

General Information

Instructor: Dr. Roberta L. Flemming: BGS 0172; Phone: 661-3143; rflemin@uwo.ca

Lecture/Lab: 3 hours once a week: Monday 9:30-12:30 in room BGS 1069

Aim of Course: Students will investigate the relationship between crystal structure and mineral behaviour by collecting and interpreting crystallographic data on their own synthetic or natural mineral specimens or rocks of research interest. Lectures will begin with fundamental crystallographic concepts and the theory and techniques of X-ray diffraction. Guest lectures will be given in spectroscopic techniques. Temperature-, pressure-, and composition-dependent changes in crystal structure are also examined. Additional topics may include cation ordering, solid solution, exsolution, and polymorphism, as determined by time and student interest.

Weekly assignments will enhance understanding of the above concepts. In the laboratory, minerals will be examined by X-ray diffraction techniques on powdered specimens and/or single crystals. The final submission for the course will be a manuscript-style report of the student's findings for their mineralogical project. This report will include a brief literature review, an explanation of experimental methods, a summary of results obtained, **including a correlation between the results obtained by XRD and existing data by other methods**. Other methods may include petrographic microscope, SEM, or various spectroscopic methods (e.g. NMR, IR, Raman, XPS, CL), depending on the mineralogical problem under investigation. The discussion will include the significance of these findings in the student's relevant field (e.g. Earth sciences, planetary science, materials science), and suggestions for further work. Students will share their results by presentation in a symposium-style session at the end of the course.

Course topics/themes - Tentative schedule

Week 1: Jan 9	No class
Week 2: Jan 16	Internal symmetry: Direct lattice, crystal systems, Bravais lattices, space groups (Lab 1)
Week 3: Jan 23	X-ray diffraction fundamental concepts: Reciprocal lattice; Miller indices (Lab 2)
Week 4: Jan 30	Powder diffraction: powder geometry, Bragg's Law vs. Laue, Ewald's sphere (Lab 3)
Week 5: Feb 6	Information from X-ray diffraction and Micro X-ray diffraction
Week 6: Feb 13	Unit cell transformations and matrix algebra, the Metric Tensor
Week 7: *****	Conference week February 20 – 24 *****
Week 8: Feb 27	Single Crystal XRD, Precession camera, Electron diffraction. Measuring this data (Lab 4)
Week 9: Mar 6	Rietveld Refinement of powder X-ray data: Structures & modal mineral analysis (Lab 5)
Week 10: Mar 13	Spectroscopy Lecture (TBA)
Week 11: Mar 20	Lab day (collect additional data for projects, write your report, prepare the presentation)
Week 12: Mar 27	Changes in mineral structure with temperature, pressure, composition. Solid solutions
Week 13: April 3	Presentations
Week 14: April 10	Presentations

Ethical Conduct: Scholastic offences are taken seriously and students are directed to read the policy, specifically, what constitutes the definition of a Scholastic Offence, at the following website:
<http://www.uwo.ca/univsec/handbook/appeals/scholoff.pdf>. Plagiarism is a serious academic offence.

Item	Evaluation
Final Exam: 3 hours TBA	30%
Lab assignments: (weekly to biweekly)	
1. Internal symmetry and space groups.	5%
2. Drawing a crystal structure from space group information.	5%
3. Powder diffraction: Data collection and unit cell refinement (CELREF).	5%
4. Unit cell transformations; metric tensor; indexing precession film; space group.	5%
5. Rietveld Refinement of crystal structures from powder diffraction data.	<u>5%</u>
Subtotal Lab assignments:	25%
X-ray Project:	
Experimental component: May include unit cell refinement (CELREF) and/or Rietveld refinement of powder diffraction data, additional micro X-ray diffraction data, additional methods (e.g. petrography), correlation to existing data (e.g. SEM, EPMA, CL).	15%
Manuscript:	20%
Presentation:	10%

Useful Texts (optional)

X-ray Diffraction:

- Azaroff and Buerger (1958) The Powder Method (Lab copy available)
- Azaroff, L.V. (1968) Elements of X-ray Crystallography, McGraw-Hill, NY (QD945.A96)
- Bloss, D.F. (1971, 1994) Crystallography and Crystal Chemistry, MSA, Washington. Ch 6, Ch 13. (Lab copy)
- Buerger, Martin J. (1964) The Precession Method in X-ray Crystallography, Wiley, NY. (QD945.B79)
- International Tables for Crystallography Vol A. Space Group Symmetry. D. Reidel Publishing Company (Taylor ref QD908.I56 1983). Abridged teaching version (QD908.I562 1985. Lab copy also available).
- Jenkins, R. and Snyder, R.L. (1996) Introduction to X-ray Powder Diffractometry, V 138, Winefordner, J.D. ed., Chemical Analysis: Monographs on Analytical Chemistry and its Applications, Wiley, NY.
- Ladd, M.F.C. and Palmer, R.A. (1993) Structure Determination by X-ray Crystallography 3rd Ed. Plenum Press NY. (QD945.L32 1993)
- Pecharsky, V.K. & Zavalij, P.Y. (2005) Fundamentals of Powder Diffraction and Structural Characterization of Materials, Springer, USA. (Available in Taylor Library on-line (2005 and 2009) or QC482.D5P43 2003).
- Rohrer, G.S. (2001) Structure and Bonding in Crystalline Materials, Cambridge (Ch 5). (QD921.R614 2001)
- Young, R.A. (1993) The Rietveld Method, IUCr Monographs on Crystallography 5. (QD945.R53 1993)

Mineralogy:

- Deer, W.A., Howie, R.A. and Zussman, J. (1992) An introduction to the Rock Forming Minerals, 2nd Ed. Addison Welsley Longman Ltd., England. (QE363.D39 1992)
- Hazen, R.M. and Finger, L.W. (1982) Comparative Crystal Chemistry: Temperature, pressure, composition, and the variation of crystal structure. Wiley, Toronto, 231 p. (QD921.H435)
- Putnis, A. (1992) Introduction to Mineral Sciences. Cambridge University Press, Cambridge, UK.

Additional information:

Accessibility:

Please contact the course instructor if you require lecture or printed material in an alternate format or if any other arrangements can make this course more accessible to you. You may also wish to contact Services for Students with Disabilities (SSD) at 661-2111 ext. 82147 if you have questions regarding accommodation.

Support Services:

Learning-skills counsellors at the Student Development Centre (<http://www.sdc.uwo.ca>) are ready to help you improve your learning skills. They offer presentations on strategies for improving time management, multiple-choice exam preparation/writing, textbook reading, and more. Individual support is offered throughout the Fall/Winter terms in the drop-in Learning Help Centre, and year-round through individual counselling.

Students who are in emotional/mental distress should refer to Western's Health and Wellness website (http://www.health.uwo.ca/mental_health) for a complete list of options about how to obtain help.

Additional student-run support services are offered by the USC, <http://westernusc.ca/services>.

The website for Registrarial Services is <http://www.registrar.uwo.ca>.

Course Website:

Students should check OWL (<http://owl.uwo.ca>) on a regular basis for news and updates. This is the primary method by which information will be disseminated to all students in the class. Students are responsible for checking OWL on a regular basis.

More on plagiarism detection:

All required papers may be subject to submission for textual similarity review to the commercial plagiarism detection software under license to the University for the detection of plagiarism. All papers submitted for such checking will be included as source documents in the reference database for the purpose of detecting plagiarism of papers subsequently submitted to the system. Use of the service is subject to the licensing agreement, currently between University of Western Ontario and Turnitin.com (<http://www.turnitin.com>).

Exams: Non-programmable calculators are allowed during the final exam. Cell phones are not allowed.

It is Faculty of Science policy that a student who chooses to write a test or exam deems themselves fit enough to do so, and the student must accept the mark obtained. Claims of medical, physical, or emotional distress after the fact will not be considered.