

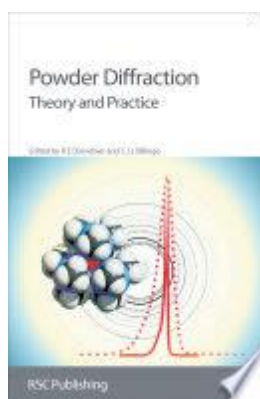
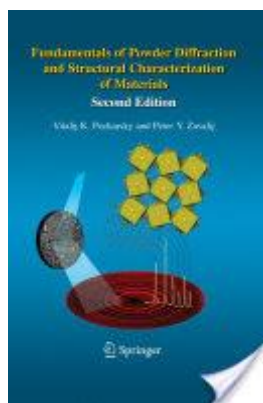
Powder diffraction course, X-ray and neutrons, 7.5 credits.
Feb 18 – March 22, 2021, Stockholm University (course code KZ8014)

Description: This course targets masters and PhD students in the fields of chemistry, physics, and engineering interested in learning and applying neutron and X-ray 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...). 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.

Textbook(s): “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). Some chapters will be taken from “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, as well as the fundamentals of diffraction. As, for example, taught in the SU course “Structure analysis by diffraction” (KZ8013). The student should be familiar with crystal structure drawing programs, like Diamond and Vesta.

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

Schedule: Feb 18 – Mar 22, 2021

Before lunch (10-12)		After lunch (13-16)
2/18	L1: Crystalline state, lattices, symmetry (AKI)	E1: Cell transformations and installation of programs (AKI)
2/19	L2: X-ray powder diffraction (JG)	E2: Search & match (AKI)
2/22	L3: Neutron powder diffraction (JC)	E3: Peak positions (AKI)
2/23	L4: Indexing (JG)	E4: Indexing (JG)
2/24	L5: Profiles, intensity extraction (LE)	E5: Pawley and Le Bail fitting (LE)
2/25	L6: Structure solution with reciprocal space methods (LE)	E6: Structure solution with EXPO (LE)
2/26	L7: Structure solution with real space methods (AKI)	E7: Structure solution with FOX (AKI)
3/1	--	--
3/2	L8: Rietveld refinement – Part I (JC)	E8: Fullprof (JC)
3/3	L9: Rietveld refinement – Part II (AKI)	E9: GSAS-II (AKI)
3/4	L10: Introduction into the Topas suite (AKI)	E10: Topas Academic (AKI)
3/5	--	--
3/8	L11: Neutron and synchrotron beamlines (AKI followed by JC)	E11: PDF/disordered structures (JC)
3/9	L12: Applications of neutron powder diffraction (JC)	Data collection for project samples (AKI)
3/10	Project	Project
3/11	Project	Project
3/12	Project	Project
3/15	Project	Project
3/16	Project	Project
3/17	Project presentation (AKI)	--
3/18	--	--
3/19	--	--
3/22	Exam	

All morning lectures (L) and afternoon exercise sessions (E) will be given online over Zoom.

Teachers and Zoom Links:

(AKI) A. Ken Inge <https://stockholmuniiversity.zoom.us/j/66343828289>
(JC) Johan Cedervall <https://stockholmuniiversity.zoom.us/j/63745976725>
(JG) Jekabs Grins <https://stockholmuniiversity.zoom.us/j/66981420874>
(LE) Lars Eriksson <https://stockholmuniiversity.zoom.us/j/68107303434>