Other presented examples represented a ceramic roller and ceramic brick exposed in furnace. After the identification of phase composition by PDF2 diffraction database, recorded data were fitted by programs using Rietveld method to determine the weight portion of phase components. Structures that can not be determined by chemical methods were found and described.

However the texture of tin coatings was determined by EBSD method, but as the sample preparation was and still is very difficult, the X-ray texture analysis was an effective and rapid solution. Obtained results showed good agreement with EBSD and also with corrected pole figures generated by MAUD program.

The measurement of residual stresses in color coated steels showed different values in various directions and asymmetric dependence through thickness of steels. Internal stresses were generated on the principle of four – point bending, which were displayed by “stress – strain” curves in form of hysteresis loop.

References

CRYSTALLOGRAPHY AT THE INSTITUTE OF INORGANIC CHEMISTRY OF THE SLOVAK ACADEMY OF SCIENCES, BRATISLAVA

L'. Smrčok, D. Gyepesová, S. Ďurovič
Institute of Inorganic Chemistry SAS, Dúbravská cesta 5, 845 36 Bratislava

The Slovak Academy of Sciences (SAS) has been founded 18 June 1863, 1953. The Chemical Institute was one of its newly created Institutes and, within it, a Department of Inorganic Chemistry was established. A three-member crystallographic group headed by F. Hanic started working at this Department, which was later transformed into a separate Institute of Inorganic Chemistry (ICH), and the crystallographic group became a basis for a Laboratory for Structural Research (Laboratory in the following). Because of lack of appropriate premises at the beginning, the individual Laboratories of the Department were “hosted” at various Chairs of the Universities in Bratislava. F. Hanic, together with I. Čakajdová and T. Veselovská were “hosted” at the Chair of Physics of the Faculty of Natural Sciences of the Comenius University (FNS CU), in the laboratory of the late J. Maďar. D. Štempelová (later Gyepesová) joined this group in 1960.

F. Hanic attended in 1951 a lecture course in “Radio-crystallography” lead by Assoc.Prof. A. Kochanovská from the Institute of Technical Physics of the Czechoslovak Academy of Sciences (ITPH CAS) in Prague, who accepted an invitation by Prof. Dr. R. Lukáč, who headed the Chair of Mineralogy and Petrography (CMP) of the Slovak Technical University in Bratislava (STU). F. Hanic, who was at the time finishing his studies at the Faculty of Chemical Technology (FCHT) STU became interested in this field and he became a PhD student of A. Kochanovská at her Institute in Prague. Under the supervision of Dr. V. Syneček, he gained a solid basis for his future work in the single-crystal X-ray structure analysis at the SAS. The Laboratory was later expanded by M. Handlovíč, I. Kaprálik, and by technicians K. Jurčo, Z. Klícovská and O. Šályová. F. Hanic headed this group until 1961 when he was appointed as a director of the IICH. F.Hanic supervised eight PhD students, who then started the X-ray structural research at various Faculties in Bratislava, but also in Brno. Together with his team he solved about 35 crystal structures, mainly those of coordination compounds but also of organic structures, the vitamin B6 being among them. It is worthwhile mentioning that, at the beginning, the structures were solved virtually “by hand”. The intensities of individual diffractions on Weissenberg patterns were estimated visually and later from integrated patterns, photometrically. The Fourier syntheses were calculated with the help of Beever-Lipson strips and a desk calculator. The situation significantly improved in 1962 when SAS purchased an East-German (DDR) computer ZRA-1, which used punched cards. Still during “hosting” at the Chair of Physics FNS CU he, together with J. Maďár and mechanician A.Kiss, constructed a prototype of a precension camera, which differèd from the Buenger model by some significant (and patentable) details. This camera was later produced also commercially. In 1970 he was expelled from the Communist party and, consequently, he lost also
his position as Director of the Institute. He worked afterwards as a rank-and-file scientist at another Department of the Institute.

His successor at the Laboratory became S. Úurovič, who became interested in structural crystallography in 1949 as a student at the FCHT STU. He attended a lecture course in structural crystallography lead by Prof. Dr. J. Novák from the Faculty of Natural Sciences Charles University in Prague. After having finished his studies, S. Úurovič became an assistant at the Chair of Prof. Lukáč. He obtained a basic knowledge in single-crystal X-ray structure analysis from V. Syneček during summer praxis at the ITPH CAS in Prague. Together with his former student V. Kupčík, he started an experimental work. Later also E. Makovický, another former student of S. Úurovič, joined them. V. Kupčík and E. Makovický started the structural investigations of sulfosalts minerals and laid down the basis for their classification. They continued in this direction also during their stays in West Germany and Canada, respectively, but, unfortunately, they could not return home during the so-called “normalization” after the Soviet-lead invasion of Czechoslovakia in August 1968. Both of them were later appointed as Professors at the Universities of Götingen (Kupčík) and Copenhagen (Makovický).

F. Hanic started also collaboration with the Institute for Structural Research of the Academy of Sciences of the German Democratic Republic in Berlin, mainly with its Director, Prof. Dr. K. Dornberger-Schiff, the founder of the theory of OD (Order-Disorder) structures. They decided that somebody from the Laboratory should learn this “craftsmanship” and have chosen S. Úurovič, who spent the three months in Berlin to learn the basic ideas and assisted afterwards at the Summer School on OD Structures. The experience thus gained helped him to solve an OD structure of $\gamma$-Hg$_2$S$_2$Cl$_2$ using diffraction data from disordered crystals, during his two-year (1966–7) Postdoctorate Fellowship at the Department of Geology McGill University in Montreal (Canada). In Montreal he also refined the crystal structure of mellite, which solved as first in 1962. Successful collaboration with K. Dornberger-Schiff resulted in an OD interpretation of basic types of sheet silicates later followed, in an efficient partnership with Z. Weiss from the Coal Reserch Institute in Ostrava, by an elaboration of a unitary geometrical theory of the polytypism of sheet silicates.

In 1979 the Laboratory was joined by L. Smrčok who just finished his studies at the FNS CU, where he was attracted to structural crystallography by L. Ulická. His main field of interest became X-ray powder structure analysis and crystallographic computing. In 1981 D. Mikloš, who joined the Laboratory in 1968, replaced S. Úurovič as the Head of the Laboratory. After 1981, three scientists of the Laboratory became functionaries of the Institute, which had a negative impact on the research work and in 1990 the Laboratory was eventually included into the Department of Theoretical Chemistry. In the nineties the Laboratory hosted two young post-doc scientists (E. Morháčová and J. Kečkéš) and later also three PhD students (M. Úrlik, O. Pritula, M. Sládkovičová).

Among the most significant achievements of the Laboratory belong solution of the crystal structure of Ge-mullite and a single-crystal study of thermal transformation of sillimanite, structure solution of Ca$_{10}$(Cr$_3$O$_4$)$_3$(Cr$_3$O$_4$)$_3$, of TiCl$_3$.3C$_2$H$_5$O and of several oxoperoxo complexes of vanadium (V), particularly sensitive to temperature. Later, in the nineties, the Laboratory started a collaboration with Prof. V. Langer (Göteborg) on crystal and electronic structure determination of chiral derivatives of saccharides, largely the amidinodervatives, which are potent ional efficacious compounds in pharmacology as well of some copper(II) complexes containing Schiff base, derived from salicylaldehyde and L-glutamic acid and $N_\circ$, or $O_\circ$ donor neutral ligands. An official collaboration has also been started with Institute of Physics CAS in Prague, the result was a refinement of the crystal structure of cronstedtite-3T and later also of the $1T$ and $2H_2$ polytypes of this mineral, with an efficient partnership by V. Petřiček, but mainly by J. Hybler. An OD interpretation of the cronstedtite structure(s) was decisive in the explanation of its twinning and parallel intergrowths. The X-ray work was greatly corroborated by a high-resolution transmission electron microscopy (HTEM) carried out by T. Kogure from Japan. Also a collaboration with M. Nespolo (Japan, France) on a relation of OD twins to general twins can be mentioned here.

In the course of years the Laboratory coordinated an extensive work on Czech and Slovak crystallographic nomenclature, S. Úurovič, D. Mikloš prepared the screenplay for educational movie “Crystals and Structure Analysis” (director J. Kořán, Krátký film, Prague). The members of the Laboratory also organized short several courses (a course on OD structures, courses on crystallography and crystal chemistry of silicates) and two annual meetings of Czechoslovak Crystallographers. S. Úurovič was a members of an ad-hoc Commission of the International Union of Crystallography for the Nomenclature of Modulated, Disordered and Polytypic Structures and participated in elaboration a proposal for the construction of descriptive polytype symbols. However, the most important contribution of a member of the Laboratory to crystallography is no doubt the chapter “Layer Stacking in General Polytypic structures” for International Tables for Crystallography, Vol. C written by S. Úurovič.