Materials 209BL: X-ray Diffraction I. Principles and Practice

Catalog Description:

The main objective of the course is to expose students to practical aspects of powder and single crystal X-ray diffraction, including the determination and refinement of crystal structures.

Teaching frequency:

Every alternate year in Spring.

Target audience:

The course should be suitable for students with little or some prior exposure to crystals and crystallography.

Goal:

Practical knowledge on how to carry out diffraction studies.

Textbooks:

C. Giacovazzo (Eds.), Fundamentals of Crystallography, Oxford University Press, 2nd Book and CD-ROM edition 2002, (ISBN 0198509588)

George H. Stout and Lyle H. Jensen, X-ray Structure Determination, a Practical Guide, 2nd Edn (ISBN 0-471-60711-8)

Other references:

The International Tables of X-ray Crystallography, Vol. I

Instructor:

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Course Website:

`http://www.mrl.ucsb.edu/~seshadri/teach.html`

Outline:

1. Classroom:

   (a) Crystal systems, Bravais lattices and Miller indices
   (b) Point groups, space groups and systematic absences
   (c) Optical diffraction and the Laue and Bragg experiments
   (d) The Ewald construction
   (e) Structure factor, integrated intensities and the phase problem
   (f) Patterson techniques and direct methods
   (g) Projecting 3D to 1D — powder diffraction
   (h) Structure refinement, least-squares, Debye-Waller factors
   (i) Rietveld analysis
   (j) Miscellaneous topics

2. Lab:

   (a) Recording powder diffraction
   (b) Correcting for systematic shifts, obtaining lattice parameters
   (c) Végard's law and alloys
   (d) Extraction of 1D intensities in layered materials and obtaining the Fourier transform
   (e) Particle size in a anisotropic material
   (f) A single crystal experiment on the CCD
   (g) Rietveld refinement of a powder pattern
   (h) Stacking faults and DIFFaX
   (i) Thin film diffraction – pole figures and rocking curves
   (j) Thermodiffractometry