



CZECH AND SLOVAK CRYSTALLOGRAPHIC ASSOCIATION

Activities in 2000 - 2001

The Czech and Slovak Crystallographic Association (CSCA) organized several conferences and 9 traditional one-day seminars in the period 2000-2001.

Seminars on problems of X-ray and neutron structure analysis (Rozhovory)

245th Seminar

Use of the synchrotron source in Trieste in materials research.

Praha 13. 1. 2000, Institute of Macromolecular Chemistry AS CR

Lectures: S. Bernstorff – Scattering and diffraction experiments at ELETTRA. Third generation synchrotron radiation center in Trieste. M. Steinhart – High pressure small and wide angle scattering measurements (HP-SWAXS) at ELETTRA. J. Baldrian, M. Horký, M. Steinhart, S. Bernstorff, H. Amenitsch - Use of the synchrotron source in material science. Polymer blends.

Organization: J. Pleštil, J. Hašek

246th Seminar

Progress in the powder diffraction.

Bratislava 28.3.2000, Faculty of Chemical Technology STU

Lectures: J. Fiala – Geometry of the powder diffraction. V. Kavečanský – Use of the Le Bail approach for the Rietveld method fitting of structural parameters of rare earth hexaferrocyanides. R. Skála – Structure relaxation of low silicon after dynamic compression. V. Jorík – The influence of free atom groups rotation at the complexes on their diffraction pattern. A. Buchal – The possibilities of amorphous phase determination in ceramic samples. M. Ďurík – The solution of crystal structure of monosaccharid using the potential energy minimalization and the Rietveld method. P. Freundlich – Fitting of WC temperature parameter using the non-plane sample surface correction. L. Smrček – The new way of the diffraction data processing - wavelet transformation.

Organization: L. Smrček, V. Jorík

247th Seminar

Praha 22. 6. 2000, Faculty of Natural Sciences, Charles University

Lectures:

Part I. Devoted to the anniversary of prof. M. Rieder

S. Ďurovič, T. Kogre, J. Hybler - Polyttypism of cronstedit $\text{Fe}_3(\text{Si}, \text{Fe})_2\text{O}_5\text{OH}_4$. XRD and HRTEM studies. M. Rieder – Mica classification and nomenclature. A view behind the scenes. M. Drábek, M. Rieder, M. Mellini, Z. Weiss – Cs-mica - crystal structure and their use for radionuclides deposit. P. Čapková – Intercalated phyllosilicates structure. Z. Weiss – Using of diffraction patterns modelling for the evaluation of kaolinite structure disorder.

Part II.

D. Havlíček, L. Dobiášová – XDR analysis of fly aerosols. I. Císařová – Structure - easily and quickly. First months with CCD detector measurements. M. Šlouf – Atomic charge experimentally determined with single crystal structure analysis.

Excursion - Nonius Kappa CCD.

Organization: Z. Weiss, I. Císařová

248th Seminar

Praha 22. 11. 2000, Institute of Physics AS CR

Lectures: M. Polcarová – In situ XRD topography using the synchrotron radiation: application on the Fe-Si bicrystals. J. Hrdý – X-ray crystal optics for synchrotron radiation. Z. Šourek – $\text{A}^{\text{III}}\text{B}^{\text{V}}$ superlattices structure characterization studied by the high-resolution XRD. M. Čerňanský – Single line methods in the diffraction profile analysis. V. Studnička – The use of X-ray phase analysis at the Rotan lab. J. Kub – HUBER diffractometer with Göbbel mirror at the Institute of Physics AS CR. V. Petříček – Refinement of difficult structures of crystals. J. Hybler – Four-circle diffractometer Xcalibur at the Institute of Physics AS CR.

Excursion to the HUBER diffractometer with Göbel mirror (Slovanka) and to the four-circle diffractometer Xcalibur (Cukrovarnická).

Organization: Z. Šourek

249th Seminar

Brno 30. 1. 2001, Institute of Materials Engineering MTU

Lectures:

Y. Jirásková – Mössbauer spectroscopy and X-ray phase analysis of the corrosion-resisting steels surface. V. Vávra – XRD quantitative analysis of the rock phases composition. O. Pritula L. Smrček, A. Buchal – Quantitative phase analysis of the Portland cement phases mixture. Z. Bochníček – The use of the high-temperature X-ray scat-



tering for the study of temperature multilayer stability. M. Meduňa – X-ray scattering on Si-Ge multilayer. M. Ďurík – Crystal structure modeling and R_{wp} factor reliability. A. Buchal – Crystal structure of partly stabilized ZrO_2 .

Excursion – Philips diffractometer.

Organization: A. Buchal

250th Anniversary seminar

Praha 1. 3. 2001, Institute of Macromolecular Chemistry AS CR

Lectures – Past, present and future of the X-ray diffraction at the labs in the Czech and Slovak Republics.

Z. Šourek, V. Petříček, Červinka – Institute of Physics Academy of Sciences (AS CR), Praha; P. Mikula – Institute of Nuclear Physics AS CR, Řež u Prahy; V. Valvoda – Faculty of Mathematics and Physics, Charles University, Praha; J. Kuběna – Faculty of Science, Masaryk University, Brno; J. Marek – Faculty of Science, Masaryk University, Brno; D. Krausová – Faculty of Science, Palacký University Olomouc; S. Ďurovič – Institute of Inorganic Chemistry SAS, Bratislava; M. Koman – Faculty of Chemical Technology STU, Bratislava; V. Kavečanský – Institute of Experimental Physics SAS, Košice; P. Šutta – Military Academy, Liptovský Mikuláš; A. Buchal – Institute of Materials Engineering MTU, Brno; J. Fiala, R. Čerstvý – ŠKODA Research Institute, Plzeň, University of West Bohemia, Plzeň; S. Vratislav, I. Kraus – Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Praha; M. Rieder – Faculty of Science, Charles University, Praha; R. Skála, K. Melka, P. Ondruš – Institute of Geology, Praha; I. Císařová – Faculty of Science, Charles University, Praha; B. Kratochvíl, J. Maixner – Institute of Chemical Technology, Praha; J. Sedláček, J. Brynda – Institute of Molecular Genetics AS CR, Praha; J. Pleštil, J. Hašek – Institute of Macromolecular Chemistry AS CR, Praha.

Organization: J. Hašek, R. Kužel

251st Seminar

Přerov 10. 4. 2001, Precheza

Lectures:

P. Pikal – Kinetics of $Fe(OH)SO_4$ decomposition. J. Balcárek, P. Pikal – The use of XRD for $Fe_2(SO_4)_3$ determination in calcined Fe_2O_3 . R. Zbořil – The use of Mössbauer spectroscopy for Fe_2O_3 identification and structural characterization. M. Mašlán – The use of Mössbauer spectroscopy for the Fe^{2+}/Fe^{3+} determination at illmenites. J. Balcárek, A. Goebel – The use of XRD for the crystallite size determination of rutil promotor. D. Novotný – Devices used for thermal analysis and microstructure of materials (Pragolab company presentation)

Organization: J. Balcárek, D. Krausová

252nd Seminar

Praha 23. 8. 2001, Institute of Macromolecular Chemistry AS CR

Lectures: A. Wlodawer – Inhibitor complexes of pepstatin-insensitive carboxyl protease from *Pseudomonas* sp.101-a serine protease with a unique catalytic triad. J. Brynda – Interaction of new inhibitors with HIV protease. J. Hašek – Role of macromolecular crystallography in anti-retroviral drug design. Mutational resistance of HIV proteases. B. Schneider – Deposition of protein structures in the Czech Republic.

Organization: J. Hašek

253rd Seminar

Mladá Boleslav 23. - 24. 10. 2001, Autoškoda, Horní Počernice, Čertousy

Lectures: E. Zinke, Z. Porkert, R. Skála – Opening and introduction of SEIFERT representation team in CR. A. Buchal – Retained austenite determination by XRD. C. Genzel – Diffraction stress-gradient analysis from surface to volume. A. Haase – Analytical X-ray diffraction systems for research and industry. Overview of SEIFERT XRD3003 innovations. B. Eigenmann – The meaning of residual stress for automotive industry and its problem orientated determination. J. Betzold – X-ray instruction parameters for stress inspections according to Volkswagen concern quality assurance.

Organization: Z. Porkert, E. Zinke, R. Skála

CSCA Colloquium - Structure 2001

Bedřichov, June 18 - 22, 2001

Traditional colloquium including the 4th student seminar.

Main topics: Physics, thin films, databases, mineralogy, powder diffraction, biological crystallography

Main lectures: Jiří Kulda (ILL, Grenoble, France): Neutron scattering; Martin Diviš (Charles University, Praha): Ab-initio calculations of structural properties of solids. Marian Čerňanský (Institute of Physics, Acad. of Sci, Praha): Coherence of X-rays. David Rafaja (Charles University, Praha): Use of X-ray diffraction and reflectivity for the study of thin films and multilayers. Stephen J. Maginn (Cambridge Crystallographic Data Centre, UK): Use of structural databases of organic and organometallic compounds. Jaroslav Fiala (ŠKODA research, Plzeň): Diffuse scattering. Miroslav Karlík (Czech Technical University, Praha): High-resolution electron microscopy. Ivan Procházka (Charles University, Praha): Positron annihilation spectroscopy.

Web page at <http://www.xray.cz/xray/csc/kol2001/> (including conference photos)

Number of participants: 92



Organization: R. Kužel, J. Hašek, L. Dobiášová, F. Eichler, L. Machonský

All abstracts are in the issue of *Materials Structure* v. 8, number 1a (<http://www.xray.cz/ms/bul2001-1a.htm>)

The 4th review of student theses from the field of X-ray and neutron structure analysis

In two days, 24 works were presented by students (results of diploma and PhD theses from the Czech and Slovak universities). Three of them were evaluated as the best and rewarded (M. Šlouf, P. Řezáčová, L. Palatinus). An extra price - scientific stay in Grenoble was given to E. Buchtelová by J. Kulda (ILL).

Workshop "The Use of the Cambridge Structural Database"

Practical demonstrations of the Cambridge structure database and related software were organized by Dr. S. J. Maginn from the CCDC center in Cambridge.

9th Regional conference on powder diffraction – RPKD – 2000

Liptovský Mikuláš, 20. 9. - 22. 9. 2000

Lectures:

J. Fiala – Polycrystalline materials XRD topography. L. Smrček – „Organic“ structure identification from powder data? Nothing easier... A. Buchal – Temperature stability and characterization of nitrid film on austenite. M. Čerňanský – One line methods in the profile analysis. V. Langer – Structure determination of κ -Al₂O₃. P. Fejdi – Consequence of the crystal morphology on the powder preferred orientation. V. Vávra - XRD determination of chemical composition of Zr minerals. Quantitative phase analysis of plant ashes and their composites. P. Šutta – The structure of Si thin layers on the ceramic substrates. D. Rafaja – Diffraction on the 2D motives. T. Havlík – XRD application on the real technological processes. D. Havlíček – Experience with „table aerosol camera“ in quantitative powder XRD. L. Čaplovič – Investigation of degradation processes in permanent magnets. O. Pritula – Quantitative phase analysis of Portland cement standards. S. Jurečka – Optimization of the diffraction line deconvolution. R. Kužel – The use of XRD for thin layers thickness determination. A. Miškuřová – The use of XRD for CaO heat resisted material related to the time of grinding. D. Krausová – Problems of desoxyephedrin quantitative determination using the powder XRD. J. Walla – Polymorphism of molecular crystal of some complex substances. M. Jergel – Multilayers for X-ray optics with extremely low interface roughness. V. Jorík – Structure refinement of [FeX₂(OPPh₃)₄][FeX₄], (X=Cl, Br) using the „rigid body“ technique. M. Ďurík – R_{wp} reliability at structure modeling. M. Škrobán – Structure from the powder data: Rietveld and/or Sheldrick? J. Marek – ODF at standard projection. Q. Jackuliak – To the problems of strain (stress) determination in the Si thin layers.

Number of participants: 40

Organization: V. Kavečanský, P. Šutta, L. Smrček, V. Jorík, R. Kužel

CSCA, Institute of Experimental Physics SAS Košice, Department of Inorganic Chemistry STU, Institute of Inorganic Chemistry SAS Bratislava, Military Academy Liptovský Mikuláš, Association of Slovak Mathematics and Physicists

10th Regional conference on powder diffraction – RPKD – 2001

Liptovský Mikuláš, 19. 9. - 21. 9. 2001

Lectures:

D. Stroz – Diffraction studies of the R-phase in the shape memory NiTi alloys. M. Čerňanský – Effects of partial coherence of X-rays. V. Jorík: Structure refinement of zeolite NaY structure - TOF neutron data. D. Havlíček – Powder diffraction on single-crystal diffractometer Bruker with position sensitive detector. A. Buchal – Relation of microstructure and mechanical properties of steel. V. Langer – Temperature dependent diffraction of layered compounds: hydrofosfite of strontium and calcium phenolphosphate. L. Smrček – Structure solution from powder diffraction pattern influenced by preferred grain orientation. L. Čaplovič – Structure and properties of parts from electrographite. V. Kavečanský – Structure and magnetic properties of selected ferrikyanides of rare compounds. O. Pritula – Quantitative X-ray phase analysis of clinks with the aid of extraction procedures. P. Šutta – Influence of diffuse scattering from strongly distorted thin interlayer on profile analysis of Si thin films deposited on SiAlON substrate. J. Vavřda – From ratio methods to Černohorský methods $\sin \phi_1 / \sin \phi_2$. J. Marek – Textures of Al alloy sheets produced by founding. M. Černík – Advantages of neutron scattering at the measurements of textures of polycrystalline materials. M. Černík – Anisotropy of steel sheets by X-ray texture analysis. J. Fiala – Structure of pyrolysis carbon in foundry forms. R. Kužel – Structural study of textured films PbTiO₃-Al₂O₃. T. Havlík Use of X-ray diffractometry at soaking of sulphides of non-ferrous metals. A. Miškuřová – X-ray diffraction study of hydration of sintered refractory CaO materials. S. Prugovecki – Commercial presentation of Phillips

Panel discussion - teaching crystallography, transformation of RPKD from regional to international conference.

Number of participants: 27

New conference Web site: <http://www.saske.sk/RPKD/>

Organization: V. Kavečanský, P. Šutta, L. Smrček, V. Jorík, R. Kužel

CSCA, Institute of Experimental Physics SAS Košice, Department of Inorganic Chemistry STU, Institute of Inorganic Chemistry SAS Bratislava, Military Academy Liptovský Mikuláš, Association of Slovak Mathematics and Physicists



X-Ray Scattering from Surfaces and Thin Layers

5th Autumn School on X-ray scattering from surfaces and thin layers, September 12 - 15, 2001, Smolenice, Slovakia

Tutorial Lectures: Vladimir Kaganer (PDI- Berlin): Kinematic theory of x-ray scattering from lattice defects in crystals and films. Frank Schreiber (MPI-Stuttgart): X-ray reflectivity and X-ray standing-waves of organic materials. Julian Stangl (University Linz): Grazing-incidence small angle scattering from surface nanostructures (GISAX). Alexei Nefedov (University Bochum): Soft-X-ray scattering from metallic multilayers. Jorg Grenzer (University Potsdam): Grazing-incidence X-ray diffraction from buried interfaces.. Nikolay Artemiev (University Prague): Progress in X-ray optics components.

30 oral contributions, 25 posters

Number of participants: 75 from 10 European countries

Organizers: U. Pietsch, V. Holý, P. Boháček

Masaryk University Brno (Czech Republic), University of Potsdam (Germany), Institute of Electrical Engineering Slovak Academy of Science Bratislava (Slovak Republic).

Fourth Heart of Europe Bio-Crystallography Meeting

Bedřichov, September 27 - 29, 2001

International presentation of PhD works in structure biology from Germany, Poland, Czech and Slovak republics. The scientific program included mainly 20-minutes talks presented mostly by PhD students

Lectures

G. Palm: The seashore of the heart: Crystallography in Greifswald. J. Ondráček: The structure of lysozyme with inorganic anions. R. Tyrrell: Rigaku/MSK. K. Anand: Crystal structure of porcine transmissible gastroenteritis viral protease. W.-D. Schubert: Structure of Glutamyl-tRNA-Reductase from *M. Kandleri*. R. Štouračová: Preliminary crystallographic study of an anti-MN/CA IX monoclonal antibody M75 Fab fragment complexed with its epitope peptide. Z. Otwinowski: HEC Lecture. D. Pal: Unusual hydrogen bonds in proteins. A. Kurzynska-Kokorniak: HIV-1 RT, as the key protein in genetic RNA recombination. Preliminary crystallographic studies. M. Huelsmeyer: Structural analysis of HLA-B27 subtypes differently associated with arthritic disease. H. Petroková: Role of conformational flexibility of the inhibitor inside of the HIV-1 protease active site. T. Skálová: HIV-1 protease in complex with tetrapeptide inhibitor - effects of mutations. S. Panjikar: Use of xenon in practise. N. Strater: A GUI for preparing figures with Molscript et al. O. Pasternak: Structural studies of *Lupinus luteus* protein of PR10.2. T. Sicker: Soft X-rays and automated structure determination. E. Fiedler: Structural determination of transketolase in complex with the reaction intermediate 2-(1,2-dihydroxyethyl)-ThDP. B. Schierbeek: Bruker

Nonius CCD detectors in the home lab: High speed, high accuracy. S. Ehinger: Crystallization of Tubulin-Tyrosine Ligase. B. Kuettner: Alliinase from garlic - the structure at last. I. Grishkovskaya: Buch Structural determinants for steroid-binding specificity of human sex-hormone binding globulin. R. Janowski: Crystal structure of wild-type zymogen of streptopain. E. Buchtelová: Product of autoproteolysis complexed with HIV-1 protease - interaction of the C-terminal carboxyl group with the active-site aspartates. J. Brynda: Structural studies in HIV protease:inhibitor complexes.

Conference Web site -
<http://www.img.cas.cz/hec/index.html>
 with the conference photos included

Number of participants: 48

Main organizer: J. Sedláček

Crystallization Course

Nové Hradky, October 5-12, 2001

Main topics: Crystallization, phase diagram, properties of solution, nucleation, crystal growth, applied crystallization, solving of structures, diffraction physics, synchrotron radiation, data collection, phasing methods, refinement

Speakers: R. Hilgenfeld, T. Klupsch, J. Mesters (Germany), J. M. Garcia-Ruiz (Spain), J. Brynda, J. Hašek, B. Schneider, P. Řezáčová, M. Hušák (Czech Republic)

Tutors: I. Kutá Smatanová, H. Petroková, R. Štouračová, L. A. González Ramírez

Conference Web site -
<http://www.xray.cz/xray/Crystallization/> with photos

Number of participants: 34 (21 students)

Organizers: I. Kutá Smatanová, R. Hilgenfeld, J. Hašek, J. Brynda

see Reports in this issue for more

Development of Materials Science in Research and Education

Kežmarské žlaby, September 9 -13, 2001

Main topics: trends in development of materials research, education in materials science at the universities, information on research programme of individual institutions, information on equipments for preparation and characterization of materials, results of materials science research, 45 lectures

Number of participants: 60

Organization: M. Koman, D. Hrivňáková, E. Dlháň

Slovak expert group of solid state chemistry and physics, Czech and Slovak Association for Crystal Growth, CSCA, Faculty of Chemical Technology, Faculty of Electrical Engineering and Information Technology, Faculty of Materials Science and Technology - Slovak Technical



University, Regional committee of Czech and Slovak Crystallographers

CSCA Information Centre

CSCA Journal

The journal "Materials Structure in Chemistry, Biology, Physics and Technology", ISSN 1210-8529. Contributions can be published in English, Czech or Slovak. Editorial board has the right to reject contributions which do not follow the editorial trends. Scientific papers are reviewed usually by two independent referees.

Accepted articles in English, Czech or Slovak languages are given under the review control. Editorial board can (has the right to) refuse the contribution that is out of the editorial plans.

Web page of the journal: <http://www.xray.cz/ms>

Other Journals and Proceedings

IUCr (International Union of Crystallography) Newsletter is quarterly distributed to all CSCA members.

CSCA Library provides:

journals concerning crystallographic aspects:

Acta Crystallographica A, B, C, D: Foundations of Crystallography, Structural Science, Crystal Structure Communications, Biological Crystallography, Synchrotron Radiation, Protein Science, Journal of Applied Crystallography, Materials Structure in Chemistry, Biology, Physics and Technology

The library also keeps conference journals and CSCA documents.

Databases installed

The latest versions of crystallographic databases are installed in Institute of Physics and Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Faculty of Mathematics and Physics, Charles University, Slovak Technical University Bratislava

INTERNET

The association has its own domain **xray.cz**.

Addresses of WWW and FTP servers:

<http://www.xray.cz>

<ftp://xray.cz>

All CSCA members are encouraged to help in improvement of the server contents or announcing of references to their own WWW pages at least.

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J. Hašek, R. Kužel

Reports

Crystallization Course CC2001

I am glad to inform you about The First Protein Crystallization Course CC2001 held in the Academic and University Center (AUC) in Nové Hradky during the second week of October (5 - 12).

In order to achieve its high level, qualified crystallographers from Germany (Prof. R. Hilgenfeld, Dr. J. Mesters, Dr. T. Klupsch of IMB Jena), Spain (Prof. J.M. Garcia-Ruiz of Instituto Andaluz de Ciencias de la Tierra, Granada) and the Czech Republic were invited to give the lectures as well as organize practices for undergraduate and postgraduate students. The CC2001 was sponsored by Photosynthetic Research Center [CR], PragoLab [CR], JenaBioScience GmbH [Germany], Molecular Dimension Ltd. [UK] and CSCA [CR]. Without their financial and/or material support the course could not be organized.

The official language of the course was English. During the morning lectures students were acquainted with standardized as well as the latest methods of protein isolation, purification and crystallization. Freshly obtained knowledge was trained during afternoon practices, which took place in the newly established Laboratory of Crystallogenesis that is unique in the Czech Republic.

Using different crystallization methods such as hanging drop and sitting drop vapour diffusion methods, crystallization in a gel, etc., students grew their own crystals of lysozyme, glucose isomerase and Concavalin A while learning how to operate a robot for protein crystallization (lent by IMB Jena). They also learnt the ways of crystal seeding and freezing as well as the work with the commercially available solution sets.

During the second part of the course students visited the Institute of Molecular Genetics in Prague, where a protein diffractometer was introduced and diffraction data of freshly produced crystals were measured. The data were later used for teaching students of solving the protein structure. These lessons took place in a new computer lab in Nové Hradky provided with all the necessary hardware and software.

The organizing committee also arranged programme for free time of all participants – such as concerts, film presentations and sightseeing.

In conclusion, I would like to address some of remaining factors that have contributed to such successful outcome. Among those, sufficient financial support and qualified scientific staff of AUC played the major role.

Considering the answers participants gave in questionnaire before leaving, I am delighted to call the first year of crystallization course very fruitful and I am looking forward to similar activities scheduled for 2002.

Ivana Kutá Smatanová