

Crystallography and Diffraction

Course Id:	CHEM 693 (3 cr.)	
Lecture:	TR 3:30 – 5:00 (Reichardt 165)	
Instructor:	Tom Trainor Rm 176 Reichardt 474-5628 tptrainor@alaska.edu	
Office Hours:	TR 1:00-3:00	
Grading:	Problem Sets	25%
	Midterm exam	25%
	Final Project	<u>50%</u>
		100%

Course web page: <http://gibbsite.cns.uaf.edu/AILwiki/Chem693-2009>

Course description and goals:

The goal of this course is to understand the structure of crystalline materials, and how to use X-ray scattering techniques to study materials structure and structural properties. Material structure topics will include crystal lattices, space-group symmetry, projections, the reciprocal lattice, and crystal chemistry. Methods for investigating the structure of materials and identification of phase will be covered in depth, including: fundamentals of X-ray scattering, diffraction from single crystals, powder diffraction, (quantitative) phase analysis, Rietveld refinements, texture analysis, and reflectivity. Students will be trained in the use of modern X-ray diffraction instrumentation and analysis software. Applications and examples will be taken from numerous disciplines including materials chemistry, mineralogy, petrology, and engineering materials, with an emphasis on methods of data collection and analysis.

Text

V.K. Pecharsky and P.Y. Zavalij, *Fundamentals of Powder Diffraction and Structural Characterization of Materials*.

Additional Sources:

- Warren B. E. (1969) *X-Ray Diffraction*. Addison-Wesley.
- IUCr *International Tables for X-Ray Crystallography, Vol A*, (2005) T Hahn, ed., Springer.
- James, R., W., (1965) *The Optical Principles of the Diffraction of X-Rays*. Cornell University Press, Ithaca.
- Als-Nielsen, J., McMorrow, D. (2001) *Elements of Modern X-ray Physics*. Wiley
- Sands, D. E. (1975) *Introduction to Crystallography*. Dover
- X-ray Data Booklet: <http://xdb.lbl.gov/>

Class Projects

Your class project will be focused on the solution of a “materials” problem using X-ray diffraction. The project should include background literature search, compilation of relevant crystallographic data, and the analysis of experimental data. The data sets may be provided by the instructor, or collected from specimens using the AIL X-ray diffraction laboratory. You will be required to submit a written report summarizing the results of the analysis (in manuscript format) and give a presentation to the class based on your topic. You will be requested to consult with the instructor early in the semester to decide on a project topic.

For performing literature searches and managing your citations I encourage the use of SciFinder Scholar, GeoRef, Endnote and other tools. If you are unfamiliar with these see: <http://www.uaf.edu/chem/Viewlets/ChemLabHowTo.html> and <http://uaflibrary.us/onlinedatabases/ui/>

Important Dates:

Sept 11 – Deadline for late registration

Sept 18 – Deadline for drop

Oct 30 - Deadline for withdrawal

Computer Lab:

Your enrollment in Chem 693 gives you user privileges in the department's computer lab.

Information and policies are available at:

<http://www.uaf.edu/chem/NewNetwork.html>

Student with Documented Disabilities:

Student with a physical or learning disability who may need academic accommodations, should contact the Disability Services office (203 WHIT, 474-7043). Disability Services will then notify the instructor of special arrangements for course work.

Ethical Considerations:

The Chemistry Department Policy on Cheating is: *“Any student caught cheating will be assigned a course grade of F. The student will not be allowed to drop the course.”*

The UAF Honor Code states: *“Student will not collaborate on any quizzes, in-class exams, or take-home exams that will contribute to their grade in a course, unless permission is granted by the instructor of the course. Only those materials permitted by the instructor may be used to assist in quizzes and examinations. Student will not represent the work of others as their own. A student will attribute the source of information not original with himself or herself (direct quotes or paraphrase) in compositions, these and other reports. No work submitted for one course may be submitted for credit in another course without the explicit approval of both instructors. Violations of the Honor Code will result in a failing grade for the assignment and, ordinarily, for the course in which the violation occurred. Moreover, violation of the Honor Code may result in suspension or expulsion”*

In this course students may collaborate on homework assignments, however, each individual should submit their own copy showing all their work. Exams and projects are to be completed independently.

I. Crystallography

- Crystal lattice and crystal structures
 - Definition of a unit cell, unit cell contents
 - Periodicity, lattice points and lattice vectors
 - Crystallographic planes, directions and indices
 - Reciprocal lattice
- Symmetry operations and symmetry elements
 - Finite symmetry elements (point groups)
 - Infinite symmetry elements (space groups)
- The International Tables, Volume A, Space Groups, and Structure Viewing Software

II. Diffraction

- Properties and sources of radiation
- Geometrical treatment of diffraction by lattices
 - Laue equations and Bragg's Law
 - Reciprocal lattice and Ewald sphere
 - Powder vs single xtal XRD
- Derivation of the structure factor
 - Scattering by electrons, atoms and lattices
 - Fourier analysis
 - Diffraction from imperfect crystals and powders (kinematic diffraction)
 - Phase problem
 - Patterson technique
 - Direct methods

III. Powder XRD

- Powder intensities and positions of diffraction peaks
 - Integrated intensities
 - Geometric factors
 - Absorption
 - Orientation
- Powder diffractometry
 - Sample preparation
 - Phase identification
 - Phase quantification
 - Unit cell refinement
 - Structure determination/refinement (Rietveld)

IV. Single crystal XRD and Materials Characterization

- Single crystal diffractometry (4-circle diffractometer)
 - Crystal orientation / alignment
- Texture analysis
- Stress analysis

V. Special Topics (possible)

- Interfaces
 - X-ray reflectivity
 - Grazing incidence diffraction
 - Truncation rods
- Anomalous scattering
- Micro-Diffraction
- Diffraction from perfect crystals,
- X-ray standing waves