

Rietveld Structure Refinement

Theory and hands-on short course

Course objective:

The course objective is to give a crystallographic and mathematical background of Rietveld method and hands-on knowledge of modern Rietveld software packages for academia, government and industry professionals.

Course description:

The course will consist of two components, the theory of Rietveld analysis and the practical application and use of software packages for Rietveld analysis. All participants will be supplied with notebook computers with installed necessary software, database, and x-ray diffraction data files of samples of various origins for structure refinement and tools for learning. The course consists of series of lectures and exercises followed by practical sessions on PCs. Teaching of tools, their usage, sharpening of skills along with required theoretical knowledge altogether is objective of this course.

Theory:

Crystal symmetry, unit cell, space groups, atom positions, thermal parameters and scattering lengths, cell transformations

Powder diffraction, Miller indexes, diffracted intensities, data reduction and formatting,

Description of profile models used for various x-ray laboratory, synchrotron sources, neutron optical configurations

Overview of parameters required in the refinement, including background, polarization, lattice constants, preferred orientation, profile and profile-shape functions, peak asymmetry, line broadening, etc.

Corrections- Lorenz, polarization, absorption, microabsorption, extinction etc.

Mathematical approach used in the refinement, use of constraints and restraints

Practical:

Overview of data collection strategies: sample preparation, beam overflow correction-long samples, capillary sample holders

Data file reading, phase identification manual and automatic Search-Match, presence of amorphous components

Working through a complete refinement of a small inorganic structures

Pitfalls in Rietveld analysis by demonstration – false minima, correlation of parameters, etc.

Checking the results

The course is intended for people familiar with powder diffraction and who want to learn how to analyze more complicated structures by this method. There are no special requirements for this course but one should understand the basic principles of powder diffraction.

After the lectures, all participants will have the opportunity to practice on PCs. Examples at different levels of complexity will be provided. Your own data sets are also welcome.

Course fee:

Academic and Government: \$1860, Industry: \$3000, which includes all course notes and CD breakfast and lunch on days 1-4 and course dinner on day 3, use of computers but excludes last day dinner, travel and accommodation.

Deadline:

Places may be reserved by submission of the application form and payment of the course fee by January 20, 2005.