Principles and Applications of X-ray Diffraction

Schouwink Pascal Alexander

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<th>Cursus</th>
<th>Sem.</th>
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<tr>
<td>Chemistry and Chemical Engineering</td>
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<td>Opt.</td>
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Contact language: English
Credits: 2
Session: Opt.
Exam: Written
Workload: 60h
Hours: 32
Lecture: 20
Exercises: 12
Number of positions: 15

Frequency
Every year

Remark
Next time: Fall 2023. Pre-registration form
https://docs.google.com/forms/d/e/1FAIpQLSd5lyrEGUar8FBwxPqnIW1JBoPB4YQjia1yRGT3E7kOL-nXQ/viewform

Summary

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/1FAIpQLSd5lyrEGUar8FBwxPqrnlW1JBoPBr4YQjiA1yRGt3E7kOL-nXQ/viewform