Fall 2021: MTSE 451 X-Ray Diffraction

Syllabus for MTSE 451

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Office hours (Tyson) are on Tuesdays from 1:00 PM to 2:00 pm. Other times by appointment
Class Web Page: https://web.njit.edu/~tyson/mtse451.html
Class Location/Time: Tiernan 408/Tuesdays 6 PM to 10 PM.

Summary
Course combines lecture and laboratory work in introducing methods of X-ray diffraction. Simple sample synthesis will be conducted to initiate experiments. Topics include fundamentals of x-ray scattering, powder and single crystal diffraction techniques and data modeling methods. Local and national laboratory facilities will be utilized for experiments.

Pre-requisites (all with grade of C or better):
Prerequisites: PHYS 234; CHEM 126; MATH 112; CS 100, CS 101, CS 115 or BNFO 135

Materials for MTSE 451:

Background
--**(Abbreviation: Y&F): "University Physics", 15th Edition, authors Young & Freedman (Pearson 2019**).
(ISBN 10: 0-135-15955-5; ISBN 13: 978-0-1351 -5955-2). Any other version of the text OK.

Powder Diffraction Methods
-- X-Ray Diffraction (Dover Books on Physics) by B. E. Warren, Available on Amazon (in Library also)
---X-Ray Diffraction A Practical Approach by C. Suryanarayana and M. Grant Norton, Available on Amazon

Single Crystal Diffraction Methods
-- X-Ray Structure Determination: A Practical Guide by G. H. Stout and L. Jensen (Wiley, 1989), Available on Amazon (in Library also)
2nd Edition 2nd Edition, Available on Amazon
-- An Introduction to X-Ray Crystallography by M. Wolfson (Cambridge University, 1970), Available on Amazon

Extra Documents/Web Pages
Commission on Crystallographic Teaching
https://www.iucr.org/education/pamphlets

MIT OpenCourseWare
https://ocw.mit.edu/courses/chemistry/5-069-crystal-structure-analysis-spring-2010/
Acknowledgment: We acknowledge use of the the MIT Open Course Ware notes as part of this course

Learning Outcomes:

You should expect to spend a minimum of 4 hrs. in outside work for each hour spent in class each week.

- You can expect to be assessed on learning outcomes by means of a midterm exam, a final exam (Project), in-class quizzes and scores on homework assignments.
- The principal learning outcome is demonstrated understanding and mastery of x-ray diffraction from crystals as random powders or oriented single crystal samples. Along this path you will reinforce you understanding of basic atomic physics, diffraction, and interference phenomena and the corresponding mathematical methods needed to describe them.
- In any/all of the above subject areas, you should be able to:
    - Recall and use the conceptual and mathematical definitions and be able to explain them.
    - Explain the conceptual and mathematical relationships between quantities used.
    - Use symmetry arguments, sketches and diagrams, graphs, and basic calculus methods in interpreting material using reasoned arguments and also to interpret and set-up problems.
    - Explain and manipulate equations and techniques developed in the text, lectures, problem examples, and in the course of working problems.
    - Critically evaluate the soundness and precision of your answers, explain and interpret your solutions to problems in a way that shows understanding, and identify and appraise the range of applicability of your results, and their limitations.
    - You should be able to index powder diffraction patterns extract the lattice parameters.
    - You should be able to solve a crystal structure using a single crystal data set by reducing the data properly, finding the space groups and refining test solutions.

Final Letter Grades will be based on a **term average** for the semester's work that includes the midterm exam score, the final exam, in-class quizzes, and the term's homework score. Here are the approximate weights to be used for calculating the term average score:

- **25%** for midterm exam
- **35 %** for the final exam (Project)
- **20 %** for homework (written)
- **20 %** for class quizzes (written weekly quizzes)

The term average values used as cutoffs for various letter grades will be in the approximate range of:

- **85 % for A, 80% for B+, 70% for B, 65 % for C+, 55% for C, and 50 % for D and < 50% for F**

Examinations: There will be one midterm Exam plus a Final Exam (Project). The schedule is:

- **Midterm Exam:** Tuesday, Nov. 9, 2021
- **Final Exam (Project):** Due Dec. 16th, 2021

Final Project (35% of Grade)

Based on the lectures and laboratory work conducted students will select a chemical (must research materials in library and discuss topic with instructor). Each student must have a different chemical compound to work with. The materials can be synthesized or purchased. (1) Powder diffraction data must be collected on the the materials and the pattern must be indexed to determine the unit cell. (2) Single crystals must be obtained for the material and a complete single crystal data set must be collected and the structure must be solved. A 10 page report including figures and methods used must be submitted at the end of the course.

Example Samples:

Aspirin
Ibuprofen
Sodium Acetate
Ammonium Acetate

Tartronic Acid
Potassium Oxylate

Quizzes

In-class quizzes covering preceding or current work will be given during lectures, and the grades will count toward your final course grade. There will be no make-up quizzes and normally no make-up exams.

Midterm Exam

Students who miss a common exam usually receive a score of zero for that exam. Students who expect to be absent from a common exam should discuss their situation with their instructor **PRIOR TO** their absence. In order to qualify for a (rare) "make-up" common exam a student needs to document the reason for not being able to take the test as scheduled. Under NJIT standard policy, the documentation should be presented to the instructor AND to the Dean of Students - (973) 596-3466, 2nd floor Campbell Entry. BOTH the instructor and the Dean of Students must concur in permitting a "make-up" common exam. Students who miss exams and do not contact and present documentation to their instructors within 7 days of the common exam will receive a score of zero for the exam.

Attendance will be taken at all classes and exams. More than 1 unexcused absences (in total) is excessive. If you have excusable absences contact your instructor or the Dean of Students.

Withdrawal: If you must withdraw from the course, do it officially through the Registrar before the last withdrawal date. If you simply stop attending and taking exams your instructor will have no option other than to assign a course grade of "F".

Honor Code Violations or Disruptive Behavior: NJIT has a zero-tolerance policy for cheating of any kind and for disruptive student behavior. Violations will be reported to the Dean of Students. The penalties range from a minimum of failure in the course plus disciplinary probation up to expulsion from NJIT. Avoid situations where your own behavior could be misinterpreted as dishonorable.

- **Students are required to agree to the NJIT Honor Code on each exam.**

Turn off all smart and cellular phones, wireless devices, computers, and messaging devices of all kinds during classes and exams. Please do not eat, drink, or create noise in class that interferes with the work of other students or instructors.

The Schedule. Do the homework problems: it is almost impossible to succeed in courses without working problems

- Read the assigned sections of the text before the lecture covering that material.
- Submit the weekly homework assignments
- **Students who do not submit homework are automatically lowering their average by ~20 %.**
- The in-class quiz solutions will be posted each week

Last Day to Drop/Add Class- September 8, 2021

Last Day to Withdraw- November 10, 2021

Thanksgiving Recess- November 25 to November 28, 2021

Last day of Classes- December 10 (Friday), 2021

Final Exam Period- December 15 to December 21

Week 1 (Sept. 6 to Sept. 12)
Chapter 15 Mechanical Waves (Transverse Waves), Young and Freeman
Chapter 32 Electromagnetic Waves, Young and Freeman
Chapter 35 Interference, Young and Freeman
Lab Work: Library workshop on use tools to finds research materials

Week 2 (Sept. 13 to Sept. 19)
Chapter 36 Diffraction, Young and Freeman
Chapters 40 and 41 Atomic Structure, Young and Freeman
Quiz1 on Week 1 Material
Lab Work: Physics Lab on Interference and Diffraction
Background on Preparation of YBCO sample

Week 3 (Sept. 20 to Sept. 26)
Math: Complex numbers, Series
Structure Factors and Fourier Synthesis (G. H. Stout and L. Jensen, Chapter 8)
Quiz2 on Week 2 Material
Lab Work: Background on Preparation of YBCO sample
In Lab power sample preparation Part 2

Week 4 (Sept. 27 to Oct. 3)
Scattering of X-Rays by Atoms (B. E. Warren, Chapter 1)
Quiz3 on Week 3 Material
Lab Work: YBCO Sample Preparation, Cycle 1

Week 5 (Oct. 4 to Oct. 10)
Crystal Axes and The Reciprocal Lattice (B. E. Warren, Chapter 2)
Quiz4 on Week 4 Material
Lab Work: YBCO Sample Preparation, Cycle 2

Week 6 (Oct. 11 to Oct. 17)
Diffraction by a Small Crystal (B. E. Warren, Chapter 3)
Quiz5 on Week 5 Material
Lab Work: YBCO Sample Preparation, Final Cycle

Week 7 (Oct. 18 to Oct. 24)
Integrated Intensity and Powder Diffraction (B. E. Warren, Chapters 4 and 5)
Quiz6 on Week 6 Material
Lab Work: Powder Diffraction Measurement at Rutgers

Week 8 (Oct. 25 to Oct. 31)
Integrated Intensity and Powder Diffraction (B. E. Warren, Chapters 4 and 5) Part 2
Quiz7 on Week 7 Material
Lab Work: Analysis of Powder Diffraction data

Week 9 (Nov. 1 to Nov. 7)
Diffraction of X-Rays (Single Crystals) (G. H. Stout and L. Jensen, Chapter 2)
Quiz8 on Week 8 Material
Lab Work: Selection of Single Crystal from Powder, Make crystal from polycrystalline sample

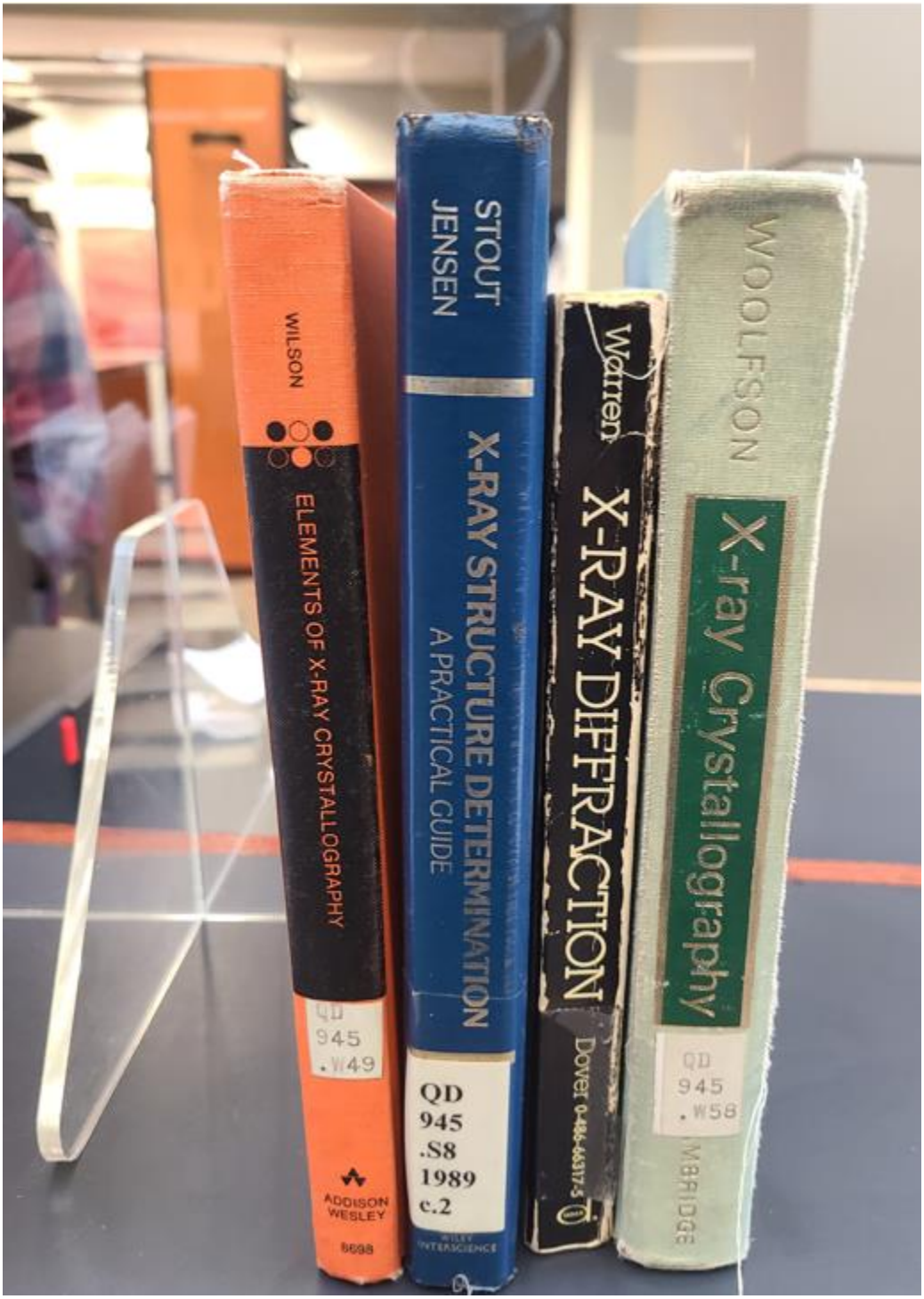
Week 10 (Nov. 8 to Nov. 14)
Crystal Symmetry and Space Groups (G. H. Stout and L. Jensen, Chapter 3)
Quiz9 on Week 9 Material
Lab Work: Symmetry Simulation-Reciprocal Space and XRD

Week 11 (Nov. 15 to Nov. 21)
Single Crystal Data Collection Pt. 1 (G. H. Stout and L. Jensen, Chapter 5)
Quiz10 on Week 10 Material
Lab Work: Measurement of Single Crystal grains from YBCO

Week 12 (Nov. 22 to Nov. 28)
Single Crystal Data Collection Pt. 2 (G. H. Stout and L. Jensen, Chapter 5)
Lab Work: Measure Student Powder samples

Week 13 (Nov. 29 to Dec. 5)
Single Crystal Data Reduction (G. H. Stout and L. Jensen, Chapter 6)
Lab Work: Measure Single Crystal samples

Week 14 (Dec. 6 to Dec. 10)
Single Crystal Structure Solution (G. H. Stout and L. Jensen, Part II (Solution Methods))
Lab Work: Measure Single Crystal samples



Books on reserve for MtSE 451 in NJIT Library