

9th European Powder Diffraction Conference

Praha, Czech Republic, August 31 - September 5, 2004

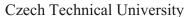
Book of Abstracts

EPDIC Organization				
List of Exhibitors and Sponsors				
Preface				
Notes to Scientific Programme				
Size-Strain workshop (August 31 - September 2)	1			
EPDIC IX (September 2 - September 5)	15			
Plenary Lectures	15			
•				
Microsymposia	19			
A1: Structure Solution and Refinement	19			
B1: Stress, Strain and Texture	23			
A2: Neutron Diffraction - Instruments	29			
B2: Phase Transitions	35			
A3: Phase Analysis	40			
B3: Non-ambient Conditions	45			
A4: Structure and Properties of Bio - Materials	50			
B4: Structure of Nanocrystalline Materials	53			
A5: Structure Solution from Powder Diffraction - Applications I	58			
B5: Materials Science (metals, alloys, intermetalics)	64			
A6: Neutron Diffraction - Applications (magnetic materials, ionic conductors)	69			
B6: Minerals	72			
A7: Indexing of Powder Diffraction Patterns, Software	79			
B7: Techniques and Instruments	84			
A8: Structure Solution from Powder Diffraction - Applications II	87			
B8: Thin Films and Multilayers	92			
Poster Topics	97			
T1: Structure Solution and Refinement	97			
T2: Real structure - Line Profile Analysis	111			
T3: Real structure - Stress, Strain and Texture	128			
T4: Real structure - Thin Films and Multilayers	148			
T5: Nanocrystalline and Disordered Materials	159			
T6: Materials Science - Metals and Alloys	169			
T7: Minerals	173			
T8: Phase Analysis	177			
T9: Phase Transitions, Non-Ambient Conditions	184			
T10: Magnetic and Ferroelectric Materials	199			
T11: Neutron Diffraction	207			
T12: Small Angle Scattering	215			
T13: Instruments and Methods	223			
Late and Special Abstracts	231			
Subject Index	233			
Author Index				



Organizing Institutions

Czech and Slovak **Crystallographic Association**



Faculty of Civil Engineering

Faculty of Mechanical Engineering

Faculty of Nuclear Sciences and Physical Engineering

Charles University

Faculty of Mathematics and Physics

Natural Science Faculty

Academy of Sciences of the Czech Republic

Institute of Physics

Institute of Macromolecular Chemistry

Conference chairman

Radomír Kužel

Department of Electronic Structures, Faculty of Mathematics and Physics, Charles University, 121 16 Praha 2, Czech Republic, kuzel@karlov.mff.cuni.cz, fax: 00420224911061

Conference secretaries

Pavlína Řezáčová

Institute of Molecular Genetics, Academy of Sciences of the Czech Republic, Prague, Czech Republic, rezacova@img.cas.cz

Ivana Kutá Smatanová

Institute of Physical Biology, South Bohemian University at České Budějovice, Nové Hrady, Czech Republic, ivas@bf.jcu.cz

Secretary for commercial exhibition and presentations

Zbyněk Šourek

Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic, sourek@fzu.cz

Conference Web site

http://www.xray.cz/epdic



Programme committee

Y. Andreev (St. Andrews, UK)

R. Cernik (Daresbury, UK)

R. Černý (Geneve, Switzerland)

 $\pmb{L.\ Cranswick}\ (Chalk\ River,\ Canada)$

J. Fiala (Plzen, Czech Republic)

H. Fuess (Darmstadt, Germany)

C. Giacovazzo (Bari, Italy)
H. Goebel (Munich, Germany)

J. Grochowski (Krakow, Poland)[†]

S. Ivanov (Moscow, Russia)

V. Kavečanský (Košice, Slovakia)

†in memoriam

B. Koppelhuber-Bitschnau (Graz, Austria)

J. Kulda (Grenoble, France)

M. Kunz (Basel, Switzerland)

V. Langer (Göteborg, Sweden)

E. J. Mittemeijer (Stuttgart, Germany)

H. F. Poulsen (Riso, Denmark)

J. Rius (Bellaterra, Spain)

P. Scardi (Trento, Italy)

S. Skrzypek (Krakow, Poland)

T. Ungár (Budapest, Hungary)

Organizing committee members

Registration

P. Řezáčová Institute of Molecular Genetics, Academy of Sciences of the Czech Republic

Treasurer

J. Hašek Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic

Accommodation

I. Císařová Natural Science Faculty, Charles University

Trips

D. Havlíček Natural Science Faculty, Charles University

Poster session

N. Ganev Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University

Exhibition

R. Gyepes Natural Science Faculty, Charles University

Z. Šourek Institute of Physics, Academy of Sciences of the Czech Republic

Refreshments, lunches

R. Králová Faculty of Mechanical Engineering, Czech Technical University

A. Župčanová Institute of Physical Biology, South Bohemian University at České Budějovice

Local arrangements

L. Kopecký Faculty of Civil Engineering, Czech Technical University
 R. Novák Faculty of Mechanical Engineering, Czech Technical University
 S. Daniš Faculty of Mathematics and Physics, Charles University

J. Hybler Institute of Physics, Academy of Sciences of the Czech Republic





List of Exhibitors and Sponsors

PANalytical B. V. www.panalytical.com

Bruker AXS GmbH www.bruker-axs.de

International Union of Crystallography www.iucr.org

International Centre for Difffraction Data www.icdd.com

Unisantis S. A. www.unisantis.com

HUBER Diffraktionstechnik GmbH & Co. KG www.xhuber.com

X-Ray Optical Systems, Inc. www.xrayoptics.com

STOE & Cie GmbH www.stoe.com

GBC Scientific Equipment www.gbcsci.com

GE Inspection Technologies, GmbH www.geinspectiontechnologies.com

INEL www.inel.fr

Osmic, Inc - A Rigaku Company www.osmic.com

Zentiva, a.s. Praha www.zentiva.cz

Anton Paar www.anton-paar.com

Oxford Cryosystems Ltd www.oxfordcryosystems.co.uk

Röntgenlabor Dr. Ermrich www.roentgenlabor-ermrich.de

Czech and Slovak Crystallographic Association www.xray.cz

to August 15

Organizers are very grateful to the above sponsors that enabled to reduce fees especially to students and scientists from developing countries as well as to cover part of the conference area rental.



Preface

The Czech and Slovak Crystallographic Association (CSCA) organized 18th European Crystallographic Meeting in 1998 at Czech Technical University. In spite of various problems, we had a feeling that the nice location of the Faculty of Civil Engineering, keeping together lectures, poster and exhibition, would be ideal for conferences. Most of a group of few people who did their best that time came to decision that they could organize another conference at this site. In 2001, we decided to submit our application for organization of popular EPDIC conference to the EPDIC committee and were happy in May 2002 shortly before the last EPDIC in Uppsala, when the EPDIC committee accepted our proposal. However, in that time, we also realized that it would be not easy to maintain the high level of all past EPDICs. Our main aims are, of course, high scientific level of the conference as well as a nice working atmosphere and pleasant time during the whole conference. I am happy that not only scientists interested in powder diffraction but also colleagues from other fields of crystallography and structure analysis as e.g. bio-crystallography are taking part at the organization of the meeting. We organized together many annual CSCA meetings and hopefully the collaboration will be successful also in this case.

The preparation started in spring 2003 when the programme committee was created. At the end of 2003 a set of 34 proposals for plenary lectures was collected. Then Internet discussion forum was opened for comments of the committee members to each candidate from the point of view of the suitability with respect to plenary lecture. After that, Internet polls were organized and each member could give points (from -5 to +5) to each candidate. All the committee members took part at this procedure. Modification of the results was planned in order to meet some criteria like avoiding topics overlapping, geographical aspects etc. Finally, the results shown clearly the first six candidates which met the criteria in quite sufficient manner and therefore the procedure was closed without changes. However, most of other candidates were then invited to microsymposia or they are among regular participants.

In the next step, the EPDIC award selection was organized in a similar way during February and March. For five candidates, their nomination letters, curriculum vitae, list of publications, other supporting material and also supporting letters of other scientists were submitted, displayed for the programme committee on the Web site and opened for their comments. The procedure was finished again by Internet voting and also in this case all the committee members gave their points (0 - 5) to the candidates. Fortunately, again the first place was quite clear and organization of the second round was found to be unnecessary. Four of the five candidates will however be present at the EPDIC anyway.

The deadline for abstracts of those authors asking for lectures was at the beginning of May. Nearly half of all abstracts came that time. The abstracts were immediately displayed in html format on the Web site under the indicated conference topics. Authors marked their classifications themselves during the abstract registration at the Web site. Three options for methods and three options for materials were possible. All programme committee members were asked for evaluation of abstracts according to their topics with the aim to select oral contributions. The criterion was not only the quality of contributions but also their suitability for a lecture. For each topics 3-4 members were asked to give their preferences. After all evaluations arrived, the chairman of the conference tried to balance the topics and distribute the abstracts into them according the evaluation. Finally, the programme of microsymposia was approved by the committee. Abstracts for posters came during June.

This was the way the programme of EPDIC IX was prepared. All the accepted abstracts for oral and poster presentations are collected in this journal. Full contributions (6 pages) will be published, if accepted by referees, in Zeitschrift für Kristallographie and its Web site.

I appreciate very much the work of all the Programme Committee members. As you could see above they were not only formal members but they were actually working and finally they will also serve as chairs and co-chairs of microsymposia.

All organizers believe that participants will have a nice time in Prague during the conference, find new ideas helping them in scientific work and, perhaps, find also new friends.

Praha, August 2004 R. Kužel



Notes to Scientific Programme

Size - Strain workshop

In autumn 2003, Paolo Scardi came with an idea to join already traditional Size - Strain meeting with the EPDIC conference in order to save time, nowadays when more and more conferences appear. It was decided to call it workshop and organize it as a meeting more focussed to the problems of line broadening analysis - main sources of diffraction line broadening, size-strain measurement and modelling, line broadening analysis for nanocrystalline materials, size - strain software.

The workshop is intended for all those interested in the X-ray powder diffraction analysis of grain size and strain including its relation to texture and stress. The analysis of powders, bulk materials as well as of thin films are of interest. Programme consists of several invited lectures and detailed discussions. The workshop follows three Size-Strain conferences that have been organized since 1995.

Software workshop

The idea of this workshop appear during the ECM conference in Durban, in August 2003, during a discussion with Lachlan M Cranswick who already organized several software workshops during the IUCr and ECM meeting and it is known by his enthusiasm in this field and also by the CCP14 site which has been created and maintained mainly by him. It was decided to pick up two topics - size - strain software and phase analysis software because there were several workshops on structure solution and refinement software in last years. He invited several lecturers and the programme covers whole day.

EPDIC programme

The EPDIC programme is more or less traditional with some modifications. It begins with an EPDIC award evening lecture. Three conference days are opened with two plenary lectures and continue with two parallel morning microsymposia. Other microsymposia are organized during afternoons. Poster sessions are organized twice after lunches but the posters should be displayed for the whole conference.

Codes of Contributions

Χ -			Y -	
	S	Size - Strain workshop	O	oral contribution
	I	Invited plenary lectures	P	poster
	An, Bn	Microsymposium	m	number of lecture within
	Tn	Poster session topics		session or poster number
	n	Number of session		