



Czech and Slovak Crystallographic Association

Brief review of activities in 2005

The Czech and Slovak Crystallographic Association (CSCA) organized or co-organized several conferences and traditional one-day seminars in 2005.

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

264th Seminar

Faculty of Mathematics and Physics, Charles University, Prague, 22. - 23. 4. 2005

Use of modern multiple-purpose diffractometers, Panalytical systems

Lecture:

R. Kužel: Diffractometer X'Pert PRO MRD, V. Holý: Mirror and diffuse reflectivity on thin films, S. Daniš: High resolution geometry - study of epitaxial thin films, rocking curve mapping of single crystals, M. Dopita, D. Šimek: Study of stresses and textures of thin films, reciprocal space mapping measured on Eulerian cradle, R. Kužel, Z. Matěj, L. Nichtová: Low-resolution parallel beam geometry - study of TiO₂ films and Au nanoparticles, V. Goliáš: Experience with X'Pert diffractometer for analysis of geological materials, P. Bezdička: Crystallization of chalcogenide glasses - what can we see with the aid of powder diffraction, T. Grygar: HTXRD as a tool for identification of expandable clay minerals in complicated mixtures, H. Petříčková: Possibilities of the use of X'Pert PRO MPD diffractometer in pharmacy, R. Kužel: The use of imaging plates and scanner VistaScan for dentists in X-ray diffraction.

Excursions in laboratories of faculty of Mathematics and Physics nad Faculty of Science, Charles University

Organization: R. Kužel, V. Holý

265th Seminar

Academy of Sciences of the Czech Republic, Prague, 20. 4. 2005

Structural Biology and Pharmacy

with the President of the International Union of Crystallography

Lectures:

W. L. Duax: Crystallography and the Noble Prize, J. Dohnálek: Enzymes - Structure and Function, J. Brynda: X-ray Crystallography in the Czech Structural Biology, I. Kutá Smatanová: Crystallization of Membrane Proteins from Higher Plants, W. L. Duax: Antisense ORFs, Codon Bias and the evolution of the Genetic Code, H. Petříčková: Applied Crystallography in Pharmacy, J. Hašek: Structure Analysis of Polymers used in Pharmacology

Organization: J. Hašek

266th Seminar

Institute of inorganic chemistry, Academy of Sciences of the Czech Republic, Řež near Prague, 25. 10. 2005

Crystallography in Řež near Prague

Lectures:

P. Bezdička: Experience with two-year work of 100 m mikrodiffrakce, T. Grygar: Use of HT XRD for the analysis of clay minerals and hydrotalcites, M. Klementová: HRTEM - a new method in the Institute of Inorganic Chemistry, examples of applications, P. Lukáš: In-situ neutron diffraction studies of deformation and transformation characteristics of metals, J. Šaroun: Study of microporosity of ceramics by SANS, J. Vacík: Neutron depth profiling and its applications, S. Vratislav: Research of structural parameters of zeolites and perovskites by neutron scattering

Excursions in laboratories (powder diffraction, electron microscopy, reactor).

Organization: P. Bezdička, P. Lukáš

267th Seminar

Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Prague, 16. 12. 2005

Lectures:

V. Janovec: Crystallography of domain structures, L. Sodomka: Crystallinity of fibres, J. Fiala: Structure of chromium-nickel high-alloyed steels, M. Rieder: Arsenic in iron pyrites from brown coal from Northern-Bohemian brown coal basin, L. Beneš: Use of powder diffraction for study of intercalates, L. Smrček: Dynamic disorder in structure of zeolite deka-dodekasil 3R, J. Kuběna: On light and X-rays, M. Polcarová: In situ synchrotron X-ray topography of bicrystals Fe-Si, P. Šutta: Transparent conducting and insulating oxides from the point of view of X-ray diffraction, R. Kužel: Study of thin TiO₂ films by X-ray diffraction and reflectivity, J. Ondráček: HipHop refinement of protein structures, J. Hašek: Structure of macromolecular system

The seminar was devoted to the speakers celebrating important life anniversaries.

Organization: J. Hašek, R. Kužel



Colloquium - Structure 2005

Castle hotel Třeš , Akademické a univerzitní centrum,
20. - 23. 6. 2005

Traditional CSCA colloquium with the 6th review of student works in the field of crystallography and structure analysis.

Main topics: Structure solution, non-diffraction methods, thin films, materials, textures, stresses, powder diffraction.

Main speakers:

L. Palatinus (Institute of Physics, CAS, Praha): Structure solution by the method of charge reversing, S. Ďurovič (Institute of inorganic chemistry, SAS, Bratislava), J. Hybler (Institute of Physics, CAS, Praha): Refinement of partially disordered OD structures, V. Petříček (Institute of Physics, CAS, Praha): Twins and multiphase single crystal systems.

M. Karlík (Faculty of Nuclear Engineerings, Czech Technical University, Praha): Ion microscopy and tomographic atom probe (FIM-TAP), P. Haušild (Faculty of Nuclear Engineerings, Czech Technical University, Praha): Application of electron diffraction in raster electron microscopy (EBSD), V. Baumruk (Faculty of Mathematics and Physics, Charles University, Praha): Infrared and Raman spectroscopy - what the vibrations can tell about biomolecules, J. Brus (Institute of macromolecular chemistry, CAS, Praha): Study of materials structure by the modern NMR methods, J. Kulda (ILL Grenoble, France): Inelastic neutron scattering, M. Kopecký (Institute of Physics, CAS, Praha): The latest results of X-ray holography, R. Kužel (Faculty of Mathematics and Physics, Charles University, Praha): Single-particle diffraction, M. Hušák (Institute of Chemical technology, Praha): Visualization of structure data by 3D stereoscopic visualization, J. Fiala (University of West Bohemia in Pilsen): Structure analysis by diffusion measurements, J. Čížek (Faculty of Mathematics and Physics, Charles University, Praha): Study of hydrogen interaction with lattice defects in solids by positron annihilation, M. Šlouf (Institute of Macromolecular Chemistry, CAS, Praha): SAXS and QELS study of colloidal solutions of gold and polyethylene particles, M. Kotrlý (Criminological institute, Praha): Structure analysis in criminological practice - interesting cases

WWW pages <http://www.xray.cz/xray/csca/kol2005/>

Number of participants: 72

Organization: R. Kužel, J. Hašek, Z. Šourek

All the abstracts have been published in Materials Structure v. 12, number 2 (<http://www.xray.cz/ms/>).

6th review of student works in X-ray and neutron structure analysis in the Czech and Slovak Republics

21 participants took part in this traditional lecture sessions. They presented mainly the results of diploma and doctoral thesis in the field of X-ray and neutron scattering obtained in the laboratories in the Czech and Slovak republics - residual stresses, thin films, structure solution, phase analysis, microdiffraction, protein crystallography, mineralogy.

The first three works (presentations) have been awarded by diplomas and financial reward - *Mariana Klementová* (Institute of Inorganic Chemistry, Academy of Sciences of the Czech Republic, Řež near Prague): Tantaloniobates in cæsiterite: inclusions or secretions?, *Jan Krčmář* (Faculty of Science, Masaryk University Brno): X-ray diffraction on thin polycrystalline films, *Martina Pokorná* (Faculty of Science, Masaryk University Brno) Crystal structure of CV-III lectin from human opportunistic pathogen

4. Discussions of structural biologists

Institute of physical biology, Nové Hradky, 10. - 12. 3., 2005

Lectures:

R. Kužel: Possibilities of modern X-ray scattering and imaging techniques in biology, T. Obšil: Regulation of 14-3-3 protein function, V. Baumruk: Solution structure and dynamics of peptides and proteins from Raman optical activity, M. Hušák: Possible use of 3D stereoscopic visualization in structural biology, I. Barák: Where the asymmetry in gene expression starts? V. Sklenář: Quo vadis? The role of NMR in structural biology

Short contributions:

J. Dohnálek, T. Skálová, V. Kopecký, L. Urbaníková, V. Suchá, J. Wolfová, J. Hašek, M. Prokop, P. Máder, L. Luley, J. Burda, P. Flecker, B. Schneider, R. Fiala, V. Sychrovský

Abstracts of lectures and poster can be found at

<http://www.xray.czs/setkani/>

Number of participants: 73

Number of posters: 32

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

Contributions in Materials Structure vol. 12 (2005), č. 1.

6th Autumn School on X-ray scattering from surfaces and thin layers

Smolenice, Slovakia, 18. 9. - 21. 9. 2005

Tutorials:

P. Zaumseil: High-resolution diffraction, P. Mikulík: X-ray Reflectometry and diffuse scattering, V. Holý: Simulation of X-ray reflectivity and diffraction curves, N. Darowski: Grazing-incidence diffraction and GISAXS, K. Walter: Texture analysis and residual strains

31 short contributions.

WWW page -

<http://cmd.karlov.mff.cuni.cz/Smolenice-2005/>

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



14th Regional conference on powder diffraction

Liptovský Mikuláš, 21. - 23. 9., 2005

Lectures:

M. Čerňanský: Single-line momentum methods, L. Smrčok: Neutron time-of-flight powder diffraction - a small introduction, E. Čaplovič: Neutron diffraction analysis of changes of phase composition at heating of fast solidified powder from high-speed steel, V. Kavečanský: Study of strongly disordered systems, J. Fiala: Use of Fourier transform in spectroscopy and quantitative microscopy, M. Kolega: Fourier analysis of azimuthal diffraction line profile, M. Jergel: X-ray analysis of ultra short period multilayers, R. Kužel: Study of inhomogeneity and thermal stability of submicrocrystalline structure of deformed materials, A. Buchal: Determination of mean crystallite size below 5 nm by X-ray diffraction, V. Jorík: Crystal structure of [Cu(3-pyacr)₂(H₂O)₂] complex from powder, some experience from solution of problems related to the nature of complex compounds, F. Laufek: Crystallochemistry of Sb-Te-Ni system, J. Marek: Textures of thin films, M. Černík: X-ray stress analysis in rolled steel sheets, M. Krupka: Presentation of the X-STRESS 3000 diffractometer - PANalytical, K. Kolařík: Diffraction study of surface integrity of high-solid alloy Incinel 718 after elektroerosive working and milling, J. Drahokoupil: Study of surface worked steel samples, Z. Pala: X-ray diffraction analysis of residual stresses of strolled steel surfaces, N. Ganey: Diffraction analysis of stress states in iron materials induced by surface working

Number of participants: 22

WWW page -

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

Organization: V. Kavečanský, S. Jurečka, E. Čaplovič, R. Kužel

Eighth Heart of Europe Bio-Crystallography Meeting

Karlovy Vary, 29. 9. - 1. 10. 2005

Main lecture:

Zbigniew Dauter (Argon, IL): Phasing on anomalous scattering: Multi- versus Single-wavelength,

32 short contributions

WWW page -

<http://www.img.cas.cz/hec/>

Abstracts published in Materials Structure, vol. 12, no. 3, 2005.

Organization: J. Sedláček

Crystallization Course

Nové Hradky, 10. 10. - 12. 10. 2005

Speakers:

Jiří Brynda (Praha, Czech Republic), Juan Manuel García-Ruiz (Granada, Spain), José A. Gavira (Granada, Spain), Rolf Hilgenfeld (Lübeck, Germany), Thomas Klupsch (Jena, Germany), Jeroen Mesters (Lübeck, Germany), Pavlína Řezáčová (Texas, USA), Lúbia Urbániková (Bratislava, Slovakia)

WWW page -

<http://www.xray.cz/cc>

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