



## Czech and Slovak Crystallographic Association (CSCA)

### Activities 2018 2019

In the period 2018-2019 the CSCA organized several meetings, seminars and conferences

### One-day seminars - Rozhovory

#### 303. ROZHOVORY

Faculty of Mathematics and Physics, Charles University Praha, 17. 5. 2018

##### Small-Angle Scattering

J. Ilavský: You got Small-Angle Scattering curve. What next? (examples), V. Ryuktin: In-situ SANS study of precipitates nanostructure in single crystal Ti15Mo, P. Strunz: The influence of C/Ta ratio on TaC precipitates in Co-Re base alloys investigated by small-angle neutron scattering, P. Hoghoj: Exploring the very small : applications of SAXS/WAXS in the lab

Excursions in labs

Organization: M. Dopita, R. Kužel, V. Holý

#### 304. ROZHOVORY

University of Jan Evangelista Purkyně, Faculty of Science, Ústí nad Labem, 11. 11. 2019

##### Structure and properties of polymers

M. Steinhart: Peculiarities of study of polymer systems and methods used in Institute of Macromolecular Chemistry, J. Hašek: X-ray diffraction for development of materials based on mixtures of chitosa with chitin fibres, A. Zhigunov: Characterization of polymer structures, M. Hřibová: Phase transitions of polymers, M. Konefal: X-Ray Reflectivity and Grazing Incidence Small Angle Scattering as tools for polymer thin films analysis, P. Čapková, P. Ryšánek: Crystallization of polymers in strong electric field

Excursions in labs

Organization: P. Čapková, P. Ryšánek

### Struktura 2018

Hotel Svornost, Harrachov

18. - 21. 6. 2018

#### Experimental methods in X-ray and neutron structure analysis

Lectures:

##### Real structure

R. Kužel: Real structure and total powder pattern fitting, P. Vertát: FitExc - program for fitting of diffraction lines in MS Excel,

K. Poruba: Universal system for management of samples: development of extended web application,

R. Pažout: Substitution limits in new mineral

Starocesekéite  $\text{Ag}_{0.7}\text{Pb}_{1.6}(\text{Bi}_{1.35}\text{Sb}_{1.35})_{2.70}\text{S}_6$

J. Capek: Comparison of residual stresses determined by different methods, K. Trojan: Effects of Advanced Laser Processing on the Microstructure and Residual Stresses of H13 Tool Steel810,

Charles Hervoche: Characterization of residual stress distribution in structural materials by neutron diffraction at CANAM infrastructure,

M. Cerník, P. Vranec: Structure Evaluation of Dual Phase Steels by EBSD Method

##### Databases, software

R. Kužel: Database of powder diffraction data - PDF-4+, phase analysis,

F. Laufek: Database of inorganic structures ICSD - Desktop,

P. Roubíček: Simple program for quantitative phase analysis,

J. Drahokoupil: Possibilities of computer simulations,

J. Hašek: Cambridge structure database of organic and organometallic compounds in 2018,

J. Rohlíček: Comparison of solvates of organic compounds with program CrystalCMP,

M. Hušák: Advances in crystal structure solution from powder diffraction data of molecular crystals,

M. Dušek: Jana2020 - the first kid's steps of program Jana2006,

J. Brynda: Solution of protein structures with program ARCIMBOLDO

##### Biocrystallography

J. Hašek: Porous catalysers of protein crystallization,

M. Marek: Crystallographic studies of inhibitor complexes HDAC8,

I. Berková: Structural studies of novel haloalkane dehalogenase DgaA from *Glaciococla agarylitica* NO2,

P. Havlíčková: Crystallographic studies of a newly prepared histidinol-phosphate phosphatase Tt82 from *Thermococcus onnurineus*,

K. Rejzková: Structural studies of haloacid dehalogenase Tt81 from *Thermococcus thio-reducens*

P. Ryšánek: Surface structure of chemically modified polymeric nanofibers studied by molecular modeling,

M. Popíšil: Structural description and properties of  $\text{Mg}_2\text{Al}$ -layered double hydroxides intercalated with the fluvastatin anions solved by molecular simulation meth-



From Struktura 2018 in Harrachov. MSTRUCT course

ods,

V. Ryukhtin: In-situ SANS study of precipitates nanostructure in single crystal Ti15Mo,

Cinthia Antunes Correa: Incommensurately modulated crystal structures and phase transitions of  $\text{Cu}_3+\text{xSi}$ ,

E. Duverger-Nédellec: Transitions toward complex electronic states and aperiodic structures in  $\text{P}_4\text{W}_{16}\text{O}_{56}$ ,

M. Meduňa: Defect study in epitaxial SiGe graded microcrystals,

P. Cejpek: Determination of content of phases L21 and B2 in alloys  $\text{Ni}_2\text{MnGa}$ ,

J. Kopeček: Destroying bulks and connecting powders in Fe-Al-Si,

#### *Instruments, commercial lectures*

Heike Ehmann: Cellulose nanocrystals - structural insights via 2D q-mapping,

Lukasz Sadowski: X-Ray Diffraction Systems – Technical advantages and Application Related Benefits,

J. Gertenbach: XRD Epyrean news,

A. Stricker: New developments in microfocus sources for X-ray diffractometry,

B. Míč: New detectors of Bruker,

P. Oberta: New Rigaku XRD SmartLab XE,

M. Čurda: Experience with powder diffractometer Bruker D8 Advance: Automatic divergent slit, „variable counting time“ method,

#### *Courses:*

Z. Matěj: MSTRUCT - real structure parameters modeling and fitting,

M. Hušák: Program, DASH



Jan Gertenbach, Panalytical

*Number of participants: 70*

Abstracts:

<http://www.xray.cz/ms/bul2018-3.htm>

Photos:

<http://www.xray.cz/xray/csca/kol2018/>

<http://www.xray.cz/ms/bul2019-3.htm>

## Struktura 2019

Hotel Jehla, Žďár nad Sázavou

10. - 13. 6. 2019

### Lectures:

Z. Matěj: Crystallographic software on malleable hardware,

J. Hybler: What's new in polytypis of cronstedtite,

M. Čurda: Application of powder X-ray diffraction for heavy mineral prospection in the Czech Republic,

E. Duverger Nedellec: Crenel or not crenel: what is the function?

A. Chauvin: Structural analysis of nanoporous gold obtain by dealloying

M. Hušák: The use of DFT calculation for salt-cocrystal distinguishing,

J. Rohlíček: Study of desolvation of organic compounds,

J. Černák: Solvatomorphism of nickel(II) complex with salen-type ligand,

E. Rakovský: Hands-on chemical crystallography course using Olex2,

Ján Moncol: Use of program packages of CSD database for teaching,

R. Kužel: New Crystal Maker X for structure visualization of structures, simulation of diffraction patterns, use for teaching

M. Jergel: Pentacen growth on graphene by in situ GISAXS and GIWAXS,

E. Dobročka: X-ray diffraction analysis of epitaxial layers with depth-dependent composition,

O. Caha: Home assembled x-ray instrumentation: rocking



curve imaging, standing wave fluorescence,  
T. Roch: Impact of substrate on preferential orientation of NbN thin layers,

E. de Prado: Hybrid multiple diffraction,

J. Kulda: What is hidden in the background of Bragg diffraction. Diffuse scattering and PDF analysis not only with neutrons,

P. Bezdička: How much is there? Difficulties of quantitative phase analysis,

J. Kašík: Utilization of high temperature X-ray powder diffraction for study of preparation of nanomaterials for environmental applications,

J. Kopeček: Spark plasma sintered alloys FeAl<sub>20</sub>Si<sub>20</sub> with ternary additions - microstructure and phase composition,

M. Čerňanský: Crystallite size and position of diffraction lines,

J. Drahokoupil: Ion implantation of titanium alloys



From Struktura 2019 in Žďár nad Sázavou.



### *Biocrystallography*

J. Hašek: Principles of dominant of adhesive mode explains why porous materials improve crystallization of biological macromolecules,

I. Kutá Smatanová: Differences in crystallization of various haloalkane dehalogenases,

J. Brynda: Directionality of dipoles of fluoregen cofactors in context of crystal structure,

P. Kolenko: Software Development for Macromolecular Crystallography,

J. Stránský: Small angle X-ray scattering of biological samples with laboratory equipment in BIOCEV

### *Instruments, commercial lectures*

P. Oberta: Rigaku news 2018/2019,

P. M. Worsch: Rheology and SAXS in one go with a laboratory SAXS system - method and applications,

B. Míč: Bruker news,

J. Maixner: Microdiffraction diffractometer Discover with 2D detector Vantec 500

### *General info*

J. Kulda: Our membership at ILL,

P. Mikulík: ESUO - European Synchrotron User Organisation,

R. Kužel: 25th Assembly and congress of IUCr



### **13th student symposium of works from the field of crystallography and structure analysis**



M. Malý



P. Veřtát

### **Biocrystallography session:**

B. Kaščíková: Avian orthoreovirus protein - NS forms pseudocapsids,

A. Shaposhnikova: Experimental and computational investigations of the human system PAPS-Synthase,

P. Havlíčková: Structural and functional studies of HAD phosphatase Tt82 from *Thermococcus thioreducens*,

A. Mazur: Preliminary crystal structure analysis of serpin 4 from tick,

F. Melicher: Structural insight into lectins from *Photobacterium asymbiotica*,

M. Malý: Estimation of diffraction limit using paired refinement

Awarded students: M. Malý, F. Melicher, P. Havlíčková

### **Materials and Physics session**

K. Trojan: Study of the real structure of the laser-cladded steel,

P. Veřtát: Thermally induced changes in modulated structure of 10M Ni<sub>50</sub>Mn<sub>27</sub>Ga<sub>22</sub>Fe<sub>1</sub> martensite,

J. Čapek: Comparison of the rolling texture of particular phases of dual-phase steel with single-phase steels,

M. Lebeda: Crystal structure and properties of SrTi<sub>1-x</sub>Mn<sub>x</sub>O<sub>3</sub> perovskites – from calculations to experiments,

T. Číž: Structural analysis of perovskite thin films and multilayers,

T. Kretková: Thermal evolution and microstructure of gas aggregation cluster source produced metal nanoparticles,

M. Pšenička: Structural analysis of clay minerals intercalated with drugs solved by classical molecular dynamics and DFT methods,

J. Škoda: Study of arrangement of intercalated organic species within layered materials by molecular simulation methods,

P. Doležal: Bound state of crystal electric field excitation and a phonon in CePd<sub>2</sub>Al<sub>2</sub>

Awarded students: P. Veřtát, T. Kretková, P. Doležal

*Number of participants: 72*

Abstracts: <http://www.xray.cz/ms/bul2019-3.htm>



CSCA was co-organizer of other meetings. This was for examples **Discussions in Structural Molecular Biology**, organized in Nové Hradý now also as annual meeting Czech Society for structural biology

[www.structbio.org](http://www.structbio.org)

### XIII Discussions in Structural Molecular Biology

Academic and university centre Nové Hradý

22. 24. 3. 2018

Abstracts:

<http://www.xray.cz/setkani/abst2018/abstracts.htm> (html)

<http://www.xray.cz/ms/bul2018-1.htm> (pdf)

### XIV Discussions in Structural Molecular Biology

Academic and university centre Nové Hradý

21.

Abstracts:

<http://www.xray.cz/setkani/abst2019/abstracts.htm> (html)

<http://www.xray.cz/ms/bul2019-1.htm> (pdf)

### "Advanced methods in macromolecular crystallization VIII"

Academic and University Center at Nove Hradý (Czech Republic)

June 10-16, 2018

The FEBS practical crystallization course has become a tradition: it has been organized biennially since year 2004. It is held in Nove Hradý, a small town in southern part of Czech Republic, a few kilometers from Austrian border in the Academic and University Center. The Center is a unique place: a historical and stylish chateau surrounded by park that offers many lecture halls, festive poster halls and laboratories. The Center provides unique opportunity to organize all of the course activities such as lectures, discussions, lab exercises, social program and accommodation under one roof.

The course is organized by Ivana Kuta Smatanova from the University of South Bohemia and Pavlina Rezacova from the Czech Academy of Sciences; under the main sponsorship of the Federation of European Biochemical Societies (FEBS). The International Union for Biochemistry and Molecular Biology supported participation of Prof. Petra Fromme from the School of Molecular Sciences of Arizona State University (Tempe, USA) as an IUBMB speaker for the 2018 FEBS course. Participants, mostly students and postdocs, were introduced to standard and advanced methods of protein crystallization. Not only to the theory, but also to practice: morning lectures were supplemented by afternoon practical sessions. Most of the students performed experiments on their own proteins. Evenings were filled with discussions, poster sessions and networking. Three poster prizes were awarded; the IUCr Journals

Poster Prize was awarded to Michal Busa from the Institute of Organic Chemistry and Biochemistry in Prague, Czech Republic.

Course webpage:

<https://macromolcryst2018.febsevents.org/>

Abstracts were published in Materials Structure vol 25, no. 3a (2018), <http://www.xray.cz/ms/bul2018-3a.htm>

Number of student participants: 38

Number of lecturers: 30 (from Europe and North America)

### Special group Solid state Chemistry and Physics

#### Development of Material Science i Research and Education

Main event organized is a seminar *Development of Materials Science in Research and Education (DMSRE)*. The first one took place in 1990 in Gabčíkovo. Since this year it is a regular meeting organized by the special group together with the Czechoslovak Association for Crystal Growth (CSACG) regularly moving between Czech and Slovak republics, usually at the beginning of September. Other organizers are Faculty of chemical and food technology STU Bratislava, Faculty of Materials and Technology in Trnava, CSCA, Regional committee of the Czech and Slovak Crystallographers and Slovak society of industrial chemistry. Conferences in 2018 and 2019 took place in 3.-7.9. i Pavlov and in 2.-6.9. in Nová Lesná, respectively.

Programme is traditionally devoted to the following items:

- Trends in development of materials research.
- Education of materials science at the universities.
- Information about the research programmes of individual institutions.
- Information about equipment for preparation and characterisation of materials.

Participation is usually close to 40. Texts to the lectures are published in proceedings IOP Conference Series: Materials Science and Engineering.

Information on activities of the special groups can be found at <http://oschftl.bts.sk>. and about the conferences on the page of CSACG

<http://csacg.fzu.cz/> resp. <https://dms.fzu.cz/>



## Scientific Board of the CSCA 2017 2021

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Ústav molekulární biologie SAV, Bratislava

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- prof. Ing. Nikolaj Ganev, CSc.  
Fakulta jaderná a fyzikálně inženýrská, ČVUT Praha

*R. Kužel, J. Hašek*

## IUCr - International Union of Crystallography

### IUCr commissions

R. Kužel is a member of the IUCr executive committee since 2014. The following CSCA members are working in the IUCr commissions

Margarida Henriques (Institute of Physics CAS, Praha) - magnetic structures, Bohdan Schneider (Institute of Biotechnology CAS, BIOCEV Vestec) - biological macromolecules, Petr Bezdička (Institute of Inorganic Chemistry, Řež u Prahy), art and cultural heritage, Michal Dušek (Institute of Physics CAS, Praha) - aperiodic crystals, crystallographic nomenclature, International tables, Lukáš Palatinus (Institute of Physics CAS, Praha) – crystallographic computing and electron crystallography, Jozef Kožíšek (STU Bratislava) – quantum crystallography.

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### International conferences organized by the CSCA

#### Current Trends and Future of Crystallography in Chemistry, Physics, Biology and Materials Science

*Prague Congress Centre and hotel Olšanka, Prague, Czech Republic, May 14 - 16, 2019*

The workshop was organized in connection with the meeting of the International Programme Committee (IPC) of the 25 IUCr congress and it summarized main topics of modern crystallography as represented by the commissions of the International Union of Crystallography. Most of contributions during the workshop was only 15 minutes without discussion. Depending on the commission type, the talk started with a characterization of the subject and possibly streams of the activity of the commission (example CAC – two basic streams: aperiodic crystals, modulated structures, or CPD – structure refinement from powder diffraction data, real structure study, in-situ studies of different types). This was followed by a few selected highlights achieved in the last years and closed by possible indication of future development. During the presentation or at their end proposed keynotes and microsymbosia for the IUCr 2020 congress could be briefly commented. Everything

was organized during one day together in the Prague Congress Centre together with excursion there. The workshop was accepted extremely well by the participants and organization of such events before next IUCr congresses is highly recommended. The workshop was open for public. Over 80 participants were registered including IPC members.

Programme:

<http://www.xray.cz/iucr/ctfc/schedule.htm>

Next two days took place in hotel Olšanka where most of participants stayed. During one and half of very intensive work the whole programme of the 25th IUCr congress was basically prepared - three plenary lectures, 35 keynote lectures and over 100 microsymbosia (titles, co-chairs). The work was quite efficient and the first day with presentations of all the commissions was very helpful for that since all the IPC members were open for compromises and easier agreement. It was necessary to cut down original proposals of keynote lectures to one third and session topics to one half.

For all the programme preparation, database driven online software was prepared. It was used also during the IPC meeting and worked basically well. Excellent work during the meeting was done mainly by both chairs of IPC and LOC (Local Organizing Committee) - Pavlína Řezáčová and Ivana Kutá Smatanová as well as by the LOC member Milan Dopita.

Workshop web page <http://www.xray.cz/iucr/ctfc/>

Proceedings

<http://www.xray.cz/ms/bul2019-2.htm>

*R. Kužel*

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### 25th congress IUCr in Prague 2020

The congress was planned for August 22-30, 2020 in Prague Congress Centre.

Main organizer is the CSCA, congress chair R. Kužel, chair of the International Conference Committee (IPC) is I. Kutá



Members of the 25th IUCr congress International Programme Committee and a few other participants of the CTFC workshop in PCC.



IPC meeting in hotel Olsanka.

Smatanová, chair of the local organizing committee is P. Malý Řezáčová and chair of the National Advisory Board is J. Hašek. We closely collaborate with Auletris (M. Haloun, [www.auletris.com](http://www.auletris.com)).

At the beginning of March, it became clear that the situation in summer could be complicated and we asked the PCC (Prague Congress Centre) about possibility of postponing to 2021 and agreed on preliminary reservation in August 2021 and we got just one week. In the second half of March, we faced the situation that this term had to be confirmed within a few days. Fast online meeting of the IUCr EC decided quickly on this so that the congress was postponed to **August 14-22, 2020**.

The programme was more or less frozen at the state from March. Unfortunately, the current situation with Covid everywhere is such that nobody knows what it will be in summer 2021. Our plans have not been changed yet. It is only clear that the congress will have to be hybrid, i.e. with both present and distant participants.

Congress website:

<https://www.iucr2020.org>  
(it should also be [www.iucr2021.org](http://www.iucr2021.org), [www.iucr25.org](http://www.iucr25.org),  
older alternative: <https://www.xray.cz/iucr>)



From the meeting of local conference committees in Prague Congress Centre, September 2019