

German Mineralogical Society

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DMG SHORT COURSES AT RUHR UNIVERSITY BOCHUM – REPORTS

DMG/MSA Short Course "Application of diffusion studies to the determination of timescales in geochemistry and petrology," 27–31 March 2023

After some years of online courses, it was the first time to meet again in-person for the diffusion modeling short course taking place at Ruhr-University Bochum. In the end of March 2023, around 35 participants made their way to the Ruhr region to learn about diffusion, and have some hands-on modeling experience, advised by the experts of that field, Sumit Chakraborty and Ralf Dohmen. The group of international scientists, ranging from student to professor level, was keen and highly motivated to learn, model, and connect!

This one-week course covers a broad mix of theoretical and practical units, which are perfectly synchronized to each other and thereby ideal for participants to learn the basics step-by-step and to dive deeper into diffusion modeling. After a quick introduction and some basic knowledge provided by Sumit Chakraborty, Ralf Dohmen introduced us to the mathematic background and some applications. Sumit taught about loads of diffusion and model theory, complex research questions, and gave further insights into fascinating case studies. In between, there were also some specialized talks from other contributors on, e.g., experimental methods (Harald Behrens), phase field theory (Julia Kundin), the application of AI (Renat Almeev, Artem Leichter), and diffusion on the isotope level (Martin Oeser-Rabe).

In the practical units, we started with some simple Excel-based approaches to model step profiles using the Gauss function and learn to fit diffusion curves in general. Afterwards, we worked on more advanced and applied tasks such as modeling the Arrhenius equation, restraining residence times of crystals or cooling rates of magmatic systems. On the last day, we were using Matlab to re-do all of the previous tackled applications, which was a challenge but definitely a highlight of the course!

A big thank you to the organizing committee at Bochum University including course-leaders Sumit and Ralf, and science coordinator Linda



The group of participants at Ruhr University Bochum. Рното: L. SOBOLEWSKI.

Sobolewski, who all did a great job to handle all kind of problems—from minor and major difficulties during the practicals to organizing the transport on Monday (public transportation strike). We really appreciate that!

The pleasant atmosphere and high-quality catering provided by Ruhr University, and especially during the Conference Dinner on Thursday (Yamas Meze restaurant in Bochum City, fantastic Greek-Mediterranean cuisine!!), were perfect conditions for networking with other young scientists, having inspiring discussions on and off-topic with colleagues, and for considering future cooperation. The course is perfect for everyone who wants to dig deeper into the field of diffusion, and is highly recommended not only for PhD candidates and students, but for everyone who is interested to work on diffusion topics and connect with other like-minded people. In summary, it was an interesting and enjoyable week in Bochum!

Anne Sturm (Heidelberg University)

20th DMG Shortcourse "Solid-state NMR Spectroscopy," 30 May-2 June 2023

A short course on NMR spectroscopy was also organized this year by the DMG/DGK. Under the direction of Dr. Michael Fechtelkord, participants from a wide variety of disciplines (e.g., cement chemistry, petrology, or chemical engineering) were able to address in detail the analytical possibilities of solid-state NMR spectroscopy.

This course offered PhD students and scientific staff the interesting opportunity to combine a repetition of the physical basics of the methodology with practical examples to obtain a comprehensible introduction to NMR spectroscopy. While the theoretical foundations and plans for the day were worked out in the morning, the afternoon was devoted to practical work. In addition to the preparation of samples to be measured, the course participants were even able to carry out measurements on the device themselves.

Using the example of the ¹H spin lattice relaxation of tetramethylammonium iodide and the calculation of activation energies and correlation times for the discovered relaxation signals of the ammonium and methyl environments, it was also shown how strong the influence of the experimental temperature can be on the obtained NMR spectra. The course day ended with drinks and food in the "Filou" pub, where the participants got to know each other better.

The next day, dipolar and chemical shift interactions were presented and their influence on the spectra obtained was explained. We were able to determine that, for example, signals from the sample cannot be easily distinguished from rotating sidebands and impurities. Here, the evaluation software DMFit2020 proved to be a very helpful tool. As in the history of NMR spectroscopy, Wednesday afternoon marked a crucial turning point in the course. The removal of anisotropy



Participants in front of the Bochum NMR Spectrometer. Рното: H.-P. SCHERTL.

effects using magic angle spinning (MAS) probe heads opened up completely new analytical possibilities. This technique was used in the practical part to study ²⁹Si, ¹⁹F, and ¹H nuclei in synthetic phlogopites. This clearly showed that NMR spectroscopy is excellently suited as a complementary technique to diffraction methods and is of particular interest when doped or naturally "contaminated" minerals are to be observed and their structural peculiarities elucidated.

The third day of the course dealt with the possible applications of multipulse techniques and the basics of the cross-polarization experiment (CP). In the practical part, a contact-time dependent CPMAS experiment

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was performed on kaolinites. Subsequently, atomic distances between Si and H nuclei were determined. This could be done with a simple spreadsheet.

The last day was dedicated to the quadrupolar nuclei (spin quantum number I > 0.5). As examples, the nuclei ²³Na and ²⁷Al were measured and analyzed in different salts and corundum.

In the theoretical part, the focus was on other NMR methods such as "double rotation" (DOR) or multi-quantum magic-angle spinning (MQMAS) and satellite transition spectroscopy (SATRAS). At this point, at the latest, it became clear that it would take four years rather than days to understand all solid-state NMR methods and to be able to apply them in practice.

However, there was enough time to develop a general idea for the different approaches and to understand which information can be obtained with which method. In general, it can be said that the overview given is very helpful for planning future projects and for evaluating scientific questions that have already been asked.

Christian Felten, Henning Kruppa, and Michael Wenzel (RWTH Aachen)

ANNUAL DMG MEETING 2023

From September 17 to 21, 2023, the joint meeting of the Austrian Mineralogical Society (ÖMG), the Slovakian Mineralogical Society (SMS), and the German Mineralogical Society (DMG) – MinWien2023 – took place in Vienna, Austria. The meeting was organized by the Institute of Mineralogy and Crystallography of the University of Vienna, among others, in honor of Josef Zemann, who had been an important member of the Mineralogical Society and the University of Vienna, and passed away late last year at the age of 99.

MinWien focused on the broad spectrum of mineralogical and petrological science and related disciplines, ranging from basic to applied research. In addition to lectures in mineralogy and crystallography; applied mineralogy; lithosphere, geochemistry, and mineralogy; and ore deposits, there were also open lectures on topics such as mineral history, gemmology and gemstones, and mineral teaching. There were also several poster sessions over the course of several days that showcased diverse research in the field of geosciences. A reception in the City Hall of Vienna, a Young Scientist meeting, the visit of the Mineralogical Collection of the Faculty, as well as excursions to the host



Participants of MinWien2023. PHOTO: R. KRICKL.



DMG awardees 2024 together with DMG president Horst Marschall. **Left to Right:** Claudia Weidenthaler, Horst Marschall, Thomas Oberthür, Roland Stalder, Eric Runge, Benjamin Walter, and Victoria Kohn. Marie Gentzmann is missing. PHOTO: M. WILDNER.

country Austria and the neighbouring country Slovakia completed the conference. A special highlight was a lecture for the public by F. Melcher (Leoben) about raw materials for the Green Deal and pointed out in detail current problems of raw material supply in Europe.

In addition to the conference, the DMG general meeting 2023 also took place, in which the list of candidates for this year's election was approved. The positive progress of the DMG was also reported and, among other things, the statutes were updated. This year the DMG again honored scientists for their outstanding work. The Paul Ramdohr Award went to E. A. Runge (Tübingen) and M. C. Gentzmann (Berlin), the Beate Mocek Prize to V. Kohn (Vienna), the Abraham Gottlob Werner Medal to T. Oberthür, the Agricola Medal to C. Weidenthaler, the Victor Moritz Goldschmidt Prize to B. Walter, and the Doris Schachner Medal to R. Stalder.

Thus, MinWien2023 showed once again how important the mentioned disciplines are for today's society. It offered an outstanding opportunity to present new research results, to discuss these or other results constructively, to establish new contacts, and to launch new projects.

Fabio Joseph, LMU Munich

DMG SHORT COURSES 2024

As before, DMG will support several short courses next year. All courses will be aimed primarily at advanced-level undergraduate and graduate students but, as always, are open to more senior researchers as well. Nonlocal student members of DMG will be eligible for travel support to the amount of \in 100. At this time five courses can be announced. Further information can be found at https://www.dmg-home.org/ aktuelles/doktorandenkurse/.

(1) **High-Pressure Experimental Techniques and Applications to the Earth's Interior**, Bayerisches Geoinstitut/University Bayreuth, Florian Heidelbach, 19–23 February 2024 (florian.heidelbach@uni-bayreuth.de)

(2) Metal Stable Isotopes as Fingerprints in the Earth and the Environment, GFZ Potsdam and FU Berlin, Geosciences, Friedhelm von Blanckenburg, Dr. Patrick Frings, 8–13 April 2024, (patrick.frings@gfz-potsdam.de, f.v.b@fu-berlin.de)

(3) **Solid-state NMR Spectroscopy**,Institute for Geology, Mineralogy and Geophysics, Ruhr University Bochum, Dr. Michael Fechtelkord, 21–24 May 2024 (michael.fechtelkord@rub.de)

(4) In situ Analysis of Isotopes and Trace Elements by Femtosecond Laserablation ICP-MS, Leibniz University Hannover

(5) Application of Diffusion Studies to the Determination of Timescales in Geochemistry and Petrology, University Bochum