CEM 913 Spring 2002

FUNDAMENTALS OF X-RAY CRYSTALLOGRAPHY

Instructor: Mercouri G. Kanatzidis

Syllabus

TEXTBOOKS: (1) Structure Determination by X-ray Crystallography, by Ladd and Palmer

(2) X-ray Structure Determination, by Stout and Jensen

These books should be purchased. They will continue to serve as useful references long after this class.

CLASS HOURS: Tu, Th 2:40 pm, Room 218 B

Assignments: Problem sets (~8-10)

Exams: There will be three exams
Exam 1 February 12 (in class)
Exam 2 March 14 (in class)
Exam 3: Final exam, May 2

Grading: Homework 20%, Exam 1 and 2:20% each, Final Exam 40%. Total: 100%.
Grade: A >85%; B>70%; C>55%; D<55%.

Web site; a website has been set up for this course. I will place course related information there such as useful crystallographic links to the internet, homework assignments, etc. http://www.cem.msu.edu/~kanatzid/CEM913Xtl.html

Course Contents

Crystal Geometry
The crystalline state
Symmetry
Miller indices
2- and 3-dimensional Point Groups
Lattices
Space Groups
Reciprocal Lattice
X-rays: origin, properties, safety
X-ray diffraction and Bragg's Law
Ewald sphere
X-ray diffraction techniques
Single Crystal techniques (Laue, Oscillation, Weissenberg and Precession Methods)

Fourier transforms (real vs reciprocal space)
Scattering of X-rays by crystals
The atomic structure factor
The structure factor (x-ray diffraction, electron diffraction, neutron diffraction)
Friedel's law
Systematic absences
Practical determination of space groups

Data reduction
Lorenz-polarization
Interpretation of intensity data
Theory of structure factors and Fourier Synthesis
The phase problem

Structure Determination
Techniques
Patterson Method
Direct Methods (intensity statistics)
Search methods
Structure refinement
Estimated standard deviations and the R value
Derived Results

Powder Diffraction
The Debye Scherrer method
Structure solution from powder data, PDF analysis, Rietveld method

The final exam will be based on oral presentations. Each student will be assigned a crystallographic topic for development and presentation to the class audience. A short paper (5-pages) on the assigned subject will be due.

Here the students will become the teachers. This is a chance for the class to expand upon a topic that I mentioned or covered only superficially in class.

Examples of Topics

1. Incommensurate Crystal Structures
2. Structures from powders by Synchrotron Radiation
3. Structures from powders by Neutron Radiation
4. Direct Methods structure solution in SHELXS
5. PDF Analysis
5. Twinning and the solution of twinned crystal structures
6. The use of Search methods in structure solution (examples)