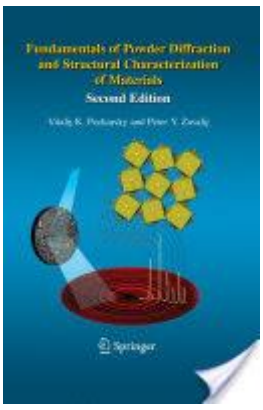
Powder diffraction course, X-ray and neutrons, 7.5 credits.
Feb 20 – March 20, 2020, Stockholm University (course code KZ7009)

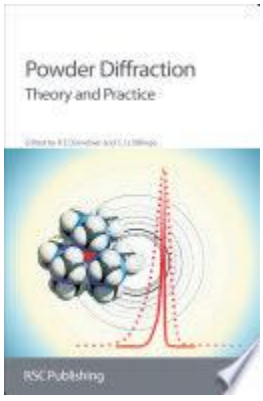
Description: This course targets masters and PhD students in the fields of chemistry, physics, and engineering interested in learning and applying neutron and X-ray powder diffraction for materials analysis and characterization. The course constitutes a theory and a project part. The theory part repeats 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 a brief report and 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: Ulrich Häussermann@mmk.su.se

Schedule: Feb 20 – Mar 20, 2020

	Before lunch	After lunch
20	Crystalline state, lattices, symmetry	Installation of programs, intro to Highscore.
21	Intensity of a Bragg reflection - X-rays and neutrons. - Magnetic neutron scattering - Magnetic form factor	Hanawalt, RIR, PDF, Qualx2
24	Data collection and correction - X-rays - neutrons (constant wavelength vs TOF) - what are "good" data ?	Peak positions, Highscore, internal standards
25	Indexing	Indexing-I, unit cell refinements
26	Profiles, intensity extraction	Indexing-II, cell transformation
27	Structure solution with reciprocal space methods	Structure solution with EXPO
28		
2	Structure solution with real space MC methods	Structure solution with FOX
3	Rietveld refinement	Fullprof
4	Rietveld refinement contd	GSAS
5	Introduction into the Topas suite	Topas
6		
9	Neutron and synchrotron beamlines	PDF/disordered structures
10	Applications of neutron powder diffraction	Data collection for project samples.
11	project	
12	project	
13	project	
16	project	
17	project	
18	Project presentation	
19		
20	Exam	

Place: Lecture room K233 (KÖL) at Arrhenius laboratory, Stockholm University.
The project will be based on in-house collected PXRD data (or provided/own data, either PXRD or neutron) and address the processing of data, structural solution from powder data and Rietveld refinement. Teachers: A.K. Inge, L. Eriksson, J. Grins, J. Cedervall.