

Quantitative Phase Analysis by Rietveld Method Theory and hands-on short course (February 22-25, 2005)

Course objective:

The course objective is to give a crystallographic and mathematical background of standardless Rietveld method and hands-on knowledge of modern Rietveld quantification 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 quantitative 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 quantification and tools for learning. The course consists of series of lectures and exercises followed by practical sessions on PCs. Vendors' representatives will present modern phase quantification software.

Theory:

Pre-Rietveld

- Unit cell, crystal symmetry, space groups, Bravais lattices, atom positions, thermal parameters and cell transformations
- Powder diffraction, Miller indexes, diffracted intensities, atomic scattering factors, anomalous dispersion
- Data collection and reduction and formatting, aberrations on Bragg-Brentano data, preferred orientation, absorption contrast, extinction corrections, particle statistics

Rietveld

- Rietveld intensity equation. Integrated intensities vs. peak shape function. Profile models used for various x-ray laboratory, synchrotron sources, neutron optical configurations
- Overview of parameters required in the refinement: phase scales, instrumental zero, cell dimensions, halfwidths parameters, preferred orientation, lineshape functions, structural parameters, peak asymmetry, split peak shape functions, line broadening and crystal size
- Corrections - Lorenz, polarization, absorption, microabsorption, extinction
- Phase quantification of amorphous materials and in absence of structural data
- Hints on refinement strategy: what to refine first, early, or later. Diagnostic features of the difference curve

Practical:

- Calculations with hand-held calculator: 1-anomalous dispersion correction, 2-powder pattern of MgO, peak positions, indexing, structure factors, and peak intensities. 3- absorption contrast correction
- Data file reading, manual and automatic phase identification, Search-Match software, presence of amorphous components
- Working through a complete quantification of specific problems, such as soil, geological, pharmaceutical, industrial samples
- Real time demonstration of SIROQUANT™, TOPAS™, RIQAS™ software packages (under guidance of software vendors)

Course fee: Academic and Government: \$2000, 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.

Course duration: 4 days (two days theory with exercises and two days practical work)

Deadline: Places may be reserved by submission of the application form and payment of the course fee by February 3, 2005.