Scattering Theory - MSE 6404

9:30 am – 10:20 am MWF Love (MRDC II) 299

Fall 2024

Professor: Hamid Garmestani
Class time: 9:30-10:20 pm, MWF
Office: 361 Love Building
Tel: (404) 385 4495
Office Hours: T, Th at 10-11am through zoom. Other times or in-person by prior appointment.
Office hours will be arranged through Zoom also and in-person (in my office by appointment).

Recorded Lectures will be prepared every M, W and F after class times and will be uploaded to Canvas by the next day.

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Course Description

The purpose of *scattering Theory* is to acquaint students with the principles and theory of diffraction/scattering of electromagnetic radiation from solids. The course serves two purposes:

A. Providing students with the kinematical formalism of x-ray scattering as a characterization tool. Reciprocal lattice concepts and Orientation Distributions are emphasized.
B. Teaching and training students to operate the three x-ray facility (Alpha-1, MPD, MRD) and learn the range of capabilities offered with various optics and in-situ high temp facility (MPD). The laboratory assignments will provide the graduate students the ability to perform (independently):
   1. Phase analysis (Alpha-1)
      i. Single Phase
      ii. Multi-phase analysis
      iii. Crystal Maker, Crystal Diffract and High Score
   2. Stress and strain
      i. Line Profile analysis for strain and particle size (Alpha-1, MPD, MRD).
      ii. Residual Stress Analysis.
   3. Texture (Pole figure) analysis
   4. SAXD

The schedule for these labs are:

Lab#1	Virtual XPS
Lab#2	Phase analysis
Lab#3	Stress and strain:
Lab#4	Texture (Pole figure) analysis
Lab#5	SAXD or EBSD To be determined.

Final Exam: Wednesday, Dec 14 8:00 AM - 10:50 AM

We will also teach popular software packages available to MSE such as Crystal Maker, Crystal Diffract, HighScore, Popla and Mtex. We have the site license for crystal maker and crystal diffract and as students registered in MSE6404, you will also get a copy of the Highscore. Popla and Mtex are freely available from the web. High Score package combines phase identification, crystallographic analysis, cluster analysis, profile fitting and Rietveld / structure calculations, all in one.

Canvas quizzes will be used as the primary mode for taking quizzes and the final. Honorlock will be used as part of the final and some of the quizzes.

Textbook: There is no textbook for this class. I will be providing lecture notes and slides.

Topics Covered

1. Overview of Microstructural Characterization Techniques
    - Optical Microscopy
    - Electron Microscopy
    - Transmission EM (TEM)
    - Scanning EM (SEM)

2. Properties of x-rays
    - Electromagnetic radiation
    - Production of x-ray (XES, XPS, …)
    - Detection of x-rays
    - Detection of x-rays

3. Crystallography
    - Crystal systems
    - Reciprocal lattice
    - Stereographic Projection
    - Pole Figures
    - Representation of Orientation (Euler, …)

4. Diffraction
    - Bragg's law
    - Laue's Equation
    - Reciprocal Lattice and Diffraction
    - Diffraction Methods
    - Scattering by an atom
    - Scattering by a Unit Cell
    - Structure factor
    - Multiplicity, Lorenz, Absorption, Temperature Factor
    - Reciprocal Space
    - Pair –correlation Functions

5. Phase Analysis by x-ray Diffraction

- Powder Diffraction
- Hanawalt Method
- Single Phase analysis
- Multi-Phase Analysis
- Indexing of Patterns (Cubic, Tetragonal,…)
- Number of atoms in a Unit Cell

6. Texture

- Texture Measurement
- x-ray diffraction (pole figures, Laue)
- Orientation Distribution
- Crystal, Sample symmetry
- Discrete vs. Continuous Representations
- Grain Boundary texture
- Lattice Curvatures (geometrically necessary dislocations)
- Spherical Harmonics
- Calculation of Orientation Distributions (OD) from Projections (pole figures)
- Analysis of OD data

7. Micro-Texture

- Electron diffraction (EBSD, OIM);
- Geometry of EBSD data acquisition

8. Stress Measurement and Crystal size

- Residual Stress
- Elasticity
- Biaxial and Triaxial Stress

9. Small Angle Scattering and reflectometry

Grading Policy

Students will be evaluated using three mechanisms:

a- Lab reports, Projects and HMW
b- Weekly Quizzes
c- Final or a Final Project

There are two options that is offered to students based on the basis of the desire in concentrating on laboratory experiments or a final project (theoretical or experimental):

Option 1:

a. Lab reports 40%
b. Weekly quizzes (and attendance): 30%
c. Final exam 30%

Option 2:

a. Final project (no labs) 40%

b. Weekly quizzes (and attendance): 30%
c. Final exam 30%

Students need to decide on the option (1 or 2) of their choice within the first two weeks of the classes.

The final letter grades are determined based on:

A: 90-100
B: 80-89
C: 70-79
D: 60-69
F: 59 and below

Main Reference:

- Cullity, B. D. S. Stock (2001). Elements of X-ray Diffraction, Addison-Wesley, Reading, Mass.
- Young, R. J. (1995). Use of Reciprocal Lattice Concepts in Power Diffraction Analysis, Georgia Institute of Technology.

Other references:

- Azaroff, Leonid V. (1968) , Elements of x-ray crystallography, , ISBN 1-878907-11-5.
- TechBooks, Kelly, A. (2000)Crystallography and Crystal Defects, , G. W. Groves and P.Kidd, Wiley
- Bunge, H. (1982). Texture Analysis in Materials Science. London, Butterworths. (located in the reference section)
- Gottstein, G. and L. S. Shvindlerman (1999). Grain Boundary Migration in Metals, CRC Press, Boca Raton, FL, ISBN 0-8493-8222-X.
- Jaffe, Howard W. (1988), Crystal Chemistry and Refractivity, Dover Publications, INC.
- Howe, J.M. (2000). Interfaces in Materials, Wiley Interscience, New York, NY, ISBN 0-471-13830-4.
- Kocks, U. F., C. Tomé, and H.-R. Wenk, Eds. (1998). Texture and Anisotropy, Cambridge University Press, Cambridge, UK.
- Nye, J. F. (1957). Physical Properties of Crystals. Oxford, Clarendon Press.
- Ohser, J. and F. Mücklich (2000), Statistical Analysis of Microstructures in Materials Science., Chichester, England: Wiley, 381pp, ISBN 0-471-97486-2.
- Randle, V. and O. Engler (2000). Texture Analysis: Macrotexture, Microtexture & Orientation Mapping, Gordon & Breach, Amsterdam, Holland, ISBN 90-5699-224-4.
- Reid, C. N. (1973). Deformation Geometry for Materials Scientists. Oxford, UK, Pergamon.
- Sutton, A. P. and R. W. Balluffi (1995). Interfaces in Crystalline Materials. Clarendon Press, Oxford, UK.
- Underwood, E. E., Quantitative Stereology, (1970), Addison Wesley Longman, ISBN: 0201076500.

Web Sites: http://www.matter.org.uk/diffraction/geometry/default.htm
http://www.uni-wuerzburg.de/mineralogie/crystal/teaching/teaching.html