CZECH AND SLOVAK CRYSTALLOGRAPHIC ASSOCIATION

Activities in 1997 - 1999

The Czech and Slovak Crystallographic Association (CSCA) organized 10 meetings and 9 traditional one-day seminars in the period 1997-1999. The most important conference organized by CSCA in 1998 was undoubtedly the 18th European Crystallographic meeting.

ECM-18
European Crystallographic Meeting, Praha, August 15-20

The conference was organized by the Czech and Slovak Crystallographic Association under auspices of the International Union of Crystallography (IUCr) and European Crystallographic Association (ECA). Co-organizers were the following: Faculty of Mathematics and Physics of Charles University, Faculty of Mechanical Engineering of the Czech Technical University, Institute of Macromolecular Chemistry and Institute of Physics of the Academy of Sciences of the Czech Republic, National Museum and Czech Engineering Academy.

The conference programme took place mainly in the buildings of the Faculty of Mechanical Engineering and Faculty of Civil Engineering (Czech Technical University). 1 059 participants came from 39 countries all over the world. The largest number of them was from Germany (185), United Kingdom (109), Russia (80), France (80), Czech Republic (70), Poland (50), Italy (41), USA (41) and Sweden (40). The programme started every conference day by three parallel invited lectures and continued with six parallel microsymposia. In total, the ECM consisted of 18 plenary lectures, 5 workshops and 48 microsymposia. 558 contributions were presented in a poster form. Five different workshops on symmetry of crystals, methods of crystal structure determination, use of databases - were organized before the conference.

The session to the 50th anniversary of the IUCr consisting of four plenary lectures on the history of IUCr and future perspectives of crystallography in physics, chemistry and biology took place in the State Opera and it was chaired by the president of the IUCr - Prof. Baker. Cultural programme included the visit of National Museum with a concert to the 25th anniversary of the ECM, crystallographic exhibition Structure of the Microworld, mineralogical collections; concert to the 650th anniversary of the Charles University in Carolinum; the Křižík´s night colourful fountains with music performances trips to different destinations around Prague and farewell party at the end.

Sponsorship of the CSCA, IUCr, two former ECM's in Lund (J. Albertsson, A. Oskarsson) and Lisboa (M.A. Carrondo) and commercial companies mostly producing X-ray equipment enabled partial financial support to 200 participants, mainly students. The companies exhibited their products in 35 exhibition stalls.

The conference programme confirmed a large scope of modern crystallography investigating structure of the matter. It goes from physics and materials sciences (e.g. phase transitions, charge densities, lattice defects, stresses and textures, thin films, low-ordered structures, structural studies under extreme conditions – pressures and temperatures), to organic and inorganic chemistry (structure determination, structure modelling, drug design) and rapidly developing biological crystallography (DNA, proteins, viruses). Several methodological microsymposia was devoted to the problems of structure determination and structure refinement, the use of synchrotron radiation, time-resolved experiments, new instruments and also to the application of Internet and teaching of crystallography. The program included following microsymposia :

A. Structure in Physics and Applied Crystallography

1. Spin, Charge & Momentum Density
2. Phase Transitions
3. Martensitic Phase Transformation
4. Defects and Microstructures
5. Texture and Stress Analysis
6. Industrial Applications at Neutron and Synchrotron Sources
7. Thin Films, Multilayers
8. Epitaxial Thin Films, Surfaces

B. Materials Science

1. Structure of Minerals
2. Structure Determination using Electron Diffraction
4. Crystallography Under Extreme Conditions
5. Optic, Electric and Magnetic Materials
6. Small Angle Scattering
7. Aperiodic Crystals and Quasicrystals
8. Low-Order and Non-Crystalline Materials, Fibre Diffraction

C. Structural Aspects in Chemistry, Chemical Crystallography

1. Materials Chemistry – Reaction in Solids
2. Structure Systematics and Structure-Function Relationships in Organic Chemistry
3. Structure Databases
4. Structure Determination by Powder Diffractometry
5. Structure of Inorganic Compounds
6. Molecular Modelling, Quantum Chemistry
7. Large Supramolecular Assemblies and Inclusion Compounds
8. Hydrogen Bonding

D. Structure and Function of Biological Systems

1. Transmission and Signalling Across Membranes
2. Metalloproteins - Structure and Function
3. DNA/RNA - Structure, Binding Modes and Function
4. Proteins and Drug Design
5. Viruses, Anti-Viral and Anti-Retroviral Treatment
6. Immunologically Active Molecules
7. Protein biosynthesis. Transcription and Translation
8. Energetics of the Cell

E. Advanced Methods for Structural Investigations and Methods for Structure Determination in Biology

1. Synchrotron Radiation
2. Neutron Scattering
3. Structure and Function in Molecular Biology
4. Time Resolved Studies
5. Ab Initio Methods for Structure Determination
6. Biological Macromolecules - Refinement, Precision, and Validation
7. Hot Biological Structures
8. Multiple Anomalous Diffraction

F. General Crystallography and Discussion Meetings

1. Purification Techniques and Crystallization of Macromolecules
2. INTERNET in Crystallography
3. Non-diffraction Techniques
4 Structural Biology in Central and Eastern Europe – Present Situation and Perspectives
5. Symmetry and Nomenclature
6. Commercial Lectures, Instruments
7. Phase Analysis
8. Teaching Crystallography

Nearly 900 abstracts of conference contributions were collected in special issues of the journal Materials Structure in Chemistry, Biology, Physics and Technology (volume 5, more than 500 pages) published by the CSCA. The Internet was preferred communication tool for the conference preparation. WWW pages on the server

www.xray.cz/ecm

still contain nearly all information, e.g. list of participants including the search, their addresses and contributions, complete conference programme, all abstracts. The post-conference book containing selected full papers as well as the conference CD-ROM is under preparation.

Crystallographic exhibition was organized in the National Museum.

CSCA Colloquium - Struktura'99

Hodonín u Kunštátu, June 14-18, 1999

Traditional colloquium including the 3rd student seminar (students thesis in the field of structure analysis). Other topics - crystallography in materials science, biology and chemistry, teaching crystallography.

Organization: A. Buchal, L. Dobiášová, J. Hašek, V. Holý, R. Kužel, L. Smrčok, Z. Weiss

All abstracts are in this issue of Materials Structure.

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

236th Seminar

Structure of biological macromolecules

Masaryk University, Faculty of Natural Sciences, Brno January 15, 1997

Lectures: LSD Bio projects in computer chemistry and molecular modelling (J. Koča), Conformational behaviour fragments of nucleic acids (E. Fadrná), Application of molecular modelling to study of biodegradation reactions (J. Damborský, M. Kutý), Study of biomacromolecular structure by NMR (V. Sklenář), Study of structure of nucleic acids by multidimensional NMR and molecular dynamics (P. Padrta).
Visit of laboratory LSD Bio, NMR laboratory (500 MHz spectrometer), X-ray (low temperature diffraction), SGI laboratory (MSI/Biosym software).

Organization: J. Koča, J. Marek, J. Hašek

237th Seminar

Selected methods of materials research

Faculty of Chemical Technology, March 5, 1997

Lectures: Methods of study of properties of construction ceramic materials (P. Šajgalík), NMR and 57Fe Mössbauer spectroscopy of minerals (P. Komadel), IR and Raman spectroscopy (D. Tunega), Analysis of real structure of polycrystalline materials (J. Kečkéš), Application of powder diffraction methods for study of zeolites (V. Jorík), Electron spectroscopy for chemical analysis (ESCA) (L. Benco).

Organization: M. Koman, M. Dunaj-Jurčo

238th Seminar

Molecular Electronics

Faculty of Electric Engineering and Information Science, STU Bratislava, May 21, 1997

Contributions concerning the study of molecular systems and their applications.

S. Nešpůrek, F. Schauer, D. Chorvát, R. Harman, G. Čík, P. Koštial, I. Thurzo, J. Cirák

Organization: J. Cirák, P. Tomčik, D. Barančok, J. Vajda

239th Seminar

Thin Films

Masaryk University, Faculty of Natural Sciences, June 5, 1997

Lectures: X-ray scattering by nanostructures (multilayers, quantum wires, self-ordering systems (V. Holý, J.Kuběna), Göbel mirror - our experience (J. Kuběna), Position sensitive detector and its application for optical reflection on SiGe/SiC multilayers (J. Grim), Possibilities of high temperature diffractometry (A. Buchal), Statistical interpretation of diffraction patterns and its use for identification of polymorphic phases (P. Súlovský), X-ray quantitative phase analysis applied to fly ash materials (V. Vávra), STOE products (L. Smrčok).

Organization: V. Vávra, V. Holý, A. Buchal

Contribution on Göbel mirror in Materials Structure, vol.4 (1997), no. 2

240th Seminar

Neutron Scattering

Institute of Nuclear Physics, Řežu Prahy,
October 10, 1997

Lectures: Centre of Fundamental and Applied Research with Thermal Neutrons in Řež (P. Mikula), High resolution small-angle scattering - application to study of porosity (J. Šaroun), Evaluation of neutron diffraction experiments by modelling and indirect transformation (P. Strunz), Powder diffractometry on zeolites and high temperature superconductors (S. Vratislav), Analysis of microstrain in metals by high resolution neutron diffraction. (P. Lukáš). Visit of reactor

Contributions in Materials Structure, vol. 4 (1997), no. 3

Organization: Pavel Mikula

241st Seminar

Textures, thin films, products of FPM Seifert

West Bohemian University, Plzeň, November 12, 1997

Visit of Department of Physics and Department of Materials and Metallurgy, demonstration of reconstructed DRON diffractometer.

Lectures: Orientierungsbestimmung durch Approximation von Texturkomponenten (K. Helming), Texture analysis of steels produced by VŠB Košice (M. Černík), Texture of two-phase mechanically unstable stainless steels (J. Zeman), Profile analysis of highly textured thin films (P. Šutta), Vorstellung eines neuen Ritveld- Programms am Beispiel von Tonmineralen (T. Taut),
Presentation of Seifert software for texture and Rietveld analysis (K. Helming, T. Taut), Produktinnovation aus dem Hause Seifert (H. Miersch), Processes on interfaces galvanic tin layer - bronze substrate (D. Jandová, J. Fiala, D. Beran, Z. Nový, Z. Kubeš), Cold-working of P900 steel (Z. Nový, M. Čepera, J. Džugan, D. Jandová).

Contributions in Materials Structure, vol. 5, no. 1 (1999).

Organization: J. Fiala, V. Bernášek, J. Vlček

242nd Seminar

INTERNET and its use in crystallography

Faculty of Mathematics and Physics, Charles University, Praha, February 17, 1998

Working on Internet

Brief introduction - PC in computer networks, choice of client software for E-mail, FCP, WWW, search on Internet, how to create own FCP and WWW servers, how to create WWW pages, crystallographic WWW servers and interesting applications, structures in VRML

Demonstration of ZDS software (powder pattern analysis) - a new version of the programme of Petr Ondruš

Organization: R. Kužel

243rd Seminar

Chemistry and physics of high-temperature superconductors

Department of Inorganic Chemistry, Faculty of Chemical Technology, Bratislava, October 10, 1998

Lectures: Substrate influence on properties of thin films (P. Kúš), MOCVD deposition of VTS thin films (K. Frohlich), Properties of VTS thin films prepared by physical methods (V.Štrbík), Preparation and properties of Tl and Hg superconductors (G. Plesch), Paramagnetic superconducting system (F. Hanic).

Organization: M. Dunaj-Jurčo, F. Hanic

244th Seminar

Thin films and surfaces

Department of Inorganic chemistry, Faculty of Chemical Technology, Bratislava, November 1, 1998

Lectures: Preparation of yttrium stabilized zirconium oxide by vacuum reactive evaporation (S. Chromík), Thin-film superlattices (I. Vávra), Magnetoresistance in multilayers (Š. Luby), Diamond and diamond-like layers (preparation and applications) (S. Bederka), Characterization of interface by DLTS method (K. Gmucová), X-ray scattering study of surfaces and interfaces (M. Jergel), Interaction of electrons with thin polymer films in electron lithography (P. Hudek), Interfaces in VTS thin films and Josephson effects (S. Beňačka).

Organization: M. Dunaj-Jurčo, M. Hartmanová

Possibilities at ESRF (European Synchrotron Radiation Facility) for technical, natural and medical sciences

Faculty of Nuclear Engineering,, Czech Technical University, January 20, 1999

Lectures: Introduction (V. Dvořák, director of the Institute of Physics, Acad, Sci), Description of the source, characteristics, applications (J. Hrdý), How to submit the proposal, practical organization of experiments (J. Vacínová), Study of structure and dynamics of proteins (J. Hašek), Study of electronic structure of solids by absorption/spectroscopic methods (J. Vacínová), X-ray topography (M. Polcarová).
Organization: V. Dvořák, J. Hrdý, J. Hašek

Student Seminar

Faculty of Nuclear and Physical Engineering, Praha, June 12.1997

Programme

Introduction. I. Kraus, L. Musílek, J. Hašek, I. Kraus: Anniversary of Laue discovery, J. Dohnálek: Structure of 6-phosphogluconate dehydrogenase from parasite Trypanosoma brucei, M. Horký: Crystallization of Polyoxyethylene - Polymethylmetacrylate polymer mixtures, D. Janeba: Study of intercalated structures, A. Kláriková: Creation of particles of hexagonal ferrites Fe_2O_3-BaO-B_2O_3 studied by Mössbauer spectroscopy, M. Kolega: X-ray diffraction analysis of grinded powders, M. Čepera: High-temperature modification of Ti in PVD thin films, P. Freundlich: Surface roughness in X-ray powder diffraction, J. Kečkéš: X-ray diffraction analysis of thermally treated InP-based Interfaces, J. Kopeček: High-temperature experiments for order investigations in Fe_3Al alloy, J. Lhotka: X-ray diffraction study of PVD deposited TiN thin films, M. Malá: Epitaxial misfit, J. Pavelka: High-temperature X-ray spectrometry of metal multilayers, E. Scholtzová: Study of structure of layered silicates by methods of quantum chemistry, I. Smatanová: Crystal structure of vanadium (V) oxoperoxo and dioxo compounds, P. Skokanová: Evolution of algorithm for phase identification from X-ray diffraction, M. Ďurík: Synthesis and characterization of complexes in the Y zeolite structure.

Organization: CSCA, Regional committee of the IUCr, Faculty of Nuclear and Physical Engineering, Czech Technical University, Faculty of Mathematics and Physics, Charles University; I. Kraus, L. Dobiášová

Contributions in Materials Structure, vol. 4 (1997), no. 1

Structure and Function of Biological Synthetic Macromolecules

June 10-12, 1997, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic

Program:

Expression, Purification and Crystallization of Proteins, Crystallization of Enzymes and Oligonucleotides, Protein Structure Database, DNA/RNA database, Software for Modelling and Crystallography, Cathepsin B - Polymeric Drug Interaction, Structure and Function of Ribonuclease, Structure Determination of Proteins, Solvation of the Phosphate Group, Protein - DNA/RNA Recognitioon, Polymers and biopolymers, Synchrotron source, Fiber diffraction, Bio-information, *Organization:* J. Hašek

X-Ray Scattering from Surfaces

3rd Autumn School on X-ray scattering from surfaces and thin layers

Smolenice, Slovakia, October 1 - 4, 1997

The school was organized as "low cost" panel meeting especially for graduate and post-graduate students and other young scientists to present their actual and often unpublished results..The discussion was very lively and fruitful.

Main Topics

high resolution X-ray specular reflectivity, high resolution X-ray reciprocal space maps, nonspecular scattering (reflection and diffraction), X-ray grazing incidence diffraction, surface rod scattering, lateral surface structure scattering.

Organizers:
Masaryk University Brno, University of Potsdam, Institute of Electrical Engineering Slovak Academy of Science Bratislava, Czech and Slovak Crystallographic Association. Supported by the Deutsche Kristallographische Gesellschaft, the International Union of Crystallography, and the Masaryk University

Programme (only tutorials are mentioned here)

Metin Tolan: X-ray reflectometry, Ullrich Pietsch: High-resolution X-ray diffraction, Juergern Haertwig X-ray topography, Tim Salditt: X-ray diffuse scattering, Sergey Stepanov: X-ray grazing incidence diffraction, Tilo Baumbach: X-ray diffraction from structurized surfaces.

Contributions in Materials Structure, vol.4 (1997), no. 3

X-Ray Scattering from Surfaces and Thin Layers

4rd Autumn School on X-ray scattering from surfaces and thin layers

Smolenice, Slovakia, September 22 - 25, 1999

Tutorial Lectures: Metin Tolan: X-Ray Specular Scattering, Leander Tapfer: High-Resolution X-Ray Diffraction, Harald Reichert: X-Ray Diffuse Scattering, Tilo Baumbach: Scattering from Gratings and Dots, Andreas Schreyer: Magnetic Scattering, Ralph Stömmer: New Apparativ Developments.

Organizers: U. Pietsch, V. Holý, D. Korytár

6th Regional conference on powder diffraction - RPDK-97

Military Academy, Liptovský Mikuláš, September 17 - 19 1997

Organization:

CSCA, Department of Inorganic Chemistry, Faculty of Chemical Technology, Slovak Technical University,

Bratislava, Military Academy Liptovský Mikuláš, Institute of Inorganic Chemistry, Slovak Academy of Sciences;
V. Jorík, P. Šutta, L. Smrčok

Lectures: P. Mikula: Neutron research laboratory in Řež near Prague, J. Fiala: Data reduction by filtration, M. Čepera: Textures -measurement and evaluation of experimental data, D. Rafaja: Depth profiles of residual stresses in ion- implanted TiN coatings, M. Jergel: Application of the Distorted-Wave Born Approximation to the X-ray interface studies, M. Černík: Deformation textures of FCC metals, R. Kužel: Anisotropy of X-ray line profile parameters and real structure of the matter, D. Krausová, R. Koďousek, V. Procházka: Crystallographic study of gall stones, V. Jorík: Use of powder diffraction methods for study of zeolites, M. Ďurík: Synthesis and characterization of Cu complex in the structure of Y zeolite, L. Smrčok: Structures of inorganic compounds from powder diffraction, J. Černák, A. Orendáčová, M. Orendáč, J. Chomič, A. Feher: Synthetic design of one-dimensional compounds using tetracyanonickellate(2-) and dicyanoargentate(1-) anions.(O), V. Šepelák, A. Buchal: X-ray diffraction study of mechanically induced disordering in inverse spinel ferrites, A. Buchal: To negative temperature expansion of DINAS bricks, Q. Jackuliak: Comparison of methods for approximation of diffraction profile, P. Šutta: Experience with the APX-63 software.

7th Regional conference on powder diffraction - RPDK-98

Liptovský Mikuláš, September 16 - 18, 1998

Organization:
CSCA, Department of Inorganic Chemistry, Faculty of Chemical Technology, Slovak Technical University, Bratislava, Military Academy Liptovský Mikuláš, Institute of inorganic chemistry, Slovak Academy of Sciences

V. Jorík, P. Šutta, L. Smrčok

Lectures: N. Ganev: On accuracy and reliability of X-ray tenzometry, I. Červeň: Holography with atomic resolution, M. Černík, P. Mikula, P. Lukáš: Textures of hot-rolled steels measured by X-ray and neutron diffraction, M. Jergel: W/Si multilayer gratings for X-UV optics, J. Fiala: Wavelet transformations, L. Smrčok: Rietveld refinement from compressed data, V. Jorík, L. Smrčok, M. Ďurík: Wavelet smoothing of powder diffraction data, M. Ďurík: Forecasting of crystal structure of two noble sugars, V. Kavečanský, A. Buchal: Limits of possibilities of quantitative analysis, T. Havlík: Application of X-ray diffraction phase analysis in hydrometalurgy, M. Škrobian: X-ray diffraction quantitative analysis of "real phases" , M. Čepera: Texture of ZrO_2 thin films, V.Kavečanský, K.Csach: X-ray diffraction study of FeCuNbSiB - finemet structure, D. Havlíček: X-ray diffraction identification of azbestos minerals in different materials.

Contributions in this issue of Materials Structure

8th Regional conference on powder diffraction - RPDK-99

Liptovský Mikuláš, September 22 - 24, 1999

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

Contributions and more information in Materials Structure, *vol 7, no 1, 2000*

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CSCA Information Centre

CSCA Journal

The title "CSCA Bulletin" was changed into "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.

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 Crystalographica A, B, C, D: Foundations of Crystallography, Structural Science , Crystal Structure Communications, Biological Crystallography, Synchrotron Radiation, Protein Science, Materials Structure in Chemistry, Biology, Physics and Technology, Structure, Macromolecular Structures

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 would like to extend the use of Internet.

A new domain - xray.cz has been registered.
Addresses of WWW and FTP servers:
http://www.xray.cz
http://www-xray.fzu.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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