

Lectures - Tuesday morning, June 10

L2

ADVANCES OF PROTEIN CRYSTALLOGRAPHY

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The General Assembly of the United Nations (UN), on its 121st plenary meeting decided to proclaim 2014 as the International Year of Crystallography. The following text contains several quotes and sentences reproduced from the 66/284 General Assembly declaration:

Recognizing the leading role of the International Union of Crystallography (IUCr), an adhering body of the International Council for Science (ICSU), in coordinating and promoting crystallographic activities at the international, regional and national levels around the world,

The humankind's understanding of the material nature of our world is grounded, in particular, in our knowledge of crystallography. The impact of crystallography is present everywhere in our daily lives, in modern drug development, nanotechnology and biotechnology, and underpins the development of all new materials, from toothpaste to airplane components. Applications of crystallography are critical in addressing challenges such as diseases and environmental problems, by providing protein and small molecule structures suited for drug design essential for medicine and public health, as well as solutions for plant and soil contamination.

Persistent flow of Nobel prizes shows that the crystallography is still fertile ground for new and promising fundamental research.

Therefore, it encourages all Member States, the United Nations system and all other actors to take advantage of the International Year of Crystallography to promote actions at all levels aimed at increasing awareness among the

public of the importance of crystallography and promoting widespread access to new knowledge and to crystallography activities.

It is also worth to commemorate the sixty-fifth anniversary of the founding of the International Union of Crystallography and the foundation of the journal Acta Crystallographica involving presently six volumes A, B, C, D, E, F devoted to specialized aspects of scientific research."

Nobel prizes awarded for crystallography or in close connection to crystallography were already listed in a short review [1]. In this paper, we concentrate especially on the last development of the protein crystallography, i.e. structure determination of large biomolecular complexes in atomic resolution where the international appreciation seems to be the highest.

Figure 1 summarizes the counts of Nobel prizes by each ten year since 1901 (the year when the first Nobel prize was awarded). In comparison with the chart published in [1], one can see here marks of oversampling. Splitting the intervals to halves makes the profiles more humped but because we know the background of each event we can follow the causes of these humps in history.

The tremendous research on development physical methods of crystallography lasting more than 40 years in the period **1895-1940 was appreciated by seven Nobel prizes.**

The high potential of X-ray crystallography for many important activities of mankind was fully recognized in the **period 1960-1980** when a completely new and economically promising insight into the micro-world of molecules and molecular machines discovered completely new view on modern technologies. New discoveries opened completely new approach to molecular biology, revealed how molecular machines work and showed basic principles behind function of living organisms. These discoveries were **rewarded with five Nobel prizes.**

Recognition of high importance of crystallography induced large investments in the field, namely in **development of technologies and crystallography methods.** Thus, we can see **four Nobel prizes in 1980-2000 for development of techniques** and also **four Nobel prizes for applications in chemistry and molecular biology** mostly due to the dissemination of new methodologies and their accessibility over the whole world.

Finally, the recent development (13 years of this century) shows that X-ray crystallography still has a

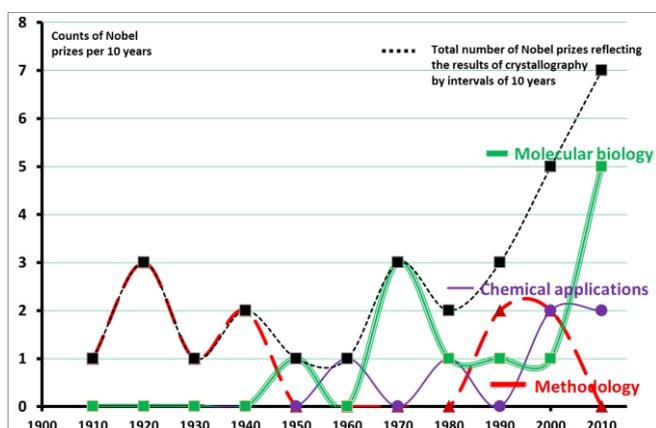


Figure 1. Numbers of Nobel prizes closely related to applications of crystallography methods in chemistry and biology in ten years intervals from 1900-1910 until now. The last points count the Nobel prizes per the period 2001-2013.

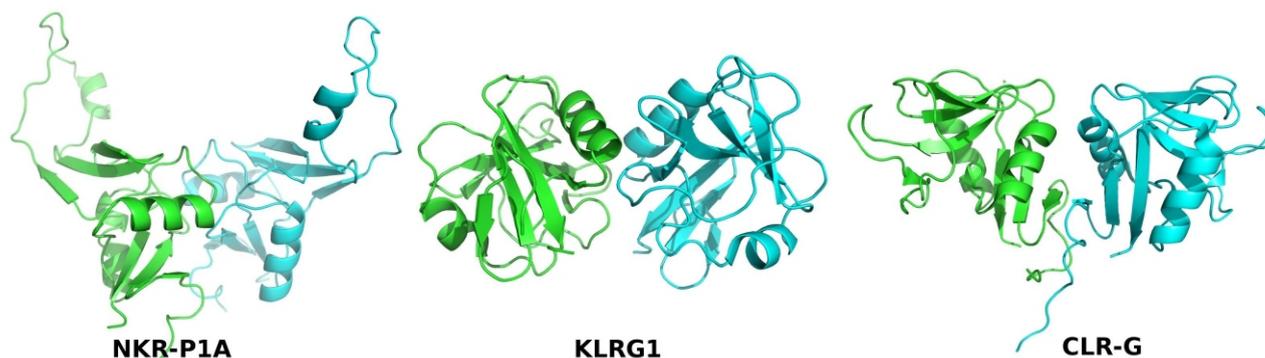


Figure 2. Comparison of dimerization modes of three mouse CTL proteins: NK receptor NKR-P1A (PDB code 3M9Z), NK receptor KlrG1(3FF9), and a ligand for NK receptor NKR-PIF: Clr-g (3RS1). Reproduced from [2].

high potential for the future of mankind. **Seven Nobel prizes awarded in the period 2003-2013** uniquely show high importance of the achievements. Particularly promising seems to be the statistics in the field of protein crystallography, where one can be fascinated by a **new Nobel prize every second year**.

Why is protein crystallography regarded so important?

Protein crystallography showed us the world of living organisms at atomic resolution for the first time. This was necessary to understand and rationally regulate the processes important for life. It allowed formation of completely new fields of research and opened our eyes to understand a huge complexity of processes in living organisms. The illustrations in the appendix show some examples answering the questions concerning:

- **exact conformation and the conformational changes of the largest known molecular complexes** as e.g. ribosomes,
- determination of **intermediate states necessary for understanding the biochemical reactions**,
- **design of completely new biomolecules** showing far better performance than their counterparts present in nature,
- **detailed elucidation of enzymatic function and design of new catalytic centers providing** biochemical reactions allowing easy production of rare or beforehand unavailable chemical products,
- **time resolved analysis of bio-chemical reactions**, even if it is presently restricted mostly to processes that can be initiated or modulated by a pulse of electromagnetic radiation,
- **analysis of intermolecular contacts, forming a base for intercellular communication and signaling** between cells in the body. The following figure showing the supposed dimerization of receptors at the surface of natural-killer cells to accept the information whether to start or suppress the attacks against other cells in its neighborhood can serve as an example.

Future applications of X-rays in structural biology?

The question about future applications of X-rays in structural biology can hardly be answered well. It seems that, after the huge progress due to better technologies (computers, advanced detectors, synchrotron sources of radiation) in the last twenty years, we need now to develop more sophisticated methods for sample preparation. Here are many points, which seem to be bottlenecks of the present research.

1. Exact structure determination of bio-macromolecular complexes in their native state. As a rule, the living entities form a special state of matter. The natural environment in living organisms where the most interesting biochemical reactions appear is not liquid, neither solid. It is molecularly overcrowded state of matter often with thixotropic properties, diffusion of molecules is overwhelmed by other transport mechanisms, intermolecular interactions do not correspond to what we can see in solutions, etc. Here, one can see a large space for new sophisticated procedures to prepare samples that could be inspected by X-ray crystallography. For example new methodic for controlled preparation of realistic multi-protein crystalline states allowing a systematic study of intermolecular contacts responsible namely for communication between cells, for immune response, for allergy, and for starting or modulation of processes in living organisms.

2. Inspection of detailed differences between similar supra-molecular complexes and their intermediate states important for life of different organisms. The final aim is for example to stop some process in harmful bacteria without influencing the human proteins or proteins in cohabiting microorganisms.

3. Time resolved studies. They are still in their beginnings. The problems here are not in the diffraction technique. Standard synchrotrons allow already much better time-resolution (~10 ns) then it is needed for biochemical reactions (μ s-ms). Shortening of the radiation pulls to femtoseconds offered by X-FEL and some new laser facilities is harmful in this sense, because each pull destroys the sample. The future problem is in **finding tools for immediate starting the reactions in the whole volume of our sample and in dealing with the multiconformational states** regularly observed in the individual time sections.

The impact of the future research is expected in many areas of human life via molecular biology, biochemistry, chemistry, health care, drug design, agriculture, food industry, chemical industry, etc.

1. J. Hašek, International Appreciation of X-ray Crystallography. *Materials Structure*, 2014, 21, 4-6.

2. T. Skálová *et al.*, Mouse Clr-g, a Ligand for NK Cell Activation Receptor NKR-P1F. Crystal Structure and Biophysical Properties, *J. of Immunology*, 2012, 189, 4881-4889.

This work was supported by the project P302/11/0855 of the Czech Science Foundation, BIOCEV CZ.1.05/1.1.00/02.0109 from the ERDF, LG14009, and MSM EE-2.3.00/30.0029BIOPOL.

L3

STRUCTURE REFINEMENT FROM DATA ACQUIRED BY ELECTRON DIFFRACTION TOMOGRAPHY

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Introduction

Structure refinement from X-ray diffraction data is a well-established method used routinely in many laboratories around the world. In contrary, structure refinement from electron diffraction data is generally considered difficult, cumbersome and restricted only to special cases. Last decade of development in the field of electron crystallography has shown, however that it is possible to solve and refine crystal structures from electron diffraction data in a way analogical to the procedures used in X-ray crystallography. Very recent progress in combining structure refinement with calculations using dynamical diffraction theory shows that such refinements have the potential to approach – although probably not yet reach – the accuracy and reliability of X-ray structure refinement. The important advantage is that the data collection can be performed on nanocrystals only a few tens of nanometers in size. This article describes the procedure from the data collection through data processing to the structure solution and refinement, pointing out the similarities and differences to the process of structure determination from X-ray diffraction data that is familiar to most practicing crystallographers.

Experiment

Electron diffraction experiments on micro- and nanocrystals are performed in a transmission electron microscope. Traditionally, electron diffraction patterns were collected from oriented crystals. However, this technique is time consuming and it is difficult to collect sufficiently complete data using only oriented patterns. An alternative is to use the method of rotating crystal that is customary in X-ray diffraction experiments. In the field of electron crystallography this method is called *electron diffraction tomography* (EDT [1,2]). A (non-oriented) crystal is tilted around the goniometer axis in small steps (typically 0.5 or 1°, but sometimes much smaller), and a diffraction pattern is recorded after every step on an area detector, typically a CCD camera. The electron microscope thus acts as a single-circle diffractometer with area detector.

The intensity of reflections is critically dependent on the exact orientation of the crystal. This makes the interpretation of the intensities difficult. A technique called *precession electron diffraction* (PED, [3]) partly removes this effect. The principle of the method is illustrated in Fig. 1. The incident electron beam is precessed around a cone with vertex on the sample and with the opening semiangle typically between 1° and 2°. The resulting diffraction pattern is then an integral over all directions of the incident beam along the cone. This technique greatly decreases the sensitivity of the diffracted intensities to the crystal orientation and on other nuisance parameters like crystal thickness and its variation. This makes the combination of PED with EDT a powerful method for crystallographic data collection.

The tilt range of the crystal in the microscope is limited by the construction of the microscope, and represents the most serious limitation of the technique. On some microscopes with some sample holders the tilt range is limited to only $\pm 20^\circ$ or even less. Such microscopes are unsuitable

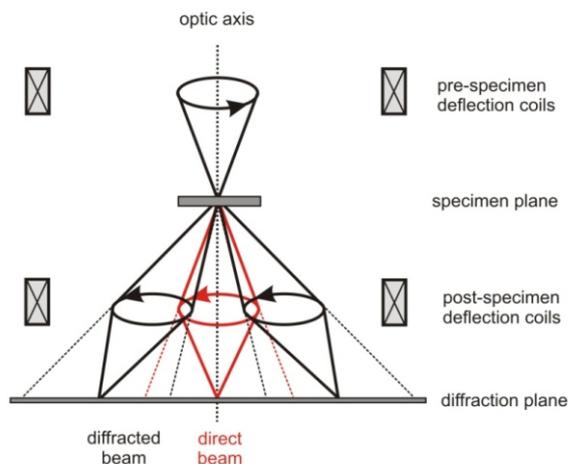


Figure 1. The principle of the precession electron diffraction technique. The incident beam is deflected by pre-specimen deflection coils to make a precessing motion (*scan*). The diffraction pattern is then focused back to the original position by post-specimen deflection coils (*descan*).

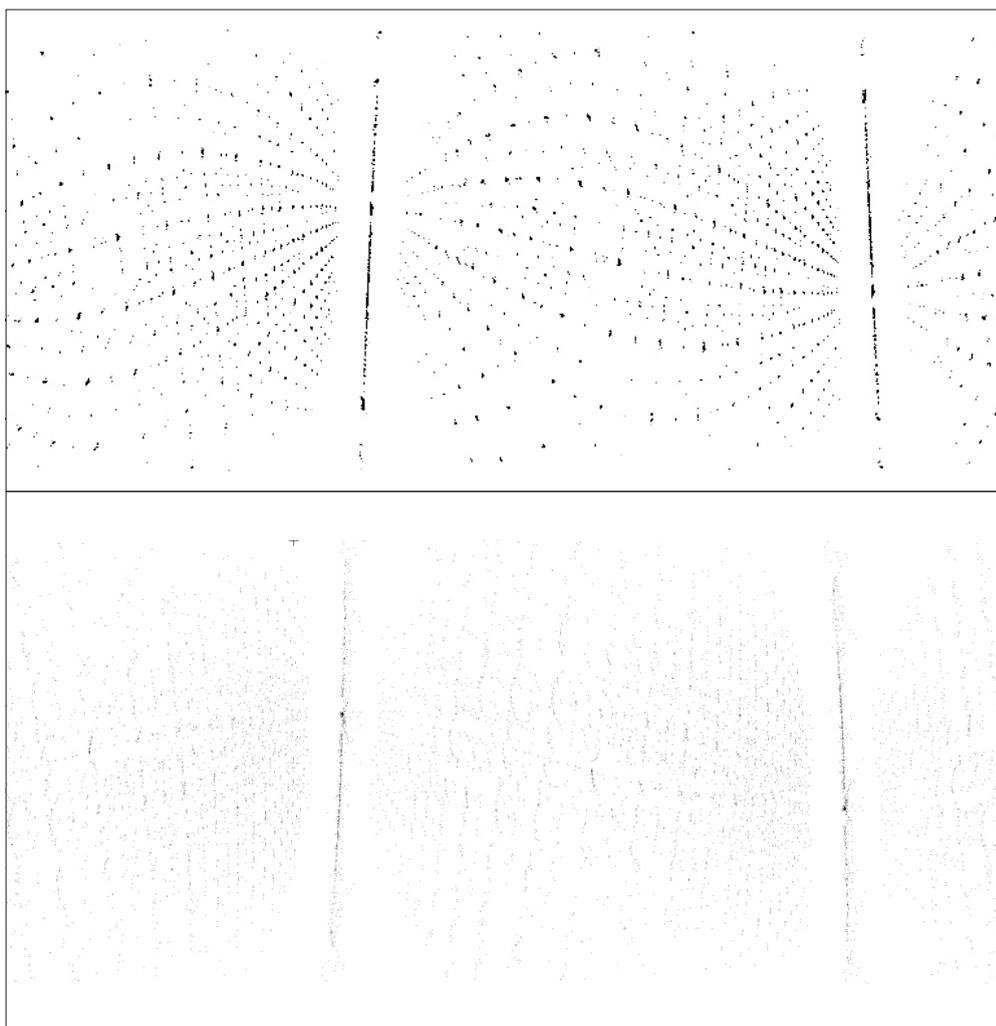


Figure 2. Cylindric projection of the distribution of points in the autoconvolution pattern using the correct (top) and 10° off-set (bottom) tilt axis position.

for collecting electron tomography data. On the other hand, some microscopes equipped with specialized tomographic sample holders allow for an almost complete $\pm 90^\circ$ tilt, and thus collection of almost a full sphere of data.

The goniometers are usually not sufficiently stable to hold the nanocrystals at a constant position during the whole data collection. Therefore it is necessary to either reposition the crystal during the experiment, or shift the beam to follow the movement of the crystal. This can be achieved manually or automatically using image analysis. The whole diffraction experiment takes usually between 15 and 60 minutes depending on the tilt range, exposure time and crystal tracking procedure.

Data processing

Once recorded, the data can be processed in a way very similar to the procedures used in X-ray diffractometer software, *i.e.* the frames are analyzed for maxima, which are stored in a “peak table” and subsequently used for finding the unit cell and orientation matrix. This matrix is then used to predict the position of all reflections on the diffraction patterns, and integrate their intensities.

Two issues require special attention. First, the electron optics is not perfectly stable, and therefore the position of

the center of the diffraction pattern may slightly change during the experiment. The data processing must therefore track the position of the primary beam. This may be non-trivial, because the primary beam is often covered by a beam stop to prevent damaging the detector by overexposure. The center can then be determined only from the positions of the Friedel pairs in the image, or by cross-correlation of subsequently recorded images.

The second issue is the position of the tilt axis. Again due to the variability in the electron optics, the projection of the tilt axis on the diffraction pattern need not be constant for every experiment. It is thus a variable that needs to be refined during data processing. The technique typically used for this purpose is the autoconvolution of the set of extracted peak positions recalculated to the 3D coordinates in reciprocal space. If the peak positions form a lattice, then their autoconvolution also forms a lattice. The peaks form an undistorted lattice only if the tilt axis is correctly determined, and this property can be used to refine the tilt axis. An example of an autoconvolution using correct and incorrect tilt-axis position is given in Fig. 2.

Table 1. Preliminary results from the refinement of the structure of orthopyroxene ($\text{Fe,Mg}_2\text{Si}_2\text{O}_6$) using kinematical and dynamical diffraction theory. Precession angle 2.0° . Data courtesy of Damien Jacob and Priscille Cuvillier, University of Lille.

	Kinematical refinement	Dynamical refinement
R1 [%]	24.4	9.3
Average atomic distance from reference structure [Å]	0.042	0.018
Maximum atomic distance from reference structure [Å]	0.070	0.035

Structure solution and kinematical refinement

As in previous sections, the basic principles of structure solution from electron diffraction data are the same as for X-ray diffraction data. The list of reflection indices with integrated intensities is submitted to a structure solution program that solves the phase problem by one of the established methods – direct methods, dual space methods or direct space methods. The difference is in the quality of the solution. While X-ray diffraction data often provide complete solutions that can be directly submitted to refinement process, electron diffraction data, being less complete and much noisier (in the sense “deviating from the expected proportionality between intensity and structure factor squared”) often result in partial solutions that require intervention of a crystallographer. However, most often the solutions are sufficiently good to allow finding the correct structure.

The structure refinement is the most problematic part of structure analysis from EDT data. The least-squares refinement can be performed against electron diffraction data using the kinematical approximation (*i.e.* using the assumption that the structure factor amplitude is proportional to the square root of the diffracted intensity). However, this approximation is very inaccurate due to the deviations from the kinematical diffraction theory caused by multiple scattering. As a result, the refined structures yield high R-values (R1 typically between 20 and 30%), inaccurate results (deviations from the correct atomic positions typically up to 0.2 \AA , but sometimes more), and non-reliable estimates of the uncertainties of the refined parameters. Despite of these problems, kinematical refinement is used with EDT data, because it is easily accessible in several refinement programs, and it provides a quick estimate of the correctness of the determined structure. For many applications, where it is the connectivity that is of in-

terest and not the accurate atomic positions, kinematical refinement provides sufficient information.

Dynamical structure refinement

An obvious remedy to the deficiencies of the kinematical refinement is to use the correct dynamical theory to calculate the expected diffracted intensities from a model structure. The underlying theory has been developed long time ago (see e.g. [4] for an overview), but the practical application was hampered by several technical problems. First of all, the dynamical diffraction theory is a many beam theory, and the intensity calculations require exponentiation of a large matrix, and are thus quite time consuming. A more serious problem is, however, that the calculated intensities are very sensitive to the crystal orientation and thickness. If the crystal is slightly mosaic, bent, or has irregular shape, the experimental intensities will strongly deviate from the theoretical calculation, which assumes a perfect crystal. A remedy to this problem is to use PED data. As already mentioned, such data are less sensitive to crystal imperfection, crystal orientation and details of the crystal shape. It is thus possible to calculate PED intensities to a better accuracy [5]. Table 1 shows a comparison of a structure refinement on pyroxene EDT data.

Conclusion

The progress in structure determination from electron diffraction data achieved over the last decade was enormous. A series of developments changed this approach from an exotic and specialized to commonly accepted and widely used. The methodological development is by no means finished, but it has reached such a state of maturity that structures can be solved from electron diffraction data by almost anybody with access to a suitable transmission electron microscope and with basic crystallographic education.

References

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Acknowledgements

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SL7

MgZn PRECIPITATES IN Mg MATRIX - ELECTRON DIFFRACTION TOMOGRAPHY STUDY

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Low density, high specific strength and the ease of recycling make magnesium and its alloys potentially good candidates for numerous structural applications [1]. One of the most common alloying elements in magnesium is Zn. Besides remarkable improvement of mechanical properties via solid solution and/or precipitation strengthening, Zn is together with Mg classified as a biocompatible element. Thus, Mg-Zn based systems can also be considered as an attractive material for implants.

Binary magnesium alloy with nominal composition Mg-12 wt.% Zn was prepared by die casting under Ar atmosphere and subsequently annealed at 320 °C for 20 hours followed by warm water quenching. The goal of this work is to describe the crystal structure of Zn based particles present in the binary magnesium alloy.

Samples were studied by transmission electron microscopy performed on a Philips CM 120 (LaB6, 120 kV) equipped with a NanoMEGAS precession unit DigiStar, an Olympus SIS CCD camera Veleta (2048x2048), and an EDAX windowless EDS detector Apollo XLTW. Precession-assisted electron diffraction tomography (EDT) in microdiffraction setup was used to acquire data for structure determination of MgZn precipitates and their orientation within the Mg matrix.

Precipitates of several micrometers in size (Fig. 1a) correspond to Mg₂₁Zn₂₅ phase with rhombohedral structure, space group R-3c, lattice parameters $a \sim 26 \text{ \AA}$, $c \sim 8.9 \text{ \AA}$ (Fig. 1b). The structure was determined from 1711 independent reflections (averaged from 13026 measured intensities, $R_{\text{int}} = 24.09$), and refined using kinematical approximation to R-value of 26.53 %. The structure model matches very well the previously reported structure of Mg₂₁Zn₂₅ [2]. The matrix is formed by hexagonal Mg, space group P63/mmc, lattice parameters $a = 3.2 \text{ \AA}$, $c = 5.2 \text{ \AA}$. Orientation relationship of MgZn precipitates in Mg matrix was observed as $(10\bar{1})\text{Mg} \parallel (010)\text{MgZn}$ and $[101]\text{Mg}$ close to $[201]\text{MgZn}$ (Fig. 1c). However, this relationship might vary significantly as the precipitates are quite coarse and therefore loss of coherency is expected.

1. T.M. Pollock, *Science*, **328**, (2010), 986-987.
2. R. Černý & G. Renaudin, *Acta Cryst.*, **C58**, (2002), 154-155.

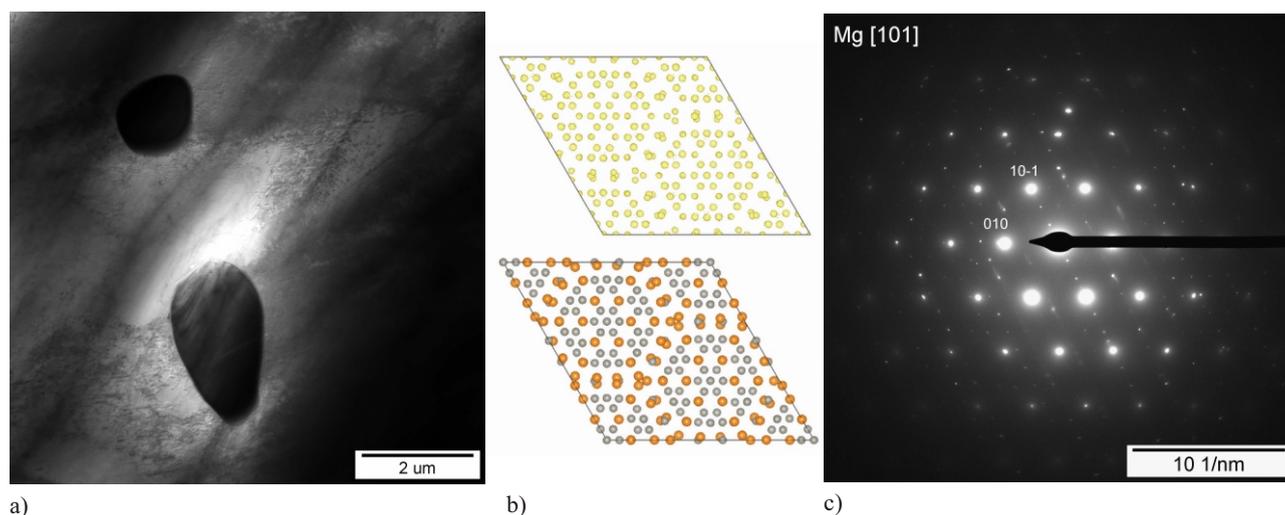


Figure 1: (a) Bright-field TEM image of MgZn precipitates in Mg matrix, (b) results of structure solution from EDT data of a MgZn precipitate viewed down $[001]$ (top - map of electrostatic potential, bottom - structural model), (c) oriented SAED pattern of a MgZn precipitate in Mg matrix viewed down Mg $[101]$.

Application of Fourier analysis for image analysis of photographs VYUŽITÍ FOURIEROVY TRANSFORMACE PŘI OBRAZOVÉ ANALÝZE MIKROFOTOGRAFIÍ

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Fourierova transformace (FT) je jedním z pokročilých nástrojů, které lze využít při obrazové analýze mikrofotografií, neboli při „převodu obrázků na čísla“. V tomto příspěvku velmi stručně shrneme teorii FT, která souvisí se zpracováním mikrofotografií. Přitom se soustředíme na metody výpočtu a interpretace FT pro tři nejčastější případy v obrazové analýze: (i) jednorozměrnou diskretní rychlou FT (1D-DFFT) čárových profilů intenzit, (ii) dvourozměrnou diskretní rychlou FT (2D-DFFT) vybraných ploch a (iii) převod vypočtených 2D-DFFT na 1D radiální profily.

Pomocí FT můžeme z LM, SEM, TEM získat informace o periodických vzdálenostech a symetrii struktury v mikroskopické škále (stovky mikrometrů – jednotky nanometrů). Pro výpočty potřebujeme dostatečně flexibilní programy, které umožní obrázky upravovat, vybírat z nich čárové profily a/nebo oblasti a následně počítat různé typy FT. V této práci využíváme dvou volně šiřitelných programů: ImageJ [1] na manipulaci s obrázky a programovací jazyk Python [2] s příslušnými moduly [3, 4] na výpočty FT.

2D-DFFT potvrdila šesterečnou symetrii a periodicitu ve vzorku blokového kopolymeru P(MMA-co-GMA)-b-PMAPOSS [5]. Ze vzorku byl připraven ultratenký řez, který byl po kontrastování v parách RuO₄ zobrazen v TEM. Nízkoúhlový rozptyl paprsků X (SAXS) naznačoval, že by polymer měl vykazovat hexagonální strukturu.

V některých oblastech TEM mikrofotografií byla hexagonální struktura zčásti patrná (obr. 1a), ale kontrast byl

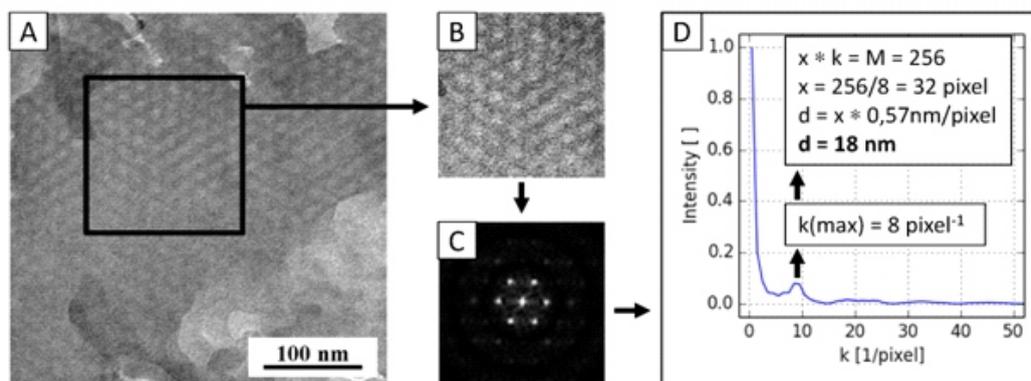
velice malý a ani úpravy v programu ImageJ příliš nepomohly (obr. 1b). Proto byl vybraný obrázek v ImageJ binarizován, v programu Python vypočtena 2D-DFFT (obr. 1c) a následně i 1D radiální distribuce (obr. 1d). Symetrie 2D-DFFT obrazu jasně potvrdila hexagonální symetrii, zatímco z 1D radiální distribuce bylo možno vypočítat průměrnou vzdálenost mezi hexagonálně uspořádanými sloupci ($d = 18$ nm), která byla ve shodě s výsledky SAXS ($d = 20$ nm).

V přednášce ukážeme ještě řadu dalších případů z praxe, včetně (překvapivě jednoduchých a krátkých) zdrojových kódů v jazyce Python pro uživatelsky definované výpočty FT z mikrofotografií.

1. Domovská stránka programu ImageJ: <http://imagej.nih.gov/ij/>
2. Hlavní stránka programovacího jazyka Python: <https://www.python.org/>
3. Distribuce WinPython, obsahující moduly pro čtení/zápis obrázků a výpočty FT: <http://winpython.sourceforge.net/>
4. Modul radial_data.py: <http://www.astrobetter.com/fourier-transforms-of-images-in-python/>
5. L. Matějka, M. Janata, J. Pleštil, A. Zhigunov, M. Šlouf, *Polymer* **55**, (2014), 126.

TAČR TE01020118, GAČR P108/14-17921S.

Rozšířený text bude publikován v dalším čísle.



Obrázek 1. Potvrzení hexagonální struktury v P(MMA-co-GMA)-b-PMAPOSS: (a) TEM mikrofotografie, (b) vybraná oblast (c) 2D-DFFT z vybrané oblasti, 4x zvětšeno a (d) 1D radiální profil s výpočtem vzdálenosti d mezi sloupci.



L4

ELI - UNIQUE LASER CENTRE IN CZECH REPUBLIC¹

Bedřich Rus

Fyzikální ústav AV ČR, Praha

The project Extreme Light Infrastructure (ELI) is part of a European plan to build a new generation of large research facilities selected by the European Strategy Forum for Research Infrastructures (ESFRI).

The main goal of ELI is to create the latest laser equipment in the world. There will be accomplished and implemented research projects covering the interaction of light with matter at intensity being 10 times higher than currently achievable values. ELI will provide ultra-short laser pulses of a few femtoseconds (10^{-15} fs) duration and give performance up to 10 PW.

ELI will bring new techniques for medical image-display and diagnostics, radiotherapy, tools for new materials developing and testing, latest in X-ray optics, etc.

ELI will also be an attractive platform for educating a new generation of PhD. students, scientists and engineers. The Czech Republic will become the host country for the top international research, which may attract further investment in advanced technologies with high added value.

ELI equals three laser centers combined under one heading.

The first facility (ELI Beamlines) will be located in the Czech Republic and will create a new generation of secondary sources for interdisciplinary applications in physics, medicine, biology and material sciences.

The second center (ELI Attosecond) is being arranged in Hungary and is to be focused on physics of ultrashort optical pulses in attosecond order.

And finally, the third center (ELI Nuclear Physics) aimed at photonuclear physics should be located in Romania.

The location of another infrastructure is currently being discussed.

ELI will be operated according to a new model designed for a consortium of European research infrastructures (ERIC). Members of the ELI-ERIC will become the Czech Republic, Hungary and Romania (founding members) as well as the major partners of the project preparatory phase (ELI-PP): Germany, Great Britain, France and other countries.

Implementation of ELI in the Czech Republic is in charge of Institute of Physics, Academy of Sciences of the Czech Republic. It coordinates a national consortium ELI-CZ comprising 14 Czech universities and research in-

stitutes. Key support is provided by the Ministry of Education, Youth and Sport and the Central Bohemia region.

ELI-CZ consortium groups together all of the Czech universities and scientific institutions interested in the ELI Project. Founded in January 2009, the Consortium stands as an evidence of a strong partnership between the academic and research institutions, and clearly demonstrates the common goal: building and operating the ELI international laser facility in the Czech Republic. Introducing new educational programmes (undergraduate, graduate, and PhD) that will be closely tied to the ELI scientific parameters, as well as raising awareness of the ELI Project and the laser sciences in general throughout the national academic community is the main mission of the Consortium ELI-CZ members.

Location

Dolní Břežany municipality in Central Bohemia region was selected as the most convenient location for the most intense laser in the world.

ELI International Beamlines will become an international infrastructure employing approx. 300 homeland and foreign member staff. In addition, it will be targeted by hundreds users and partners from all over Europe. Reasonable distance from the Prague airport and main highways were considered to be essential criteria whereas domestic scientific and industrial base is concentrated in the capital.



Design of the center by <http://www.boglearchitects.com/>.

¹ The above text can be found on the Web page of ELI - www.eli-beams.eu.

L5

USE OF DIFFRACTION ON PERFECT CRYSTALS FOR SHORTENING OF FEL PULSES AND MEASUREMENT OF THEIR LENGTH

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Since the first lasing of the hard X-ray FEL facility LCLS in 2009 engineers and physicists were looking for new optical devices and set-ups with the simple goal of preserving the unique properties of the next generation synchrotron sources. It is extremely important to preserve the unique time structure of the hard X-ray FEL pulse or even to have the possibility to change the parameters of the pulse. If we speak of changing the pulse parameters we are speaking of pulse compression. Currently, mostly grating schemes are used for pulse compression and correlation and auto-correlation schemes incorporated in delay lines are used for pulse length measurements. Crystal optics was not so much used in the application of hard X-ray FEL sources because of their narrow acceptance range. With the introduction of seeded FEL sources the FWHM of single pulses is now equal or smaller than the acceptance of commercially used crystal optics (Si, Ge, ...). Using dislocation free silicon crystals we have introduced two new methods for pulse compression. One is based on the use of an asymmetrically cut crystal and the second on the use of inclined crystals. Both methods are based on the fact that finite wavelength range of the impinging radiation diffracts under different angles depending on the wavelength, even if the impinging beam is parallel. Using a properly chirped pulse, the inclined cut crystal generates a path length difference, which leads to pulse compression, fig.1.

We have also introduced two new methods enabling the measurement of pulse lengths. One is based on the use of multi-beam diffraction and the other on the novel design of a pure BBBB interferometer.

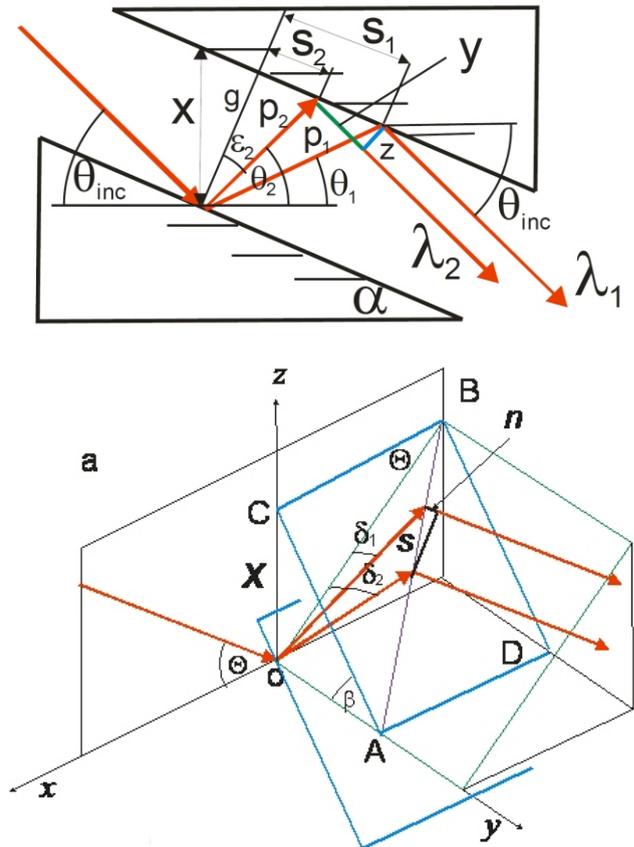


Figure 1. To generate a path difference with the goal of pulse compression we have explored a symmetrical cut crystal (top) and an inclined geometry crystal (bottom).