

Scattering Theory MSE 6404

Professor: Hamid Garmestani

Class time: 9:30 am – 10:20 am, MWF

Office: Room 361, Love Building

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Office Hours: M, W at 8:30-9:20 a.m. and any other time by prior appointment. Office hours will be arranged through bluejeans. Lectures will be prepared every M, W and F and will be uploaded to Canvas in the early afternoons.

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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

Expectations:

- 1- Attendance in lectures: Lectures will be delivered online (synchronous) through blueJean.
- 2- Online canvas quizzes (during class time and ...) and exams using proctoring tools like lockdown browser.
- 3- Lab reports: Labs are performed through Virtual tools (with optional labs attendance.)

Virtual Labs and Online classes:

Students will attend all classes online and perform virtual labs. Students can also choose to attend a portion of the labs in groups of 3 or less.

The schedule for these labs are:

Lab#1	Phase analysis	September 7th
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Lab#2	Stress and strain:	September 21
Lab#3	Texture (Pole figure) analysis	September 28th
Lab#4	SAXD or EBSD	October 5th

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.

Textbook: There is no text book 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
- 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, Lorentz, 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:

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

Grade Distribution:

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|---|-----|
| a. Lab reports (1) or the final project (2) | 40% |
| b. Weekly quizzes (and attendance): | 30% |
| c. Final exam | 30% |

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 Powder 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: Macrotecture, 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>

Timing Policy

- The Modules follow a logical sequence
- Assignments are announced but not collected but may/will be included in the daily or weekly quizzes
- Quizzes must be completed during the time allotted and all lectures and quizzes should be completed by the end of the Sunday prior to the following week.
- You will have access to the course content for the scheduled duration of the course.

Attendance Policy

- This is a **live** fully online course.
- Log in on a regular basis to complete your work, so that you do not have to spend a lot of time reviewing and refreshing yourself regarding the content.

Plagiarism Policy

- *Plagiarism is considered a serious offense. You are not allowed to copy and paste or submit materials created or published by others, as if you created the materials. All materials submitted and posted must be your own.*

TOOLS Needed:

We will be using tools such as Respondus Lockdown browser or the Proctortrack for the exams. So, please make sure that you are prepared:

- 1- Have a computer with a webcam. The webcam should have a large field of view for the exams.
- 2- Installed the proper tools on your computer
- 3- Contact OIT if you have any issues
- 4- Make sure that you have a reliable internet connection

Student Honor Code

All learners are expected and required to abide by the letter and the spirit of the Georgia Tech honor code.

- Review the Georgia Tech Student Honor Code www.honor.gatech.edu.
- You are responsible for completing your own work.
- Action will be taken against any learners found in violation of the Georgia Tech Honor Code.

Office of Disability Services

If needed, we will make accommodations for students with documented disabilities. These accommodations must be arranged in advance and in accordance with the Office of Disability Services (<http://disabilityservices.gatech.edu>).

Communication

- All learners should ask questions, and answer their fellow learners' questions, on the course discussion forums. Often, discussions with fellow learners are the sources of key pieces of learning.

Netiquette

- Netiquette refers to etiquette that is used when communicating on the Internet. Review the [Core Rules of Netiquette](#). When you are communicating via email, discussion forums or synchronously (real-time), please use correct spelling, punctuation and grammar consistent with the academic environment and scholarship¹.
- Learners who do not adhere to this guideline may be removed from the course.

1. Conner, P. (2006-2014). Ground Rules for Online Discussions, Retrieved 4/21/2014 from <http://teaching.colostate.edu/tips/tip.cfm?tipid=128>

Course Materials/Textbook

- All content and course materials can be accessed on Canvas.

Technology/Software Requirements

- Internet connection (DSL, LAN, or cable connection desirable)
- Adobe Acrobat PDF reader (free download; see <https://get.adobe.com/reader/>)