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Original article text and available illustrations

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LETTER FROM THE PRESIDENT

President's Letter – Spring 2024



Santiago García-Granda (front row, third from right) surrounded by IUCr staff and Journal Editors at the Journals Management Board meeting in Chester, UK, in March 2024.

Santiago García-Granda

As the year progresses, the IUCr is forging ahead, actively shaping its future to increase its appeal to new generations, its engagement in scientific solutions to global problems and its contribution to the maintenance and improvement of the condition of the planet, being an instrument of peace, freedom and respect for the environment.

Writing this first letter of 2024, I'm filled with optimism for the future of our Union. The recent commemoration of our 75th General Assembly, held in Melbourne, Australia, the 26th in our triennial series, was a jubilant occasion where we celebrated our illustrious history. It is important to recognise, learn from and even imitate the pioneers, but perhaps it is just as important to look to the future through the new generations, in the same way that scientific objectives have evolved from classical crystallography to all aspects of structural science, as highlighted by the theme of our next Congress and General Assembly, IUCr27 in Calgary, Canada, in August 2026: 'Embracing Structural Science'. New times call for new ways and new people, and generational change is the key factor in any organisation that intends to endure. That is why the IUCr needs to put its efforts into offering leadership opportunities to young people and integrating all structural scientists in a transversal way in our plans for scientific cooperation with the widest possible transversality.

One of the aspects that should differentiate our renewal, in the current social context, is the incorporation of female leadership in a natural way in our activity. By fostering a culture where female leadership thrives naturally, we're not just evolving; we're paving the way for a brighter, more inclusive future for all.

A second aspect is the identification of the IUCr as a global scientific organisation, with local representation through the Regional Associates and National Committees. They must have the capacity to operate with broad autonomy but have a clear identification with the global parent IUCr. Our five Regional Associates cover in a very reasonable and convenient way the five continents. It is important that all of them participate in a rational way in the leadership of the IUCr and that they strengthen the links of collaboration between them.

On the other hand, the 55 National Committees, which make up the General Assembly, should also, both through their Regional Associates and through their representation in the IUCr, make their voice heard, participate actively in the IUCr's activities and establish multinational collaborations. One of the objectives of the Executive Committee (EC) is to increase the number of National Committees to include

countries where crystallography and structural science are developing so that they can contribute to the enrichment of the IUCr with their input.

The aim is to create a more cohesive image of the IUCr and also to take advantage of the capacity of the Regional Associates and the National Committees to raise awareness of the IUCr. In particular, it is important to show via social media a coherent and close image to society from a scientific analysis of the main challenges we face as a global society, and the specific effects in a community or nation or in a given geographical area.

The sustainability of resources for life on the planet – in all its diversity – is a key issue that humanity is not satisfactorily resolving. The International Year of Basic Sciences for Sustainable Development 2022/2023 (IYBSSD) has provided a new look at sustainability from a scientific point of view, and managed to capture the attention of the highest global institutions, such as the United Nations, UNESCO and the ISC, and especially, gave a voice to the new generation of scientists to address the problems and provide sustainable solutions.

The natural follow-up to the success of IYBSSD is the International Decade of Sciences for Sustainable Development (IDSSD), which was launched by the United Nations on 25 August 2023 and will run until 2033. The broad period of the Decade, beyond 2030, will allow progress to be assessed and for the SDGs (Sustainable Development Goals) to be modulated using the tools of basic science. It will also allow the integration of efforts to train new generations of scientists increasingly concerned with solving global problems, in a cross-cutting and cooperative way, and give female scientists the chance to be protagonists, contributing to and leading the paradigm shift. Structural scientists can apply their developments to environmental remediation and recovery as well as to the optimal reuse of resources or the production of clean energy, solving global environmental problems by seeking an optimal distribution of the planet's limited resources. The exploration of off-planet resources is another avenue in which the experience and knowledge of structural scientists will be extremely valuable. These people should be ready to be fully involved in changing the priorities and the way of life of humanity in the following decades.



The IUCr is proud to support IDSSD, as it did IYBSSD. See a short video about the IUCr's role in the Decade here.

In early March, after the EC bimonthly meeting, the Journal Management Board met in Chester on 7 and 8 March, and on 11 and 12 March, the spring meeting of the Finance Committee (FC) took place in Lund, Sweden. At both meetings important decisions were taken about the most important area of activity of

our Union, our 10 journals, which, as we all know, are undergoing major changes due to the influence of new forms of publishing and the emergence of new practices of publishing business. In this regard, the EC, in connection with the Editor-in-Chief and the Executive Managing Editor, is devising new ways to revitalise our publications, with initiatives such as the setting up of an independent working group to provide a vision for the future development of our publishing activity in the new environment. In parallel, the FC is analysing the impact of the publishing section on the Union's finances and the initiatives that can be implemented to strengthen the Union's funds.



The current IUCr FC consists of Santiago García-Granda and, shown above from left, Malcolm Cooper, Bo Brummerstedt Iversen, Joe Ferrara, Alex Stanley (*ex officio*), Hanna Dabkowska, Mike Glazer, Andrew Allen, Peter Strickland (*ex officio*) and Trevor Forsyth. Photo courtesy of LINXS Institute of advanced Neutron and X-ray Science.

As announced last summer, the International Science Council (ISC) voted for its new statutes on 29 February in a virtual extraordinary General Assembly. After initial fears about their position and a unanimous action by the scientific unions, the unions – the IUCr among them – have maintained their full capacity for scientific initiative and influence at the global level and in the decisions of the ISC. Hanna Dabkowska, IUCr Immediate Past President and IUCr Representative on ISC, and I attended meetings with the ISC President on 28 February.

The Chester office is doing its job as professionally as ever, with the only recent change being the appointment of Kezia Bowman in January as a Marketing Executive. Kezia is already also doing a fantastic job settling into the role, as progress is being made towards the implementation of a customer relationship management system and a new website.



Kezia Bowman on her first day at the IUCr.

Further to the workshop at the Melbourne Congress last August, the EC has confirmed the Purpose, Vision and Values statements and is working on a Mission statement that covers all the important issues the IUCr will deal with to achieve its Vision and Purpose. This will be circulated to members in due course. This refocussing of the Union's objectives is reinforced by a brand refresh where we are working on updating the Union's logo and colour scheme.

Furthermore, a Memorandum of Understanding has been formalised with the Organisation of Islamic Cooperation (OIC) Ministerial Standing Committee for Scientific and Technological Cooperation (COMSTECH), as a framework of cooperation. This formal framework will facilitate the organisation of joint activities and increase the mobility of young scientists and collaboration on unique scientific projects and infrastructures, with the aim of strengthening structural science research with the Islamic scientific community.



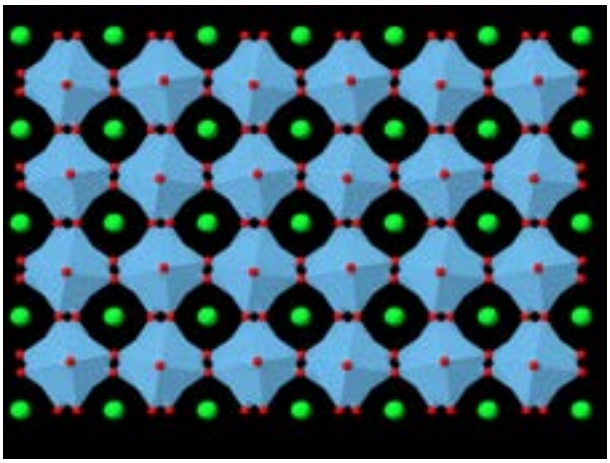
The Memorandum of Understanding (MOU) was signed by Professor Iqbal Choudhary (Coordinator General COMSTECH) (front right) during the Opening Ceremony of Pakistan's OIC-SESAME Users Meeting held at the COMSTECH Secretariat in Islamabad in January 2024. Photo courtesy of Professor Samar Hasnain, who can be seen receiving the MOU on behalf of the IUCr.

Once again, many thanks to all those who form and make our organisation work: the Regional Associates, the IUCr Commissions and Committees, Editors, Co-editors, referees and authors of our journals, our Chester staff and all individual crystallographers, women and men. Thanks to *IUCr Newsletter* Editor Mike Glazer, his team and all contributors for making possible, every quarter, a new issue and for continuing to be the communication reference for our community. Many thanks to all for contributing to the sustenance and reinvention of the IUCr from anywhere in the world.

All the best!

EDITORIAL

Editorial



$SrTiO_3$: Mesmerising picture of a low-frequency distortion mode for a wave vector at the *R* point of the cubic Brillouin zone (*CrystalMaker 11*: Phonons Explorer).

Mike Glazer

Spring is here in the UK at last! I am always glad when winter is on its way out. I have just returned from a two-day IUCr Finance Committee meeting in the city of Lund (Sweden), where I heard about the creative work carried out by our new Marketing Executive, Kezia Bowman. Kezia will be involved in developing marketing strategies to promote the IUCr and its publications and initiatives, and creating engaging content for diverse audiences. I wish her success in this important role.

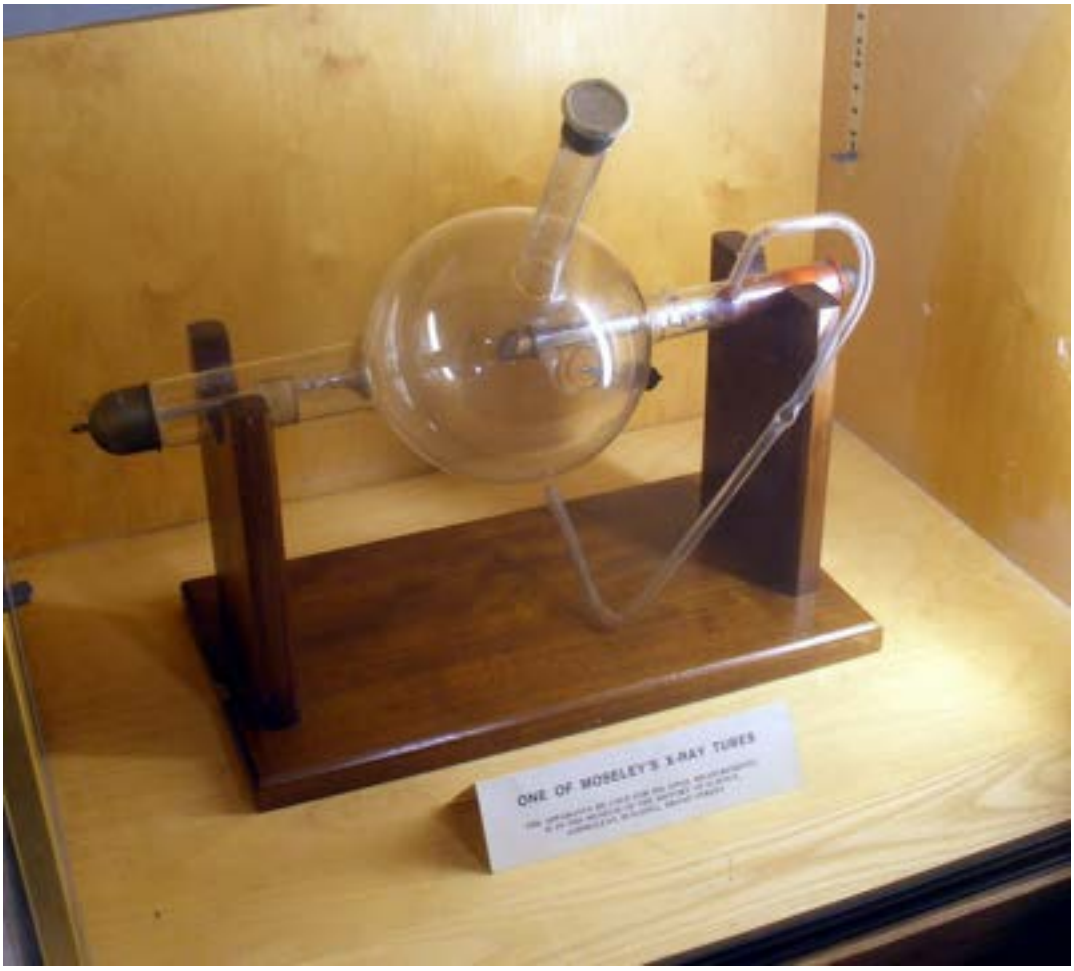


Kezia Bowman (right) interviewing Tina Weigel (left) and Florian Meurer, Immediate Past Chair and Chair of the DGK Young Crystallographers, respectively, at DGK2024 in Bayreuth, Germany.

In this issue of the *Newsletter*, we have two articles from the Hargittais, one on the Russian crystallographer Vladimir A. Koptsik, who was an important contributor to symmetry groups, especially the so-called Shubnikov groups. These groups, sometimes called colour groups, explore all the possible symmetry operations in which alternating colours (say black and red) can be included. Most crystallographers will already be familiar with the 230 space groups, which relate possible atomic positions subject to symmetry constraints in three dimensions. The Shubnikov groups add the possibility of positions for species with alternating properties, such as up and down electron spins. This is important for the study of magnetic crystal structures. There are 1651 such groups, and these were tabulated and illustrated by Koptsik in a weighty book (Шубниковские группы, published by Moscow University in 1966). I actually have a copy in front of me and I have to admire the enormous body of work that Koptsik achieved.

The other Hargittai article is on Johannes Kepler, he of planetary fame. Whereas his work on planetary orbits is well known, he was also interested in crystals and why they formed such symmetric shapes. Why, for example, were snowflakes hexagonal in shape? In 1611, he conjectured that there must be some underlying regularity in their internal structure, though he could not know what this structure actually was. He, along with others, such as Robert Hooke, considered the close packing of spheres as a way of explaining the external morphology of crystals: today we know that it is periodic arrangements of atoms and molecules that are responsible for the external shapes of crystals. Kepler famously considered, for instance, the three-dimensional packing of spheres (this was related to the problem of how to keep cannon balls from rolling around the deck of a warship). Kepler's conjecture was that the so-called cubic and hexagonal close packings were the most stable arrangement (think of the way oranges can be stacked together on a fruit stall). Surprisingly, his conjecture was not fully proved until very recently by T. Hales, S. M. Adams, G. Bauer *et al.* ["A Formal Proof of the Kepler Conjecture" (2017). *Forum Math. Pi*, **5**, e2]. So that took just over 400 years to solve!

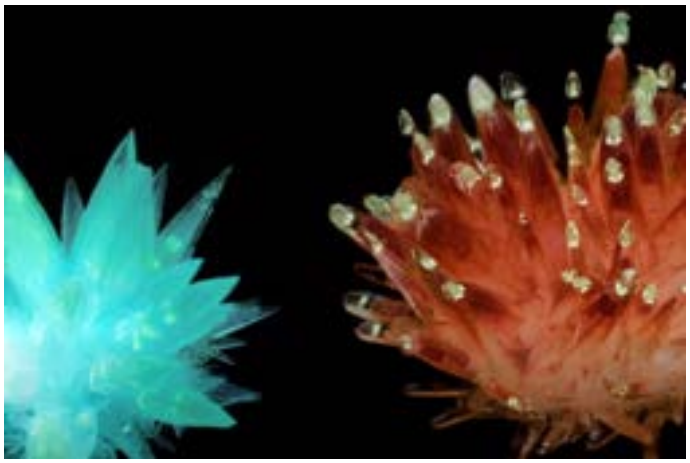
I was intrigued when a friend of mine in India sent me a poem that she had found that mentioned a famous scientist who played an important role in our understanding of X-rays and atomic physics, namely Harry Moseley. He was killed in battle at Gallipoli in 1915 and this poem was published 10 years after. Many years ago, I went into the office of one of our secretaries and noticed a cardboard box in the corner behind the door. I also saw that every time someone entered the room, the door was slammed against the box. I looked inside the box, and there was one of Moseley's original X-ray tubes, very similar to the one seen being held by Moseley in my article about the poem. Miraculously, despite its fragility, it had survived despite its rough treatment. It can now be seen in the small museum at the Clarendon Laboratory.



One of Moseley's X-ray tubes found in the Clarendon Laboratory, Oxford, UK.

OUTREACH

Winners of the 2023 IUCr Crystal Growing Competition



Pupils from IES Alfaguara in Loja, Spain, showed the effects of including phosphorescent substances when growing ammonium dihydrogen phosphate crystals.

We are delighted to announce the winners of the 2023 IUCr Crystal Growing Competition.

Schoolchildren were invited to convey their experiences of growing crystals through a video. The entries were judged on their creativity, aesthetic value, description of the working plan and experimental work, clarity of explanation, scientific background and safety by an international panel. The winners, who receive a certificate and medal, are as follows:

Category: 15–18 - GOLD: Ejercito de los Andes, Catriel (Argentina); SILVER: IRIS School, Thai Nguyen City (Vietnam); BRONZE: Escuela No. 751 "Dr Luis Federico Leloir", Trelew (Argentina)

Category: 11–15 - GOLD: Marie Curie Science Club, HNUE, Hanoi (Vietnam); SILVER: IES Alfaguara, Loja (Spain); BRONZE: Global Science Journey, Nguyen Tat Thanh School, Hanoi (Vietnam)

and the winning videos can be watched here.

Many thanks to all those who took part. Once again, the quality of the entries was extremely high, making the decisions difficult for the judges. We are looking forward to receiving more sparkling videos in the 2024 competition!


YOUNG CRYSTAL GROWER CERTIFICATE
IUCr Crystal growing competition 2023
GOLD MEDAL AWARD
Category: 11–15 (high-school mid
BY AIR MAIL
VERY MANY CONGRATULATIONS
IUCr Crystal growing competition 2023

EDITORIAL

Welcoming five new Co-editors



Our new Co-editors: Svetlana, Evangelia, Rhys, Jiawei and Hongyi.

Charles S. Bond, Elspeth F. Garman, Randy J. Read

Acta Cryst. D continues to welcome articles covering all aspects of structural biology, especially structures of biological macromolecules or the methods used in their determination. Growth of new areas remains a focus including cryoEM and electron crystallography. This month we are delighted to welcome five new Co-editors to *Acta Cryst. D* to help cover the breadth of structural biology we hope and aim to publish.

Dr Svetlana Antonyuk is a Reader at the Institute of Integrative Biology, University of Liverpool, UK, and has particular expertise of metalloenzymes, glycoproteins and membrane proteins. She plays an integral role in the neutron and X-ray structural communities, and complements her research with cryoEM.

Professor Evangelia D. Chrysina is the Research Director at the Institute of Chemical Biology, National Hellenic Research Foundation, Athens, Greece. She has over 20 years of experience spanning crystallization, crystallographic data processing, protein structure determination and wider biochemical studies.

Dr Rhys Grinter is a Laboratory Head based at the University of Melbourne, Australia, and has a background in structural microbiology. He brings to the journal sound cutting-edge practical knowledge of crystallography and cryoEM as well as an interest in the use of *AlphaFold* as a tool in 21st century structural biology.

Professor Jiawei Wang is an Associate Professor in the School of Life Sciences, Tsinghua University, Beijing, China. He has a strong background in structural biology, having worked on both X-ray crystallography and cryoEM. In addition to his work solving structures of membrane proteins and studying bacteriophage lambda, he has a strong interest in computational methods.

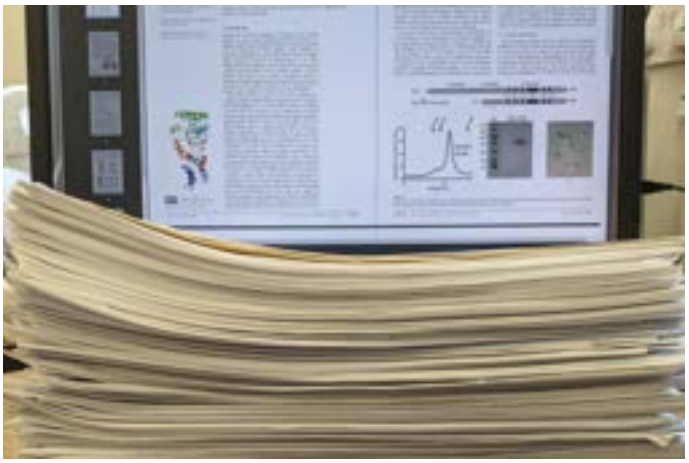
Dr Hongyi Xu is both a Principal Investigator in the Department of Materials and Environmental Chemistry, Stockholm University, Sweden, and a Senior Lecturer in Electron Diffraction, School of Chemistry and Molecular Biology, University of Queensland, Australia. He has a high level of expertise in electron diffraction, particularly in methods of sample preparation and data collection.

These appointments will enhance and renew the *Acta Cryst. D* Editorial Board while increasing the representation from different disciplines and different geographical regions around the world.

This article was originally published in *Acta Cryst*. (2024). D**80**, 147.

EDITORIAL

The unbearable burden of peer review?



Mark J. van Raaij

In conversations between researchers and on social networks the slowness and pickiness of peer reviewing is often decried. Journal editors often have difficulty securing the desired number of reviews for a manuscript. Anecdotal evidence suggests that some scientists do not pull their weight in reviewing, often not even taking the trouble to reply to a legitimate review request. After all, logic suggests that if we want our own manuscripts to be reviewed, we should review several times the number of manuscripts that we submit to scientific journals. In cases where a scientist really does not have time and receives more than their fair share of reviewing requests, it is also helpful to decline quickly, so that alternative reviewers can be sought as soon as possible. Suggesting names of alternative reviewers is also helpful. In many cases, an experienced postdoc in the same laboratory may be able to provide a timely and thoughtful review.

At the same time, reviewers that do accept sometimes submit exaggerated requests for changes and additional experiments. They are perhaps doing to others what has been done to them, while they should really do to others what they wish would be done to them. Here, it is important that journal editors step in decisively to limit these requests in their letter to the authors, rather than just sending a generic letter requesting a revision in line with the attached reviews.

In our journal we are not immune to these trends and have also experienced difficulties at times. However, our impression is that, for scientific society journals, finding reviewers is easier than many other editors report. We also do not seem to receive that many exaggerated requests for unreasonable changes or additional experiments. This is probably related to a greater feeling of community than with non-society journals, and the fact that any profits that IUCr journals generate are returned to science, in the form of subsidising conferences, workshops, fellowships and prizes for example.

We have a committed team of Co-editors, covering a wide range of structural biology specialties. Details can be found on our webpage https://journals.iucr.org/f/services/editors.html. On the same page, you will see that we also run a Review Board. The Review Board consists of experienced scientists (currently 31), who have agreed to referee up to twelve papers a year, to reply to requests promptly and to return reports within two weeks. During the coming months, we plan to update the Review Board, so volunteers are welcome!

The Section Editors also keep a non-public list of junior, but reasonably experienced, researchers who have expressed their specific interest to review manuscripts for our journal (even if it is with the clear thought to obtain merits for their academic CV, for a citizenship application or similar). The Section Editors welcome enquiries from researchers volunteering to be on this list.

Together, the Co-editors, Review Board and volunteer reviewers have helped to keep our average manuscript publication time down to just over three months (from first submission to final publication). We feel this is a reasonable standard, although we aim to get it down further — without compromising review quality of course.

Finally, at *Acta Crystallographica F – Structural Biology Communications* we are happy to receive more manuscripts, have them reviewed by knowledgeable scientists — and edit them efficiently and speedily to a high scientific and technical standard.

This article was originally published in *Acta Cryst*. (2024). F**80**, 52.

EDITORIAL

Private glycan investigations and public video content



The *Privateer* web app.

Mark J. van Raaij

In this issue of *Acta Cryst. F – Structural Biology Communications* we publish an article describing a web app in which the carbohydrate software *Privateer* (Agirre *et al.*, 2015; https://privateer.york.ac.uk) can be run (Dialpuri *et al.*, 2024). Although this self-updating and easy-to-use web app will be used by seasoned sugar-wranglers, it promises to be particularly useful for non-specialists who 'encounter' a glycan in their electron density. It should allow the structural biology community to easily inspect, refine, analyse and validate glycan modifications and carbohydrate ligands. The availability of this tool will hopefully help improve the current situation with many missing or wrong carbohydrate residues in the PDB (Joosten & Lütteke, 2017). The *Privateer* web app runs on the user's computer and keeps all data local, making these investigations truly private (https://www.youtube.com/watch?v=P9K27HvhDxA).

The communication is accompanied by a video in which the corresponding author Jon Agirre (also one of the Section Editors of *Acta Cryst. F*) succinctly explains the main features and usefulness of the web app. In addition to being available from the journal website the video can also be found on the IUCr YouTube channel (https://youtu.be/WDnmfgI_zB8). In future issues of our journal, we plan to solicit and include more video content. This could take the shape of a brief explanation like here, or structured interviews with one of more of the authors of published articles. Apart from interesting aspects of the papers, these interviews may also treat backgrounds of the authors or salient details of how the paper came about. In certain cases a `how-to' video might also be appropriate. As examples we can think of new ways to handle protein crystals or electron microscopy grids, but also novel ways to produce biological molecules or step-by-step instructions on how to install and run innovative software. We gladly welcome suggestions for video content made by our authors!

References

Agirre, J., Iglesias-Fernández, J., Rovira, C., Davies, G. J., Wilson, K. S. & Cowtan, K. D. (2015). *Nat. Struct. Mol. Biol.* **22**, 833–834.

Dialpuri, J. S., Bagdonas, H., Schofield, L. C., Pham, P. T., Holland, L., Bond, P. S., Sánchez Rodríguez, F., McNicholas, S. J. & Agirre, J. (2024). *Acta Cryst.* F**80**, 30–35.

Joosten, R. P. & Lütteke, T. (2017). *Curr. Opin. Struct. Biol.* **44**, 9–17.

This article was originally published in *Acta Cryst*. (2024). F**80**, 28–29.

EDITORIAL

A new era is emerging at scientific user facilities



Dimitri Argyriou

One of the features of the culture of science is the exchange of ideas and the sharing of advances. This typically happens by scientists and their students travelling to conferences, collaborating labs or large-scale user facilities to participate and contribute to discussions and experiments. Such travel is a wonderful way to not only expose each other to new work and ideas but also shape and share culture and habits. Most importantly it has been a great way to educate and train the next generation of scientists to the scientific method and to advance ideas, techniques and equipment.

However, this global scientific exchange has been profoundly perturbed by the COVID-19 pandemic. Changes in user travel behaviours, the use of remote access greatly perfected and adopted during the pandemic, combined with the advent of remarkable advances in artificial intelligence (AI), are aligning in such a way that they may possibly change how large-scale scientific facilities operate. This transformation is still ongoing and the new normal is still evolving.

Most scattering facilities report that while the number of submitted user proposals for experiments is slowly recovering toward pre-pandemic levels, the physical presence of users is recovering at a much slower pace while telepresence is increasing. The implications of this pattern are significant for facility operators. Experiments that were once performed by the users themselves are now dependent more so than before on the local beamline staff, thus pressuring the facility’s operational staff levels. And, while one can argue that remote presence in experiments may indeed expand the user base of facilities, the reality is that this emerging user base may be less able to conduct experiments in the future as students are not hands-on trained as rapidly as in the past. This again places increasing pressure on the local staff needed to support physically experiments at the facility.

This shift in user behaviour is taking place while scientific facilities are generating increasing amounts of data and experiments are becoming more demanding. Upgrades to ESRF and LCLS and planned upgrades at APS, ALS and Diamond facilities as well as the many new facilities that are coming online such as ESS, will add even further to the significant deluge of high-quality data. Innovations in the manipulation of the radiation, use of complex sample environments and other add-ons at the beamlines increase the demands on the experimental team to provide real-time support during the experiment as well as substantial support in the processing and analysis of the data post-experiment.

So how do facilities adjust to the reality that while experiments are growing more demanding and generating more data, user physical participation is slow to recover and shifting more to telepresence?

There is no doubt in my mind that the evolving trend at photon and neutron facilities is destined towards a hybrid model — a blend of traditional onsite work with enhanced remote participation in experiments. Already many facilities are investing heavily to enable this mode of user engagement. While the pandemic accelerated the adoption of remote access and AI tools, the value of in-person collaboration and hands-on experimentation remains irreplaceable. The future most likely holds a coexistence, leveraging the strengths of both virtual and physical realms to drive scientific progress. AI will also be part of that future and this will further add to the shift in the mix of skills needed at the beamline to incorporate the AI/data expertise needed when running an experiment, alongside the increasing numbers of beamline scientists who will be needed to mitigate the smaller number of physically participating users.

The future, where a user proposal will be read by an AI chatbot, its content and purpose understood sufficiently to configure a beamline and predict the initial data from the sample examined, is well within reach (Hexemer *et al.*, 2023). An autonomous AI-driven beamline that will perform routine measurements for users is not that far away either.

So where does that leave user facilities, that community watering hole, bringing scientists and ideas together, fostering collaboration and scientific progress?

Here, we need to remember that the science is in the sample. Scientists who made and understand the sample are irreplaceable when conducting experiments and their collaboration with the beamline staff is essential to success. It is no surprise therefore that the scientific community remains deeply committed and engaged in the future of large-scale facilities. A recent personal example was the user meeting of the Advanced Light Source which focused on the capabilities that users will harness with its upcoming upgrade. It is clear that the user community fully recognizes the value brought by user facilities and is fully invested in their success, irrespective of changing trends in user presence.

The brightest future lies in fully embracing AI to harness automation and autonomy at beamlines where it is useful and adds operational value. Deploying AI in harvesting all essence from the PTBs of data collected is unavoidable, given the volumes that we'll soon face. Remote participation in experiments must be supplemented by hands-on training to provide sufficient experience to users so that the results obtained are put into the right context. Nothing still replaces the value of getting your *hands dirty* on a beamline and engaging in strong collaborations with the local staff.

The COVID-19 pandemic together with the advent of AI is acting as a catalyst for change within large-scale scientific facilities, reshaping user behaviours and accelerating the role of AI in beamline automation and the analysis of ever-growing volume of data. As we navigate this transformative landscape, we cannot take much of the past for granted. Training of the next generation of users needs to be a community priority. We need to find new ways to support collaboration and user engagement at the beamline so as to perform the most challenging and impactful experiments and drive innovation. Incorporating AI-driven advances to deal with data will be needed to harvest value from experiments and fuel future breakthroughs. To succeed, facilities will need to collaborate widely with the AI community, access infrastructures to manage and process data and work with sponsors to manage the shift in skills needed in staff at the beamline. This is a significant transformation that is best embraced head-on.

Acknowledgements

Ashley White, Andreas Scholl and Simon Kimber are thanked for helpful comments and discussions.

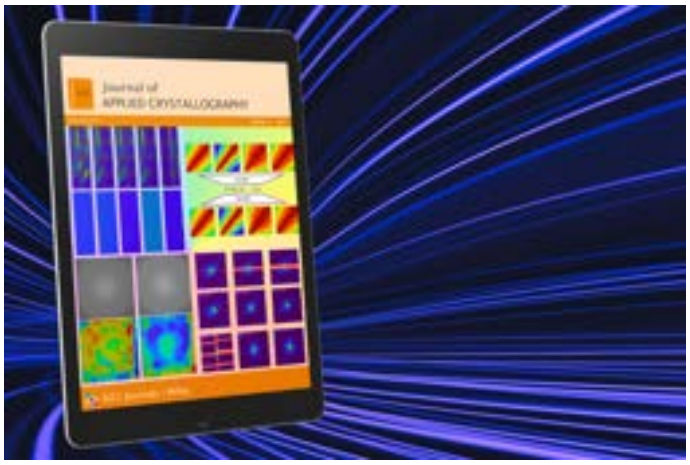
References

Hexemer, A., Pham, V., Köpp, W., White, A. & Rotenberg, E. (2023). ALS User Meeting September 11–15, 2023, poster.

This article was originally published in *IUCrJ* (2024). **11**, 1-2.

EDITORIAL

Introduction to the virtual collection of papers on Artificial neural networks: applications in X-ray photon science and crystallography



Tomas Ekeberg

Artificial intelligence (AI) is more present than ever, both in our society in general and in science. At the center of this development has been the concept of deep learning, the use of artificial neural networks (ANNs) that are many layers deep and can often reproduce human-like behavior much better than other machine-learning techniques.

This development has been going on for a long time, and it is ambiguous to identify a specific starting date for it. Possible candidates might be the first ANNs in 1943 (McCulloch & Pitts, 1943), the popularization of backpropagation to train many layers in a network at once in 1985 (Rumelhart *et al.*, 1986) and the application to identify human handwriting in 1989 (Le Cun *et al.*, 1989).

Today the growth of this field is seemingly exponential, with major breakthroughs being reported almost every year. Some of the most notable examples are

(1) beating a professional player at the game of go (Silver *et al.*, 2016),

(2) residual neural networks (ResNets) for image recognition (He *et al.*, 2016),

(3) AlphaFold protein structure prediction (Jumper *et al*., 2021),

(4) ChatGPT and other large language models (LLMs) (https://gluebenchmark.com/leaderboard).

During the same time frame, deep learning has also seeped into our society in many less prominent cases such as

(1) automatic image processing of photographs from our cell-phone cameras,

(2) recommendations for music or movies on streaming services,

(3) optimization of server hall power efficiency.

It is certainly no understatement that AI has become a foundation for society as we know it today. And so far, the technology has mainly been developed by big tech companies.

With this knowledge, many scientists have started to investigate what these new tools could mean for their field of research. While some areas of science were fairly slow to adopt these methods, we are now

seeing a rapid spread of AI applications in many different fields, and the contributions in this collection of articles from *Journal of Applied Crystallography* (https://journals.iucr.org/special_issues/2024/ANNs) manifest that observation for X-ray photon science and crystallography.

Most applications of AI are, however, not of the transformative kind, comparable to the effect that AlphaFold had on the field of structure prediction. Instead, we have examples such as preprocessing that gives smaller improvements to data quality, or automation of a mundane task that would otherwise have to be done by a researcher.

Classification. One of the first applications of machine learning was to classify data. Famous examples include recognizing handwritten digits and letters or identifying human faces. In photon science this is also a common use case, and recently we have, for example, seen it being used for femtosecond X-ray imaging patterns (FXI) (Assalauova *et al.*, 2022), X-ray photon correlation spectroscopy (Timmermann *et al.*, 2022) and serial femtosecond crystallography (Rahmani *et al.*, 2023). This is often a convenient way to speed up a researcher's work by automating an otherwise labor-intensive task, by classifying a small set of patterns by hand and then training a machine-learning algorithm to classify a bigger dataset in a similar fashion.

Another example is from neutron diffraction (Hao *et al.*, 2023) where a neural network approach was used not only to filter out relevant data but also to label regions of interest in each diffraction pattern.

A common critique towards neural network approaches is their black-box nature — that we usually have very limited understanding of the analysis that a trained network actually performs. A particularly interesting development is, therefore, the attempts to understand the internal workings of our networks. One such example is reported by Nawaz *et al.* (2023).

Data analysis. A more recent development is that neural networks take a more active role in data analysis in addition to classification. We see cases in the entire pipeline of data processing. A successful example is data preprocessing where, for example, missing regions of data can be recreated using deep neural networks. This has been shown for both small/wide-angle X-ray scattering (SAXS/WAXS) (Chavez *et al.*, 2022) and FXI (Bellisario *et al.*, 2022) experiments.

It is still fairly rare for neural networks to perform the bulk of the analysis. One such case is, however, a study of band gap structures in metal–organic frameworks where an ANN trained on a large set of simulated data was applied to experimental data with remarkable success (Gómez-Peralta *et al*., 2022). In another example by Lim *et al*. (2023), subsurface temperatures are estimated during laser melting comparing experimental data with ANN-based simulations.

Parameter estimation. A more common application is the use of neural networks to provide parameters to an analysis that is otherwise using conventional methods or to reduce the search space for an existing algorithm. Chitturi *et al.* (2021) use neural networks to estimate lattice parameters for X-ray powder diffraction data, which can reduce the search space for this time-consuming algorithm by more than a factor of 100. A similar example comes from X-ray reflectivity, where a neural network was used to estimate model parameters in a fraction of the time required for traditional methods (Mareček *et al*., 2022). Recently, a web-service called *CrystalMELA* was also released, which can estimate the crystal system using several machine-learning methods (Corriero *et al*., 2023).

In addition to direct applications, AI is mentioned by a vast number of articles, and it is clear that there is a curiosity and optimism about AI techniques within the field. The implementation of AI techniques is, however, most likely in its infancy. Most examples included here are the work of small talented teams of researchers using relatively modest hardware. The effects are already tangible, by speeding up research, identifying hidden patterns and freeing up time for researchers by automating tasks. Given the success so far, more effort and more computational power could potentially have the same transformative effect in our field as AlphaFold has had on protein structure prediction.

References

Assalauova, D., Ignatenko, A., Isensee, F., Trofimova, D. & Vartanyants, I. A. (2022). *J. Appl. Cryst.* **55**, 444–454.

Bellisario, A., Maia, F. R. N. C. & Ekeberg, T. (2022). *J. Appl. Cryst.* **55**, 122–132.

Chavez, T., Roberts, E. J., Zwart, P. H. & Hexemer, A. (2022). *J. Appl. Cryst.* **55**, 1277–1288.

Chitturi, S. R., Ratner, D., Walroth, R. C., Thampy, V., Reed, E. J., Dunne, M., Tassone, C. J. & Stone, K. H. (2021). *J. Appl. Cryst.* **54**, 1799–1810.

Corriero, N., Rizzi, R., Settembre, G., Del Buono, N. & Diacono, D. (2023). *J. Appl. Cryst.* **56**, 409–419.

Gómez-Peralta, J. I., Bokhimi, X., García-Peña, N. G., Quintana-Owen, P. & Rodríguez-Gattorno, G. (2022). *J. Appl. Cryst.* **55**, 1538–1548.

Hao, Y., Feng, E., Lu, D., Zimmer, L., Morgan, Z., Chakoumakos, B. C., Zhang, G. & Cao, H. (2023). *J. Appl. Cryst*. **56**, 519–525.

He, K., Zhang, X., Ren, S. & Sun, J. (2016). *2016 IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 770–778, https://doi.org/10.1109/CVPR.2016.90. Piscataway: IEEE.

Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., Tunyasuvunakool, K., Bates, R., Žídek, A., Potapenko, A., Bridgland, A., Meyer, C., Kohl, S. A. A., Ballard, A. J., Cowie, A., Romera-Paredes, B., Nikolov, S., Jain, R., Adler, J., Back, T., Petersen, S., Reiman, D., Clancy, E., Zielinski, M., Steinegger, M., Pacholska, M., Berghammer, T., Bodenstein, S., Silver, D., Vinyals, O., Senior, A. W., Kavukcuoglu, K., Kohli, P. & Hassabis, D. (2021). *Nature*, **596**, 583–589.

Le Cun, Y., Jackel, L. D., Boser, B., Denker, J. S., Graf, H. P., Guyon, I., Henderson, D., Howard, R. E. & Hubbard, W. (1989). *IEEE Commun. Mag*. **27**, 41–46.

Lim, R. E., Mukherjee, T., Chuang, C., Phan, T. Q., DebRoy, T. & Pagan, D. C. (2023). *J. Appl. Cryst.* **56**, 1131–1143.

Mareček, D., Oberreiter, J., Nelson, A. & Kowarik, S. (2022). *J. Appl. Cryst.* **55**, 1305–1313.

McCulloch, W. & Pitts, W. (1943). *Bull. Math. Biophys.* **5**, 115–133.

Nawaz, S., Rahmani, V., Pennicard, D., Setty, S. P. R., Klaudel, B. & Graafsma, H. (2023). *J. Appl. Cryst.* **56**, 1494–1504.

Rahmani, V., Nawaz, S., Pennicard, D., Setty, S. P. R. & Graafsma, H. (2023). *J. Appl. Cryst.* **56**, 200–213.

Rumelhart, D., Hinton, G. & Williams, R. (1986). *Nature*, **323**, 533–536.

Silver, D., Huang, A., Maddison, C. J., Guez, A., Sifre, L., van den Driessche, G., Schrittwieser, J., Antonoglou, I., Panneershelvam, V., Lanctot, M., Dieleman, S., Grewe, D., Nham, J., Kalchbrenner, N., Sutskever, I., Lillicrap, T., Leach, M., Kavukcuoglu, K., Graepel, T. & Hassabis, D. (2016). *Nature*, **529**, 484–489.

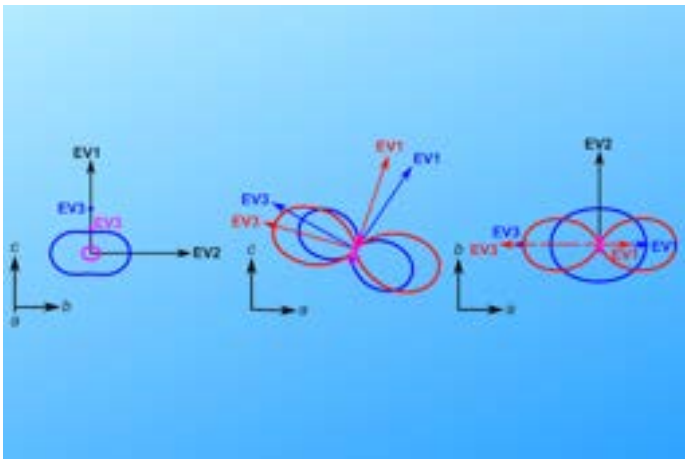
Timmermann, S., Starostin, V., Girelli, A., Ragulskaya, A., Rahmann, H., Reiser, M., Begam, N., Randolph, L., Sprung, M., Westermeier, F., Zhang, F., Schreiber, F. & Gutt, C. (2022). *J. Appl. Cryst.* **55**, 751–757.

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An overview of a related virtual collection of AI/machine-learning papers that have been published in *Acta Crystallographica* (*Sections A*, *B* and *D*), *IUCrJ* and *Journal of Synchrotron Radiation* can be found here.

COMMENTARY

Radiation damage as a source of information



Elena V. Boldyreva

It has long been known that X-ray radiation can damage samples. This phenomenon was extensively investigated in protein crystallography as something unwanted and detrimental for data quality. The main efforts were focused on developing experimental strategies that minimize the damage (Garman, 2010; Bourenkov & Popov, 2010). That radiation damage has been observed much more in macromolecular crystallography than for small-molecule samples can be attributed not only to the higher sensitivity of macromolecular crystals to radiation but also to the fact that synchrotron radiation was used much more when studying the crystals of biomolecules than when studying small-molecule crystals.

The advent of new synchrotron sources with increased brightness made synchrotron experimentation very attractive for structural research. As more synchrotron experiments are now performed with small-molecule crystals, radiation damage is becoming more and more frequently reported for these systems too (Christensen *et al.*, 2019; Bogdanov *et al.*, 2021; Collings, 2021; Collings & Hanfland, 2022). Radiation damage may affect structural data and lead to wrong conclusions on the properties of materials. Serious damage is disturbing, but at least it can be easily detected both by watching for a single crystal with a hole burnt in it by the beam (Fig. 1) and/or by poor quality of diffraction data.

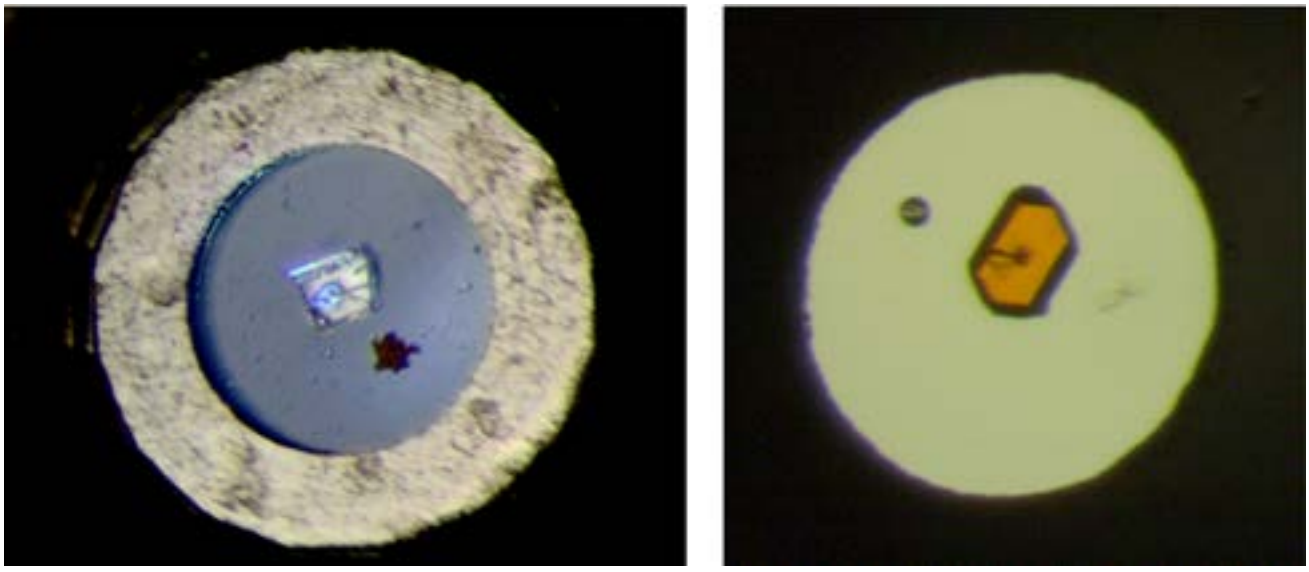


Figure 1. Samples of small-molecule crystals beam-drilled by synchrotron radiation during diffraction experiments. Courtesy of Professor Boris Zakharov.

Radiation damage may be less obvious and easily overlooked, especially during the early stages of the experiment, when the data as well as refined structural parameters and *R* factors look 'normal' at first sight. Data collection at a single temperature may reveal no suspicious effects. Multi-temperature data collections starting with the highest temperature and then decreasing may suggest that something 'strange' happens, if structural data deteriorate and atomic displacement parameters (ADPs) increase on cooling. If a negative bulk thermal expansion is observed, this also may look suspicious. Such is the case with glycinium phosphite (Bogdanov *et al.*, 2021). Should the same series of multi-temperature data be collected on heating the crystal from the lowest temperature upwards, no radiation damage effect would be, most likely, even suspected, since an increase in the ADPs, a slight deterioration of structural data and positive thermal expansion would look natural. At the same time, one may note that in some rare cases even a structural contraction on cooling may be masked by structural contraction due to radiation damage (Coates *et al.*, 2021; Boström *et al.*, 2022).

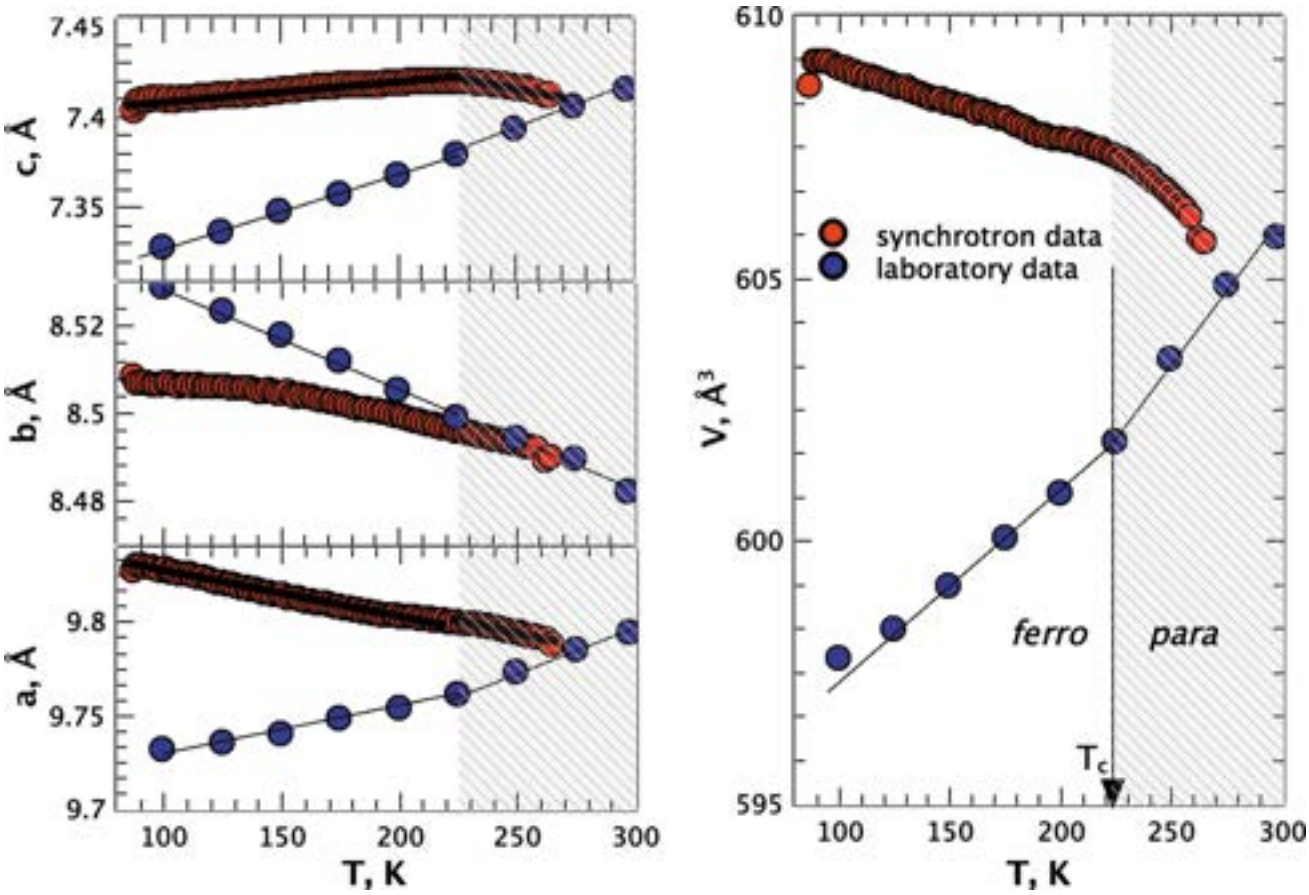


Figure 2. Unit-cell parameters and volume of glycinium phosphite versus temperature from synchrotron and laboratory data. The error bars, if they appear missing, are smaller than the symbols. The shaded zone indicates the temperature domain for the paraelectric phase. The temperature in the experiments changed from the higher to lower values. Reproduced from Bogdanov *et al.* (2021).

What really helped to detect the radiation damage in glycinium phosphite was a comparison of the synchrotron data with the results of the low-dose measurements at a laboratory source. The differences in the temperature dependencies of the unit-cell parameters and volume obtained in a synchrotron experiment and at a laboratory source were really striking and convincing (Fig. 2). The final proof of the radiation-induced structural expansion was obtained later in additional isothermal experiments (Fig. 3) (Bogdanov *et al.*, 2022).

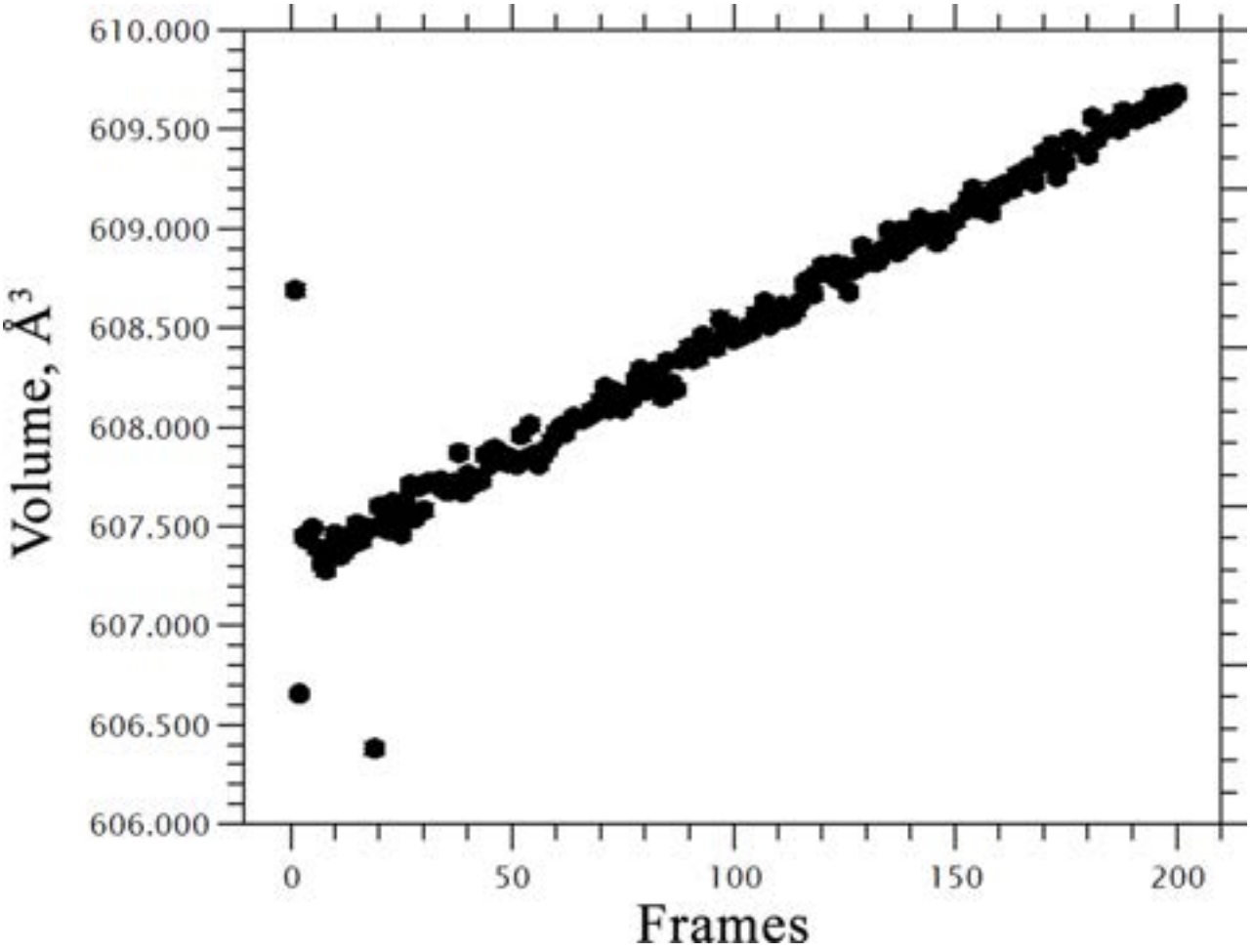


Figure 3. Changes in the unit-cell volume of glycinium phosphite at constant temperature over time resulting from radiation damage. Data collected by Professor Dmitry Chernyshov at SNBL ESRF (Bogdanov *et al.*, 2022).

The earlier work by Bogdanov *et al.* (2021) has not only illustrated how important it may be that a synchrotron experiment is compared with that at a laboratory source. Bogdanov *et al.* have suggested that the radiation damage may be considered as a tool to tune structural disorder and associated properties, and here synchrotron experiments with the additional option of data collections at different energies may provide new and yet unexplored opportunities.

A recent publication by McMonagle *et al.* (2024) provides an excellent illustration of this. The authors have compared the radiation-induced strain in a series of compounds with thermal expansion of the same crystals. A second-rank tensor of radiation-induced lattice strain was proposed to characterize the structural susceptibility of the crystal to radiation. Such tensors were calculated and compared with the corresponding tensors of thermal expansion (Fig. 4).

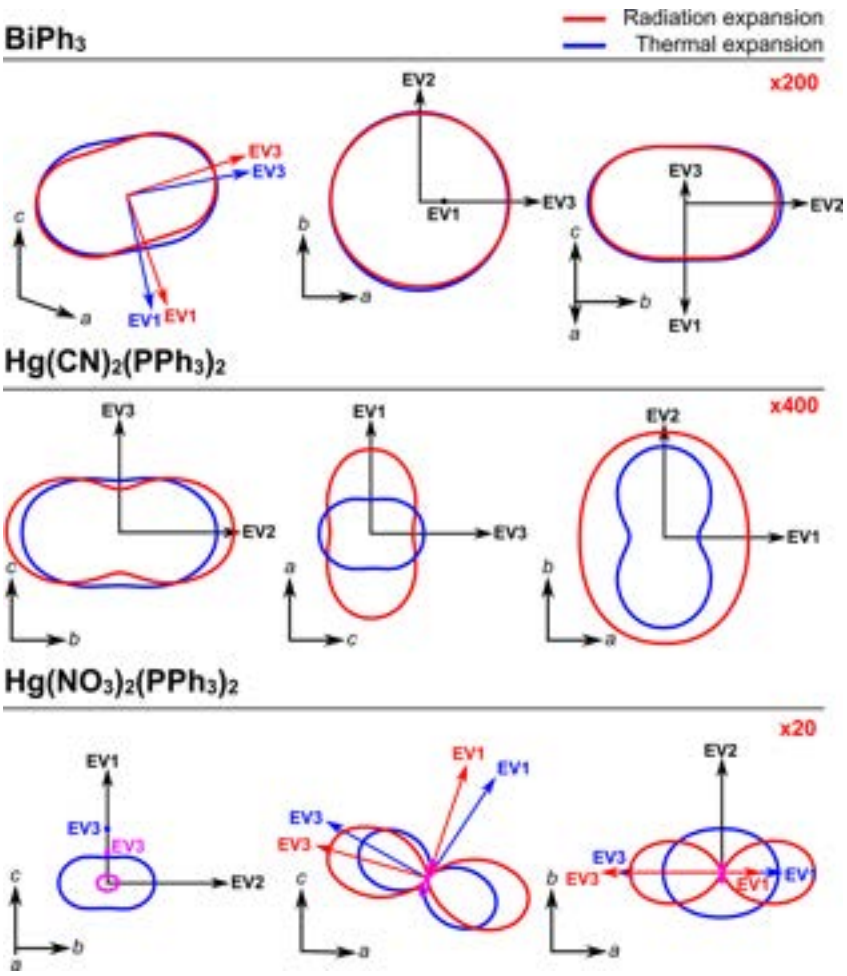


Figure 4. Expansion indicatrices of three compounds. Each panel shows three sections of the indicatrix, viewed along each of the Cartesian coordinates, with the corresponding unit-cell vectors and expansion eigenvectors (EV) labelled. Blue sections show thermal expansion and red the expansion due to radiation. The pink lines indicate negative expansion induced by radiation. Where the thermal and radiation expansion share the same eigenvectors, these are shown in black, otherwise they are shown in blue and red, respectively. To make the thermal expansion (in K^{-1}) and radiation expansion (in Gy^{-1}) a comparable size in the diagram, the radiation expansion has been multiplied by the figure given in red in the top right of each panel. Reproduced from McMonagle *et al.* (2024).

The associated eigenvalues and eigenvectors showed that for $Hg(NO_3)_2(PPh_3)_2$ and $Hg(CN)_2(PPh_3)_2$ [PPh_3 = triphenylphosphine, $P(C_6H_5)_3$; Ph = phenyl, C_6H_5] the two tensors were not the same and therefore probed truly different structural responses, whereas for $BiPh_3$ they were quite similar.

The authors emphasize that at the level of elastic response, radiative expansivity relates to deformations induced by the insertion of anisotropic defects while thermal expansion is defined by anisotropy of elastic stiffness and Grüneisen parameters. Structural deformations induced by temperature (‘phonon pressure’) and radiation damage (‘defect pressure’) are not necessarily correlated with each other. For two out of three materials studied by McMonagle *et al.* (2024), deformations induced by phonon and defect pressure were directionally different from each other. To determine the exact nature of the defects one would want to look at the local and not an average structure. The authors supposed that different bonds and intermolecular contacts are affected by anharmonic phonons and radiation-induced defects. Therefore, thermal and radiative expansion have different underlying structural mechanisms.

These findings should be taken into account when studying thermal expansion with synchrotron light, since the true picture may be ‘masked’ by the radiation-induced strain. But the importance of this work is more significant than that. Many physical properties of small-molecule crystals, in particular their ferroelectric and piezoelectric phase transitions, are related to structural strain on temperature or pressure variation. Synchrotron radiation can be also used to manipulate structural strain and in this way it can be used as a tool to affect also the temperature- and pressure-induced phase transitions: to prevent them or to shift the transition point. Examples of the effect of radiation on phase transitions in

ferroelectrics have been already documented in the literature (Chernyshov *et al.*, 2022; Grzechnik *et al.*, 2023). The paper by McMonagle *et al.* (2024) shows clearly how more light on the problem may be shed by a quantitative comparison of the anisotropic thermal and radiation expansions. Complementary multi-temperature studies of materials by synchrotron light and at laboratory sources may also be very important in order to reveal radiation strain effects reliably.

References

Bogdanov, N. E., Zakharov, B. A. & Boldyreva, E. V. (2022). In *Synchrotron Radiation Techniques for Catalysts and Functional Materials*, II International Conference, Book of Abstracts, pp. 66–67. BIC SB RAS.

Bogdanov, N. E., Zakharov, B. A., Chernyshov, D., Pattison, P. & Boldyreva, E. V. (2021). *Acta Cryst*. B**77**, 365–370.

Boström, H. L., Cairns, A. B., Chen, M., Daisenberger, D., Ridley, C. J. & Funnell, N. P. (2022). *Phys. Chem. Chem. Phys.* **24**, 25072–25076.

Bourenkov, G. P. & Popov, A. N. (2010). *Acta Cryst*. D**66**, 409–419.

Chernyshov, D., Dyadkin, V. & Törnroos, K. W. (2022). *Acta Cryst*. B**78**, 392–396.

Christensen, J., Horton, P. N., Bury, C. S., Dickerson, J. L., Taberman, H., Garman, E. F. & Coles, S. J. (2019). *IUCrJ*, **6**, 703–713.

Coates, C. S., Murray, C. A., Boström, H. L. B., Reynolds, E. M. & Goodwin, A. L. (2021). *Mater. Horiz.* **8**, 1446–1453.

Collings, I. E. (2021). *Acta Cryst.* B**77**, 307–308.

Collings, I. E. & Hanfland, M. (2022). *Acta Cryst*. B**78**, 100–106.

Garman, E. F. (2010). *Acta Cryst*. D**66**, 339–351.

Grzechnik, A., Petříček, V., Chernyshov, D., McMonagle, C., Geise, T., Shahed, H. & Friese, K. (2023). *Acta Cryst*. B**79**, 104–113.

McMonagle, C. J., Fuller, C. A., Hupf, E., Malaspina, L. A., Grabowsky, S. & Chernyshov, D. (2024). *Acta Cryst.* B**80**, 13–18.

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COMMENTARY

A new approach for serial electron diffraction data collection

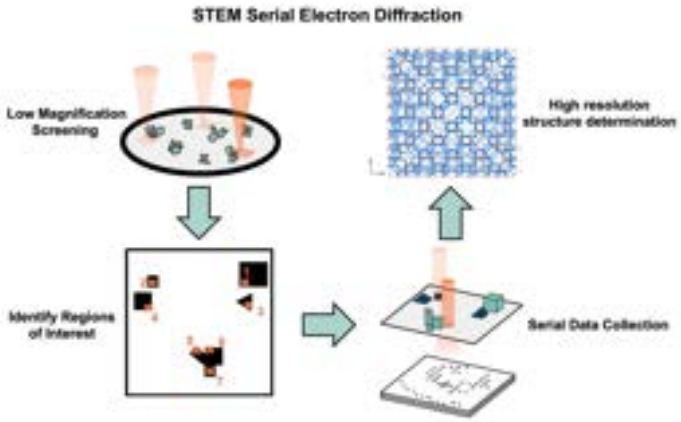


Figure 1. Overview of the scanning transmission electron microscopy (STEM) serial electron diffraction workflow presented by (and adapted from) Hogan-Lamarre *et al.* (2024).

Brent L. Nannenga

From materials characterization to the study of biological materials, electron crystallography has played a key role in the structural sciences (Zou *et al.*, 2011; Glaeser, 2007). The wider field of electron crystallography has always been driven forward by advances in methodology. In recent years, electron crystallographic methods that make use of three-dimensional micro- and nanocrystals have come to the forefront (Nannenga & Gonen, 2019; Gemmi *et al.*, 2019). Currently, the most common method of data collection is continuous rotation of the crystal in the electron beam, which produces electron diffraction datasets analogous to single-crystal X-ray diffraction datasets (Nannenga *et al.*, 2014; Cichocka *et al.*, 2018; Gemmi *et al.*, 2015). This robust approach for continuous rotation electron diffraction data collection has led to an explosion in popularity of the technique and it has been successfully applied to a variety of samples including nanomaterials, organic molecules, pharmaceuticals, peptides and proteins.

Despite growing interest in the field, there are portions of the data collection pipeline that are the focus of continued methods development. For example, when studying samples that are beam sensitive and require large amounts of data to be collected, structure solution can prove to be difficult. Therefore, improvements to data collection throughput, automation of the data collection process and minimizing the exposure of crystals during collection of diffraction datasets are areas of interest.

In this issue of **IUCrJ**, Hogan-Lamarre *et al.* (2024) directly address these issues by utilizing scanning transmission electron microscopy (STEM) to rapidly collect serial electron diffraction patterns with low dose to determine high-resolution structures of nanomaterials. This work builds on previous serial electron diffraction methodology that made use of a customized STEM setup and hybrid pixel detector to determine the structures of model proteins from nanocrystals (Bücker *et al.*, 2020). A major benefit of this new method (Fig. 1) is that, in contrast to the previous study, it does not require specialized STEM hardware, makes use of the microscope scripting software provided and can be performed using more widely available electron microscope camera systems. These improvements will make the implementation of this technique more broadly accessible to the electron crystallography community. The STEM serial electron diffraction workflow starts by screening the grid at low magnification with minimal dose delivered to the sample. Using the low-magnification screening, regions of interest (*i.e.* potential crystals) are identified and selected. Each region of interest is then targeted, and a single electron diffraction pattern is collected. The data are then processed and combined to produce serial

electron diffraction datasets for subsequent data processing and structure determination efforts.

As a proof of concept for this new serial electron diffraction workflow, the authors of the study used two zeolite samples. The first sample, zeolite Y, was used to benchmark the new serial diffraction methodology as it could be directly compared with data collected by standard continuous rotation data collection. With both approaches, a high-resolution structure of zeolite Y was determined with similar quality, thereby validating the serial diffraction approach on this model target. The next target chosen for validation was the zeolite ZSM-25, which represented an exciting sample for the new methodology as electron diffraction had not yet been able to produce datasets of sufficient quality for *ab initio* structure solution. With the new approach in hand, the authors were able to collect serial electron diffraction data from ZSM-25 and ultimately generate a 99.8% complete dataset to 0.90 Å, which facilitated structure solution by direct methods. This demonstration of the first ever *ab initio* structure solution of ZSM-25 highlights the power of STEM serial electron diffraction data collection, and the more user-friendly implementation promises to allow more users to take advantage of the technique.

Serial electron diffraction data collection using STEM is an important new approach for the field of electron crystallography. It will be exciting to follow future work in this area including the continued streamlining of the STEM workflow, the extension of the technique to an even broader range of STEM and detector combinations, and the structure determination of more novel targets using the methodology. The possibilities of further combining STEM serial electron diffraction with existing continuous rotation methods will also be interesting to developers and users. Overall, STEM serial electron diffraction has the potential to provide highly automated and rapid structures from nanocrystalline materials that may have proven difficult to study using other structural methods.

References

Bücker, R., Hogan-Lamarre, P., Mehrabi, P., Schulz, E. C., Bultema, L. A., Gevorkov, Y., Brehm, W., Yefanov, O., Oberthür, D., Kassier, G. H. & Dwayne Miller, R. J. (2020). *Nat. Commun*. **11**, 996.

Cichocka, M. O., Ångström, J., Wang, B., Zou, X. & Smeets, S. (2018). *J. Appl. Cryst.* **51**, 1652–1661.

Gemmi, M., La Placa, M. G. I., Galanis, A. S., Rauch, E. F. & Nicolopoulos, S. (2015). *J. Appl. Cryst.* **48**, 718–727.

Gemmi, M., Mugnaioli, E., Gorelik, T. E., Kolb, U., Palatinus, L., Boullay, P., Hovmöller, S. & Abrahams, J. P. (2019). *ACS Cent. Sci.* **5**, 1315–1329.

Glaeser, R. M. (2007). *Electron Crystallography of Biological Macromolecules*. Oxford University Press.

Hogan-Lamarre, P., Luo, Y., Bücker, R., Miller, R. J. D. & Zou, X. (2024). *IUCrJ*, **11**, 62–77.

Nannenga, B. L. & Gonen, T. (2019). *Nat. Methods*, **16**, 369–379.

Nannenga, B. L., Shi, D., Leslie, A. G. & Gonen, T. (2014). *Nat. Methods*, **11**, 927–930.

Zou, X., Hovmöller, S. & Oleynikov, P. (2011). *Electron Crystallography: Electron Microscopy and Electron Diffraction*. Oxford University Press.

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FEATURE ARTICLE

Johannes Kepler – the first scientific crystallographer



Istvan Hargittai, Magdolna Hargittai

Johannes Kepler's (1571−1630) best-known contribution to science is his three laws of planetary motion. He was a pioneer in model building, which he extended into the third dimension, though his famous planetary model proved to be a non-discovery. He discussed the stacking of equal spheres when examining snowflakes and advanced the notion that internal structure determines the external shape. This was relevant to a fundamental issue in crystallography, and he has been considered the first scientific crystallographer.



Johannes Kepler, line engraving by N. Dietz (Wellcome Collection).

Science has made great use of Kepler's works over the centuries, but little is known of the man himself. Galileo did not give him much recognition, and Newton did not mention him in most parts of his *Principia* or did so only in passing [1]. Kepler's principal languages were German and Latin, and his penetration into English literature was slow. Then, in the 19th century, two monographs in English were devoted to Kepler [2, 3]. The first complete biography of Kepler was published in German by the great Keplerian scholar Max Caspar and translated into English in 1959 [4]. Arthur Koestler's monumental book, *The Sleepwalkers*, also appeared in 1959 [5]. Part of it is a biography of Johannes Kepler, which was also published separately as a little volume entitled *The Watershed* [6]. These publications broke the ice and did a great deal to make Kepler better known. Since then, there has been a growing amount of literature about Kepler.

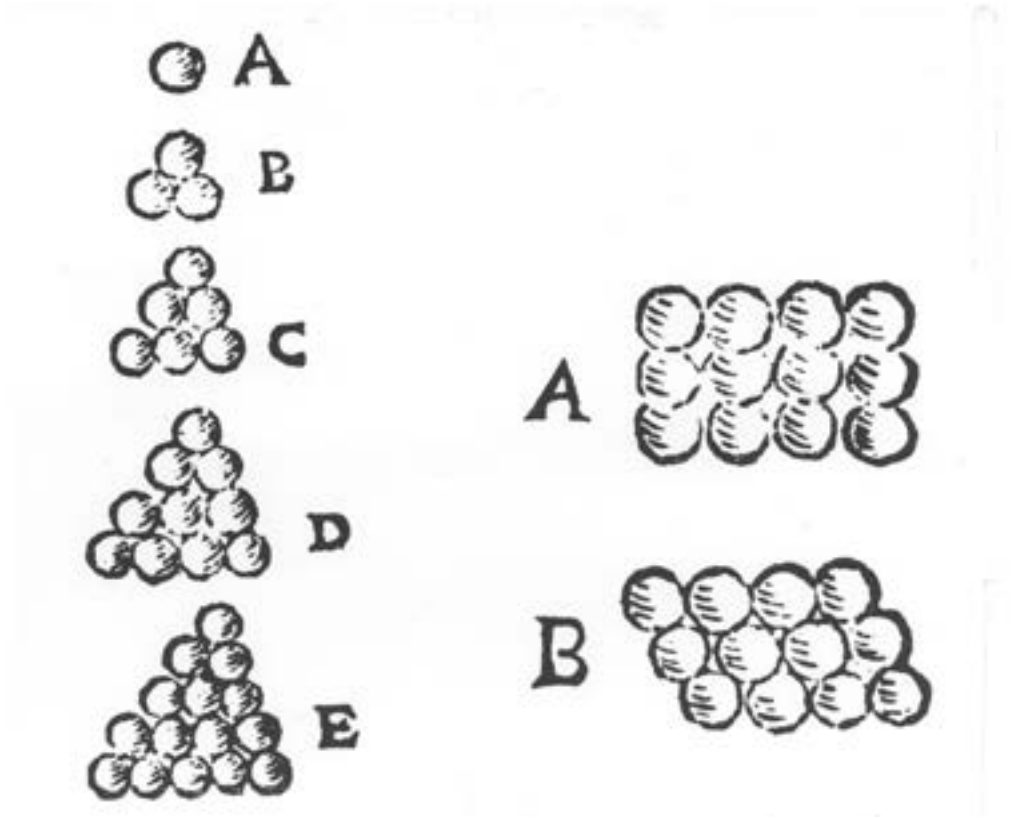
Kepler's three laws of planetary motion have earned him a solid place in the domains of physics and astronomy. Just as a reminder:

The orbit of a planet is an ellipse, with the Sun at one focus.

The line joining a planet to the Sun sweeps out equal areas in equal times.

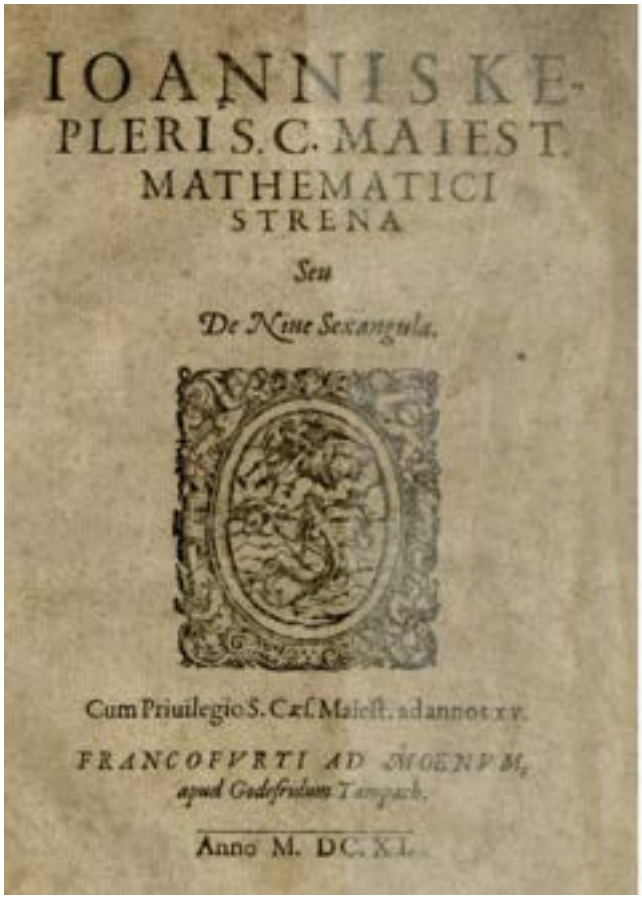
The squares of the periods of the planets are proportional to the cubes of their mean distances from the Sun.

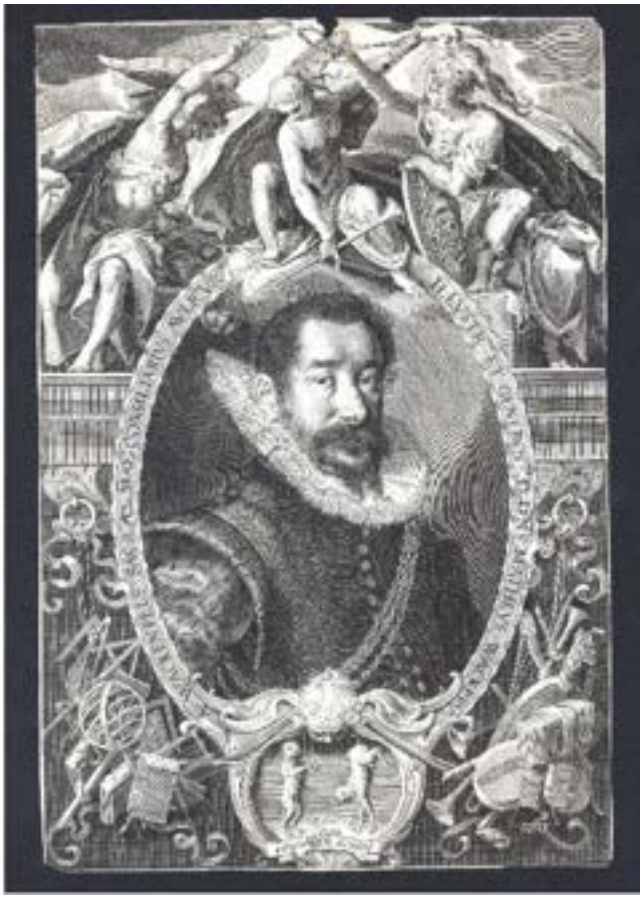
Kepler's work relevant to crystallography is documented in the *Historic Atlas of Crystallography* [7] and more extensively in our volume about the role of symmetry in scientific discoveries, giving emphasis to model building [8].



Closely packed spheres by Kepler [9].

Kepler's treatise, *De Nive Sexangula* (*The Six-Cornered Snowflake*), was published in 1611 in Latin [9], followed by an English translation 355 years later.





The cover of *De Nive Sexangula* and J. M. Wacker von Wackenfels' portrait by Aegidius Sadeler in the Scientific Library of the City of Trier, Germany (in the public domain; file: Johann Matthäus Wacker von Wackenfels.jpg - Wikimedia Commons).

Kepler wrote this 24-page treatise as a New Year's gift to his patron, J. M. Wacker von Wackenfels (1550−1619), thereby making his name immortal in science history. Wacker von Wackenfels was a scholar and author interested in philosophy and history. He originated from modest circumstances and worked himself up the societal ladder through scholarship, hard work and advantageous marriages. He received support for his studies and earned hereditary nobility and a position in the high court of the Holy Roman Empire.

Kepler was the first credited with discussing the problem of packing equal spheres. In this work, he discussed the structure of the honeycomb and, when trying to figure out why snowflakes have hexagonal shapes, he considered the question in three dimensions. This contrasts with Descartes, who, when discussing snowflakes a quarter of a century later, considered them only in a plane [10].

In *De Nive Sexangula* [9], Kepler realized that external shape is correlated with internal structure. The external polyhedral shape grows naturally because of the internal regular arrangements of the building elements. In contrast, a symmetrical polyhedral shape does not necessarily mean an ordered internal structure. This is obvious today, yet even some widely used introductory chemistry texts state that crystals and amorphous bodies differ in their shapes: it is easy to cut a piece of glass to look perfect, but it will still remain amorphous. Alan L. Mackay called our attention to the importance of this knowledge for the courtesans in sixth-century India, according to the *Kama Sutra* by Vatsyayana [11]. They had to learn mineralogy as they were often paid in precious stones. They had to be able to distinguish genuine crystals from paste.

Kepler felt the excitement of discovery when looking at snowflakes in cold, dry weather. They were all hexagonal in their full shape and symmetry, but they came in a great variety, and no two looked the same. As he was considering the origin of these perfect shapes, he concluded that the uniform arrangement of their elemental building particles must be the reason for these shapes. These building

particles were water molecules, but of course, he could not know this. However, he correctly assigned the formation of shapes to very dense internal packing. Furthermore, he correctly described cubic closest packing, hexagonal packing and simple cubic packing. He could not explain why the snowflakes have sixfold symmetry but conjectured that hexagonal packing would provide the maximal close packing. Thomas C. Hales referred to Kepler's conjecture as "No packing of congruent balls in Euclidean three-space has a density greater than that of the face-centered cubic packing". Hales published his proof of Kepler's conjecture in 2005 in the *Annals of Mathematics* [12] and dedicated his work to the memory of the Hungarian geometer László Fejes Tóth.



Statue of Sir Walter Raleigh by William McMillan in Greenwich (photograph by the Hargittais) [13] and portrait of Thomas Harriot, 1602, by an unidentified painter from the collection of the University of Oxford (in the public domain; file: ThomasHarriot.jpg - Wikimedia Commons).

Kepler's discovery is considered a foundation of modern crystallography, though he may not have been the first to recognize how the densest packing of congruent spheres is accomplished. As often happens in science, there was another person, Thomas Harriot (*ca* 1560−1621), who, in England in 1599, came up with a similar observation of the arrangement of densest packing. He was an astronomer, mathematician and ethnographer; he improved navigational techniques and created advanced maps and participated in expeditions. He was the scientific advisor on one of Sir Walter Raleigh's (1552 or 1554−1618) expeditions around 1587. Raleigh posed Harriot the question about the most economical means of storing cannon balls in his ship. This was thus a question about the densest packing of equal-size spheres. Both the question poser and the one who responded deserve our note. Harriot corresponded with Kepler about optics, but there is no information on whether their exchange contained any reference to densest packing.

Kepler's treatise inspired Alan L. Mackay to respond in 1981, 370 years later, with his paper *De nive quinquangular* [14]. Mackay predicted then what were later to be called 'quasicrystals'. For a beautiful computer-automated drawing of a 'Pentagonal snow crystal' by Robert H. Mackay in 1975, see [15]. Philip Ball celebrated the fourth centenary of Kepler's publication about the six-cornered snowflake with an essay in *Nature* [16]. There and elsewhere, see for example [17, 18], are presented the attempts over centuries to understand and explain the hexagonal shapes of snowflakes. Shafranovskii called attention to Kepler's attempt to create a pattern of fivefold symmetry [19].

Kepler graduated as a theologian, but his first position, at the age of 20, was as a teacher of mathematics and astronomy in Graz, Austria. He was unhappy with this job and found an escape in thinking about Copernicus' new ideas concerning the solar system, the six planets and their distances from the Sun. Then, while drawing some figures on the blackboard, a new idea suddenly came to his mind. It was like a lightning bolt, and he was so shaken that he noted the date when this happened: 9 July 1595. The idea never left him for his entire life. He started with a large circle with a triangle in it and another circle within the triangle. He suddenly realized that the ratio of the two circles was the same as that of the orbits of Saturn and Jupiter, the two outermost planets. He continued inscribing into the next interval between Jupiter and Mars a square, between Mars and Earth a pentagon, and between Earth and Venus a hexagon. He calculated the ratios of the radii of the subsequent circles and compared them with the results of Copernicus. He was soon disappointed because they did not match. At that point came yet another lightning bolt, the realization that he should expand his considerations into the third dimension, just as the planets exist in three dimensions, in space rather than merely in the plane. So, he used spheres rather than circles and polyhedra rather than polygons.



Kepler's planetary model based on regular solids [20], and a Hungarian postage stamp with Kepler's portrait and his model.

The five regular polyhedra of Plato were the perfect solution, matching the six planets that were known at the time. Except for the orbits of Saturn and Mercury, his results mostly agreed with those of Copernicus. To eliminate the discrepancies, he gave some thickness to his orbits, and this approach improved the agreement. This is also how he arrived at the great discovery of the elliptical orbits of the planets. Kepler wrote a small book, *Mysterium Cosmographicum* [20]. This was in 1597, when he was 26 years old. This book already contains the seeds of all of Kepler's later discoveries. It also shows him as a modern scientist who knew that his model could be right only if it were consistent with observation. It was in this connection that he introduced the concept of observational error. Later in his life, when he realized that his model still had problems, he extended his considerations to general harmonies. He augmented his geometrical model with the principles of harmony. By doing this, he returned to ancient notions, which was a retreat, but he had no other recourse, as at the time, there was no other recourse. Kepler expressed the complementary nature of geometry and harmony in his *Harmonices Mundi* (1619) [21].

Kepler's planetary model was incorrect. Some considered it childish. Others recognized its fertility for a host of other scientific endeavors. This was not a unique case in science history when an incorrect model paved the way to correct results. Aaron Klug quoted the philosopher A. N. Whitehead, who co-authored *Principia Mathematica* with Bertrand Russell: "It is more important that an idea be fruitful than that it be correct." When Klug compiled his Nobel lecture for publication, he included a picture representing his

original idea of nucleation, which turned out to be erroneous. Klug wanted to include it because it showed how science was a *process* of establishing the truth (emphasis by Klug) [22]. Klug's notion reflected what Kepler himself noted: "The roads by which men arrive at their insights into celestial matters seem to me as worthy of wonder as those matters in themselves" [23].

In conclusion, let us quote Koestler concerning this matter ([6], p. 61):

"That some of his answers were not right does not matter. As in the case of Ionian philosophers of the heroic age, the philosophers of the Renaissance were perhaps more remarkable for the revolutionary nature of the questions they asked than for the answers they proposed. Paracelsus and Bruno, Gilbert and Tycho, Kepler and Galileo formulated some answers that are still valid; but first and foremost, they were giant question masters. *Post factum*, however, it is always difficult to appreciate the originality and imagination it required to ask a question which had not been asked before. In this respect, too, Kepler holds the record."

References

[1] Holton, G. (1973). *Thematic Origins of Scientific Thoughts: Kepler to Einstein*, p. 89. Cambridge, MA: Harvard University Press.
[2] Small, R. (1963). *An Account of the Astronomical Discoveries of Kepler*, a reprint of the 1804 text, with a foreword by W. D. Stahlman. Madison: The University of Wisconsin Press.
[3] Brewster, D. (1847). "Life of John Kepler". In *The Martyrs of Science Or, The lives of Galileo, Tycho Brahe, and Kepler*, pp. 187−240. New York: Harper & Brothers.
[4] Caspar, M. (1959). *Kepler*, translated and edited by C. D. Hellman. New York: Abelard-Schuman Ltd.
[5] Koestler, A. (1959). *The Sleepwalkers*. London: Hutchinson and Co.
[6] Koestler, A. (1960). *The Watershed: A Biography of Johannes Kepler.* Garden City, NY: Doubleday and Co.
[7] Lima-de-Faria, J. (1990). Editor. *Historical Atlas of Crystallography*. Dordrecht: Kluwer Academic Publishers.
[8] Hargittai, I. & Hargittai, M. (2000). *In Our Own Image: Personal Symmetry in Discovery*, ch. 3, pp. 26−51. New York: Kluwer Academic/Plenum.
[9] Kepler, J. (1966). *De Nive Sexangula*. English translation: *The Six-Cornered Snowflake*. Oxford: Clarendon Press.
[10] Descartes, R. (1637). *Discours VI*, *Les Meteores*, Leiden; cited in J. V. Field (1988). *Kepler's Geometrical Cosmology*, p. 173. University of Chicago Press.
[11] Vatsyayana (1963). *Kama Sutra: The Hindu Ritual of Love*, p. 14. New York: Castle Books.
[12] Hales, T. C. (2005). "A proof of the Kepler conjecture", *Ann. Math.* **162**, 1065–1185.
[13] Hargittai, I. & Hargittai, M. (2021). *Science in London: A Guide to Memorials*, p. 34. Springer Nature.
[14] Mackay, A. L. (1981). "De Nive Quinquangula: On the Pentagonal Snowflake", *Sov. Phys. Crystallogr.* **26**, 517–522.
[15] Hargittai, I. & Hargittai, B. (2020). "Penrose–Mackay–Shechtman and bringing down the dogma about fivefold symmetry", *IUCr Newsletter*, Vol. 28, No. 4.
[16] Ball, P. (2011). "On the Six-Cornered Snowflake", *Nature*, **480**, 455.
[17] Hargittai, M. & Hargittai, I. (2009; 2010). *Symmetry through the Eyes of a Chemist*, 3rd ed., pp. 40−53. Springer.
[18] Danzer, L., Grünbaum, B. & Shephard, G. C. (1982). "Can All Tiles of a Tiling Have Five-fold Symmetry?", *Am. Math. Mon.* **89**, 568–585.
[19] Shafranovskii, I. I. (1975). "Kepler's Crystallographic Ideas and His Tract *The Six-Cornered Snowflake*". In Beer, A. & Beer, P. (Editors), *Kepler, Four Hundred Years, Vistas in Astronomy*, Vol. 18, pp. 861−876. Oxford; New York: Pergamon Press.
[20] Kepler, J. (1981). *Mysterium Cosmographicum (The Secret of the Universe)*, translated by A. M. Duncan. New York: Abaris Books.
[21] Kepler, J. (1997). *The Harmony of the World*, translated into English with an introduction and notes by E. J. Aiton, A. M. Duncan and J. V. Field, *Memoirs of the American Philosophical Society*, Vol. 209, p. 490. Philadelphia, PA: American Philosophical Society.
[22] Hargittai, I. (2002). *Candid Science II: Conversations with Famous Biomedical Scientists*, edited by M. Hargittai, ch. 20, pp. 306−329 (the actual reference is made to the top of p. 313). London: Imperial College Press.
[23] Kepler, J. (1609). *Astronomia Nova*, summary of ch. 45, cited in *The Watershed*, p. 59 (which served as our source for this quote).

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REGIONAL NEWS

Recent news from the European Crystallographic Association



In early February 2024, the ECA's Executive Committee had the chance to visit the Poznań Congress Center, where ECM35 is envisioned to be held, and to speak not only with the main local organisers Grygoriy Dmytriv (second from right) and Maciej Kubicki (fourth from right) but also with people from Adam Mickiewicz University (AMU), the Professional Congress Organisation (AMU Foundation) and the Poznań Convention Bureau.

Arie van der Lee

European crystallographers usually hold their Crystallographic Meeting (ECM) in Europe in years when the IUCr does not organise its triennial congress. 2023 was such a year without an ECM when the worldwide crystallographic community, including Europe, gathered in Melbourne, Australia. The ECA Council meeting was held remotely in two different sessions, on 20 and 22 September 2023, to ensure as high an attendance as possible. Meetings of the Executive Committee were organised remotely just before the Council Meeting on 11 and 12 September 2023, and in Poznań, Poland, from 2 to 4 February 2024.

A considerable part of the business at the ECA Council Meetings naturally concerns the planning of future ECMs and European Crystallographic Schools (ECSs), and Councillors receive progress updates on the planning of upcoming meetings as well as the opportunity to vote for the location of future ECMs and ECSs. Due to the ongoing conflict in Ukraine, where ECM35 was due to be held in 2025, a proposal was made by the Polish Crystallographic Association in collaboration with ECM35 organisers and other Ukrainian colleagues, to move the location of the conference to Poznań, which the Council approved. A bid from Czech colleagues to hold ECM36 in Prague (at the same location as the 25th IUCr Congress in 2021) was also presented and approved.

The Prizes awarded by the ECA were also discussed in detail. The oldest Prize is the Max Perutz Prize, which is awarded in recognition of meritorious achievements in any branch of crystallography, and the Erwin Félix Lewy Bertaut Prize, which is awarded jointly with the European Neutron Scattering Association to a young scientist in recognition of notable experimental, methodological or theoretical contributions to the investigation of matter using crystallographic or neutron scattering methods. The Alajos Kálmán Prize was created more recently and is awarded jointly with the Hungarian Chemical Society in recognition of outstanding scientific contributions in the field of structural sciences. At the Council meeting in September, proposals were heard and approved for the incorporation of two new prizes related to the ECA: the George M. Sheldrick Prize (awarded to a non-tenured researcher for outstanding scientific contributions in the field of structural sciences) and the Lodovico Riva de Sanseverino Prize (awarded in

recognition of notable contributions to the dissemination of crystallography in the field of education at all levels). More information is available here. All five prizes will be awarded this year at ECM34 in Padova, Italy, in August.

Finally, of interest to younger members of the crystallographic community, the ECA Council heard the report on ECS8, which took place in person in Berlin, Germany, in June 2023. ECSs combine lectures and hands-on tutorials to provide attendees with a fundamental understanding of the principles underpinning crystallography. Each school is unique, however, and offers a variety of topics to cater to a broad range of interests. ECS9 will take place in 2024 in Nancy, France, and a successful bid takes ECS10 to Ohrid, North Macedonia, in 2025. For further information about the ECS, please go here.



Group photo of ECS8 held in Berlin (June 2023). Photo contributed by Manfred Weiss.

The ECA finances were discussed extensively: it was decided to increase the part of the budget allocated to support schools, workshops and congresses, in particular for the ECA's own ECSs.

The ECA's General Interest Group 3 (GIG-03: Education in Crystallography) received a grant from the Royal Society of Chemistry (£5k), for the preparation and dissemination of a series of ten video interviews to celebrate the importance of women in the field of crystallography and science, while, at the same time, raising awareness about the pitfalls and obstacles on the way to reach gender parity in science. The first video will be launched in June 2024. GIG-03 is also preparing a Crystallography Video Competition (using a grant obtained from the Cambridge Crystallographic Data Centre) for schools in different European countries. The aim is to present the winning videos at ECM34.

European crystallographers continue to meet during the ECA's monthly lunchtime webinars, a successful series of online seminars covering all sub-disciplines in crystallography and organised by the ECA's young crystallographers. Eight lunchtime webinars took place from April 2023 until March 2024. Another series of webinars, the *Distinguished Lectures on Quantum Crystallography and Complementary Fields*, initiated by the ECA's Special Interest Group 2 (SIG-02: Quantum Crystallography) and the IUCr Commission on Quantum Crystallography continued as well: eight webinars took place, usually with two lectures during the same webinar.

MEETING REPORT

80th Annual Pittsburgh Diffraction Conference



Simone Brixius-Anderko, Uta Ruett, Matthias Zeller

The 80th Annual Pittsburgh Diffraction Conference took place from 15 to 17 October 2023 at the Wyndham Hotel situated on Pittsburgh's Oakland Campus, PA, USA. Nestled amidst the University of Pittsburgh and Carnegie Mellon University, Schenley Park, Phipps Conservatory and Botanical Gardens, and the Carnegie Museums of Art and Natural History, this location provided an excellent setting for this event.

The Pittsburgh Diffraction Society (PDS) is a non-profit organization dedicated to advancing fundamental and applied diffraction and crystallographic research, and fostering the exchange of ideas and information. The PDS was founded by Surain S. Sidhu, who organized the first Pittsburgh Diffraction Conference at the University of Pittsburgh 80 years ago in 1943.

The 2023 conference was attended by 127 registered participants, and featured 48 oral presentations and 20 poster presentations in sessions focused on all areas of diffraction, from applied science to protein crystallography. The conference was chaired by Simone Brixius-Anderko (University of Pittsburgh), who was supported by a team of over 16 organizers and session chairs from all over the country.

Preceding the main conference, a workshop on *Phenix*, which is a comprehensive software package for macromolecular structure determination, gathered 20 attendees led by the experts Dorothee Liebschner (LBNL), Tom Terwilliger (New Mexico Consortium), Pavel Afonine (LBNL) and Christopher Williams (Duke University).

The conference commenced with an opening reception on 15 October, followed by keynote lectures delivered by two former winners of the PDS Sidhu Award, which is given to outstanding scientists within six years of earning a PhD or equivalent. Erica Ollmann Saphire (the 2003 Sidhu awardee, now the head of the La Jolla Institute for Immunology) presented on the role of diffraction and CryoEM in fighting diseases in her talk "Antibodies against Emerging Infections: a Global Collaboration". Chong-Yu Ruan, awarded the Sidhu prize in 2005, reviewed recent developments in ultrafast electron diffraction in his talk on "Femtosecond Electron Crystallography and Microscopy: Recent Advances and Applications". The keynote lectures were followed by a Young Investigator Platform that allowed the upcoming researchers Tyra Douglas (ANL), Jordan Kelly (Duquesne), Vanessa Moresco (UC Riverside), Ari Selzer (Pitt), Sylwia Pawledzio (ORNL) and Giancarlo Gonzalez-Areizaga (Pitt), selected from student and postdoc poster submissions, to present their projects and findings in short presentations.

In the spirit of the 80th jubilee of the Pittsburgh Diffraction Conference were the closing sessions of the first day, provided by William Furey (Pitt) and John P. Rose (University of Georgia), with recollections from 46 years of Pittsburgh Diffraction Conferences, opening the birthday party, reception and cake, which was generously sponsored by Rigaku. The following karaoke session brought out sides of people very few expected.



William Furey (Pitt, right) and John P. Rose (University of Georgia), who gave the two presentations on the history of the Pittsburgh Diffraction Conference, with the 80th anniversary birthday cake.

The following day started with a keynote session presented by Andrew Kruse of Harvard ("Structural Basis for Antibody Fragment Modulation of a G Protein-Coupled Receptor"), after which the conference continued with two parallel sessions covering both physical and life sciences (also known as 'structural biology'). The structural biology section featured sessions on "Structure-Based Drug Design", "Synergy of Computation and Crystallography for Structural Biology" and "Crystallography meets CryoEM". The Physical Sciences sessions covered "Latest Developments at Light Sources", "Spins, Phonons, and Disordered States in Complex Materials" and "Investigating Materials' Structures and Properties using X-ray Diffraction Microscopy". Short presentations by vendors and sponsors, and poster sessions and presentations complemented the sessions, and the day ended with the traditional Banquet Dinner and some fun activities.

A keynote lecture by Daniel Shoemaker (UIUC) titled "Inorganic Quantum Crystallography: Discovering Materials in the Computer and in the Lab" started sessions on the 17th, followed again by parallel sessions covering "Structure-Property Relationships in Quantum and Layered Materials" and "Materials under High Pressure – Using Diffraction Techniques to Understand Synthesis Pathways, Phase Transitions and Phase Behaviors" for the Physical Sciences, and "High Pressure in Macromolecular Crystallography" and "General Interest and Cool Techniques" on the bio-side of crystallography. Short vendor presentations and more opportunities to meet at posters and talk to vendors enabled inspiring discussions. Cora Lind-Kovacs delivered a presentation on behalf of the American Association to Advance

Powder Diffraction (AAAPD), outlining preliminary results that compared worldwide high-resolution powder diffraction at user facilities. The presentation raised concerns regarding the competitiveness of the user facilities within the United States.



The karaoke session. From left to right: James Weng (ANL), Alexis Paskach (University of Alabama, Huntsville), Tyra Douglas (ANL) and Stephany Webb (Pitt). In the front (back to audience) is Cora Lind-Kovacs (Toledo) taking a break from 'singing'.

The meeting was concluded by the Society's business meeting. The Chung Soo Yoo poster awards, established by the PDS in his honor, were given to the graduate students who presented the best posters at the conference: Michael P. Dalton (Stony Brook University) and Jordan Kelly (Duquesne). Simone Brixius-Anderko gave a summary of the conference and announced the winners of the vendor raffle, and Matthias Zeller gave an overview of the Society's finances in the Treasurer's report. Elections for positions on the PDS board were announced, and candidates for the offices of Treasurer and Secretary, as well as for Chair-Elect for 2025, were asked to come forward. The President of the PDS, Uta Ruett (ANL), asked for nominations for next year's Sidhu Award and for future hosts for the upcoming conferences. The business meeting was closed by next President-Elect Jeney Wierman, who invited the attendees to next year's Annual Pittsburgh Diffraction Conference at CHESS on the Cornell Campus in upstate New York, in October 2024. Please see the PDS website for upcoming details.

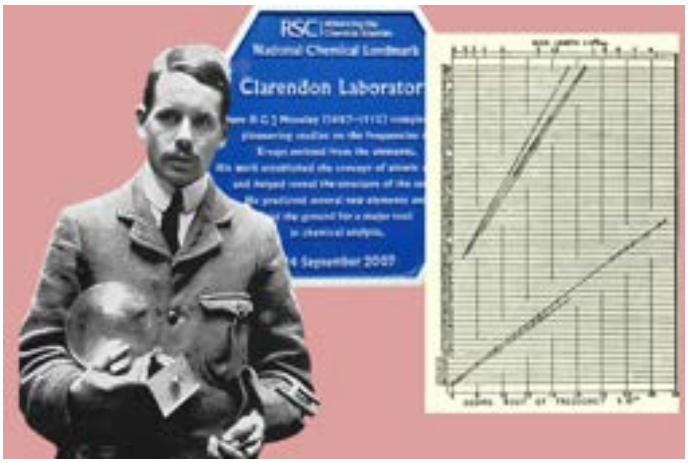


Eric Reinheimer (left) and Joe Ferrara (both from Rigaku), also with the 80th anniversary birthday cake (which Rigaku sponsored).

We would like to thank all our sponsors and exhibitors: University of Pittsburgh School of Pharmacy, Argonne National Laboratory, MiTeGen, Art Robbins Instruments, Formulatrix, Crystal Positioning Systems, Rigaku Americas, Dectris, Anton Paar and STP Labtech, without whose support the conference would not have been possible. A special thanks also goes to Burroughs Wellcome Fund, which granted generously a proposal sent in by Denise Okafor (Penn State University) requesting travel support for selected attending students, postdocs and early career scientists for the conference.

HISTORY OF CRYSTALLOGRAPHY

A curious poem



Mike Glazer

Recently, a friend of mine in India came across a strange poem originally published in the *Journal of Chemical Education* in 1925, having noted that it seemed to have some relevance to crystals and, in particular, to the name Moseley. This immediately struck me as interesting, especially as Moseley's name has a special connection with Trinity College at the University of Oxford and the Clarendon Laboratory, UK. So who was this chap, Moseley?

Well, he was Henry Gwyn Jeffreys Moseley, known usually as Harry Moseley. And his claim to fame, especially in the field of crystallography, was indeed profound. He graduated from Oxford in 1910, spent some time in Manchester with Ernest Rutherford and then returned to Oxford to carry out his research in 1913.

Now, it is important to recall that, at the beginning of the 20th century, one of the outstanding questions that needed settling had to do with the nature of X-rays (originally discovered in 1895 by Wilhelm Roentgen). The burning question for physicists then was: are X-rays particles or are they waves? Most scientists believed the wave theory, but some, including William Henry Bragg (WHB), thought they consisted of neutral particles. Then, in April 1912, an important experiment was carried out at the suggestion of Max Laue, a Privatdozent at the Institute of Theoretical Physics in Munich, but without the agreement of Arnold Sommerfeld, the head of the institute. The actual experiment was carried out in secret[1] one night by Walter Friedrich, an assistant of Sommerfeld, and Paul Knipping, a student of Roentgen. The experiment consisted of shining a beam of X-rays onto a crystal and then recording the scattering of the X-rays on photographic film. After several failed attempts, they finally obtained photographs that indicated that the X-rays were deviated by the crystal and even formed sharp spots on the film. This seemed to demonstrate that the X-rays had been diffracted by the atoms in the crystal, thus proving that X-rays were wave-like. Laue, later ennobled as von Laue, received the Nobel Prize in Physics in 1914. Although Friedrich and Knipping did not share the prize, Laue divided up the prize money between them. You can read Laue's amusing account of the experiment here.

In the summer of 1912, word of this important experiment reached WHB, then Professor of Physics at the University of Leeds. He then set about trying to show that he could explain the effect with his particle theory. His son, William Lawrence Bragg (WLB), had just graduated from Cambridge University, and he joined his father in conducting experiments to demonstrate the viability of the particle theory. The experiments all failed, but in August that year, WLB, while back in Cambridge, suddenly realised that Laue's results actually supported wave theory rather than his father's corpuscular theory.[2] WLB's theory was remarkably simple as it drew upon well known theories of the reflection and scattering of light.



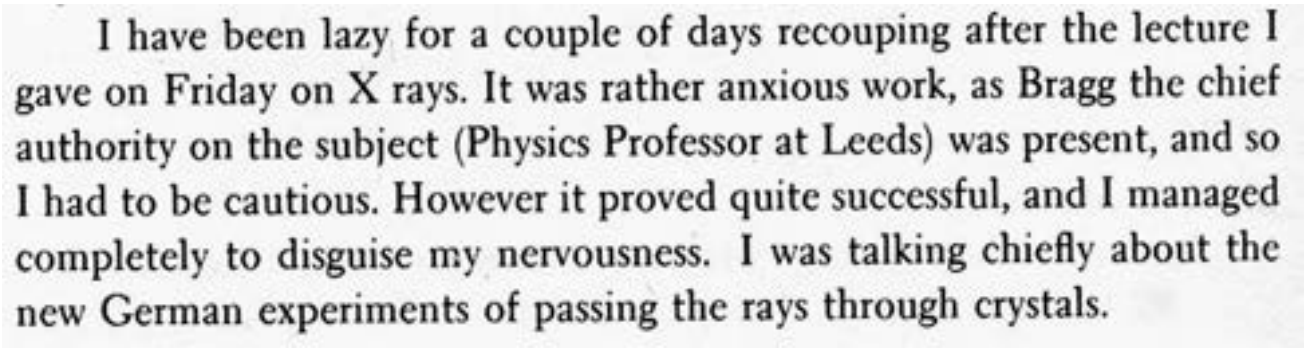
WLB's 1912 notebook showing the first statement (near the top) of what was later to be called Bragg's law (courtesy of the Royal Institution).

From this, WLB produced the equation that later, after modification, became known as Bragg's law. This took the form of a cosine function, where the angle q referred to the angle of incidence of X-rays on planes of atoms in the crystal. In this formula, l is the X-ray wavelength and *d* is the distance between the planes. Whenever this equation was satisfied for all three terms l, *d* and q simultaneously, the scattered X-ray left a spot on the film. WLB was able to show that it was possible to use this to derive information about the structures of crystals, and that he could explain all the spots seen on the Laue diagrams as arising from diffracted X-rays with different wavelengths and from different planes within the crystal. He wrote a paper on this discovery that was read by J. J. Thomson on 11 November 1912 at the Cambridge Philosophical Society. Following this, he worked closely with his father to show how to solve crystal structures in numerous materials throughout 1913 and 1914 until all research was interrupted by the First World War. In 1913, WLB made use both of Laue's film method and of WHB's recently developed ionization spectrometer. The spectrometer gave more precise measurements than the film method (by the way, WHB's ionization spectrometer can be seen as the forerunner of the automatic diffractometers universally used today in crystallographic research). I suggest that it was the use of WHB's spectrometer that led in 1913 to changing Bragg's formula to the more familiar sinusoidal function that we use now

$\lambda = 2d\sin\theta$.

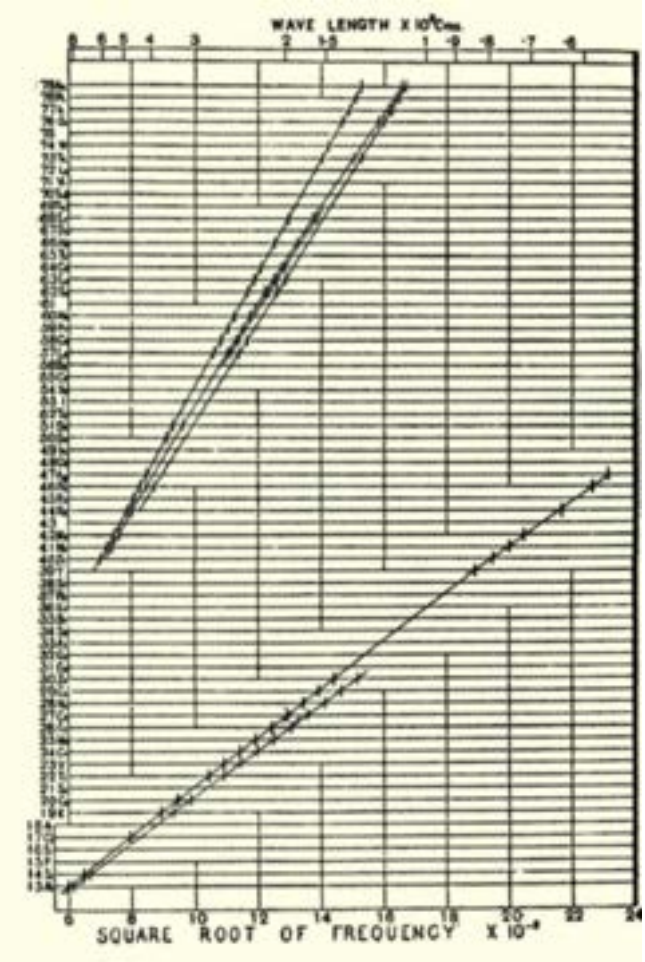
This is because it is more natural when using a spectrometer to measure angles from the incident beam direction, thus 90° minus WLB's original angle q. Both father and son shared the 1915 Nobel Prize in Physics during the war.

Now, this is where Harry Moseley comes into the story. At the time, Harry was working in Manchester under Rutherford and one day gave a talk to explain the Laue experiment.


I have been lazy for a couple of days recouping after the lecture I gave on Friday on X rays. It was rather anxious work, as Bragg the chief authority on the subject (Physics Professor at Leeds) was present, and so I had to be cautious. However it proved quite successful, and I managed completely to disguise my nervousness. I was talking chiefly about the new German experiments of passing the rays through crystals.

Letter from Moseley to his mother, 4 November 1912.

WHB was present at the talk and afterwards told Harry that his son, WLB, had also developed similar ideas. However, as far as I know, Harry's talk was not recorded, so we do not know if he had been able to gain as much insight as WLB. Harry later said that he was confused by crystal structures and that WLB had gone further. WHB was initially more interested in studying the characteristics of X-rays rather than pursuing crystallography, but after a difficult discussion with Rutherford, he reluctantly agreed to leave this field to Moseley and, instead, to concentrate on crystallographic research. WHB then magnanimously offered to help Moseley by explaining the tricks he had developed from his experience in using the spectrometer. At the time, it was not known for sure what the wavelength distribution of X-rays was and that it contained both a broad white component (a continuum of wavelengths) and sharp characteristic lines. In using the spectrometer, it was essential to change the detector angles through very fine steps to avoid missing the sharp lines. Moseley was able to measure the frequencies of the characteristic lines of X-rays for a number of elements, discovering that the square root of the frequency was proportional to the atomic number (the number of protons in the atom). If you ever visit Oxford, you can see his original diagram in the Clarendon Laboratory. This discovery was important because it established the importance of the atomic number and supported the concept of the periodic table, earlier proposed by Dmitri Ivanovich Mendeleev in Russia. It also enabled Harry to fill in some of the gaps in the list of elements in the then known periodic table (see the gaps at atomic numbers 43, 61 and 75).



Moseley's graph for the *K* and *L* lines, Clarendon Laboratory, Oxford.

Moseley had a prestigious talent and was almost certainly destined for a Nobel Prize. However, with the outbreak of the world war in 1914, research ended. Harry decided to show his patriotic duty by enlisting in the army, despite entreaties against this by his family. Calamity struck on the morning of 10 August 1915 during the botched battle of Gallipoli when 30,000 Turks, 'calling upon the name of God', streamed down a hill towards the British lines. According to General Sir Ian Hamilton:

...our men stood to it, and maintained, by many a deed of daring, the old traditions of their race. There was no flinching. They died in their ranks where they stood.[3]

Thus ended the life of a promising young man.

Coincidentally, WHB's other son, Robert, was also wounded at Gallipoli on 1 September 1915 and died from his wounds the next day. The effect on WHB and his wife was devastating, something neither of them ever overcame. After the war, in 1920, WHB and WLB were invited to Stockholm for the Nobel Prize ceremony. But WHB refused to go because "there will be Germans there!" His son also did not attend, presumably because of his father's influence, but he did go in 1922.

So, finally, we now come to the poem. Here it is.

Ballad of Ryerson

Reprinted with permission from Edwin H. Lewis (1925). *J. Chem. Educ.* **2**, 610. Copyright 1925 American Chemical Society.

Lo, Paris and Cambridge and Ryerson were needed to make one thought

Till on the final droplet-star, the massiest, tiniest sphere,

The moon-grain lingered a moment and told the secret here.

Now take the charge and the crystal! Young heroes, unlock the lead,

And kindle a rose for mother ere the rose of her hearth be dead.

O planet, ridged with Calvaries and rimmed with Suvla Bays,[4]

Not all your nights are reined with fire, not all of your lightning slays,

Then why have you slain your darlings? And why did your heart disclose

Fury and flame and the flash of lead when your dearest brought you a rose?

Ah, the rose! The expectancy and the rose!

The beat of the harp is broken, the heart of the gleeman is fain

To call him back from the grave and rebuild the shattered brain

Of Moseley dead in the trenches, Harry Moseley dead by the sea,

Balder slain by the blindman there in Gallipoli.

No longer the towers of Oxford whisper the middle age,

But the dearest of hopes destroyed and the great unwritten page.

No longer the Trinity meadows bloom as in other days

But the sunlight dreams of violets beyond the violet rays.

Beyond the violet seek him, for there in the dark he dwells,

Holding the crystal lattice to cast the shadow that tells

How the heart of the atom thickens, ready to burst into flower,

Loosing the bands of Orion with heavenly heat and power.

He numbers the charge on the center for each of the elements

That we named for gods and demons, colors and tastes and scents,

And he hears the hum of the lead that burned through his brain like fire

Change to the hum of an engine, the song of the sun-grain choir,

As it spins the chaliced lightning to banish shadow and shade,

Or drives the heavy hammers by the sun-grain cannonade,

Or wears the wings of the humming birds that flash through heaven afar,

Or grinds the golden barley by the voltage of a star.

Now, if they slay the dreamers and the riches the dreamers gave,

They shall get them back to the benches and be as the galley slaves.

So, what are we to make of this? The author appears to be Edwin Herbert Lewis (1886–1939), a rhetorician, novelist, poet and professor of English at the Lewis Institute of Chicago. It seems to me that the poem is a lament for a promising life cut short, for it was written 10 years after Moseley's death. Why Lewis wrote it, I don’t know, but I assume the 10th anniversary of the loss of Moseley must have been keenly felt by many at the time. And why the name Ryerson? There is a Ryerson Laboratory in the Physics Department at the University of Chicago, but what is the connection with Moseley?



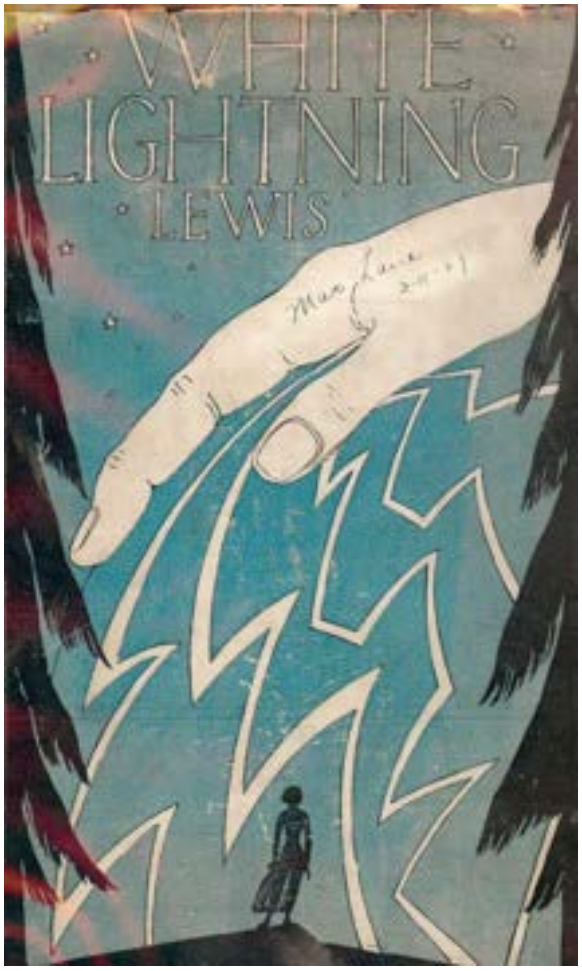
Edwin Herbert Lewis, University of Chicago Photographic Archive (apf1-03859), Hanna Holborn Gray Special Collections Research Center, University of Chicago Library.

I see that in his book *White Lightning*, published in 1923, Moseley is mentioned thus:

And it was in Jimmy's house in June of 1914 that Marvin picked up the Phil. Mag. and read the most important article he had ever read in his life. The author was quite unknown to him – one of Rutherford's men who signed himself H. G. J. Moseley. This man was reporting some measurements that he had made by the use of crystal gratings and short rays. He asserted that the method gave a spectrum of two dark lines for each element, and that the frequency of vibration increased definitely, step by step.

Marvin laid down the magazine and reflected. This unknown Moseley had found it – a sure way to determine the amount of electricity concealed in the heart of any atom. In ten years chemistry would be a new science. In much less than that time every chemical element would receive a number indicating the charge on the nucleus.

Moseley had already numbered some thirty elements, beginning with aluminum as 13, and calculating gold at 79.



Note Max Laue written on image of the hand.

So, if anyone out there can fill in more details and throw more light on the reasons for this poem, please let me know.

Addendum: Many years ago (as mentioned in my Editorial), I went into the office of one of our secretaries and noticed a cardboard box in the corner behind the door. I also saw that every time someone entered the room, the door was slammed against the box. I looked inside the box, and there was one of Moseley's original X-ray tubes, very similar to the one seen being held by Moseley in the image at the beginning of this article. Miraculously, despite its fragility, it had survived despite its rough treatment. It can now be seen in the small museum of the Clarendon Laboratory.

Notes

1 Probably because Laue's idea for the experiment was not agreed upon by Sommerfeld.

2 In fact, WHB was well ahead of his time because later in the 1920s, quantum theory showed that both the wave and the particle theories applied to X-rays.

3 Quoted from *Prof: The Life of Frederick Lindeman*, by Adrian Fort, published in 2003 by Jonathan Cape (Random House).

4 The landing in 1915 at Suvla Bay was an amphibious landing made at Suvla on the Aegean coast of the Gallipoli peninsula in the Ottoman Empire as part of the August Offensive.

HISTORY OF CRYSTALLOGRAPHY

Remembering Vladimir Koptsik, a theoretician of crystallography and co-author of a famous symmetry book, on his centennial

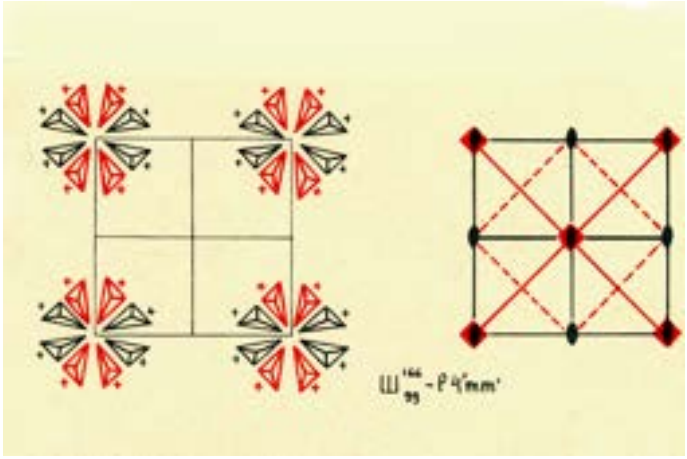


Image from Koptsik's famous book on color symmetry (Шубниковские группы, published by Moscow University in 1966).

Istvan Hargittai

Vladimir A. Koptsik (1924−2005) was born in Ivanovo, an industrial town and educational and regional administrative center some 250 km north east of Moscow. He attended school in Moscow and completed the ninth grade in June 1941, just as Germany was about to attack the Soviet Union. First, he helped in building anti-tank barriers around Moscow, then, for three years, he worked in the defense industry. While working, he completed his school education and enrolled on the correspondent course of the Faculty of Physics of Moscow State University (MSU). In 1944, he became a full-time student of the Geophysical Department of the Faculty of Geology of MSU. In 1949, he graduated in the Department of Crystallography and Crystal Chemistry, and stayed on for PhD-equivalent graduate studies in the same department. Noted crystallographers, such as G. B. Bokii, A. I. Kitaigorodskii and A. V. Shubnikov, were among his professors, and Shubnikov acted as his mentor. Koptsik defended his candidate of science (PhD equivalent) dissertation in 1953. When MSU expanded hugely and took possession of its new campus on Lenin Hills, Koptsik followed Shubnikov to the Faculty of Physics of MSU and helped his mentor in organizing the new Department of Crystallography and Crystal Physics.



Vladimir Koptsik lecturing in front of Alexei Shubnikov's portrait at the Shubnikov Centennial Meeting, 1987, Moscow, and Vladimir Koptsik at the "Symmetry 2000" meeting in Stockholm, Sweden. Both photographs by Istvan Hargittai.

In 1963, Koptsik acquired the higher degree of Doctor of Science, a prerequisite for professorial appointment, which he soon received. In 1968, he became head of the department, by now called the Department of Crystal Physics. His principal research activities covered theoretical crystal physics, theory and applications of color symmetry, structural phase transitions and theory of real crystals. He authored and co-authored about 300 publications of original research. He is, however, best known for his co-authorship, with Shubnikov, of the monograph *Symmetry in Science and Art*, whose Russian original appeared in 1972 [1]. This is also how I came across his name in my symmetry studies and especially while working on the monograph *Symmetry through the Eyes of a Chemist* [2]. It was indeed our shared interest in symmetry that initiated our interactions.

Koptsik remained active in research of the theoretical aspects of crystallography throughout his career. He published monographs, had 27 pupils that earned the PhD-equivalent candidate of science degree, and creatively contributed to the efforts of the crystallography community both at domestic and international levels, among others, as a member of the IUCr Commission on International Tables from 1963 to 1983. I met Koptsik in person for the first time in 1987 during a conference in Moscow celebrating the 100th anniversary of Shubnikov's birth. His contribution was a panoramic review about generalized symmetry in crystal physics [3]. Our second meeting happened at the "Symmetry 2000" conference where he was one of the invited speakers. Characteristic of his broad interests, Koptsik's presentation at the Stockholm meeting was about symmetry compositions in the great Russian poet Alexander Pushkin's works [4].

References and literature

[1] Shubnikov, A. V. & Koptsik, V. A. (1974). *Symmetry in Science and Art*. New York: Plenum Press. [Russian original: Симметрия в науке и исскустве. (1972). Moskva: Nauka. This monograph is a substantially expanded version of Shubnikov's original volume: Симметрия (Закони симметрии и их применение в науке, технике и прикладном исскустве). The title in English translation: *Symmetry (Principles of Symmetry and their Applications in Science, Technology and Applied Art)* (1940). Moskva-Leningrad: Izd AN SSSR.]

[2] Hargittai, I. & Hargittai, M. (1986). *Symmetry through the Eyes of a Chemist*. Weinheim: VCH. [Hargittai, M. & Hargittai, I. (2009). *Symmetry through the Eyes of a Chemist.* 3rd ed. Springer.]

[3] Koptsik, V. A. (1988). *Crystal Symmetries: Shubnikov Centennial Papers*, edited by I. Hargittai & B. K. Vainshtein, pp. 407–424. Oxford: Pergamon Press. [To make this project viable, the materials of this book were first published in a journal of the same publisher: *Comput. Math. Appl.* **16**, 351−669; the book retained the pagination of the journal version.]

[4] Koptsik, V. A. (2002). *Symmetry 2000*, Part 2, edited by I. Hargittai & T. C. Laurent, pp. 585–596. London: Portland Press.

AWARDS AND PRIZES

Yvonne Mascarenhas wins Fifth Carolina Bori “Science & Woman” Award



Photo of Yvonne Mascarenhas from an interview by Fabrício Marques published in *Pesquisa FAPESP*. Image credit: Léo Ramos Chaves / Revista Pesquisa FAPESP.

Yvonne Mascarenhas, a pioneering Brazilian crystallographer, has won the Fifth Carolina Bori "Science & Woman” Award in the area of Engineering, Exact and Earth Sciences. The award, a tribute from the Brazilian Society for the Advancement of Science (SBPC) and named after the society's first female president, recognises outstanding Brazilian scientists and future Brazilian scientists of notable talent.

The Award ceremony, which was part of the celebrations of the centenary of Carolina Bori's birth, took place on 6 February 2024 in São Paulo and was broadcast on the SBPC YouTube channel. In the video, Professor Mascarenhas, who was nominated for the award by the Brazilian Association of Crystallography and the Brazilian Societies of Physics and Research in Materials, gives a message of encouragement to young women who wish to pursue a scientific career.

When talking about her work as a professor, Mascarenhas told the SBPC how happy she was to have trained a “reasonable” number of masters and doctors who work in Brazil and around the world, and who helped to found and establish a community in this multidisciplinary area. “This is my immediate and most important contribution to society,” she said.

Reflecting on her career, Professor Mascarenhas said she feels privileged. “I didn’t need to break the famous glass ceiling, because my laboratory was the only one – with support from CNPq (National Council for Scientific and Technological Development) and FAPESP (Fundação de Amparo à Pesquisa do Estado de São Paulo) – of crystallography in Brazil and, as a result, I had to interact with many areas and this interaction opened doors for me. People liked my work and so I progressed in my career very smoothly, without any setbacks and often with the support of other people. Even for administrative positions, such as IFSC Management, I was approached and asked if I would like to take over. But it’s not like that for everyone,” she admitted, recognizing the struggle of many women to pursue a scientific career. “We have had fantastic women. Therefore, I recommend that young women, when making their choices, do so in the best way possible, analyzing their options. And, more than anything, we need to focus, because life, especially for us women, is not peaceful. We cannot give up on starting a family and having children, because this is all part of life. But, if a person wants to have a scientific career, they need to have focus and persistence, even in the face of difficulties”, she concluded.

At the age of 92 Professor Mascarenhas is still active, as a collaborator and retired professor, at the São Carlos Physics Institute (IFSC). See more information about her career here.

This article is an abridged version of "Focus and persistence" published in the 5 February 2024 edition of *JC Notícias*, the electronic edition of SBPC's *Jornal da Ciência*.

AWARDS AND PRIZES

Eminent Polish–American scientist Alexander Wlodawer honored



Alexander Wlodawer.

Mariusz Jaskolski

Our colleague and eminent crystallographer Alexander Wlodawer (National Cancer Institute, Frederick, MD, USA) has been awarded the prestigious Casimir Funk Award by the Kosciuszko Foundation (KF) and the Polish Institute of Arts and Sciences of America (PIASA).

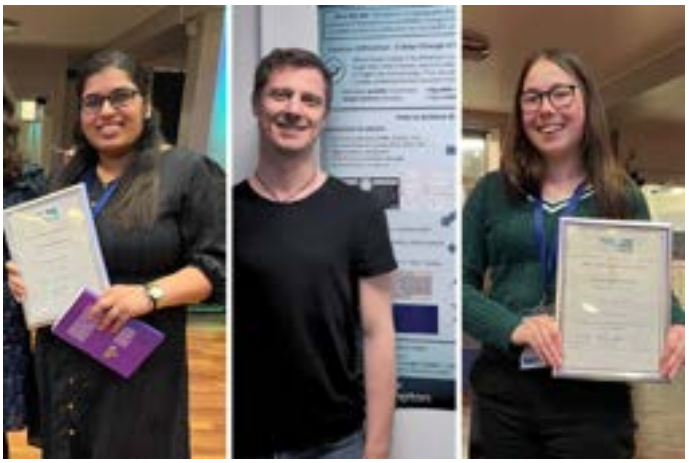
For historical record, Tadeusz Kosciuszko ("pure son of liberty" in the words of his friend, Thomas Jefferson) is a national hero in Poland and the United States. Kazimierz (Casimir) Funk is the discoverer of vitamines (later called vitamins).

The award ceremony and lecture took place on 5 April 2024 in the KF headquarters in New York.

For more information about Dr Wlodawer's lecture “What can structural biology do for human health and the environment?” see here.

AWARDS AND PRIZES

IUCr Journals Poster Prizes at BCA 2024



IUCr Poster Prize Awardees, from left: Shivani Grover (photo courtesy of Claire Hobday), Daniel Rainer and Cicely Tam.

Three IUCr Journals Poster Prizes were awarded at the annual conference of the British Crystallographic Association (BCA), held at the University of Leeds, UK, just before Easter 2024. The judges were looking for the three best posters from an undergraduate, postgraduate or postdoctoral researcher with up to three years' experience in distinct areas of crystallography such as structural biology, structural chemistry and applied crystallography. The judging panel was chaired by Dr Briony Yorke (University of Leeds). The prize winners were as follows, in alphabetical order:

Dr Shivani Grover, a Postdoctoral Research Associate at the University of Edinburgh, UK, whose poster was entitled “Understanding the barocaloric effect in choline based plastic crystals from *ab initio* molecular dynamics”.

Dr Daniel Rainer, Specialist Technician for Electron Diffraction at the National Electron Diffraction Facility, University of Southampton, UK, whose poster was entitled “The National Electron Diffraction Facility – what, where, and how for 3DED now”.

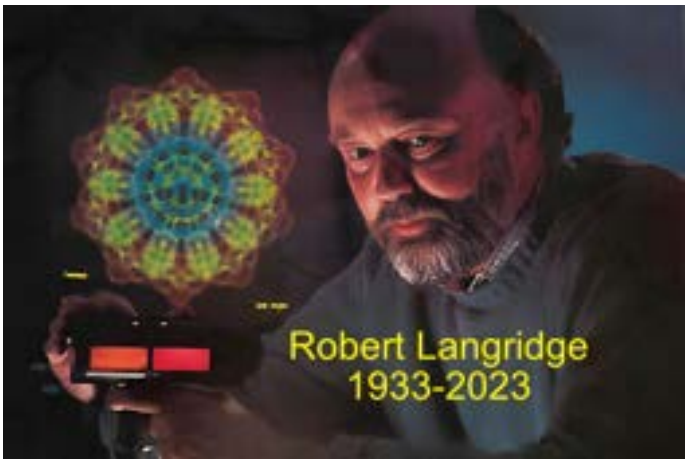
Cicely Tam, an Industrial Placement Student at Diamond Light Source, Didcot, UK, whose poster was entitled “Optimising and automating microcrystallisation methods for serial crystallography”.

The prize comprised a copy each of the IUCr’s *Little Dictionary of Crystallography* 3rd edition, a complimentary three-year membership of the IUCr Associates Programme and a certificate.

The IUCr would like to take this opportunity to thank the previous Chair, Professor John Helliwell, for filling this role so enthusiastically and to Dr Yorke for taking over the task.

OBITUARY

Robert Langridge (1933–2023)



Credit: Christopher Springmann, 1985.

Suzan Revah

Robert Langridge, PhD, professor emeritus in the Department of Pharmaceutical Chemistry, University of California San Francisco (UCSF), CA, USA, and an icon in the field of molecular computer graphics, passed away just a few weeks after his 90th birthday on 11 November 2023.

Langridge was honored in 2018 with the UCSF Medal, the University's highest honor, for ushering in a new era of biological experimentation and drug discovery. He received the award along with Peter Andrew Kollman, PhD, and Irwin "Tack" Kuntz, PhD, in recognition of the group's collaborative spirit and pioneering research in pharmaceutical science and computational chemistry.

In the 1950s, there were two approaches to visualizing molecular interactions: scientists built wire models, sketched them, and did mathematical calculations. In 1956, Langridge obtained access to an IBM 650 computer. Even though the machine had miniscule memory by today's standards, Langridge loved programming and was able to reduce the computation time of his calculations from two weeks to thirty minutes.

Langridge became convinced that computers were here to stay. "Although there are many stories about Bob's work on the beginnings of molecular computer graphics and how he became this amazing pioneer who recognized the potential of computers, he did that despite the scientific community not being very receptive," said his wife Ruth Langridge, MAT, MA, PhD, a researcher at the University of California, Santa Cruz.

Langridge's 1970 grant for a computer graphics lab at Princeton University established one of the first Research Resource Centers created by the National Institutes of Health. In 1976, he was recruited to UCSF, where he founded and directed the computer graphics lab until he retired in 1994. He pushed the field of pharmaceutical chemistry into the computational era – a daunting task in a time of room-sized computers.

"If you want to see with your own eyes the results of Bob's work, pick out any magazine, video or movie dealing with science or with many other features of everyday life," said Professor Emeritus of Pharmaceutical Chemistry Kuntz.

Probing biology at the atomic level

Born in the small English village of Froyle in 1933, Robert Langridge was the first in his family to attend university, receiving his BSc in physics at the University of London with first-class honors in 1954. In 1955, he published his first important paper in *Nature*, detailing the molecular structure of DNA based on X-ray diffraction data.

In 1957, Langridge received his PhD in crystallography from the University of London. His research was guided by Maurice Wilkins, who was studying the structure of DNA using the technique of X-ray diffraction. Wilkins shared the 1962 Nobel Prize with James Watson and Francis Crick for their discovery of the molecular structure of DNA.

As a graduate student, Langridge showed how the Watson and Crick DNA model could be modified to agree with X-ray diffraction studies of DNA. His dissertation on X-ray crystallographic model-building and computational studies of the structure of DNA included the first application of a stored-program digital computer (the IBM 650) to the analysis of DNA structure.



Becoming a computational revolutionary

After coming to the United States in 1957, Langridge worked as a postdoc in biophysics at Yale University and in biology at the Massachusetts Institute of Technology (MIT). In 1961, he set up a lab to study the structures of DNA and viruses at the Children's Cancer Research Foundation in Boston, with faculty appointments at Harvard University and Harvard Medical School. Concurrently, in 1964 he collaborated on the original work in molecular graphics at Project MAC (now the Laboratory for Computer Science) at MIT.

In 1966, Langridge joined the University of Chicago as a professor of biophysics and then moved to Princeton in 1968 as a professor of chemistry and biochemical sciences. He established the first

Computer Graphics Laboratory, the name and concept of which he brought with him to UCSF in the fall of 1976.

"When he came to UCSF from Princeton, he didn't bring any other personnel with him, and he didn't bring any computer hardware with him," said Professor of Pharmaceutical Chemistry Tom Ferrin, PhD, who took over UCSF's Computer Graphics Lab when Langridge retired.

At UCSF, he developed a computer graphics system that produced some of the first pictures of molecular interactions in three dimensions, with the ability to rotate an image on the screen. Among the field's milestones, Ferrin recalled the advent of color graphics as a quantum leap that allowed scientists to identify different chemical components and proteins. "He had to build everything from the ground up, which required a lot of bravery on his part."

"Bob was the son of a gardener who bootstrapped himself up from the ground," added Ferrin, who remembered Langridge as not only a pioneer of molecular computer graphics, but also as an ambassador for the technology. "He had the vision, and he knew that if he was going to realize the vision for his future and make his mark in science, he needed to do that in the United States, which also required a lot of bravery."

The advent of interactivity

The ability to interact with graphic images was the breakthrough that allowed the viewer to gain insight into both molecular structure and function. This resulted from significant effort to develop software that could "meaningfully" display large molecular structures, like DNA and proteins.

"Interactive molecular graphics has always been the key to what we've done at UCSF, which is to make the user part of the graphics system…and allow the user to apply their knowledge and investigate parts of the molecular structure," said Ferrin. "That wouldn't be possible if you're just looking at a drawing or an image on a printed page."

Today's UCSF scientists carry Langridge's legacy forward with computational innovations allowing them to screen millions of potential drugs simultaneously and observe molecular interactions in virtual reality.

"Bob's expertise was in visualization because computations alone just yield columns and columns of numbers. The insight comes from understanding what these computations mean," Ferrin said. "There are countless antecedents along the way, but some brilliant scientists have come to the graphics lab, and they just haven't yet seen the molecules that they're so familiar with in an interactive 3D fashion, and then they'll get some flash of insight from being immersed inside these complex 3D molecules, so it's a very powerful technique."

Inspiration and impact



Langridge's work continues to have an enormous impact on scientific discovery. "He was a giant here at UCSF, and his legacy will be long and fondly remembered," said UCSF Chancellor Sam Hawgood, MBBS.

"Looking back, it seems like Bob was always spreading the word about molecular graphics, and he was the perfect person to do it because he was there from the very beginning," said Ferrin.

Langridge served on the Computer and Biomathematics Research Study Section of the National Institutes of Health (NIH) and the Science and Educational Advisory Committee at Lawrence Berkeley Laboratories. He was a member of the NIH Computer Science & Telecommunications Board of the National Research Council and the NIH Council of the National Center for Research and the council representative on the Advisory Committee to the NIH director.

In 1983, Bob collaborated with Industrial Light & Magic, the motion picture visual effects company founded by George Lucas, and used real-time, interactive graphics of DNA to generate the intro to the "Genesis" segment of Star Trek II. In 1989, he was elected fellow of the American Association for the Advancement of Science and in 1990 to the Institute of Medicine of the National Academy of Sciences. In 2005, he was highlighted by Smithsonian Magazine as an innovator who made a difference.

"Computer graphics has become the paintbrush that colors it all," Kuntz said. "I can't tell you what an honor it was to work with him, day after day, for so long."

Teri Klein, PhD, a faculty member in the Department of Biomedical Data Science at Stanford University, described Bob as an incredible mentor and a wonderful human who "was one of a kind, and I have emulated him throughout my academic career."

"He was my inspiration for our center, in science, in leadership, and in humanity," said Ken A. Dill, PhD, distinguished professor at Laufer Center for Physical & Quantitative Biology at Stony Brook University. "I

am forever grateful for his brilliant and inspiring vision."

Langridge is survived by his wife; three daughters, Elizabeth, Catherine and Suzanne; and five grandchildren.

Suzan Revah is at the UCSF School of Pharmacy.

OBITUARY

Patrick J. McArdle (1945–2024)



Anuradha Pallipurath, Andrea Erxleben

Professor Patrick J. McArdle from the University of Galway, Ireland, passed away unexpectedly but peacefully, at home in Galway, surrounded by his family on 2 January 2024, and was laid to rest in Rahoon Cemetery, Galway, on 5 January 2024.

Pat was a professor of inorganic chemistry with expertise in X-ray crystallography and nuclear magnetic resonance (NMR), and has published over 400 papers on a range of topics, from small-molecule pharmaceuticals and organometallics to carbohydrates. Born and raised in Drogheda, County Louth, Pat's first job was at his family hotel, The White Horse. He pursued his BSc and PhD (1962–1969) from University College Dublin (*Tautomerism in Some Binuclear Metal Carbonyl Derivatives*) and a DSc (1989) from the National University of Ireland Galway (now University of Galway), where he worked until his passing. Pat was also the last academic staff member in Galway to give chemistry lectures in Irish until he retired (as the Head of the School of Chemistry) from teaching in 2010. He was elected to the Royal Irish Academy on his first application in 1998.

Pat's research work initially concentrated on the organometallic chemistry of iron and later included the synthesis and reaction kinetics of quadruply bonded metal complexes. He started working in crystallography in the early 1980s when the first four-circle diffractometer in Ireland was set up in Galway. He was one of the five founding principal investigators of the Science Foundation Ireland (SFI)-and industry-funded Synthesis and Solid State Pharmaceutical Centre (SSPC) in 2007. The setting up of this Research Centre, led by Kieran Hodnett at the University of Limerick, was very important for chemistry in Ireland as it was the first research centre funded by SFI that did research in chemistry. At the SSPC, Pat's work concentrated on solid-state analysis of pharmaceutical solids, the use of sublimation for crystal growth and cocrystal synthesis, crystal growth mechanisms and theoretical analysis of solid-state interactions. Together with Pavel Karen (University of Oslo, Norway) and Josef Takats (University of Alberta, Edmonton, Canada), starting in 2009, he worked on an IUPAC project that examined the use of the oxidation state in chemistry. After 10 years of effort, the first comprehensive definition of the oxidation state was produced together with an 86-page technical report. He was also a member of the International Program Committee for the 2017 IUCr Congress in Hyderabad, India.

Pat's passing is a great loss for the crystallography community as well as the University of Galway. Having trained under eminent scientists – such as Jack Lewis at University College London, UK, and Massachusetts Institute of Technology, Cambridge, USA (1969–1972), during his postdoctoral work; Frank Albert Cotton at Texas A&M (1978) and Jack Norton at Princeton and Columbia, USA; and Guy Dodson at the University of York, UK (1991), on sabbatical – Pat developed a passion for crystallography and contributed several computational methods for structural analysis. In 1996, he developed and published the *ABSEN* program to predict all possible space groups in different orientations from an HKL file. He also

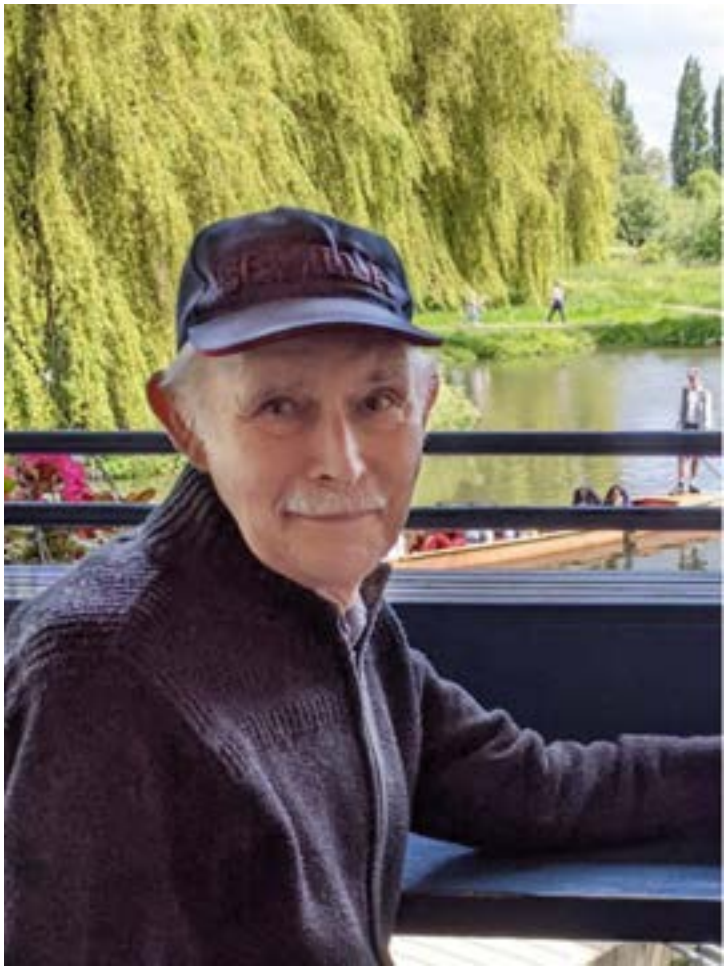
developed the *ORTEX* program to visualise *ORTEP* diagrams interactively. His interest in computing and crystallography led him to develop the *OSCAIL* software that integrated several crystallographic tools and is widely used in Ireland to date.

Pat was a very hands-on researcher. When he and his colleague Desmond Cunningham sourced Ireland's first diffractometer in 1981, a second-hand Hilger & Watts Y290 four-circle diffractometer from Canada, Pat had the confidence to take it all apart and put it back together in a functioning form. He believed in innovation but also respected heritage. True to this, he never got rid of older goniometer setups when the diffractometers were upgraded, and used them to train his students. This equipment is still on display in the crystallography labs in Galway and is soon to be added to the National Museum of Ireland's National Scientific Instruments Collection. Pat sought to bring a modern influence on the direction of capital spending on facilities in the new Science building in Galway, which opened in 1974. In collaboration with Professor R. N. Butler, this effort also brought the first 100 MHz NMR spectrometer to Ireland, which was followed by a ^{13}C spectrometer and the first high-field NMR spectrometer.

Pat was also an innovator who was not afraid of drilling a hole through a vacuum oven to modify it in order to control the temperature of his sample for the sublimation process to generate single crystals. He believed in sharing the knowledge he gathered. To that end, his YouTube channel has tutorial videos for the tools he has incorporated in *OSCAIL* on how to set up a cyclone vacuum at home for cleaning, and as an avid cyclist, on how to prevent your cycle chain from falling out.

In his colleague Niall Geraghty's words, "Pat is a renaissance man", who could talk about any topic from molecular orbital theory to history, art, opera, film, theatre and politics. He was a man of outstanding intellect and someone who was interested in everything till the end. His very humble and gentle approach made him a great mentor and a great teacher. Reading through his Condolence Book reveals how many lives he touched and how many people owe their careers to his training.

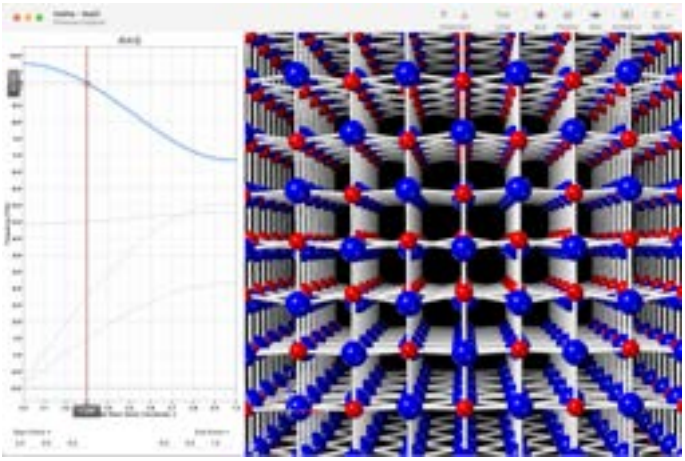
His dedication was not just to science but also to his family. Pat is survived by his wife Aideen, children Orla, Eoin, Aideen Óg and their families, as well as his siblings and their respective families.



IUCr note: Professor McArdle was a valued Co-editor of *Acta Cryst. E* from 2010 to 2019. For a list of the papers he published in IUCr Journals, please click here.

PRESS RELEASE

CrystalMaker Software launches all-new software for Mac and Windows



Visualizing an optical phonon mode in the crystal structure of halite (displacements exaggerated for clarity).

CrystalMaker Software Ltd has just launched all-new versions of its award-winning crystallography products, designed to provide fast crystal-energy modelling, Rietveld structure refinement, 3D diffraction visualization, plus interactive crystal shape building.

The flagship program, ***CrystalMaker 11***, is the culmination of a 10-year research project, working with leading academics to open up the world of computational materials chemistry: empowering scientists to understand crystal properties on their Mac or Windows computers — without the need for arcane workflows or energy-wasting supercomputers.

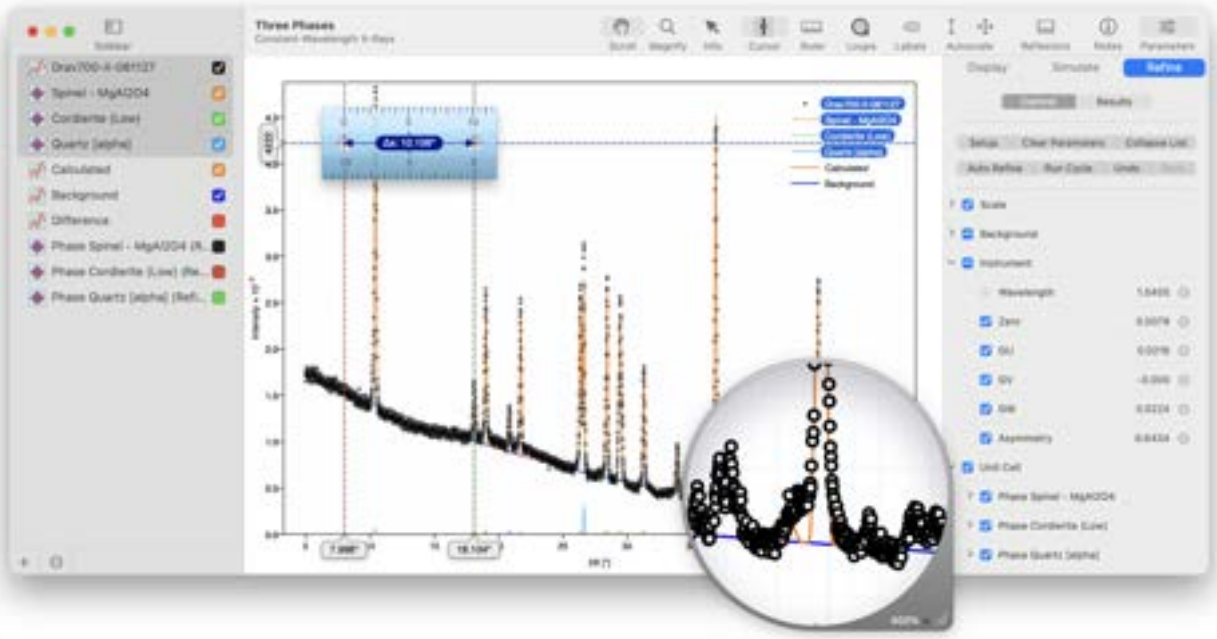
The new software features full crystal-energy modelling, with lattice dynamics, phonon visualization, plus physical and thermodynamic properties predictions. These build on the existing software's ease-of-use and elegant design, delivering the best visual understanding of complex structures and properties.

Other new features include dynamic "out-of-the-screen" 3D red/blue stereo, auto perspective, crystal range optimization, an interactive molecular-crystal packing explorer, silicate & phosphate framework automation and AI-powered hand tracking that leverages the "Neural Engine" built into Apple M-series processors.

CrystalDiffract 7 is a new powder diffraction program that features multi-phase "Rietveld" structures refinement and comprehensive Phase ID.

Not content with third-party software, the company created its own refinement engine from scratch: extensively optimized for multi-core performance and ease-of-use. An "Auto Refine" command provides a streamlined refinement process, with full manual control overrides.

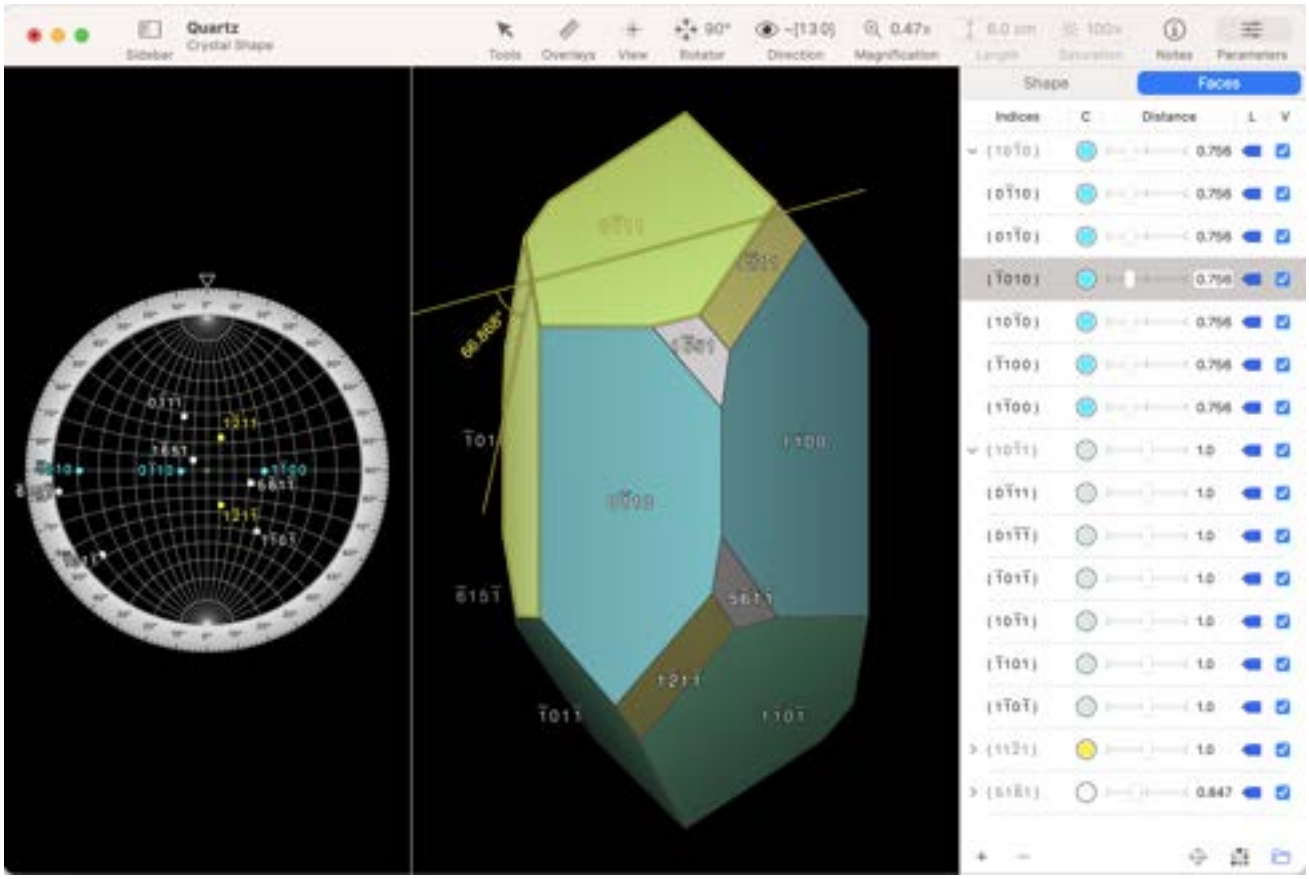
Other new features include integrated Phase ID (no external database required), as well as automatic background subtraction, peak detection, integrated structures library and numerous user interface improvements.



Multi-phase Rietveld refinement of a hydrothermal synthesis run (data courtesy of Professor Vincent van Hinsberg).

SingleCrystal 5 is a new program for working with single-crystal diffraction data. New features include interactive visualization of diffraction properties and Brillouin Zones in 3D. The software also provides interactive crystal shape building with on-screen measurement of faces, vertices, edges and angles. Multiple shapes can be precisely oriented and combined to show twinning and topotactic relationships.

SingleCrystal 5 can now import data from Gatan DM3 and DM4 files and includes automatic detection (and measurement) of observed peaks, as well as auto-indexing of Laue patterns. An instant "snap-to-grid" command facilitates auto-indexing of TEM diffraction patterns. Real-time fast Fourier transforms provide interactive "optical diffraction" on the desktop: an invaluable reference for teaching and research (a reference library is included, for teaching).



Measuring faces and angles for the crystal shape of right-handed α-quartz.

CrystalMaker, *CrystalDiffract* and *SingleCrystal* are developed *natively* for Mac or Windows computers and can be downloaded directly from the company website, https://crystalmaker.com. Education and multi-user discounts are available.

IUCR SUPPORTED EVENTS

IUCr supported meetings

These forthcoming meetings are supported by grants from the IUCr Calendar Committee.



11th Oct 2026 - 16th Oct 2026

Indaba10

Skukuza, Kruger National Park, South Africa



5th Dec 2026 - 10th Dec 2026

African Materials Research Society (AMRS 2026)

Nairobi, Kenya

MEETINGS CALENDAR

Meetings calendar

This is a list of meetings of interest to crystallographers occurring within the next twelve months, as recorded in the IUCr Calendar of Events. Please let us know of any that are missing by completing this form or sending an email to forthcoming.meetings@iucr.org.



Indaba10 South Africa 11th Oct 2026 - 16th Oct 2026



Synchrotron Radiation: Science, Knowledge, Innovations, Future (SKIF-2026) Russian Federation 18th Oct 2026 - 23rd Oct 2026



CCP-EM/Diamond Icknield Workshop United Kingdom 9th Nov 2026 - 13th Nov 2026



Instruct-ERIC hands-on workshop on Advanced cryo-FIB-SEM methods Germany 9th Nov 2026 - 13th Nov 2026



Crystal36-AXAA 2026 Meeting Australia 26th Nov 2026 - 2nd Dec 2026

African Materials Research Society (AMRS 2026) Kenya 5th Dec 2026 - 10th Dec 2026

Joint Polish-German Crystallographic Meeting 2027 Germany 15th Feb 2027 - 18th Feb 2027