

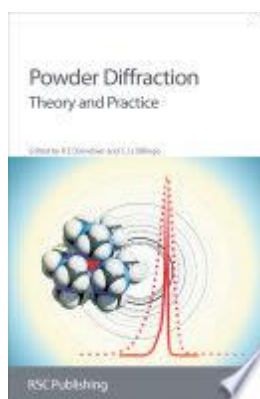
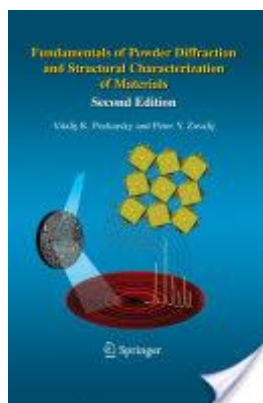
Powder Diffraction with X-rays and Neutrons in Materials Chemistry, 7.5 credits.
Feb 19 – March 20, 2026, Stockholm University (course code KZ8014)

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: Course notes will be provided. Additional 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. Students should be familiar with crystal structure viewing programs like Diamond, Mercury, Crystal Maker or Vesta.

Contact for registration: andrew.inge@su.se

Schedule: Feb 19 – Mar 20, 2026

	Before lunch (10:00-12:00)	After lunch (13:15-16:00)
2/19	L1: Crystals, lattices & symmetry (AKI)	E1: Installation of programs (AKI)
2/20	--	--

2/23	L2: X-ray powder diffraction (AKI)	E2: Search & match (AKI)
2/24	E3: Peak positions (AKI)	L3: Neutron powder diffraction (LE)
2/25	Data collection for project (optional)	Project
2/26	L4+E4: Indexing (LE) (C545)	Project
2/27	Data collection for project (optional)	Project

3/2	L5+E5: Pawley and Le Bail fitting (LE)	Project
3/3	L6+E6: Structure solution in reciprocal space (LE)	Project
3/4	L7: Structure solution in real space (AKI)	E7: Structure solution with FOX (AKI)
3/5	L8: Rietveld refinement – GSAS-II (AKI, C516)	E8: GSAS-II (AKI)
3/6	Project	Project

3/9	L9: Rietveld refinement – TOPAS (AKI)	E9: TOPAS-Academic V6 (AKI)
3/10	L10 + E10: Rigid bodies (AKI)	Project
3/11	Project (or Bruker XRD User Meeting)	Project (or Bruker XRD User Meeting)
3/12	L11+E11: Sequential refinements (AKI, C516)	Project
3/13	L12: Synchrotron & neutron facilities (AKI)	L13: Introduction to PDF analysis (LE)

3/16	Project	Project
3/17	Project	Project
3/18	Project	Project Presentations
3/19	--	--
3/20	Exam 10:00-15:00 (Room C516)	

Lectures (**L**), Exercise sessions (**E**)

All lectures and exercise sessions will be held in **room C513** unless otherwise stated

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

Address: Svante Arrhenius väg 16C, Stockholm 114 18