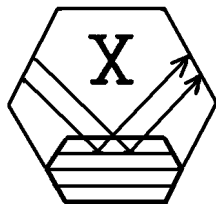


## CZECH AND SLOVAK CRYSTALLOGRAPHIC ASSOCIATION

### Activities in 2002



The Czech and Slovak Crystallographic Association (CSCA) organized or co-organize several conferences and traditional one-day seminars in 2002.

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

#### 254<sup>th</sup> Seminar

#### State of art and perspectives of teaching crystallography in universities.

Bratislava 6. 2., Faculty of chemical and food technology

*Lectures:* survey of crystallography teaching at different universities

D. Barančok (Faculty of Electrical Engineering, Slovak Technical University, Bratislava), A. Buchal (Faculty of Mechanical Engineering, Technical University Brno), L. Čaplovič (Faculty of Materials and Technology, Technical University Trnava), J. Černák (Faculty of Nature Safarik University, Košice), P. Fejdi (Faculty of Nature, Komensky University, Bratislava), J. Fiala (West Bohemian University, Plzeň), N. Ganev (Faculty of Nuclear Engineering, Czech Technical University, Praha), J. Kameníček (Faculty of Nature, Palacky University Olomouc), V. Kavečanský (Institute of Experimental Physics, Slovak Academy of Sciences, Košice), M. Koman (Faculty of Chemical and Food Technology, Slovak Technical University, Bratislava), R. Kužel (Faculty of Mathematics and Physics, Charles University, Praha), J. Marek (Faculty of Nature, Masaryk University Brno), F. Pavelčík (Faculty of Nature, Komensky University Bratislava), S. Ďurovič (Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava)

*Organization:* M. Koman

#### 255<sup>th</sup> Seminar

Plzeň, 24. 10., West Bohemian University

*Lectures*

P. Zuna: Engineering Academy of Czech Republic, J. Rosenberg: New Technologies – Research Center in West-Bohemian region, J. Fiala: Materials and their degra-

ation, J. Hubka: X-ray analytical Bruker AXS, D. Šimek, R. Kužel, J. Kub, F. Kunc: X-ray structural study of textured thin films by reciprocal space map fitting. A. Buchal, R. Foret: Evaluation of structural stability of steels from X-ray line broadening. E. Bekker: Scanning Electron Microscope Quanta 200 FEI for Applications in Materials Science and Engineering. J. Marek, M. Kolega: Comparison of texture measurement in the Faculty of Nuclear Engineering of the Czech Technical University and Research Center New Technologies in Plzeň. P. Šutta: Microstructure of sputtered films of yttrium oxide with various content of oxygen. R. Čerstvý: X-ray laboratory of Department of Physics in West Bohemian University and its modernization. J. Kasl, P. Zuna, J. Fiala: Reversible processes at recrystallization. *Excursion in New Laboratories of the Research Center - New Technologies.*

*Organization:* J. Fiala

#### 256<sup>nd</sup> Seminar

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

#### Inhibition of Serine and Aspartic Proteases

*Lectures:*

J. Hašek: Complex Study of HIV proteases, M. Jaskolski: Atomic Resolution Structures of Trypsin Inhibitors, G. Bujacz, N. Ziolkowska: Structural investigation of HIV-1 protease inhibitors, J. Brynda: High Resolution Structure of HIV1 Protease – Inhibitor Complex, T. Skálová: Structural and Energy Comparison of Ethyleneamine Inhibitor Binding to the Wild and Mutant HIV Proteases, K. Zimmermann: Soft Block Constraints in Energy Minimization – HIV protease experiments, E. Buchtelová: Product of Autoproteolytic Cleavage Found in the Active Site of HIV Protease by X-ray Crystallography, K. Huml: Computer Model of DNA B - poly(L-lysine) Interaction

*Organization:* J. Hašek

#### 257<sup>th</sup> Seminar

Trnava, 3. 12., Faculty of Materials and Engineering

*Lectures:*

K. Wetzig: Application on Analytical Electron Microscopy in Materials Research. I. Hrivnák: M-A (martensite-austenite) component in construction steels. M. Čaplovičová: Use of convergent beam electron diffraction in crystallography. M. Ožvold: Metal multilayers for spin electronics. M. Dománková: EELS and its application in materials science of CN ultrathin films. T. Kuníková: Principle and use of back scattered electrons diffraction. S. Jurečka: Study of microstructure CaCO<sub>3</sub> powder by the Rietveld method. L. Čaplovič: Structure and properties of electrographite. *Excursion in laboratories.*



## CSCA Colloquium - Experimental Methods in X-ray and Neutron Structure Analysis

Ostravice, June 17 - 21

Traditional colloquium organized as a course. State of art of experimental techniques in structure analysis, their use and possibilities for obtaining information on crystal structure in biology, chemistry, physics and mineralogy.

*Main Topics:* sources, detectors, monochromators, powder diffraction: sample preparation, diffractometry, topography of polycrystalline materials, tensometry, textures, quantitative phase analysis; single crystal diffraction - film methods, diffractometry; crystallization of proteins, cryocrystallography, protein diffractometry, neutron scattering, small-angle scattering, multiple crystal diffractometry, diffuse scattering, structure of surfaces and thin films, high-pressure diffraction, high temperature diffraction, low-temperature diffraction, X-ray holography, magnetic structures, modulated structures, charge densities.

*Lecturers:* J. Brádlér (FzÚ AVČR, Praha), J. Kulda (ILL, Grenoble, Francie), N. Ganey (FJFI ČVUT, Praha), J. Marek (PřF MU, Brno), J. Hybler (FzÚ AVČR, Praha), M. Dušek (FzÚ AVČR, Praha), R. Kužel (MFF UK, Praha), Z. Weiss (VŠB Ostrava), J. Fiala (ŠKODA výzkum, Plzeň), J. Marek (FJFI ČVUT, Praha), P. Lukáš (ÚJF AVČR, Řež u Prahy), P. Strunz (ÚJF AVČR, Řež u Prahy), M. Steinhart (Univerzita Pardubice, ÚMCH AV ČR, Praha), V. Holý (PřF MU Brno), J. Kub (FzÚ AVČR, Praha), J. Hrdý (FzÚ AVČR, Praha), M. Polcarová (FzÚ AVČR, Praha), Z. Šourek (FzÚ AVČR, Praha), I. Kutá Smatanová (ÚFB JČU České Budějovice), P. Řezáčová (ÚMG AVČR, Praha), J. Brynda (ÚMG AVČR), J. Hašek (ÚMCH AVČR, Praha), E. Buchtelová (ÚMCH AVČR, Praha), M. Šlouf (ÚMCH AVČR, Praha), K. Prokeš (MFF UK, Praha), M. Dušek (FzÚ AVČR, Praha), D. Rafaja (MFF UK, Praha), Z. Bochníček (PřF MU Brno), A. Buchal (VUT Brno), M. Dopita (MFF UK Praha)

WWW pages <http://www.xray.cz/xray/csca/kol2002/> (including conference photos and videos)

Number of participants: 92

*Organization:* R. Kužel, J. Hašek, Z. Weiss, L. Dobiášová

*All the abstracts published in a special issue:*

*Materials Structure v. 9, number 1a*

(<http://www.xray.cz/ms/bul2001-2a.htm>).

## 11. Regional conference on powder diffraction – RPKD – 20002

Liptovský Mikuláš, September 20 - 22

*Lectures:*

M. Čerňanský: XRD determination of dislocation density in steel samples, L. Čaplovič: Changes of phase composition in the process of preparation of construction ceramics, M. Kolega: X-ray tensometry of laser treated steel 12050, R. Kužel: Study of submicrocrystalline materials by XRD

and diffuse scattering in the transmitted wave, V. Langer: Determination of symmetry in thin epitaxial films TI-2201, M. Dopita: Diffraction study of thin films AlN, J. Fiala: Evaluating corrosion resistance by means of X-ray diffraction, D. Havlíček: Mineralogic composition of solid fraction of aerosol on Milešovka and its comparison with height profiles from Kopisty near Most and Dlouhá Louka near Litvínov, D. Šimek: Measurements and fitting of reciprocal space maps, V. Jorík: XRD results of characterization of heterogeneous catalysts, O. Pritula: Quantitative phase analysis of the mixture of pure phases of Portland cement. M. Lukáčová: Magnetism and structure of selected molecular magnets, F. Glatt: Ion nitridation of austenitic steels, P. Sedlák: Experimental study of residual deformation in steel samples, J. Marek: Textures of thin MgO films M. Černík: Influence of pressing on the texture of steel sheets, J. Bednarčík: Phase formation and properties of mechanically alloyed CoFe, S. Jurečka: Study of microstructure evolution of CaCO<sub>3</sub> powder in vibration mill.

Number of participants: 30

Conference Web page:

<http://www.saske.sk/RPKD/>

*Organization:*

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

Military Academy, organizers: 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

## 1<sup>st</sup> meeting of the Czech and Slovak structural biologists

Institute of physical biology, Nové Hrady,  
March 14 - 16

*Lectures:* J. Sedláček: Protein Crystallography at the Department of Gene Manipulations of Inst. Molecular Genetics I, J. Brynda: Protein Crystallography at the Department of Gene Manipulations of Inst. Molecular Genetics II, I. Barák: Differentiation and cell division in *Bacillus subtilis*: Genetic and structural studies of proteins involved, P. Flecker: Molecular recognition and misrecognition in complex molecular systems, L. Janda: Preparation of the actin binding domain of plectin for crystallization, T. Kubičárová: Structural biology of telomeres, R. Hrabal: NMR structural study of proteins from Mason-Pfizer monkey virus, P. Padrta: Structure Refinement of Nucleic Acids Using Very Small Residual Dipolar Couplings, M. Munzarová: A Quantum Chemical Study of the Structure-NMR Relationships in Nucleic Acids: Spin-Spin Coupling Constants across the Glycosidic bond vs. Glycosidic Torsion Angle, E. Fadrná: Computer modeling and simulations of nucleic acids at NCBR, Z. Kříž: Computer modeling and simulations of peptides and proteins at NCBR, M. I. Otyepka: Proteins and their interactions with small molecules studied by computer simulations, V. Sychrovský:

Determination of structure, energy, and spectroscopic parameters by means of quantum chemistry, J. Vondrášek: Calculation of interaction energy of inhibitor - enzyme complexes and studies of HIV-1 protease structure and flexibility as a function of its mutations, R. Kužel a J. Hašek: The role of the Czech and Slovak Crystallographic Association in Structural Biology, J. Vévodová: Applications of methods of protein crystallography at NCBR, J. Damborský: Protein Engineering of Dehalogenating Enzymes, J. Hašek: Structural studies of enzymatic reactions, B. Brzobohatý: Laboratory of molecular physiology at Masaryk University, Brno, J. Marek: Laboratory of numerical protein crystallography, teaching bio-crystallography for Brno and beyond, V. Bouda: Live cell as a colloidal system. Muscle contraction, V. Baumruk: Use of vibrational spectroscopy for study of biomolecules, K. Bezouška: Chemistry and mass spectroscopy applied to resolution of the complete covalent structure of small proteins, D. Štys, L. Nedbal: Structural studies at the South Bohemian University.

Web page -

<http://www.jh-inst.cas.cz/~setkani/>

Number of participants: 90

Organization: B. Schneider, I. Kutá Smatanová, D. Štys, J. Hašek

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## 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, 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.

#### Domain - **xray.cz** has been registered.

Addresses of WWW

<http://www.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.

### CSCA Scientific Board

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 Faculty of Chemical Technology,  
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*J. Hašek, R. Kužel*

