MGML

Materials Growth and Measurement Laboratory

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Editors: Martina Rážová, Pavel Javorský

Scientific Advisors: Jan Prokleška, Martin Žáček, Jiří Pospíšil, Jiří Prchal, Martin Míšek

Production team: Martina Rážová, Štěpán Sechovský

Further copies can be obtained from:

Martina Rážová

KFKL, MFF UK

Ke Karlovu 5

121 16 Prague 2, Czech Republic

www.mgml.eu

m.razova@mag.mff.cuni.cz

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Foreword

The year 2020 has been quite intense for the MGML management, as it was overshadowed by the worldwide spreading of Covid-19 pandemic. MGML had to perform the required measures and restrictions to maintain the functionality of the research infrastructure with a limited on-site staff and no on-site users outside the Czech Republic. Even more challenging was to continue the progress in increasing the research landscape of MGML, despite the limited funding situation in 2020.

The Scientific Advisory Committee (SAC) of MGML met via a video conference in September 2020, at which the MGML management presented an update of the year's MGML activities. The SAC was very pleased that the MGML management with enthusiasm and great efforts has successfully overcome such challenges and extremely satisfied with the well targeted and coordinated activities to move forward in developing the infrastructure. The MGML management made major progress to broaden the research landscape by optimizing existing infrastructure activities as well as creating new structural elements.

In this respect, I would like to highlight the clever and effective incorporation of advanced structural analysis for structural characterization of complex and new materials. The former has been achieved by integrating a variety of new instrumentations together with excellent groups of experts from the Department of Structure Analysis of the Institute of Physics and x-ray group of the Department of Condensed Matter Physics at Charles University in Prague. Such a useful extension of structural characterization facilities is very important not only to satisfy the growing demands of the users, but also to provide services for users from the industry.

Also, increasing national and international collaborations, e.g. NanoEnviCZ (nanomaterials), and in particular ISABEL (high magnetic fields) is very positive step that goes in line with increasing the research landscape of MGML.

In 2020, the MGML and its users produced an impressive number of high level publications, many of them presenting novel findings in new materials for fundamental science and for technological applications, thereby reflecting the impact of the continuous scientific progress of this excellent infrastructure. Details about the progress of MGML infrastructure and other scientific activities are documented in this annual report.

Finally, I would like to thank scientific and technical staff members, users, and cooperating partners for their enthusiasm and excellent work.

Mohsen Abd-Elmeguid, Chair of MGML Scientific Advisory Committee

Dear colleagues and MGML users, we have experienced very difficult year 2020. The COVID-19 epidemic situation and subsequent restrictions influenced all our lives including the operation of our laboratories. We tried our best to keep all the laboratories running for the users. The remote online access is possible for majority of our instruments, our staff can even perform some user experiments after detailed discussion with the user(s). Our traditional weekly meetings are organized also in online form only. On the other hand, many users and collaborators who are not currently present in Prague can join such online meetings, what is in some sense a positive consequence of the restrictions. Perhaps we should think about such a form also in the future.

Despite the unusual situation around all of us, MGML reached several important milestones. Extensive progress was achieved in offered portfolio of services by **incorporating advanced structural analysis**. In the past several years, the materials synthesis portfolio significantly extended beyond the original focus on metallic systems. The oxide materials, fluorides or two-dimensional van der Waals materials are now routinely synthesized. This is, however, associated with an extended demand for structural characterization of complex materials, not available in MGML. This was temporary solved by mediating the contact between the users and (i) Department of Structure Analysis, IoP CAS, and (ii) The X-ray Group, Department of Condensed Matter FMP CU. Reflecting this growing user demand for advanced structural analysis, the MGML board has negotiated to incorporate the experimental equipment already working at the above mentioned groups into MGML portfolio of services. This is very positive as the infrastructure gains not only the instrumentation (its overview is given also in this Annual Report), but also the huge scientific know-how of these groups. (i) Has long term tradition in crystallography of standard, modulated and magnetic structures. It belongs to world top recognized groups in the field of structure solution from x-ray data. The group members are authors of crystallographic computing program Jana. (ii) Is focused on x-ray studies of bulk, polycrystalline, nanocrystalline, amorphous and organometallic compounds, as well as on the investigation of low-dimensional system as thin polycrystalline and epitaxial layers, multilayers, quantum dots, wires and tubes. Personally, I believe that this is a huge step forward in the development of our Research Infrastructure.

On the level of collaborations with other LRI in the Czech Republic, the **close cooperation with the NanoEnviCz** Large Research Infrastructure (www.nanoenvicz.cz) led to a conclusion of a Joint Declaration on Cooperation between MGML and NanoEnviCz, signed at the beginning of August 2020. Both sides confirmed their intention to work closely together in the liaison areas of science and research. The mutual collaboration aims to optimize the operation of the two Research Infrastructures and maximize usage of available resources (financial, material and human). Cooperation in services, sharing of knowledge, technical know-how and apparatuses, preparation of joint projects as well as development of a joint user portal are all anticipated. We should be active to get all these aims into reality.

On the international level, I was very happy that the **EU Framework Programme Project ISABEL** (Improving the sustainability of the European Magnetic Field Laboratory, www.emfl.eu/Isabel) was approved for financing within the call H2020-INFRADEV-2018-2020. The ISABEL project started on November 1st 2020 and will last for 48 months. It is focused on collaboration in research in high magnetic fields through the realization of following objectives:

- strengthening the EMFL structure by enlarging its membership and by improving several organizational aspects, such as data management, outreach and access procedures.
- strengthening the socio-economic impact by bridging the gap with industry.
- strengthening of the role of high magnetic field research in Europe.

Seventeen European institutions representing the significant centers of research in high magnetic fields are involved in ISABEL. The scientific partners are Centre National de la Recherche Scientifique (CNRS, France), Helmholtz-Zentrum Dresden-Rossendorf (HZDR, Germany), Stichting Katholieke Universiteit / Radboud Universiteit (Netherland), University of Nottingham (UK), University of Oxford (UK), University of Warsaw (Poland), Université de Genève (Switzerland), Universidad Autonoma de Madrid (Spain), Charles University (Czech Republic), National Institute of Chemical Physics and Biophysics (Estonia), Commissariat d'Energie Atomique et Energie Alternative (CEA, France), University of Salento (Italy) and European Magnetic Field Laboratory (EMFL) itself. The industrial partners are represented by Oxford Instruments (UK), I-Cube Research (France), Bilfinger Noell (Germany), Metel (Netherland) and Ampulz (Netherland). Czech Republic is formally represented by Charles University as a legal entity, but all activities are provided by MGML and only its personnel is involved in the project.

The involved institutions form a European network of magnetic field facilities. MGML acts here as a regional partner of EMFL for the Central European region involving Czech, Slovak, Austrian and Hungarian scientific community of potential users. MGML participates in two work packages: WP2 Community building and WP5 Access improvement. The work package Community building focuses on development of networks of regional partner facilities, user community meetings or training of early career researchers. MGML will organize (in 2022 or 2023) a regional workshop focused on materials research in high magnetic fields. Beside the workshop, user community meetings or training of early career researchers are expected user profits. The project for example enables our users to participate in specialized schools organized by EMFL. The work package Access improvement focuses on improving the user access and novel access modes including access to regional partner facilities. Here, the new dual-access mode to regional partner facility and subsequently to the EMFL facilities will be implemented and evaluated. The main purpose of this access mode is to better serve the user community. In case of positive feedback, this access mode will continue after the end of ISABEL, which perfectly corresponds to our focus. I consider the ISABEL project to be a huge step forward in the international visibility of MGML.

Very close collaboration exists especially with the **Dresden High Magnetic Field Laboratory** (HLD) at HZDR. In 2020, the Memorandum of Understanding between Charles University and HZDR aiming to broaden and deepen the scientific and technological cooperation as well as extend the collaboration towards various new activities between MGML and HLD has been signed. This includes also collaboration within ISABEL, where both Large Infrastructures are involved.

Our thanks go to the members of our Scientific Advisory Committee. In 2020, we had one SAC meeting, this time only in online form. I believe we will welcome them again in Prague in 2021 or in 2022at the latest.

I hope that the year 2021 will represent a path towards a normal life not only in our laboratories, although the beginning is still very difficult. I wish success to all of you and especially to our users who make the Research Infrastructure meaningful.

Pavel Javorský, Head of MGML

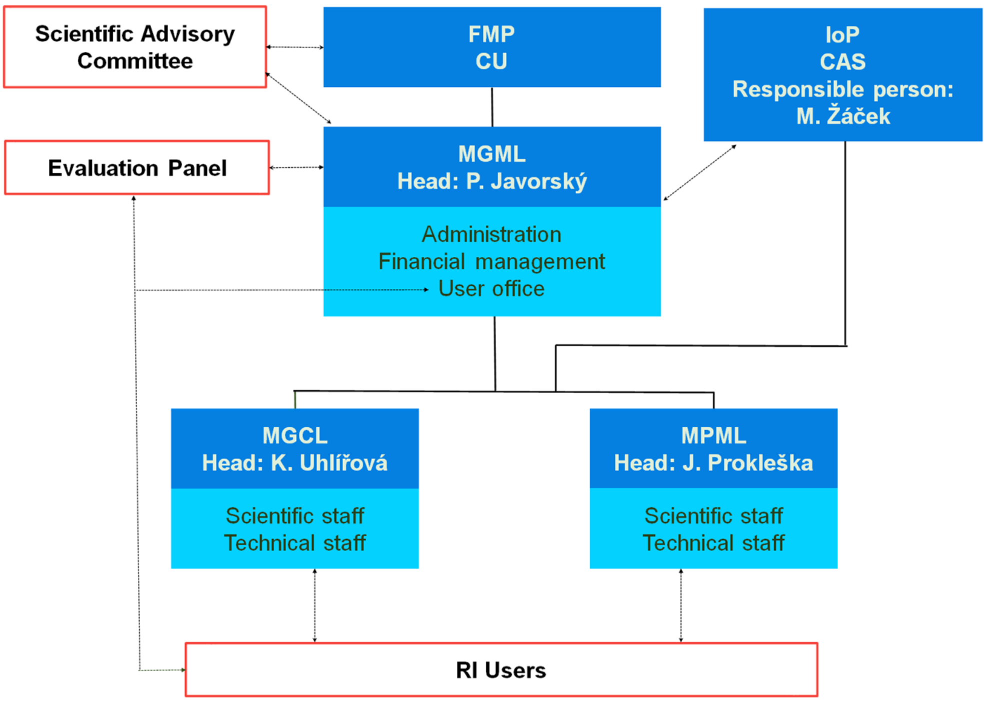
About MGML

MGML is a research infrastructure financed by the Ministry of Education, Youth and Sports within the program of Large Infrastructures for Research, Experimental Development and Innovation of CR (project No. LM2018096). It is an open access research infrastructure available to all users from CR and abroad.

The research infrastructure is hosted by the Faculty of Mathematics and Physics of Charles University with the Institute of Physics of the Czech Academy of Sciences, v. v. i. as the partner institution.

MGML provides a laboratory base for advanced material research. Within its two closely co-operating units, Material Growth and Characterization Laboratory (MGCL) and Material Properties Measurement Laboratory (MPML), MGML offers open access for external users to a vast experimental instrument suite as well as high-level expertise of its scientists. MGCL has state-of-the-art facilities for metal refinement, synthesis of new materials, and the preparation of high-quality single crystals with several different techniques. The unique combination of different crystal growth methods allows users a great deal of flexibility and optimization of the technology of producing entirely new materials. Modern X-ray diffraction and electron microscopy instruments allow detailed structural and phase characterization of samples. MPML offers the measurement of a wide portfolio of physical (magnetic, transport, thermal, acoustic and elastic) properties of materials through several complementary experimental methods. The extensive range of MGML instruments makes it possible to carry out the measurements in the temperature range from mK up to several hundred degrees Celsius, magnetic (up to 20 T) and electric (from -50V to + 50V) fields, hydrostatic and uniaxial pressures up to 15 GPa. Important is the possibility of preparation, characterization and measurement of uranium materials, for which the institution has the appropriate license. Interconnection of this wide range of experimental techniques for the preparation, characterization and measurement of physical properties makes MGML a unique research infrastructure in the Czech Republic, fully comparable with the world's leading laboratories.

Organizational chart of MGML



Our laboratories are located at three places in Prague:

The MGCL technology laboratories are located in the building of the Faculty of Mathematics and Physics - Ke Karlovu 5. You can find also the administration unit here.

The measurements of material properties are performed mostly in the cryo-pavilion of the Faculty of Mathematics and Physics in Troja, V Holešovičkách 2. The helium liquefier located in this building supplies all the cryogenic needs of the laboratory.

Some instruments for measurements of material properties and structural analysis are situated in the building of the Institute of Physics, Cukrovarnická 10.

Scientific Highlights

Magnetic moments on geometrically frustrated pyrochlore lattice

The rare-earth oxides of the general formula $A_2T_2O_7$, with *A* being a rare-earth ion and *T* a transition metal, have been extensively studied for their frequently exotic electronic properties. The majority of $A_2T_2O_7$ oxides crystallize in cubic ordered pyrochlore structure (space-group *F d -3 m*, n. 227). The pyrochlore structure with both *A* and *T* sites separately forming lattices of corner sharing tetrahedra, represents a canonical example of a frustrated lattice. When magnetic ions reside on the *A* or *T* sites, the formation of long-range ordered magnetic ground-states is suppressed due to competing exchange interactions. This suppression can lead to the formation of strongly-correlated unconventional ground-states. The pyrochlore oxides have been found to host a wide range of exotic states ranging from spin-glasses, to spin-liquid and spin-ices [1], with spin-ices capable of hosting magnetic monopole-like excitations [2]. The geometrical frustration or competing spin interactions can cause also the freezing of spins, spin glass [3] or spin liquid state, i.e. the system with distinct dynamics of correlated non-ordered spins fluctuating down to the lowest temperature [3].

In case of $A_2Ir_2O_7$ iridates, the subject of our study, the magnetic Ir^{4+} ions on *T*-site play a crucial role - influencing the rare-earth magnetism - in formation of (especially) low-temperature properties of $A_2T_2O_7$. Moreover, spin correlations, a strong entanglement of spin and orbital degrees of freedom of its 5d electrons and a comparable strength of electron Coulomb repulsion and SOC [4] make pyrochlore iridates attractive for both theoretical and experimental studies. Beside mentioned complex low-temperature states, pyrochlore iridates exhibit highly interesting electronic properties, connected to the iridium sublattice, also at higher temperatures (> 100 K). The iridium sublattice is supposed to order magnetically with the all-in-all-out (AIAO) long-range structure (between 30 and 140 K, depending on the *A* ion, no ordering found for Pr analogue) [4]. Metallic (*A* = Pr, Nd) or semi-metallic/non-metallic (*A* = heavier rare-earth element) $A_2Ir_2O_7$ become insulators at (similar) temperature, below which the Ir^{4+} ions start to be correlated [5].

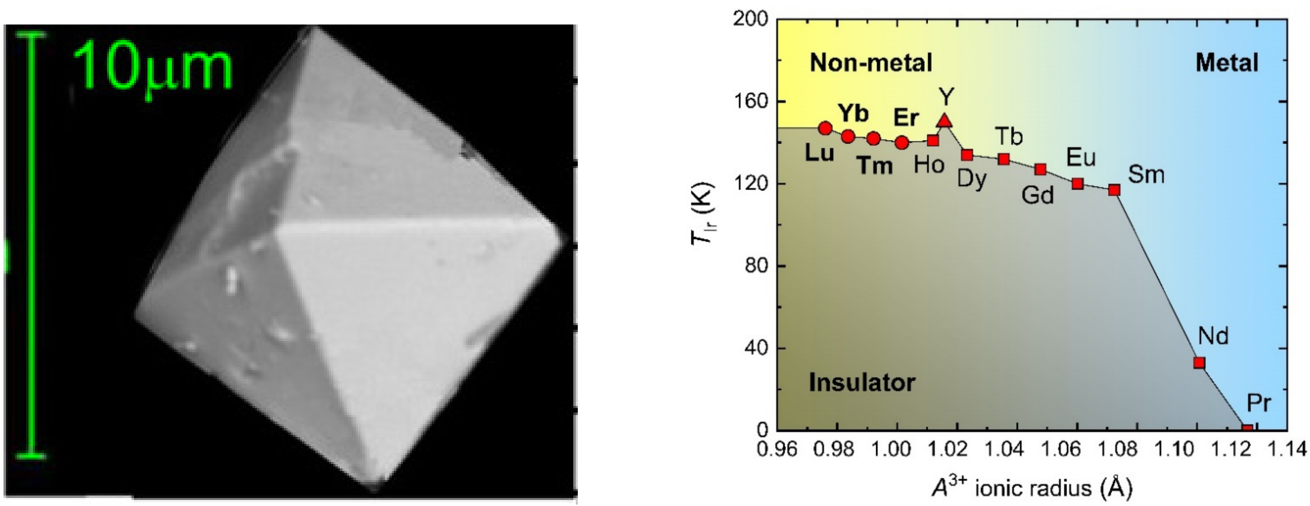
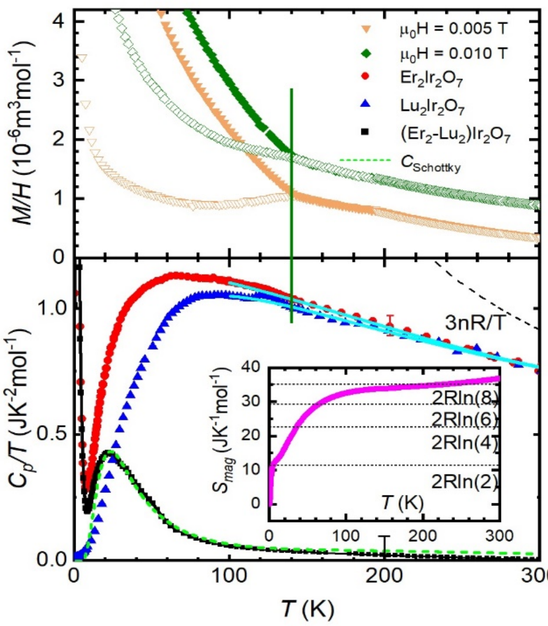


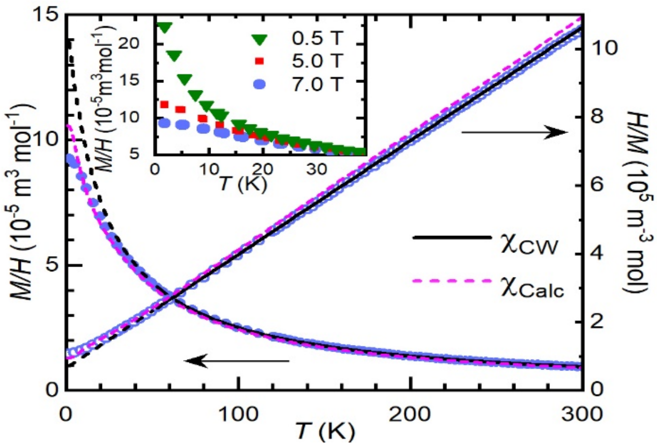
***Fig. 1**: Prepared $Tm_2Ir_2O_7$ single crystal, an example of back-scattered electron image (left panel). Phase diagram of $A_2Ir_2O_7$ pyrochlores - the dependence of ordering temperature of the Ir sublattice on the ionic radius of rare-earth A with the 8-coordination number [6] (right panel).*

Our systematic investigation of magnetic properties of heavy rare-earth $A_2Ir_2O_7$ pyrochlore oxides, including the, so-far-unreported, $Tm_2Ir_2O_7$, consisted of (i) sample preparation, a non-trivial task itself. A large number of preparation attempts and multiple synthesis routes have been employed, including hydrothermal synthesis, solid-state reaction, flux-growth etc. A large quantity (grams) of individual materials were prepared - further investigated in polycrystalline form only as the dimensions of crystals were small (Fig. 1); (ii) sample characterization, confirming a good quality of prepared samples. A number of experimental techniques was used to fully characterize the samples, including bulk properties measurements; (iii) microscopic experiments, synchrotron radiation, muon and neutron scattering techniques, were performed on selected compositions, leading to substantial insight into their properties; (iv) discussion of the data with previous results and theory predictions/calculations.

Among a number of results, published in Refs. [6-9], we highlight (i) a study of the development of iridium sublattice ordering with heavy rare-earth ion A^{3+} radius, resulting in a completed magnetic phase diagram (Fig. 1). And (ii) an investigation of the low-temperature magnetic properties of rare-earth sublattice by means of macroscopic and in selected cases by microscopic techniques, leading to better understanding of their ground state. The fitted magnetic excitations in energy spectra of $Er_2Ir_2O_7$ led to crystal field parameters perfectly in agreement with macroscopic magnetization and specific heat data, evidencing, somewhat surprisingly, a negligible impact of Ir sublattice magnetism on rare-earth sublattice (Fig. 2).

This work is a part of the junior research project financed by the Czech Science Foundation Grant No. GACR 18-09375Y. Sample preparation and characterization were performed on the ground of Department of Condensed Matter Physics of Charles University, and Materials Growth and Measurement Laboratory MGML, while microscopic experiments were done at international facilities, namely Institute Laue-Langevin, Grenoble; Rutherford Appleton Laboratory, Didcot; and Helmholtz Zentrum Berlin.





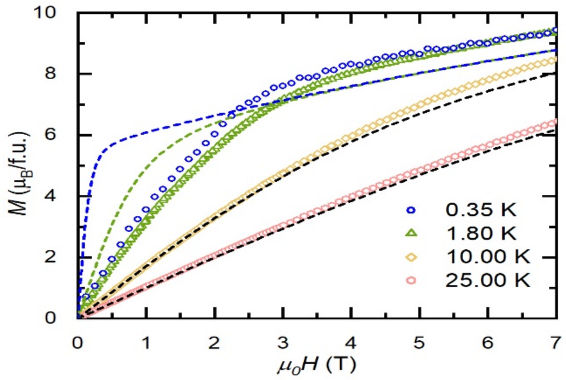


***Fig. 2**: Magnetization and specific heat data measured on Er2Ir2O7. Perfect agreement of measured and calculated (Refined crystal field parameters from inelastic neutron scattering experiments were used.) values is observed [7].*

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A new phase of nanoconfined water discovered

Researchers discovered a new phase of nanoconfined water; separate water molecules that are confined within nanocavities formed by ions of the cordierite crystal lattice. The first reliable experimental observation of a phase transition in a network of dipole-dipole coupled water molecules is an important fundamental breakthrough. Apart from that, the discovered phenomenon can also find practical applications in ferroelectrics, artificial quantum systems, and biocompatible nanoelectronics.

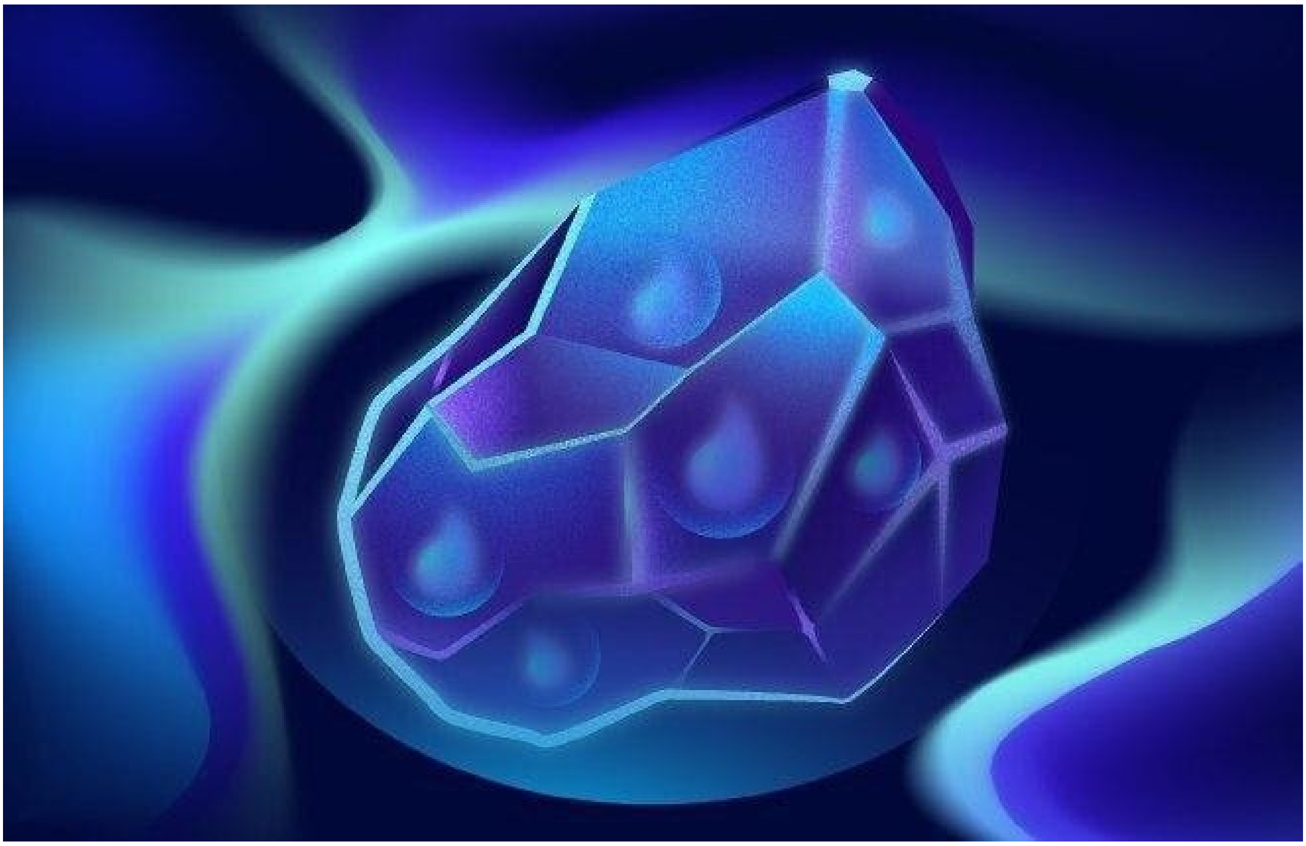


Fig. 1: *Water molecules inside a crystal. Credit: Daria Sokol, MIPT.*

The study was a joint effort of MIPT scientists and researchers from Shubnikov Institute of Crystallography, A. M. Prokhorov General Physics Institute of RAS, Skoltech, Sobolev Institute of Geology and Mineralogy, and Novosibirsk State University, as well as their colleagues from Germany (Stuttgart University), the Czech Republic (Prague Institute of Physics and MGML), and Japan (University of Tokyo). The results of the study have been reported in Nature Communications.

“We are searching for new phases of electric dipole lattice, i. e. an ensemble of interacting point electric dipoles,” explained Mikhail Belyanchikov, one of the study’s initiators and a junior researcher at MIPT Laboratory of Terahertz Spectroscopy. “A great number of different magnetic dipole phases have been discovered but the research of material phases related not to magnetic but rather to point electric dipoles is still in its early stages. Moreover, electric dipole lattices are a type of ferroelectrics that may have promising microelectronic applications.”

It is known that to experimentally realize a lattice of point electric dipoles is a challenging task. Usually, physicists use the so-called interferometric optical lattice – a periodic structure of fields that is created as the result of laser beams interference. Ultracold atoms of materials to be studied are placed into the lattice points. But researchers at MIPT Laboratory of Terahertz Spectroscopy found a more efficient way. They place separate water molecules that possess a rather high electric dipole moment into a so-called dielectric matrix, in this case, a zeolite crystal lattice with periodically distributed nanoscale voids formed by lattice ions. One then gets an easily handled sample (a crystal) with practically free water molecules trapped in these voids during crystal growth – the so-called nanoconfined water. This sample can be studied in a wide range of temperatures including room temperature and in different environments (electric fields, pressure, etc.).

However, the key result of the study was achieved at rather a low temperature of 3 K (–270 °C). The researchers observed an order-disorder ferroelectric phase transition in a three-dimensional nanoconfined water molecular network at the temperature of 3 K. “It was challenging to find an instrument which can cool our sample down to sub-kelvin temperatures and simultaneously allow high-frequency dielectric measurements. 20T MGML cryomagnet is ideal for that due to robust coaxial wiring down its low temperature stage,” explained Maxim Savinov who performed the measurement in the MGML.

“Not only does studying nanoconfined water molecules have fundamental importance for the field of electro-dipolar lattices but it also contributes to a deeper understanding of natural phenomena and may even potentially enable the construction of biocompatible nanoelectronic devices. This is a rapidly developing field that promises new and extremely efficient electronics based on biological materials,” comments Boris Gorshunov, who heads MIPT Laboratory of Terahertz Spectroscopy.

Publication: https://doi.org/10.1038/s41467-020-17832-y

Original featured article (edited): https://phys.org/news/2020-08-phase-nanoconfined.html

Technical Developments

Progress in CVT single crystal growth method

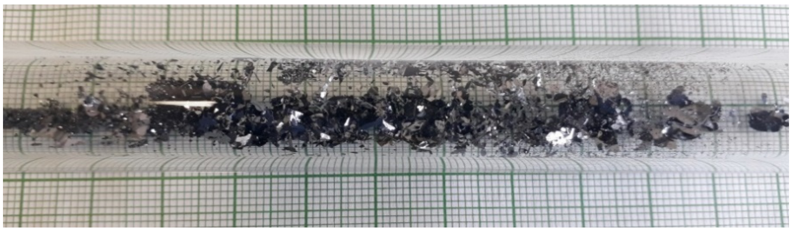


Fig. 1: *Chalcogenide single crystals grown by CVT in MGML.*

Fig. 2*: New two-zone gradient furnace.*

The users demand for technical instrumentation reflects the actual scientific subjects in the field of condensed matter physics. There is a continuous and clearly increasing trend of the single crystals growth of non-metallic materials. In particular, the chemical vapour transport (CVT) method is frequently used for the growth of various new layered materials (magnetic vdW halides, chalcogenides). For this purpose one four-zone furnace was available in MGCL. However, the working capacity of the furnace was found to be insufficient due to the time length of the CVT processes. In addition, requirements for this single crystal growth method are expected to increase further. Therefore, a second two-zone gradient furnace was installed in MGCL laboratory made by Clasic Company. Each zone is operated independently with maximum operation temperature 1200°C. It is maximum accessible temperature for quartz tubes, in which growth process is mostly realized. The chamber fits for all available quartz tube diameters used in MGCL. For future applications, the furnace is constructed also for implementation of the controlled growth processes by external gass flow.

Installation of new high temperature and high vacuum sapphire furnace

The recently installed optical furnaces with implemented floating zone method have provided unique opportunity of single crystal studies of oxide based materials. The research of this class of materials continues and has clearly increasing trend not only in fundamental science requested by academic users, but also in field of perspective materials in applications. MGCL has established collaboration with Crytur Company which is a global leader in industrial growth of photonic single crystals based on yttrium-aluminum garnet, perovskite and wide series of their substituted derivate.

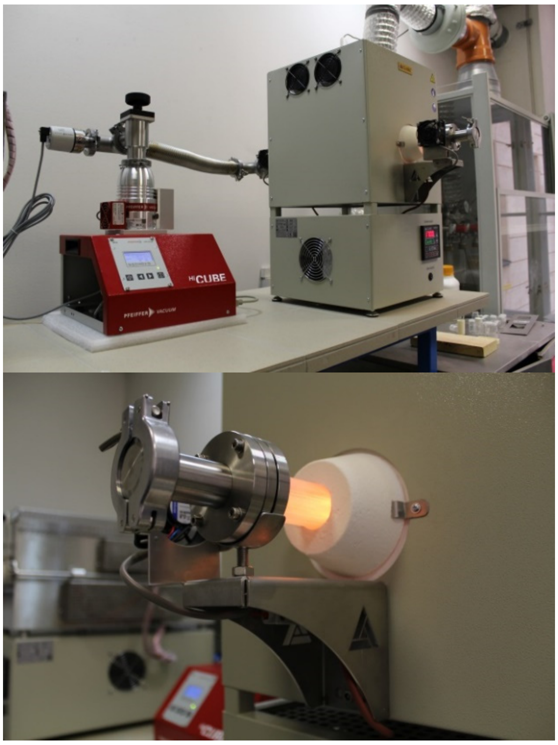


***Fig. 3**: Sapphire high temperature and high vacuum furnace for sintering of oxide-based materials.*

MGCL was implemented to the company development program to investigate new compositions of photonic single crystals to improve their properties for laser applications and detectors.

The single crystal quality strongly depends on quality of the polycrystalline feeding precursor. We have developed new feeding form for preparation of the rod precursors, which contains more powder materials as well as its diameter is precisely preserve along whole length. The pressing forms of various diameters (10, 9, 8 and 5 mm) are available in MGML. The final proper sintering of the precursor rods is crucial step to avoid the presence of bubbles and cavities inside the single crystal. For this purpose a new high vacuum and high temperature super-kanthal furnace was installed in MGML. The chamber of the furnace is made of sapphire single crystalline tube in which temperature 1800°C can be reached under the vacuum 10^{-6} mbar, which is created by turbomolecular pump. The inner diameter of the chamber is 32 mm and length of the hot zone 20 cm. The furnace can be operated also on air.

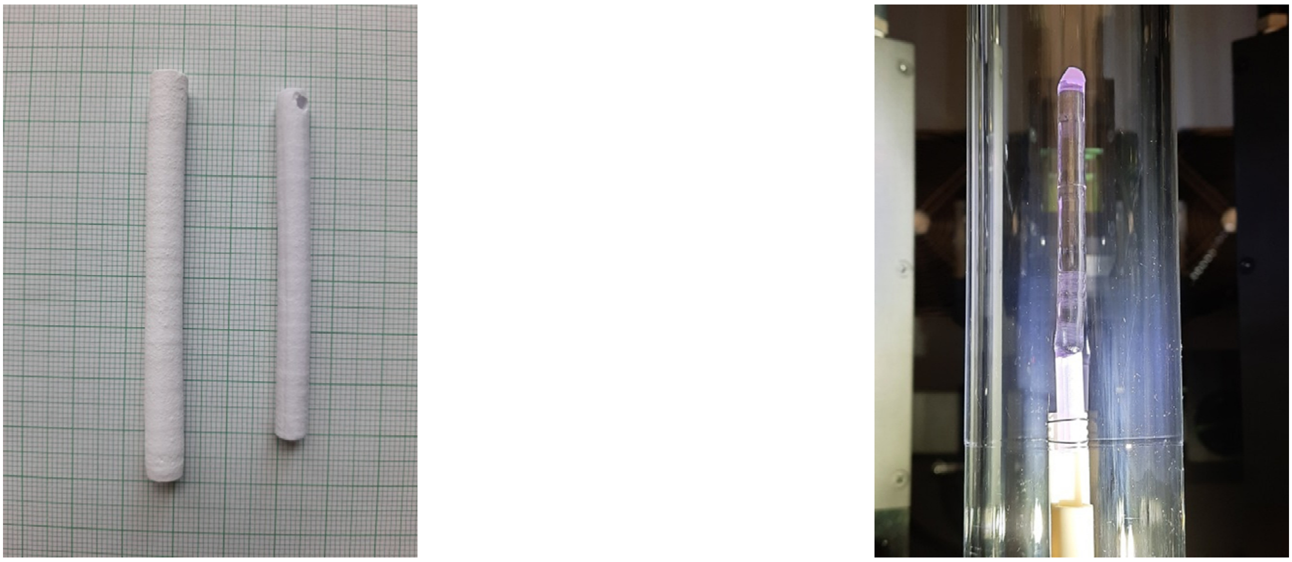


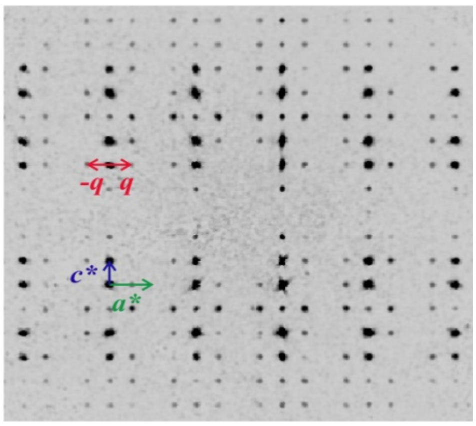
***Fig. 4:** Polycrystalline rod prepared in the new pressing form before (left) and after (right) sintering in the new sapphire furnace. Example of YAG single crystal.*

Extension of structural characterization possibilities

Until recently, the MGML instrumental equipment utilizing an x-ray scattering processes for a structural characterization supported only several basic characterization techniques. Namely these techniques were restricted to Laue method used for orientation of single crystals, x-ray powder diffraction in Bragg-Brentano geometry, and a medium-resolution diffraction in a parallel beam geometry; though the latter two available for sample temperatures down to impressive 3 K. Since the previous upgrades of technology laboratories extended the sample preparation methods by floating zone technique, chemical vapor transport or hydrothermal synthesis, it made it possible to prepare materials of a larger diversity and a higher complexity and thereby a necessity of more advanced structural characterization techniques arose. In 2020, the MGML users could utilize such techniques requiring top level instruments due to the cooperation with Department of Structure Analysis, IoP CAS, and with the X-ray Group, Department of Condensed Matter FMP CU. Newly available methods consisted of single crystal diffractometry, (grazing incidence) small angle x-ray scattering, pair distribution function analysis, high-resolution diffractometry and in-plane x-ray diffractometry; all of them with possibility to measure in non-ambient conditions. The MGML users could also benefit from the instrument operational know-how and the data evaluation support provided by the local staff. In summary, the current characterization possibilities were extended for instance by structure refinement, phase-, stress-, and texture analysis, crystallite and particle size determination, all applicable now on variety of (standard and nonstandard) sample types such as small/bulk single-crystals, nano-particles in powders/liquids, thin/epitaxial (multi-)layers, quantum dots and further complex low dimensional systems. The overview of accessible instruments and the brief specification follows.

Single crystal x-ray diffractometer

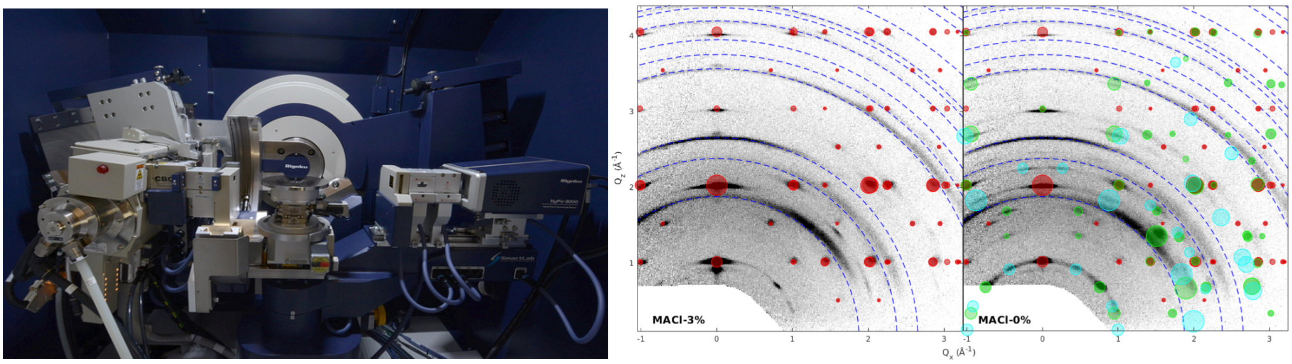
Single crystal diffractometer SuperNova (Agilent Technologies, Rigaku Oxford diffraction) with dual wavelength (Cu and Mo) micro-focus x-ray source is equipped with Kappa goniometer and CCD detector. It is capable to measure samples in temperature range 80—500 K using Cryostream 800 cooler. The diffractometer is dedicated to the single crystal diffraction measurements allowing to solve and refine standard and modulated structures.



Left: SuperNova diffractometer. Right: Example of reconstructed reciprocal space section for $CePt_2Al_2$ crystal measured with this SuperNova. Adapted from P. Doležal, et al, Inorganic Chemistry ***2020*** *59(17), 12263-12275*

Universal high-brilliance x-ray diffractometer

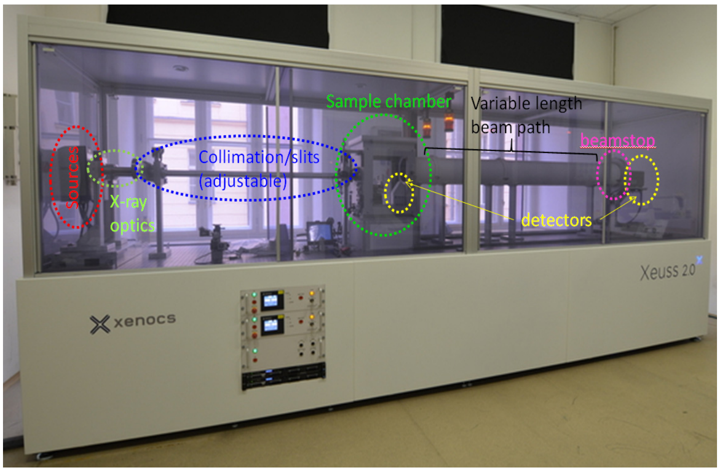
Rigaku Smartlab equipped with 9 kW rotating Cu anode and Θ-Θ vertical goniometer is a multi-purpose diffractometer suitable for measurement of wide range of sample types including polycrystalline powder and bulk samples, thin coatings, epitaxial and other low dimensional structures. All standard measurement techniques such as x-ray reflectometry, powder diffraction in Bragg-Brentano and parallel beam geometries, high-resolution reciprocal space mapping benefit from the combination of a high brilliance source and a fast single-photon counting 2D detector that allows producing high-quality data at no additional expense of exposure time. Besides all standard diffraction techniques following quite extraordinary diffraction techniques are also available. Firstly, optionally mountable optical module (Johansson K-alpha1 monochromator) produces a divergent monochromatic beam for a powder pattern measurement in Bragg-Brentano geometry in order to do highly precise peak profile analysis. Secondly, the detector arm of the vertical goniometer has also possibility of horizontal movement that allows performing of in-plane diffraction measurements giving an access to the lattice planes perpendicular to the sample surface. Thirdly, an easily changeable sample to 2D detector distance makes it possible to switch from a high resolution mode to a low resolution super-fast reciprocal space mapping that can be used for rapid pre-characterization of the samples; well suitable for instance to reveal a crystallographic orientation of a single-crystalline epi-layer, which is generally undoable using conventional Laue method and it is quite time consuming using a high-resolution space mapping.

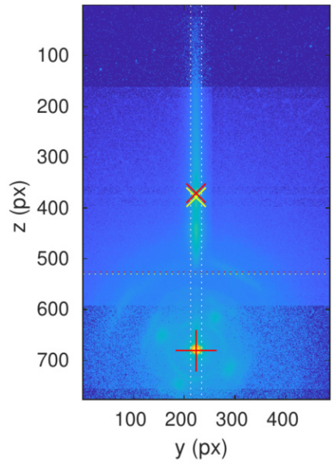


*Left: Rigaku Smartlab. Right: Measured with this diffractometer, low-resolution reciprocal space maps for FAPbI3 thin coating crystallized with assistance of different MACl additive concentration. Already one-hour measurement can reveal the complicated texture composition in the coating. Adapted from Supplementary materials for A. Amalathas, et al., ACS Applied Energy Materials **2020** 3 (12), 12484-12493.*

Small angle x-ray scattering apparatus

Xenocs Xeuss 2.0 equipment for small angle x-ray scattering (SAX) and grazing incidence small angle scattering (GISAXS) is equipped with Cu and Mo micro-focus x-ray sources, toroidal x-ray mirror optics producing the parallel beam, motorized scatter-less slit system and evacuated sample chamber. Two hybrid single photon counting detectors Dectris Pilatus 3R 200k and 100k are combined to measure simultaneously both SAXS signal and a wide angle x-ray scattering (WAXS) signal (diffraction angle between 15°and 45°). A changeable sample to detector distance together with a possibility to switch between two different wavelengths make accessible a reciprocal space between 0.003 Å-1 and 0.5 Å-1. This range allows studying nanomaterials and low dimensional structures of sizes between 1.3 nm and 209 nm. The samples can be measured at non-ambient conditions using Linkam THMS 600 (-195°C to 600°C) and Linkam TS 1000 (ambient to 1000°C) chambers. Deformation stage (MTI) can be mounted for in-situ measurements as well.

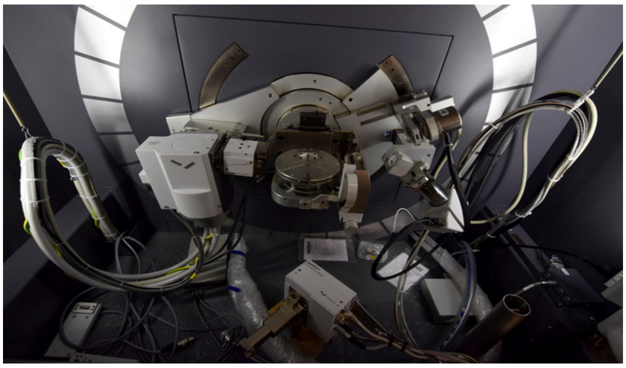


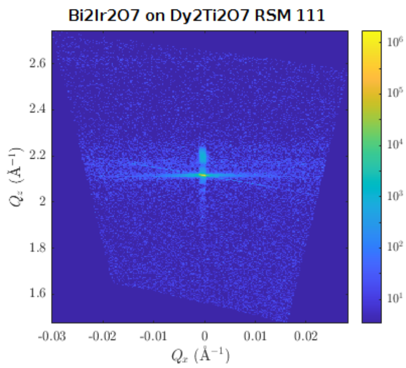


Left: Xenocs Xeuss 2.0. Right: GISAXS image from the presented instrument measured for thin coating of $LuFeO_3$ on Pt island-like electrode deposited on sapphire.

High energy x-ray diffractometer

Panalytical Empyrean II diffractometer is equipped with Θ-Θ vertical goniometer and with substitutable x-ray sealed tube sources: Cu, Mo, and Ag radiation. For low energy radiations (Cu and Mo), parallel beam optics, high resolution setup (hybrid monochromator and crystal analyzer) and Bragg-Brentano high definition optics (plane mirror) are available. With high energy radiation (Ag), the diffractometer can be used for optics-free Bragg-Brentano measurements, however the main purpose is a measurement of diffraction pattern for a Pair distribution function (PDF) analysis when mounted with elliptic focusing mirror for Ag radiation (focusing on the detector). High detector efficiency (<98%) for all three wavelength is achieved using 2D detector GaliPix (hybrid pixel, single photon counting technology with CdTe chip). The goniometer is mounted with a standard Eulerian cradle. The diffractometer can be equipped with reactor chamber XRK 900 (Anton Paar) allowing the measurements up to 900°C and pressure of 10 bar. Eventually, Cryostream 800 cooler (Oxford Cryosystems) for x-ray studies between 80 – 500 K and a deformation stage for in-situ measurements are available as well.

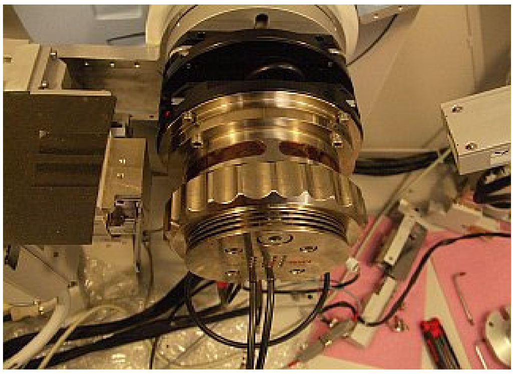


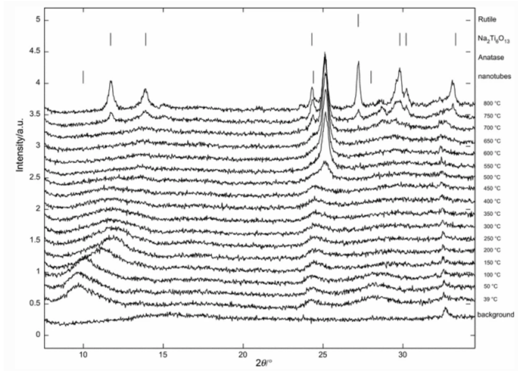


Left: Panalytical Empyrean. Right: Measured with this diffractomter in high resolution mode, reciprocal space map of $Bi_2Ir_2O_7$ epilayer deposited on $Dy_2Ti_2O_7$ substrate.

High temperature x-ray diffractometer

Powder diffractometer Panalytical MPD equipped with Θ-Θ vertical goniometer, Cu sealed tube source and 1D Pixcel detector can be mounted with high temperature chamber allowing measurements from room temperature up to 1600°C. In Bragg-Brentano geometry automatic variable slits controls the irradiated area of the sample to be constant. For parallel beam geometry with an incident parallelizing parabolic mirror, two possible analyzers can be mounted: first, a parallel plate analyzer for a grazing-incidence and/or symmetric diffraction, second, a secondary receiving parabolic mirror for a symmetric and/or grazing-exit diffraction.

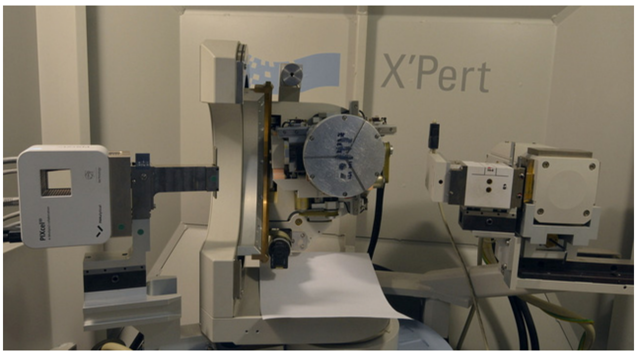


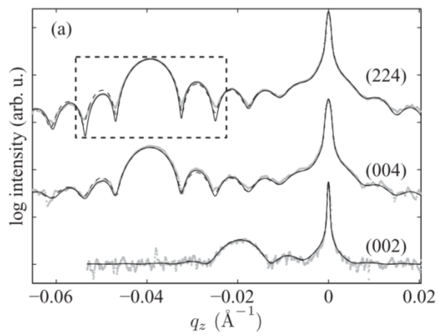


Left: Panalytical MPD mounted with high temperature chamber. Right: PXRD patterns for Ti-NT system during heating in air.. Measured with the presented diffractometer and adapted from T. Vaclavů. Et al., J Therm Anal Calorim ***128****, 779–785 (2017).*

High-resolution x-ray diffractometer

Panalytical MRD diffractometer with a sealed x-ray tube (Cu radiation) is equipped with a horizontal goniometer and 2D Pixcel single photon counting detector. As a low resolution primary optics can be mounted x-ray polycapillary well suitable for stress and texture measurements; or parallelizing parabolic mirror for grazing incidence diffraction and x-ray reflectometry. For high-resolution measurements, a hybrid monochormator (x-ray mirror + channel cut Ge crystal) or combination of x-ray mirror and Bartels (4bounce) monochromator are available on a primary beam side. On the diffracted beam side, the 2D detector or 3-bounce analyzer crystal can be used. The diffractometer is equipped with Anton Paar Doomed Hot Stage allowing elevating the sample temperature up to 1100°C.



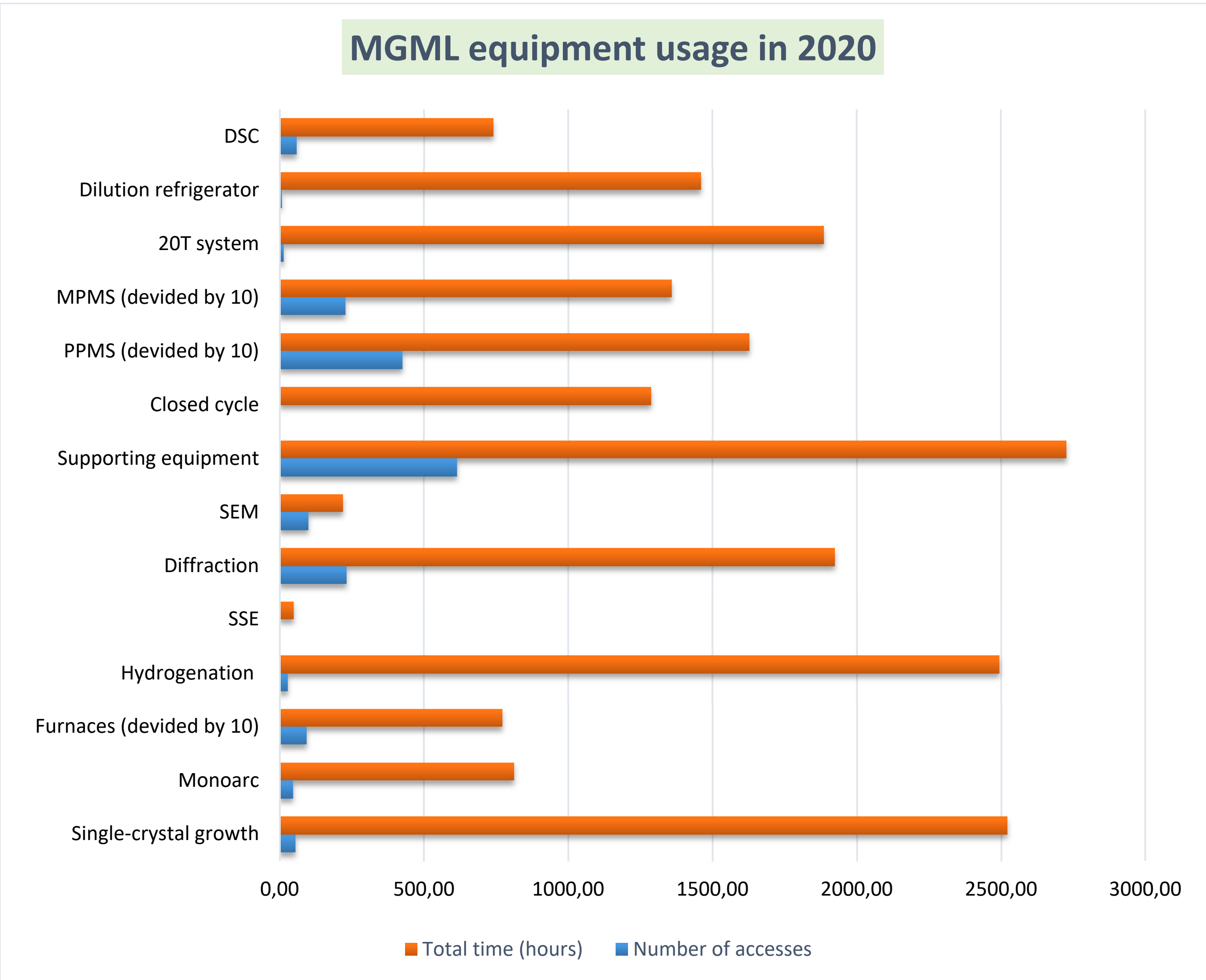


Left: Panalytical MRD diffractometer. Right: measured with the presented diffractometer in high-resolution mode, several diffraction curves for GaMnAs epitaxial layer on GaAs substrate. Adapted from L. Horák, et al., Phys. Rev. B ***83****, 245209 (2011).*

User Programme

Reflecting the epidemic restrictions, MGML enables to perform most of the experiments online without personal presence of the user in the laboratory. In total, 52 experimental proposals were accepted, among them 29 long-term proposals, 9 standard and 14 test proposals. Experiments were performed by users from 5 different countries. Namely, Czech Republic, Slovakia, Germany, Ukraine and United Kingdom. Majority of experiments were performed by users from Czech Republic.

The usage of individual equipment is depicted in the following Figure. Despite the restrictions due to the epidemiological situation, practically all the equipment is frequently used. In some cases (dilution refrigerator) even considerably more than in the previous year. It is thanks to the fact, that most of the instruments can be operated online and do not require physical presence of the user. Users can just send their samples, the measurement is then performed by the MGML staff. The PPMS, MPMS, 20T system, furnaces and crystal-growth equipment together with the X-ray diffraction analysis are the most used ones, similar to 2019.



Conferences, Workshops, Events

Kick off meeting – ISABEL project

On the 20th of November, all the participants of the project ISABEL gathered online to officially start the beginning of the project ISABEL and to organize the actions which will be implemented within the four next years.

As usual in 2020, the meeting was held only in an online form (instead of planned meeting in Toulouse). Nevertheless, it was a great opportunity for everyone to meet as a team, sharing their ideas and defining the coming agenda. All the participants are rather enthusiastic and we are looking forward to the collaboration.

The large-scale facilities mini-school through a virtual format

Before the current crisis, a mini-school for budding physicists was planned and organized by scientists at the Technical University of Munich and MGML, Charles University – a cooperation project funded by the Bayerisch-Tschechischen Hochschulagentur. But as it has turned out, Corona forced the event to be held in a virtual format. The silver lining is that this format has allowed a larger number of people from around the world to participate.

The aim of this **Czech-Bavarian mini-school**, held from the 18th to the 22nd of October, was to introduce the junior researchers to the large-scale facilities ELI (Extreme Light Infrastructure) beamlines, the Charles University, and Heinz Maier-Leibnitz Zentrum. Through these introductions, participants could gain valuable insights into these laboratories as well as opportunities for networking and socialisation.

An online event does have a few clear advantages – instead of the original 20 participants from Munich and Prague, close to 100 scientists from 20 different countries registered for the various different lecture series.

In spite of the restrictions imposed by the current conditions, the highlights of the mini-school were the guided tours through the different large-scale facilities. The ELI beamlines near Prague, reconstructed their laboratories virtually, allowing for a complete online tour to take place. Similarly, Dr. Johanna K. Jochum organized a tour which led the students through the FRM II using a webcam. In addition, the students received a detailed look through the Materials Growth & Measurement Laboratory.

Hands-on data evaluation

In addition to guided tours and lectures, the students from Prague and Munich were able to demonstrate their presentation skills and give a short introduction to their research topics during the student flash talk competition. The participants delivered impressively clear and creative talks, even under the pressure of strict time constraints.

During the last day of the mini-school, the participants were apprised of an important current trend in the documentation of scientific research: Open Data based on the “FAIR” principles of “findability, accessibility, interoperability, and reusability” of data for the good of the entire scientific community. After an extensive introduction to the topic and several open data tools, the participants were given a chance to immediately apply these tools to a dataset made available by the Institut Laue-Langevin.