

DMG/DGK Ph.D. student course

Basics and Applications of the Rietveld Method



R. E. Dinnebier



DECTRIS®

March 6 – 9, 2017

Max Planck Institute for Solid State Research
Heisenbergstrasse 1
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in cooperation with the
universities of Tübingen and Stuttgart
and



the working committee Powder Diffraction of the DGK

<http://www.fkf.mpg.de/xray>



Course description

It is the aim of this intensive course to impart the Rietveld method in theory and practice. Using selected examples the entire process from profile fitting using fundamental parameters towards crystal structure determination and refinement will be explained. In particular the following topics will be covered:

- Basics of powder diffraction and Rietveld Refinement
- Whole Powder Pattern-Fitting (WPPF), fundamental parameters (FP), complex reflection profiles
- Determination of the Instrument Resolution Function (IRF) for powder diffractometers
- Angular and intensity corrections (LP-Faktor, absorption, microabsorption, extinction, preferred orientation, sample height, zero error, ...)
- Methods to develop a starting model for crystal structure determination
- Penalty-functions, constraints, restraints
- Rigid Bodies (RB) (flexible polyhedra, molecules, z-matrices)
- Strategies for structure determination, global optimization in direct space, Charge-Flipping (CF)
- Difference-Fourier-analysis in combination with Rietveld refinement
- Isotropic and anisotropic microstructural parameters
- Quantitative Phase Analysis (QPA) with the Rietveld method
- Different methods for quantifying the amorphous content
- Symmetry and rotation modes as alternatives ways of describing crystal structures
- Parametric Rietveld refinements (includes basic macro-programming)
- Local and global optimization of stacking faulted superstructures
- Local and global optimization of the Pair-Distribution-Function (PDF)
- The making of Rietveld-Plots for publications

Place and Time:

Meeting point at Monday March 6th, 2017 at 8:30 am in front of the seminar room 2P4 of the MPI-IS (Heisenbergstrasse 3). Please be there in time.

Duration of the course approx. 9.00 am – 4:00 pm

Tutors:

Robert E. Dinnebier, Sebastian Bette, Luzia Germann, Roland Zenn (MPI-FKF, Stuttgart), M. Etter (Petra III)

Alan Coelho (Brisbane)

Course Fee:

Researcher from industry: 400 Euros

Students/ post-docs : 60 Euros

Student members of the DMG: 10 Euros (due to 50 Euro grant by the DMG)

Payable in cash at the reception. Please bring the exact amount.

Language

Lectures in English. Exercises in English and German.

Computer

No computers can be supplied by the organizer. For the exercises, a contemporary laptop (Windows 7, 8, or 10) with administrator rights is necessary. The licenses of Topas will be supplied using WiFi. If you have your own license dongle for Topas, please take it with you. A sufficient number of power outlets will be supplied. Bring an adapter if needed.

All programs and course material need to be downloaded and installed before the course. Installation instructions will be sent in due time.

Due to the large number of participants, there is no time for individual installation support.

Information

More information and an application form are available at : <http://www.fkf.mpg.de/xray>

Food

The MPI canteen serves breakfast and lunch.

Evening buffet with finger food on Tuesday is included.

Lunch vouchers for the canteen might be distributed free of charge (depends on the funding situation).

ECTS

2 ECTS (European Credit Transfer System) points can be awarded after passing a written test after the course.

Housing

There is no support from the organizers but a limited number of rooms in the MPI guest house is available on a „first-come-first- served” base (Tel: +49-(0)711-689-1241).

Inexpensive accomodation is limited, therefore book you accommodation sufficiently early.

Here are some suggestions for nearby hotels:

RELEXA Waldhotel Schatten (15 min walking distance)

<http://www.relexa-hotel-stuttgart.de/en/hotel>

Commundo Tagungshotel (5min bus ride, however heavily booked)

<http://www.commundo-tagungshotels.de/stuttgart/stuttgart.html>

ARCONA MO.HOTEL (15 min bus ride)

<http://stuttgart.arcona.de>

Hotel Römerhof (convenient by car, 5 min)
<http://www.roemerhof-vaihingen.de/index.php/en>

Pullmann Stuttgart Fontana Hotel (20 min bus ride, high budget)
<http://www.pullmanhotels.com/gb/hotel-5425-pullman-stuttgart-fontana/index.shtml>

Akzent Hotel Möhringer Hof (convenient by car, 20 min)
<http://www.hotel-moehringerhof.de/en/hotel/rooms-in-hotel>

Hotels in Stuttgart:
<http://www.stuttgart-tourist.de/en/hotels-stuttgart>

The internet is also a good resource: e.g.
<http://www.booking.com/Unterkunft-Stuttgart?>
<http://www.hrs.de>
<http://www.homeapartments.de/>
<http://www.nd-bed-breakfast.de/?>
<http://bbhappy.de/home>

Transportation

How to find us: <http://www.fkf.mpg.de/92750/40> [How to find us](#)
Public transportation is quite good with a frequent bus stop close to the institute (stop: Max-Planck-Institute):
<http://www.vvs.de>

Number of participants

Approx. 80

This and that:

- If you like to bring your own data, please contact the organizer in time before the course starts. No guarantee though.
- The DMG travel grant of 50 Euro/person is for non-local student members of the DMG. It is possible to fill out an application form for the DMG during the registration in order to get the grant.
- **Should you not be able to attend the course, please notify the organizer in time. The course is pro-bono. If you cancel your participation later than February 15th, you will be charged the full amount !**
- **Out of respect for the other participants and the waiting list, participation for the full 4 days is mandatory.**

Contact details

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Preliminary schedule (time estimates):

Monday March 6, 2017

8:00 – 9:00 Registration in front of 2P4 lecture hall

9:00 – 9:15	Welcome, organization
9:15 – 10:00	Introduction to the Rietveld method Information content of a powder diffraction pattern
10:00 – 10:30	Break (coffee/tea/water/cookies)
10:30 – 11:15	Theory of the Bragg reflection: position, peak shape, intensity
11:15 – 12:00	Concept of convolution, fundamental parameters versus phenomenological peak shape functions, isotropic and anisotropic peak broadening, microstructural properties
12:00 – 13:00	Lunch (canteen)
13:00 – 13:45	Single peak fits, Whole Powder Pattern-Fitting (Pawley, LeBail, Rietveld), powder pattern calculation
13:45 – 14:30	Exercises
14:30 – 15:00	Break (coffee/tea/water/cookies)
15:00 – 16:30	Determination of the instrumental resolution function

Tuesday March 7, 2017

9:00 – 10:00	Indexing, space group determination (with exercises).
10:00 – 10:30	Break (coffee/tea/water/cookies)
10:30 – 11:15	Crystal structure determination in direct space (simulated annealing) and reciprocal space (charge-flipping)
11:15 – 12:00	Exercises
12:00 – 13:00	Lunch (canteen)
13:00 – 13:45	Correction functions (LP-factor, absorption, microabsorption, extinction, preferred orientation etc. (with exercises)
13:45 – 14:30	The pair distribution function (PDF) and its combination with Rietveld analysis
14:30 – 15:00	Break (coffee/tea/water/cookies)
15:00 – 16:30	Exercises
16:30 – 17:00	Success in structure solution as a result of specific data collection strategy (Dubravka Sisak Jung, Dectris GmbH)
17:30 – 21:00	Evening buffet with beverages
21:00 – 22:00	Scientific discussion I

Wednesday, March 8, 2017

9:00 – 10:00	Penalty-functions in global and local minimization (constraints, restraints and rigid bodies (with exercises)
10:00 – 10:30	Break (coffee/tea/water/cookies)
10:30 – 11:15	How to set up rigid bodies (flexible polyhedra, molecules, z-matrices)
11:15 – 12:00	Exercises
12:00 – 13:00	Lunch (canteen)
13:00 – 13:45	Combining Rietveld refinement with difference Fourier analysis and global optimization
13:45 – 14:30	Exercises
14:30 – 15:00	Break (coffee/tea/water/cookies)
15:00 – 16:00	Quantitative Phase Analysis (QPA) with the Rietveld method Quantifying the amorphous content (with exercises), PONCS

Thursday, March 9, 2017

9:00 – 10:00	Refinement of crystal structures with stacking faults using Rietveld analysis (exercises)
10:00 – 10:30	Break (coffee/tea/water/cookies)
10:30 – 11:15	Symmetry/distortion mode analysis
11:15 – 12:00	Exercises
12:00 – 13:00	Lunch (canteen)
13:00 – 13:45	Sequential and parametric Rietveld refinement in dependence on external variables. Macro programming
13:45 – 14:30	Exercises
14:30 – 15:00	Break (coffee/tea/water/cookies)
15:00 – 16:00	Macro programming/ Making of Rietveld plots/ Critical analysis of results
16:00 -	Scientific discussion II – The future