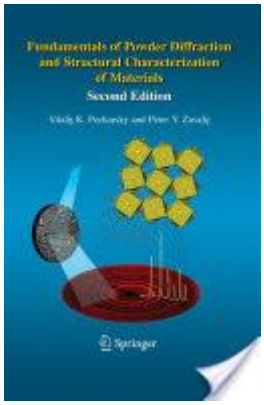
Powder Diffraction with X-rays and Neutrons in Materials Chemistry, 7.5 credits.
Feb 20 – March 21, 2025, Stockholm University (course code KZ8014)

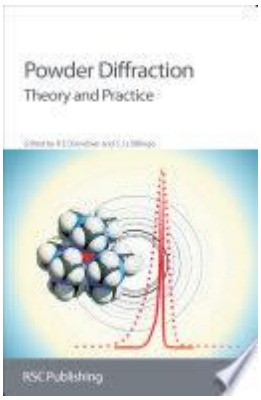
Description: This course targets masters and PhD students in the fields of chemistry, physics, and engineering interested in learning and applying powder diffraction for materials analysis and characterization. The course constitutes a theory and a project part. The theory part repeats briefly principles of crystallography (description and analysis of crystal structures, symmetry, lattices and space groups) and principles of diffraction (single crystal and powder, nuclear and magnetic) and then focuses on the specifics of powder diffraction (background of patterns, peak positions and shape, indexing, intensity extraction, Rietveld refinement, etc.). The project part deals with the application of powder diffraction to real problems (data sets).

Learning goal: the student should obtain a good understanding of the principles of diffraction and the application of diffraction techniques for phase and structural analysis of crystalline materials. The aim of the project part is to provide the student with tools and experience to independently perform advanced analysis of powder diffraction data.

Grading: Grading will be based on a written exam covering the contents of the lectures and an oral presentation of the project work.

Recommended reading: "Fundamentals of powder diffraction and structural characterization of materials" by V.K Pecharsky and P. Y. Zavalij. 2nd edition, 2006, Springer (ISBN: 978-0-387-09578-3). "Powder Diffraction, Theory and practice" by R.E. Dinnebier and S.J.L. Billinge, RSC publishing, 2008 (ISBN: 9778-0-85404-231-9).





Both books are available as e-books via the SU library.

Requirement: The student should possess basic knowledge of the crystalline state, crystal lattices, (space group) symmetry, systematic absences, as well as the fundamentals of diffraction as, for example, taught in the SU course "Structure analysis by diffraction" (KZ8013). Students should be familiar with crystal structure viewing programs like Diamond, Mercury, Crystal Maker or Vesta.

Contact for registration: andrew.inge@mmk.su.se

Schedule: Feb 20 – Mar 21, 2025

	Before lunch (10:00-12:00)	**After lunch (13:15-16:00)**
2/20	**L1**: Crystals, lattices & symmetry (AKI)	**E1**: Installation of programs (AKI)
2/21	--	--

2/24	**L2**: X-ray powder diffraction (AKI)	**E2**: Search & match (AKI)
2/25	**L3**: Neutron powder diffraction (HB)	**E3**: Peak positions (AKI)
2/26	**L4**: Indexing (LE)	**E4**: Indexing (LE)
2/27	Data collection for project (optional)	Data collection for project samples (optional)
2/28	Project	Project

3/3	**L5**: Profiles, intensity extraction (LE)	**E5**: Pawley and Le Bail fitting (LE)
3/4	**L6**: Structure solution in reciprocal space (LE)	**E6**: Structure solution with EXPO (LE)
3/5	**L7**: Structure solution in real space (AKI)	**E7**: Structure solution with FOX (AKI)
3/6	**L8**: Rietveld refinement – GSAS-II (AKI)	**E8**: GSAS-II (AKI)
3/7	Project	Project

3/10	**L9**: Rietveld refinement – TOPAS (AKI)	**E9**: TOPAS-Academic V6 (AKI)
3/11	**L10**: Rigid bodies and restraints (AKI)	**E10**: Rigid bodies in TOPAS (AKI)
3/12	Project	Project
3/13	Project	Project
3/14	**L11**: Sequential refinement (AKI)	**E11**: Sequential refinement in TOPAS (AKI)

3/17	**L12**: Introduction to PDF analysis (HB)	**L13**: Synchrotron & neutron facilities (AKI)
3/18	Project	Project
3/19	Project	**Project Presentations**
3/20	--	--
3/21	**Exam 10:00-15:00 (Room C516)**	

Lectures (**L**), Exercise sessions (**E**)
All lectures and exercise sessions will be held in room C513, Arrhenius Laboratory 16C

Teachers: (AKI) A. Ken Inge, (HB) Hanna Boström, (LE) Lars Eriksson