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British Crystallographic Association

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BCA Spring Meeting 2012

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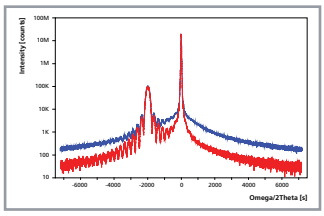

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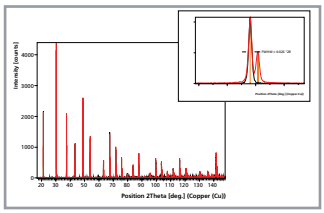

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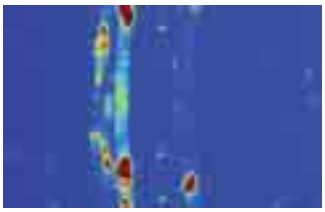

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This month's cover:

Scenes from the BCA 2012 Spring Meeting

From the President

I'VE discovered that you have to hit the ground running when you take on the role of President of the BCA. As I was leaving the AGM I was grabbed by the CN Editor and informed that my first Crystallography News "From the President" column was due within a week. Carl then softened the blow somewhat by suggesting that I should write about what I had just talked about in the meeting, so it was just as well that I was using notes…

I should perhaps start by introducing myself. I have been working at ISIS for over 20 years, first on SXD, the single crystal diffractometer and more recently on the GEM powder diffractometer. From 2000 I spent five years as an EPSRC advanced research fellow in Oxford and I have been fortunate to be able to continue these links with Oxford as a visitor in the Physics Department. Scientifically I am interested in structural disorder in all its guises. Indeed my PhD supervisor exclusively worked on liquids until he took me on and I've slowly become more ordered – and I hope a better crystallographer – as my career has progressed. In another sense my career has developed in a way that might be typical for a crystallographer: a physicist by training; much of my work could be labelled 'chemistry' or 'materials science'; and I have even dabbled in protein crystallography! Working at a facility is a brilliant place to broaden your crystallographic perspectives.

When **Elspeth** asked me to consider standing for President some months ago I spent some time considering what I might bring to the role. Amongst many other things, she has done a brilliant job in sorting out the structures of the BCA and BCA 'housekeeping' (she has even remaindered the polyester BCA ties!) and the Association is in pretty good shape. I believe that I am the type of person who can build on what she has achieved and consolidate; I don't plan to be initiating any major changes. This is not to say that there aren't challenges. Our conferences are well attended and popular, but our membership numbers are falling. We also need to see a smooth transition from Northern Networking Events to HG3 and I'm pleased that maintaining (and chasing potentially 'lost') members' details is a high priority in this.

I also believe that this is a period when we should be working together to look outward. We are awash with crystallographic centenaries: Laue's first diffraction measurements in 1912; the Braggs' seminal work in 1913; Laue's Nobel Prize in Physics in 1914, followed by the Braggs' in 1915. These are all excellent opportunities to show the importance and relevance of crystallography today and are coupled with our hosting of the European Crystallographic Meeting in Warwick University next August and the IUCr's International Year of Crystallography in 2014. Education, outreach, mutual support and co-operation will all be key to the success and purpose of the BCA over the next few years. With this in mind, I have asked **Ross Harrington** from Newcastle to act as our Education and Outreach Co-ordinator for the next three years. Ross will be working with our recently appointed and enthusiastic Group Education representatives (**Airlie McCoy** (BSG), **Liana Vella-Zarb** (CCG), **Richard Morris** (IG), **Mike Glazer** (PCG) and **Robert Young** (YCG)) to co-ordinate the BCA's outreach and public engagement activities during these important few years. Please do contact him or your group representative if you have any good ideas for outreach or would like to be involved in this work.

Please take a while to look at the details of meetings coming up over the coming months in the rest of this issue of *Crystallography News*. We have the European Crystallographic Meeting (ECM27) in Bergen, Norway this August, following hot on the heels from the ACA2012 meeting in Boston at the very end of July. The European Powder Diffraction Conference (EPDIC13) is being held on October in Grenoble, France. I would also like to make a personally biased recommendation for the reverse Monte Carlo meeting (RMC5) in Budapest, Hungary at the end of September. If you are at all interested in total scattering or pair distribution function methods then this will be an excellent opportunity to discuss this work with other experts in this area in a very informal environment. Please see **www.szfki.hu/~nphys/rmc5/rmc5.html** for further information.

I will finish this with two very pleasant tasks. First, I want to invite nominations for new Honorary Members of the BCA. Honorary Membership is the highest membership accolade of the BCA, and is awarded to a small number of colleagues who have contributed significantly both to crystallography and to the work of the BCA. This year **Professor Jack Dunitz** became our latest Honorary Member, joining a small but distinguished group of people (see **crystallography.org.uk/honorary-members**). In the coming year we anticipate electing one or two new Honorary Members so please send your nominations, together with a short (one page) supporting case and the endorsement of at least three other BCA members to me by 31st January 2013.

Secondly I want to express my thanks to a number of people. As I write this, many of us have just returned from a very good Spring Meeting in Warwick with a number of highlights (although the performance of the present President attempting to dance with the far more graceful past President was probably not one of them). I want to thank all those involved in the excellent scientific programme and in the general organisation, smoothly coordinated by **Kirsten Christiansen**. I also thank Northern Networking Events for their care of us over the past twelve years, and – in anticipation – for their continued support for ECM28 next year. Finally, it is a pleasure to thank Elspeth for her excellent work in leading our association over the past three years. I am sure that over the coming weeks and months I will come to appreciate with ever greater clarity how much she has done for us; I am especially grateful that she is staying on Council for a further year to look after this "newbie" president!

David Keen

BCA Council 2012

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Full committee details on the BCA website
www.crystallography.org.uk

From the Editor

PLEASE forgive me if this column seems to be a travelogue. Some recent meetings have impressed me in ways I want to share. Already in March I had been to Munich for the Laue Day and the annual meeting of the German Crystallographic Society. The pre-meeting announcements stated that the official language would be English, and this message was reinforced by a large banner over the main entrance giving the Society's name in English. Would anyone care to estimate the attendance at a BCA (or ACA) meeting if our official language were German? Of course, this is not just a case of the Germans avoiding any trace of unseemly nationalism. Since international meetings use English, this national meeting provided an additional opportunity to practice the effective use of English in talks and posters. A very high standard was achieved, as is reported elsewhere in this issue.

The venue for this meeting was the main building of the Ludwig-Maximilian University, with many commercial exhibits and refreshment points occupying the great glass-domed atrium pictured on our March cover. The address of this building is Geschwister-Scholl (Scholl Siblings) Platz, and Professor-Huber-Platz is just across the street. I had only a vague idea about the significance of these names until I studied the memorial exhibition in this building. Hans Scholl was a medical student at the University. To deal with mounting casualties on the Russian front in 1942 the Nazi government extended the summer vacation and sent medical students to help out in field hospitals. Hans Scholl made firm friendships with a number of lightly wounded German soldiers whom he helped to patch up. When they had recovered, they were sent back to the front. From there they wrote letters about their harrowing experiences, and most of them perished at Stalingrad that winter. Hans Scholl also did what he could to help wounded Russians, becoming aware of how badly the Germans were treating them and how much hatred this would engender. Upon his return to Munich he related his experiences to his sister Sophie, and they discussed the ethical issues with Professor Huber. Knowing that it would most likely cost their lives but feeling an ethical imperative, Hans and Sophie clandestinely printed a manifesto calling for a return to democracy and an end to the war. They posted copies to people they considered sympathetic and scattered the remainder in the atrium court. Inevitably they were arrested by the Gestapo and guillotined. When Professor Huber interceded for them, he too was executed. However, sympathisers in Berlin who had received a leaflet reproduced it. One of these reached Sweden and was sent on to Britain, where for the first time it became clear that not all Germans had been brainwashed into following Nazi orders. Four million copies of the manifesto were made and dropped over Germany by the RAF. Durable copies of the manifesto have been set into the floor of the entrance hall and the paths outside.

From the Laue Day commemoration I learned a lot more about Max von Laue. Most aspects of the additional information reinforced my admiration for his generosity. He felt that Friedrich and Knipping, who practically implemented the experiments for which he provided the basic principles, deserved equal credit. Therefore he shared his Nobel Prize money with them. Considering himself purely a physicist, he was happy to give the Braggs helpful information as they sought to use X-ray diffraction to determine chemical structures. However, his memoirs appear to give an unfair impression of his boss, Arnold Sommerfeld. He implied that Sommerfeld was so implacably opposed to his idea of X-ray diffraction that he, Friedrich and Knipping had to go behind Sommerfeld's back and do the research mostly in evenings and weekends. Apparently the truth is that Sommerfeld told them that it would never work (the wavelength of the X-rays being too poorly defined to give coherent diffraction); but if they were determined to waste a few weeks on this crazy idea, they could go ahead. The result was a rift with Sommerfeld that lasted for a number of years.

My next trip was to London at the beginning of April for the annual open meeting of CPOSS (Control and Prediction of the Organic Solid State). Recent meetings have shown a rapid rate of progress. Last year the progress was most evident in the area of prediction, the latest Blind Test of prediction methods having demonstrated an ability to deal with more complicated systems than ever before. This year was noteworthy for our enhanced ability to control the outcome of crystallization. A report is presented in this issue.

Two weeks later we returned to Warwick University for the BCA's big event, the Spring Meeting. If anyone might have doubted the value of having a BCA instead of independent subject groups, the extensive integration achieved at this meeting would have dispelled such doubts. A trial session in which a panel of experts in biological and chemical crystallography answered questions from the audience attracted so much interest and so many pertinent questions that it could have continued far beyond the allocated time. It was obvious that the largest "chemical" structures now approach macromolecular structures in size and complexity and are often being tackled with the aid of similar techniques, though sometimes under different names. In the area of hydrogen bonding where I have particular research interests, I found it very instructive first to hear three physicists describing hydrogen bonding at a fundamental level and applying computational methods to the simulation of water. In the second part of the session two chemical crystallographers observed and rationalised the hydrogen bonding actually adopted from a multitude of possibilities in series of organic molecules. Most likely because of the sartorial elegance of my BCA tie, I was chosen to conclude this session. On the last day of the meeting a joint session encompassing not just the physicists and chemists but also the industrial crystallographers considered distortion and disorder in crystals, moving away from the view that these phenomena are a plague for the unfortunate crystallographer towards the idea that they are interesting subjects for study. This Spring Meeting provided a good test

for Warwick as the venue for next year's European Crystallographic Meeting. From the adequately sized lecture theatres with good sight lines to the tasty conference dinner followed by an enjoyable ceilidh, Warwick triumphantly passed the test. The only complaint I heard from several people was that the sparse signage around the campus left us with a considerable challenge in real-space navigation.

This issue includes a number of pictures taken at the Spring Meeting. I thank **Allan Pang** for many of the best photographs. Please take particular note of the pictures of exhibitors which appear across the centrefold. We should be doubly grateful to them: their payments for display space help to reduce the cost to conference participants, and their dedication to research and development even in a difficult economic environment keeps providing improved equipment that enables us make progress in crystallography. I am also pleased to include photographs of our Prize Winners. Several of them were invited to give presentations during the meeting; these talks were noteworthy for exciting science explained with clarity and enthusiasm. Because of the short time interval between the conclusion of the main meeting and the publication deadline, detailed reports of the scientific sessions will appear in the next issue.

I also wish to draw your attention to *"Central Facility News"*, which this time describes the European Photon and Neutron Science Campus in Grenoble. Since the UK is an important shareholder in the facilities on this campus, and a major upgrade programme is further enhancing their usefulness, it is important that UK researchers are aware of the opportunities they offer. I am grateful to **Edward Mitchell** for communicating this information to us.

Carl Schwalbe

Puzzle Corner

EACH of the following 12 words is a Cambridge Structural Database refcode that follows the standard convention, consonant-vowel-consonant-consonant-vowel-consonant.

BASSET, BULGAR, CARBON, CARNAL,
CARPET, CITRUS, DOGSEX, FARMER,
MUPPET, POSSUM, SURFER, WASHED.

Only one of them refers to the chemical name of the compound it represents. Which one is it?

Do SURFER and WASHED contain any water?

March Puzzle Corner: *Since I have not yet received solutions to the crossword, it will be held over.*

BCA Corporate Membership

The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA offers Corporate Membership. Corporate Membership is available on an annual basis starting from 1 January to 31 March and includes the following benefits:

- Up to 10 free BCA memberships for your employees.
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CPOSS Open Meeting 3 April 2012

As with previous meetings, comprehensive series of slides have been provided by the speakers and are accessible on the website www.cposs.org.uk .

THIS year's title was "Crystal or Not, Where Do We Go from Here?" My general impression was one of good progress. Our capability used to be limited to the preparation of crystalline materials by trial-and-error, the determination of their structures and then the rationalisation and "retrodiction" of these structures. Now we are starting to achieve the objectives of control and prediction, not just of "ordinary" crystals but also of less ordered material.

Sally Price began by reminding us of the naive intention behind crystal structure prediction in the early 1990s: to predict THE crystal structure. This term can be interpreted to mean "the thermodynamically most stable structure," as indicated by the global minimum in the static lattice energy for a perfect infinite lattice. We now have enough experience of predicting crystal energy landscapes to know that the global minimum is accompanied by other local minima that also have low energy and high density. In fact, we over-predict polymorphs. If we (or our computers) are to identify which local minima are practically important, we need an understanding of the kinetics of crystallisation. Closely related structures on crystal energy landscapes will not be observed as polymorphs because they are insufficiently distinct during crystallisation. Large flexible molecules like many pharmaceuticals may take considerable time to rearrange to the appropriate conformer and docking orientation. Sally presented a wealth of examples where computation of the crystal energy landscape clarified the experimental situation: structures of homochiral and racemic naproxen, the lack of cocrystals between succinic acid and p-dicyanobenzene, discrimination between salts and cocrystals when the gross structure was determined from X-ray powder data, dimer versus catemer formation. We are even acquiring some ability to predict disorder and hydro-gel formation.

Alastair Florence described the use of prediction and experiment in selecting the optimal form (which could be a polymorph, salt, solvate, cocrystal or even amorphous) of a new chemical entity for a given application. The predicted energy landscape can suggest feasible additional forms, which can be sought experimentally by a variety of screening techniques. As well as conventional crystallisation from solution, the "toolbox" includes growth from slurries, emulsions, or supercritical fluids, elevated pressure, addition of impurities or polymers, mechanical methods, and thermal methods like hot stage microscopy and sublimation. The results can be surprising, as demonstrated by attempts at growing cocrystals that produced polymorphs of the components instead. Alastair reminded us of two events that will take place at the University of Strathclyde: the 4th European Conference on Crystal Growth from the 17th to the 20th of June 2012, and also the first Annual Open Day of the EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation on the 13th of September.

Simon Gaisford turned our attention to characterisation, describing techniques of thermal analysis that can be used on crystalline and amorphous forms. As a technique for pharmaceutical analysis, differential scanning calorimetry is second only to high performance liquid chromatography. It can be used for identification, purity determination, characterisation of physical form, excipient compatibility and processability. Detection of polymorphs is probably the most important application. Different polymorphs will have different melting points and different heats of fusion. The heating rate is important: fast heating increases signal response and broadens the peak. While the determination of melting temperature is not affected by the heating rate, the crystallisation endotherm changes with heating rate due to kinetic effects, and a very rapid heating rate may not allow time for a metastable polymorph to recrystallise. At the "highest-tech" end of instrumentation, the lab is a test site for equipment that can heat as fast as 2000 °C min^{-1}. At the "economy" end, an ink-jet printer purchased from a high street store has been adapted to mix solutions of cocrystal components, e.g. benzoic acid and isonicotinamide. The printed samples can be examined by DSC to detect cocrystal polymorphs. DSC can also provide information about amorphous materials, which have no melting point but usually do have a glass transition temperature.

Matthew Habgood addressed the challenging topic of growth-stage selection of polymorphs, real or imaginary, with the awkward case of tetrolic acid as the example. Its energy landscape from default crystal structure prediction reveals the 2 known polymorphs at reasonably high density and low energy, but several other predicted structures have similar or slightly better stability. To ascertain whether and when any of the predicted structures could appear as metastable polymorphs one needs to model nucleation and growth. The methods chosen were molecular dynamics for the solution, and simulation of clusters. Matthew found that among the 13 low-energy structures in the landscape there are only 4 types of packing and hydrogen bonding. Therefore it is sufficient to select 4 representative structures, the 2 experimental polymorphs and 2 "imaginary" ones that have not (yet?) been found. The most stable structure on the landscape is an "imaginary" catemer with antiparallel stacking. The second most stable structure is an observed catemer with parallel stacking. Slightly less stable is an

"imaginary" dimer structure, with the metastable observed dimer still less stable. This polymorph crystallises from chloroform, whereas the catemer structure forms from ethanol. Because infrared spectra as well as molecular dynamics calculations indicate more dimers in chloroform than in ethanol, this is evidence that solution species may assist nucleation and growth. However, these techniques provide no information about packing. Nanocrystal stability calculations on spherical crystals with radius *ca.* 1.25 nm containing about 70 molecules reverse the order of bulk stability, placing the observed catemer or dimer lower in energy than their "imaginary" counterparts, suggesting the former may be more stable during growth.

Jonathan Steed and **Sharon Cooper** provided a double act on the use of gels and emulsions to control crystallisation. The first aim is to use knowledge of supramolecular chemistry to produce organogels for which the rheology can be controlled by using switchable competing interactions. For instance, the dominant hydrogen bonding motif in urea is the tape based on $R_2^1(6)$, which promotes rapid growth in one dimension leading to fibrils. A stronger acceptor such as an anion can switch off the urea tape, breaking down the gel and allowing crystals grown in it to be harvested. Proof of this principle was achieved by growing carbamazepine crystals. It is envisaged that gelators can be designed to mimic part of a drug molecule.

Microemulsions can help with the control of polymorphism. With stabilisation by a surfactant it is possible to prepare relatively monodisperse droplets 2-10 nm in size. Energetic collisions may enable the droplets to exchange their contents, and crystallisation can start if the colliding droplet provides a nucleus. If the droplets are only slightly supersaturated with a solute, nuclei of the thermodynamically stable polymorph will be longer-lived than metastable ones, and thus the likelihood of crystallising the most stable polymorph is enhanced. Challenging materials that have been studied include the thiophene derivative ROY, mefanamic acid and glycine.

Philippe Fernandes illustrated the application of techniques learned in academia (particularly structure solution from powders and polymorph screening) to real-world problems in industry. One important difference is the need to work on a faster timescale. Working for a small company employing about 50 people, he had to make the burdensome investment in laboratory facilities pay off. At the heart of the screening setup is an automated platform for doing chemical manipulations and measuring X-ray powder diffraction patterns. This has enabled cost-effective contract research to be performed for customers requiring selection and control of the most suitable solid form and satisfaction of regulatory requirements.

Doris Braun beautifully illustrated the successful combined use of *in silico* and *in vitro* solid form screening for organic hydrates. Of 960 solid organic drug compounds in the European Pharmacopoeia, only 36% are monomorphic while 64% can exist as polymorphs, hydrates or solvates. Hydrates pose particular problems since contact with water is unavoidable during the manufacturing process. Changes in temperature or relative humidity may result in the loss or uptake of water. Doris performed experimental screening and calculations on four organic molecules with a benzene ring bearing OH or COOH substituents: 2,4- and 2,5-DHB (dihydroxybenzoic acid), phoroglucinol and gallic acid. A crystalline hydrate should form if and only if the lattice energy of the hydrate is more negative than the sum of (negative) lattice energies of the anhydrate and ice. The observation that 2,4-DHB forms a hemihydrate and a monohydrate while 2,5-DHB forms no hydrate at all is consistent with calculations of lattice energy of the anhydrates that come out 5.5 kJ mol^{-1} more negative for 2,5-DHB than for 2,4-DHB. In the anhydrous state 2,4-DHB is less stable and less dense; thus hydrate formation is preferred. In addition, the 2,4-DHB hemihydrate is predicted with the correct compound:water ratio. Experimental screening supported by calculations showed that phoroglucinol could undergo a transition between anhydrate and dihydrate, the latter demonstrating diffuse X-ray scattering. Gallic acid monohydrate was chosen as a subject for the 2010 Blind Test since it was already known to form 2 polymorphs. The crystal energy landscape studies (which were very sensitive to the choice of wavefunction used) stimulated by this test led to the discovery of a 5th monohydrate polymorph, in addition to the two blind test and two previously known polymorphs!

Chick Wilson concluded the meeting by describing progress on the Directed Assembly Network, DAESTP. This network has grown to encompass over 400 contributors, working towards the eventual goal of controlling assembly of matter to create materials with tuneable properties and functions. This bottom-up approach going from molecules to products has 5 themes: (1) molecular frameworks and hybrid materials, (2) crystallisation and nucleation, (3) biological and biomimetic systems, (4) surfaces and (5) evolving systems. Theme 2 in particular, but also themes 4 and 5, build on the achievements of CPOSS and are complementary to the recently established EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation described earlier by **Alastair Florence**. The combination of modelling and experiment is crucial, and secondments between academia and industry will be encouraged.

Carl Schwalbe

Speakers (from left to right) ***Prof Chick Wilson*** *(University of Bath),* ***Dr Philippe Fernandes*** *(formerly University of Strathclyde),* ***Dr Sharon Cooper*** *(University of Durham),* ***Prof Sally Price*** *(UCL),* ***Prof Jon Steed*** *(University of Durham),* ***Prof Derek Tocher*** *(UCL),* ***Dr Matthew Habgood*** *(UCL),* ***Dr Doris Braun*** *(UCL),* ***Prof Alastair Florence*** *(University of Strathclyde).*

Laue Day and 20th Annual Meeting of the German Crystallographic Society

THE Laue Day, Monday the 12th of March, was planned to start with presentations by scholars with expertise in the history of science about the life of Max von Laue (1879-1960), his colleagues and his discovery of X-ray diffraction. The first lecture was to be given by Michael Eckert from the Deutsches Museum in Munich. However, his unexpected illness necessitated major rearrangements. Wolfgang Schmahl, the cheerful local chairman, announced that Dieter Hoffmann from Berlin would bring his presentation forward. By way of thanks he quoted a report of the Prussians coming to the rescue at the battle of Waterloo. This was generous indeed since the Bavarians relate to the Prussians in a similar way as the Scots to the English.

The conference venue

In his talk on the optical properties of X-rays **André Authier** provided an interesting insight into Laue's thought processes. Laue originally believed that the incoming X-ray beam would excite fluorescence in the specimen, and the monochromatic radiation thus produced would undergo interference phenomena. Although inapplicable to the diffraction experiments pioneered in 1912, this was not a stupid idea. Kossel lines arise when fluorescent radiation from one type of atom in a crystal is Bragg-reflected by the lattice planes in that crystal. First observed with electrons as the primary energy source by Kossel's group in 1935, it was then also observed with X-rays by **Gerhard Borrmann**. The long-lived Borrmann (1908-2006) went on to predict double refraction of X-rays, which was subsequently observed by Authier. André also gave a lucid account of the early efforts to find a satisfactory theory of X-ray diffraction and develop the dynamical theory of diffraction. His article, along with an introduction and three other articles, has appeared in Part 1 of Volume 68 of *Acta Crystallographica, Section A*.

Under the title "Max von Laue – knight without fear or fault" **Dieter Hoffmann** enlightened us in particular about Laue's later career. Laue did not seem to be at all spoiled by making a great discovery at the age of 33 and receiving the Nobel Prize for it just a year later. He developed a firm friendship with Einstein in the 1920's and maintained it after the Nazis came to power. Laue steadily resisted the blandishments and threats of the Nazis. Neither did he emigrate, although beyond question he could have walked into a prestigious academic job almost anywhere. He did not want to take such a position that another more endangered exile would have needed, and he wanted to help rebuild German science after the inevitable catastrophe that he foresaw. After the war he did his best to maintain some contact with the scientists of East Germany. He delighted in driving, often scaring his passengers with his love of speed. Ironically, he perished in an accident that was not his fault.

We then enjoyed a guest appearance by Laue's great-grandson **Christian Matthei**, who continued the theme of Laue's love of driving. Laue kept a guest book for passengers. Among the signatories was **Otto Hahn**.

Dieter Schwarzenbach took us on a fascinating tour through diffraction based crystallography, showing how topics addressed in the early days still provide fertile ground for research today. For instance, by 1914 **Peter Debye** had worked out the influence of thermal motion on the intensities of diffraction. Nowadays we are addressing questions such as the "second phase problem": are thermal motions correlated or anticorrelated? Already in 1939 Brill and co-workers collected data of sufficient quality to demonstrate interatomic bonding density. Now we are well aware of the

the original apparatus used by Friedrich and Knipping to carry out Laue's experiment

The conference dinner

arbitrariness of partitioning the electron density into atoms and succeeding with many charge density studies.

After lunch (we were exhorted to think of the Braggs and have an "English" lunch so that we could reassemble within an hour) the talks were devoted to modern developments. **Helmut Dosch** from the DESY synchrotron described 1912-2012 as the "Crystalline Century" which enabled us to understand important phenomena such as metallic conduction, crystal optics and magnetism. The new challenges are disordered structures, non-equilibrium phenomena and transient states. Because Laue had highly ordered material, he could get away with incoherent radiation. With disordered material we must have coherent radiation. X-ray free-electron lasers (XFEL) give us the promise of "quantum cinema."

Henning Friis Poulsen presented multigrain crystallography. We hear much about microfocus sources today, but already in 1951 Hirsch and Kellar developed a micro-beam technique to study grain size and grain perfection. Recent work by **K. S. Paithankar** & **E. F. Garman** at Oxford was particularly commended. Multigrain crystallography involves four steps: (1) determining the space group from the pseudo powder pattern, (2) indexing, to find vertices in orientation space, (3) integration and filtering, (4) structure solution and refinement by one's favourite software such as SHELX, JANA or MOSFLM. A demonstration on $Cu(C_2O_2H_3)_2.H_2O$ with 70 grains of size < 1 μm gave better distances and displacement parameters than could be obtained from powder data. With XFEL irradiation of single crystals 3 shots are insufficient to give good statistics, but 3 shots at 20 microcrystals will be much better. In the future, with coherent beams, ptychography will become possible. *(Editor's query: how do you pronounce ptychography'? Is the 'p' like the 'P' in 'Ptolemy"?)*

The main meeting covered a wide variety of topics in 18 microsymposia stretching over 2 ½ days. There were some distinctive differences in coverage between this meeting and a typical BCA meeting. For instance, there was relatively little about pharmaceutical compounds: besides mine there were only two other posters on this topic. **Peter Luger** did give a very interesting talk on the contribution of electron density to drug discovery, using the invariom database to provide a fixed contribution to the aspherical electron density. It would be very difficult to determine electron density around a complete protein, but reduction to the region around the active site is more realistic, provided that the protein structure is completely reliable and the choice of active site region is appropriate. If there is any doubt, it is wiser to stick to electrostatic potential and Hirshfeld surfaces. However, small-molecule charge density determination, e.g. on donepizil, is now routine.

On the other hand, three microsymposia dealt with materials. Obviously there is great interest in Germany in understanding structure-property relationships and designing new materials, which reaches out to other countries as well. A very lively plenary lecture on "Bio-inspired crystallisation: challenging single crystal shape and structure" was given by **Fiona Meldrum** from the University of Leeds. Focusing on $CaCO_3$, she and her group have sought to control polymorph and morphology. Biological samples contain curved crystals which nevertheless give single crystal diffraction patterns. Whereas a conventional single crystal of $CaCO_3$ cleaves easily, these do not. The two key strategies for control in the laboratory are confinement in a matrix of insoluble macromolecules and admixture of soluble additives. Confinement affects nucleation rate, polymorph selectivity, degree of crystallinity and orientation. Biominerals often contain macromolecules with repeating blocks of acidic amino acids. Organic macromolecules embedded in calcite make it stronger and stiffer.

The conference dinner was held in the Augustiner Keller. A large vaulted basement room had been reserved for our exclusive use. There we sat at long tables where we were served typical Bavarian fare family-style, accompanied by as many refills as we wished of the excellent brew. This convivial evening assisted our insight into the reasons for Laue, Friedrich, Knipping and Sommerfeld to choose to live in Munich and to come up with brilliant science!

Carl Schwalbe

an Art Nouveau screen exhorting students and crystallographers that hard work conquers everything

Growth and Form: Request for Images

KEVIN Lotery is a project researcher working with exhibition organizers from the Tate and elsewhere on the potential reconstruction of *Growth and Form*, an exhibition mounted by British artist Richard Hamilton (1922-2011) in 1951. The exhibition consisted of several sections. These contained images gathered from various different scientific disciplines (often from particular scientists or departments that Hamilton visited personally). One goal was to bring together some of the most cutting edge image technologies then available and examine them on aesthetic grounds (electron-micrographs, photomicrographs, X-ray diffraction patterns, etc.). He is now in the process of trying to locate repositories of similar images at various universities and institutions in the UK.

Some of the most prominent images in the exhibition were crystallography images of various types (all from the middle of the century of course). He is looking, therefore, for high-resolution images or original negatives/prints of images from around this period.

He is based in London and can be reached via the information below.

Kevin Lotery
Ph.D. Candidate
History of Art and Architecture, Harvard University
+44(0) 75 2823 8040 (UK)

We thank the Museum of London for permission to reproduce the handbill promoting the original exhibition. Many more fascinating images are available on the website www.museumoflondonimages.com

BCA Spring Meeting, Warwick, 2012

Scenes from Award Lectures, Ceilidh and Conference Dinner

Prize Winners

ONCE again our judges had a very daunting task to select the winners from a very strong field of entries, in scientific content as well as presentation. Our thanks go to the sponsors, and our congratulations go to the winners of prizes given by the Groups of the BCA; most of the winners have been pictured receiving their awards at the BCA Spring Meeting.

The Biological Structures Group awarded the beautiful trophy for the David Blow Poster Prize to **Stephen Carr** for the crystal structure of a complex which participates in the Fanconi anaemia pathway. This year's greatly expanded BSG presence merited the award of two runner-up prizes, to **Stephen Harper** and **Yonca Yüzügüllü**.

Among the chemical crystallographers, the Chemical Crystallography Group Prize was won by **Alexis Munn**, the CrystEngComm prize by **Peter Galek** for methods of assessing hydrogen-bonding landscapes; and, although we couldn't afford a luminescent gold medal, **Chris Woodall** received the IUCr Prize for studies of the luminescent behaviour of gold(I) trimers.

The glory of the Industrial Group Young Crystallographer Award, accompanied by the "butterflies-in-the-stomach" experience of giving a Prize Lecture was capably received by **Andrew Maloney**. Earlier, an excellent CCDC/CCG Prize Lecture had been given by **Gareth Lloyd**.

The Physical Crystallography Group PANalytical Thesis Prize is always a highlight because of the amount of sustained work it honours. This year's winner, **Lucian Pascut**, carried out the PhD research at Bristol University and is now at Rutgers University in the USA. The IoP-sponsored PCG-SCMP Physical Crystallography Prize was won by **Jonathan Wright**. He also took the opportunity to give a stimulating lecture, starting with the memorable line, "How do you spend 10 years on one crystal structure?"

Joe Paddison experienced the satisfaction of winning the RSC Solid State Chemistry Group Prize for his studies of frustration in beta-MnCo and MnO. The Young Crystallographers Poster Prize was won by **Emma McKinley**. The Durward Cruickshank Prize, named for a great crystallographer whose refinement procedures have helped a multitude of other crystallographers, appropriately went to **Robin Owen** for his fine individual and collaborative research at the Diamond Light Source. Finally, the Rigaku Poster Prize was awarded to **Nick Funnell** just before the onset of the ceilidh for his study of the onset of disorder in solid cyclohexane.

Carl Schwalbe

Jonathan Wright

Andrew Maloney

Robin Owen

Stephen Carr

Stephen Harper

Peter Galek

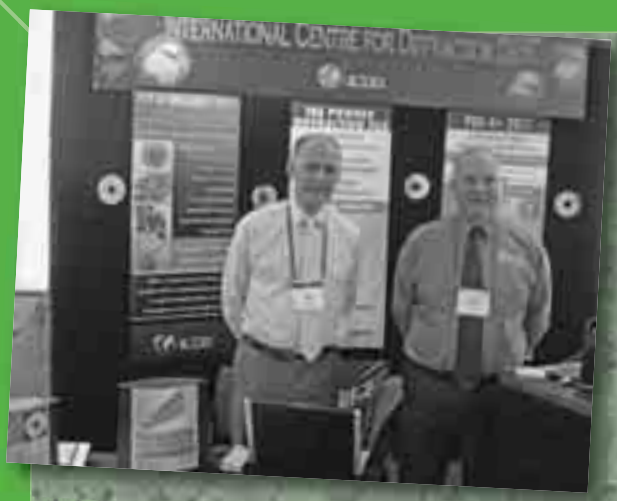
Chris Woodall

Emma McKinley

Nick Funnell

Yonca Yüzügüllü

Spring
Exhi



Meeting
ibitors

From Small Molecules to Proteins: Bridging the Gap

AS an experiment Kirsten Christensen, Amber Thompson and Arwen Pearson organised this 1-hour early evening forum at the BCA Spring Meeting. For further expertise they recruited Elspeth Garman and Bill Clegg, and then they hoped that people would (1) turn up, and (2) ask questions from the floor. In this attempt they were triumphantly successful. There was a very large attendance; and, long before people had run out of questions, the session had to be terminated on humanitarian grounds so that participants could get to the food and wine at the poster session before these essential supplies ran low. Although reports on the other scientific sessions will appear in our September issue, I include this one now because our experience here will be very relevant to Microsymposium 42 at the forthcoming European Crystallographic Meeting: 'Big "small molecules" and small "macromolecules" – learning techniques from each other'.

Amber convincingly demonstrated the development of small-molecule crystallography from a well-behaved structure like diazepam, determined in 1972, to the brute described by Sprafke et al. in 2011 in their paper, J. Am. Chem. Soc. 133 (43), 17262-17273. This structure had most of the "macromolecular" attributes: high molecular weight, 60-70% solvent content and lots of disorder. The techniques used by macromolecular crystallographers to overcome such impediments can be very relevant. On the other hand, the skills acquired by small-molecule crystallographers in handling twins and split crystals can be helpful with macromolecules.

Elspeth reminded small-molecule crystallographers that with such high solvent content the radiolysis of water becomes a serious problem and radiation damage becomes a limiting factor for data collection. On the other hand, macromolecular crystallographers need to know some inorganic chemistry. For instance, cacodylate buffers often are efficacious in promoting protein crystallisation, but the high absorption of X-rays by arsenic leads to radiolysis. After crystals have formed, back-soaking to remove the As can improve crystal lifetime. Incorporation of selenomethionine is good for phasing, but Se also increases absorption and radiolysis. Even a change of wavelength is not much help: short wavelengths lead to low absorption but also low diffraction. Changing to a longer wavelength increases both the undesirable absorption and the desirable diffraction. As a general procedure Elspeth suggested to calibrate the available beam in photons/sec, test the lifetime of a sacrificial crystal, measure sample crystals for a length of time based on that value and merge the data. Bill reported that radiation damage has begun to appear during small-molecule data collection with synchrotron sources, but it still affects fewer than 10% of samples. Amber mentioned that problems of radiolysis that appeared at 150 K became far more tractable at 100 K. Elspeth ascribed this effect to OH radicals, which are immobile at 100K but become mobile at 130 K. However, even at 90 K a protein chain serves as a motorway for electrons.

Claire Murray mentioned a characteristic of CheckCIF that can be disturbing. Groups that are mobile even at the lowest available temperature lead to error messages. Bill responded that it is not the responsibility of authors, referees or editors to ensure that published structures are free of CheckCIF alerts. Rather, CheckCIF points out features that need careful examination. If, in the case of mobile groups, the atom types are verified and any previously undetected disorder has been found, then it should be safe to publish. The Validation Reply Form enables the author to respond to CheckCIF alerts. The criterion that referees and editors should use is fitness for purpose, not any specific R factor or ratio of observations to parameters.

Roy Copley spoke from the point of view of a small-molecule crystallographer working with protein people. At the IUCr Congress in Madrid he attended a session where ligands attached to proteins were classified as probably correct, probably wrong or certainly wrong. Most ligands in published protein structures fell into the latter two categories!

The discussion moved on to the topic of resolution with a question about how bad the resolution of a small-molecule structure can be, still permitting structure determination. Amber answered that 1.3 Å resolution is needed for direct methods to work. Bill gave us two more numbers: 0.84 Å is the routinely desirable resolution to give a good description of bonds, while 0.5 Å is needed for charge density studies. He added that charge flipping can *sometimes* solve a structure from data with worse resolution than 1.3 Å. Amber sought to pin down the definition of resolution in the small-molecule context, suggesting that it should not be defined by the highest single reflection but rather by the shell where I / sigma is equal to a threshold value, traditionally 2.

A series of points about methodology were raised. Amber mentioned that with 50–70 % solvent one uses SQUEEZE extensively, but with a wrong or incomplete model SQUEEZE would eliminate parts of the molecule. In answer to a question about whether one should take a "large small-molecule" crystal to a macromolecular beamline, Bill replied that there is not really much difference between beamlines

Arwen Pearson makes a point which elicits intense concentration from Bill Clegg

nowadays. Bill and Amber pointed out that small molecules may need better corrections for absorption, which is less often a problem for proteins. Elspeth described methods used to speed up macromolecular refinement. Maximum likelihood can be used in place of least squares.

The discussion returned to radiation damage, this time specifically with respect to metals in small-molecule structures. Elspeth explained that an X-ray can knock out a highly energetic photoelectron, which in its progress creates up to 500 secondary electrons. Because of exposure to such electrons, most metalloproteins in the PDB actually have their metal in reduced form. **John Helliwell** explained how care was taken with the data collection protocol to produce a solvable and plausible structure in the context of photosystem PS2: use of a large crystal which was frequently stepped through a small beam. Bill stated that he was not aware of any reduction of the metal in Cu(II) MOFs. MOFs benefit from a low ratio of solvent to metal; and if the solvent is, say, chloroform rather than water, it is a less efficient source of photoelectrons.

I asked the final question of the session, stating that small-molecule crystallographers lose so much sleep over "getting Marshed" (missing a symmetry element) that an "inverse Marsh effect" has begun to appear (wrongly treating non-crystallographic symmetry as crystallographic). John recapitulated some findings from Richard Marsh's last paper, that 10 % of structures in the CSD published in P1 and 5 % of those in Cc have been misreported (the symmetry should have been higher). The most common mistake was to miss an inversion centre, but protein crystallographers could be serene in the knowledge that their crystals cannot have one. Arwen said that concern arises when an apparently non-crystallographic symmetry element in a macromolecular structure comes close to a crystallographic axis.

Carl Schwalbe

Central Facility News

CONTINUING the series on UK User Facilities, in this issue of Crystallography News, we turn our attention to the UK participation in the European centres in Grenoble, France with particular reference to resources for structural biology. Materials crystallography will be looked at in a future article.

The EPN (European Photon and Neutron) Science Campus in Grenoble, France hosts three major European institutes all co-funded by the UK, which together provide a unique centre of excellence in basic and applied scientific research: the world's most powerful neutron source, the Institut Laue Langevin (ILL), the world's most productive photon source, the European Synchrotron Radiation Facility (ESRF), and the Grenoble Outstation of the European Molecular Biology Laboratory (EMBL). The EPN Science Campus is home to 1500 staff.

The United Kingdom is an important shareholder in the ESRF, the ILL and the EMBL. The UK-funded user facilities in Grenoble welcome around 1,100 visits by researchers from British universities and institutes per year, and they also serve a wide range of British companies.

Major Facility Upgrades Underway

Both ESRF and ILL have been continuously upgrading their facilities in the past to meet the evolving needs of academic science and industrial R&D. Currently, two large-scale updates are running: the 180MEuro ESRF Upgrade Programme and the 85MEuro ILL Millenium Programme.

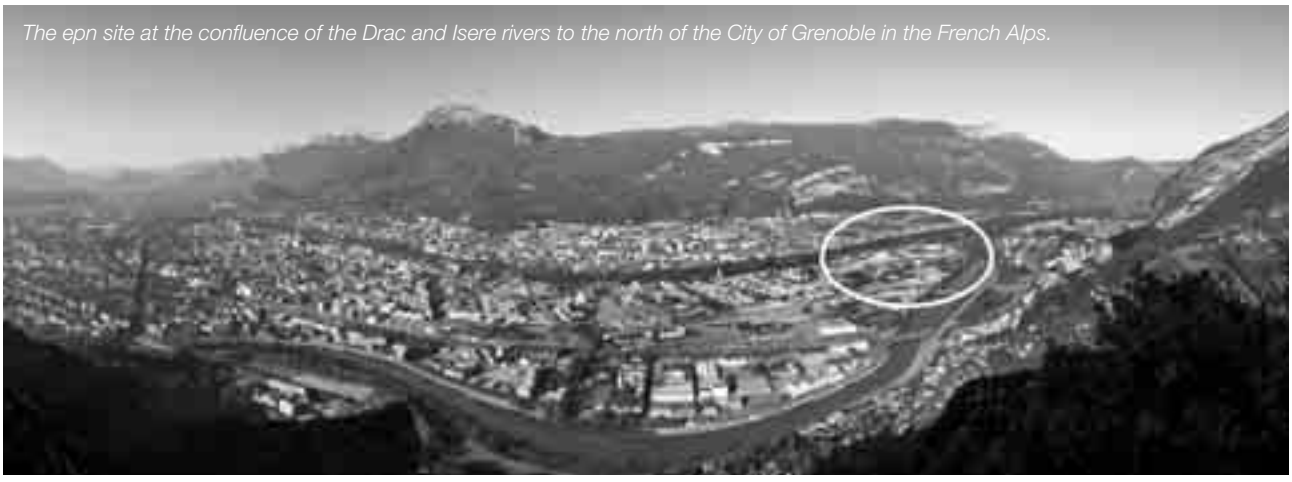
The ESRF Upgrade Programme is approaching the half-way mark of Phase I (2009-2015) with a peak in building activity and the restart of the ESRF after an exceptional 5-month shutdown. The most visible part of the ongoing works is the construction of the new premises for long beamlines in the eight beamline sectors ID01-ID02 and ID27-ID32. Phase I covers construction of 17 new or completely refurbished beamlines; the first of these are in user operation since the end of 2011. Phase II of the Upgrade (2015-2020) is now in preparation. A major task this year is to consult our user communities about their scientific and technical needs, a process that began at the 2012 Users' Meeting. The final proposal for Phase II will be submitted to Council in time for its Spring meeting in 2013 with a decision hopefully taken later in the year.

The Institut Laue-Langevin also is undergoing an ambitious upgrade plan. The *Millennium Programme*, founded on new scientific opportunities as well as exciting developments in instrument design, was officially launched in 2000 and the first phase completed in 2008. Six new instruments have been delivered and a further eight have been extensively upgraded. These developments are impacting strongly on the life sciences capability at the EPN Science Campus – with a number of powerful new instruments becoming available over the next 6 to 18 months. These include new instruments for crystallography and small-angle neutron scattering, with applications for the study of large scale structures in chemistry, biology and solid state physics.

Biological Crystallography on the epn

At the ESRF

Protein crystallography has a long history at the ESRF; the first experiments were made in 1994 with a single data collection taking a shift of beam time or more. Nowadays, data collection times are down to seconds and minutes and in 2011 the six ESRF MX beamlines handled over 140,000



The epn site at the confluence of the Drac and Isere rivers to the north of the City of Grenoble in the French Alps.

samples. In Phase I of its Upgrade Programme and building on the well-known advances made with the EMBL in beamline automation, the ESRF is creating an enhanced suite of facilities for structural biology.

The hub at the heart will be the ***MASSIF*** complex with three highly intense fixed wavelength beamlines which will offer a completely automated toolset for high-throughput sample evaluation, prioritisation, sorting and data collection. The three stations will each with a flux of ca. 10^{13} ph sec^{-1} (equivalent to ID23-1 or -2) and photon energy just above the selenium K-absorption edge (12.8 keV), but with complementary beam sizes:

- *MASSIF*-1 and *MASSIF*-2 with a 100 µm beam diameter
- *MASSIF*-3 with about 10 µm beam diameter

Automation will allow *MASSIF*-1 and *MASSIF*-2 to screen up to 1000 crystals a day. Advanced software protocols and workflows using the beamlines in parallel will allow the full characterisation and most effective use of crystal volumes, and the most efficient use of beam time. The microfocus station will also be equipped with high capacity sample changing robotics and allow samples to be screened in a variety of mounts such as plates and micro-fluidic chips. In addition to the *MASSIF* stations, a fully tunable beamline with variable beam size at the sample position, **ID30B**, will be constructed on the same sector to complete the ESRF's capacity for MX. The first user operation of the *MASSIF* stations is expected in May 2013, and for ID30B a year later.

The existing MX beamlines will also evolve: the iconic ID14 complex of four stations, which ID30 replaces, is being closed progressively; tunable **ID29** will have an enhanced micro-focus MAD and SAD capability – particularly at lower X-ray energies where the line will be made UHV compatible; tunable **ID23-1** will have a Pilatus 6M-F pixel detector installed later in 2012 to complement that already installed on ID29 and move to a continuously variable beam size using advanced compound refractive lens focussing; **ID23-2** will have a 1 x 1 micron beam focus option available with a very high precision data collection spindle. Finally, the bioSAXS activity has already been moved from ID14 to its new sector at **BM29**, right in the heart of the BM29-ID29-ID30 "structural biology village". BM29 is tunable and has an intensity enhanced by ten-fold over ID14-3 - allowing a faster throughput - and an on-line HPLC facility added to the existing sample changer robotics to allow SAXS spectra of samples to be recorded as they are purified.

The ESRF hosts several Collaborative Research Group (CRG) beamlines funded by member countries or consortia. One of these is **BM14**, a bending magnet beamline dedicated to macromolecular crystallography. The beamline optics, completely renewed during year 2011, are ideal for the multiple anomalous diffraction method that enables *de novo* phasing of diffraction data. The experimental hutch is equipped with cutting edge instrumentation, which will soon enable users to perform data collections from samples still in crystallisation plates as well as a microfocussing system to create a 30 micron beam. BM14 operation is funded by the EMBL and the Indian Department of Biotechnology (DBTP) for the benefit of both European and Indian MX communities.

At the ILL

Neutron macromolecular crystallography is a growing field that is making strong and unique contributions to structural biology thanks to a number of key aspects. Firstly, the **LADI-III diffractometer** has had a major impact. Since its installation in 2007, it has been responsible for wide range of unique contributions providing important information on the protonation states of biological macromolecules and on specific hydrogen bond interactions. LADI-III has just been refurbished and relocated and is expected to come on-line in May with a gain factor of around five. It is now a heavily sought-after instrument and oversubscribed by a factor of two to three. Secondly, the new **D19 diffractometer**, developed with EPSRC funding as part of the first phase of ILL's Millennium Programme is now demonstrating the scope of monochromatic neutron crystallography. A study on xylose isomerase was published in 2010 as a cover article in *Structure*, with a follow-up article in *Angewandte Chemie* describing the first observation of hydronium ions in a protein. Additionally, a new multimodal (monochromatic/polychromatic) diffractometer called **OCTOPUS** is being planned: The new instrument will deliver major efficiency gains as well as offering greatly extended flexibility through the option of several easily interchangeable modes of operation. This will build upon the demonstrable need to extend ILL's capacity for high resolution structural studies of protein systems, as well as the need to widen the scope of biological crystallography. The development will be carried out in close collaboration with structural biologists at the ESRF, and engineered in such a way that the user interface of the instrument (from sample to software) will be transparently identifiable to a large, dynamic, and driven community of European synchrotron X-ray macromolecular crystallographers.

ILL's capabilities for neutron macromolecular crystallography are strongly complemented by the developments for SANS. A third SANS machine (**D33**) has just been built – this will allow new types of SANS studies and also relieve the serious overload that is occurring for **D22** and **D11**. ILL's biological SANS work is now carried out in close collaboration with ESRF SAXS studies, with both approaches benefiting from the joint SANS/SAXS platform.

The success of recent crystallographic and SANS work owes much to the availability of deuterated protein provided by the **Deuteration Laboratory**, which is a part of ILL's Structural Biology/Life Science Group. It allows routine availability of perdeuterated protein crystals, and now provides more than 90% of the samples that are used on LADI-III. Perdeuteration greatly alleviates the crystal volume requirement and enhances the quality of the crystallographic analysis. The provision of deuterated protein is also of crucial value to the development of SANS work at the ILL, with a large fraction of SANS experiment using samples from the Deuteration Laboratory.

Partnership for Structural Biology (PSB)

Set up ten years ago by the ILL, the ESRF and the EMBL together with local partners the Partnership for Structural Biology (PSB) hosts a set of technical platforms that complement the capabilities of each of the individual partners.

The French Institut de Biologie Structurale (IBS), one of the local PSB partners, will in 2013 move into new premises on the EPN Science Campus, which will bring even more platforms into close vicinity of the European institutes.

There is increasing recognition of the fact that biological systems have to be studied in a far more integrated fashion, using methods that span resolution boundaries from atomic to cellular levels, and employing a wide range of techniques for sample preparation and *in vitro* and *in vivo* biophysical and structural characterisation. Within this overall vision is the idea that individual users coming to the ILL and ESRF are able to benefit from the capabilities of the other members of the Partnership. The PSB contains a powerful range of technology platforms including state-of-art instrumentation for crystallography, small-angle scattering, NMR, electron microscopy, as well as novel capabilities such as the Deuteration Laboratory (see above), an automated soluble expression platform, a eukaryotic expression facility and a high-throughput crystallisation platform. The PSB operates in such a way that ESRF and ILL users can benefit from these platforms and therefore enhances greatly the value of traditional facility access. The PSB is also making joint X-ray/neutron facility usage routine – not just for macromolecular crystallography but also for small-angle solution scattering – the PSB SANS/SAXS platform is now accessible through a single proposal mechanism, with users able to record both SANS and SAXS data during the same visit to the site.

1. ESRF structural biology facilities

Current	New	Technique	Beam size (µm)	Energy [keV]	Flux [ph/sec]	Key features
ID14-1 →	***MASSIF-1/-2***	MX	100	12.8	~10^{13}	Full automation
ID14-2 →	***MASSIF-3***		10x10	12.8	~10^{13}	Full automation and microfocus
ID14-3 →	**BM29**	SAXS	700 / 100	7-15	~$3x10^{12}$	Tunability, focus and detector, on-line HPLC
ID14-4 →	**ID30B**	MX	20-200	6-20	~10^{13}	Low divergence, variable beam size
–	**ID23-1**		30-150	6-20	~10^{12}	Variable beam size, pixel detector
–	**ID23-2**		1x1, 5x5	14.2	~10^{12}	1 micron focus
–	**ID29**		50x30 10x10	5-20	~10^{13}	Long wavelength, pixel detector

2. ILL structural biology facilities

Instrument	Technique	Data collection	Detector type	Key features
LADI-III	MX	Quasi-Laue ($\delta\lambda/\lambda \approx$ 25%, typical λ_{range} = 3-4 Å)	Cylindrical neutron-sensitive image plate (coverage > 2π sr)	Small crystals (>0.1mm^3) Large unit-cells (<1.5 x 10^6 Å^3) Fast data collection
D19	MX	Monochromatic (λ choice from 0.8-2.4 Å)	120° x 30° position-sensitive detector, gas: ^{3}He (5 atm) + CF_4 (1 atm)	High-resolution (d_{min} better than 1 Å)
OCTOPUS	MX	1. Quasi-Laue ($\delta\lambda/\lambda$ options from 5-35%) 2. Monochromatic (λ choices from 2.4-7.5 Å)	Octagonal array of neutron CCD/Scintillator detectors	Optimisation of data collection (S/N) Sample environment options, *in situ* Raman
D22	SANS	$\delta\lambda/\lambda$ = 10% (standard) 4.5 Å < λ < 25 Å	Reuter-Stokes multitube (^{3}He) detector (active area 1 m^2)	Large dynamic range (Q_{max}/Q_{min} in one instrument configuration) Polarised neutrons

Working together

The ESRF and ILL are working increasingly in concert for both academic and industrial use of X-ray and neutron facilities. ILL's neutron crystallography experiments are now routinely carried out in parallel with synchrotron X-ray studies, allowing neutron crystallographic data to be complemented directly by X-ray data. In all areas relevant to biology, the ESRF and ILL are making a major effort towards common sample and data processing procedures in a way that maximises the combined exploitation of the two facilities.

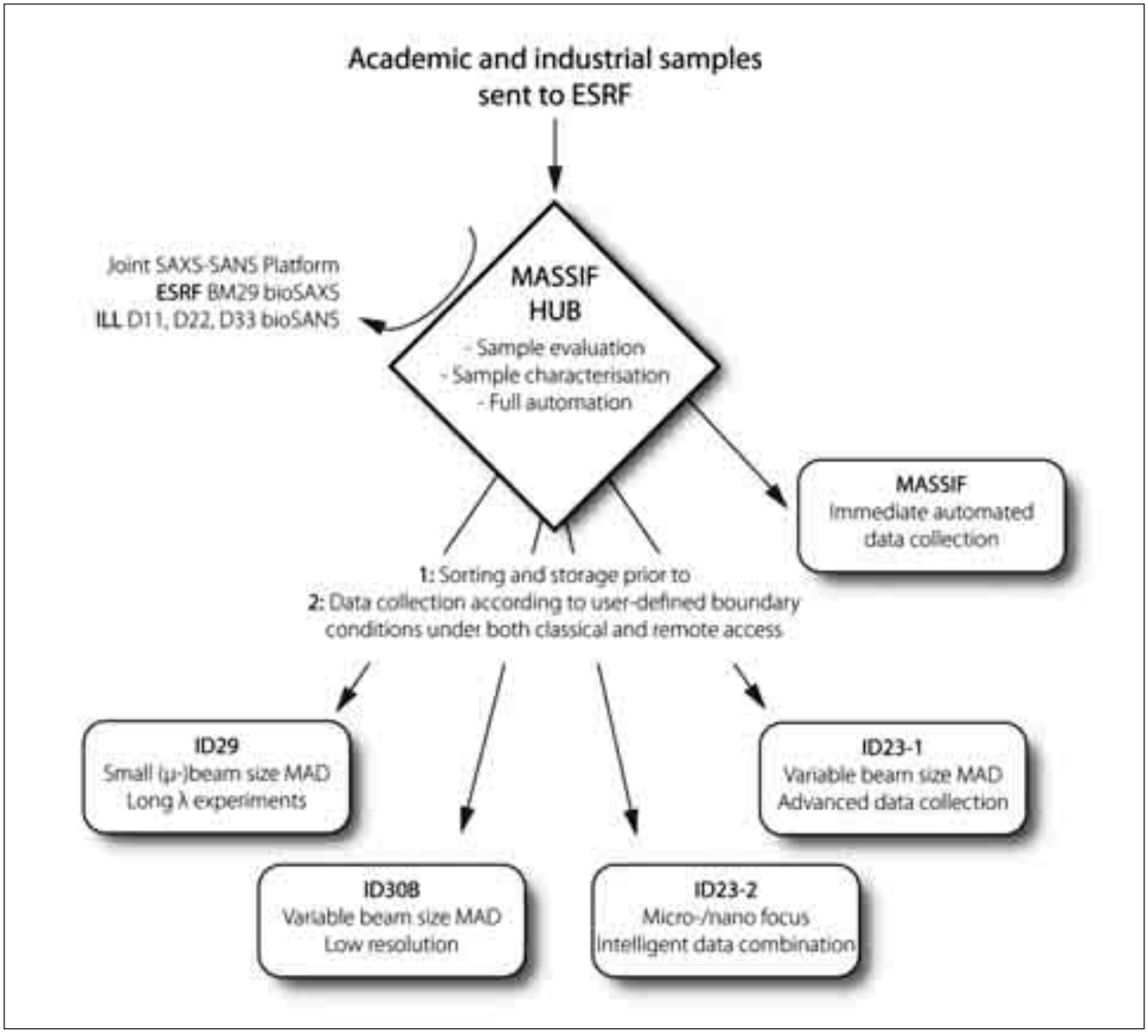
The instrumentation technologies - both in the hard- and software fields - developed at the European research infrastructures are available to all national facilities in the funding countries. Feedback by users will remain the most important driver for making these developments and for their implementation across the various user facilities.

Contacts

Should you have any queries regarding access and use of the ESRF or ILL facilities, please do not hesitate to contact the structural biology teams at both institutes:

- **ESRF Structural Biology** (go.esrf.eu/MX): Sean McSweeney (Group Head, mcsweeney@esrf.fr), Gordon Leonard (Deputy Head, leonard@esrf.fr), David Flot (Beamline Operations Manager, flot@esrf.fr), Christoph Mueller-Dieckman (Project Manager MX Upgrade, muellerd@esrf.fr)
- **ESRF CRG BM14 (www.bm14.eu):** Dr Hassan Belrhali (belrhali@embl.fr)
- **ILL Structural Biology Beamlines** (www.ill.eu/instruments-support/instruments-groups/), **Deuteration Laboratory** (www.ill.eu/sites/deuteration) and **Industrial Access:** Trevor Forsyth (tforsyth@ill.eu)
- **Industry access and collaborations at the ESRF:** Elspeth Gordon and Stephanie Monaco (Industry Liaisons for Structural Biology, gordon@esrf.fr and monaco@esrf.fr)

The future ESRF suite of facilities for structural biology with MASSIF as the central hub for sample evaluation, characterisation and sorting

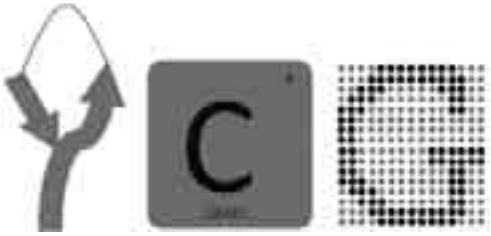


Young Crystallographers Satellite meeting

THIS year's Young Crystallographers Satellite meeting took place immediately before the main BCA Spring Meeting at the University of Warwick. It was great to see so many new and old faces at the meeting with a very high standard of talks being presented. There were a significant number of abstracts submitted for the satellite, with only 14 slots to fill; it was great to have such an enthusiastic interest in the meeting. Due to the vast number of abstracts submitted, we were really pleased to have some YCG representatives invited to speak at the main meeting. These people were Allan Pang, James Hall and Elena Marelli, their talks were very well received.

The second Parkin Lecture was this year presented by **Dr Lynne Thomas** from the University of Bath, entitled 'A Diffractometer's Tale - Exploring the Frontiers and Forests'. Lynne delved into the frontiers by describing her work educating undergraduate students about crystallography, from crystallisation through to structure solution and refinement. She then followed on to talk about the forests, which involved her research on crystalline fibres in wood and what effect strain or hydration on the wood had on the diffraction patterns.

Each year the YCG committee award the Durward Cruikshank prize to a Young Crystallographer who has made an outstanding contribution to crystallography. Although the winner this year was just outside the remit of a Young Crystallographer, it was decided by the committee and BCA council that the person's outstanding achievements deserved recognition. This year's recipient was **Dr Robin Owen** from Diamond Light Source. He has been heavily involved in beamline and method development of synchrotron beamlines since graduating in 2006, as well as supervising PhD students and carrying out outreach activities. He also presented a plenary talk at this year's satellite meeting.



At this year's AGM there were a number of new committee members appointed as well as a shuffle in the committee. **Duncan Sneddon** stood down as chair, being replaced by **Anna Warren** whose term as secretary/treasurer had come to an end. Duncan has been co-opted onto the committee as an ordinary member for a year to help the committee in an advisory capacity. **Claire Murray** remains as vice-chair and **Lauren Hatcher** has moved from IG representative to secretary/treasurer. There are also two retirements in the committee, **Peter Byrne** as CCG representative and **Sam Callear** as PCG representative. Their posts have been filled by **Helen Mason** and **Anthony Phillips** respectively. The role of BSG representative remains as **Soshichiro Nagano** and the IG representative was filled by **Kate Wittering**. Due to the re-shuffling in the committee one post remained open for a new ordinary member, which was filled by **Issy Kirby**. She joins our existing three ordinary members **Robert Young**, **Geoffrey Masuyer** and **James Hall**. Last but not least, the committee is completed by **Allan Pang**, our webmaster who over the past year has made an excellent YCG website (http://ycg.crystallography.org.uk/) and a recently developed Facebook page (http://www.facebook.com/YCG.BCA) to keep all the YCs up to date with our latest news.

In **Duncan Sneddon's** final report as chairman, he reported on the excellent outreach activities the YCG have been carrying out, led by **Claire Murray**. This involved a Café Scientifique in Reading, presented by **Prof. Chick Wilson**, and also holding a public engagement activity in March entitled 'The Structure of Stuff is Sweet' in a pub as part of Reading Science Week. The YCs had also been contacted by **Ruth Doherty** from CrystEngComm to see if anyone from the committee would be interested in becoming a web writer for the journal. **Claire Murray** enthusiastically took on this role and her posts can be found at http://blogs.rsc.org/ce/.

Anna Warren gave an account of the secretary's report and commented on the funding issues over the last year. The YCG applied for a small awards scheme through the STFC but were unfortunately unsuccessful. The next year will give the committee a chance to think about other funding bodies that can be approached. We are happy to hear feedback or suggestions from any YCs to: ycg@crystallography.org.uk.

Anna Warren
YCG Chair

YCG Satellite Meeting: Scientific Sessions

KENNETH Shankland from the University of Reading opened the Young Crystallographers Satellite meeting with his talk on structure solution from powder data. Quasi-Newton runs produced surprisingly successful rates for structure solution, and this is very useful for structures with accidental reflection overlap, where the net intensity is known, but the individual contribution to each intensity is not.

Soski Nagano from Queen Mary University, London, presented his work on the light-sensitive protein phytochrome. By troubleshooting with the "surface entropy reduction" strategy, it was possible to crystallise the model phytochrome Agp1 in the Pfr form, by modifying the cofactor to block conversion.

Ed Pyzer-Knapp from the University of Cambridge reported his use of computational chemistry to the issue of predicting molecular porous crystals. Boldly declaring that "MOFs were out", he used a series of computational methods to successfully predict the crystal structures of a series of tetrahedral imine cages.

Karim Sutton from the University of Oxford discussed his work on using anomalous diffraction to improve small molecule structures, using X-ray fluorescence data to determine chemical changes in the crystal. This includes discriminating between multiple oxidation states for atoms with near-identical X-ray scattering factors.

Alex Graham from the University of Edinburgh reclaimed "a victory for MOFs" by discussing his work on zeolitic imidazolate frameworks and incorporation of FC-77 into the pores using a combined experimental high-pressure and computational approach.

Thembaninkosi Gaulle from the University of Leeds then spoke about probing molecular interactions in copper amine oxidases. She explored the role of buried and surface metal sites by generating mutations in *Escherichia coli* copper amine oxidase, observing these by kinetic and crystallographic studies.

Claire Murray from the University of Reading highlighted some of the outreach work that the YCG have been carrying out. (See the outreach report, which follows this one.) The free unit cell building tools (aka marshmallows) proved to be very popular with the audience.

The biological plenary this year was given by **Robin Owen** from Diamond Light Source and discussed the development of the use of tomography to visualise very small or hard to see samples on the beamline. Also discussed was the use of UV/visible absorbance spectroscopy to obtain data complementary to the diffraction experiment.

Callum Young from the University of Oxford presented his work on magnetite, focusing on the atomic and magnetic ordering of the structure at low temperatures (10 K). With total neutron scattering data and reverse Monte Carlo refinements, large box atomic configurations were produced, consistent with experimental data.

Marco Llamas from the University of Manchester discussed his work on the interactions of counter ions with proteins correlated with enzyme activity. By replacing the usual counter ions with ones based on heavier elements (but with similar size and chemistry), counter ion interactions with the proteins could be identified.

Karun Arachchige from the University of St Andrews spoke about the synthetic and crystallographic studies of novel organotin acenaphthene compounds, where variation of the peri-substituents on the ligand provides an insight into weak non-covalent interactions.

Montha Meepripruk from Suranaree University of Technology, Thailand, presented her work on the tricyclic acyclovir crystal structure and the very disordered nature of the water molecules.

Lynne Thomas from the University of Bath gave the Parkin lecture in recognition of her outstanding contribution to science communication and crystallography. She highlighted some of the outreach work with undergraduates that they had carried out at the University of Bath, and also discussed some of her work on the fibre diffraction from wood.

Ioana Sovago from the University of Glasgow began the Tuesday session with a talk discussing the challenges associated with estimating the stability of polymorphic materials in charge density studies. This included the use of data from both neutron and X-ray diffraction to assist in calculations.

Richard Martin from the University of Portsmouth then spoke about the molecular basis of protein-DNA recognition in a bacterial genetic switch, using mutagenesis to determine the interactions between the protein and DNA sequence.

Alan Martin from the University of Bath gave his talk on the difficulties encountered during the crystallization of reactive compounds and how to overcome them, along with an example of a crystallized peroxy-acid.

Andrew Maloney from the University of Edinburgh then finished the session with a discussion on the PIXEL method which has been expanded to take account of transition metal species. The PIXEL method uses semi-classical density sums to calculate intermolecular interactions, which can be missed by taking a purely geometric approach.

Jessica Bland from the Royal Society gave an interesting talk on the history and importance of science outreach in society. This included a very interesting discussion on the various methods that scientists can use to advertise their work to the general public.

Claire Murray and **James Hall**
(University of Reading)

The Structure of Stuff is Sweet

DURING National Science and Engineering Week March 2012, the YCG held an outreach event on Crystallography in Reading, in association with the Thames Valley Branch of the British Science Association. We lured local pubgoers with the promise of sweets in exchange for an evening of crystallographic entertainment. Many people took the chance to try their hands at the dark art of crystal growing, observing their very own lysozyme crystals growing under a microscope.

Others took advantage of the diffraction gratings, lasers and slinkies to learn about waves and the fundamentals of diffraction. The construction of unit cells was particularly popular, with marshmallows, Toblerone and Maltesers as staple building materials (for scientific purposes of course!).

We had more than 40 participants show up, and lots of interest from teachers who expressed interest in bringing the workshop into their classrooms. We have also had interest in hosting the event again in London in collaboration with Science London. We would like to thank the British Science Association Thames Valley branch for funding and for publicity. We feel it was a very successful event and would like to thank all of the volunteers for their hard work to make this possible.

FRIENDS and colleagues of Professor Dame Louise Johnson will be very saddened to learn that she suffered a serious and very incapacitating heart attack with complications in August 2011 and has been in hospital since then. Louise is visited daily by members of her family, and, starting very recently, by a small number of friends. Cards and messages can be sent to Louise c/o Department of Biochemistry, South Parks Road, Oxford, OX1 3QU, from where they will be passed on to the family and communicated to Louise.

Please do not email Louise directly. As and when there is further news I will let everyone know via Crystallography News and the CCP4 Bulletin Board.'

Elspeth Garman

27th European Crystallographic Meeting

IN what promises to be a very exciting scientific programme, details of keynote speakers and microsymposia at the forthcoming meeting in Bergen have now been published.

Keynote Speakers and tentative titles:

- **Danny Shechtman**, Technion, Israel Institute of Technology, Haifa, Israel: *The Discovery of Quasi-Periodic Materials*
- **Michael Rossmann**, Purdue University, Purdue, USA: *EM X-ray interface*
- **Jacqueline Cherfils**, LEBS, CNRS, Gif sur Yvette, France: *The many roles of small GTPases*
- **Randy Read**, University of Cambridge, Cambridge, UK: *Extending the reach of molecular replacement*
- **Henry Chapman**, DESY/University of Hamburg, Hamburg, Germany: *Femtosecond protein nanocrystallography with an X-ray free-electron laser*
- **Jens Preben Morth**, University of Oslo, Oslo, Norway: *Membrane transporters*
- **Ross Angel**, University of Padova, Padova, Italy: *High Pressure Minerals and Materials*
- **Olivier Mentré**, UCCS, University of Lille, Villeneuve d'Ascq, France: *Phase Homology and Structural Prediction in Extended Series of Inorganic Bi-based Compounds*
- **Björn Winkler**, University of Frankfurt, Frankfurt, Germany: *Computational Crystallography*
- **Mark Spackman**, University of Western Australia, Crawley, Australia: *Charge densities and crystal engineering*
- **Paul Midgley**, University of Cambridge, Cambridge, UK: *Towards Routine Structure Solution using Precession Electron Diffraction*
- **Paola Gilli**, University of Ferrara, Ferrara, Italy: *Towards the unification of intermolecular forces: The hydrogen bond as a charge-transfer interaction*
- **Simone Techert**, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany: *Time Resolved Crystallographic Processes for Molecular Systems*
- **Maryjane Tremayne**, University of Birmingham, Birmingham, UK: *Structure solution from powder diffraction; new developments, applications and avenues*
- **Neil Champness**, University of Nottingham, Nottingham, UK: *Metal-Organic Frameworks: Synthesis and Applications*
- **Knut Urban**, Peter Grünberg Institute, Jülich, Germany: *Picometre electron microscopy*
- **Simon Parsons**, University of Edinburgh, Edinburgh, Scotland: *Absolute Structure Determination*

Microsymposia

1 Protein crystallization and sample preparation
2 MX at Synchrotron Sources, including X-FELs and time-resolved crystallography
3 Getting the best data from your crystal(s)
4 Phasing challenges. Bootstrapping from a poor start
5 Advances in refinement and validation. Ligand chemistry
6 Bioinformatics informs MX
7 Pharmaceutical crystallography - Drug design: success and failures
8 Membrane proteins
9 EM and MX for viruses, assemblies and biological nano-machines
10 Infection and Disease
11 Frontiers in Structural Enzymology
12 Molecular recognition
13 Energy related materials
14 Materials in operando and in situ crystallography of materials
15 Structural complexity of minerals and inorganic materials
16 Minerals from Scandinavia: a unique crystal chemistry and inspiration for new materials
17 Structural and crystal-physical studies in large volume high-P devices
18 New perspectives for charge density analysis: materials properties from inorganics to macromolecules
19 The importance of low temperature in charge density studies: history and future
20 Probing crystal structures at the nanoscale by quantitative electron crystallography
21 Crystal chemistry of aperiodic crystals and frustrated systems
22 Quasicrystals, their approximants and surfaces: from the atomic to the nanoscale
23 Intermolecular interactions at ambient and extreme conditions
24 Polymorphism and chirality in molecular crystals
25 Design, structure, and function of multi-component crystals
26 Porous materials for gas storage and other applications
27 Molecular structures in catalysis and magnetism
28 Imaging using diffraction, spectroscopy or coherent signals
29 Likely to be useful: Statistical software packages
30 Buy one, get one free: Software for twin handling
31 "How-to"
32 Optimizing the use of Databases
33 Neutrons and high-resolution X-ray diffraction for bio-crystallography
34 Aperiodic, short-range ordered and non-crystalline materials at ambient and non-ambient conditions
35 Ferroic and multiferroic materials
36 Towards megabar pressures: complex and geo-materials
37 Electron Crystallography on functional materials
38 Structure solution of minerals and inorganics by electron crystallography
39 Electron diffraction and X-ray powder diffraction: getting the best of both worlds
40 Structure prediction for crystalline and amorphous molecular solids
41 Dynamics in crystals: experimental techniques and software
42 Big "small molecules" and small "macromolecules" – learning techniques from each other
43 Hot topics and structures in molecular chemistry
44 Controlling and Monitoring crystal growth and quality
45 Advances at lower resolutions: new experimental and modeling approaches
46 Advances in powder diffraction: structure solution and structure-property relationships
47 3rd Generation Synchrotrons – Radiation Damage/Impact on Crystals
49 Crystallographic teaching
50 X-ray or neutron optics and instrumentations

Obituary

DAVID Sayre, a pioneer crystallographer, a member of the team that wrote the original FORTRAN compiler, and a visionary leader in X-ray microscopy, died on February 23, 2012.

David received his B. S. from Yale at the age of 19. During the last year of World War II he worked on Radar at the MIT Radiation Laboratory, before going to graduate school. He received his Ph. D. from Oxford University in 1951, working with Dorothy Hodgkin. It was during this time that David and his wife Anne got to know Rosalind Franklin, another young crystallographer, working at Kings College, London.

David wrote some of his seminal papers during the 1951-52 period. It was then that he discovered what is known today as Sayre's equation, and which was the first and critical step in the development of direct methods in crystallography. His half-page 1952 paper "Some implications of a Theorem due to Shannon" forms the foundation of diffraction microscopy, and 50 years later is still frequently cited in the literature.

Between 1956 and 1990 Sayre worked for IBM, where he was Assistant Manager of the Fortran Development Group and later Corporate Director of Programming. In the 1960's he lead the Programming Research Group that developed the first virtual memory operating system. In 1971 he proposed that IBM's newly developed electron beam microfabrication technique be used to make Fresnel zone plates for X-ray microscopy. It took a decade for this idea to be realized, but it is now the basis of the rapidly growing field of X-ray microscopy at synchrotron light sources world wide, and of commercial laboratory instruments made by the company, Xradia, founded by one of Sayre's first Ph. D. students, Wenbing Yun.

In 1972-73 the Sayres returned to Oxford where David once again worked in Dorothy Hodgkin's lab. This was after the publication of the book by James Watson, the Double Helix, in which the author treated the contributions of Rosalind Franklin to DNA structure determination in a scandalously dismissive way. This inspired Anne Sayre to write the book "Rosalind Franklin and DNA", a book that became a best seller, and went a long way toward setting the record straight.

Subsequently David turned his attention to X-ray microscopy. He realized that due to the short wavelengths involved, X-rays could reach higher resolution than standard visible light microscopes, and due to the penetrating nature of the radiation, they would not be limited to ultrathin samples as electron microscopes are. He worked on contact microscopy at IBM, and later became involved with the development of microscopes using the National Synchrotron Light Source at Brookhaven National Laboratory.

After his retirement from IBM, he served as Adjunct Professor at Stony Brook University. Sayre's last great scientific contribution was Diffraction Microscopy, or Coherent Diffraction Imaging. In 1980 he realized that synchrotron lightsources may be powerful enough to provide sufficient coherent X-rays so that the diffraction pattern of non-crystalline specimens could be recorded. These patterns would be continuous, and not restricted to Bragg peaks. He conjectured that even though only the intensity could be recorded and not the phase, the information could be sampled on a much finer grid than Bragg peaks from crystals, and this may make the phase reconstruction possible.

In the 1980's he succeeded in recording the first diffraction patterns from non-crystalline samples. In the 1990's, working with Henry Chapman (then a Stony Brook postdoc) and John Miao (then a graduate student), he was able to apply James Fienup's iterative algorithm to find the phases for a computer generated diffraction pattern. The final breakthrough came when Miao succeeded in reconstructing an experimentally recorded diffraction pattern. This achievement opened up the field of diffraction microscopy, now practiced in different forms at many lightsources around the world, and which is playing a critical role in the experimental program at recently developed free electron lasers such as the Linac Coherent Lightsource at SLAC.

During his career, Sayre served on numerous committees. In 1983 he was President of the American Crystallographic Association. He received the organization's Fankuchen Award in 1989. In 2008, at the triennial Congress in Osaka he received the highest award of the International Union of Crystallography, the Ewald Prize. David was a superb scientist, a warm hearted colleague, and an exceptional mentor. He was preceded in death by his wife, Anne. He is greatly missed.

Chris Jacobsen, Argonne National Laboratory and Northwestern University

Janos Kirz, Lawrence Berkeley National Laboratory

John Miao, UCLA

(Reprinted by permission from *Physics Today*)

David Sayre receiving the Ewald Prize in 2008 (IUCr)

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, c.h.schwalbe@hotmail.com . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

3-6 June 2012
23nd Conference on Crystal Growth and Epitaxy - West (2012 AACGE-west), Fallen Leaf 3-8 June 2012 Lake, CA, USA.
http://www.crystalgrowth.us/accge_west23/

3-8 June 2012
Electronic Processes in Organic Materials. Exploring the Fundamentals of Organic Electronics. Gordon Research Conference, Lucca, Italy.
http://www.grc.org/programs.aspx?year=2012&program=elecproc

3-8 June 2012
Multiphoton Processes. Attoseconds, Intense Fields, and Ultrafast Imaging. Gordon Research Conference, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=multiphot

4-8 June 2012
ICDD Clinic on X-ray Powder Diffraction. Session I - Fundamentals of X-ray Powder Diffraction, Newtown Square, PA, USA.
http://www.icdd.com/education/xrd.htm

7-14 June 2012
Bombannes 2012. 11th European School on Scattering Methods Applied to Soft Condensed Matter, Gironde, France.
http://www.ill.eu/news-events/events/bombannes-2012/

9-10 June 2012
Plasmonics. Light--Matter Interaction at the Nanoscale. Gordon Research Seminar, Waterville, ME, USA.
http://www.grc.org/programs.aspx?year=2012&program=grs_plsmnc

10-15 June 2012
Plasmonics. Light--Matter Interaction at the Nanoscale. Gordon Research
Conference, Waterville, ME, USA.
http://www.grc.org/programs.aspx?year=2012&program=plasmonics

11-14 June 2012
10th International Workshop on Crystal Growth of Organic Materials, University of Limerick, Limerick Ireland.
www.cgom2012.com/

11-13 June 2012
Geo-Raman Xth Meeting, Nancy, France.
http://georaman10.uhp-nancy.fr/georaman/scope.html

11-15 June 2012
ICDD Clinic on X-ray Powder Diffraction. Session II - Advanced Methods in X-ray Powder Diffraction, Newtown Square, PA, USA.
http://www.icdd.com/education/xrd.htm

14-16 June 2012
Raman Spectroscopy Applied to Earth Sciences and Cultural Heritage, International School, Nancy, France.
http://georaman10.uhp-nancy.fr/internationalschool/scope.html

16-17 June 2012
Noble Metal Nanoparticles. New Understanding in Synthesis, Characterization and Applications of Noble Metal Nanoparticles, Gordon Research Seminar, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=grs_noble

16-24 June 2012
Seventh International Topical Meeting on Neutron Radiography, Kingston, ON, Canada.
http://itmnr-7.com

17-20 June 2012
European Conference of Crystal Growth 2012, University of Strathclyde, Glasgow.
http://eccg4.org/

17-20 June 2012
Electron Crystallography School - Methods and Applications, Stockholm, Sweden.
http://www.mmk.su.se/electron-crystallography

17-22 June 2012
Noble Metal Nanoparticles. Gordon Research Conference, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=noblemetal

18-21 June 2012
Coherence 2012. International Workshop on Phase Retrieval and Coherent Scattering, Fukuoka, Japan.
http://rsc.riken.jp/coherence/

18-21 June 2012
Ultrafast X-ray Summer School, Menlo Park, CA, USA.
http://www-conf.slac.stanford.edu/uxss/

18-21 June 2012
Nanotech Conference and Expo 2012, Santa Clara, CA, USA.
www.techconnectworld.com/Nanotech2012

18-22 June 2012
European Conference on X-ray Spectrometry (EXRS 2012), Vienna, Austria.
http://www.ati.ac.at/EXRS2012/

18-23 June 2012
Summer School on the Fundamentals of Neutron Scattering, Gaithersburg, MD, USA.
http://www.ncnr.nist.gov/summerschool/ss12/index.html

20-22 June 2012
International Symposium on X-ray and Electron Crystallography – from Materials Sciences to Structural Biology. Celebration of Professor Sven Hovmöller's Scientific Career, Stockholm, Sweden.
http://www.mmk.su.se/electron-crystallography

21 June 2012
100 Years of Diffraction: Historical Highlights and a Look into the Next 100 Years. Meeting of the Swiss Society for Crystallography, Zürich, Switzerland.
http://www.oci.uzh.ch/group.pages/linden/sgk2012/

21-22 June 2012
Applied Mineralogy of Cement and Concrete. MSA Short Course, Trondheim, Norway.
http://www.icdc2012.com/

24-28 June 2012
ACNS2012. 6th American Conference on Neutron Scattering, Washington, DC, USA.
http://www.mrs.org/acns-2012/

24-29 June 2012
Research at High Pressure. Gordon Research Conference, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2012&program=highpress

24-29 June 2012
Correlated Electron Systems. Correlations and Topology in Electron Systems, Gordon Research Conference, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=correlec

25-28 June 2012
IWPCPS-14 (International Workshop on Physical Characterization of Pharmaceutical Solids), Barcelona, Spain.
http://www.iucr.org/news/notices/meetings/meeting_2011_252

25-29 June 2012
WLMI-2012. International Workshop on Laser-Matter Interaction, Porquerolles, France.
http://www.pks.mpg.de/~wlmi12/

2-6 July 2012
NSS-7. 7th International Workshop on Nano-scale Spectroscopy and Nanotechnology, Zurich and Villigen, Switzerland.
http://indico.psi.ch//event/nss7

4-6 July 2012
3rd Workshop on Simultaneous Combination of Spectroscopies with X-ray Absorption, Scattering and Diffraction, ETH Zurich, Switzerland.
http://www.psi.ch/csx2012

7-8 July 2012
Ion Channels. Excitable Cells and Electrical Signaling. Gordon Research Seminar, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=grs_ion

8-13 July 2012
Ion Channels. Gordon Research Conference, South Hadley, MA, USA.
http://www.grc.org/programs.aspx?year=2012&program=ionchan

8-13 July 2012
UP2012. XVII International Conference on Ultrafast Phenomena, Lausanne, Switzerland.
http://www.up2012.org/

9-11 July 2012
Neutron Delivery Systems, Grenoble, France.
http://www.ill.eu/news-events/events/nds-2012/

15-17 July 2012
ISMB 2012. 20th Annual International Conference on Intelligent Systems for Molecular Biology, Long Beach, CA, USA.
http://www.iscb.org/ismb2012

15-19 July 2012
4th International Congress on Ceramics (ICC4), Chicago, IL, USA.
http://ceramics.org/4th-international-congress-on-ceramics-icc4

15-20 July 2012
35th Annual British Zeolite Association Meeting, Chester, UK.
http://chemweb.bham.ac.uk/~hriljaja/bza2012/index.htm

15-20 July 2012
Sagamore XVII. Great Potentials from Advanced Probes, Kitayuzawa, Japan.
http://rsc.riken.jp/sagamore/home/

16-24 July 2012
Canadian Synchrotron Summer School: Synchrotron Techniques in Materials Research, Saskatoon, SK, Canada.
http://www.lightsource.ca/education/summerschool/

22-27 July 2012
15th International Conference on Experimental Mechanics, Faculty of Engineering, University of Porto, Porto, Portugal.
http://paginas.fe.up.pt/clme/icem15/

28-29 July 2012
Radiation Chemistry. Radiation Driven Processes in Physics, Chemistry, Biology and Industry. Gordon Research Seminar, Andover, NH, USA.
http://www.grc.org/programs.aspx?year=2012&program=grs_rad

28 July - 1 August 2012
ACA Meeting 2012, Westin Waterfront Hotel, Boston, MA, USA.
http://www.amercrystalassn.org/2012-meeting-homepage

29 July - 2 August 2012
Microscopy & Microanalysis (M&M 2012), Phoenix, AZ, USA.
http://www.microscopy.org/MandM/2012/

29 July - 3 August 2012
Radiation Chemistry. Radiation Driven Processes in Physics, Chemistry, Biology and Industry. Gordon Research Conference, Andover, NH, USA.
http://www.grc.org/programs.aspx?year=2012&program=radchem

29 July - 3 August 2012
Stereochemistry, Newport, RI, USA.
http://www.grc.org/programs.aspx?year=2012&program=stereochem

29 July - 3 August 2012
Scientific Methods in Cultural Heritage Research Non-Destructive Imaging and Micro-Analysis in Cultural Heritage. Gordon Research Conference, West Dover, VT, USA.
http://www.grc.org/programs.aspx?year=2012&program=heritage

6-10 August 2012
61st Annual Denver X-ray Conference, Denver, CO, USA.
http://www.dxcicdd.com/

6-11 August 2012
27th Meeting of the European Crystallographic Association, Bergen, Norway.
http://ecm27.ecanews.org/

12-17 August 2012
Defects in Semiconductors. Gordon Research Conference, Biddeford, ME, USA.
http://www.grc.org/programs.aspx?year=2012&program=defects

13-17 August 2012
XXI International Materials Research Congress (IMRC) 2012, Cancun, Mexico.
http://www.mrs-mexico.org.mx/imrc2012/index.php

19-23 August 2012
ACS Fall 2012 Meeting. Materials for Health & Medicine, Philadelphia, PA, USA.
http://portal.acs.org/portal/PublicWebSite/meetings/nationalmeetings/CNBP_029137

24-27 August 2012
International Workshop on New Developments of Methods and Software for Protein Crystallography, Xi'An, China.
Professor Xiao-Dong Su (e-mail: xdsu@pku.edu.cn).

27 August - 1 September 2012
International Summer School on Crystal Growth and Photovoltaic Materials, Brasov, Romania.
http://rocam.unibuc.ro/intschool/index.html

2-6 September 2012
First European Mineralogical Conference (EMC2012), Frankfurt, Germany.
http://emc2012.uni-frankfurt.de/

2-6 September 2012
XXII Conference on Applied Crystallography (XXII CAC), Targanice/Andrychów, Poland.
http://www.cac.us.edu.pl/

2-6 September 2012
ECSCRM2012. 9th European Conference on Silicon Carbide and Related Materials, Saint Petersburg, Russia.
https://www.ecscrm-2012.org/

2-7 September 2012
Aperiodic 2012, Cairns, Queensland Australia.
http://www.iucr.org/news/notices/meetings/meeting_aperiodic_2012

3-7 September 2012
CMD-24, ECOSS-29, ECSCD-11 and CMMP-12. European Condensed Matter Conferences, Edinburgh, UK.
http://www.cmd-24.org/Home

4-9 September 2012
22nd IUBMB and 37th FEBS Conference, Seville Conference and Exhibition Centre, Seville, Spain.
http://www.iubmb-febs-2012.org/IUBMBFEBS2012/

11-14 September 2012
Mc Phase School 2012, Grenoble, France.
http://www.ill.eu/news-events/events/mc-phase-2012/

13 September 2012
First Annual Open Day of the EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation, University of Strathclyde, Glasgow, UK.
www.cmac.ac.uk

14-15 September 2012
Applications of Precession Electron Diffraction, Manchester, UK.
http://www-hrem.msm.cam.ac.uk/events/Precession_Meeting/main.xhtml

15-20 September 2012
6th European Charge Density Meeting, Štrbské Pleso, Slovakia.
http://ecdm6.stuba.sk/?page=home

16-19 September 2012
MOF2012. 3rd International Conference on Metal-Organic Frameworks and Open Framework Compounds, Edinburgh, UK.
http://events.dechema.de/en/mof2012

16-21 September 2012
50th EHPRG Meeting, Thessaloniki, Greece.
http://www.ehprg.org/meetings/

17-20 September 2012
7th International Sample Environment Workshop, Amora Hotel Jamison, Sydney, Australia.
http://www.ansto.gov.au/research/bragg_institute/current_research/conferences_and_workshops/sample_environment_at_neutron_scattering_facilities

17-21 September 2012
E-MRS 2012 Fall Meeting, Warsaw, Poland.
http://www.emrs-strasbourg.com/index.php?option=com_content&task=view&id=500&Item=172

20-22 September 2012
The first 24 years of reverse Monte Carlo Modelling, Hotel Normafa, Budapest, Hungary.
http://www.szfki.hu/~nphys/rmc5/rmc5.html

23-28 September 2012
ICCBM 14. 14th International Conference on the Crystallization of Biological Macromolecules, Huntsville, AL, USA.
http://iccbm14.org/

24-28 September 2012
SR Summer School 2012, Oxford and Didcot, Oxon, UK.
http://www.diamond.ac.uk/Home/Events/SR-Summer-School-2012.html

1-3 October 2012.
Basic Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA
http://www.icdd.com/education/rietveld-workshop.htm

4-5 October 2012
Advanced Rietveld Refinement & Indexing Workshop, Newtown Square, PA, USA.
http://www.icdd.com/education/rietveld-workshop.htm

7-9 October 2012
ICRS-9. Ninth International Conference on Residual Stress, Garmisch-Partenkirchen, Germany.
http://www.mf.mpg.de/en/abteilungen/mittemeijer/icrs9/index.htm

14-18 October 2012
2012 AAPS Annual Meeting and Exposition, Chicago, IL, USA.
http://www.aaps.org/annualmeeting/

14-19 October 2012
IWN2012. International Workshop on Nitride Semiconductors, Sapporo, Hokkaido, Japan.
http://iwn2012.jp/

16-18 October 2012
Handheld XRF Workshop, Newtown Square, PA, USA.
http://www.icdd.com/education/handheld-xrf-workshop.htm

20-27 October 2012
BioCrys2012. Fundamentals of Modern Methods of Biocrystallography, Oeiras, Portugal.
http://www.febs.org/index.php?id=652

22-26 October 2012
Crystal structure prediction using the USPEX Code, Lausanne, Switzerland.
http://www.cecam.org/workshop-0-635.html

28-31 October 2012.
EPDIC13. 13th European Powder Diffraction Conference, Grenoble, France
http://epdic13.grenoble.cnrs.fr/

28-31 October 2012
7th International Workshop on Modeling in Crystal Growth (IWMCG-7), Taipei, Taiwan.
http://iwmcg7.ntu.edu.tw/

18-23 November 2012
International Small-Angle Scattering Conference (SAS2012), Sydney, Australia.
http://www.sas2012.com/

26-30 November 2012
2012 MRS Fall Meeting and Exhibit, Boston, MA, USA.
http://www.mrs.org/fall2012/

2-5 December 2012
AsCA 12/CRYSTAL 28, Adelaide, Australia.
http://www.sapmea.asn.au/conventions/crystal2012/index.html

6 December 2012
Bragg Symposium: Celebrating 100 years of Crystallography, Adelaide, Australia.
http://www.sapmea.asn.au/conventions/crystal2012/bragg.html

4-10 August 2013
ISSCG-15. 15th Summer School on Crystal Growth, Gdansk, Poland.
http://science24.com/event/isscg15/

11-16 August 2013
ICCGE-17. 17th International Conference on Crystal Growth and Epitaxy, Warsaw, Poland.
http://science24.com/event/iccge17/

25-29 August 2013
28th European Crystallographic Meeting, University of Warwick.
http://www.crystallography.org.uk/

5-12 August 2014
IUCr2014. 23rd Congress and General Assembly, Montreal, Quebec, Canada.
http://www.iucr2014.org/

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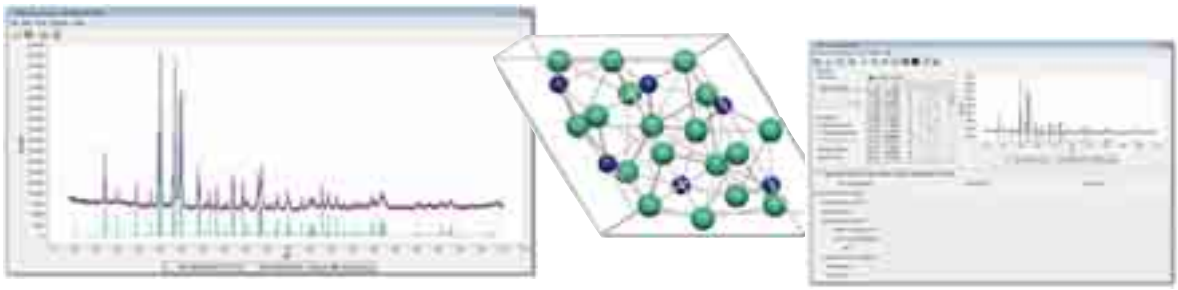

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