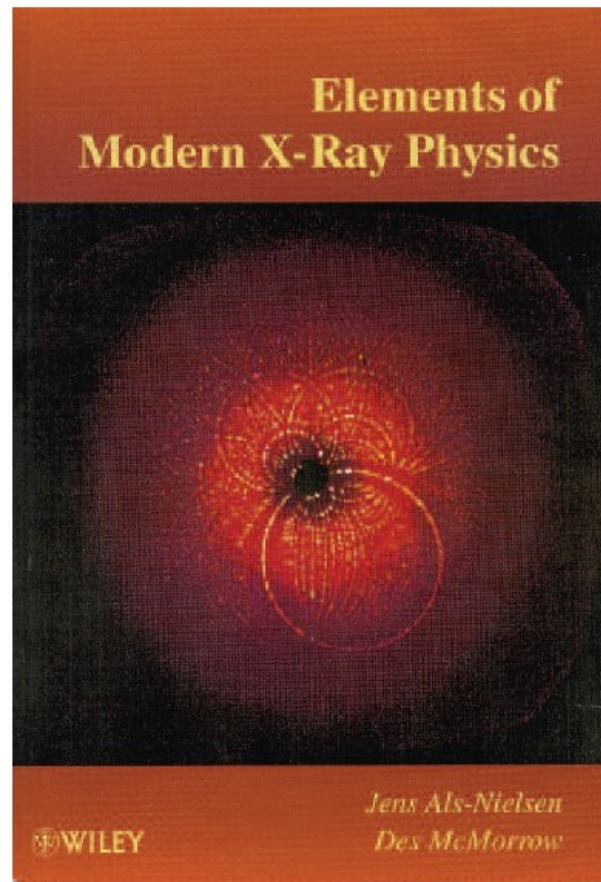
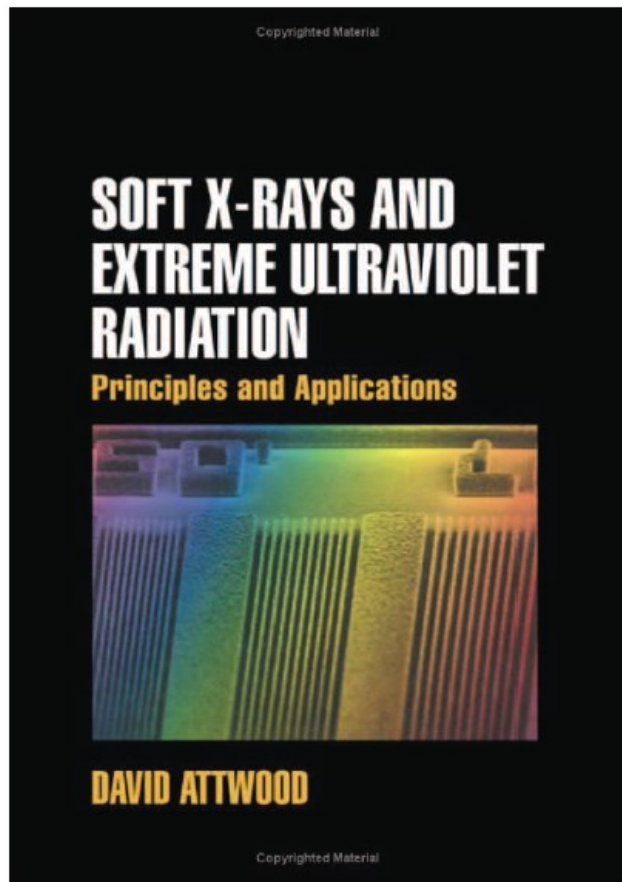
### Physik der Teilchenbeschleuniger und Synchrotronstrahlungsquellen

K. Wille, Teubner Studienbücher 1996

# Lecture Notes

[http://photon-science.desy.de/research/studentsteaching/lectures\\_\\_seminars/ss16](http://photon-science.desy.de/research/studentsteaching/lectures__seminars/ss16)





\* 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, ...

# Methoden moderner Röntgenphysik II: Streuung und Abbildung

## Part II:

### Soft Matter

by Stephan Roth (SR)

#### What is Soft Matter

What are the Properties and Which Properties can be Investigated by X-rays: Example Bulk Polymer and Diffuse Scattering

#### Soft Matter and Biological Multilayer Membranes

Investigation by X-ray Reflectivity (Born Approximation)

#### Soft Matter and Biological Multilayer Membranes

Investigation by X-ray Reflectivity (Parratt-, Abeles-Formalism), Examples

#### Structures Surfaces/Gratings and Molecular In-plane Ordering, Off-specular Diffraction

#### Capillary Waves

What are Capillary Waves, Correlation Functions, Power Spectral Density

#### Capillary Waves, Diffuse X-ray Scattering

# Methoden moderner Röntgenphysik II: Streuung und Abbildung

## Part III:

## Surfaces and Interfaces

by Oliver Seek (OS)

### Introduction

- Concepts of surfaces
- Scattering (Born approximation)

### Crystal Truncation Rods

- The basic idea
- How to calculate

### Reflectivity

- In Born approximation
- Exact formalism (Fresnel)

### Grazing Incidence Diffraction

- The basic idea
- Penetration depth

### Diffuse ScatterinG

- Concepts of rough surfaces
- Correlation functions
- Scattering Born-approximation
- DWBA



# Methoden moderner Röntgenphysik II: Streuung und Abbildung

## Part IV:

### Macromolecular Crystallography

by Thomas Schneider (TS)

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## Macromolecular Crystallography

by Thomas Schneider (TS)

### 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.