Geology 9516B: Advanced Mineralogy and Crystallography Winter 2025

General Information

Instructor: Dr. Roberta L. Flemming: BGS 0172; Phone: 519-661-3143; rflemmin@uwo.ca

Lecture/Lab: 3 hours once a week - Thursdays @ 1:30 pm – 4:30 pm

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 or diffraction techniques. Temperature-, pressure-, and composition-dependent changes in crystal structure are also examined. Additional topics may include cation ordering, solid solution, exsolution, or 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), computer modelling, or machine learning, 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	Introductions – Survey
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
Week 5: Feb 6	Information from X-ray diffraction and Micro X-ray diffraction (Lab 3)
Week 6: Feb 13	Unit cell transformations and matrix algebra, the Metric Tensor
Week 7: **********	Reading week - February 17 - 21 **********
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	Independent work on your project (Flemming & some students will go to LPSC in Texas)
Week 11: Mar 20	Guest Lecture (TBA) (covering a spectroscopic or diffraction technique)
Week 11: Mar 27	Changes in mineral structure with temperature, pressure, composition (solid solution)
Week 12: Apr 3	Presentations
Week 13: Apr 10	Exam period - Final Exam to be scheduled sometime over this period (TBA)

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. Assignments and X-ray project may be submitted to Turnitin, to check against plagiarism.

Artificial Intelligence Statement: Students may not use generative AI (e.g. ChatGPT) to write any written component of your labs/reports for this course. You may use machine learning for data analysis if applicable.

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 (e.g. CELREF). 5%
4. Unit cell transformations; metric tensor; indexing precession film; space group. 5%
5. Rietveld Refinement of crystal structures from powder diffraction data. 5%

Subtotal Lab assignments: **25%**

X-ray Project:

Experimental component: Will include X-ray diffraction (powder or micro-XRD data), and may include unit cell refinement, Rietveld refinement of powder diffraction data, additional methods (e.g. optical, modeling, machine learning), correlation to existing data (e.g. EPMA, XRF, Raman). 15%

Manuscript: 15%

Presentation: 10%

Subtotal X-ray Project: **40%**

Participation: **5%**

Useful Texts (optional) – Excerpted portions used by Flemming in lectures

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., Palmer, R.A. (1993) Structure Determination by X-ray Crystallog. 3rd Ed. Plenum Press NY.
- 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. Wiley, Toronto, 231 p. (QD921.H435)
- Putnis, A. (1992) Introduction to Mineral Sciences. Cambridge University Press, Cambridge, UK.