GEOLOGY 9516B: Advanced Mineralogy and Crystallography Winter 2014

General Information

Instructor: Dr. Roberta Flemming: B&G 0172; Phone: 661-3143; rflemmin@uwo.ca

Lecture/Lab: 3 hours once a week: Wed 9:30-12:30 in B&GS room 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 08	No class
Week 2: Jan 15	Internal symmetry: Direct lattice, crystal systems, Bravais lattices, space groups (Lab 1)
Week 3: Jan 22	X-ray diffraction fundamental concepts: Reciprocal lattice, Ewald's sphere (Lab 2)
Week 4: Jan 29	Powder diffraction: Bragg's Law, powder geometry (Lab 3)
Week 5: Feb 5	Microdiffraction. In situ measurement, texture, crystallinity, strain
Week 6: Feb 12	Unit cell transformations and matrix algebra, the Metric Tensor (Lab 4 or 5)
Week 7: **********	Conference week February 17 – 21 **********
Week 8: Feb 25	Laue equations: Single Crystal XRD, Precession camera, Electron diffraction (Lab 4 or 5)
Week 9: Mar 5	IR and Raman spectroscopy (Guest lecturer Dr. Sean Shieh)
Week 10: Mar 12	Changes in mineral structure with temperature, pressure and composition
Week 11: Mar 19	Lab day (collect additional data for projects, continue with lab assignments)
Week 12: Mar 26	Solid solutions: Examining their stability
Week 13: April 2	Presentations
WeeK 14: April 9	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 (and VOLCAL?). 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. 5%

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 (QD921.H435)
- Putnis, A. (1992) Introduction to Mineral Sciences. Cambridge University Press, Cambridge, UK.