Submit original with signatures + 1 copy + electronic copy to UAF Governance.

See <a href="http://www.uaf.edu/uafgov/faculty/cd">http://www.uaf.edu/uafgov/faculty/cd</a> for a complete description of the rules governing curriculum & course changes.

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		TRI	AL CO	URS.	E OR	NEW (	COUF	RSE P	ROP	OSAL							
BMITTED BY:																	
Department						College/School				CNSM							
Prepared	Tom Trainor				Phone												
by	Tom Traine	om Tramor								5628							
Email Contact	tptrainor@alaska.edu					Faculty Contact				Tom Trainor							
								Contact									
1. ACTION D	CHECK ON	E):	T	rial	l Cour	se				New	Cour	se	X				
2. COURSE I	DENTIFICATIO	N:	Dep	t	СН	EM	С	ourse #		618		No. Cred			3		
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3. PROPOSED COURSE TITLE:			Crystallography and Diffraction														
4. CROSS LISTED? YES/NO			No If yes, Course # Dept:														
	approval of bores.)	oth d	lepartm	nents	and d			lved.	Add	i line	s at	end o	of for	m for	such		
5. STACKED? YES/NO			No If yes, Course # Dept.														
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OTHER FORM (specify)	AT																
Mode of de (specify l field trip etc)	ecture,	Lecture and laboratory based course (3cr). Laboratory assignments will involve the use of XRD instrumentation, and data modeling / analysis using a variety of crystallography software packages.															
9. CONTACT	HOURS PER WE	EK:		2	177	TURE	eks	3	LA	B urs /v	veek		100	ACTIC	CUM week		
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OTHER HOURS			t Suit	1.50	FLAN								Re	ce	ive		

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FEB 17 2010

Dean's Office College of Natural Science & Mathematics 618

10. COMPLETE CATALOG DESCRIPTION including dept., number, title and credits (50 words or less, if possible):

#### CHEM 693 Crystallography and Diffraction 3 Credits Offered Fall Odd-numbered Years

The structure of solid-state materials and the analysis of materials using X-ray scattering techniques. 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. Special fees apply. *Prerequisite: Graduate standing or permission of the instructor.* (2+3)

11.	COURSE CLASSIFICATIONS: (undergraduate courses only. Use approved criteria found on Page 10 & 17 of the manual. If justification is needed, attach on separate sheet.)  H = Humanities  N = Natural X S = Social Sciences  Will this course be used to fulfill a requirement for the baccalaureate core?  IF YES, check which core requirements it could be used to fulfill:					
12.	O = Oral Intensive, Format 6 W = Writing Intensive, Format 7 Natural Science, Format 8 COURSE REPEATABILITY:					
	Is this course repeatable for credit?  Justification: Indicate why the course can be repeated (for example, the course follows a different theme each time).					
	How many times may the course be repeated for credit?  If the course can be repeated with variable credit, what is the maximum number of credit hours that may be earned for this course?  CREDITS					
13.	GRADING SYSTEM:  LETTER: X PASS/FAIL:					
REST	TRICTIONS ON ENROLLMENT (if any)					
400						
14.	PREREQUISITES Graduate standing or permission of the instructor					
14.	PREREQUISITES Graduate standing or permission of the instructor  These will be required before the student is allowed to enroll in the course.					
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1 C: 15.	These will be required before the student is allowed to enroll in the course.  RECOMMENDED					
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15. CON 16. Has	These will be required before the student is allowed to enroll in the course.  RECOMMENDED  lasses, etc. that student is strongly encouraged to complete prior to this course.  SPECIAL RESTRICTIONS, NDITIONS  PROPOSED COURSE FEES \$70  s a memo been submitted through your dean to the Provost & VCAS for YES approval? Yes/No					
15. CON 16. Has	These will be required before the student is allowed to enroll in the course.  RECOMMENDED  lasses, etc. that student is strongly encouraged to complete prior to this course.  SPECIAL RESTRICTIONS, NDITIONS  PROPOSED COURSE FEES \$70  s a memo been submitted through your dean to the Provost & VCAS for YES					

#### 18. ESTIMATED IMPACT

WHAT IMPACT, IF ANY, WILL THIS HAVE ON BUDGET, FACILITIES/SPACE, FACULTY, ETC.

None. The course has been worked into the Department of Chemistry and Biochemistry 3 year teaching plan (it was recently offered as special topics). Facilities for the course already exist (XRD equipment was purchased on a NSF-MRI grant).

#### 19. LIBRARY COLLECTIONS

Have you contacted the library collection development officer (ffklj@uaf.edu, 474-6695) with regard to the adequacy of library/media collections, equipment, and services available for the proposed course? If so, give date of contact and resolution. If not, explain why not.

No

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Yes

No special materials needed

#### 20. IMPACTS ON PROGRAMS/DEPTS

What programs/departments will be affected by this proposed action? Include information on the Programs/Departments contacted (e.g., email, memo)

This course will be covered by the Department of Chemistry and Biochemistry. Based on the enrollment in the trial course (Fall 2009), we suspect students from Chemistry, Environmental Chemistry, Biochemistry and Molecular Biology, Geology, Geophysics, Physics, Soils Sciences, and Engineering will all be served by this course. T. Trainor has been in contact with numerous faculty on campus regarding the trial course, and training in the use of the UAF XRD laboratory, and has found a high level of interest.

#### 21. POSITIVE AND NEGATIVE IMPACTS

Please specify positive and negative impacts on other courses, programs and departments resulting from the proposed action.

There are negative impact associated with this course. Positive impacts include offering an advanced course in a topic area that is currently not covered at UAF. The material is highly relevant to Natural/Physical Sciences and Engineering Students and will better prepare our students for future careers. This course will also train individuals and promote use of the UAF XRD laboratory.

#### JUSTIFICATION FOR ACTION REQUESTED

The purpose of the department and campus-wide curriculum committees is to scrutinize course change and new course applications to make sure that the quality of UAF education is not lowered as a result of the proposed change. Please address this in your response. This section needs to be self-explanatory. Use as much space as needed to fully justify the proposed course.

Currently there is no course at UAF covering this material. There is however a demand for a crystallography/diffraction course (which are traditionally taught in Chemistry and/or Geology departments) to meet the needs of current graduate students and faculty. In particular, we have recently acquired and installed a new diffraction system as part of the suite of materials analysis equipment housed within the UAF Advanced Instrumentation Laboratory (AIL). As with many of the more complicated instruments within AIL, use is limited unless there is specific and dedicated user training. Since graduate students are typically the dominant users of the instrumentation, the best method / most efficient methods of training is through the offer of a graduate course. The proposed course will provide students with the required background for successful application of diffraction in their research and train them in modern topics and methods of materials analysis needed for future careers.

APPROVALS:						
John ey coll	Date 2-15-10					
Signature, Chair, Program/Department of:						
	Date 2/23/10					
Signature, Chair, College/School Curriculu Council for:	N8M					
Janly Large	Date 2/23/10					
Signature, Dean, College/School of:						
	Date					
Signature of Provost (if applicable) Offerings above the level of approved programs must be approved in advance by the Provost.						
ALL SIGNATURES MUST BE OBTAINED PRIOR TO SUBMISSION	TO THE GOVERNANCE OFFICE					
	Date					
Signature, Chair, UAF Faculty Senate Curriculum Review Committee						
ADDITIONAL SIGNATURES: (If required)						
	Date					
Signature, Chair, Program/Department of:						
	Date					
Signature, Chair, College/School Curriculu Council for:						
	Date					
Signature, Dean, College/School of:						

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# **Crystallography and Diffraction**

CHEM 18 (3 cr.) Course Id:

Graduate Standing or permission of instructor **Prerequisites:** 

Lecture/Lab:

Instructor: Tom Trainor

Rm 176 Reichardt

474-5628

tptrainor@alaska.edu

Office Hours: TBA

Problem Sets/Labs 35% Grading:

Midterm exam 20% Final Exam 20% Final Project 25%

100%

Course web page: TBA

### Course description and goals:

The goal of this course is to understand the structure of crystalline materials, and how to use Xray 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/

#### **Instructional Methods:**

#### Lecture

Two lecture periods per week will be used to deliver the core materials. Focus will be on theory and background required for understanding the structure of crystalline materials, the use of x-ray diffraction instrumentation and interpretation of data. Lecture topics will be complimented by problem sets and tested via written exam.

### <u>Laboratory</u>

Students will be given hands on training in the use of XRD instrumentation and analysis software. Assignments will build upon lecture topics using practical examples. Students will be expected to complete laboratory assignments working in groups.

#### 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: <a href="http://www.uaf.edu/chem/Viewlets/ChemLabHowTo.html">http://www.uaf.edu/chem/Viewlets/ChemLabHowTo.html</a> and <a href="http://uaflibrary.us/onlinedatabases/ui/">http://uaflibrary.us/onlinedatabases/ui/</a>

### **Important Dates:**

Sept XX – Deadline for late registration Sept XX – Deadline for drop Oct XX - Deadline for withdrawal

#### Computer Lab:

Your enrollment in Chem 618 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.

### **Topics**

### I. Crystallography

- Crystal lattice and crystal structures
  - o Definition of a unit cell, unit cell contents
  - o Periodicity, lattice points and lattice vectors
  - o Crystallographic planes, directions and indices
  - o Reciprocal lattice
- Symmetry operations and symmetry elements
  - o Finite symmetry elements (point groups)
  - o 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
  - o Laue equations and Bragg's Law
  - o Reciprocal lattice and Ewald sphere
  - o Powder vs single xtal XRD
- Derivation of the structure factor
  - o Scattering by electrons, atoms and lattices
  - o Fourier analysis
  - o Diffraction from imperfect crystals and powders (kinematic diffraction)
  - o Phase problem
    - Patterson technique
    - Direct methods

#### III. Powder XRD

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

### IV. Single crystal XRD and Materials Characterization

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

# V. Special Topics (possible)

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



Department of Chemistry and Biochemistry 900 Yukon Drive 194 Reichardt Building PO Box 756160 Fairbanks, AK 99775-6160 (907) 474-5510 Fax (907) 474-5640

February 12, 2010

To:

Through:

Paul Layer, Interim Dean, CNSM
John Keller Chair

From:

Tom Trainor. Professor

Re:

Lab Fee for Proposed Course Chem 618, Crystallography and Diffraction

Chem 618 is a 2-credit lecture + 1-credit lab course that is being submitted for curriculum council approval this spring, and which will be offered with the 618 moniker in the fall 2011 semester. The course will be taught by Tom Trainor who taught a similar course in the fall 2009 semester as a 3-credit special topics lecture course. Last fall the assignments in the course involved mostly hands-on use of the new diffraction instrument installed in 2009 in the Advanced Instrumentation Laboratory in the Reichardt Building. Tom found that there were significant expenses for consumables, and therefore it would be appropriate to assign laboratory credit for the course, and charge a lab fee.

We propose a fee of \$70 which is consistent with the recently approved lab fee schedule for various chemistry laboratory courses. We anticipate that the revenue generated from this fee would cover most of the incidental expenses for the course. approved: (and fay