## EPDIC IX -European Powder Diffraction Conference and Size-Strain Workshop

The 9th European Powder Diffraction Conference together with two-days Size-Strain IV workshop held at the beginning of September 2004 in Prague. The conference site was at the Czech Technical University, Faculty of Civil Engineering.

The Size-Strain workshop (August 31 - September 2) followed the tradition of past Size-Strain conferences. The first one was organized in August 1995 in Liptovsky Mikulas, Slovakia, the second one in November 1998 in Freiberg, Germany and the third one in December 2001 in Trento, Italy. They were devoted to the problems of real structure analysis mainly by diffraction methods. This time only the workshop was organized for all those interested in the X-ray powder diffraction analysis of grain size and strain including its relation to texture and stress. Invited lectures given by R. Kuzel, N. Armstrong and P. Scardi were devoted to the reviews of dislocation and size diffraction line broadening as well as whole powder pattern modeling for the study of nanocrystalline and imperfect materials. Unfortunately, two lectures on disclinations and stacking faults had to be cancelled. Anyway, about 90 participants could listen to other interesting lectures. The XRD analysis of nanocrystalline powders and thin films as well as severely deformed materials was discussed (D. Rafaja,

R. Pielaszek, Z. Kaszkur, J. Gubicza, A. Leineweber, J. Rodriguez-Carvajal, A. Borbély, A. Boulle). At the end, discussion on problems of line profile analysis was organized by Paolo Scardi, the chair of the workshop.

The EPDIC IX started with another workshop organized by Lachlan M Cranswick. He is famous by his enthusiasm in the field of (mainly free) crystallographic software distribution, maintaining the CCP14 site as the CCP14 secretary for many years and organizing software workshops during the IUCr and ECA meetings. After several workshops on structure refinement, this time the programme was splitted into two half-day sessions - size-strain software and phase analysis software. The workshop was free for the Size-Strain and EPDIC registered participants and more than 150 participants could listen to 14 short presentations. Both commercial (Bruker Topas, Panalytical HighScore, Bergmann BGMN) and free software were presented. Some of it is of general purpose including size-strain and phase analysis, other is rather special. Both phenomenological size-strain and phase analysis are included in the Rietveld type programs like Fullprof (Rodriguez-Carvajal) or Maud (Lutteroti). Nowadays, also in the case of line profile analysis, the whole powder pattern modeling (fitting) including physically realistic microscopic description seems to be the most appropriate. This approach was presented by M. Leoni (PM2k) and G. Ribárik (CMWP - fit).

The third workshop - ICDD was organized by J. Faber during the evening of the second conference day. He in-



EPDIC IX - Poster and Exhibition Area





David Rafaja, R. Kužel



Vincent Favre-Nicolin, the EPDIC award winner



Conference secretary Pavlína Řezáčová

formed about the new trends in development of PDF databases.

Three-days EPDIC programme started with two plenary lectures each day: Andy Fitch (ESRF, Grenoble) on high-resolution diffraction, Udo Welzel (Stuttgart) on diffraction stress analysis, Lynne McCusker (Zurich) on exploiting preferred orientation to resolve overlapping reflections, Tamas Ungar (Budapest) on nanocrystalline materials, Gavin Vaughan (ESRF) on multicrystal approach to crystal structure solution and Helmut Ehrenberg (Darmstadt) on in-situ characterization of materials.

Then two parallel sessions were running in the morning and also twice in the afternoon. All posters were displayed during the whole conference in the Poster and Exhibition area (Atrium of the Faculty building). In this way, two poster sessions during and after lunch time gave enough time for discussion. Topics of parallel microsymposia were the following: structure solution from powder diffraction methods and application, stress, strain and texture analysis, neutron diffraction - instruments and applications, phase transitions, non-ambient conditions, phase analysis, structure and properties of bio-materials, nanocrystalline materials, metals and alloys, minerals, thin films, techniques and instruments, indexing powder patterns and software. Topics of posters were similar.



Jordi Rius - a new chairman of the EPDIC committee

Participation of companies was very helpful for organization of the conference. Commercial exhibition was opened most of the conference time right in the conference center together with posters. Most of sponsors had their booths there. Two general sponsors - Panalytical and Bruker supported the conference so that organizers could assist participation of quite many scientists. Participation of especially young scientists was supported by the IUCr fund. Strong support was also given by the ICDD and Unisantis. However, organizers would like to thank to all of the sponsors - Huber, GBC, Stoe, XOS, GE Inspection Technologies, Inel, Osmic, Zentiva, Anton Paar, Oxford Cryosystems and Roentgenlabor Dr. Martin Ermrich.

Two meetings were held during the conference: CPD (Commission for Powder Diffraction of the IUCr), EPDIC committee (identical with a SIG8 - of the ECA). In the latter meeting a new chairman of the committee was elected - Jordi Rius from Barcelona, Spain as well as two vice-chairs - Paolo Scardi from Trento, Italy and Robert Cernik (Manchester, UK). Paolo Scardi is also the secretary of the committee.



Poster and Exhibition Area



Refreshment





Poster and Exhibition Area



H. Fuess - the ECA president and S. Cherepanova



R. Dinnebier - CPD (IUCr Commission for Powder Diffraction) chairman



P. Scardi - EPDIC committee vice chairman, M. Leoni



Pilsen brewery



Volunteers



Organizers

The scientific programme was accompanied with social programme. The conference was opened with a welcome evening in the Prague Congress Center by the traditional EPDIC award lecture. The award was given by Panalytical and this year the winner was Vincent Favre-Nicolin who is well-known author of FOX programme and Crystal Object system. The EPDIC award selection was done by the whole programme committee that evaluated all materials



R. Černý - chairman of next EPDIC X

submitted by five candidates - their nomination letters, curriculum vitae, list of publications, other supporting material and also supporting letters of other scientists. The lecture was followed by music performance of the Z-band mixed voice Prague children choir.

On the last day of the conference, Sunday, September 5, a special train trip to Pilsen was organized. Participants had a dinner directly in the famous Pilsen brewery and took part at the excursion in the brewery. The train returned to Prague right in the midnight and we hope that most of participants enjoyed the evening.

Participation at the conference was comparable with last EPDIC in Uppsala, even though we expected a little more. However, there is a permanent difficulty with the selection of the conference time with respect to the IUCr and ECA meetings. In this case, it has been decided to attach it to Budapest ECA meeting, since both locations are quite close. It was convenient for some participants and companies and inconvenient for others. There is no ideal solution, if both meetings are organized in one year. According to the opinion of the EPDIC IX organizers it would be very reasonable, if between the IUCr congresses one year only the ECA meeting - ECM while in next year EPDIC and other specialized conferences and meetings are organized. It is also a task for future EPDIC organizers to attract more people from industry because this was the original idea of EPDIC. Anyway, participation of more than 320 people from 36 countries of Europe, North and South America, Africa, Asia and Australia was quite good. In addition to 54 Czech participants, the highest number of participants



H. Goebel, T. Baumbach



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came from Germany (49), France (19), Sweden (18), UK (16), Hungary and Austria, the Netherlands (13), Italy and USA (12) and Poland (10).

All the information about the conference together with photos and a few video clips are available at the Web site http://www.xray.cz/epdic. All the conference abstracts in html format including search engine can be found there too. About hundred six-pages papers have been submitted for publication in the conference proceedings. They should appear within one year in a special issue of Zeitschrift für Kristallographie.

Next conference - EPDIC X will be held in September 2006 in Geneve, Switzerland. Information is available at the address of main organizer: Radovan Cerny, Laboratoire de Cristallographie, 24, quai Ernest-Ansermet, CH-1211 Geneva 4, Switzerland, Phone: [+[41] 22] 37 964 50, FAX: [+[41] 22] 37 961 08, E-mail: Radovan.Cerny@cryst.unige.ch





## **Credits:**

I would like to acknowledged excellent work of the whole organizing committee. Namely, secretaries Pavlína Řezáčová and Ivana Kutá Smatanová, treasurer: Jindřich Hašek, secretary for commercial presentations: Zbyněk Šourek, to members of the committee responsible for other things: accommodation - Ivana Císařová, refreshments: Rudolfa Králová, Anita Župčanová, trips: David Havlíček, poster session: Nikolaj Ganev, also to Stanislav Daniš, Robert Gyepes, Rudolf Novák, Lubomír Kopecký. Lot of work was done by the team of volunteers which created also a nice atmosphere for participants.

> R. Kuzel Chairman of the EPDIC IX conference

