# Crystallography in the Czech and Slovak Republics now


The first use of X-rays in Czechoslovakia shortly after their discovery were restricted to medical applications and testing of materials. The applications of XRD in *materials science* was probably the leading stream of crystallography and structure analysis in this territory and still plays an important role. However, simultaneously mineralogical, chemical and physical crystallographies were developing and in the last years biocrystallography has been growing quickly as well. Several scientific centra supported from EU funds have arised now. Examples of a few of the most important groups with only a few person selected are briefly listed below.

## Crystallography in Materials Science, Applied Crystallography, Physics

Applications closely related to industry were developed in famous Czechoslovak enterprise **Škoda** in Plzeň and its research institute. Nowadays, the work is concentrated in the **New Technologies - Research centre in the West Bohemia region** (P. Šutta, J. Fiala) equipped with modern powder diffractometers. The current research is concentrated on research and development of materials for photovoltaic cells of second and third generations, on materials for photonics and on microsystems technology.The work in the *Department of Physics at the Faculty of Applied Sciences,* **University of West Bohemia** (R. Čerstvý) is aimed in investigation of a new generation of thin-film materials with unique physical properties and a high application value. These materials are produced by modern physical technologies using mainly plasma discharges of various kinds (DC, RF, and MW discharges in a continuous or pulsed mode)

In **Škoda car factory** (Mladá Boleslav) the diffraction is daily used as an output control of compressive stress profiles in parts of gear units. Another famous company is **Precheza Přerov**, the biggest producer of inorganic pigments in the Czech Republic, one of the three producers of titanium dioxide within the countries of CEFTA and an exporter of technological knowledge. Diffraction is routinely used in several cement works.


M. Černík

The most advanced *texture measurements* are currently performed in **U. S. Steel Košice** (Research and Development, M. Černík) with the aid of a new texture goniometer detectors as well as several modern texture sotware, is well complemented with the EBSD. Rolled steel sheets, coatings, ceramics, sediments, dusts, sludges, different slags, casting powders, entry ores, etc. are analyzed.


Ľ. Čaplovič

In Slovakia, XRD in materials science is most developed now in **Institute of Materials, Faculty of Materials Science and Technology in Trnava** (L. Čaplovič, M. Kusý)**.** The institute received the EU project and the research is directed to complex metal alloys, corrosion resistivity of austenitic alloys, steels for cutting tools prepared by powder metallurgy and equipment for nuclear industry. Stresses and thermophysical properties are studied as well.


N. Ganev

Scientific development of the X-ray methods related to materials science is located mainly in universities and the Academy. One of the places with long history is the Department of Solid State Engineering, **Faculty of Nuclear Sciences and Physical Engineering, Czech Technical Univer-sity in Prague** (now mainly N. Ganev, L. Kalvoda). X-ray laboratory has the reputation for being the leading work-place for X-ray diffraction tensometry and has strived to meet the growing demands for knowledge of surface and depth distributions of macroscopic and microscopic residual stresses resulting from wide range of material manufacturing and surface treatments. Neutron diffraction group cover the range from location of light atoms and cation distributions to magnetic structures and phase transitions.

Not only pure applications of XRD should be mentioned but also developing units. There is a long tradition in development and production of X-ray optical elements and detectors, cameras (e.g. **Rigaku Innovative Technologies Europe, s.r.o. in Prague** or **Crytur in Turnov**).

***Nanomaterials*** are studied at several different places. For example at the **Nanotechnology centre, Technical University of Ostrava** (M. Valášková, G. Simha Martynková), where nanomaterials based on modified inorganic layered structures (phyllosilicates and hydrotalcites), metal nanoparticles and their oxides, silicate nanoparticles are prepared by different techniques and investigated. **Regional Centre of Advanced Technologies and Materials** was founded at **Faculty of Science, Palacky University, Olomouc** (R. Zbořil, J. Filip) and it is focussed to research of metal oxide nanoparticles for catalytic, magnetic and biomedical applications, carbon nanostructures based on graphene and carbon quantum dots, metal nanoparticles for antimicrobial treatments and water treatment technologies, medical, computational and coordination chemistry and photonics. Research infrastructure **NanoEnviCz at the University of J.E. Purkyně in Ústí nad Labem (**P. Čapková, P. Ryšánek) is focused on the research of nanomaterials, surfaces and nano-composites for environmental and related applications including the controllable syntheses, complex characterization, tuning their functional properties, monitoring their potential toxicity and developing their application in advanced technologies.


J. Filip

**Brno University of Technology** has a long tradition in collaboration with industry and development of advanced ceramics for medical purposes. In the **Institute of Physics of Materials in Brno** (O. Schneeweis, P. Roupcová) structure and properties of metallic and oxidic magnetic materials prepared by non- traditional technologies and role of defects in electrical, magnetic and mechanical properties of ordered intermetallic systems are studied for example


P. Roupcová

Several laboratories are oriented between materials science and physics
Department of Condensed Matter Physics**, Faculty of Mathematics and Physics, Charles University in Prague** (mainly V. Holý, R. Kužel, M. Dopita, S. Daniš) well-equipped with several modern diffractometers deals with broad spectrum of topics. In addition to study of materials with interesting magnetic properties, nanocrystalline powders and thin films and their thermal stability, crystallization process, nanotubes, nanorods, self-ordered surface structures like quantum dots, ultrafine-grained materials prepared by sever plastic deformation, strongly oriented thin films, epitaxial thin films, multilayers, shape-memory alloys. Software for total powder pattern fitting related to real structure characterization has been developed. Large attention is devoted to modern materials like new semiconductors with ordered magnetic moments - ferromagnetic and antiferromagnetic (LiMnAs, NaMnAs, CuMnAs), hexagonal ferrites, topological insulators. Neutron diffraction mainly at ILL is highly used also for studies of magnetic structures.


V. Holý


P. Mikulík

Traditional X-ray group, Department of Physics, **Faculty of Science Masaryk University in Brno** (P. Mikulík, M. Meduňa, O. Caha, J. Novák) has long-time collaboration with semiconductor industry and improved significantly equipment with several modern powder and thin films diffractometers also for in-situ measurements. The studies include now structure of single crystal films and multilayers, interface roughness in superlattices, quasi-periodic superlattices, defects in semiconductors and their nano-structures, mainly for optoelectronic and magnetic applications. The group is also involved in large CEITEC project.

**Institute of Physics, Academy of Sciences of the Czech Republic** (IP ASCR) always belonged to the main crystallographic centres in Czechoslovakia and it has several X-ray laboratories nowadays.

The ***Laboratory Rotan*** (D. Šimek, Z. Šourek, J. Kub, M. Čerňanský, V Studnička) is now equipped with two X-ray rotating anode generators and contributes to further technological research in many fields. The structural problems of condensed matter physics are solved in a wide spectrum of materials by different and often unique techniques. For example - nanoscopic ferroelectric and nanoscopic ferromagnetic films real structure of surface of mechanically treated materials, depth gradients of macro- scopical strain, crystallite size and microstrains. High resolution X-ray diffraction and reflectometry were used for example for studies of metal and semiconductor superlattices.


Z. Šourek


D. Šimek

***Department of structure analysis*** is quite large and famous group nowadays. The main activity consists now in development of crystallographic computational methods. System Jana (V. Petříček, M. Dušek, http://jana.fzu.cz)) has become a world standard for complicated structures and covers vast regions of crystallography - service crystallography, incommensurate modulated structures, commensurate structures, composite and magnetic structures. Its remarkable feature is the ability of combination of different data and structural model can be refined simulatenously with single crystal and powder data. New direction is precession electron diffraction tomography (L. Palatinus, M. Klementová) used for structure determination of microcrystals and nanoparticles. The group has modern both single crystal and powder diffractometers.


V. Petříček


M. Dušek

**Institute of Physics, Slovak Academy of Sciences (SAV), Bratislava** (M. Jergel, P. Šiffalovič, K. Végsö, E. Majková). The department of multilayers and nanostructures is focused on preparation and study of thin films, multilayers and nanostructures for X-ray optics, spintronics and sensors. It also investigates processes of growth and self-assembling of nanoparticle ensambles prepared by modified Langmuir-Blodgett technique. Different techniques are used - non-specular reflectometry, SAXS with MetalJet and GISAXS. The diffuse scattering is studied for characterization of surfaces and interfaces. For GISAXS a new equipment was constructed that allowed in-situ studies of 2D nanoparticle crystals on the interface liquid-air and test models of paracrystal. Other equipment of GISAXS with microfocus source enables in-situ studies of thin films growth at dual-ion beam deposition. Department of metal physics (P. Švec, D. Janičkovič, M. Krajčí, M. Mihalkovič) was one of the first where the rapid cooling technology was developed for preparation of strips of amorphous metal alloys with unique combination of mechanical and magnetic properties. Now, it develops the technique for new microcrystalline and bulk materials with desired properties. The group contributed significantly to the theory of intermetallic alloys and quasicrystals.

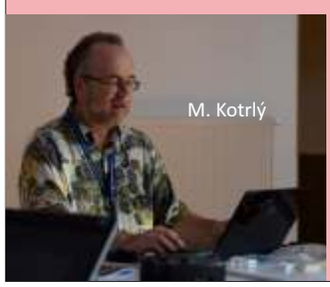
A consortium **MULTIDISC** for multidisciplinary research of materials was established in Slovak Academy of Sciences and the first X-ray diffractometer with rotating anode in Slovakia serves now for a large scale of studies including coplanar reciprocal space mapping, phase analysis, strains and stresses. The common laboratory of the Institute of Physics and Inst. of Electrical Engineering (E. Dobročka) collaborate also on development of new elements of X-ray optics. Studies in Faculty of Mathematics, Physics, and Informatics of the Comenius University in Bratislava (T. Roch) are focussed on analysis of different polycrystalline thin films.


M. Jergel

## Crystallography in Art and Forensic Science


P. Bezdička

Applications of X-ray diffraction in the field of art, archaeology, forensic science have become very popular in last years. A new insight into the material microanalysis of painted artworks in Prague was opened in 2004 when the **Academic Materials Research Laboratory of Painted Artworks (ALMA)**, (P. Bezdička) joint workplace of the Academy of Fine Arts in Prague and the Institute of Inorganic Chemistry of the ASCR was established. Combining the branches of the natural sciences, art and history, it pursues deepening the knowledge of painting materials and techniques. ALMA Laboratory develops instrumental materials analysis methods and interprets the results in the context of art history and history of materials technology. In particular, for XRD analysis the aim is to reduce the amount of material to be analysed and sample size. The labora-tory cooperates with PANalytical.


M. Kotrlý

The **Institute of Criminalistics in Prague** (M. Kotrlý). The history of XRD there goes back to 60's last century. In last years, stress is imposed to the verification of analysis by at least two independent methods. In this connection the role of XRD phase analysis is crucial.

## Mineralogy

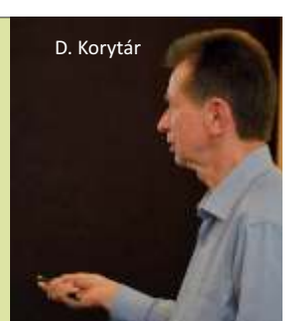
The origin of mineralogic crystallography is connected with B. Ježek (see history) and in recent time with M. Rieder. Nowadays, the major portion of mineralogical investigations in Czech Republic originates in the **National Museum** (Prague), **Czech Geological Survey** (F. Laufek), **Geological Institute** (R. Skála) and **Faculties of Science of Charles University in Prague** (V. Goliáš) , **Masaryk University in Brno** (V. Vávra) and **Palacký University in Olomouc** and also in other institutions, where the X-ray powder diffraction is used mainly as routine analytical method. Bohemian region is famous for its mining centers with many localities and deposits of base metal, silver, gold and also uranium ores (like Kutná Hora, Příbram or Jáchymov). About ninety new mineral species were described from these localities and were approved by International mineralogical association. Every year, there are few additional descriptions and crystal structure determinations of the new natural crystalline phases. From the latest findings we can mention for example a new phase vavřínite from Northern Bohemia, litochlebite from the northern Moravian uranium deposit, pale green slavkovite or orange-yellow sejkoraite-(Y) from Jáchymov deposit.


F. Laufek

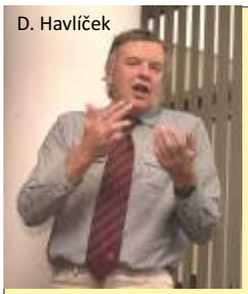

R. Skála

## X-Ray Optics

The **X-ray optics group of IP AS CR** (J. Hrdý, P. Oberta) in cooperation with local industry (ABB s.r.o.) works successfully in the field of design, testing and production of cooled monochro-mators for synchrotron radiation facilities. Another achievement is the development of X-ray crystal monochromators with curved (not bent !) working surface based on the diffractive-refractive optics. 1-D and 2-D monolithic crystal optics using asymmetric flat diffractors is being developed at the Department of Technology and Diagnostics of Semiconductors (DTDS) of the **Institute of Electrical Engineering, Slovak Academy of Sciences in Piestany, Slovakia** (D. Korytár). In-line optics with the input and outgoing X-ray beams being mutually parallel have been devised, realized and tested with laboratory and synchrotron sources.


D. Korytár

## Chemical Crystallography


D. Havlíček

The Center of Molecular and Crystal Structures at the **Faculty of Science**, **Charles University, Prague** (I. Císařová, D. Havlíček, P. Vojtíšek) was established in 2000. In average, three structures are solved daily. The main topics are: organo-elemental chemistry and catalysis, coordination and bio-inorganic chemistry, chemistry of solids and nanomaterials. The lab is equipped with modern single crystal and powder diffractometers now.


B. Kratochvíl

**Institute of Solid State Chemistry, Institute of Chemical Technology Prague** (B. Kratochvíl, M. Hušák, J. Čejka) deals mainly with applications of XRD in pharmaceutical industry, in particular correlation of structure and properties, monitoring of polymorphism of pharmaceutical compounds (anhydrates, hydrates, salts, co-crystals). The group contributed largely to promotion of XRD techniques in several pharmaceutical companies. Characterization of new materials for catalysis, ecological applications, geopolymers also belong to important topics. X-ray lab of the Central Laboratories of the institute (J. Maixner, R. Pažout), a service center for phase analysis and XRD and XRF data analysis also deals with structure determination of small organic molecules, crystal growth and single crystal diffraction on individual grains. The group of inorganic solids deals new materials for catalysis and geopolymers.

**Molecular simulations laboratory at the Faculty of Mathematics and Physics, Charles University** (M. Pospíšil, J. Burda) was established in 1997. The simulations by Materials Studio are mainly used for calculations of various types of silicates intercalated with organic species, anionic clays like layered double hydroxides (LDH) with positive layer charge intercalated with benzoic acid and its derivatives and porfyrin molecules.

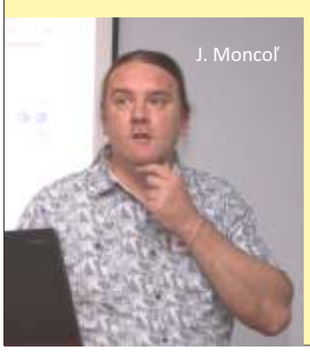
Other groups connected to chemical crystallography are – **University of Pardubice; Faculty of Science, Masaryk University Brno and Faculty of Science, Palacky University Olomouc** (Department of Inorganic Chemistry, Z. Trávníček), is oriented on new complex compounds of transition elements, new biologically active compounds with application in medicine, materials for molecular magnets, sensors etc.


L. Smrčok

In Slovakia, three places should be mentioned. **Institute of Inorganic Chemistry, Slovak Academy of Sciences** (L. Smrčok, 1954-2016). Activities are related to the development of advanced computational methods of electron interactions in molecules and solids, magnetic and electric properties of medium-size systems, organometallic and biologically and catalytically active compounds. Precise DFT calculations are combined with different experimental techniques.

Development of crystallography in Slovakia has been closely connected to coordination chemistry. This is now most related to the **Faculty of Chemical and Food Technology, Slovak Technical University** (M. Koman, J. Kožíšek, J. Moncoľ, V. Jorík), where a modern single-crystal X-ray laboratory was established able to solve the structure of very small, weak diffracting crystals, merohedric twins and the absolute structure of small organic molecules and also to study electronic structures of solids. Main orientation is in complex functional objects, in particular materials and catalysts in live organisms or those in ecological applications. This includes preparation, study of structure, chemical and biological reactivity of materials with applications in medicine and used as precursors for preparation of new materials. The research of biocoordination compounds, namely carboxylate complexes of copper and iron with biologically active ligands are of interest now, first of all.


J. Kožíšek


J. Moncoľ

Small molecules based on coordination compounds (mainly cyanido-complexes based on Ni, Cu, Pd and Pt, along with zinc complexes containing biologically active ligands are studied at the **Department of Inorganic Chemistry of P. J. Šafárik University in Košice** (J. Černák).

## Biocrystallography


J. Hašek

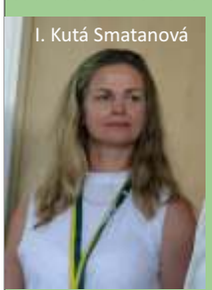
Czech and Slovak scientists published their work containing results of protein crystallography already before 1990. However, the principal crystallographic works were done only in cooperation with foreign laboratories. The first real investment into the protein crystallography was a joint project of the **Institute of Molecular Genetics** (now e.g. P. Řezáčová, J. Brynda**)** and the **Institute of Macromolecular Chemistry of the Academy of Sciences in Praha** in 1998 (J. Hašek, J. Dohnálek**)**. Now, the former group of structural biology has developed labs significantly and carries out structural studies on various proteins of biological or medicinal interest in a joined laboratory of Institute of Molecular genetics and Institute of Organic Chemistry and Biochemistry CAS. Among main targets, protease from HIV, antibody fragments as well as other human enzymes take a prominent position.


P. Řezáčová

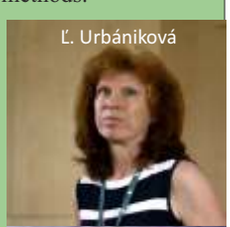

J. Dohnálek


J. Brynda

The latter group moved to the **BIOCEV** and new **Institute of Biotechnology** (B. Schneider, J. Dohnálek, J. Hašek). The *Laboratory of structure and function of biomolecules* is focused on application of XRD analysis on the problems of structure-function relationships in biological macromolecules, mainly structure elucidation of new and novel enzymes, receptors, or complexes. The *Laboratory of biomolecular recognition* studies interactions between proteins and nucleic acids with the goal to understand the mechanisms of their specific mutual recognition. Computational and experimental approaches are combined. The *Centre of Molecular Structure* offers services in biological crystallization, X-ray diffraction and structure solution, advanced structural mass spectrometry and biophysical characterisation of biomolecules and their complexes.

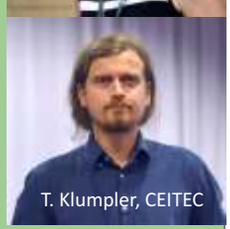

I. Kutá Smatanová

**Laboratory of Structural Chemistry at the Faculty of Science, University of South Bohemia** (I. Kutá Smatanová) does the basic research in the field of isolation and purification of proteins and their crystallization, structural studies of proteins and develops alternative and advanced crystal-lization techniques. There is a strong collaboration with **Center for Nanobiology and Structural Biology, Institute of Microbiology, Nové Hrady** (R. Ettrich) focused on relationship between the structure and function of the proteins and their complexes by experimental and computational methods.


Ľ. Urbániková

**Laboratory of Prokaryotic Biology, Institute of Molecular Biology SAS in Bratislava** (L. Urbániková) studies genomics, proteomics and transcriptomics of bacteriophages and relations structure-function of the enzymes degrading the cell walls.

Relatively broad spectrum of crystallographic methods is present in **CEITEC (Central European Institute of Technology) in Brno** including core facilities *Biomolecular Interactions and Crystallization* (M. Wimmerová) with services leading to structure characterization of biomolecules and to study (bio)molecular interactions in a real time using mainly biosensor and calorimetry-based methods. Modern top equipment is in *X-ray Diffraction and Bio-SAXS Core Facility* (J. Marek) and *Cryo-electron Microscopy and Tomography* (J. Nováček).

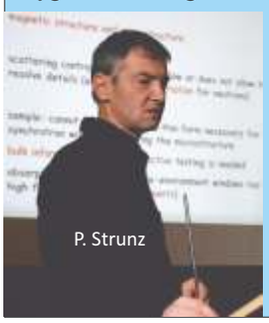

T. Klumpler, CEITEC

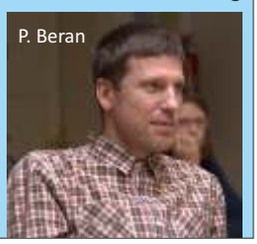
Among other groups, the **1st Medical faculty and Faculty of Natural Sciences of the Charles University in Praha** (T. Obšil) **and Palacky University in Olomouc** (Z. Trávníček) should be mentioned.

The variety of institutions also means a variety of topics ranging from medical, agricultural applications (drug design, genetic deseases, cell receptors, transmembrane transport, bio-compatible materials, etc.) to food production and industrial applications (enzyme engineering, new products, activity under extreme conditions, etc.). Studies are also oriented on theoretical explanation of self-organization and effectivity of processes in macromolecular systems. The sources of synchrotron radiation used most frequently for measurements are ESRF, BESSY, DESY, MAX laboratory.

## Neutron Scattering

The centre of neutron scattering is at the **Nuclear Physics Institute ASCR**, v.v.i., **Řež near Prague** (P. Mikula, P. Lukáš, J. Strunz, J. Šaroun, P. Beran). Studies of ***neutron optics*** are at present focused on studies of multiple reflections in bent perfect crystals or in a sandwich like bent perfect crystal and includes also development of Monte Carlo simulation software RESTRAX. A complete apparatus for ***neutron interferometry*** was developed and built up. Efficient focusing monochromators and new position sensitive detectors opened new possibilities in materials science as ***residual stress*** mapping (weld joints, composites and functionally graded ceramics) and investigation of stresses in situ upon mechanical loading (different kinds of modern steels, martensitic transformation in shape memory alloys). New type of small-angle neutron scattering (**SANS**) instrument was designed and constructed: original high-resolution double-bent-crystal diffractometer MAUD useful for for characterization of inhomogeneities of the dimension of 20 nm - 1 μm (e.g. large precipitates in superalloys, porosity of ceramics, cavities in superplastic ceramics). Modern powder diffractometer MEREDIT is equipped with an efficient multidetector system, changeable mono-chromators and variety of sample environment devices (vacuum and radiation furnace, deformation rig, close-cycle cryostat). This is used now for studies of archeological artifacts, oxygen conducting materials for fuel cells and hydrogen storage materials, crystal and magnetic structure of magnetocaloric materials, identification of magnetic structure in meteorite compounds and new semiconducting anti-ferromagnets.




## Central European Institute of Technology CEITEC

Scientific centre in the fields of life sciences, advanced materials and technologies whose aim is to establish itself as a recognized centre for basic as well as applied research. It is a consortium whose partners include the most prominent universities and research institutes in Brno, and it benefits from the support of the Region of South-Moravia and the City of Brno. The research is divided into 61 groups and 7 programmes: Advanced Nanotechnologies and Microtechnologies, Advanced Materials, Structural Biology, Genomics and Proteomics of Plant Systems, Molecular Medicine, Brain and Mind Research, Molecular Veterinary Medicine. www.ceitec.cz.

## BIOCEV

BIOCEV is a joint project of six institutes of the Academy of Sciences of the Czech Republic and two faculties of Charles University in Prague. The project's goal is to establish European Centre of Excellence in biomedicine and biotechnology. Main aim is detailed study of cellular mechanisms at the molecular level, research and development of novel therapeutic strategies, early diagnostics, biologically active agents including chemotherapeutics, protein engineering and other technologies with impact on the quality of life. www.biocev.cz

## ELI - Extreme Light Infrastructure

The project ELI is part of a European plan to build a new generation of large research facilities selected by the European Strategy Forum for Research Infrastructures (ESFRI). The main goal of ELI is to create the latest laser equipment in the world. ELI will provide ultra-short laser pulses of a few femtoseconds (10-15 fs) duration and give performance up to 10 PW. Central Bohemia region was selected as the most convenient location for the most intense laser in the world (www.eli-beams.eu).

# 25th General Assembly and Congress of the International Union of Crystallography

**Venue:** **Prague Congress Centre, Czech Republic**

**Time:** August 22 – August 30, 2020

**Main Organizing Body:** Czech and Slovak Crystallographic Association

Czech and Slovak Crystallographic Association
www.xray.cz

www.iucr25.org

CzechTourism

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