



Session IV, Wednesday, June 24

L12

CRYSTAL X-RAY OPTICS FOR METROLOGY AND IMAGING

M. Jergel, K. Végso, P. Šiffalovič, Y. Halahovets, D. Korytár, Z. Zápražný, P. Vagovič

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L13

INTEGRATION OF 2D DETECTOR DATA IN SCANNING POWDER DIFFRACTION EXPERIMENT

Z. Matěj, F. J. Martínez-Casado, D. Haase, O. Balmes

MAX IV Laboratory, Lund University, Ole Römers väg 1, 223 63, Lund, Sweden
zdenek.matej@maxlab.lu.se

Powder X-ray diffraction (PXRD) patterns can be collected in few minutes with common laboratory diffractometers using position sensitive detectors (PSDs) and even within few milliseconds at synchrotron instruments with large PSDs banks [1]. In another standard experimental setup diffraction images of whole diffraction rings (Fig. 1) can be taken with *area (2D) detectors* and by azimuthal *integration* using available software (e.g. Fit2D [2], PyFAI [3]) the images are reduced into 1D diffraction patterns. Whereas the finite length of PSD strips implies asymmetry of diffraction lines due to an axial divergence of the X-ray beam accepted by the detector [4, 5], integrated patterns from 2D detectors principally do not suffer from this effect. Good quality data at very low diffraction angles are important for (organic) structures with very large unit cells or if high energy X-rays are used. Recording large azimuthal fraction of diffraction rings is advantageous for intensity and grains statistics too. Disadvantages of static area detectors are limited angular range ($2\theta_{\max}$) and resolution ($\Delta 2\theta$). This can be bypassed by continuously scanning 2θ range with the detector, as e.g. in the powder diffraction beamline 11-BM at APS [6]. We have implemented a similar solution using hybrid pixel detector Pilatus100K in the powder diffraction beamline I711 at MAX-II ring that allows to collect moderate resolution PXRD data of high quality.

The basis of the underlying powder diffraction data reduction procedure is rebinning of intensities in pixels of thousands (~10k) of diffraction images taken with high frequency (~50 Hz) during continuous scanning of the detector axis (Fig. 2). Our solution provides powder diffraction data in a *real time* as one is used from laboratory measurements with PSD. We discuss necessary instrumental corrections and calibration procedures which should be included as e.g. in *xrayutilities* [7].

Setup in I711 gives PXRD patterns with moderate resolution (Fig. 3) in both transmission mode with capillaries and reflection mode with solid samples. It is well suitable for microstructure analysis as well as structure solution (Fig. 4).

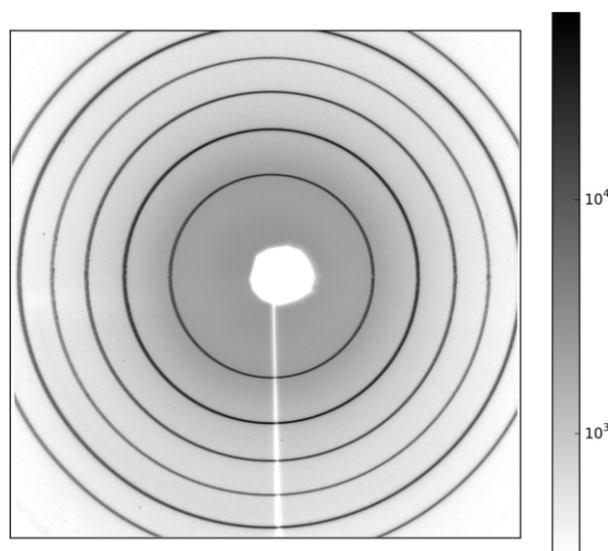


Figure 1. Diffraction image from LaB_6 taken with a large CCD.

1. A. Bergamaschi, A. Cervellino, R. Dinapoli, F. Gozzo, B. Henrich, I. Johnson, P. Kraft, A. Mozzanica, B. Schmitt, X. Shi, *J. Synchrotron Rad.*, **17**, (2010), 653. doi:10.1107/S0909049510026051.
2. A. P. Hammersley, S. O. Svensson, A. Thompson, *Nucl. Instr. Meth.*, **A346**, (1994), 312. doi:10.1016/0168-9002(94)90720-X.
3. G. Ashiotis, A. Deschildre, Z. Nawaz, J. P. Wright, D. Karkoulis, F. E. Picca, J. Kieffer, *J. Appl. Cryst.*, **48**, (2015), 510. doi:10.1107/S1600576715004306.
4. R. W. Cheary, A. A. Coelho, *J. Appl. Cryst.*, **31**, (1998), 851. doi:10.1107/S0021889898006876.
5. *Axial Divergence in Powder Diffraction at APS Beamline 11-BM*, <https://youtu.be/Slz6Ng6UzAw> (June 1, 2015).
6. B. H. Toby, T. J. Madden, M. R. Suchomel, J. D. Baldwin, R. B. Von Dreele, *J. Appl. Cryst.*, **46**, (2013), 1058. doi:10.1107/S0021889813013824.
7. D. Kriegner, E. Wintersberger, J. Stangl, *J. Appl. Cryst.*, **46**, (2013), 1162. doi:10.1107/S0021889813017214.

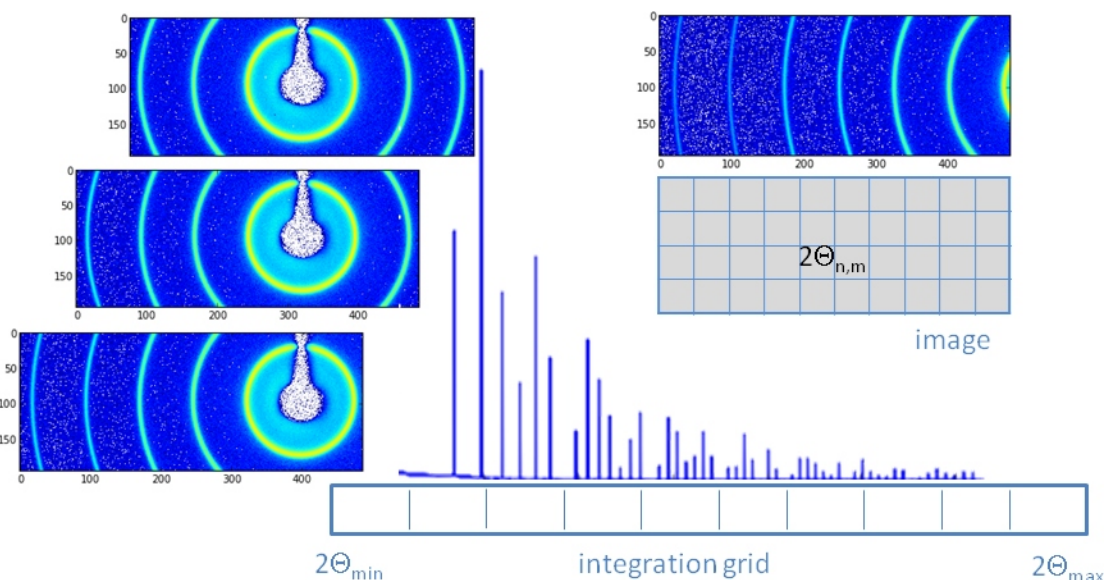


Figure 2. Schematic integration of a series of PXRD images (on the left): intensities from all pixels of each image are moved (rebinned) to appropriate integration bins of the final 1D powder diffraction pattern.

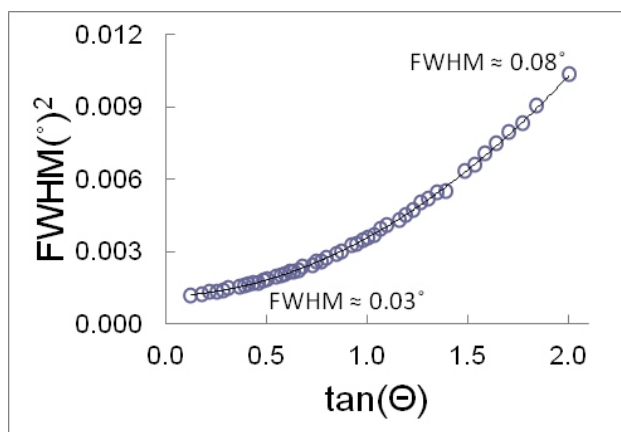


Figure 3. Caglioti plot of the resolution function for the Pilatus100K setup in I711.

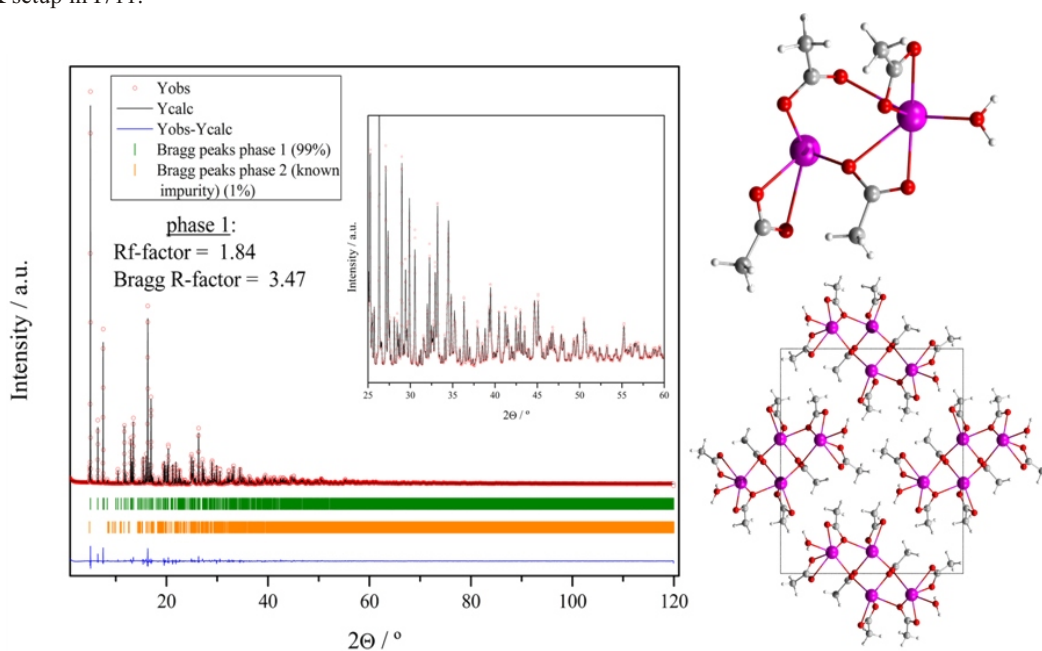


Figure 4. Lead acetate hemihydrate ($\text{Pb}_2\text{C}_8\text{O}_9\text{H}_{16}$) structure solved from PXRD data from I711.



L14

THE EFFECT OF SOME PHYSICAL FACTORS ON THE PHASE STRUCTURE OF ISOTACTIC POLYBUTENE -1

M. Hřibová, F. Rybníkář, J. Jakubiček

Department of production engineering, Tomas Bata University in Zlin

Full paper on p. 133.

L15B

INTERNATIONAL YEAR OF CRYSTALLOGRAPHY – IYCr INTERNATIONAL UNION OF CRYSTALLOGRAPHY – IUCr

R. Kužel

Charles University in Prague, Faculty of Mathematics and Physics, Ke Karlovu 5, 121 16 Praha 2

International Union of Crystallography organized many activities for the International Year of Crystallography - IYCr. They were summarized and discussed during the meeting *Crystallography for the next generation: the legacy of IYCr*, that was held in Rabat, April 22-24, 2015 <http://www.iycr2014.org/legacy/conference>. Many discussions were focussed more to the future.

The official objectives of the IYCr were:

- to **increase public awareness** of the science of crystallography and how it underpins most technological developments in our modern society
- to **inspire young people** through public exhibitions, conferences and hands-on demonstrations in schools
- to illustrate the **universality of science**
- to intensify the programme **Crystallography in Africa** and create similar programmes in **Asia and Latin America**
- to foster **international collaboration** between scientists worldwide, especially North–South contributions
- to **promote education** and research in crystallography and its links to other sciences

- to involve the large **synchrotron and neutron radiation facilities** worldwide in the celebrations of IYCr2014, including the SESAME project set up under UNESCO auspices.

One of the main activities were the so-called **OpenLabs**, which should continue also in future. The IUCr-UNESCO OpenLabs is a network of operational crystallographic laboratories based in different countries worldwide, many in less endowed regions of Africa, South and Central America and South Asia.

The purpose of the OpenLab project is

- to encourage the birth of new research centres or the start of research projects in crystallography in already established research centres;
- to increase the technological base and spark interest in youngsters;
- to favour international cooperation by transferring the expertise and knowledge from countries with a strong tradition in the field to those where crystallography must still be developed.

Summary with links can be found at

<http://www.iycr2014.org/openlabs>. These were mainly courses on powder or single crystal diffraction and each OpenLab was sponsored by one company.



Figure 1. From the Rabat IYCr Legacy meeting, the hall (left), Gilberto Artioli and Michele Zema, the IYCr manager (right).

The IUCr-UNESCO summit meetings were intended to bring together scientists from countries in three widely separated parts of the world, using a common crystallographic theme. <http://www.iycr2014.org/summits>. They were organized in Karachi (Pakistan), Campinas (Brazil) and Bloemfontein (South Africa).

A photo competition <http://www.iycr2014.org/participate/photo-competition> was organized in collaboration with Agilent. Amateur and professional photographers were invited to submit stunning images that capture the spirit of crystallography in the places, objects and experiences of everyday life. 254 entries were submitted to the competition. Two winners received a USD 1000 bursary, sponsored by Agilent Technologies, to attend the IUCr Congress in Montreal in August 2014. A third prize winner was selected as the “Crystallographers’ Choice” of the 29th Biennial Conference of the Society of Crystallographers in Australia and New Zealand in April 2014. The 3 winning and 13 most highly commended entries were used in a celebratory Agilent/IYCr2014 Academic Calendar for 2014/2015. The winning and other noteworthy entries were exhibited during the Montreal Congress.

Very successful appeared to be the Crystal Growth Competition <http://www.iycr2014.org/participate/crystal-growing-competition> for school children. Finally, it was decided that each participant would have to either send a video or essay. The winners were announced during the Rabat meeting. The winning videos and essays can be found at <http://www.iycr2014.org/participate/crystal-growing-competition/winners>.

A new competition has been open for 2015 with a deadline on November 22. The aim of the competition is to grow participant’s own crystals (whether involved in a regional/national competition or not) and to convey her/his experience through a video. Each contribution should clearly show or mention the experimental work carried out by the participants during the growing of their single crystals (compounds and methods used are free of choice). Furthermore the contribution should reflect in a creative way on the experimental work and theoretical background and/or applications.

Commemorative postage stamps have been released in 17 countries http://www.iycr2014.org/events/postage_stamps including Slovakia.

The **Crystallography365** project sets out to blog a crystal structure every day <http://www.iycr2014.org/learn/crystallography365>

Voyage dans le cristal. A family of 36 panels in A0 format, highlighting the different aspects and applications of crystallography have been exhibited in several places. They are available for download in 13 languages, 12 of them also in Slovak. <http://www.iycr2014.org/resource-materials/voyage>. The main author and coordinator is Jean Louis Hodeau.

In connection with the IYCr, many other things have been developed. For example, thanks mainly to the current IUCr president, Marvin Hackert, the history of crystallography can be nicely viewed in Timelines of Crystallography <http://www.iycr2014.org/timeline> now.

A book *Little Dictionary of Crystallography* was written by André Authier and Gervais Chapuis. The online crystallographic dictionary can be found at http://reference.iucr.org/dictionary/Main_Page.

A section of news <http://www.iucr.org/news/whats-new> and calendar of events has been redesigned <http://www.iucr.org/calendar/calendar-of-events> and become much more useful.

World Directory of Crystallographers was initiated in 1957 and since then it has continued to grow and is now available online for all researchers associated with crystallography, the database currently has 20,000 entries.

To sign-up is free, and members of the directory have access to large network of scientists practising in similar and related fields of interest, trying together research topics, scientists and institutions in one easy to search database. There are plans to extend its use largely.

In the last year, already the ninth volume of International Tables for Crystallography was issued, volume H – Powder Diffraction as well as some promotional booklets and books for school teachers.

The IUCr publishes two journals that are fully open access, *i.e.* all articles are made available free of charge to the reader. An open-access fee is charged to authors of articles published in these journals to cover the costs of peer review, journal production, and online hosting and archiving. These journals are:

- *Acta Crystallographica Section E: Structure Reports Online*
- *IUCrJ*

Other journals are **hybrid open-access** journals. The authors can choose to make their article open access by paying an open-access fee. Funds generated from open-access payments are used to keep subscription costs as low as possible. The journals are also by far the main source of finances for the IUCr. In addition to the IUCrJ, these are: *Acta Crystallographica A-F*, *Journal of Applied Crystallography* and *Journal of Synchrotron Radiation*. Most of professional staff of the IUCr in Chester is working on the journals with their own editorial system. Since the last year, all the publications are only electronic except a few sample copies. There is also IUCr Newsletter. It is published 4 times per year, available online only subscribe by signing up to the World Directory of Crystallographers. It is circulated to over 200 different countries around the world. The newsletter contains many different article types, of interest to the diverse international scientific community involved in understanding the basic structure of matter.

The electronic form of journals allows to build-in some features of structural databases and online structure visualization. Supplementary materials to the papers are available free.

The IUCr currently sponsors scientific activities and meetings in a number of ways:

- Bursary scheme for meetings of Regional Associates
- Visiting Professorships. The IUCr Visiting Professorship scheme aims to support some of the costs of having internationally recognized scientists as lecturers for short courses at workshops or schools organized in developing countries.



Figure 2. Building of the IUCr office in Chester, UK.

- Scientific conferences and workshops
- Journal subscriptions
- Crystallography in Africa
- The IUCr is on facebook now as well - [facebook.com/iycr2014.org](https://www.facebook.com/iycr2014.org).

International Union of Crystallography has currently 50 adhering bodies including 4 regional associates: ACA – American Crystallographic Association, AsCA - Asian Crystallographic Association, ECA - European Crystallographic Association and a new LACA – Latin American Crystallographic Association

<http://www.iucr.org/iucr/ab.html/adhering-bodies>,

and 24 commissions

<http://www.iucr.org/iucr/commissions>.

The IUCr main aims are –

- to promote international publication of crystallographic research
- to promote international cooperation in crystallography
- to form a focus for the relations of crystallography to other sciences
- to facilitate standardization of methods, units, nomenclatures and symbols
- to contribute to the advancement of crystallography in all its aspects including related topics concerning the non-crystalline state.

The main IUCr event is the Congress and General Assembly, with usual participation of 2000-3000 people. The 24th congress will take place in Hyderabad, India in 2017



Figure 3. Current IUCr president Marvin Hackert (USA) in Rabat.

and we can be proud that the anniversary 25th congress should be hold in Prague in 2020.