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NEXT ISSUE OF CRYSTALLOGRAPHY NEWS

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President's Remarks

Cover pictures left to right:

Chis Cardin local organiser of Reading Meeting

Bob Gould leads the singing of Arnold Beevers favourite (My Bonnie lies over the ocean) at the Conference Dinner

Claire Wison receiving the CCDC award from Frank Allen

Kate Crennell at the Education in Crystallography Discussion

The BCA Spring Meeting organised by Chris Cardin and Northern Networking was superb from the point of view of both science and the administration. The groups had all been allocated extra funds to invite top speakers from Europe and further afield. They spent it well with the result that the scientific programme was as good as any BCA Meeting I have attended, and everyone involved is to be congratulated. The scope of the programme was especially notable with major talks at all the sessions. We were, however, a little disappointed by the number of people attending (about 270); this was probably due to the use of a weekend (which are becoming ever more precious), the cost, and problems with bursaries - more of this later. The new newsletter format was, in general, also very well received.

The AGM saw the election of a new Vice President in Paul Fewster, and a new Secretary, Chris Cardin (who was obviously hooked on BCA administration after her conference experience!). We also said 'thank you' to Frank Allen and Hilary Muirhead who have finished their terms as BCA officers. As I frequently remark, the BCA is well served by its Council members and officers, and Hilary and Frank have done a fine job. We also welcomed Kate Crennell back into the fold as Education Officer which is a new, and important post for the BCA. Kate chaired a lively and well-attended discussion on education in crystallography at Reading, and has come away from the meeting with some good ideas for ways forward in this vital area.

On a related topic, the AGM expressed the desire for a re-appraisal for the way in which bursaries are awarded, and this has been taken on board by Council with establishment of a bursary fund, substantially funded by the BCA in honour of Arnold Beevers. Bob and Sheila Gould write about this on page 4. Your support will be very welcome. We are also investigating other ways of raising finance for students to attend our meetings.

The final payment of about £31K from the profits of the Glasgow IUCr Meeting was also handed over to the BCA at Reading. This brings the total to about £104K so we should be awash with money one would think. Life and money are never quite that simple, and our treasurer, Dave Taylor, explains our financial position and where this money is going on page 5.

Have a good summer.

CGilmore

Chris Gilmore
June 2001

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Full committee details on the BCA website
http://bca.cryst.bbk.ac.uk/BCA/

The second issue

Judging by the comments I have received since the issue of the March newsletter the majority of BCA members are happy with the new format. I welcome any feedback 'positive or negative' so that we can continue to produce a newsletter that you the members enjoy reading. A large section of this issue is devoted to the reporting of the Spring Meeting at Reading University. This year we have pictures as well as text, due to the efforts of Christine Cardin and helpers who took many photographs at the meeting. In the March issue I included several technical articles courtesy of CLRC and in this issue there is one technical article which I think will interest. I hope that some of you, whether in Industry or Academia, will be inspired to put pen to paper and produce similar articles for inclusion in future issues of the newsletter.

Jo Jutson
April 2001

Arnold Beevers Bursary Fund

The BCA Council at the Reading Meeting agreed to set up a substantial Bursary Fund. This is in response to a need, expressed at many AGMs, to increase the participation of young Scientists in our meetings. We are particularly pleased that Council have decided to name this fund in honour of the late Dr Arnold Beevers, and we know he would have thoroughly approved of this move.

Arnold was a firm believer in the free and open exchange of scientific ideas and information. He was also a founder member of the BCA and thrived on getting together with people of all ages there and at IUCr and ECM meetings. Everyone who came across him at one of these could immediately sense how much sheer fun he got from them. He was particularly keen to meet young scientists and to encourage their participation. In addition, he spent much of his life working with disabled people and helping them to develop their full potential. With all this in mind, Council has decided to devote the main support to students, but post-docs will also be considered. Special consideration will be given to disabled applicants.

Council is starting the fund by placing £20 000 in it, and further donations in memory of Arnold will be most gladly received. These may be sent to the BCA Office, with cheques made payable to the "British Crystallographic Association" and marked "Arnold Beevers Bursary Fund" on the reverse. A form for making a donation is enclosed with this newsletter. Further opportunity to contribute will be given with next year's subscription. Applications for bursaries should be made as in the past.

Bob and Sheila Gould

Acknowledgements
BCA Sponsors

The British Crystallographic Association is grateful to Birkbeck College, University of London, who host and manage the server for our Website.

BCA Prize

BCA Council has approved a BCA Prize Lecture to be awarded each year except when there is a Dorothy Hodgkin award or another named lecture. (To see further details on the origins and frequency of BCA lectures see: http://bca.cryst.bbk.ac.uk/BCA/CNews/1997/Sep97/namel.html)

1. It is to be called the 'BCA Prize Lecture' and can be awarded to any crystallographer in the world, but is named in honour of a prominent British crystallographer; *this name would change with each award*. So we would have, for example, 'The BCA Prize Lecture in honour of XXX'.
2. The crystallographer in whose honour it is given would attend the BCA Meeting and present the prize. Their expenses would be paid for by the BCA. There should be some link between the work of the two people involved.
3. The recipient would receive full travel costs, and would give a lecture at the BCA Meeting. They would also receive a trophy of some sort rather like the quaichs given to the Dorothy Hodgkin award winners.

Nominations for this award, to be presented at the Nottingham BCA Spring Meeting are now sought. They should be sent to the Secretary, Dr Chris Cardin whose address can be found in the list of BCA officers. They should be received by October 1st 2001. Nominations should include a summary of the achievements of the two crystallographers involved.

Chris Gilmore

IUCR Windfall

What is happening to the donations received from Crystal Congress 1999? A cheque for £32,114 was handed over at the AGM in Reading making a final total of £108,000. The souvenir colour supplement of the 1999 meeting cost £5K to produce. The AGM ratified a proposal to invest £50K for the long term to provide income with growth. This will buffer the present £45K BCA investments which mature over the coming years. Council has approved the following spending programme. To establish a £25K IUCr meeting loan fund requested by Crystallography Congress 1999. This money is to be lent to the next IUCr Meeting to provide bursaries. It is to be repaid from the profits of the congress, and there is a hope that they will provide such a loan to the 2005 congress. The Arnold Beevers Bursary Fund (see elsewhere in this issue) will be established with £5K of operating funds and £15K invested to provide income into the operating fund for future years. This makes a total spend of £100K split between securing future income to fund the charitable work of the BCA and direct charitable expenditure on supporting the next generation of crystallographers and currently leaves the BCA with unrestricted working cash funds of £15K.

Dave Taylor

Obituary

Clifford G Shull 1915-2001

MIT Professor Emeritus Clifford G. Shull died on March 31, 2001 aged 85. He was co-recipient of the Nobel Prize in physics in 1994, awarded for his pioneering work in neutron scattering. Professor Shull started in work in 1946 at what is now Oak Ridge National Laboratory. He teamed up with the late Ernest Wollan, and for the next nine years they explored ways of using the neutrons produced by nuclear reactors to probe the atomic structure of materials. In his opinion the most important problem he worked on at the time dealt with determining the positions of hydrogen atoms in materials.

As he refined the scattering technique, Professor Shull studied the fundamental properties of the neutron itself. He also initiated the first neutron diffraction investigations of magnetic materials. This yielded information about the magnetic properties of materials at the atomic level, opening up an entirely new field of study. Professor Shull's awards include the Buckley Prize, which he received from the American Physical Society in 1956, and election to the American Academy of Arts and Sciences (1956) and to the National Academy of Sciences (1975). In 1993 he received the Royal Swedish Academy of Sciences' Gregori Aminoff prize for his "development and application of neutron diffraction methods for studies of atomic and magnetic structures of solids."

BCA Spring Meeting - Reading 2001

From the Local Organiser, BCA Reading 2001

Here in Reading we are still feeling the excitement of having hosted a highly successful and enjoyable meeting. For those thinking of doing this in the future, it is absolutely exhausting, even with the excellent professional support of Northern Networking, but very worthwhile. We took large numbers of photos, which can be accessed through the Web (www.chem.rdg.ac.uk/bca) and which capture some of the spirit of the occasion. A big thank you to all helpers, session organisers and chairs, local committee members and sponsors/exhibitors for your many contributions and enthusiasm. Without you all there would have been no meeting. Please enjoy reading the reports of the sessions which follow, many of which had the great merit of bridging some of the gaps between the BCA groups.

The main regret I have is that this meeting was not more affordable for students and young postdocs, but I am happy to say that we have already taken action to change things for next year, and I am looking forward to seeing far more students next year in Nottingham. My best wishes to Sandy Blake and his committee.

Christine Cardin

Visualisation (Plenary Lectures)

Crystallographers collect a lot of data, and use it to generate a lot more. We have been immensely pro-active in our development of computer graphics and databases, so a plenary session on visualisation has a relevance to all branches of the subject.

The session started with Rod Hubbard (University of York) who looked at the problem from a macromolecular viewpoint and from an historical perspective. His main example involved exploring the structure and reactivity of the oestrogen receptor and the molecular biology of oestrogen action. As you would expect, he drew upon the full graphical resources employed by macromolecular crystallographers, but concluded that not much has changed with regard to graphics techniques in the last five years apart from faster and cheaper computers.

Sam Motherwell (CCDC) followed with a talk on 'Visualisation of Molecular Interactions in Crystals'. The graphics were simpler than those used by Rod Hubbard but they were put to new uses. These included hydrogen bonding networks, visualisation of the strongest interactions, the use of voids and relationships between molecules when there is more than one molecule in the asymmetric unit. Many of these ideas have found their way into CCDC software.

This was followed by Phil Withers (Manchester University) exploring visualisation techniques in texture, stress and tomography. Much of his work concerned electron backscatter experiments to obtain high definition maps of grains and sub-grains in alloys. The use of visualisation tools was very convincing; they allowed quick detection of grain boundaries, and there was a lot of scope for new methods and software development.

The last speaker was Martin Dove form Cambridge University with a talk on 'Visualisation of dynamics of disordered crystalline materials'. This talk used animations of molecular dynamic simulations to visualise atomic motions in disordered materials. As an example, he showed the diffusion of Na through quartz in an electric field and radiation damage in ZrSiO4. The insights that graphic gave were clear and tangible.

This was a continually varied and interesting session. The distance we have travelled in the last decade is immense, and there is clearly a lot of scope for new ideas and development.

Chris Gilmore

Bragg Lecture

Bragg Lecture – Bragg Reflections illuminate the structure of some perfidious viruses – Professor David Stuart.

The first Bragg lecture was given by P. Ewald in 1962, the centenary of the birth of W. Lawrence Bragg's father, W.H. Bragg and the jubilee of the discovery of X-ray diffraction by crystals. A fund administered by the Royal

Institution provides a small honorarium and travelling expenses for a lecture every two or three years which was hosted by the BCA at the Spring meeting this year. The committee could not have known when they invited Professor David Stuart to give the lecture how timely their choice would be, in the midst of the worst Foot and Mouth Disease outbreak since 1967. Professor David Stuart has specialised in the application of crystallography to viruses. In his introduction, he quoted David Baltimore who said in his 1976 Nobel lecture "The study of biology is partly an exercise in natural aesthetics". Add a crystallographer's delight in symmetry, and what could be more appropriate than an icosahedrally symmetric virus particle.

His first excursion into virus structure was the determination of the structure of Foot and Mouth disease virus (published 1989) in collaboration with Brown, Roland and Fox. The structure of the virus was as beautiful as expected, but initially did not reveal the details of a surface loop which is crucial for immune recognition of the virus. A chemical trick, reducing a disulphide bond in the loop, allowed its visualisation. Further work including cryo-electron microscopy confirmed that the loop had multiple conformations, but some structural integrity which could potentially be harnessed in vaccine design. There had been some success in presenting the loop in this particular conformation as a virus-free vaccine that had some protective effect, when their collaborators' group was disbanded and the work stopped.

Prof. Stuart went on to describe the structure of the Reverse Transcriptase from HIV-1, a success story for rational drug design. 90 structures have been solved, including complexes and mutants, which have provided information used to design a series of chemical inhibitors, resulting in a compound which is undergoing trials.

For the majority of the talk Prof. Stuart described how he has gone about piecing together how double stranded RNA (ds-RNA) viruses function. Bluetongue virus (MW 10^8 Da) has two concentric icosahedral protein shells which protect 10-12 different RNAs and the transcription machinery to duplicate them. The highly parallel X-ray beam third generation synchrotron sources provide is crucial in the resolution of the densely populated images (50,000 reflections on a 0.2 degree oscillation image). The redundancy provided by non-crystallographic symmetry allowed phases to be determined so accurately that electron density maps calculated at 3.5-Å resolution were of sufficient quality to identify errors in the protein sequence. 60 dimers form icosahedral shell of the bluetongue virus core particle. Rather than make 'quasiequivalent' interactions (Caspar and Klug), a single protein building block switches between two different conformations in formation of a dimer. The outer shell consists of 780 copies of VP7. The symmetries of the shells match at the icosahedral 3-fold axes, with the rest of the shell being formed in a 2-D 'crystallisation' of trimers out across the shell surface. The particle functions as a molecular factory, secreting mRNA which the host cell machinery translates into proteins to form new virus particles. The polymerase is not observed in detail in crystal structures of the whole capsid. The active polymerase subunit was isolated from dsRNA bacteriophage _6, and its crystal structure solved in complex with oligonucleotide and/or nucleoside triphosphates, allowing a mechanism for genome replication and transcription to be proposed. Experiments on BTV crystals including soaking in oligonucleotides to identify where the mRNA must emerge (five-fold axis) and crystallisation in a state that allows transcription (revealing wide ranging conformational changes) put the mechanism in a viral context.

The lecture exemplified how far crystallography has travelled since Lawrence Bragg described a method to determine the structure of NaCl (28 Da) in 1912. He can little have imagined that within a century it would be possible to use the same methods, along with clever choice of biological experiment, to visualise the atomic structure of a virus particle of 108 Daltons in the act of transcription.

Biological Structures Sessions

The David Blow Poster Prize

There were 19 BSG posters on display. Most poster presenters made use of the opportunity to provide a short oral summary of their poster on the Sunday morning. The posters were judged by Neil McDonald (ICRF), Peter Moody (Leicester), Elspeth Garman (Oxford) and Siân Rowsell (AstraZeneca) during the poster session itself on Sunday evening, which was made rather enjoyable by plentiful free wine supplied by Bruker. Both posters and oral presentations were of high standard and the poster judges were faced with the difficult task of selecting a winning poster from a very interesting and professional set of posters. Although the prizes are intended for the posters rather than the oral presentations, an 'honourable mention' was given to Fiyaz Mohammed from the University of Southampton for his exceptionally clear and comprehensible oral presentation based on his poster on the crystal structure of bovine inositol monophosphatase at 1.65Å resolution. Two "runners-up" poster prizes, each a set of crystallisation screen solutions, were generously donated by Tony Savill of Molecular Dimensions Ltd. These were awarded to Kieron Brown from Marseille for his poster entitled "Domain swing upon His to Ala mutation in the nitrite reductase from *Pseudomonas Aeruginosa"*, and to Wilf Horn from the University of Leeds for "Structural determination of an RNA translational operator incorporating 2'-deoxy-2-aminopurine complexed with bacteriophage MS2 coat protein". The main poster prize, which is a trophy known as the David Blow poster prize (a beautiful piece of Blue John crystal) as well as a cash supplement, was presented to Andrew Carter from the LMB, Cambridge for his poster entitled "Crystal structure of an initiation factor bound to the 30*S* ribosomal subunit". The awards were presented immediately after the BCA AGM, just before the Bragg Lecture by Dave Stuart, and all recipients smiled when photographed along with their prize.

Sian Rowsell presenting the biological poster prize to Andrew Carter from the Laboratory of Molecular Biology in Cambridge

"Looking at Structure"

Plenary lecture by Rod Hubbard (York).

Rod started his lecture by describing how wire and plastic models were used during the seventies for displaying structures of biological macromolecules. These models were of limited use for studying flexibility and conformational change. In those days, the co-ordinates of atoms had to be measured manually from map sections or with a Richards Box. The first demonstration of the power of computer graphics for displaying molecular structures was by Levinthal during the early sixties. During the 1970's a number of programmers made significant headway in developing portable code that allowed other groups to take advantage of molecular graphics, as a tool for protein crystallography and also for drug design. In those days, the software relied heavily on expensive Evans and Sutherland (E&S) vector graphics equipment. Rod recalled how in 1982 the protein crystallography groups of York, Leeds and Sheffield shared one such E&S PS2 system costing £180k. The graphics system was transported to each lab in turn. Many groups had to wait until the mid-80's when a major boost in UK funding allowed them to purchase their own graphics equipment. The general demise of vector graphics systems stemmed largely from the much lower cost of raster graphics equipment which currently dominates the market. Rod described work on the development of stereo visualisation and also efforts to make use of virtual reality although one problem with this is the fatigue suffered by users! Rod ended his talk by looking at the binding of steroids to the oestrogen receptor as an example of the importance of graphics work in understanding biological processes and outlined the challenges that macromolecules continue to present in terms of visualisation.

"How MAD can you get?"

The first of the main BSG sessions dealt with the increasingly important role of anomalous scattering in the structure determination of macromolecules. Neil McDonald (ICRF) started the session by explaining why the use of SeMet proteins is the most popular route to MAD structure determination. He described the relative merits of using methionine auxotrophs or inhibiting the Met biosynthetic pathways for standard *E. coli* strains, and highlighted the possible use of cell free transcription/ translation systems for toxic proteins. For proteins that cannot be expressed in *E. coli*, possible alternatives are yeast, insect cells or mammalian cells. While there are successful examples in all three systems, the yields are generally low and consumable costs are high. He concluded his talk with a very useful summary of practical problems (lack of Met in native sequence, slow growth, oxidation, difficulties in crystallisation) and a variety of possible solutions.

Sean McSweeney (ESRF) dealt with the practical aspects of data collection at the ESRF, where they have been focusing particularly on the use of relatively small anomalous signals to provide the phase information. Typically one Se per 20kDa provided excellent phasing, while one Se per 30kDa was more difficult but achievable. Radiation damage is a serious problem at third generation sources, and a data collection strategy was essential. Attenuation of the beam is not uncommon, and the phasing data need not be collected to the diffraction limit of the crystal. A single wavelength (SAD experiment) was often sufficient to solve the structure when combined with density modification, and may be the favoured route in the future. In all cases, collection of a complete data set at the peak wavelength was recommended in the first instance, followed by additional data at other wavelengths. Anomalous scattering from sulphur, at λ=1.77 Å, had been successful, but the very small signal (0.72e-) required very careful data collection.

Pierre Rizkallah (Daresbury) went on to describe the possibilities of using longer wavelength radiation from second generation sources to collect the anomalous signal from xenon and sulphur. He illustrated the technique with the example of lobster apocrustacyanin, an enzyme involved in producing the colour changes which allow the lobster to blend into different backgrounds. The sites for the xenon derivative were located with Shake'n'Bake, and the resulting phases used to locate the sulphur atoms. A final map calculated using the anomalous signal from both the Xe and S was readily interpreted. Pierre ended his talk with a traditional Aramaic blessing for Palm Sunday.

Following coffee, Thomas Schneider (Göttingen) described the latest software available for solving the anomalous atom substructures, focusing particularly on SHELXD and SnB (Shake'n'Bake). Both of these rely on multi-trial algorithms, and an alternation of phase refinement (shaking) in reciprocal space and density modification or map interpretation (baking) in real space. Computation time was reduced by only using reflections with high E values (~15% of all reflections) and extensive use of Fast Fourier Transforms. The algorithms in SHELXD differ from those of SnB in several respects, perhaps the most significant being in the choice of the starting model, where SHELXD uses Patterson superposition methods rather than a set of randomly placed atoms. An important practical point was to limit the resolution to include only the strong data, but substructures of up to 60 Se atoms can be solved routinely.

ZbyszekZbigniew Dauter went on to describe a novel procedure for incorporating the anomalous scatterers. Soaking crystals for very short periods (10-40 seconds) in high concentrations of halides, such as 1M NaBr or 0.5M KI, resulted in the incorporation of large numbers of bromine or iodine atoms. Although many sites have low occupancy, the major sites could be located using standard software (SHELXS, SHELXD or SnB) and phases based on these sites could be used to locate minor sites in difference Fourier maps. The procedure has now been used for over twenty proteins, some of which were test cases but others were unknown structures. Bromine

substitution provided the best opportunity for MAD data collection, with an edge of 0.92 Å, while iodine was best suited for SIRAS or SAD phasing, and provides a good anomalous signal with CuKα radiation. The use of halides provides an alternative to classical heavy atoms or Se, and is very straightforward to use. Strongly diffracting crystals (2 Å) improved the chances of success, but there were some examples at resolutions between 2.8 Å and 3.0 Å.

Jan Löwe (LMB, Cambridge) gave the final talk to illustrate that MAD can be successful when the crystals diffract poorly (3.1 Å), have a high mosaicity (2.0°) and the resulting data have a high Rmerge (10%). In spite of these problems, a 3 wavelength Se MAD data set collected using inverse beam geometry on ID29 at ESRF gave a readily interpretable map. The sites were correctly located with SnB although the solution did not stand out. The resulting structure of the SMC (Structural maintenance of chromosomes) head domain showed a fold similar to the ABC transporters. In concluding a fascinating session, the chairman drew attention to the recently acquired MAD beamline (BM14) at the ESRF, which is now being run as a joint UK/Spanish CRG. Applications for beamtime can be submitted electronically via www.bm14.ac.uk

"Stretching the limits - proteins at atomic resolution"

The first talk in this session was by Elspeth Garman (Oxford) who spoke on techniques for data collection on proteins at atomic resolution. Elspeth explained how data collection to resolutions around 1.0Å allows refinement of anisotropic displacement parameters for each atom, dual conformations of disordered residues and hydrogen atom positions. Standard deviations for the refined parameters can be estimated and, in general, such studies lead to a much improved water structure for the molecule under study. Use of cryogenic temperatures is essential for data collection at atomic resolution requiring the experimenter to optimise the use of cryo-protectant to avoid ice formation and excessive mosaic spread. Elspeth covered various practical aspects of data collection to atomic resolution such as the need to carry out several i.e. low, medium and high resolution passes to avoid the problem of strong reflections overloading the detector. Elspeth emphasised the importance of knowing the wavelength and crystal-to-detector distance for accurate cell determination and refinement. Atomic resolution work on proteins often takes a long time to get into the literature due to the effort required to complete the refinement.

Keith Wilson (York) then reviewed current progress with atomic resolution studies of proteins. One of the major breakthroughs was the advent of the image plate detector. Keith described the advantages of atomic resolution protein work e.g. how it has allowed the stereochemical criteria for structure validation to be improved and how it can contribute to mechanistic studies of enzymes. Keith speculated that much information remains to be derived from TLS tensor analysis using atomic resolution data. Keith then described a computer program (ACORN) which has been developed in York (Jia-Xing Yao) for *ab initio* structure protein determination using atomic resolution data. The method relies on a seed structure which can be derived either from anomalous data or by molecular replacement using a short polypeptide fragment. A new dynamic density modification algorithm has been implemented in ACORN which also uses tangent refinement for structure determination. The program obviates the need for manual rebuilding of the molecule and has been successful in solving a number of structures where other direct methods packages failed.

Dean Myles (EMBL Grenoble) spoke on the value of neutron diffraction in detecting hydrogen or deuterium positions both for studies of protein dynamics and enzyme catalytic mechanisms. Dean described the recently developed neutron quasi-Laue image plate detector (LADI) at Institut Laue-Langevin which was designed to solve the problems of low flux at monochromatic neutron sources and the small

size of most protein crystals. The detector consists of a cylindrical drum coated with a neutron sensitive image plate and now has a cryo-cooling facility. Dean outlined recent work using this instrument, including work on an aspartic proteinase, which demonstrated its potential in addressing mechanistic questions.

Alberto Podjarny (Strasbourg) then described X-ray structural studies on recombinant human aldose reductase which has been solved at sub-atomic resolution (0.66 Å) using data from an inhibitor complex collected at APS (Argonne). Alberto described how micro-seeding was required to avoid problems of twinning in the crystallisation. The structure was refined using X-PLOR and SHELX. Intriguingly, refinement of the anisotropic thermal ellipsoids of water molecules showed that their long axes are oriented parallel with the protein surface. Within the protein itself, density due to valence electrons in covalent bonds was visible throughout the map. One of the crucial mechanistic questions concerned the nature of the proton donor during the reaction. The visibility of hydrogen atoms in the map was found to be correlated negatively with the temperature factors of the atoms to which they are bonded. Nevertheless, density for a catalytic hydrogen atom was visible on the side chain of an active site histidine and the protonation state of this residue was confirmed by inspection of bond lengths obtained from unrestrained refinement. This work allowed an improved mechanism to be proposed. Finally, Alberto described MAD studies using atomic resolution data.

The final lecture in the session was given by Peter Moody (Leicester) who described atomic resolution (0.8 Å) studies of pentaerythritol tetranitrate reductase (affectionately known as 'bangase' in the lab). This enzyme can degrade many highly explosive compounds and has potential in engineering micro-organisms for decontamination of explosive dumps. Peter emphasised the value of atomic resolution studies, since inspection of maps at lower (1.5 Å!) resolution had erroneously led to speculation that an active site tryptophan side chain might be covalently modified, which would have had a major bearing on the mechanism. However, the atomic resolution studies subsequently showed that this residue was instead disordered, occupying two conformations in the active site.

"Hot structures"

This was a crammed session on recent exciting results in which the chairman called on the assistance of various bells and whistles to keep the speakers to time. The first talk was given by Jim Naismith (St Andrews) who described the biosynthesis of the sugar rhamnose in bacteria. Rhamnose is one of many bacterial carbohydrates not found in man and is a common component of the cell wall and recently believed to be essential to bacterial survival, hence of therapeutic interest; Jim mentioned tuberculosis in particular. Conversion from glucose-1-phosphate to rhamnose involves four enzymes, RmlA, RmlB, RmlC, RmlD. Jim's talk focused in the third, RmlC, which catalyses a unique dual epimerization reaction. The structure had been solved by SAD methods and reveals that the mechanism of action, which was studied through ligand-binding and mutagenesis studies, appears to be entirely novel.

The second talk was given by Katjusa Brejc (Amsterdam) who described the fascinating structure determination of a molluscan acetylcholine binding protein that has significant homology with the extracellular domain of the nicotinic acetylcholine receptor (α-subunit). This has considerable impact since it reveals for the first time the structure of the binding site in the ligand-gated ion channel superfamily and therefore is of major pharmaceutical interest. The protein, which was expressed in yeast, is soluble since it lacks the trans-membrane domain of the homologous receptor. The structure was solved by SAD analysis of a lead derivative and 20-fold NCS averaging as well as averaging between 3 crystal forms. The subunits have a modified immunoglobulin fold and form a pentameric assembly with the ligand binding pockets at the subunit interface. All residues which form the ligand binding site (occupied by a HEPES buffer molecule in the structure) are conserved in the receptor. Katjusa showed some crystals

which would certainly appear to have originated in Amsterdam.

Erhard Hohenester (Imperial College, London) described the structure of a fragment of the extracellular matrix protein nidogen. This so-called G2 fragment is involved in binding other extracellular proteins including perlecan and collagen. Such interactions allow cells to adhere and ultimately form complex tissues. Intriguingly one of the two domains in the G2 fragment was found to have a fold very similar to that of green fluorescent protein (GFP). The structure consists of an 11-stranded ß-barrel with a helix running through the middle, where the chromophore of GFP is located. The G2 fragment forms a tight complex with another extracellular matrix protein perlecan and the complex has been crystallised and solved.

Eui-Jeon Woo (Queen Mary College, London) described the structures of two plant proteins which were found to have similar folds as part of the cupin (little cup) superfamily: oxalate oxidase (germin) and the auxin receptor ABP1. The highly thermostable oxalate oxidase enzyme is manganese dependent and was found to have a ß-jellyroll fold with an active site having a strong resemblance to Fe/Mn superoxide dismutases (SODs). Accordingly, oxalate oxidase was itself found to have appreciable SOD activity, and the protection against superoxide is suggested to be an additional role in its stress defence function. The oxalate oxidase is a dimer of trimers, while the auxin binding protein has two homodimers in the asymmetric unit, sharing the monomer fold. The metal site is the auxin binding site.

The 2.1Å resolution structure of ß-acrosin, a serine proteinase located in sperm heads, was elegantly described by Becky Tranter (Bristol). The enzyme was isolated from ram sperm; in addition, a 2.9 Å structure from boar sperm was also determined - both in complex with an inhibitor, p-amidobenzamidine. The structure is confirmed as a trypsin-like serine protease with considerable homology to two-chain proteases such as Factor Xa. Since antibodies against this protein render sperm inactive, the enzyme is thought to be involved in binding and degrading the zona coating the egg. The enzyme has two basic patches on its surface and one of these surrounds the active site. These patches are in all likelihood important for binding to the acidic zona glycoproteins on the egg surface.

Finally, Jonathan Hadden (Leeds) described the structure of the Holliday junction resolvase (endonuclease I) produced by bacteriophage T7. The function of this 149 residue protein is to allow the phage DNA to integrate with the host cell chromosome. The absence of endogenous methionine residues in the sequence and lack of success of MIR methods meant that methionine would have to be introduced by mutagenesis to be able to carry out a MAD experiment. Leucine and Isoleucine residues tend to be good candidates for replacement, and one successful mutation (Ile92Met) was found from several experiments. Cross-seeding the selenomethionine-substituted protein with native enzyme crystals was required for crystallisation. Selenomethionine MAD allowed the structure to be solved revealing that the monomers of this protein associate via long arms that dimerise to form a long connecting ß-sheet. The location of the DNA binding site was suggested by mutations which affect DNA binding and activity.

All speakers in all sessions are thanked for their excellent contributions to an excellent programme, compiled by Jon Cooper, who is thanked for his considerable efforts as local BSG organiser.

Chemical Crystallography Sessions

Hot and Cold Structures

The main CCG session chaired by Paul Raithby on 8th April was entitled "Hot and Cold Structures", and dealt with methods and results obtained from unusual low temperature methods as well as "hot" results.

Judith Howard (Durham) started the session with a discussion on "New Developments in Low Temperature Crystallography; Methodology and Applications". She emphasized the applications of low temperatures in electron

density studies, phase transitions and crystallography of unstable samples. The two common methods of cooling samples are the gas stream method (useful down to around 80K) and by conduction using a Joule-Thompson device (9K can be achieved). Gas streams are easy to use, and are also useful for flash freezing samples, but some phase changes can be missed. Conduction uses no refrigerant, but the equipment is bulky, often homemade and time-consuming to set up; further, the crystal is often hidden from view. More recently, a helium gas stream method has been developed which can cool to ~25K but it can be expensive to run.

New insights into problems can be obtained below 100K; disorders can often be resolved, and different ordering at low temperatures can manifest itself in phase transitions. Several examples of the use of very low temperatures were topological analysis of experimental charge densities in phosphorus ylides, following the reaction pathway for C-H activation, and very low temperature studies to determine initial stages of hydride migration. Reducing the temperature from 100K to 30K removes much of the disorder and anisotropic thermal motion.

She continued by describing a selection of devices at neutron sources (e.g. the LADI and VIVALDI (to be commissioned in 2001) cameras at the ILL (for studying Laue diffraction) and the new SXD at ISIS (a multiple detector)), and finished with a mention of some high pressure devices, e.g. a Bordeaux cell operating at 293K using a diamond anvil on a SMART detector. In Edinburgh, a variable temperature (20-300K) pressure cell has been developed for mounting on the Fddd diffractometer. A cell using nitrogen gas pressure already exists at ISIS and can operate at 5kBar. A new device, to be built at Durham for use with X-rays will operate between 100 and 3kBar.

Russell Morris (St Andrews) moved onto the "hot" structure part of the session with a talk entitled "Unusual Properties of Zeolites Studied by single Crystal Synchrotron X-ray Diffraction" in which he described several structures which could only be determined with the use of synchrotron radiation (SR). The primary building unit of zeolites and other nanoporous materials is a tetrahedron of MO_4 (M = Al, Si, etc). They are synthesized by templating reactions, but it is very difficult to grow large crystals - 0.4mm is considered giant.

The specific impact of Daresbury Station 9.8 on this field has in three main areas, viz., new structures, synthesis studies, and the study of properties. While zeolite STT-SSZ-23 had been known for 10 years, its structure was unknown. Synthesis gave crystals ~20 x 20 x 5 microns; the structure determination showed that these were essentially pure silica, with 9 atoms in one ring and 7 in the other. This work overturned the paradigm of even numbered rings but modelling studies did not show why.

Another zeolite, IFR, is centrosymmetric when the template is removed by heating and shows no second harmonic generation (SHG). As made, however, it shows strong SHG (glowing green under IR laser light). This is explained by the symmetry being broken by part filling the cages with fluorides according to a set of well-defined structural requirements. IFR displays negative thermal expansion, which is common in zeolites through twisting of the MO_4 tetrahedra; this gives rise to shrinking of the pores and decrease in size on heating in all 3 dimensions.

Philip Coppens (SUNY, Buffalo) gave an insight to "Combining Crystallography and Photochemistry in the Study of Light-induced Metastable States and Transient Species". Historically, photochemistry of transition metal nitrosyls has been performed on frozen gas matrices at 20K, and analysed with IR spectroscopy. Modern equipment allows the study of crystalline systems with simultaneous laser irradiation and diffraction. At liquid helium temperatures metastable species have essentially infinite lifetimes, and the experimentalist can tune the experiment to isolate different species by changing the wavelength of the laser or the temperature. Calculation of photodifference maps shows that the nitrosyl-metal linkage is changed by irradiation. Low temperature IR difference spectroscopy shows that the same effects occur for NO in iron

porphyrins and isotopic substitution confirms that it is an NO phenomenon.
Pulsed lasers (time structure of ~5KHz) and pulsed X-rays (~0.1 - 1 MHz) allow this work to be extended to other species. During the experiment, the population of excited states rises to a pseudo steady state with a sawtooth distribution. Early experiments with small crystals (50x50x50 mu) of $(TEA)_2Pt_2(P_2O_5H_2)_4$ at 16 - 18K have been performed. T can be measured accurately by measuring the lifetime of the species. First results show a reduction for 5% of the population of Pt-Pt distance from 2.91 to 2.61 Å, but the standard deviation is ~0.1Å, so further study is necessary. "Solid state dilution", i.e. embedding molecules of interest in a supramolecular framework allows the excitation of a larger fraction. However, sometimes framework needs time to recover from irradiation, so the observed photochemistry can be affected.

Simon Parsons (Edinburgh) finished the session with a lively talk on "Low Temperature Crystal Growth". The need for this arises from the desire to study samples which are gases or liquids at ambient temperatures. He covered the practicalities for both low temperature and high pressure crystallisation. Both gases and liquids tend to be simple compounds. They often have different structures in different phases, e.g. $BGaH_6$ has the diborane structure in the gas phase but not as a solid. Simple systems have several advantages, e.g. solid and gas phases can be compared, high level QM calculations are feasible, there are minimal steric effects and archetypal behaviour for a class of compounds can be derived.

Crystal growth is achieved by establishing a stable solid-liquid equilibrium in a capillary, and cooling slowly to induce crystal growth. An IR laser can supply local heating to move the position of the solid-liquid equilibrium; this was illustrated by reference to Me_3PbSMe. The laser can be used to create a polycrystalline powder from a glass, followed by zone melting to give a single crystal; slow growth tends to eliminate formation of twins. Those twins which are encountered are usually of the TLQS type or simply multiple crystals.

Pressure can also be used to produce crystals from compounds which are normally liquids or gases under ambient conditions. However, the pressure cell can shade some regions of reciprocal space. The diffraction pattern is recorded of sample, Be windows and diamond anvil, so this can cause some problems in data collection. Problems can arise in reaching the global minimum structure. He finished by illustrating both low temperatures and high pressures with a study of acetone; three types of interactions of carbonyl group found in CSD. The high pressure structure gives one of these, whereas low temperature gives the other two.

CCDC Prize Award and Lecture

Claire Wilson receives the CCDC award from Frank Allan

Before giving her lecture Dr Claire Wilson, who now holds a research post in the Department of Chemistry, at the University of Nottingham, was presented with the Cambridge Crystallographic Data Centre Prize by the Scientific Director of the CCDC, Dr Frank Allen. As Dr Allen mentioned this is the second occasion that the Prize has been awarded, the inaugural award having been made at the BCA Spring Meeting last year. The Prize is awarded to the young scientist, normally under the age of 35 years, who, in the view of the CCG Committee, has made an outstanding contribution to Chemical Crystallography.

Claire's lecture was entitled "It's the way that you twist that counts: Mechanisms in Molecular Magnetism". In her presentation she described a series of variable temperature single crystal X-ray and neutron studies on a series of di-copper complexes and related the structural changes to changes in their magnetic properties. The archetypical complex was $[Cu_2(PAHAP)(H_2O)_6](NO_3)_4$, where PAHAP is an open chain diazine ligand that has flexible N-N single bonds that affords a range of co-

ordination modes to a transition metal. Magneto-structural studies on this system show a linear relationship between the rotation of the copper-containing magnetic planes about the N-N bond and the exchange integral. This relationship is observed over a 105° angular range, with a change from ferromagnetic coupling at angles less than 80° to antiferromagnetic coupling at angles greater than 80°. Variable temperature crystallographic studies, including charge density investigations at 35 K, showed a catastrophic change in crystal quality at around 270 K, and significant changes in cell dimensions between 35 K and room temperature. In all data sets were collected at eleven temperatures between 35 and 295 K, and the key structural feature observed was an approximately 3° change in the angle between the magnetic planes over this temperature range.

CRYSTALS Workshop

A CRYSTALS workshop was held as part of the BCA Spring Meeting at the Department of Chemistry in Reading. Jim Thorpe arranged for the April release of CRYSTALS to be installed on sixteen PCs, and for data-projection facilities for real-time demonstrations and a short presentation. Although only 20 people originally signed up for the workshop, about 50 ended up crowding into the computer room!

In the first of the presentations Richard Cooper explained the design aims behind the current release and gave a real-time demonstration of a structure analysis. Broadly speaking, the software aims to provide tools which will enable a synthetic chemist to make a reasonable attempt at performing a structure analysis on data that they have either collected themselves, or which has been provided for them. The rationale for this approach is that modern CCD diffractometers have a massive potential data throughput, which would completely overwhelm one structure analyst. For example, the Nonius KCCD instruments in Oxford are run in 3-shifts, and can be booked by authorised users for 9am-1pm, 1pm-5pm or over night 5pm-9am. There are about 20 chemists registered as authorised users and one structural service analyst. With this number of structures passing through the instruments, it is clearly important that the software tries to ensure that crystallographically sound decisions are made, and that the user-interface enables professional chemists to use their skills and knowledge to help the program when necessary.

The second presentation by David Watkin was an overview of some of the crystallographic model building, manipulation, and analysis tools in CRYSTALS. These have been created over the years to assist in the handling of big or difficult structures, and are probably of most interest to professional analysts and research crystallographers.
Finally, Horst Puschman (Durham) gave a brief unscheduled demonstration of a structure archiving and tracking suite that he is developing to assist in record keeping for these high productivity systems.

The second part of the workshop gave people the opportunity to get hands-on experience with CRYSTALS. Handouts were provided for two small organic structures, and users were guided step-by-step through typical 'routine' analyses. To demonstrate that twins are not necessarily difficult, the second example was of a twinned material for which a trial structure was readily obtained by SIR92. The refinement converged to an R-factor of about 25%, but tumbled to 3% once the twin law was identified and applied.

As maintainers and developers of the software, one of the main benefits of running the workshop was that it gave us the opportunity to see how a diverse group of people, mostly unfamiliar with CRYSTALS, got on with the program. Some people took to it immediately, while others had difficulties adapting to the interactive response. We came away with a number of ideas about how the system could be improved, and we are grateful to everyone who participated. The CRYSTALS package is available free to academic and not-for-profit institutions from

http://www.xtl.ox.ac.uk/crystals.html

We must record our thanks to Jim Thorpe and Rick Hobson for all their help installing the system for us, and to Christine Cardin and Ann Chippindale for arranging and publicising the workshop.

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PCG/CCG Joint Symposium on Advanced Sources

Session I - New X-ray Sources

The first talk of this session was given by Mike Poole (Daresbury) and gave an overview of the history of the DIAMOND project. The role of DIAMOND as a medium energy facility to compliment existing high energy facilities was explained and the possibility of using DIAMOND to fulfil the low energy requirements that were to be satisfied by the abandoned SINBAD project was described. A number of design decisions were explained. These included the somewhat controversial option not to use in-vacuum undulators, but retain the option of a later upgrade to these. The related problems and benefits of top-up injection were also discussed. Top-up injection will not be implemented on day one, but the option to include this at a later date will be retained. In the discussion that followed the talk it was pointed out that the 'goalposts' may well move over the next decade as detectors and other equipment improve. Mike also explained some of the very difficult technical challenges which the design has to meet; such as nonlinear electron dynamics and orbit control.

The discussion of DIAMOND was continued by Colin Norris (Leicester; DIAMOND Interim Director, Physical Sciences), who encouraged the use of the DIAMOND website (see the end of this article), which is due to be greatly improved in the near future. Colin then explained the structure and organisation of the DIAMOND project. The first beamlines to become available to users at DIAMOND should complement the facilities available at ESRF, for example by allowing complex experiments that are hard to set up (and so not possible at ESRF) to be carried out. Proposals for the 'day one' beamlines were described and input from the community was encouraged. Forms will be soon be available for prospective users to give their opinions on the facilities that should be made available.

The final speaker before coffee was Bill Clegg (Newcastle/ Daresbury), talking about New Opportunities for Chemical Crystallography with Synchrotron Radiation in the U.K. For the most part the talk was concerned with opportunities for research that are available now or will be available in the very near future, principally at the SRS. By way of an introduction, some of the challenges that can now be met and some of the technology that is making this possible, were introduced. This was followed by a brief consideration of the pros and cons of dedicated versus multipurpose beamlines. After describing a few of the results that have been obtained by using synchrotron radiation (at station 9.8 at SRS), Bill talked about upcoming improvements to the station. These improvements will lead to increased capacity, opportunities for new experiments, and hopefully a reduction in over subscription. Access to facilities like station 9.8 was explained. The application for an extension of the national service at Southampton to include station 9.8 is still, at present, undecided.

All three speakers encouraged the community to make their views felt, in order to ensure that the facilities that are needed are provided. There was a lot of discussion after each talk, and the co-chair, Paul Raithby, managed well with the unenviable task of keeping the progress of the session to schedule.

After coffee Jochen Schneider (DESY-HASYLAB) spoke about Free Electron Laser X-ray Sources. This interesting talk covered the ideas behind free electron laser X-ray sources as well as the new experiments that they will make possible. Such experiments include the chance to study non equilibrium states and possibly real time studies of bond formation and formation of condensed matter. The TESLA laser X-ray source is expected to have a peak brilliance more than 100 million times that of currently available synchrotron sources. The TESLA web page is given at the end of this report.

The session was completed by Uli Arndt (Cambridge) speaking about X-ray Optics for use with Laboratory X-ray Sources. The changes in the requirements of equipment over time was highlighted. A number of approaches to solving the problems of focusing X-rays were covered including monocapillaries, polycapillaries

and toroidal mirrors. We were warned to beware the claims of manufacturers, for example, because placing the focus mirror close to the source increases intensity but also increases the divergence.

DIAMOND website:
http://www.diamond.ac.uk/
TESLA website:
http://tesla.desy.de/

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Session II - Diffraction at the Edge - Part I

This joint CCG/PCG session began with a lecture by Georgina Rosair (Heriot-Watt) entitled "Structural Chemistry from the Edge(s); an Introduction" where she outlined how absorption edges contain information not only on the local structure of any material – whether crystalline, amorphous or liquid – but also on local electronic and magnetic structure. The processes involved in EXAFS and XANES were described and related to the elucidation of the number and type of surrounding atoms. Although the Fourier transform of an EXAFS spectrum is a radial distribution function giving a direct representation of interatomic distances, the requirement for an accurate initial refinement model was also stressed. Anomalous data collected at two or more wavelengths can be used to distinguish elements with similar atomic numbers, probe disorder or determine valence states. Georgina finished with some wide-ranging examples such as studies of excited states; the uses of XANES and *X-ray* MCD, the latter showing antiferromagnetic coupling between V and Cr; the study of metal environments in metalloproteins; studies at the S *K*-edge to establish the degree of covalency in metal-ligand bonds and the discovery of an explanation for the enhancement by Ge of the catalytic activity of Pt: interaction between these elements and alloy formation are seen above 540K.

In her lecture "At the Edge of Microporous Materials" Madeleine Helliwell (Manchester) detailed the main applications of anomalous dispersion in chemical crystallography, before describing the essential features of phosphate-based molecular sieves. Incorporation of metal changes their chemical and physical properties and to understand these changes it is necessary to know the framework geometry and the sites of incorporation. Although NiAPO can be studied using laboratory data from Mo and Cu sources, discrimination is greatly enhanced with synchrotron radiation of 1.488 Å, which should allow detection of lower levels of incorporation. For CoZnPO-CZP, Cu data did not show any significant site preference for Co, but SR data from fluorescence scans of both metal edges showed most of the Co was located on one particular site. Improved instrumentation will make these techniques more powerful, for example by increasing the available resolution. Combined XRD/EXAFS can provide several different handles to study oxidation and reduction processes: Madeleine described how it was possible to show the preference for particular sites in MeAPO. Finally, referring to ongoing work on ZnULM-5, she noted that although features such as unitcell expansion and changes in bond lengths were useful indicators, it would be necessary to obtain data at the Zn and Ga edges.

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The remainder of this session will be reported in the next Crystallography News.

Philips Analytical Physical Crystallography Award

The 2001 Philips Award was given to Dr Jens Kreisel of the ENS de Physique de Grenoble, for his work on phase transitions in perovskite and related phases, much of which was carried out while at Oxford.

A full report of the Prize lecture "A Peculiar Relaxor Ferroelectric, $Na_{0.5}Bi_{0.5}TiO_3$ (BZT)" will be included in the next issue of Crystallography News.

Jan Kreisel receiving the Philips Analytical Crystallography Award from Robin Aird

CCG/PCG/IG Oral Poster Sessions

The CCG/PCG/IG joint oral poster sessions were led in inimitable fashion by Bob Gould and his gong, assisted by Chick Wilson. The presentations were of high quality and enthusiastic. It is noticeable that the previous trend of over-running time (now stifled by the deterrent effect of the gong) has been replaced by a worrying trend towards presentations which do not take full advantage of the two-minute allowance. Sanctions to penalise presentations which are too short may well be devised!

The oral presentations formed part of the deliberations of the poster prize adjudicators, and this lively session continues to educate and entertain.

The group poster prizes were awarded as follows:

CCG: Pam MacGregor (Edinburgh) for poster CP-8 (the High Pressure Crystal Structure of Ethylene Glycol)

PCG: Matthias Gutmann (ISIS, RAL) for poster PP-11 (Charge Inhomogeneities in $La_{2-x}Sr_xCuO_4$ Evidenced from Pulsed Neutron Diffraction)

IG: Helen Thompson (Heriot-Watt) for poster IP-2 (the Dehydration of a-Lactose Monohydrate).

Paul Raithby, the current Chairman of the CCG, presenting the CCG Poster Prize to Dave Allan from Edinburgh who received it on behalf of his student, Miss P.A. McGregor

Coherence Workshop

The Coherence workshop at the BCA Spring Meeting offered an opportunity for all, including non-experts, to learn more about this important trend in X-ray science.

The session opened with *Coherence: A Tutorial* by Dr. D. Laundy (CCLRC Daresbury). Dr Laundy explained what *lateral* and *temporal* coherence are, and then went on to described how both could be measured via synchrotron radiation. This was followed by a talk from Prof. P. Fewster (Philips Analytical, Redhill) entitled *How the final observed diffraction profile is formed.* Techniques for determining coherence length were discussed - one method involves using randomly distributed blocks of a planar surface. Prof. Fewster introduced the idea of thinking about the coherence length as the effective 'length' of the photon. It was noted that effects such as Mossbauer and sending a photon through a monochromator, lengthen photons. Prof. Fewster's talk gave rise to lots of contributions, the first of several *Impromptu Open Forums* in this lively Workshop!

Prof. B. Tanner (Durham) then spoke about *using grazing incident surface scattering to determine near surface density*. The diffuse scattering is measured as a function of the sample orientation in the beam. Plots were shown of diffuse scattering, containing the Yoneida wings and specular peak. This technique has now been applied to polished alumina - polishing has an effect on the surface density ratio. Due to the fact that in low angle scattering the X-rays are effectively 'seeing' an average surface density, for this technique to be successful the coherence length needs to be larger than the grain size of the sample. Prof. A. Lang (University of Bristol) then spoke on *Assessment of Lateral Coherence at Station 7.6 Daresbury Lab. by X-ray Biprism Interference Pattern Production.* This talk focused on an experiment originally carried out in the 1930s, that Prof. Lang had repeated. The set-up was described and the theory explained - Fresnel fringes are observed if the experiment is successful. The 'wobble' of the electron beam at a synchrotron was then discussed - this would obviously decrease the coherence of the X-ray beam, so experiments that are carried out over large time scales must expect a reduced coherence length than the one expected.

Open Forum

Dr Collins (CCLRC Daresbury) stated that if the last point was so, then a time factor should be included into the coherence length of a station. Discussion as to whether vibrational analysis of a station would yield any information on possible effects on the coherence length, i.e. if the station is near a motorway such as the ESRF. Prof. Hart stated that coherence length is a function of sample/set-up/ apparatus etc.

Dr. C. Nave (CCLRC Daresbury) then gave an introduction to

Biological Crystallography with highly-coherent sources. Dr. Nave started by describing the structures that he studies: ribosomes, huge viruses and large protein structures. These molecules are up to 1000Å in size, and consequently are very difficult to crystallise. Such crystal mosaics that are crystallised are often so disordered that they cannot be used for structural analysis, however if one can achieve a large coherence length, the entire molecule can be studied in situ (via different orientations). Dr. Nave showed a table of when various properties of the beam would be required to be optimised for a particular study. For example, in certain biological studies a high-flux is essential, whereas coherence is relatively unimportant. He then listed various studies that require high-coherence, e.g. protein crystallography. The topic of "speckle", caused by path differences in highly coherent rays from a source (e.g. the stars 'twinkling'), was also touched upon. Speckle can also be used to study biological systems, and Prof. J. L. Finney (University College London) quickly contributed that systems on the microsecond range could be studied via speckle.

Prof. M. Hart started his talk, *Phase-contrast imaging – the wheel re-invented?* by suggesting various titles that he could have used, 'Phase-contrast imaging: The Hype and the Lope', and 'Coherence is in the eye of the Beholder'. In his opinion the whole topic of what coherence length is and can be used for is a very confused area. This, he said, was due in no small part to certain textbooks, which don't clearly state what is meant by 'coherence length'. To start with he went through a background literature survey, concluding that the best work was *Optical Physics* by Lipson & Lipson. He then ran through formulae for spatial and temporal coherence and stated that if you are to understand what coherence is then you must consider that only one photon enters experiment at a time and that coherence can be thought of as space-time averages for data collected. He then showed the 'coherence volume' for several sources, from an X-ray tube to undulators and wigglers on a synchrotron beam. He concluded that all were of a comparable magnitude, and that the coherence volume will always be bigger than your unit cell parameter.

Open forum

At this point Dr Vladimir Dmitrienko (Institute of Crystallography, Moscow) talked about the theoretical use of polarisation tensors. He explained that manipulation of the polarisation tensors could sometimes by more useful than the Darwin equations when trying to understand diffraction in mosaic crystals.

Dr. G. Fraser (Bede Scientific) then spoke on *Phase-contrast imaging with micro-sources of X-rays.* This technique required a very simple apparatus, comprising of a source, then sample and then film or image plate. An electron beam is focused on an X-ray producing target; the X-ray beam size is controlled by the electron beam optics. This system can be used for looking at low-density composite materials, producing low contrast images. The primary use of this technique is non-destructive testing and here two impressive phase-contrast images of a housefly were handed around.

Dr. P. Thomas (University of Warwick) led the final discussion including the answers to the coherence quiz. Prof. A. Lang was the only entrant but had answered all questions correctly, and so was awarded the prize of book tokens.

Thomas Lyford
(phryv@warwick.ac.uk)

Industrial Sessions

Why Industry uses Crystallogaphy

The Alun Bowen Industrial Lecture

Crystallography in the Aerospace industry – Colin Small (Rolls Royce plc, Derby)

The Crystallographic Section (Colin) at Rolls Royce provides engineering answers from interpreted crystallographic data – phase identification, texture analysis (for titanium), residual stress in metallic materials – and any service Colin is unable to provide himself, is obtained from ISIS, Daresbury, various

Universities and commercial organisations. These answers are provided for engineering colleagues who, although well qualified themselves, are unfamiliar with aspects of crystallography such as texture analysis and pole figures.

Colin's talk began with an entertaining video presentation of aero engine testing. Engines such as the Trent 890, fitted to the Boeing 777, undergo rigorous ground tests to ensure that failure will never result in disintegration, rather containment of any components within the engine body. To the relief of the audience, especially those facing a return flight across the Atlantic, the engine passed all tests (crosswinds, icing, bombardment with hail, water, 2.5lb chickens and 8lb Canada geese) with flying colours!

Thermal paints are used to show (by colour changes) the temperature to which certain parts of a jet engine rise during operation. No really systematic attempt had been made to establish a sound scientific basis for these colour changes. So, one of Colin's first jobs was to analyse the ingredients of the thermal paint, look at their high temperature chemistries, and then analyse their reaction products, in order to explain the colours produced at high temperatures.

One aircraft operating in the Middle East had suffered engine failure during take-off. Subsequent investigation revealed turbine blades coated in an orange-brown substance, which had blocked the blades' cooling holes. Phase analysis of the brown substance by XRD showed diopside ($CaMg(SiO_3)_2$), $CaSO_4$, quartz, $Fe2O_3$, and $CaCO_3$. Analysis of dust from the tarmac accounted for all these compounds except diopside. Diopside had been formed from some of the other compounds when they had struck the hot turbine blades. Reference to the diopside phase diagram suggested that the engine's operating temperature would cause the formation of solid diopside which had then blocked the turbine blades' cooling holes, causing overheating, resulting in engine failure. On the basis of this work, advice was given to raise the engine's operating temperature such that diopside would be present as a supercooled *liquid* phase rather than as a solid. As a result, the liquid diopside was blasted through the cooling holes and no further blockages occurred. A superb piece of all-round science!

The underlying theme of this year's Alun Bowen Lecture was really one of communication and education. Colin's response to engineers' dislike of complicated information about pole figures was to provide them initially with a simplified scheme consisting of a sketch and 3 numbers. However, when a titanium wide chord fan blade (WCFB) had failed a bird test, and yet there appeared to be no changes in the chemistry and microstructure of the blade, the texture was checked. A 0002 pole figure revealed dramatic differences between the texture of the failed blade and that of a normal blade and it was apparent that on this occasion a simple explanation would not suffice. Some change in the manufacturing process must have occurred, and to convince the engineers, Colin supplemented a more detailed explanation with some 3-D pictures of the pole figures. Further investigation then revealed that in this particular forging process, it had taken 5 minutes longer than normal to take the ingot to the rolling mill and this time delay had caused the texture change. The lecture highlighted just how important it is for a crystallographer (or any scientist for that matter) to be able to translate his/her analytical results into meaningful information for the customer who may then act upon it. The examples quoted above illustrate the point admirably.

Pharmaceutical R&D: Protein Crystallography – David Brown (Pfizer, Sandwich, Kent)

In today's approach to drug design, teams of structural biologists are formed to develop screening methods and to look for compounds that form the basis for effective treatments for a disease. Compounds are made based on structural information from computer modelling of the biochemical targets. Thousands of compounds from existing compound libraries can be screened by high speed robots (high throughput screening, HTS), and those which show promising biological activity, called "leads", are then optimised by chemical modification. If these lead

compounds pass early safety tests, they become development candidates and move forward into the exploratory development phase.

In terms of target molecules, the requirements for structure-based drug design (SBDD) are: (a) a source of high yield protein, (b) high purity proteins, (c) crystallisable proteins, (d) high resolution diffraction patterns <2.5Å, and (e) stability to solvents such as DMSO, MeOH and EtOH. It is apparent that there is great value in data from protein crystallography for understanding the modes of protein binding in high throughput screening (HTS). There are currently some 14,000 structures stored in the protein data bank and use is made of virtual screening in which 3-D structures of target protein and small molecules are screened for docking or selectivity.

Pharmaceutical R&D: How to make an impact with small molecule crystallography – Roy Copley (GlaxoSmithKline Pharmaceuticals, Harlow, Essex)

Single crystal studies are used at all stages of the Drug Discovery Process, for protein crystallography and for the drug itself. They are used for molecular conformation and absolute configuration studies (NMR is used almost exclusively for molecular connectivity) and are also used in conjunction with powder diffraction, solid state NMR, IR and Raman spectroscopy, DSC and TGA for studies of bulk properties and polymorphism.

A particularly interesting example of the use of crystallography concerned Augmentin, an oral antibacterial containing sodium amoxycillin. It was important to see if the crystals were solvated with methyl acetate, to determine why methanol is needed for crystallisation, and to explain the powder pattern. The space group was $P2_12_12_1$ and the asymmetric unit contained sodium amoxycillin, methyl acetate and methanol. The sodium ions and solvent molecules lay in channels parallel to the *a* axis, and methyl acetate did not bind to the Na ion. However, the predicted powder pattern did not match that of the bulk material. Another crystal was selected, and in this structure there was no methanol, the methyl acetate molecule was bound to the Na ion, but still the powder pattern did not match the predicted one. A moment of inspiration resulted in the production of a calculated powder pattern derived from a 2:1 mixture of the two crystal structures, which matched the experimental pattern.

X-ray diffraction in the Minerals Industry – Nick Elton (Exeter Advanced Technologies)

Analysis in the minerals industry is used in all stages from exploration through extraction, comminution, separation, blending, storage and transport. Chemical analysis is done by wet chemistry and XRF, and phase analysis is undertaken by XRD.

Typical problems arising with quantitative XRD analysis are: (a) complex mixtures, (b) variable phases (solid solution polymorphs), (c) poor crystallinity, (d) low concentration, (e) preferred orientation, and (f) speed of analysis. The cement industry is a prime example of where these problems occur and they are compounded by lack of standards and peak overlaps in the XRD patterns. The best approach would seem to be Rietveld or whole pattern analysis. Sophisticated approaches such as these are unheard of at the moment in the minerals industry! XRD is usually only used for semi-quantitative analysis in troubleshooting, but now some European plants are using on-line XRD for clinker analysis. For on-line work, the diffractometer is literally assembled at a suitable place in the process. Phase analysis is achieved at both ambient and non-ambient temperatures, and crystallite size distribution (especially for the oil exploration industry) can be measured. Another recent advance has been the prediction of 3 & 28 day compressive strength from XRD data using only 2 measurements from the XRD pattern.

In the aluminium industry too, bauxite processing suffers from lack of good standards, variable crystallinity and preferred orientation. As a consequence, the XRD/XRF mass balance approach is used. The conversion of goethite-diaspore to haematite is related to the amount of Al substitution, the solid solution obeying Vegard's Law. Preferred orientation is solved by spray drying methods of sample preparation. In the China Clay industry,

quantification of quartz, feldspar, kaolinite and mica is achieved through Peter Salt's Quanticlay software.

XRD will continue to be a key analysis tool in terms of QA and QC, but a fast throughput is needed, because as is the case with all industries, cost reduction is essential.

David Rendle

New and Future possibilities in Powder Diffraction

The second IG symposium of the Reading Spring Meeting took place on the morning of Tuesday April 10th in room 104 of the Palmer Building. A very substantial number of people managed to shake off the previous evening's revelries - that evening having seen the Conference Dinner and an extension until 1am at the bar - and attended the session, indeed filling the room to capacity for much of the time. Chairing duties were ably fulfilled by Steve Norval and Phil Holdway, deputising for Chris Frampton who was unable to attend for happy reasons.

The session's theme was designed to review recent developments and look forward to near-future developments in a number of key fields in powder diffraction. Three talks covered specific application areas, with two more technology-based presentations from diffractometer manufacturers to round off the morning.

The session was kicked off by Rob Delhez of Delft University, with a talk on Line Broadening Analysis; Yesterday and Tomorrow. Rob described a subject in a "transition state" - his title did not contain the word "today". He described established methods of size and strain analysis, such as the Warren-Averbach approach, and how these have now been supplemented by methods for accounting for the concentrations of different kinds of lattice defects. However, so far there is little evidence for the practical application of these methods to real materials problems, although much theoretical work has been published. Rob made a plea for the rectification of this situation.

John Faber from ICDD (the International Centre for Diffraction Data) described some recent and ongoing developments in the Powder Diffraction File (PDF), which is very much a staple of many powder diffractionists' work. There are now links with structural database providers; the PDF is now growing rapidly, replete with calculated patterns from the Inorganic Crystal Structure Database and the Cambridge Structural Database. A new relational structure to the database will also accompany the launch of new, targeted subsets of the PDF, the first of which - metals and alloys - is already available. John described some examples of datamining using the new systems, including looking at phases of the oxides of lanthanides, and determination of atomic co-ordinates for beta-tantalum through examination of isostructural compounds.

Jeremy Cockcroft (Birkbeck College) gave a splendid overview of the broad subject of Rietveld refinement. His description of the subject's history pointed out the evolution of different aspects of the topic, such as the kinds of radiation sources used, the computing power applied, the peak shape parameters applied, etc. Moving on to the present, he gave examples of the kind of complex organic and organometallic compounds that are now being refined by the Rietveld method (albeit with restraints and constraints), sometimes having been determined ab initio from powder data. There are now dynamic studies being carried out as a function of temperature and pressure, and there is now even application in structural molecular biology, with recent reports of polypeptide structure refinements and refinement of the T3R3 human insulin zinc complex. Into the future, Jeremy posed some tough questions - more structures will be solved and refined ab initio with better data from better sources, but how can we weed out the errors? And exactly what information and/or data should we archive?

Technical presentations from Philips and Bruker AXS wound up the session. Anna Widdowson from Philips described the capabilities of their new X'Celerator system, which uses a new detector technology called RTMS - "real time multiple strip". Frank Stowasser of Bruker AXS described the many

arrangements of Goebel mirrors and beam expanders or compressors that can be used to optimise beam optics for a range of different X-ray diffraction applications. So an entertaining and informative session came to an end at lunchtime. Many thanks are due to all the speakers and to the organisers for putting together such a worthwhile morning.

Dr. Stephen J. Maginn.

Basic Powder Diffraction Workshop

The Basic Powder Diffraction Workshop was made up of three half-day sessions and was aimed at people relatively new to the field of powder diffraction. Many graduates enter the field of powder diffraction with very little knowledge of crystal structure or how a diffractometer functions. This workshop aimed to correct those deficiencies. The first session provided a well-balanced introduction to the principles of crystallography relevant to an understanding of powder diffraction. In the second session the X-ray diffractometer and sample preparation were described and in the third session the problem of sample identification was covered. Each of the Workshops sessions was well attended.

Introduction to Crystallography
The speaker for this session was Jeremy Cockcroft (Birkbeck College) who covered the crystallographic principles underpinning powder diffraction. Topics discussed included symmetry groups and crystal systems, space group diagrams, factors affecting peak position, peak intensity and line profiles in a powder diffraction pattern and reflection multiplicity. The principles and practice of indexing reflections by assigning hkl values to each diffraction peak, various indexing methods, the choice of reflections for indexing and indexing problems were also covered. Other topics ranged from unit cell refinement (including the need to take into account zero errors and instrumental aberrations), space group determination and whole pattern fitting. Finally Jeremy discussed reflection conditions for the various crystal classes including conditions for glide planes and screw axes.

Powder Diffraction Instruments
Judith Shackleton (Manchester Material Science Centre) started the second session with an introduction to the production of monochromatic radiation, X-ray tube construction and choice and the correct tube settings to use. This was followed by a discussion on diffraction geometry, including the Bragg-Brentano geometry which is generally used in powder diffractometers. Other topics included the choice of filters and monochromators to remove unwanted radiation and the use of Soller slits and divergence slits and of primary and secondary optics in general. Judith then talked about the sources of errors in powder diffraction data. These included systematic errors such as instrumental design and errors caused by the instrument being incorrectly set up. Sample errors were also discussed and included sample preparation, sample height, surface roughness, particle statistics, transparency of sample, crystal size and texture.

Phase Identification
The speaker for this session was John Faber (ICDD) who began with a brief history of the development of powder diffraction data bases in qualitative analysis up to the present day and the introduction of the more versatile Relational Data Base (RDB). The ICDD powder diffraction file (PDF) currently contains about 130,000 entries. John demonstrated the Boolean search system and the Hanawalt and Fink search methods for qualitative analysis and followed this with a discussion of fully automated search methods, which are based on these. The latest developments in automated search methods now include programs, which have total pattern matching. Finally John demonstrated the Relational Data Base (RDB) version of the PDF which gives a more flexible search environment and allows easier updating of information.

Jo Jutson

Particular thanks to Geoff Mitchell, Jim Thorpe and Jeannette Hobbs, Local Committee of BCA Reading 2001 for providing the pictures here and on the front cover.

The British Crystallographic Association

Summary of the consolidated BCA accounts for year ended 31 December 2000

The full BCA accounts for 2000 are available on request as an E-mail attached rich text file from the BCA admin office.

Examining Accountant: R A Young,
The Young Company, Lakeview Court, Ermine Business Park, Huntingdon PE29 6XR

These are consolidated accounts and include the BCA, BSG, CCG and IG funds.

INCOME:

	31.12.00	31.12.99
Glasgow 1999	76,000	4,000
Annual Conference	56,635	-
Meetings of Groups	3,471	16,961
Newsletter	13,230	12,624
Membership subs.	9,302	8,444
Course fees	-	14,044
Grants and sponsorship	537	9,181
Net income from trading	63	138
Donations	256	207
Investment income	4,275	4,275
Interest received	2,980	1,221
Other	-	237
TOTAL INCOME	**166,749**	**71,332**

EXPENSES:

	31.12.00	31.12.99
Direct charitable expenditure (1)	86,034	58,499
Management and administration (2)	14,983	4,663
TOTAL EXPENDITURE	**101,017**	**63,162**

	31.12.00	31.12.99
NET INCOME (EXPENDITURE)	65,732	8,170
Unrealised gains (losses) of investment assets	70	(4,758)
NET MOVEMENT IN FUNDS	**65,802**	**3,412**
Balances brought forward at 1 January 2000	113,101	109,689
Balances carried forward at 31 December 2000	178,903	113,101

ASSETS:

Fixed Assets	**2000**	**1999**
Tangible assets	81	216
Investments	49,838	49,768
	49,919	49,984
Current Assets		
Stocks	3,264	3,324
Debtors	4,870	10,549
Short term deposits	100,630	40,654
Cash at bank and in hand	30,028	13,040
	138,792	67,567
LIABILITIES: amounts falling due within one year	7,480	2,000
LIABILITIES: amounts falling due after more than one year	2,328	2,450
NET ASSETS	**178,903**	**113,101**

INCOME FUNDS		
Restricted funds (3)	38,327	39,491
Unrestricted funds (BCA)	140,576	73,610

BCA CASH FLOW STATEMENT FOR YEAR ENDED 31 DECEMBER 2000

	2000	1999
Net cash inflow (outflow) from operating activities	76,964	(9,050)
Increase (decrease) in cash and cash equivalents	76,964	(9,050)
Cash and cash equivalents at 1 January 2000	53,694	62,744
Cash and cash equivalents at 31 December 2000	130,658	53,694

NOTES TO THE ACCOUNTS:

1. DIRECT CHARITABLE EXPENDITURE

	31.12.00	31.12.99
Glasgow 1999	-	2,359
Subscription to International bodies	1,175	2,493
Annual Conference	61,883	-
Meetings of Groups	2,056	12,179
Newsletters	10,516	10,119
Colour supplement	5,212	-
Course fees and accommodation	1,000	17,646
Grants and sponsorship	1,000	500
Prizes	1,413	65
Awards and bursaries		
- Chemical	25	25
- BCA Bursary Fund	1,520	13,050
- Industrial Group	234	63
	86,034	58,499

2. MANAGEMENT AND ADMINISTRATION

General expenses		
- Depreciation	135	136
- Administration fee	8,812	-
- Accounting fee	1,527	1,410
- Insurance	175	169
- Bank and security charges	116	153
- Other	364	220
- Special Interest Group administration	649	898
- Transfer of Physical Group fund	180	-
	11,958	2,986
Council Expenses		
- Council	317	1,119
- Officers	833	171
- Administration expenses	459	114
- Printing, stationery and postage	893	111
- Telephone	523	162
	3,025	1,677
Total	14,983	4,663

The British Crystallographic Association

Summary of the consolidated BCA accounts for year ended 31 December 2000

3. Restricted Funds

	Physical Group	Biological Structure Group	Industrial Group	Chemical Group	CCG Teaching School	Dorothy Hodgkin Prize	Bursary Fund	Totals 2000	Totals 1999
Balances at 1.1.00	180	16,026	8,158	1,596	6,526	7,005	-	39,491	31,145
Donations	-	-	-	-	-	156	100	256	207
Interest received	-	368	126	44	150	206	-	894	741
Transfers	(180)	-	-	-	-	-	1,420	1,240	12,984
Net income (expenditure)	-	999	(1,831)	384	(98)	(75)	-	(621)	7,464
Bursaries awarded	-	-	-	-	-	-	(1,520)	(1,520)	(13,050)
Dorothy Hodgkin Prize	-	-	-	-	-	(1,413)	-	(1,413)	-
Balances at 31.12.00	-	17,393	6,453	2,024	6,578	5,879	-	38,327	39,491

Treasurer's Report

2000 Accounts

The 2000 accounts see some major changes to the Associations funds. In April the BCA gratefully received a donation of £75,000 from Crystal Congress 99. A further donation is expected in the near future as the company is wound up. This has been a major contribution to the massive increase in the net movements of funds up from £3,412 to £65,802. The fixed interest investments are giving very good returns. However, as they start to mature over the next few years it will be impossible to find similar high returns for the capital without increased risk. There is also a need to invest some of our surplus funds for better long-term returns.

Financial administration of the Physical Crystallography Group has been transferred to the Institute of Physics where the group is known as the Structural Condensed Matter Physics Group.

The level of general bursary funding of £1520 is a little lower than usual. However, the Bursary Committee turned down only one application for funding, which breached the rules. The administration of the Bursary fund has been overhauled and consequently a donation of £500 to the Glasgow Protein Workshop, which would previously have been recorded as bursary funding, is this year recorded in the grants and sponsorship figure. The Heriot-Watt Spring Meeting gave bursary funding of £4481. However, the meeting made an overall loss of £5248 when deposits accrued from previous years are included.

The Newsletter made a profit of £2714 this year, slightly up on last year, which helped to defray some of the £5625 cost of the additional IUCr Colour supplement. The stock of extra colour supplements should contribute to future sales income. We will see the production costs of our Newsletter rise over the next year as we change style and format. However, increased advertising revenue should help maintain a small profit.

The new arrangements for the provision of Administration Services from Northern Networking under an initial 3 year contract are starting to impact on our expenditure with nine months charges reflected this year. Also included are the expenses incurred in the period when the new administration services worked hand in hand with Stephanie Harris during the transition.

We have had no success this year in obtaining payment of £540 from X-ray Associates (A Spectrolab Company) for advertisements placed in Crystallography News in 1999.

An effort to increase donations to help contribute to over £8000 expenditure on "good works" this year brought little success. Donations totalling £256 were received up from £207 last year. Many of our members have now signed Gift Aid declarations and it is hoped that refunds due from the revised legislation will make an impact in next years accounts and contribute to our charitable expenditure.

Education in Crystallography

Report of a discussion meeting held in Reading at the Spring Meeting, 2001

This discussion was prompted by the Presidential letter from Henk Schenk in an IUCr newsletter early last year. He suggested that we should all try to show younger children the excitement of crystallography. Since I am not a teacher myself I did not want to limit this discussion, merely to ask BCA members what they thought should be done.

We clearly have a problem with the image of crystallography as portrayed by the National newspapers and TV, phrases such as 'crystal balls' or 'crystal clear' are often seen, but there is rarely more technical news; David Stuart's image of the structure of the 'foot and mouth' disease virus has adorned recent copies of 'The Sun', but sadly not in response to how the structure was determined. As part of the IUCr Congress in Glasgow in 1999 our Press officer issued 'news items' related to the exciting 'breakthroughs' to be reported that day. The National media paid no attention. This ignorance extends to all walks of life, including rather surprisingly, some University Physics Departments which we were told, know nothing of modern crystallography and its importance in a technological society. Should we worry about this?

Members of the audience thought we should, because changes in the teaching practise in Universities mean that few now offer specialist courses in crystallography. Most students have very few lectures devoted to the fundamentals of crystallography as part of their undergraduate chemistry, physics, geology or materials science courses. A disturbing trend to 'Modularisation' is also squeezing out crystallography. The mathematical background of undergraduates coming up to University today is lower than it used to be. Should our 'Summer Schools' begin with remedial maths which would help the students understand crystallographic concepts?

Modern manufacturers supply 'black boxes' with their X-ray diffractometers, so that little detailed knowledge is now needed to solve a structure. Students should be taught to realise the limitations of the methods used in the algorithms within these 'black boxes'. Chris Hammond, University of Leeds, thought that we should put greater emphasis on the understanding of symmetries in two dimensional patterns; he finds materials science students who really understand plane groups have much less trouble with the 3D space groups. Phil Withers, University of Manchester, had suggested in his earlier lecture that some of his striking texture patterns of materials would make good designs for 'Liberty' fabrics. He pointed out that the Research Councils and others now make funds available for the Public Understanding of Science. We might seek a collaboration with Design Schools on using crystallographic patterns for wallpapers and fabrics. (I will maintain a list of such funding agencies and possible projects on the BCA website. Send me news preferably by email to bca@isise.rl.ac.uk). Guy Orpen, University of Bristol, thought we should emphasise the excitement of discovery in crystallography, he still remembers an old 'BBC TV Horizon' program on the discovery of the structure of DNA. BCA members are not skilled film makers, but granting agencies such as the Wellcome Foundation are currently calling for collaborative projects between scientists and film makers to bring bio-medical dramatisations to live acting or video or film. Please send me news of any dramatisations or novels about crystallographers.

The consensus on educating secondary school children was that we should try to get some crystallography into special training courses for teachers; these are often run in school holidays by organisations such as the Institute of Physics, The Royal Society of Chemistry (R.S.C) and the EPSRC. The teachers attending these courses tend to be the more enthusiastic ones; hopefully, they will go back to their schools and spread the word to their colleagues. Sometimes they write in to say how much they enjoyed these courses, we might publish such letters in 'Crystallography News'. Please let me know details of such 'Update' courses, and your ideas of what crystallography

should be in them.
Harry Powell described the 'Crystal Growing' projects organised by Phil Smith of the R.S.C. in the Thames Valley area. The crystals were on display upstairs in the commercial exhibition for members to see. Judging was to take place later during this meeting. Many schools enjoy these competitions. Others are less enthusiastic because 'Crystals' do not form part of the National Curriculum. There is a 'Materials' section, where we might try to insert a little about crystals. Does anyone know how we might get changes in the National Curriculum? Young children enjoy growing crystals and become very enthusiastic about it because it is something they can do for themselves.

There was general agreement that we should make more interesting pages on the BCA web site for the general public. We can try to make 'Picture Galleries' ourselves or can link to others who may have more resources than we have to make the images. Although photographs of beautiful crystals are needed, we should try to include additional information about the structure of the crystal, and probably allow people to rotate the structures over the web. Please send me news of any good websites and your ideas of what the BCA should be doing to improve the UK education in crystallography.

Kate Crennell
BCA Education Officer, April 2001
email: BCA@isise.rl.ac.uk

Crystallography in Forensic Science

Crystallography in forensic science [1] usually implies the use of X-ray powder methods (XRD). Single crystal diffraction methods are rarely used, because full structural analyses are seldom required, and the expense of maintaining or leasing a facility for this purpose could not be justified. Qualitative phase analysis of polycrystalline organic, inorganic and metallic substances is the bread and butter work of the forensic diffractionist, who may be dealing with anything from microgram specimens to kilogram seizures of drugs. Apart from one-off samples to be identified by reference to a database of powder patterns such as the ICDD Powder Diffraction File, most forensic analyses involve identification and comparison of "control" with "suspect" samples, to establish whether or not they have a common origin. XRD is used mainly in "contact trace" analysis. So-called contact traces (paint flakes, slivers of metal, polymers (plastics), soils, building materials, stains of any description, corrosion products and loose powdered materials) appear in the traditional areas of forensic science. Identification and comparison of trace quantities of material can help in the conviction or exoneration of a person suspected of involvement in a crime.

Brass is one of the most common alloys that each of us encounters on a daily basis, and its analysis is usually quite straightforward. However, the following instance shows that this is not always the case. A man had attempted to cut up a ship's propeller, which had been removed for the purposes of cleaning. He had used a gasoline-powered abrasive disc cutter, which unfortunately ran out of gasoline, before he had completed the job. He was seen running away from the dockyard repair shop and was arrested some time later. Sweepings from his clothing and control metal from the propeller were analysed by XRD. Both metals were a duplex (a + b) brass of approximate composition 60:40 Cu:Zn, but the ratios of a to b brass in the two specimens were different. After annealing both specimens, these ratios were identical. Reference to the CuZn phase diagram offered a clue and an *ad hoc* experiment proved useful—brass from the propeller was held against an abrasive wheel in the laboratory, and the resulting brass grindings collected and analysed. The d's and I's agreed with those found in the XRD patterns of the original grindings from the suspect's clothing. The discrepancy between control and suspect analyses was due to phase transformation at the high temperatures, produced during the grinding operation, followed by rapid cooling (quenching) as the grindings flew through the air.

Similarly, drug analysis should be a straightforward affair – and in most cases it is. In this instance, crystallinity, or lack of it was the problem. A sample known to contain heroin was submitted for

XRD analysis to establish the form of heroin (hydrochloride or base) and the identity of its excipients. Analysis showed the presence of calcium carbonate (calcite) and glucose monohydrate, but no heroin! In this case the heroin had been extracted and recrystallised to clean it up prior to submission for analysis with the excipients. Analysis of the original (non-recrystallized) sample showed calcite, glucose monohydrate and heroin hydrochloride. Heroin hydrochloride crystallizes as a monohydrate and its powder pattern is very weak, with rather broad, diffuse, diffraction peaks. Attempts at recrystallisation usually mean loss of the water molecule and this results in a sample of heroin that is virtually amorphous – hence its "absence" from the recrystallised sample.

An example of the importance of XRD in identifying specific phases where polymorphism exists was the case of a burglary at a company warehouse. As there were no signs of a forced entry, it was concluded that entry had been gained by someone using a key. There were three keyholders in the company, and one was under suspicion of having provided an accomplice with his key in order to have a duplicate made. All three original keys were examined, and the one belonging to the man under suspicion had minute traces of a white substance on it. Analysis by XRD revealed aragonite (one of the polymorphs of calcium carbonate). This also happens to be the major constituent of cuttlefish bone, something commonly used to make impressions of keys.

Powder diffraction's versatility is one of its greatest attributes. Its ability to analyse mixtures of inorganic, organic and metallic substances is very useful indeed. A smouldering object was pushed through the letterbox of an elderly man's house. He stamped on it and managed to extinguish it, and then called the police. Children found in the vicinity had in their possession some large pellets resembling theatrical smoke pellets. Analysis of the partially burnt pellet and an unburned one by XRD revealed that they were of similar composition, containing potassium chlorate, ammonium chloride, a-lactose monohydrate, and traces of sodium chloride.

Although the strict definition of forensic science is that science which is used in the law courts, in many respects industries which use analytical methods for troubleshooting or problem-solving purposes, are undertaking work of a forensic nature - sometimes with, but usually without, the court-going aspect. They are using analytical techniques in "detective" fashion to find out, for example, why a machine or a process has failed (corrosion, incorrect ingredients, wrong conditions?), or why a product is not what it is supposed to be. Analytical applications of this nature are always interesting, whether or not they be undertaken in a *bona fide* forensic science laboratory. Forensic science applied to high profile criminal cases, however, will generally capture the public's imagination, to the point where science may even feature on the front page of the tabloid newspapers!

[1] D.F. Rendle (2000). Forensic Science: Every Contact Leaves a Trace, in *Industrial Applications of X-ray Diffraction*, Eds. F. H. Chung & D.K. Smith, Marcel Dekker Inc., New York/Basel, pp. 659-675.

PS How would *you* explain powder diffraction to a jury?

David Rendle
Forensic Science Service, London Laboratory, UK

Book Review

Diffuse Neutron Scattering from Crystalline Materials

by Victoria M.Nield and David A.Keen

Publisher Oxford University Press 7 December 2000 UK price £65 hardback
Series Oxford Series on Neutron Scattering in Condensed Matter
ISBN 0-19-851790-4 336 pages 5 halftones, 80 line figures, 234mm x 156mm

The authors begin their preface with these sentences: *"The existence of diffuse scattering in diffraction data has confounded and fascinated crystallographers for over eighty years. For some it is an inconvenience, increasing 'background' and obscuring weak Bragg peaks whereas others may harness it to reveal the subtle details of structures".*

In the rest of the book they explain in detail the theory and experimental techniques to do

this and give examples of applications in many materials. The book is aimed at research workers in crystallography and can probably be understood by graduate students with some mathematical training since the authors explain their terminology clearly in the introduction and include a brief historical overview of the subject. Did you know that in the middle of the Second World War, in early 1941, many eminent crystallographers, including Kathleen Lonsdale, both Braggs and Max Born, attended a workshop on diffuse scattering held at the Royal Society in London? The front cover of the September 1990 issue of 'Crystallography News' carried an example of a surface plot representing the coherent diffuse elastic scattering from a single crystal of cubic zirconia. This was about the time that R.L.McGreevy and W.Hayes at Oxford University were doing pioneering work on computer modelling as an aid to data analysis with their D.Phil students, who are the authors of this book, which was started some 5 years ago. Although this is a book mainly concerned with neutron scattering there is a short section on the uses of X-rays and electrons in diffuse scattering. Topics such as magnetism and quasielastic neutron scattering are not covered since they are the subjects of other recent books in this series.

Later chapters cover neutron scattering formalism, diffuse scattering theory and experimental techniques. Instruments are not usually designed with diffuse scattering experiments in mind; however, the authors suggest some possible compromises in design which would make diffuse scattering experiments easier. Existing instruments are described which are at the ISIS pulsed neutron source in the UK and at the Institute Laue Langevin reactor source in Grenoble and there is a paragraph on the types of sample environment needed. Further chapters cover data correction and computer simulation and modelling of the defect structures in the crystals. This has much in common with the simulation of liquids; the techniques covered are molecular dynamics, Monte Carlo simulations, Reverse Monte Carlo (RMC) simulations and the pair distribution function (PDF) analysis methods.

Later chapters cover applications of diffuse scattering theory to binary systems, examples of diffuse scattering experiments on alloys, other binary materials and on superionic conductors. Diffuse scattering can also be used to study the internal structure of molecules such as that of ice at very low temperatures; experiments are described which used the SXD instrument at ISIS over a range of temperatures from 10 to 250K. Large crystals were needed (of the order 10mm diameter by 10mm height) in order to measure the weak diffuse scattering with sufficient statistics in a limited time. Organic molecules and even proteins can also be studied. The final chapter concerns framework structures using the tetrahedral phases of silica as an example. This book is the first comprehensive account of diffuse neutron scattering and should be available to anyone working on neutron scattering.

Kate Crennell,
Note from the publisher A few early copies of this book had misprints on the x-axes of some of the diagrams; these have been corrected in later printings."

Biological Structure Group Logo Competition

The BSG is currently lacking a logo. To rectify this, we are holding a logo design competition. A cash prize will be awarded for the chosen design at the Biological Structure Group Winter meeting. The logo should identify our group clearly, and designers should bear in mind that it will be used both in printed media (including Crystallography News, two tone only) and on the BCA website. Entries should be submitted to the group secretary, electronically (a.t.hadfield@bris.ac.uk), by December 1st.

PCG Bursaries

The PCG welcomes bursary applications from BCA or IoP members who are affiliated to the PCG or to the Structural Condensed Matter Physics Group of the IoP. These are intended mainly to help young scientists (students and post-docs) to attend meetings and conferences relevant to PCG/SCMPG areas of interest. Bursaries can be applied for at any time, through the PCG/SCMPG Secretary (C.C.Wilson@rl.ac.uk) and will be considered by the Group Committee. However, each year we expect to target selected meetings as highly relevant for the award of bursaries.

The next targeted meeting for PCG bursaries will be ECM-20 in Krakow. Applications for bursaries are expected to be received by the PCG Secretary **at least two weeks** prior to any early registration deadline - more details of deadlines will be publicised on the PCG Website. Recipients of bursaries are expected to write a brief report on the relevant meeting, and may be asked to report on a particular session. Reports received from bursary awardees to the BCA Spring Meeting (Thomas Lyford & Vincent Jennings) can be found among the Meeting reports in this issue of Crystallography News.

PCG Website:
http://bca.cryst.bbk.ac.uk/bca/PCG/pcg.html

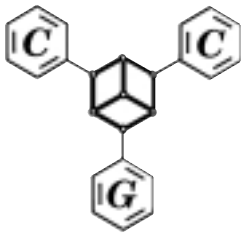
BCA Meetings

Industrial Group: Autumn Meeting - Crystallography in Industry

Thursday 1st November 2001 - Pilkington, Lathom, Lancashire

An Industrial Group Award will be made to Dr Ian Langford at this meeting.

Offers of contributions to this meeting should be addressed to:
Ms J Shackleton, Manchester Materials Science Centre, Grosvenor Street, Manchester M1 7HS
Tel: 0161 200 3581
Fax: 0161 200 3586
Email: judith.shackleton@man.ac.uk



Chemical Crystallography Group: Autumn Meeting

Mesomolecular crystallography
Wednesday November 14 - 2001
Aston University

The meeting will focus on methods and experiences of structure solution, refinement and results for large small molecules. Invited speakers include;

Dr Andrew Burrows (University of Bath)
'Co-ordination and Hydrogen Bond Interplay in Supramolecular Network Formation'

Professor Martin Schroder (University of Nottingham)
'Construction of Framework Polymers: Catenates, Helicates and Porous Materials'
Dr Jonathan Steed (King's College, London)
'Crystal Frustration - and how to Avoid It'
Professor Richard Winpenny (University of Manchester)
'Studies of High Nuclearity 3d-Metal Cages with Unusual Magnetic Properties'

Full details including a registration form will appear in the September edition of Crystallography News and on the CCG pages of the BCA website. The local organiser is Carl Schwalbe (e-mail: c.h.schwalbe@aston.ac.uk).

Offers of short presentations (particularly by post-graduates and post-doctoral workers) at the meeting should be sent to the scientific session organiser, Professor Paul R. Raithby, Department of Chemistry, University of Bath, Bath BA2 7AY, Tel: (01225) 826444 Fax: (01225) 826231
E-mail: p.r.raithby@bath.ac.uk

PCG Rietveld refinement workshops Introduction to the principles and practice of Rietveld refinement

Rutherford Appleton Laboratory, Oxfordshire
17-18 October 2001

In Autumn 2001, the PCG will begin a series of tutorial workshops on powder diffraction profile refinement methods. This technique, much used and a vital component of much of physical crystallography, is very powerful but if improperly used can lead to problems both in the refinement process itself and in the resulting structural models. The aim of these workshops is to provide a general introduction to the method and its applications. They are aimed both at those new to the technique, particularly research students and post-docs, and those who feel the need for a refresher. The first of these workshops will be hosted by ISIS and held on 17 & 18 October 2001 at the Rutherford Appleton Laboratory, and will be two-day event introducing the basics of profile refinement using the Rietveld method. The workshop will include introductory lectures, demonstrations and hands-on examples. Topics will include:

- principles of Rietveld refinement, including minimisation;
- crystal structure refinement and what it achieves, including the use of constraints and restraints;
- data collection strategies, including angle- and energy-dispersive techniques with both X-ray and neutrons;
- basic refinement strategies - how to give yourself the best chance to get the right result;
- an introduction to some of the software suites available.

Speakers will include Bill David (ISIS/UCL), Jeremy Cockcroft (Birkbeck) and Kevin Knight (ISIS). Registration will be free and local accommodation will be available. Further details will be announced on the meeting Web site as they develop.

Contact Chick Wilson (C.C.Wilson@rl.ac.uk) for more details or check the meeting website:

http://www.isis.rl.ac.uk/Crystallography/RietveldWorkshop.htm

PCG Autumn Meeting Applications of high pressure in structural studies

Daresbury Laboratory, 5 December 2001

The Autumn 2001 meeting of the PCG will be a one-day meeting covering the wide-ranging applications of high pressure techniques in the study of crystal structure, to be held at the Daresbury Laboratory on 5 December 2001. The meeting will include scientific presentations, accounts of the latest technical advances in pressure techniques for both X-ray and neutron diffraction, and a chance to view some of the advanced high pressure kit currently being made available on laboratory and central facility sources. Topics will include:

High pressure single crystal diffraction in the laboratory using point and area detectors;
Developments in high pressure single crystal neutron diffraction;
State-of-the-art high pressure powder diffraction at synchrotron sources;
Status of high pressure powder diffraction at laboratory sources;
High pressure EXAFS;
Possibilities in high pressure spectroscopy.
More details will be available on the PCG Website. For more information on the meeting contact the organiser: Dr David Allan (University of Edinburgh; dra@ph.ed.ac.uk) or the PCG Secretary Chick Wilson (C.C.Wilson@rl.ac.uk).

Summer School in Protein Crystallography

St. Andrews

CCP4 will be in large part sponsoring the summer school in protein crystallography held in St. Andrews. Provisional dates are Sunday 9th of September to Saturday 15th September. A call for applicants will be issued by email to CCP4BB and on http://speedy.st-and.ac.uk
The course is intended for either 1st year Ph.D. students or post-docs who have transferred into Structural Biology. Numbers are limited. Your supervisor will have to send a letter of nomination to either Jim Naismith (naismith@st-and.ac.uk) or Garry Taylor (glt2@st-and.ac.uk)

Other Meetings of Interest

If you have news of any meetings to add to list please send them to the BCA Web Master cockcroft@img.cryst.bbk.ac.uk or to the Editor, josephinejutson@beeb.net

July 9-12, 2001
Scattering Methods for the Investigation of Polymers, Institute of Macromolecular Chemistry, PRAGUE, [Details from Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, P.M.M. Secretariat, Heyrovskeho nam. 2, 162 06 Praha 6, Czech Republic, Tel: +420-2-204 03 332, Fax: +420-2-35 35 79 81, e-mail: sympo@imc.cas.cz

July 24 - 29, 2001
ISSCG-11 School on Crystal growth, KYOTO, Japan [e-mail: info@iccg.doshisha.ac.jp]

July 29 - August 3, 2001
ICVGE-11 International Conference on Crystal Growth 13 in conjunction with Vapour growth and Epitaxy - 11, KYOTO, Japan [email: info@iccg.doshisha.ac.jp]

July 30 - August 3, 2001
Denver X-ray Conference, STEAMBOAT SPRINGS, CO, USA [Details at http://www.dxcicdd.com/]

August 1 - 3, 2001
Neutron and Hard X-ray Optics and Applications, San Diego, CA, USA [See IUCr Web site]

August 25 - 31, 2001
ECM 20, XXth European Crystallographic Meeting, KRAKOW, Poland [email; ECM2001@chemia.uj.edu.pl]

August 27 - September 6, 2001
7th Oxford Neutron Scattering Summer School, Mansfield College, Oxford and Nuclear Physics Laboratory, Oxford. [Contacts c.c.wilson@rl.ac.uk, bertram.willis@chemcryst.ox.ac.uk and carlile@ill.fr]

September 1 - 3, 2001
Crystallography and Drug Design Lódz, Poland. [e-mail: marekglo@ck-sg.p.lodz.pl]

September 4 - 9, 2001
International Workshop on Crystallography at High Pressures - 2001, Orsay, France [See IUCr website]

September 5 - 9, 2001
Fourth International Conference on Molecular Structural Biology. VIENNA, Austria. [e-mail: andreas.kungl@kfunigraz.ac.at]

September 9 - 12, 2001
2001 Meeting of AK ChenKrist: Crystal Growth - Data Collection - Crystal Engineering and Polymorphism, Essen, Germany [See IUCr website]

September 9 - 13, 2001
ICNS 2001, International Conference on Neutron Scattering, MUNICH, Germany [See web site]

September 9 -13, 2001
Philips 22nd International Durham Conference on X-ray Analysis, DURHAM, UK [Sally Fuller +44 (0) 1223 468 888 e-mail: sally.fuller@philips.com]

September 17 - 21, 2001
Crystallogenesis and Mineralogy, Saint Petersburg, Russia [See IUCr website]

March 25 - 28, 2002
BCA Annual Meeting, Nottingham University, last day is Maundy Thursday

May 21 - June 2, 2002
From Genes to Drugs via Crystallography, the 33rd Crystallographic Course at the Majorana Centre, ERICE, Italy [Paola Spadon, fax +390 49 8275 239, email paola@chor.unipd.it]

August 6 - 15, 2002
XIX Congress of the International Union of Crystallography, GENEVA, [e-mail: iucr@kenes.com]

e-Science Centre Appointment

Professor Paul Durham, Computational Science and Engineering, Daresbury Laboratory has been appointed Head of the CLRC e-Science Centre.

New Chief Executive for CCLRC

Professor John Wood has succeeded Gordon Walker as CCLRC's new Chief Executive. His appointment is for four years from 1st April 2001. Professor Wood became Dean of the Department of Egineering at the University of Nottingham in 1998 and is a Fellow of the Royal Academy of Engineering. He is the Chairman of the Office of Science and Technology's Foresight Panel on Materials and has held a number of directorships and consultancies with industry and has acted as an advisor on material issues to governments.

Corporate Members

Astex Technology

Bede Scientific Instruments Ltd

Bruker/Nonius

Cambridge Crystallographic Data Centre

Hampton Research

International Centre for Diffraction Data

Molecular Structure Corporation

Oxford Cryosystems

Philips Analytical

BCA Corporate Membership

The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA is pleased to announce that they are now offering Corporate Membership.

Corporate Membership is available on an annual basis running from 1 January to 31 December and includes the following benefits:

- Up to 10 free BCA memberships for your employees.
- A 10% discount on exhibition stands at the annual Spring Meeting.
- Free insert in the annual Spring Meeting delegate bag.
- Two free full registrations to the annual Spring Meeting.
- Ten complimentary copies of the quarterly BCA Newsletter.
- Corporate Members will be listed in every BCA Newsletter and on the BCA Web Site with links to your corporate site.

The cost of this membership is £600.00 per annum

To apply for Corporate Membership, or if you have any enquiries, please contact:

BCA Administrative Office
Northern Networking Ltd
Bellway House
813 South Street
Glasgow
G14 0BX

Phone 0141 954 4441
Fax 0141 954 2656
e-mail BCA@glasconf.demon.co.uk

Retirement -

Ron Jenkins

Dr. Ron Jenkins, Executive Director of the ICDD has announced his retirement after 40 years experience in X-ray powder diffractometry and X-ray fluorescence and 16 years of service with ICDD. His particular areas of interest have been instrument development and design, software and teaching. He was Principal Scientist for ICDD for 11 years before becoming Executive Director. This year he was awarded the title of Distinguished Fellow, an award that is only given to ICDD members who have given long and meritorious service.

In his role as teacher, Ron has participated in many BCA meetings, organising and speaking at workshops designed to inform and educate young crystallographers in the UK. He is also an honorary member of the BCA.

Bursary Reports

There has been no space in this issue to print the Bursary reports held over from the March issue of Crystallography News. All the reports, including those already printed will be posted on the BCA website. If any member would like a copy of the reports I can e-mail them in the form of a MSWord97 document or send a hard copy by post

Jo Jutson
Editor

2002 Ludo Frevel Crystallography Scholarship Award

The Ludo Frevel Crystallography Scholarship Fund was established in 1991 by the International Centre for Diffraction Data (ICDD) to encourage promising graduate students to pursue crystallographically-oriented research, Applications for the 2002 awards are now invited and must be received by the ICDD no later than 31 October 2001.
The applicant should be a graduate student seeking a degree with major interest in crystallography, e.g. crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification and materials characterization. There are no restrictions on country, race, age or sex. The term of the scholarship is one year, however award recipients may reapply for one scholarship renewal. For more information contact:
Helen M. McDonnell
mcdonnell@icdd.com

Quasicrystals

Would you like to know more about Quasicrystals? For an introduction to Quasicrystals log onto
http://members.nbci.co/_XOOM/steffenweber/index.html or
http://www.nirm.go.jp/~weber/index.html.
The site also contains information on books, articles, software and other websites related to Quasicrystals, and links to research groups working on structure refinement.

Standards for Diffraction

Many diffraction users (including myself) are not fully aware of all the standards available to help them in their work. It is the aim of the Industrial Group to put together a list of all the available standards and some hints and tips on their use. In fact it is really two lists as we can consider physical standards or Standard Reference Materials (SRM's) as one list and Standard Operating Procedures (SOP's) as a separate list. The list can be found on the Industrial Group pages at the BCA web site in the July 1999 copy of the Industrial Group Newsletter. It is not exhaustive and I rely on you to let me know of any that are not included. The lists will be stored and updated on our Web site with links to the various suppliers hopefully into a growing and useful resource.
(http://bca.cryst.bbk.ac.uk/BCA/ig/news/n99t2.htm#Std)

David Taylor

Making Matter- The atomic structure of crystals

Making Matter- the atomic structure of crystals- is at the ILL website
http://www. ill.fr/dif/3D-crystals/
There is an introduction explaining the importance of atomic structure and pages for related topics. These include close packing, compounds, bonding, gems and minerals, layered structures and superconductors. All the pages are illustrated with clear, colourful images of 3D structures. of inorganic materials in the ILL's ICSD-for-WWW database.

The Online Macromolecular Museum (OMM)

The Online Macromolecular Museum (OMM) at http://www.clunet.edu is a site for the display and study of macromolecules. The OMM's exhibits are interactive tutorials on individual molecules with explanations of important biochemical features are linked to illustrative images of molecules. In order to view the macromolecular exhibits at the OMM you will need two, free items which you can access from the web site:

1. A FRAMES-capable browser. Netscape Navigator 4.73 strongly recommended but NOT Navigator 6 and NOT MS IE

2. MDL Chemscape Chime(v.2.0+ recommended),

The Student Zone, EPSRC Website

For information relating to EPSRC postgraduate training logon to the Student Zone on the EPSRC website, http://www.epsrc.ac.uk. The topics covered are:

- Options for postgraduate study
- Research
- Jobs
- Advice
- Money