MATERIALS SCIENCE & ENGINEERING

MSE 8803F – Advanced X-ray Diffraction and Scattering

(3 credit hours)
Instructors: R. Snyder, and H. Garmestani
Lecture: 3:05 pm - 3:55 pm MWF Instr Center 109
Laboratory: Monday-Friday

The purpose of Scattering and *diffraction in Materials* is to acquaint students with the principles and theory of crystallography and diffraction analysis of materials. The course will be focused primarily on qualitative and quantitative phase analysis of materials but topics include small angle scattering theory, texture, residual stress, line profile analysis and electron back scattered diffraction analysis in SEM for micro-texture analysis. Reciprocal lattice concepts and the peculiarities of the different methods will be presented. The intent is to bring the student close to the state of the art in these characterization methods and to illustrate the general approach to characterization problems based on scattering and diffraction. In addition both the hardware and software aspects of modern automated instrumental procedures will be covered.

Lecture Topics

1- (20 Lectures) Snyder
Powder Diffraction Methods and calibration techniques
The modern Automated diffract meter
Applications of the Powder Method.
Qualitative phase analysis.
Crystallography and space group analysis
Indexing and lattice parameter determination, refinement and identification.
Powder pattern calculation
Crystal structure determination - The Rietveld method.
Single Crystal Methods
Quantitative X-ray Diffraction
Interaction of X-rays with matter: absorption and EXAFS (time?)
X-ray reflectometry analysis

2- Small Angle Scattering (5 lectures) Bucknall, Kumar
a. Patterson Function
b. Pair correlation functions and linkage to structure function
c. Application to spherical, elliptical and needle shape inclusions
d. Debye's function
e. Application to amorphous structures, nano-composites.

3- (20 lectures) Garmestani
Particle size and strain analysis – line profile and Fourier techniques.
Texture, Micro-texture and Residual stress
Pole figure in x-ray (single crystal and area detector)
Electron Diffraction (Orientation Imaging Microscopy)
Fourier Analysis of Distributions
Euler angle definition of orientation space (Bunge's notation)
Orientation Distribution Function
Fourier analysis of Orientation Distribution Function and quantification of texture
Stress (residual stress analysis)

Text: No text.

References:

1- R. Jenkins and R. L. Snyder, Introduction to X-ray Analysis Diffractometry, John Wiley and Sons (1996)
2. Jens Als-Nielsen, DesMorrow, Elements of Modern X-ray Physics, Wiley
3. D. L. Bish and J. E. Post ed., Modern Powder, Diffraction Reviews in Mineralogy Vol. 20, Mineralogical Society of America, (1989).
4- John Mc. Cowley Diffraction Physics,
5- Klug and Alexander, X-ray Diffraction Procedures, J. Wiley and Son, New York (1972)
6- B. D. Cullity, Elements of X-ray Diffraction, Addison Wesley Publishing Company, Reading, Mass. (1956)

Basis for Grading: Laboratory 50%
2 exams @ 50%

Class Attendance: Three lecture periods and one laboratory per week based on the schedule distributed in class. All laboratory work must be completed.

Labs:

08/18 1- Alignment and Calibration of automated diffractometers (1 week)
08/25 2- Phase identification – multiphase unknown (2 weeks)
09/08 3- Internal Standard Method: Lattice parameter refinement and Accuracy assessment (1 weeks)
09/15 4- Indexing of powder patterns and identification via the Crystal-Data data base (1 week)
09/22 5- Crystal Structure Analysis via the Rietveld Method (2 weeks)
10/06 6- Profile fitting and deconvolution techniques. Size and strain analysis from profile deconvolution (2 weeks)
10/20 5- Residual Stress Analysis (2 weeks)
11/03 6- Nanostructures, thin films and Reflectometry (2 weeks)
11/17 7- Pole Figure Texture Analysis (2 weeks)
12/01 8- Small angle scattering (1 week)

Class schedule:

Class 1 Accuracy in XRPD: X-ray Diffractometry to slide #42 of L1-3
Class 2 Diffraction geometries
Class 3 Intensity measurement and Calibration to slide #134 end
Class 4 Qualitative Analysis XRF Qual and Quant to slide #31 of L 4-5
Class 5 Qualitative Phase Analysis XRPD to end of L4-5
Class 6 Crystallography Space Group Theory 3 to slide #23 of L6-7
Class 7 Finish L6-7 generation of equipoints
Class 8 Fundamental Diffraction Theory, Laue Conditions, Reciprocal lattice L8-9 #27
Class 9 Fundamental Theory 2 Structure Factor to Slide #50 in L8-9
Class 10 Calculated PD and generalized F, finish L8-10
Class 11 Crystal Structure Analysis and Rietveld Refinement L11
Class 12 Workshop on Rietveld – Jung-Il?
Class 13 Computer indexing and lattice parameter refinement workshop Jung-Il & Ken
Class 14 Quantitative analysis
Class 15 Reflectometry and thin film analysis
Class 16 Non-ambient analysis
Class 17 Workshop on non-ambient – Melanie
Class 18 Interference function and size and strain broadening
Class 19 Line Profile analysis – demo by Ken
Class 20 Test take home?

Schedule

Week#		Monday		Wednesday		Friday	Lab
1- Aug	18	RS	20	RS	22	RS	
2-	25	RS	27	RS	29	RS	
3-Sep	1	School Holiday	3	RS	5	RS	
4-	8	RS	10	RS	12	RS	
5-	15	RS	15	RS	17	RS	
6-	22	RS	24	RS	26	RS	
7-Oct	29	RS	1	RS	3	RS EXAM	
8-	6	SAX	8	SAX	10	SAX	
9-	13	Recess	15	SAX	17	SAX	
10-	20	HG	22	HG	24	HG	
11-	27	HG	29	HG	31	HG	
12-Nov	3	HG	5	HG	7	HG	
13-	10	HG	12	HG	14	HG	
14-	17	HG	19	HG	21	HG	
15-	25	HG	27	School Holiday	29	HG	
16-Dec	1	HG	3	HG	5	HG	
17	8	HG & SAX	10		12		

		Exams					

Class Schedule I take first 20

Aug 18 Powder diffraction and instrumentation
20 Calibration and accuracy
22 Crystallography 1

25 Crystallography 2
27 Crystallography 3
29
Sept 03
05
08
10
12
15
17
19
22
24
26
29
October 01
03 Exam