

- Lecturer; CHAN PARK (880-9324, 33-320, pchan@snu.ac.kr)
- Grading; **Mid-term exam (20%), Final exam (15%)**
Experiment (20%), Term project (35%)
Attendance (10%)
No attendance of the 1st class (-5%), Assignments (+5%)

- Class hours/class room; Monday & Wednesday, 0930 ~ 1045 / 33-330
- No class – TBD
- Supplementary lecture class - TBD
- Evaluation; absolute assessment
- Lecture info – ETL

- This course is to provide students with a thorough grounding in the **theory and applications of crystal structure analyses using diffraction and spectroscopy.**

- Fundamentals of crystallography are first covered briefly, followed by advanced diffraction and scattering methods which include both theory and application.

- The principles of crystal structure analyses emphasizing powder techniques are covered.

Prerequisite of this course

- Need basic knowledge of crystallography.
- Need to have the license to use any XRD inside SNU (those in Research Institute of Advanced Materials (RIAM)(Sin-Gong-Yeon) is recommended)
- Need this for experiment. The XRD runs for the experiment have to be done by the students themselves.
 - ✓ Those who do not have the license have to get one before the 1st class.
 - ✓ Those who do not have the license in the 1st class cannot take the course.

Exams/Presentation Schedule

- Midterm (take-home exam)
 - ✓ Problems out **April 17**
 - ✓ Solutions due **May 1**
- Final exam
 - ✓ **May 29**
 - ✓ Problems from those handed out
- Presentation
 - ✓ Starts @ **May 13**

Tentative schedule

Mar 4	intro, xtallography		Apr 24	EVA, TOPAS demo	
Mar 6	symmetry, point group		Apr 29	residual stress	
Mar 11	reciprocal lattice		May 1	projection	Mid-term due
Mar 13	PDF, Inter' Table, diffractometer		May 8	texture	
Mar 18	diffraction		May 13	Presentation1	Term paper due
Mar 20	interaction, Bragg, Laue		May 15	Presentation2	
Mar 25	intensity		May 20	Presentation3	Experiment report due
Mar 27	Error, Accuracy, precision		May 22	Presentation4	
Apr 1	phase ID, profile fitting		May 27	Presentation5	
Apr 3	quantitative phase analysis		May 29	Last class	Final exam
Apr 8	quantitative phase analysis				
Apr 10	Broadening, order-disorder				
Apr 15	thin film				
Apr 17	Rietveld	Mid-term out			
Apr 22	Rietveld, residual stress				

5 CHAN PARK, MSE, SNU Spring-2019 Crystal Structure Analyses

Extra classes

- **Class starts @ 0900** → 30 X 20 = 600 min
- 600 / 75 = 8
- 6/14 end of semester → no class on 6/12, 6/10, 6/5, 6/3
- Presentations 5/13, 5/15, 5/20, 5/22

6 CHAN PARK, MSE, SNU Spring-2019 Crystal Structure Analyses

Term paper & presentation

- Choose two out of the subjects given below and let me know. I will choose one for you.
- Describe the principle, data collecting procedures, sources of error, limits of accuracy, etc.
- Find **two** papers which used that analysis, explain why they used that analysis, how they prepared the specimen, how they collected the scattering data, what they did to improve the accuracy/precision of their data (if any), how they used that information for their research.
 - ✓ Reciprocal space mapping
 - ✓ EDS/WDS quantitative elemental analyses (comparison of WDS & EDS, discussions on energy resolution needed)
 - ✓ Quantitative phase analysis
 - Internal/External standard method, External standard method, Direct comparison method, Spiking method
- Term paper due --- **2017-05-13, both hardcopy and file (e-mail)**
- Scoring criteria - the depth of understanding and the way they are summarized.
- **Do not repeat what we cover in the class.**
- Had better be as easy to read as possible → **most important scoring criterion**
- Size < 20 pages (penalty in case more than 21 pages), Term paper in Korean or English

7 CHAN PARK, MSE, SNU Spring-2019 Crystal Structure Analyses

Term paper & presentation

- When you find two papers on the subject of your term project, please send me those files before **April 8**.
- Work on the papers only after we discuss.
- I want to check whether some of the students are working on the same papers.
- In case the papers you send to me includes the papers which another student already sent to me, I will ask you to change the paper(s).
- **Do not repeat what we cover in the class.**

8 CHAN PARK, MSE, SNU Spring-2019 Crystal Structure Analyses

Presentation

- **(15 + 5) minutes/students including Q&A**
- **Ppt file has to be e-mailed to me TWO days before presentation. (this will greatly affect the 35% of the total grade)**
- Hard copy has to be submitted to me on the day of presentation.
- Penalty in case the presentation lasts longer than the amount of time allocated. (up to 2 minutes is OK)
- All the info on the sources of the data used has to be written on the slide.
- No background. (pure white background)
- Presentation in Korean or English
- Font size has to be large enough to be seen when 4 slides are printed in one page
- Scoring criteria
 - ✓ the depth of understanding/contents and the way they are summarized
 - ✓ how much the audience can understand the presentation
 - ✓ **do not repeat what we cover in the class.**
 - ✓ the contents of slides, how the contents of slides are organized, presenting attitude

9 CHAN PARK, MSE, SNU Spring-2019 Crystal Structure Analyses

XRD Experiment

Powder mixture will be provided (1 per each or 1 per two)

- Phase ID (qualitative phase analysis)
 - ✓ Need to find out which phases are included in the powder mixture
- Quantitative phase analysis (quant)
 - ✓ Need to find out the quantity (percentage) of each phase in the powder mixture
 - ✓ Have to use **two** methods (one has to be Rietveld method)
- The report has to be < **4 pages**
- **Report due May 20**

- e-mail Title ; name – XSA
- File name; name – XSA.xls

- Make an excel file with the info in the table below and send it to pchan@snu.ac.kr & lilyjulie5@gmail.com
- Whether you have ever taken crystallography or XRD related course before – title of the course, textbook

name	Course (e.g. master 3 rd semester)	advisor	Related course taken before	Undergraduate univ (major, dept)	Textbook used when you took the related course before	Cell- phone	E- mail

Sources of info

- www.iucr.org
- www.icdd.com/resources
- www.uni-wuerzburg.de/mineralogie/crystal/teaching/teaching.html
- journals.iucr.org/cww-top/crystal.index.html
- phycomp.technion.ac.il/~sshaharr/intro.html
- www.softdisc.co.kr
- super.gsnu.ac.kr
- icsd.ill.fr/icsd
- home.wxs.nl/~rienv025
- www.ncnr.nist.gov/programs/crystallography/software/expgui/expgui.html