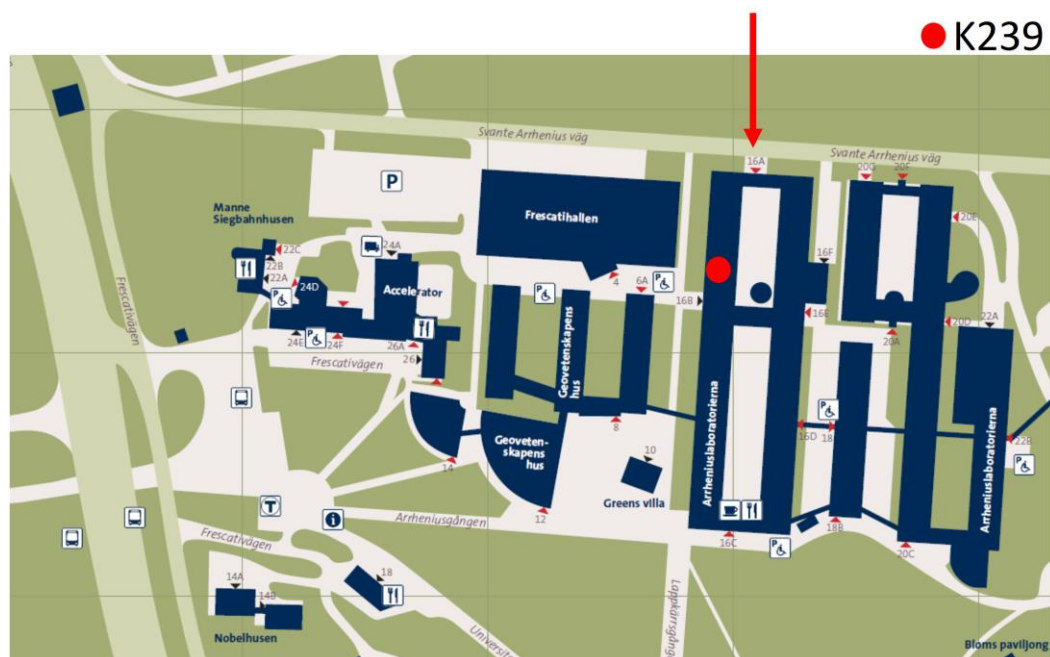**Powder diffraction course, X-ray and neutrons, 7.5 credits.**
**Feb 20 – March 20, 2020, Stockholm University (course code KZ8014)**

Start: February 20 (Thursday) 10 am

Place: Lecture room K239 (KÖL) at Arrhenius laboratory, Stockholm University. (Note, that without SU access card you can enter K233 only from entrance 16A)

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).
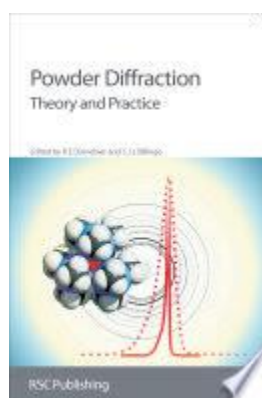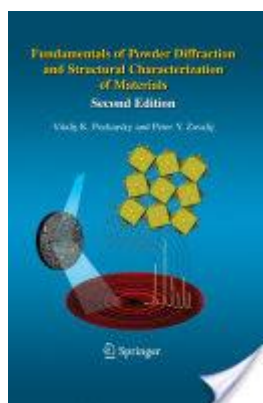
Please make sure that you have access to these books, e.g. as e-books via your university library.

Other course materials: Lecture notes, software, exercises, datasets, etc will be distributed via a dropbox. You are requested to bring a laptop for performing exercises, project work, etc. Note, that this course is very practice-oriented. *Make sure to have an eduroam account for internet access.*

Schedule: Feb 20 – Mar 20, 2020

	10 – 12	13 -16
20	Crystalline state, lattices, symmetry (LE)	Installation of programs, intro to Highscore.
21	Intensity of a Bragg reflection (JG JC) - X-rays and neutrons. - Magnetic neutron scattering - Magnetic form factor	Hanawalt, RIR, PDF, Qualx2

24	Data collection and correction (JG) - X-rays - neutrons (constant wavelength vs TOF) - what are "good" data ?	Peak positions, Highscore, internal standards
25	Indexing (JG)	Indexing-I, unit cell refinements
26	Profiles, intensity extraction (LE)	Indexing-II, cell transformation
27	Structure solution with reciprocal space methods (LE)	Structure solution with EXPO
28		

2	Structure solution with real space MC methods (AKI)	Structure solution with FOX
3	Rietveld refinement (JC)	Fullprof
4	Rietveld refinement contd (JG)	GSAS
5	Introduction into the Topas suite (AKI)	Topas
6		

9	Neutron and synchrotron beamlines (JC AKI)	PDF/disordered structures
10	Applications of neutron powder diffraction (JC)	Data collection for project samples.
11	project	
12	project	
13	project	

16	project	
17	project	
18	Project presentation	
19		
20	Exam	

Teachers: A.K. Inge (AKI), L. Eriksson (LE), J. Grins (JG), J. Cedervall (JC).

Course set up: Mornings are more lecture- and afternoons more exercise/practice-oriented. Aspects and components of powder diffraction will be taught by working with actual datasets. In the project, acquired knowledge of processing data, structure solution and Rietveld refinement

will then be applied to different data, either in-house collected PXRD data or data you may have collected previously (either PXRD or neutron diffraction).