# Principles and Applications of X-ray Diffraction

Schouwink Pascal Alexander

Cursus	Sem.	Туре	l anguage of	English
Chemistry and Chemical Engineering		Opt.	teaching	Ligist
			Credits	2
			Session	
			Exam	VVritten
			VVORKIOAD	60n
			Lecture	<b>32</b> 20
			Exercises	12
			Number of positions	15

### Frequency

CH-632

Every year

#### Remark

Next time: Fall 2023. Pre-registration form https://docs.google.com/forms/d/e/1FAIpQLSd5lyrEGUar8FBwxPqnIW1JBoPBr4YQjiA1yRGt3E7kOL-nXQ/viewform

#### Summary

Basic theoretical aspects of Crystallography and the interaction between X-ray radiation and matter. Experimental aspects of materials-oriented powder and single crystal diffraction. Familiarization with modern X-ray diffractometers.

#### Content

The course will consist of various modules. Students will be introduced to the fundamentals of Crystallography (symmetry, groups, lattice theory) and the basic theoretical aspects of X-ray diffraction (Generation of X-rays, interaction with matter, principles of interference functions and diffraction, scattering of periodic arrays, fourier transform and structure factors).

The basic theoretical aspects of structure solution will be taught (phase problem, reciprocal and direct space methods, absolute structure, twinning) as well as of structure refinement, with a focus on the theory of Rietveld refinement on powders.

Basic experimental aspects will be taught for single crystal, powder and thin film X-ray diffraction (Anomalous dispersion, Debye-Scherrer and Bragg-Brentano measurements, grazing incidence diffraction, in-plane diffraction) aiming at providing a solid knowledge on a large spectrum of methods relevant to diffraction studies on materials.

Students will be familiarized with different modern X-ray diffractometers, instrumental optics and experiment strategies. This course is open both to PhD students and PostDocs, passing the oral exam will give PhD students 2 ECTS credits.

# Keywords

XRD, Powder diffraction Materials

## **Learning Prerequisites**

#### **Required courses**

No particular prequisites, notions of very basic concepts of scattering and the solid state (inorganic materials) would be advantageous.

#### Learning Outcomes

By the end of the course, the student must be able to:

basics of Crystallography

- basic theoretical and experimental aspects of the discussed x-ray diffraction methods
- basic data analysis on materials

# **Assessment methods**

exercises (computer-based)

# Resources

# Websites

• https://docs.google.com/forms/d/e/1FAIpQLSd5lyrEGUar8FBwxPqnIW1JBoPBr4YQjiA1yRGt3E7kOL-nXQ/viewform