Rietveld Structure Refinement

Theory and hands-on short course

Program

Day 1

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 ***Introductory crystallography:*** unit cell, symmetry elements of macro- and microcrystallography, crystal structures, seven crystal systems, 14 Bravais lattices, space groups, Miller indices

10:30 – 11:50 Coffee Break

11:50 – 13:00 ***X-ray diffraction:*** X-ray sources, choice of radiation, wavelength, resolution, atomic scattering factors, diffracted intensities, thermal parameters, anomalous dispersion; mass absorption,

13:00 – 14:00 Lunch

14:00 – 15:30 **Profile models.** Profile models for x-ray, synchrotron and neutron diffraction, profile functions

15:30 – 15:50 Coffee Break

15:50 – 17:00 ***Description of Background:*** functions and limitations

Day 2

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 ***Least square fitting:*** zero, unit cell, background, halfwidths, peak shape, proffered orientation, polarization

10:30 – 11:50 Coffee Break

11:50 – 13:00 ***Mathematic approach vs. chemical approach:***

13:00 – 14:00 Lunch

14:00 – 15:30 ***Restrains and constraints:*** geometrical and chemical

15:30 – 15:50 Coffee Break

15:50 – 17:00 ***Parameter correlations:***

Day 3

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 ***Practical session***

10:30 – 11:50 Coffee Break

11:50 – 13:00 ***Practical session***

13:00 – 14:00 Lunch

14:00 – 15:30 ***Practical session***

15:30 – 15:50 Coffee Break

15:50 – 17:00 ***Practical session***

Day 4

8:00 – 8:30 Continental Breakfast

08:30 - 10:30 ***Practical session***

10:30 – 11:50 Coffee Break

11:50 – 13:00 ***Participant examples***

13:00 – 14:00 Lunch

14:00 – 15:30 ***Participant examples***

15:30 – 15:50 Coffee Break

15:50 – 17:00 ***Practical session***

Standardless quantitative phase analysis of X-ray powder diffraction data by the Rietveld method-why benefits:

Rietveld analysis of X-ray powder diffraction data can be utilized for the determination of the quantitative phase composition of inorganic crystalline raw materials, materials of natural origin (soils, rocks), intermediate products, precursor phases or of final products

It helps:

- To manufacture ***products with reproducible quality*** for producing and processing industries.
- To ensure a constant quality the ***specific properties of the material*** have to be defined and controlled.
- Often the ***mineralogical phase composition*** is one of the most decisive and measurable factors of quality.
- To control by the supplier of the raw materials during the process
- To control of the producer of half wares or final products during (**process control**) and after the production (**quality control of the product**).
- Control by the customer of raw materials, half wares or final products (**income control of the material**).

For academic research, government and industry

Cement clinker and cement
Limestone and lime based products
Gypsum- and anhydrite based products
Mixtures of different building materials
Intermediate and final ceramic materials
Refractory materials
Natural and synthetic inorganic raw materials
Pharmaceutical Industry
Active pharmaceutical ingredient or testing of the pharmaceutical product
Polymorphic purity, state of hydration, degree of crystallinity and/or particle size of the active pharmaceutical product
Analysis of the composition of a tablet or tablet components