

Syllabus "Crystal Structure Analysis" (445.616) Spring 2022

Professor Chan Park

Location: 33-330

Lecture time: Tuesday & Thursday 14:00-15:15

Language of the class: English

Class web page: ETL

Teaching staff:

Instructor: **Chan Park** Office: 33-219 Tel: 02-880-9324 Email: pchan@snu.ac.kr

Office hours/place: **Tuesday & Thursday 13:00- 1400, 15:30-17:00 / 33-219**

Teaching assistant: TBD

Prerequisite of this course:

- Need basic knowledge of crystallography.
- Need to have the license to use any XRD (can be one in Research Institute of Advanced Materials (RIAM, Sin-Gong-Yeon) or anywhere else). (this applies without any exception)
 - You need this for the experiment (see below).
 - Those who do not have the license have to get one before taking this course.
 - Those who do not have the license should take this course after getting one.

Text: Lecture notes and additional reading materials. Information on the additional reading materials will be provided in each section.

Books which are included in the "reading materials" of the lecture notes :

- V.K. Pecharsky & P.Y. Zavalij, Fundamentals of powder diffraction and structural characterization of materials
- C. Hammond, The Basics of Crystallography and Diffraction
- D. Sherwood & J Cooper, Crystals, X-rays, and Proteins
- M. Birkholz, Thin Film Analysis by X-ray Scattering
- B. D. Cullity, S. R. Stock, and S. Stock, Elements of X-ray Diffraction
- A. D. Krawitz, Introduction to Diffraction in Materials Science and Engineering,
- R. Jenkins & R. L. Snyder, Introduction to X-Ray Powder Diffractometry
- D. L. Post & J. E. Bish, Modern Powder Diffraction, Reviews in Mineralogy (Reviews in Mineralogy)
- R. A. Young, The Rietveld Method

Course Description:

- The objective of this course is to provide students with a thorough grounding in the theory and applications of crystal structure analyses using X-ray diffraction.
- Fundamentals of crystallography are first covered briefly, followed by advanced diffraction and scattering methods which include both theory and application.
- Modern instrumentation and automation techniques are addressed.
- The principles of crystal structure analyses emphasizing powder techniques are covered.

Lecture contents will include:

- Fundamentals of crystallography
- Nature of X-rays (generation & detection)
- Interaction of X-rays with matter
- Diffraction theory and diffractometers
- Powder diffraction methods and calibration techniques
- Powder diffraction pattern and profile analysis
- Qualitative & quantitative phase analysis
- Residual stress analysis
- Size and strain analysis
- Texture analysis
- Rietveld method
- Structure of thin films

Components of Your Grade:

(1) class attendance* (10%) (2) mid-term exam (20%) (3) final exam (25%)

(4) experiment (20%); Powder sample which consists of 4 different phases will be handed out, and you are expected to find out what they are and carry out the quantitative analysis of the 4 phases with two different methods.

(5) term paper & presentation (25%); Several subjects will be announced, and you are expected to choose one subject and prepare an in-depth term paper on that subject together with a 20 minute presentation in the class.

* The attendance of the 1st class is mandatory (5% out of 10%).

Evaluation; absolute assessment (in case the number of students is larger than 21, relative assessment will be used)

Both on-line and off-line class will be provided. The plan is that the lectures of week 1, 6-15 will be off-line and those of other weeks will be on-line. This plan is subject to change. The final plan will be announced at the 1st class.