



## Announcement

# Basics of Structure Physics: Probing the atomic structure by electrons, (X-rays and neutrons) – including hands-on problem solutions

Prof. Kaiser, Prof. Rose

## Description

The objective of this course is to teach fundamental principles and introduce the state-of-the-art instrumentation for probing atomic (and electronic) structure with electrons (X-rays, neutrons), along with the skill to transfer the theory taught during the course to practical computer code or talk. Each student will have to solve a dedicated problem related to one of the topics addressed during the lectures. These problems will be addressed in a student talk, along with a detailed explanation of the background of the implemented theory or a numerical solution. The student will also perform two experiments on our Cs-corrected TITAN80-300 on high-resolution TEM.

## Content

1. Introduction into structure physics (Bragg and Laue, history, instrumentation)
2. The symmetry of crystals – space groups
3. Basics of geometrical optics – paraxial approximation, Scherzer theorem, aberrations, correction of aberrations
4. Basics of Fourier optics – Sommerfeld diffraction, basics for Abbe imaging theory
5. Basics of contrast in TEM – scattering amplitude, scattering cross section, electron optical refraction index, Born approximation, high energy approximation, multislice algorithm, propagation and image formation, image intensity
6. Basics of HRTEM imaging – experiment and calculation

Student's project: Evaluate one of the problems below, document the problem and the approach used to solve it. Present and discuss the project during the exercises.

- Generate atom positions within the unit cell from symmetry operators and replicate this unit cell a given amount of times, building a crystal – build in pre-defined space group numbers
- Calculation of the electron paths in a magnetic field
- Chromatic and spherical aberration, calculation of the influence and different accelerating voltages
- How a hexapole corrector works? Calculation of ray paths.
- Fresnel and Fraunhofer diffraction in TEM
- Calculation of the scattering amplitude and the scattering cross-section in first Born approximation and high-energy approximation
- Compute an electron diffraction pattern and the projected potential and the image contrast using the multislice algorithm for a defined structure
- Calculation of the amplitude and phase contrast transfer function of different objects and imaging conditions.

## Prerequisites

Undergraduate physics and mathematics, some experience in programming would be helpful

## Literature

Links to relevant literature and programming guides will be provided on the course website <http://www.uni-ulm.de/einrichtungen/hrem/lehre/lehreaching/>

**Additional information**

Two block for 1 week each (corresponding to 3 hours per week)

Seminars/Exercises/Experiment (2 hours per week)

6 ECTS credits

**Dates**

First meeting: Tue, 2.5.17, 16:00, N27/glas box

Introductory seminar: Wed, 3.5.17, 16:00, N27/glass box

Lectures: 4.5. - 9.5.17, daily 9 – 12 and 8.6. - 13.6.17, daily 9 - 12

Lab course: 10.7. - 13.7.17

**Assessment**

The final grade will be composed as follows: 50% for the student's project + 50% for the exam.

**Lecturer**

Prof. Kaiser, Prof. Rose, Electron Microscopy Group of Materials Science